

# *Ab Initio* Nuclear Theory for Tests of Fundamental Symmetries

SMEFT meets ChEFT

TRIUMF, September 29 - October 3, 2025

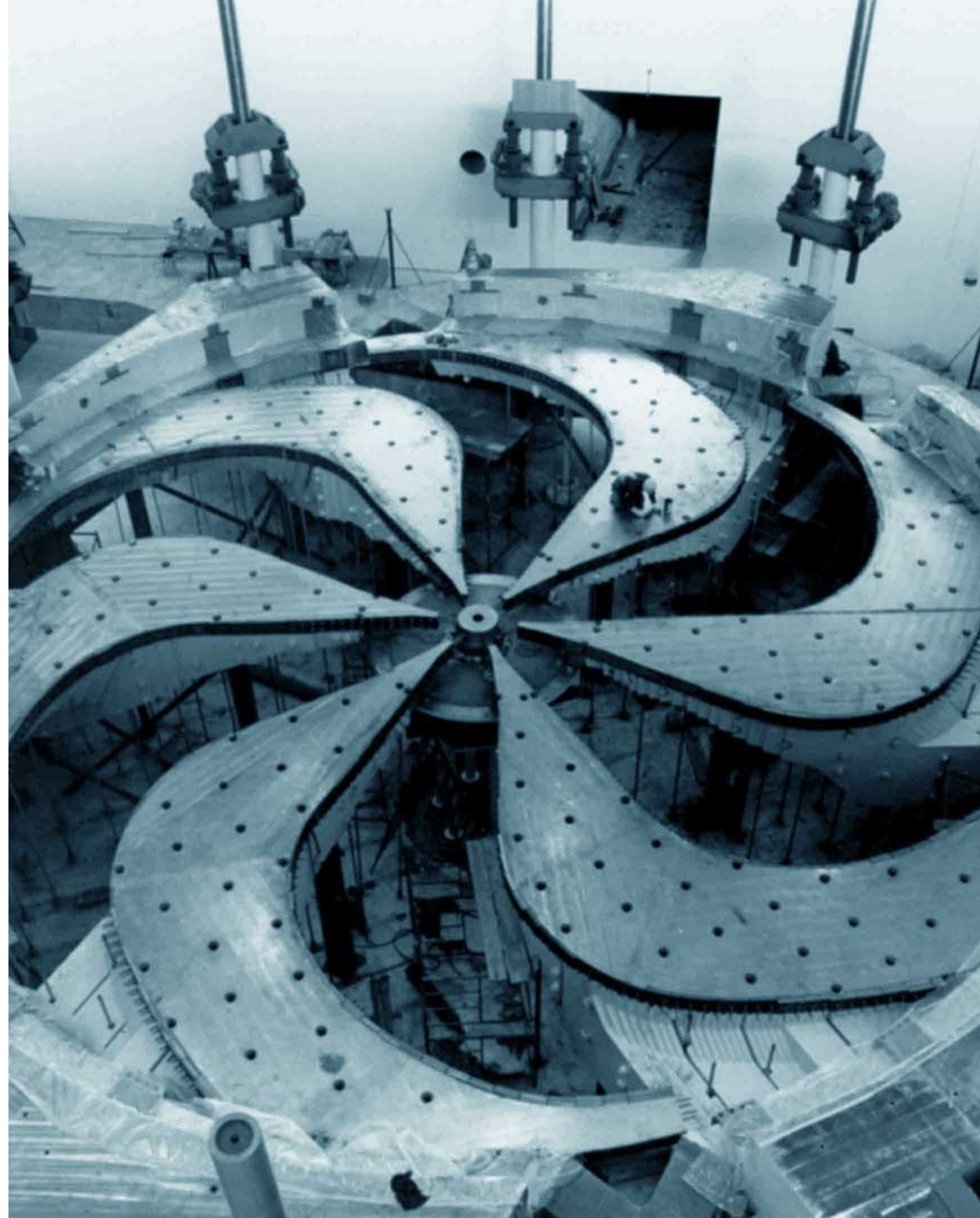
Petr Navratil

TRIUMF


Collaborators:

Michael Gennari (Mainz), Mehdi Drissi (TU Darmstadt), Stephan Foster (TRIUMF/McMaster), Chien-Yeah Seng (Tennessee), Misha Gorchtein (Mainz), Kia Boon Ng (TRIUMF), Stephan Malbrunot (TRIUMF), Lan Cheng (Johns Hopkins), Ayala Glick-Magid (INT), Doron Gazit (Hebrew U), Christian Forssen (Chalmers UT), Daniel Gazda (NPI Rez), Peter Gysbers (FRIB)

2025-09-30



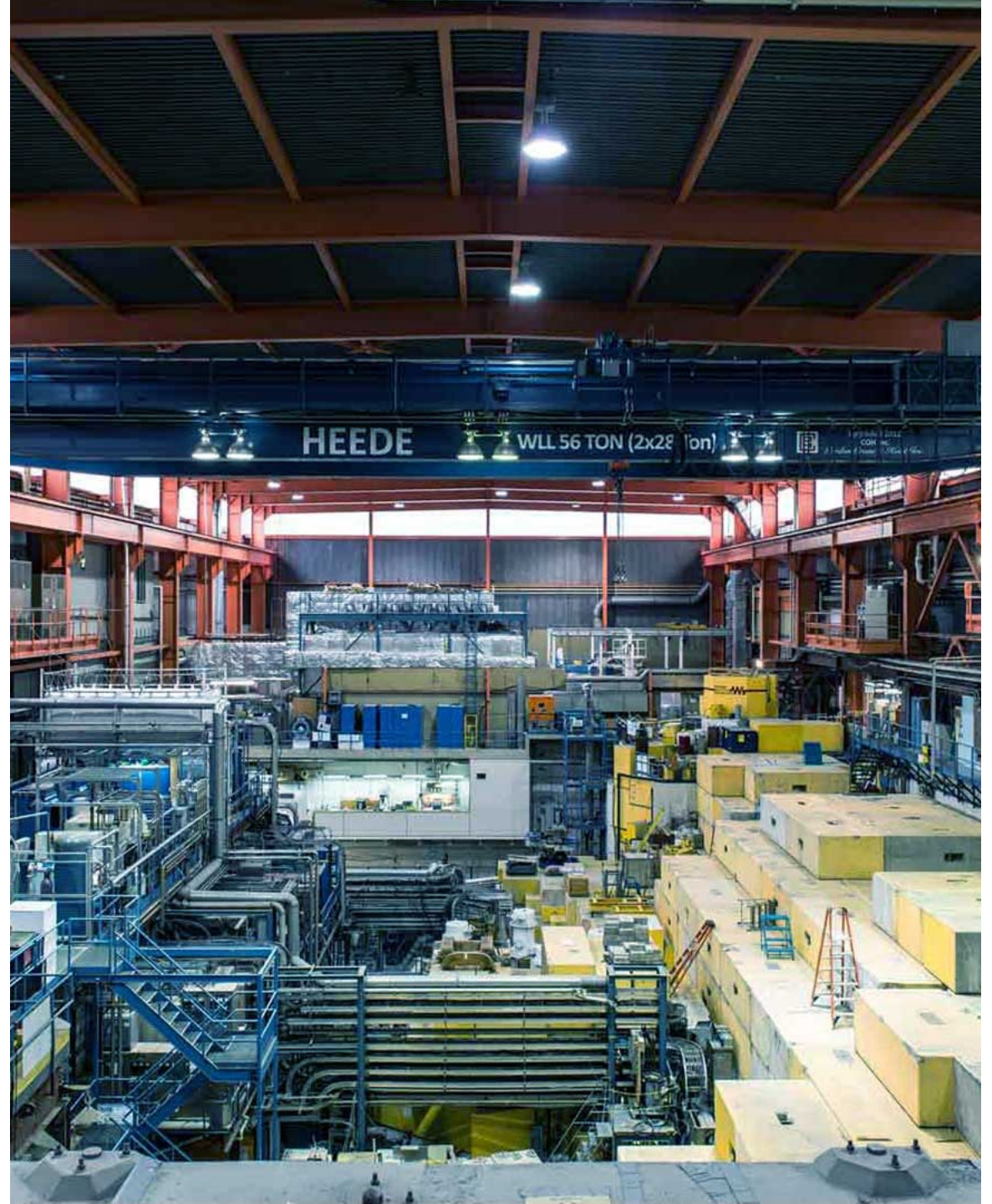
# Outline

- Introduction – *Ab initio* nuclear theory – no-core shell model (NCSM)
- *Ab initio* calculations of parity-violating moments 

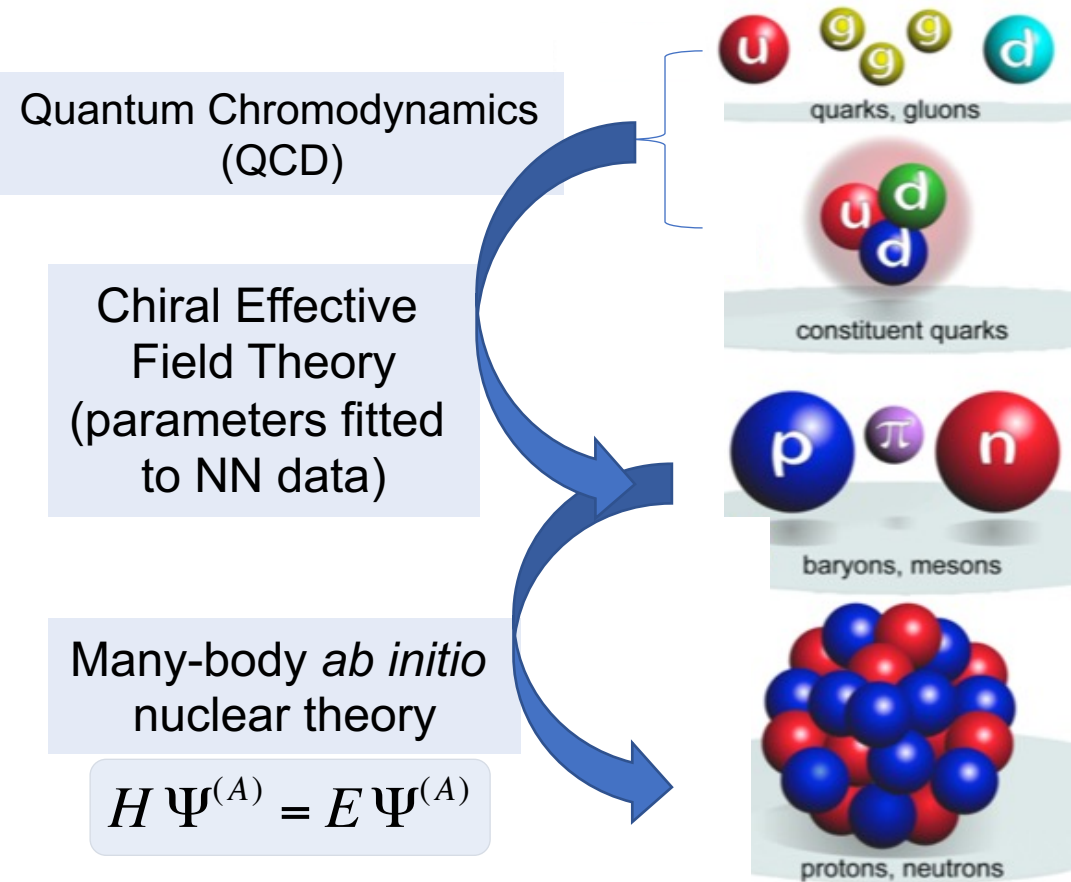
Lanczos strength method
- Parity violating and parity & time-reversal violating NN interactions
- Calculations of anapole, electric dipole, and nuclear Schiff moments
  - Experimental limits on the Schiff moment of  $^{19}\text{F}$
- Search for beyond the standard model physics in  $^6\text{He}$   $\beta$  decay
- Conclusions

# *Ab initio* nuclear theory - no-core shell model (NCSM)

2025-09-30



# First principles or *ab initio* nuclear theory



	NN force	NNN force	NNNN force
$Q^0_{LO}$			
$Q^2_{NLO}$			
$Q^3_{N^2LO}$			
$Q^4_{N^3LO}$			
	+ ...	+ ...	+ ...



Review

*Ab initio* no core shell modelBruce R. Barrett<sup>a</sup>, Petr Navrátil<sup>b</sup>, James P. Vary<sup>c,\*</sup>

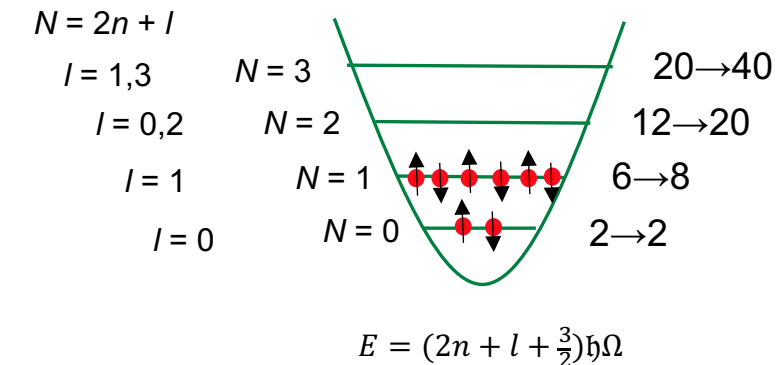
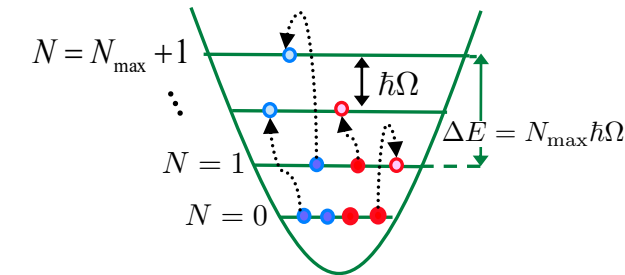
5

## Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

- Basis expansion method (CI)
  - Harmonic oscillator (HO) basis truncated in a particular way ( $N_{\max}$ )
    - HO frequency variational parameter
  - Why HO basis?
    - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 –  $^4\text{He}$ ,  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ )
    - Equivalent description in relative(Jacobi)-coordinate and Slater determinant basis – **nuclei self-bound**,  $[\mathbf{H}, \mathbf{P}_{\text{CM}}]=0$ 
      - Exact factorization of CM and intrinsic eigenfunctions at each  $N_{\max}$

$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_{A-1})$$

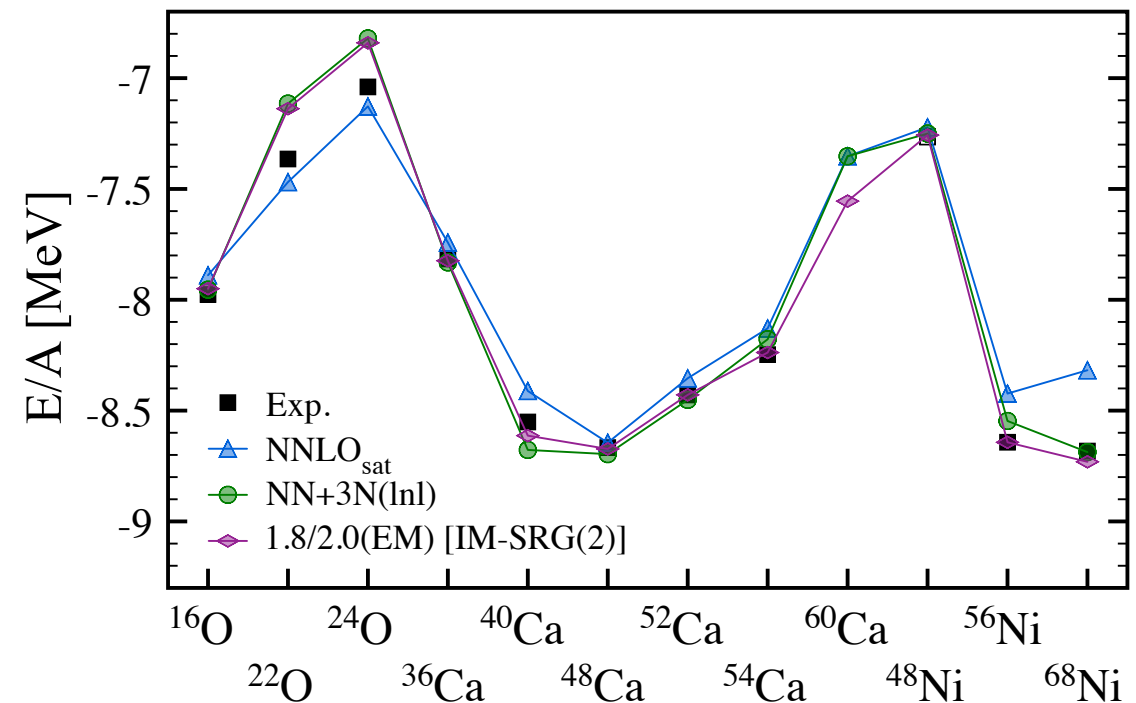
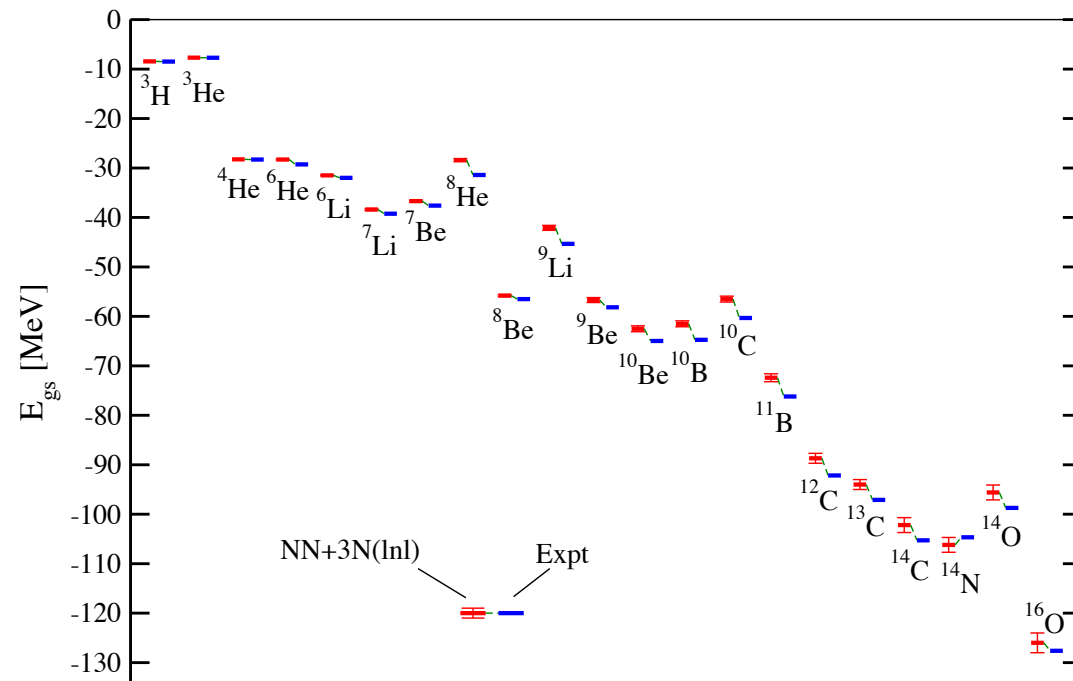
$$\Psi_{\text{SD}}^A = \sum_{N=0}^{N_{\max}} \sum_j c_{Nj}^{\text{SD}} \Phi_{\text{SD}Nj}^{HO}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{\text{CM}})$$



## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Medium mass nuclei – Self-Consistent Green’s Function method

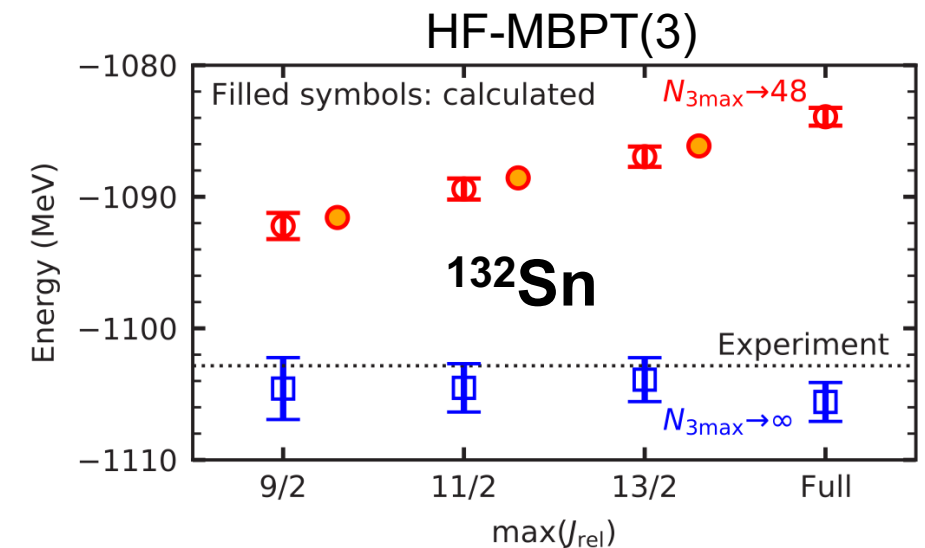
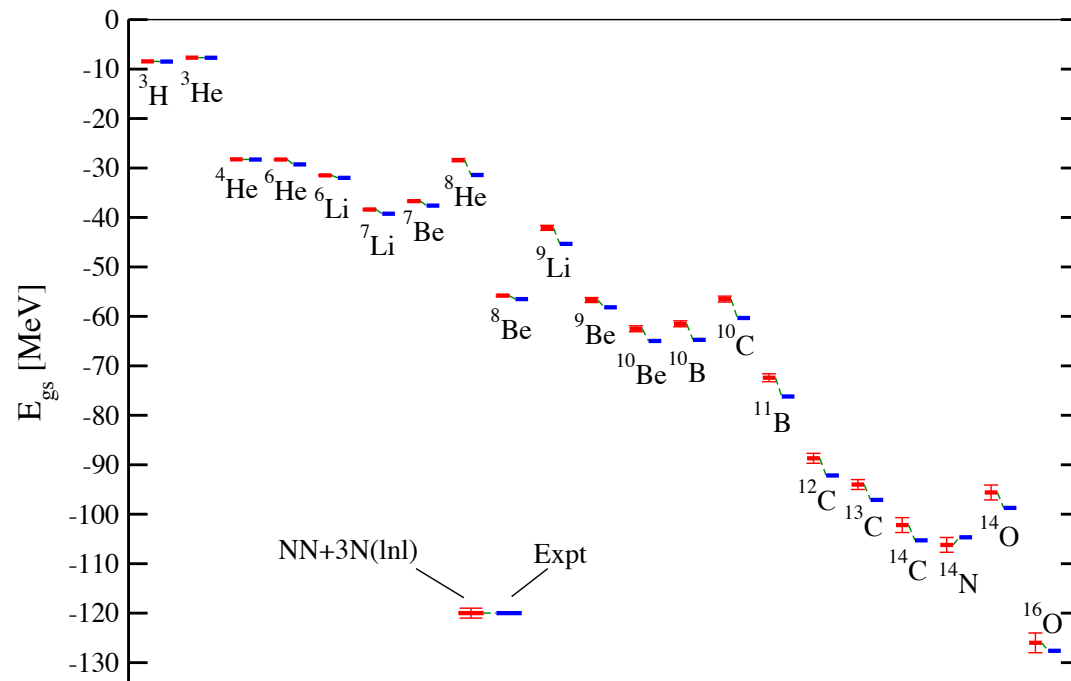
NN N<sup>3</sup>LO (Entem-Machleidt 2003)  
3N N<sup>2</sup>LO w local/non-local regulator



## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Heavy nuclei – HF-MBPT(3)

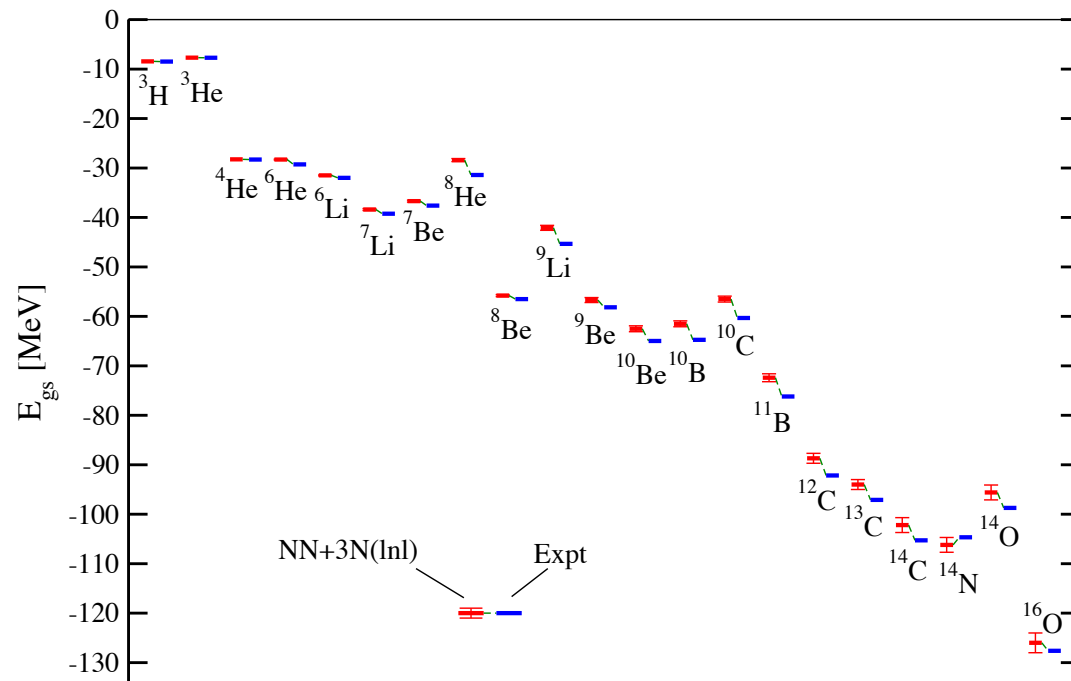
NN N<sup>3</sup>LO (Entem-Machleidt 2003)  
3N N<sup>2</sup>LO w local/non-local regulator



## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Denoted as NN N<sup>3</sup>LO + 3N<sub>lnl</sub> - applied here for the PV moment calculations

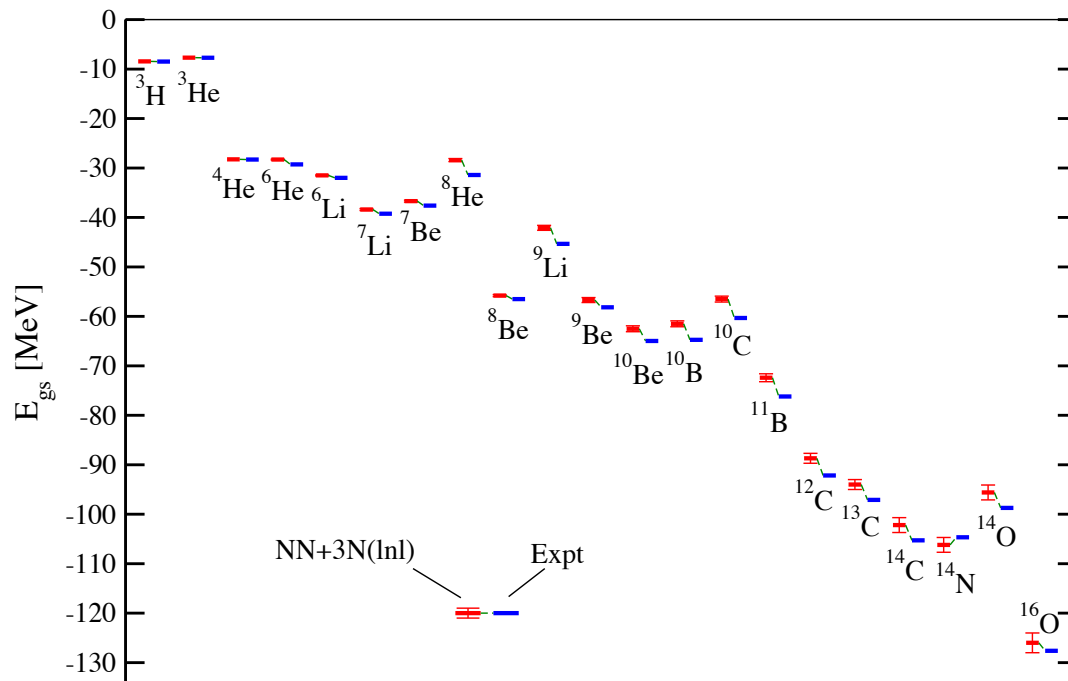
NN N<sup>3</sup>LO (Entem-Machleidt 2003)  
3N N<sup>2</sup>LO w local/non-local regulator



## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Denoted as NN N<sup>3</sup>LO + 3N<sub>Inl</sub> - applied here for the PV moment calculations

NN N<sup>3</sup>LO (Entem-Machleidt 2003)  
3N N<sup>2</sup>LO w local/non-local regulator

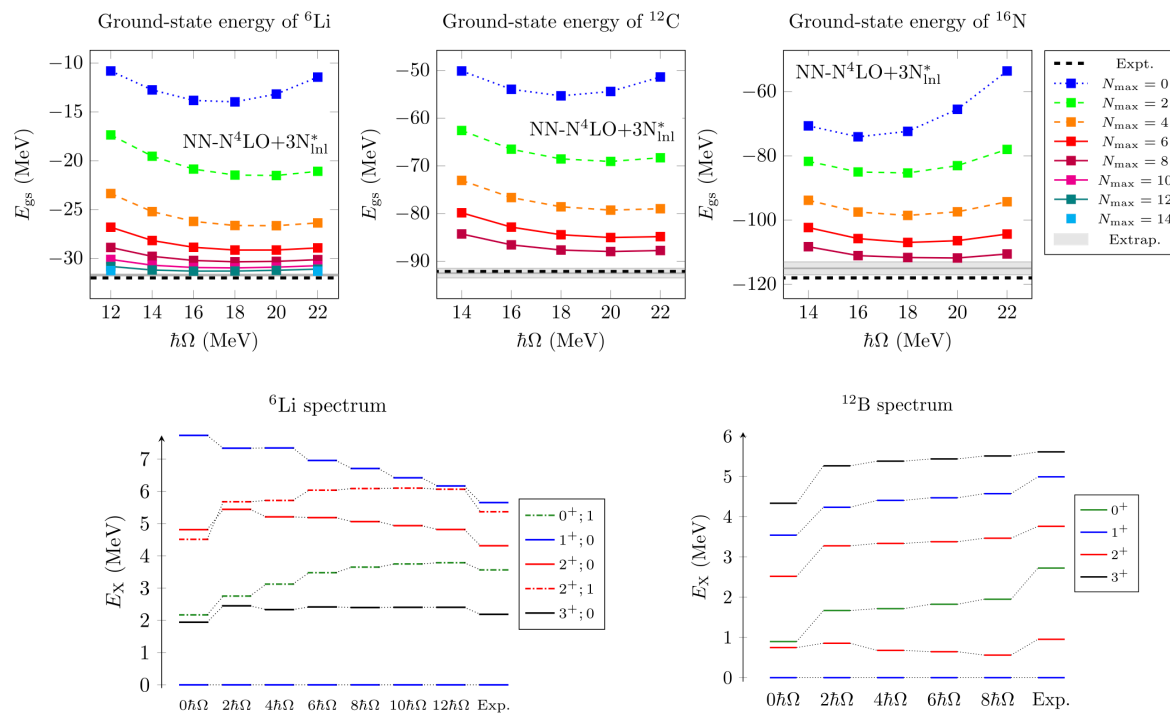


- A new version denoted as NN N<sup>4</sup>LO + 3N<sub>InlE7</sub>
  - NN N<sup>4</sup>LO 500 (Entem-Machleidt-Nosyk 2017)
  - 3N N<sup>2</sup>LO w local/non-local regulator
  - 3N subleading spin-orbit contact term (Girlanda 2011)
    - new LEC ( $E_7$ ) fitted to improve excitation levels in  $^6\text{Li}$
    - reproduces well  $P$ -wave resonances in  $^5\text{He}$
- Successfully applied to  $^7\text{Be}(p,\gamma)^8\text{B}$  (PLB 845,138156) and muon capture on  $^6\text{Li}$ ,  $^{12}\text{C}$ , and  $^{16}\text{O}$  (PRC 109, 065501)
- Applied here for  $^{19}\text{F}$  EDM, Schiff moment calculations

## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Denoted as NN  $N^3\text{LO} + 3N_{\text{Inl}}$  - applied here for the PV moment calculations

NN  $N^3\text{LO}$  (Entem-Machleidt 2003)  
3N  $N^2\text{LO}$  w local/non-local regulator



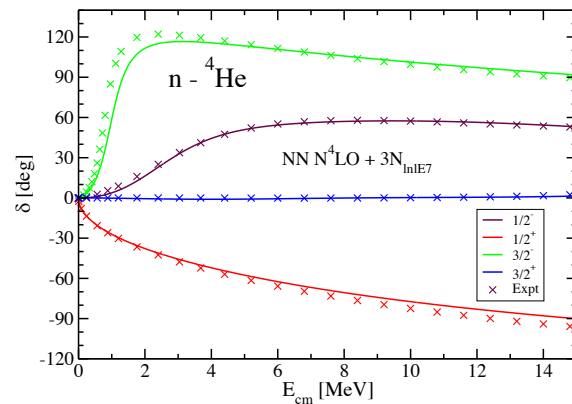
- A new version denoted as NN  $N^4\text{LO} + 3N_{\text{InlE7}}$

- NN  $N^4\text{LO}$  500 (Entem-Machleidt-Nosyk 2017)
- 3N  $N^2\text{LO}$  w local/non-local regulator
- 3N subleading spin-orbit contact term (Girlanda 2011)
  - new LEC ( $E_7$ ) fitted to improve excitation levels in  $^6\text{Li}$
  - reproduces well  $P$ -wave resonances in  $^5\text{He}$
- Successfully applied to  $^7\text{Be}(p,\gamma)^8\text{B}$  (PLB 845,138156) and muon capture on  $^6\text{Li}$ ,  $^{12}\text{C}$ , and  $^{16}\text{O}$  (PRC 109, 065501)
- Applied here for  $^{19}\text{F}$  EDM, Schiff moment calculations

## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

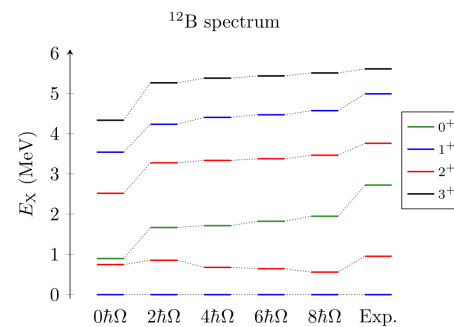
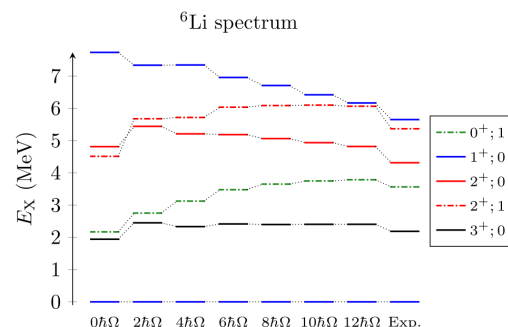
- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Denoted as NN N<sup>3</sup>LO + 3N<sub>Inl</sub> - applied here for the PV moment calculations

NN N<sup>3</sup>LO (Entem-Machleidt 2003)  
3N N<sup>2</sup>LO w local/non-local regulator



- A new version denoted as NN N<sup>4</sup>LO + 3N<sub>InlE7</sub>

- NN N<sup>4</sup>LO 500 (Entem-Machleidt-Nosyk 2017)
- 3N N<sup>2</sup>LO w local/non-local regulator
- 3N subleading spin-orbit contact term (Girlanda 2011)
  - new LEC ( $E_7$ ) fitted to improve excitation levels in  $^6\text{Li}$
  - reproduces well  $P$ -wave resonances in  $^5\text{He}$

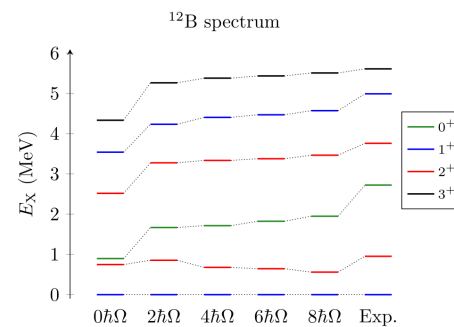
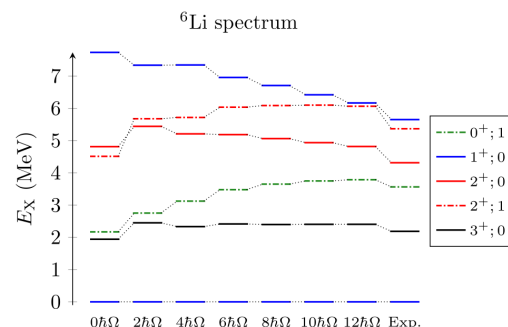
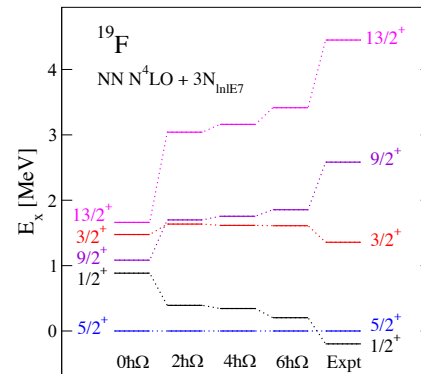
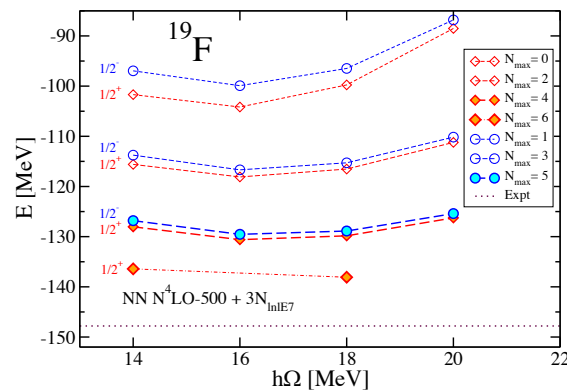


- Successfully applied to  $^7\text{Be}(p,\gamma)^8\text{B}$  (PLB 845,138156) and muon capture on  $^6\text{Li}$ ,  $^{12}\text{C}$ , and  $^{16}\text{O}$  (PRC 109, 065501)
- Applied here for  $^{19}\text{F}$  EDM, Schiff moment calculations

## Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in  $A=2$  and  $A=3,4$  systems**
    - Nucleon–nucleon scattering, deuteron properties,  $^3\text{H}$  and  $^4\text{He}$  binding energy,  $^3\text{H}$  half life
  - Light nuclei – NCSM
  - Denoted as  $\text{NN N}^3\text{LO} + 3\text{N}_{\text{InI}}$  - applied here for the PV moment calculations

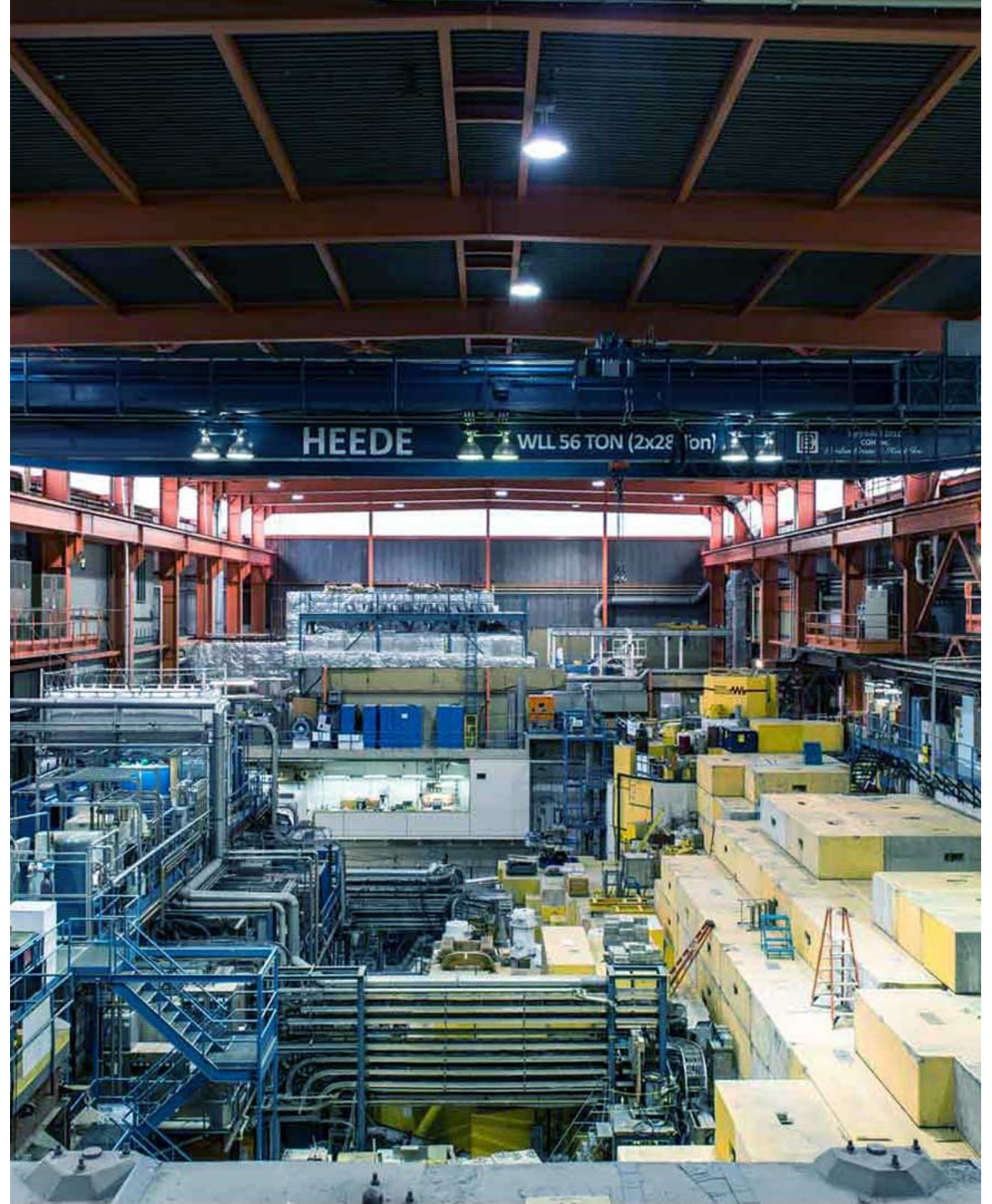
NN  $\text{N}^3\text{LO}$  (Entem-Machleidt 2003)  
 3N  $\text{N}^2\text{LO}$  w local/non-local regulator



- A new version denoted as  $\text{NN N}^4\text{LO} + 3\text{N}_{\text{InIE7}}$

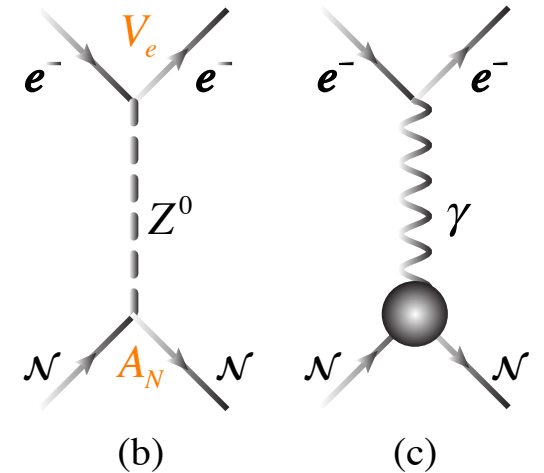
- NN  $\text{N}^4\text{LO}$  500 (Entem-Machleidt-Nosyk 2017)
- 3N  $\text{N}^2\text{LO}$  w local/non-local regulator
- 3N subleading spin-orbit contact term (Girlanda 2011)
  - new LEC ( $E_7$ ) fitted to improve excitation levels in  $^6\text{Li}$
  - reproduces well  $P$ -wave resonances in  $^5\text{He}$
- Successfully applied to  $^7\text{Be}(p,\gamma)^8\text{B}$  (PLB 845,138156) and muon capture on  $^6\text{Li}$ ,  $^{12}\text{C}$ , and  $^{16}\text{O}$  (PRC 109, 065501)
- Applied here for  $^{19}\text{F}$  EDM, Schiff moment calculations

*Ab initio* calculations  
of parity-violating moments  
-  
anapole moment  
electric dipole moment (EDM)  
Schiff moment



## Why investigate parity violation in atomic and molecular systems and the nuclear anapole moment?

- Parity violation in atomic and molecular systems sensitive to a variety of “new physics”
  - Probes electron-quark electroweak interaction
  - Best limits on the  $Z'$  boson parity violating interaction with electrons and nucleons
- Spin dependent parity violation
  - Z-boson exchange between nucleon axial-vector and electron-vector currents (b)
  - Electromagnetic interaction of atomic electrons with the nuclear anapole moment (c)
- Experiments proposed for triatomic molecules  $^9\text{BeNC}$ ,  $^{25}\text{MgNC}$



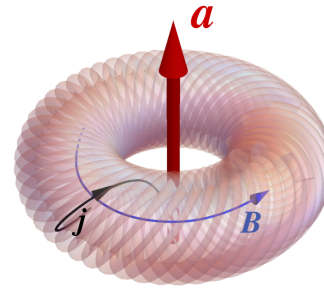
Anapole moment measurements also planned in  $^{137}\text{BaF}$  and  $^{88}\text{SrF}$  molecules

To extract the underlying physics, atomic, molecular, and **nuclear** structure effects must be understood  
→ *Ab initio* calculations

## What is the nuclear anapole moment?

- Anapole moment is a parity-odd and time-reversal-even electromagnetic moment – transverse E1 multipole

$$\mathbf{a} = -\pi \int d^3r r^2 \mathbf{j}(\mathbf{r})$$



- Arises in nuclei due to the parity-violating nucleon-nucleon interaction
- Anapole moment operator dominated by spin contribution

$$\hat{\mathbf{a}}_s = \frac{\pi e}{m} \sum_{i=1}^A \mu_i (\mathbf{r}_i \times \boldsymbol{\sigma}_i)$$

$$\mu_i = \mu_p(1/2 + t_{z,i}) + \mu_n(1/2 - t_{z,i})$$

# Why investigate the Electric Dipole Moment (EDM) and nuclear Schiff Moment (NSM)?

16

- Unsolved problem in physics: matter-antimatter asymmetry of the universe
- Standard model predicts some CP violation, not enough to explain this asymmetry
- The EDM and nuclear Schiff moment is a promising probe for CP violation beyond the standard model, as well as CP violating QCD  $\bar{\theta}$  parameter

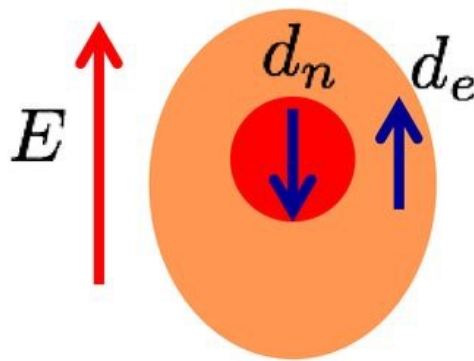
Proposal to measure  $^8\text{Li}$  EDM in ion trap at ISOLDE

- Nuclear EDMs can be measured in storage rings (CERN feasibility study: arXiv:1912.07881)
- Nuclear Schiff moments can be measured using (radioactive) molecules

Nuclear Schiff moment measurements planned in  $^{227}\text{ThF}^+$ ,  $\text{RaF}$ , and  $\text{FrAg}$  molecules

To understand the nuclear EDM and Schiff moment, nuclear structure effects must be understood

## What is the nuclear Schiff moment?



Schiff Moment

$$\vec{S} = \frac{\langle er^2 \vec{r} \rangle}{10} - \frac{\langle r^2 \rangle \langle e \vec{r} \rangle}{6}$$

Leonard Schiff's Theorem (1963):

- Any permanent dipole moment of the nucleus is perfectly shielded by its electron cloud
- True for point-like nuclei, non-relativistic electrons

However, the “Schiff moment” is not shielded by this effect

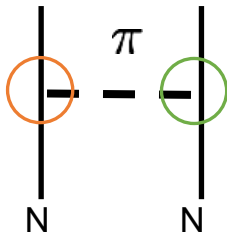
- Zero for point-like, spherical nuclei
- Arises from deformations in the nucleus or its constituent nucleons
- Very large in nuclei with both a quadrupole and octupole deformation

**Look for heavy nuclei with large quadrupole and octupole deformations!**

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{NN}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components

Meson-exchange picture – one vertex PC strong force, one vertex PV (weak) force



$$\begin{aligned} \mathcal{H}_{MNN}^{\text{p.v.}} = & (2)^{-1/2} f_\pi \bar{N} (\vec{\tau} \times \vec{\phi}^\pi)^3 N \\ & + \bar{N} \left[ h_\rho^0 \vec{\tau} \cdot \vec{\phi}_\mu^\rho + h_\rho^1 \phi_\mu^{\rho 3} + h_\rho^2 \frac{(3\tau^3 \phi_\mu^{\rho 3} - \vec{\tau} \cdot \vec{\phi}_\mu^\rho)}{2(6)^{1/2}} \right] \gamma^\mu \gamma_5 N \\ & + \bar{N} [h_\omega^0 \phi_\mu^\omega + h_\omega^1 \tau^3 \phi_\mu^\omega] \gamma^\mu \gamma_5 N \\ & - h_\rho^1 \bar{N} (\vec{\tau} \times \vec{\phi}_\mu^\rho)^3 \frac{\sigma^{\mu\nu} k_\nu}{2M} \gamma_5 N. \end{aligned}$$

$$\begin{aligned} \mathcal{H}_{MNN}^{\text{p.c.}} = & ig_{\pi NN} \bar{N} \gamma_5 \vec{\tau} \cdot \vec{\phi}^\pi N + g_\rho \bar{N} \left( \gamma_\mu + \frac{i\chi_V}{2M} \sigma^{\mu\nu} k_\nu \right) \vec{\tau} \cdot \vec{\phi}^\rho N \\ & + g_\omega \bar{N} \left( \gamma_\mu + \frac{i\chi_S}{2M} \sigma^{\mu\nu} k_\nu \right) \phi_\mu^\omega N \end{aligned}$$

Include  $\pi$ ,  $\rho$ ,  $\omega$  meson exchanges

ANNALS OF PHYSICS 124, 449–495 (1980)

### Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES\*

*Institut de Physique Nucleaire, Division de Physique Théorique, 91406 Orsay Cedex—France*

JOHN F. DONOGHUE†

*Center for Theoretical Physics, Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

AND

BARRY R. HOLSTEIN

*Physics Division, National Science Foundation, Washington, D. C. 20550*

PHYSICAL REVIEW C 70, 055501 (2004)

### P- and T-odd two-nucleon interaction and the deuteron electric dipole moment

C.-P. Liu\* and R. G. E. Timmermans†

frontiers  
in Physics

REVIEW  
published: 21 July 2020  
doi: 10.3389/fphy.2020.00218



### Parity- and Time-Reversal-Violating Nuclear Forces

Jordy de Vries<sup>1,2</sup>, Evgeny Epelbaum<sup>3</sup>, Luca Girlanda<sup>4,5</sup>, Alex Gnech<sup>6</sup>, Emanuele Mereghetti<sup>7</sup> and Michele Viviani<sup>1\*</sup>

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

19

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{NN}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components

Meson-exchange picture – one vertex PC strong force, one vertex PV (weak) force

$$H_{PV} \propto \left[ \frac{\vec{p}}{M}, y_x(r) \right] \dots + \dots \left\{ \frac{\vec{p}}{M}, y_x(r) \right\}$$

$$H_{PTV} \propto i \left[ \frac{\vec{p}}{M}, y_x(r) \right]$$

$$y_x(r) = e^{-m_x r} / (4\pi r)$$

Include  $\pi$ ,  $\rho$ ,  $\omega$  meson exchanges

ANNALS OF PHYSICS 124, 449–495 (1980)

### Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES\*

*Institut de Physique Nucleaire, Division de Physique Théorique, 91406 Orsay Cedex—France*

JOHN F. DONOGHUE†

*Center for Theoretical Physics, Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

AND

BARRY R. HOLSTEIN

*Physics Division, National Science Foundation, Washington, D. C. 20550*

PHYSICAL REVIEW C 70, 055501 (2004)

### P- and T-odd two-nucleon interaction and the deuteron electric dipole moment

C.-P. Liu\* and R. G. E. Timmermans†

frontiers  
in Physics

REVIEW  
published: 21 July 2020  
doi: 10.3389/fphy.2020.00218



### Parity- and Time-Reversal-Violating Nuclear Forces

Jordy de Vries<sup>1,2</sup>, Evgeny Epelbaum<sup>3</sup>, Luca Girlanda<sup>4,5</sup>, Alex Gnech<sup>6</sup>, Emanuele Mereghetti<sup>7</sup> and Michele Viviani<sup>1\*</sup>

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

20

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{NN}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components

Meson-exchange picture – one vertex PC strong force, one vertex PV (weak) force

$$H_{PV} \propto \left[ \frac{\vec{p}}{M}, y_x(r) \right] \dots + \dots \left\{ \frac{\vec{p}}{M}, y_x(r) \right\}$$

$$H_{PTV} \propto i \left[ \frac{\vec{p}}{M}, y_x(r) \right]$$

$$\bar{G}_{\pi}^t = g_{\pi NN} \bar{g}_{\pi NN}^t \quad (g_{\pi NN} \sim 13.3)$$

$$y_x(r) = e^{-m_x r} / (4\pi r)$$

Include  $\pi$ ,  $\rho$ ,  $\omega$  meson exchanges

ANNALS OF PHYSICS 124, 449–495 (1980)

### Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES\*

*Institut de Physique Nucleaire, Division de Physique Théorique, 91406 Orsay Cedex—France*

JOHN F. DONOGHUE†

*Center for Theoretical Physics, Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

AND

BARRY R. HOLSTEIN

*Physics Division, National Science Foundation, Washington, D. C. 20550*

PHYSICAL REVIEW C 70, 055501 (2004)

### P- and T-odd two-nucleon interaction and the deuteron electric dipole moment

C.-P. Liu\* and R. G. E. Timmermans†

frontiers  
in Physics

REVIEW  
published: 21 July 2020  
doi: 10.3389/fphy.2020.00218



### Parity- and Time-Reversal-Violating Nuclear Forces

Jordy de Vries<sup>1,2</sup>, Evgeny Epelbaum<sup>3</sup>, Luca Girlanda<sup>4,5</sup>, Alex Gnani<sup>6</sup>, Emanuele Mereghetti<sup>7</sup> and Michele Viviani<sup>1\*</sup>

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

21

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{NN}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components
  - Admixes unnatural parity states in the ground state

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{NN}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

ANNALS OF PHYSICS 124, 449–495 (1980)

### Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES\*

*Institut de Physique Nucleaire, Division de Physique Théorique, 91406 Orsay Cedex—France*

JOHN F. DONOGHUE†

*Center for Theoretical Physics, Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

AND

BARRY R. HOLSTEIN

*Physics Division, National Science Foundation, Washington, D. C. 20550*

PHYSICAL REVIEW C 70, 055501 (2004)

### *P*- and *T*-odd two-nucleon interaction and the deuteron electric dipole moment

C.-P. Liu\* and R. G. E. Timmermans†

frontiers  
in Physics

REVIEW  
published: 21 July 2020  
doi: 10.3389/fphy.2020.00218



### Parity- and Time-Reversal-Violating Nuclear Forces

Jordy de Vries<sup>1,2</sup>, Evgeny Epelbaum<sup>3</sup>, Luca Girlanda<sup>4,5</sup>, Alex Gnech<sup>6</sup>, Emanuele Mereghetti<sup>7</sup> and Michele Viviani<sup>1\*</sup>

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

22

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{\text{NN}}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components
  - Admixes unnatural parity states in the ground state

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- Anapole moment calculation:

$$\kappa_A = \frac{\sqrt{2}e}{G_F} a_s \quad \kappa_A = -i4\pi \frac{e^2}{G_F} \frac{\hbar}{mc} \frac{(II10|II)}{\sqrt{2I+1}} \sum_j \langle \psi_{\text{gs}} I^\pi | \sqrt{4\pi/3} \sum_{i=1}^A \mu_i r_i [Y_1(\hat{r}_i) \sigma_i]^{(1)} | \psi_j I^{-\pi} \rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

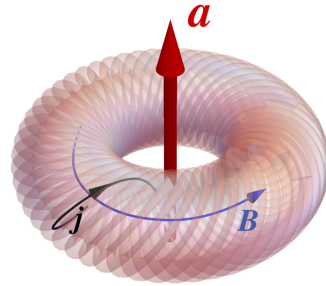
- Anapole moment operator dominated by spin contribution

$$\mathbf{a} = -\pi \int d^3r r^2 \mathbf{j}(\mathbf{r})$$

$$\hat{\mathbf{a}}_s = \frac{\pi e}{m} \sum_{i=1}^A \mu_i (\mathbf{r}_i \times \boldsymbol{\sigma}_i)$$

$$\mu_i = \mu_p(1/2 + t_{z,i}) + \mu_n(1/2 - t_{z,i})$$

$$a_s = \langle \psi_{\text{gs}} I I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{\text{gs}} I I_z = I \rangle$$



## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

23

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{\text{NN}}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components
  - Admixes unnatural parity states in the ground state

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- Anapole moment calculation:

$$\kappa_A = \frac{\sqrt{2}e}{G_F} a_s$$

$$\kappa_A = -i4\pi \frac{e^2}{G_F mc} \frac{\hbar}{\sqrt{2I+1}} \sum_j \langle \psi_{\text{gs}} I^\pi | \sqrt{4\pi/3} \sum_{i=1}^A \mu_i r_i [Y_1(\hat{r}_i) \sigma_i]^{(1)} | \psi_j I^{-\pi} \rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

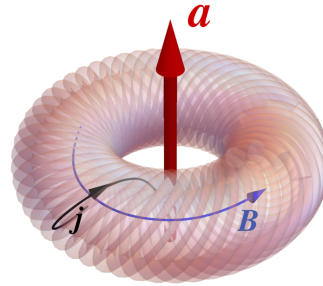
- Anapole moment operator dominated by spin contribution

$$\mathbf{a} = -\pi \int d^3r r^2 \mathbf{j}(\mathbf{r})$$

$$\hat{\mathbf{a}}_s = \frac{\pi e}{m} \sum_{i=1}^A \mu_i (\mathbf{r}_i \times \boldsymbol{\sigma}_i)$$

$$\mu_i = \mu_p(1/2 + t_{z,i}) + \mu_n(1/2 - t_{z,i})$$

$$a_s = \langle \psi_{\text{gs}} I I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{\text{gs}} I I_z = I \rangle$$



Low lying states of opposite parity can lead to enhancement!

## Parity violating (PV) and parity & time-reversal (PTV) violating nucleon-nucleon (NN) interaction

- Anapole moment arises due to PV NN interaction (weak force - imaginary), EDM and Schiff moment due to PTV NN interaction (real)
- Parity non-conserving PV or PTV  $V_{\text{NN}}^{\text{PNC}}$  interaction
  - Conserves total angular momentum  $I$
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components
  - Admixes unnatural parity states in the ground state
- EDM and Schiff moment operators

$$\hat{D}_z = \frac{e}{2} \sum_{i=1}^A (1 + \tau_i^z) z_i$$

$$\mathbf{S} = \frac{e}{10} \sum_{i=1}^Z \left( r_i^2 \mathbf{r}_i - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \mathbf{r}_i \right)$$

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- EDM and Schiff moment calculation
  - Nuclear EDM is dominated by and the Schiff moment determined by the polarization contribution:

$$D^{(pol)} = \langle \psi_{\text{gs}} I^\pi | \hat{D}_z | \psi_{\text{gs}} I \rangle + c.c.$$

$$\mathbf{S} = \langle \psi_{\text{gs}} I^\pi | \mathbf{S} | \psi_{\text{gs}} I \rangle + c.c.$$

**NCSM applications to parity-violating moments:**  
**How to calculate the sum of intermediate unnatural parity states?**

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

**NCSM applications to parity-violating moments:**  
**How to calculate the sum of intermediate unnatural parity states?**

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

Sum over all possible  
intermediate states

**NCSM applications to parity-violating moments:**  
**How to calculate the sum of intermediate unnatural parity states?**

27

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- Solving Schroedinger equation with inhomogeneous term

$$(E_{\text{gs}} - H)|\psi_{\text{gs}} I\rangle = V_{\text{NN}}^{\text{PNC}}|\psi_{\text{gs}} I^\pi\rangle$$

- To invert this equation, we apply the Lanczos algorithm

## NCSM applications to parity-violating moments: How to calculate the sum of intermediate unnatural parity states?

28

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- Solving Schroedinger equation with inhomogeneous term

$$(E_{\text{gs}} - H)|\psi_{\text{gs}} I\rangle = V_{\text{NN}}^{\text{PNC}}|\psi_{\text{gs}} I^\pi\rangle$$

- To invert this equation, we apply the Lanczos algorithm
  - Bring matrix to tri-diagonal form ( $\mathbf{v}_1, \mathbf{v}_2 \dots$  orthonormal,  $H$  Hermitian)

$$\begin{aligned} H\mathbf{v}_1 &= \alpha_1 \mathbf{v}_1 + \beta_1 \mathbf{v}_2 \\ H\mathbf{v}_2 &= \beta_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \beta_2 \mathbf{v}_3 \\ H\mathbf{v}_3 &= \beta_2 \mathbf{v}_2 + \alpha_3 \mathbf{v}_3 + \beta_3 \mathbf{v}_4 \\ H\mathbf{v}_4 &= \beta_3 \mathbf{v}_3 + \alpha_4 \mathbf{v}_4 + \beta_4 \mathbf{v}_5 \end{aligned}$$

- $n^{\text{th}}$  iteration computes  $2n^{\text{th}}$  moment
- Eigenvalues converge to extreme (largest in magnitude) values
- $\sim 150$ - $200$  iterations needed for 10 eigenvalues (even for  $10^9$  states)

Journal of Research of the National Bureau of Standards Vol. 45, No. 4, October 1950 Research Paper 2133  
An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators<sup>1</sup>  
By Cornelius Lanczos

## NCSM applications to parity-violating moments: How to calculate the sum of intermediate unnatural parity states?

29

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

- Solving Schroedinger equation with inhomogeneous term

$$(E_{\text{gs}} - H)|\psi_{\text{gs}} I\rangle = V_{\text{NN}}^{\text{PNC}}|\psi_{\text{gs}} I^\pi\rangle$$

- To invert this equation, we apply the Lanczos algorithm

$$|\mathbf{v}_1\rangle = V_{\text{NN}}^{\text{PNC}}|\psi_{\text{gs}} I^\pi\rangle$$

$$|\psi_{\text{gs}} I\rangle \approx \sum_k g_k(E_0)|\mathbf{v}_k\rangle$$

~100 iterations

$$\hat{g}_1(\omega) = \frac{1}{\omega - \alpha_1 - \frac{\beta_1^2}{\omega - \alpha_2 - \frac{\beta_2^2}{\omega - \alpha_3 - \beta_3^2}}}$$

...

Lanczos continued  
fraction method  
or  
Lanczos strength  
method

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 17, 1974. Printed in Great Britain. © 1974

### The inverse of a linear operator

Roger Haydock

Few-Body Systems 33, 259–276 (2003)  
DOI 10.1007/s00601-003-0017-z

Few-  
Body  
Systems  
Printed in Austria

### Efficient Method for Lorentz Integral Transforms of Reaction Cross Sections

M. A. Marchisio<sup>1</sup>, N. Barnea<sup>2</sup>, W. Leidemann<sup>1</sup>, and G. Orlandini<sup>1</sup>

*Ab initio* calculations of electric dipole moments of light nuclei

Paul Froese\*  
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada  
and Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

Petr Navrátil†  
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

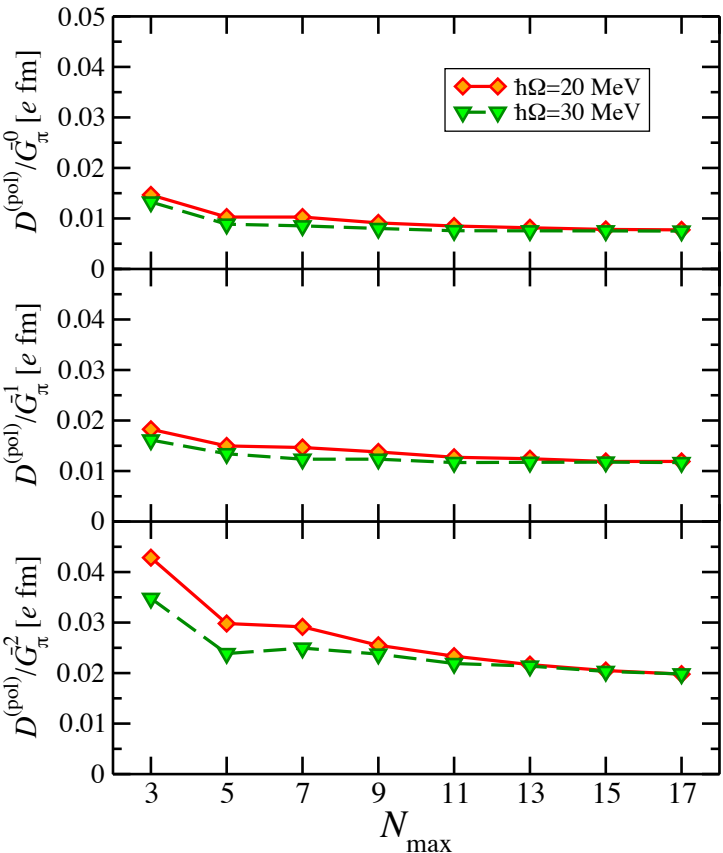
**<sup>3</sup>He EDM Benchmark Calculation**

Discrepancy between calculations?

	PLB 665:165-172 (2008) (NN EFT)	PRC 87:015501 (2013)	PRC 91:054005 (2015)	Our calculation (NN EFT)
$\bar{G}_\pi^0$	0.015	(x 1/2)	(x 1/2)	0.0073 (x 1/2)
$\bar{G}_\pi^1$	0.023	(x 1/2)	(x 1/2)	0.011 (x 1/2)
$\bar{G}_\pi^2$	0.037	(x 1/5)	(x 1/2)	0.019 (x 1/2)
$\bar{G}_\rho^0$	-0.0012	(x 1/2)	(x 1/2)	-0.00062 (x 1/2)
$\bar{G}_\rho^1$	0.0013	(x 1/2)	(x 1/2)	0.00063 (x 1/2)
$\bar{G}_\rho^2$	-0.0028	(x 1/5)	(x 1/2)	-0.0014 (x 1/2)
$\bar{G}_\omega^0$	0.0009	(x 1/2)	(x 1/2)	0.00042 (x 1/2)
$\bar{G}_\omega^1$	-0.0017	(x 1/2)	(x 1/2)	-0.00086 (x 1/2)

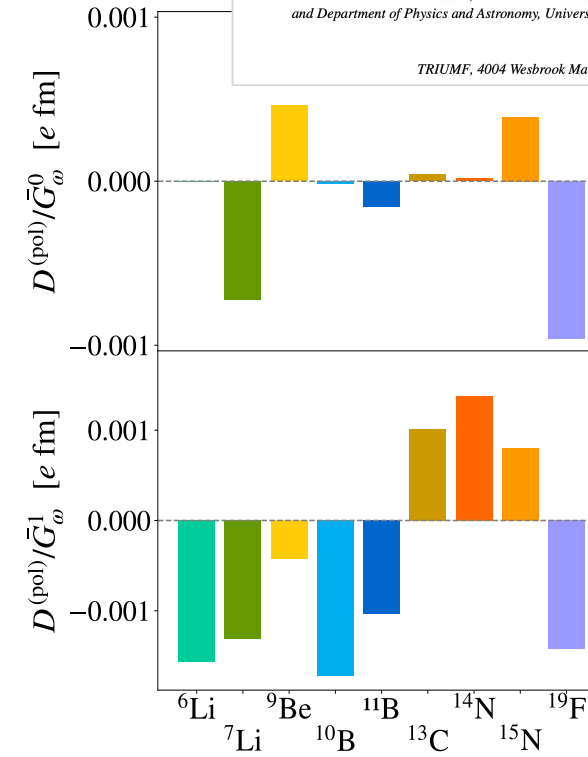
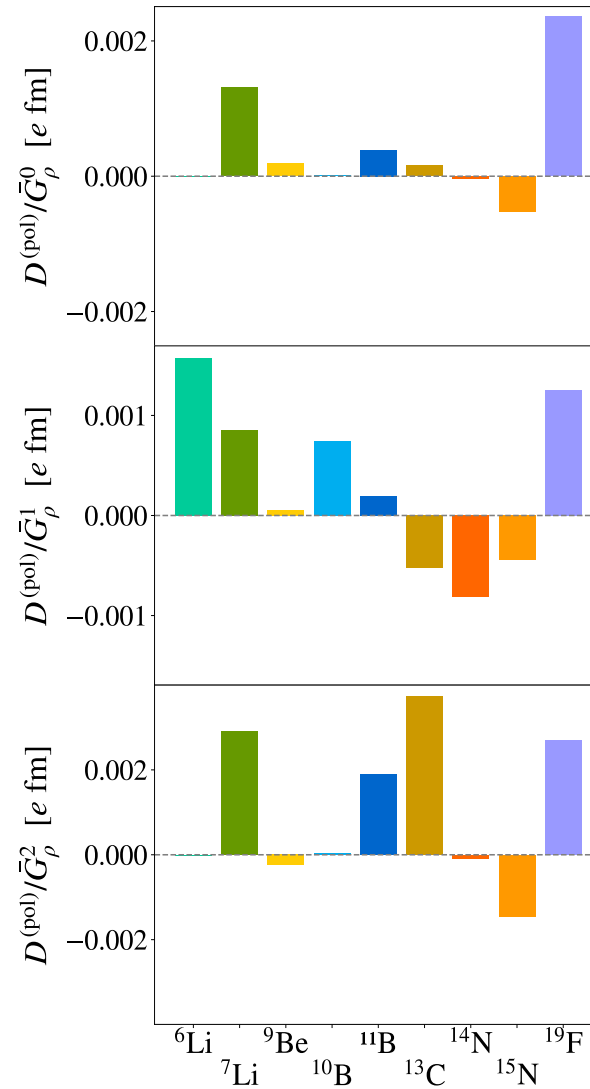
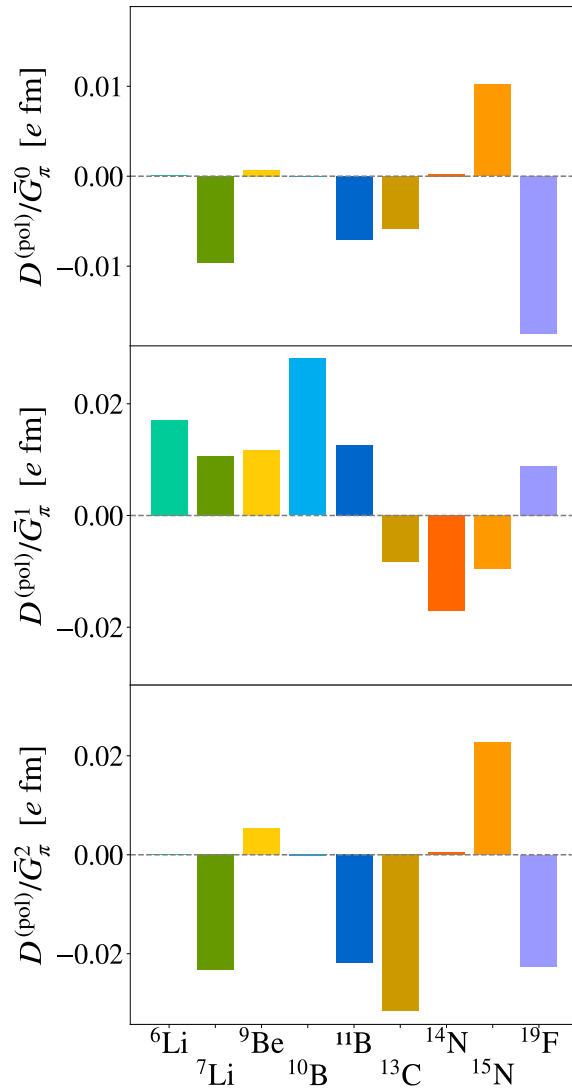
**$N_{\max}$  convergence for <sup>3</sup>He**

N<sup>3</sup>LO NN

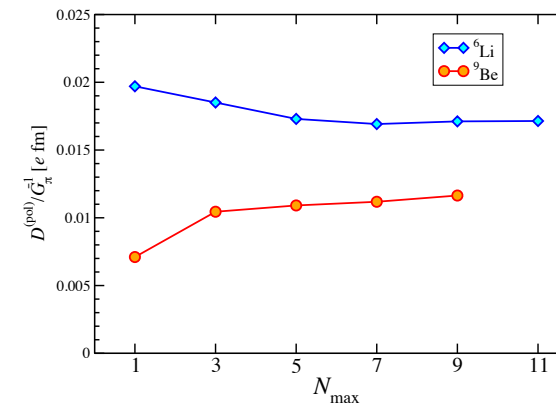


Our results confirm those of Yamanaka and Hiyama, PRC 91:054005 (2015)

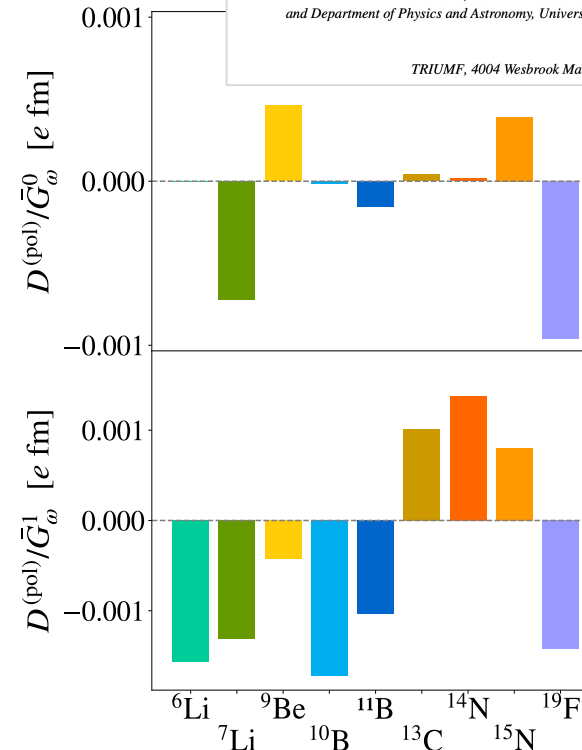
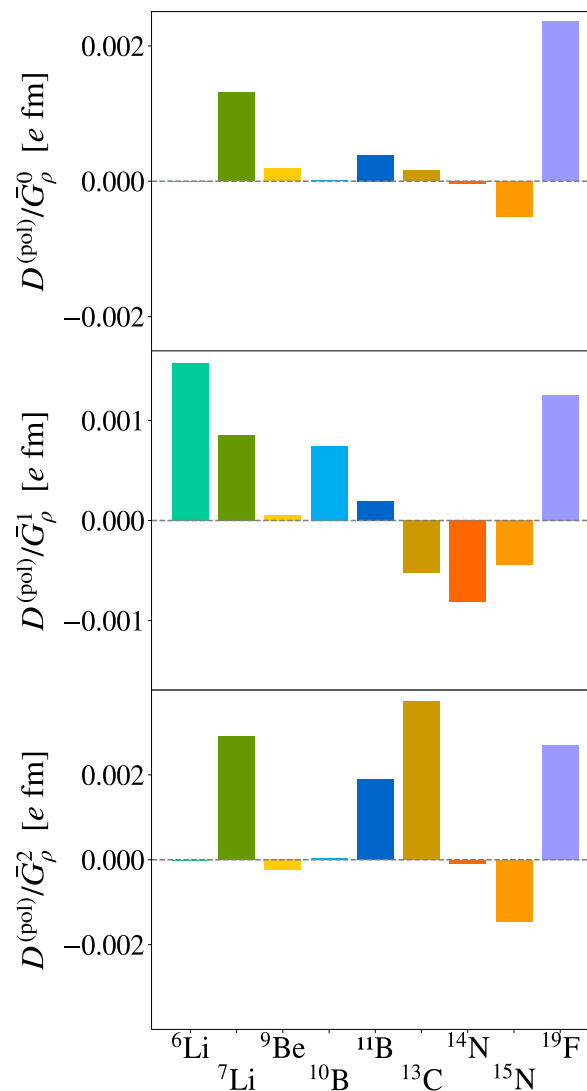
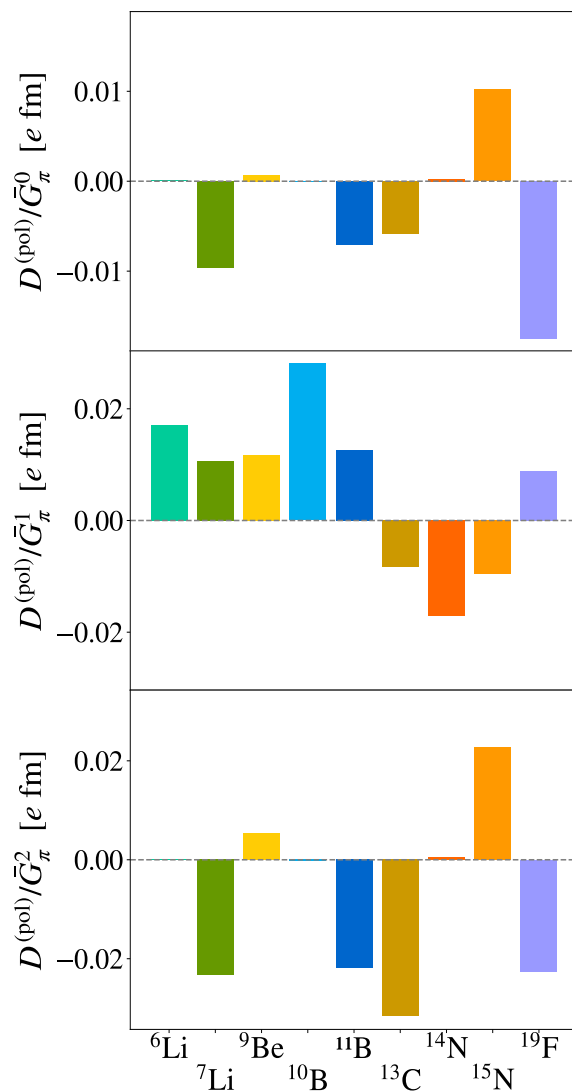
# NCSM applications to parity-violating moments: EDMs of light stable nuclei



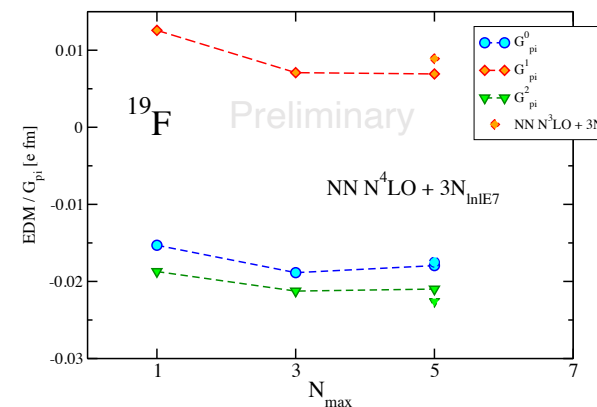
## Examples of $N_{\max}$ convergence



# NCSM applications to parity-violating moments: EDMs of light stable nuclei

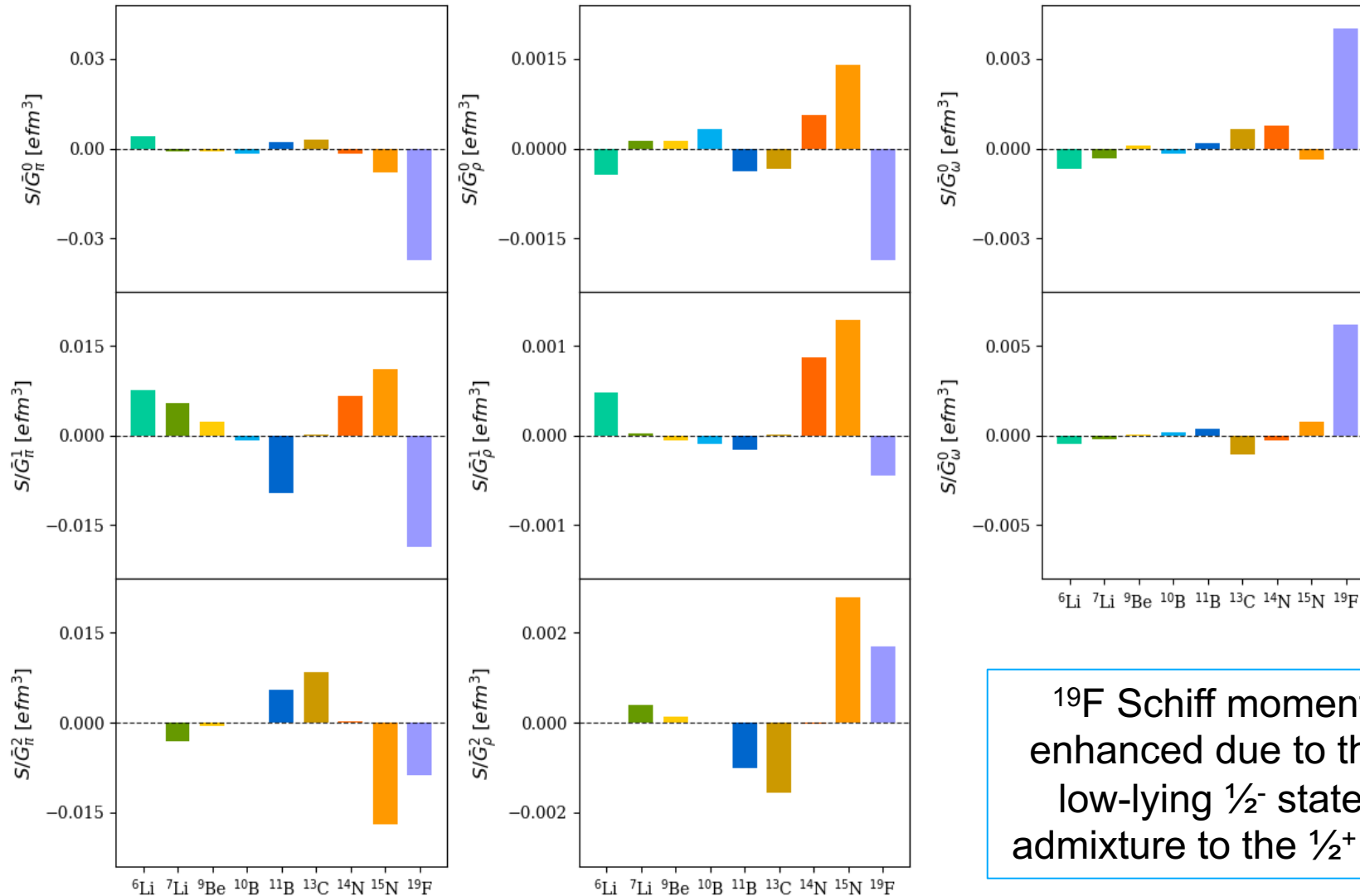


## Examples of $N_{\max}$ convergence



# NCSM applications to parity-violating moments: Schiff moments of light stable nuclei

Results preliminary

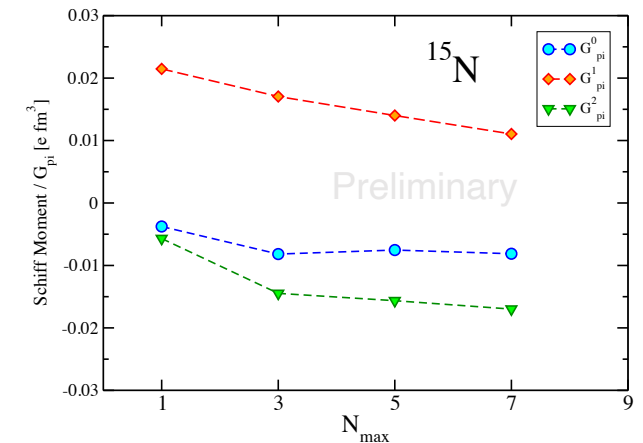


$^{19}\text{F}$  Schiff moment enhanced due to the low-lying  $\frac{1}{2}^-$  state admixture to the  $\frac{1}{2}^+$  gs

Work in progress  
with Stephan Foster,  
McMaster University  
undergraduate student

33

Examples of  $N_{\max}$  convergence



Convergence more challenging due to a destructive contribution of the two terms and the long-range  $r^3$  dependence

$$s = \frac{e}{10} \sum_{i=1}^Z \left( r_i^2 \mathbf{r}_i - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \mathbf{r}_i \right)$$

# NCSM applications to parity-violating moments: Schiff moment of $^{19}\text{F}$

Results preliminary

Calculated  $1/2^-$  state energies shifted to match the  $1/2^-_{-1}$  excitation energy

Relevant for planned nuclear Schiff moment measurements in  $^{227}\text{ThF}^+$  at TRIUMF

34

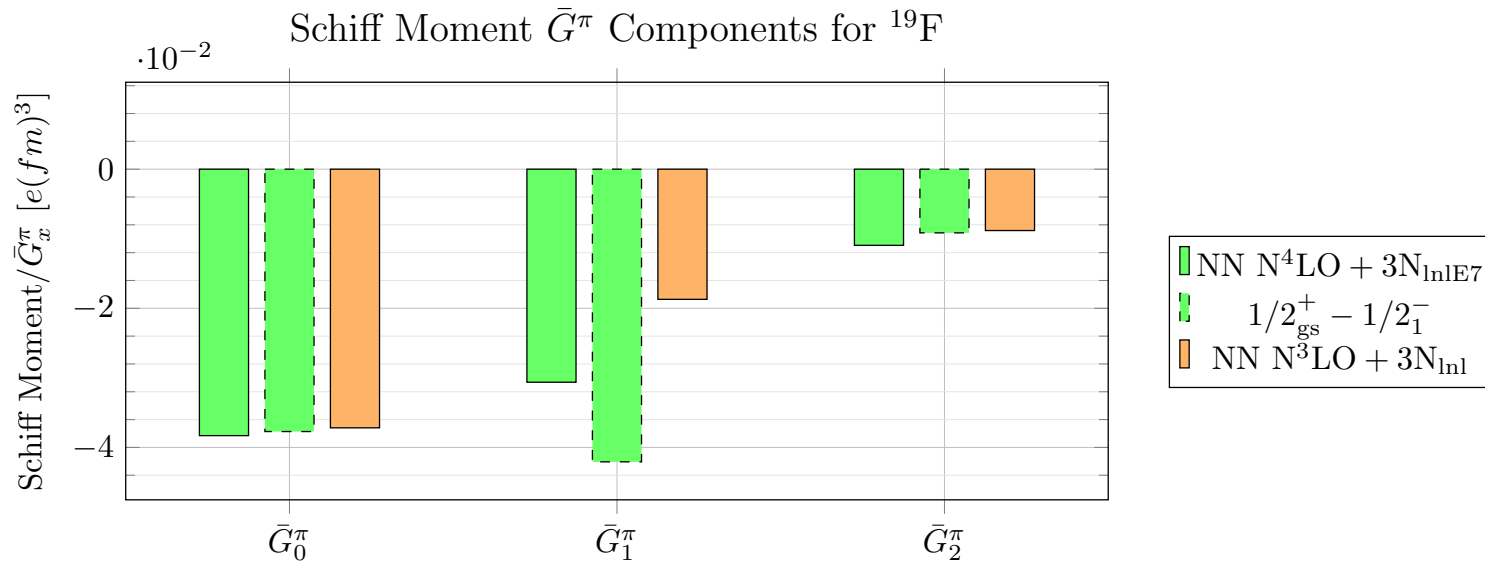
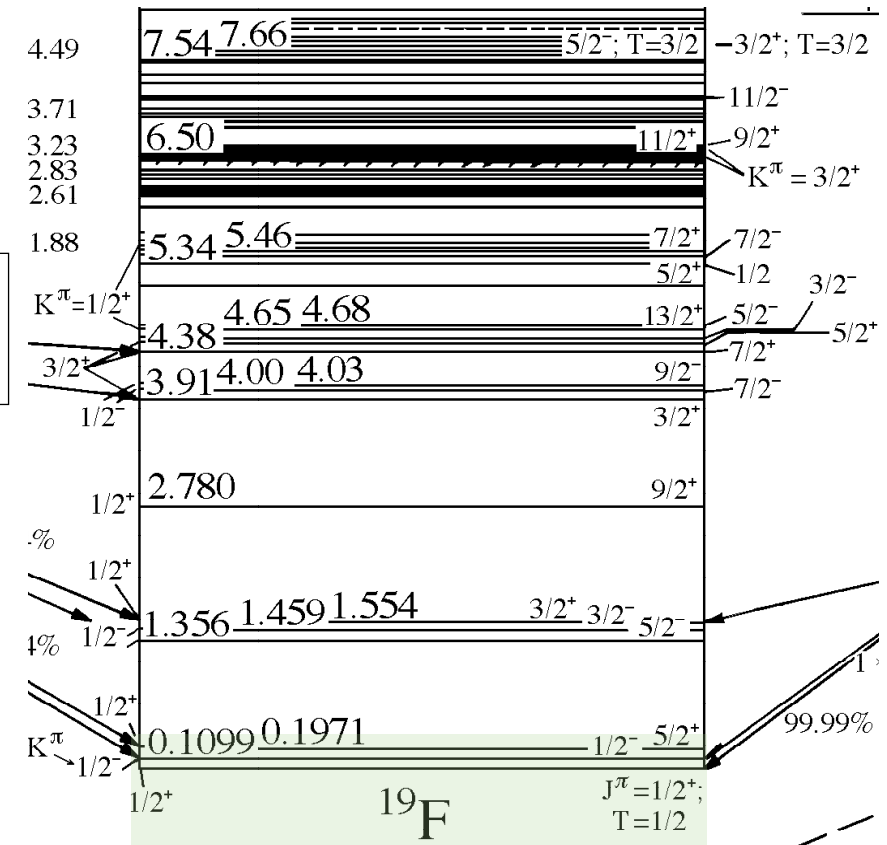


Figure 1: Comparison of  $^{19}\text{F}$   $\bar{G}^\pi$  components for different interactions and included states.

$$S = \langle \psi_{\text{gs}} I^\pi | S | \psi_{\text{gs}} I \rangle + c. c.$$

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

$^{19}\text{F}$  Schiff moment enhanced due to the low-lying  $1/2^-$  state admixture to the  $1/2^+$  gs



$$s = \frac{e}{10} \sum_{i=1}^Z \left( r_i^2 \mathbf{r}_i - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \mathbf{r}_i \right)$$

## Schiff moment of $^{19}\text{F}$

## Results preliminary

Calculated  $\frac{1}{2}^-$  state  
energies shifted to match  
the  $\frac{1}{2}^-_{1}$  excitation energy

Relevant for planned nuclear  
Schiff moment measurements in  
 $^{227}\text{ThF}^+$  at TRIUMF

35

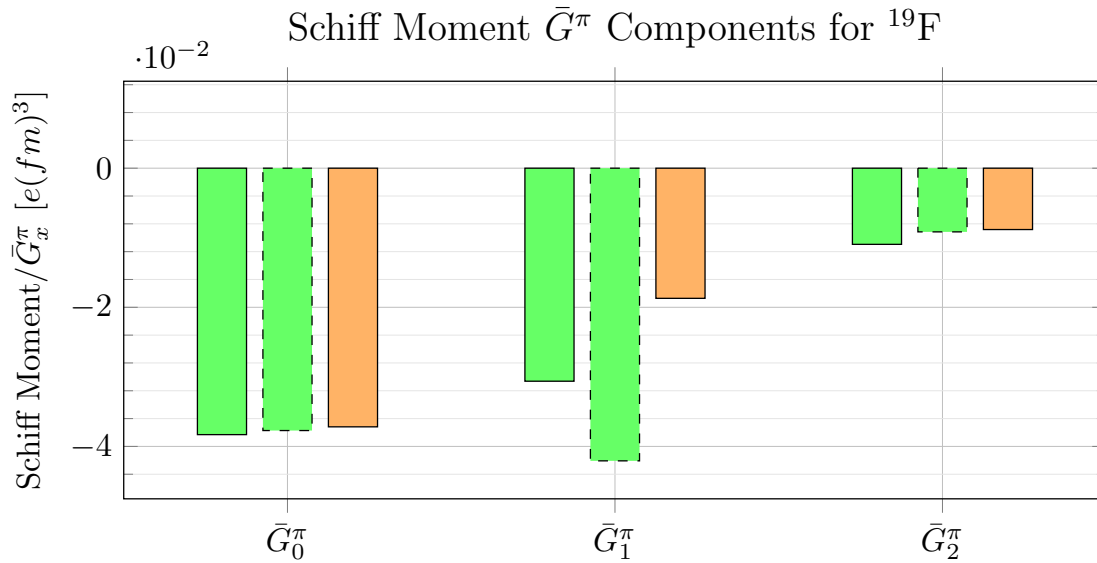
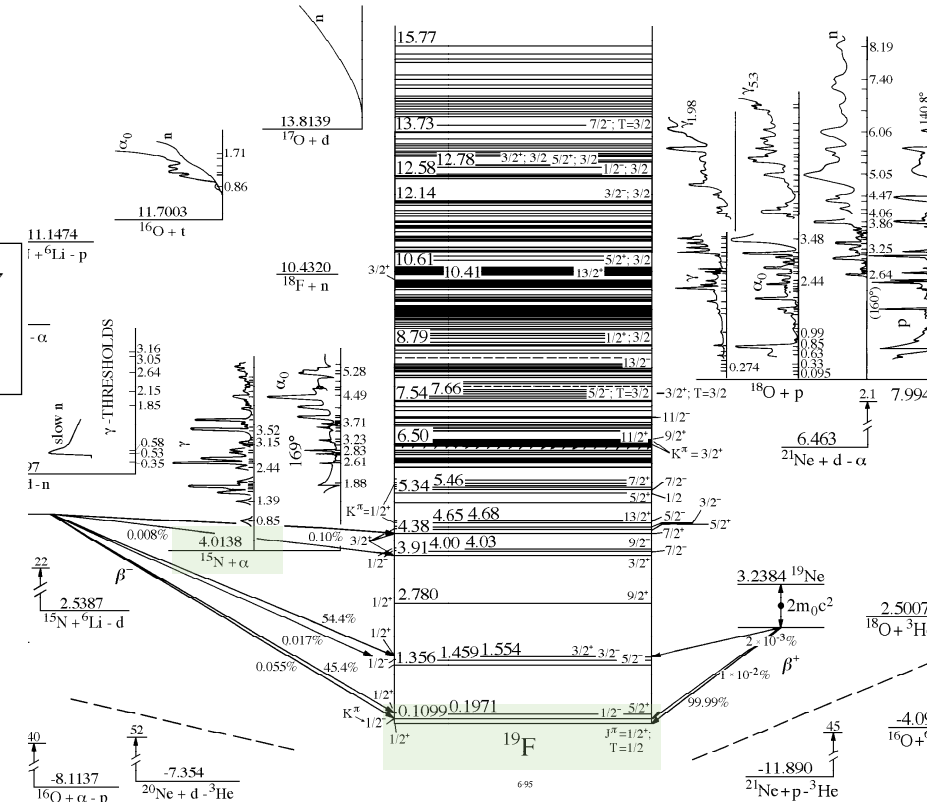


Figure 1: Comparison of  $^{19}\text{F}$   $\bar{G}^\pi$  components for different interactions and included states.

$$S = \langle \psi_{\text{gs}} I^\pi | \mathbf{S} | \psi_{\text{gs}} I \rangle + c.c.$$

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

<sup>19</sup>F Schiff moment  
enhanced due to the  
low-lying 1/2<sup>-</sup> state  
admixture to the 1/2<sup>+</sup> gs



$$\mathbf{S} = \frac{e}{10} \sum_{i=1}^Z \left( r_i^2 \mathbf{r}_i - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \mathbf{r}_i \right)$$

# NCSM applications to parity-violating moments: Schiff moment of $^{19}\text{F}$

Results preliminary

Calculated  $\frac{1}{2}^-$  state energies shifted to match the  $\frac{1}{2}^-_{-1}$  excitation energy

Relevant for planned nuclear Schiff moment measurements in  $^{227}\text{ThF}^+$  at TRIUMF

36

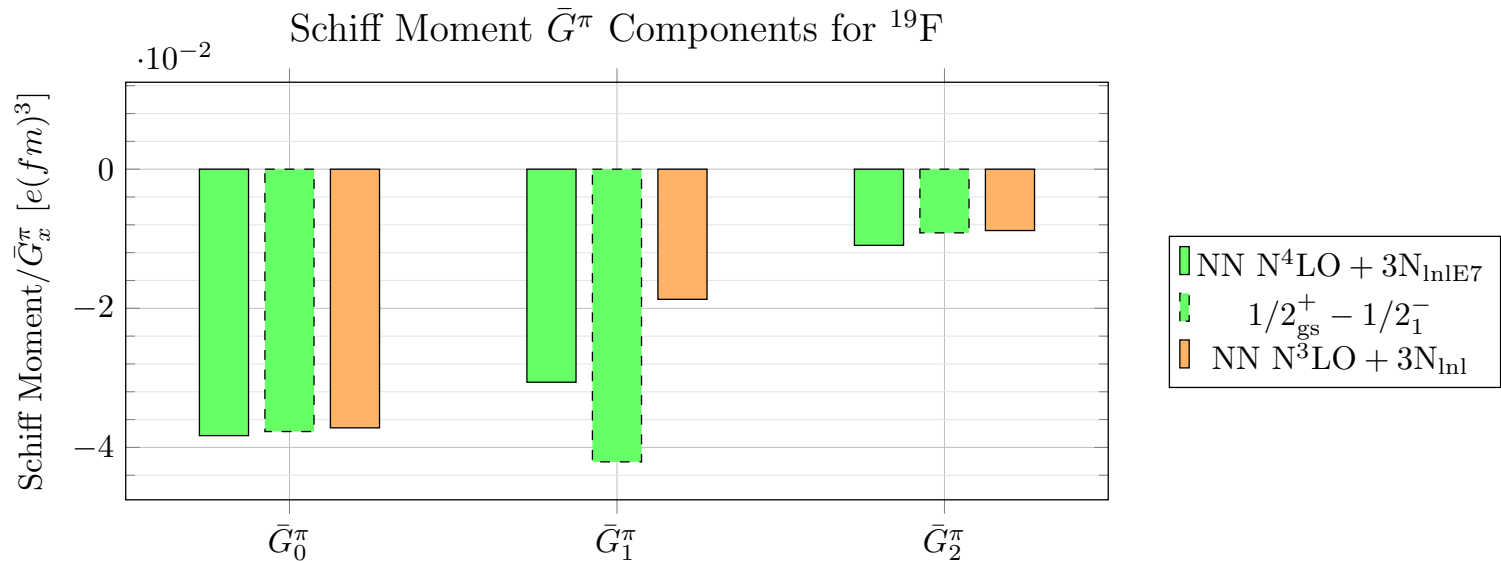


Figure 1: Comparison of  $^{19}\text{F}$   $\bar{G}^\pi$  components for different interactions and included states.

$$S = \langle \psi_{\text{gs}} I^\pi | S | \psi_{\text{gs}} I \rangle + c. c.$$

$$|\psi_{\text{gs}} I\rangle = |\psi_{\text{gs}} I^\pi\rangle + \sum_j |\psi_j I^{-\pi}\rangle \times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

$^{19}\text{F}$  Schiff moment enhanced due to the low-lying  $\frac{1}{2}^-$  state admixture to the  $\frac{1}{2}^+$  gs

$^{19}\text{F}$  Schiff moment comparable to  $^{129}\text{Xe}$  Schiff moment calculated within the nuclear shell model

PHYSICAL REVIEW C **102**, 065502 (2020)

Large-scale shell-model calculations of nuclear Schiff moments of  $^{129}\text{Xe}$  and  $^{199}\text{Hg}$

Kota Yanase<sup>\*</sup> and Noritaka Shimizu<sup>†</sup>

TABLE II. The NSM coefficients of  $^{129}\text{Xe}$  in units of  $10^{-2} e fm^3$ . Our final results are given in bold.

	$a_0$	$a_1$	$a_2$
IPM ( $m_\pi \rightarrow \infty$ )	-9.9	-9.9	-19.8
IPM	-4.6	-4.6	-9.2
LSSM (SN100PN, $m_\pi \rightarrow \infty$ )	-8.7	-8.2	-15.8
LSSM (SNV, $m_\pi \rightarrow \infty$ )	-8.6	-8.3	-16.2
LSSM (SN100PN)	-3.7	-4.1	-8.0
LSSM (SNV)	<b>-3.8</b>	<b>-4.1</b>	<b>-8.1</b>
IPM ( $m_\pi \rightarrow \infty$ ) [35,36]	-11	-11	-22
IPM [38]	-6	-6	-12
RPA [38]	-0.8	-0.6	-0.9
PTSM [41]	0.05	-0.04	0.19
PTSM [42]	0.3	-0.1	0.4

$$S = \frac{e}{10} \sum_{i=1}^Z \left( r_i^2 \mathbf{r}_i - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \mathbf{r}_i \right)$$

# NCSM applications to parity-violating moments: Schiff moment of $^{19}\text{F}$

Results preliminary

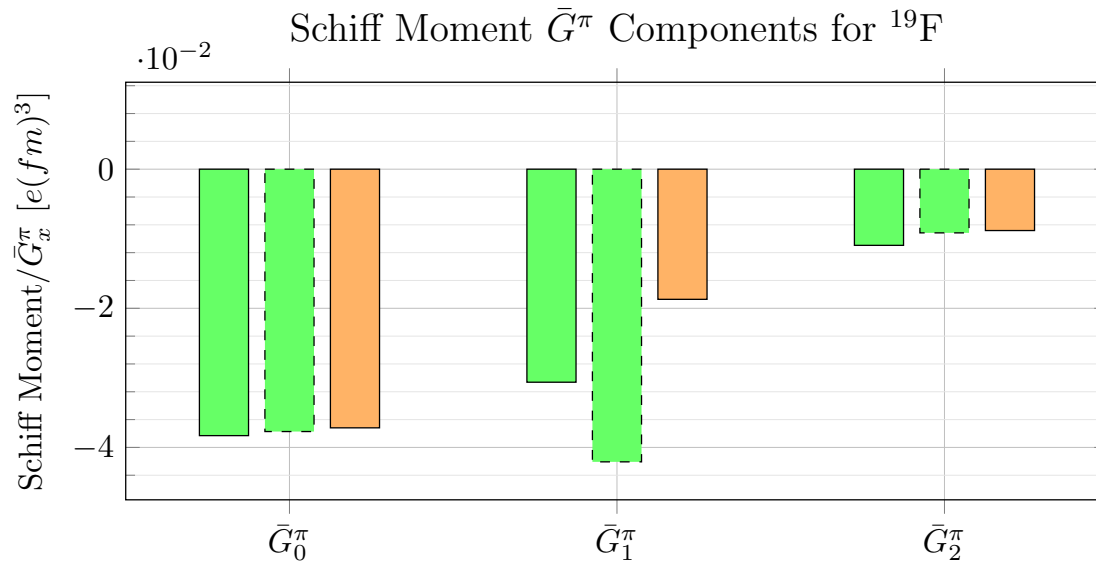


Figure 1: Comparison of  $^{19}\text{F}$   $\bar{G}^\pi$  components for different interactions and included states.

$$S = \langle \psi_{\text{gs}} I^\pi | S | \psi_{\text{gs}} I \rangle + c.c.$$

$$| \psi_{\text{gs}} I \rangle = | \psi_{\text{gs}} I^\pi \rangle + \sum_j | \psi_j I^{-\pi} \rangle$$

$$\times \frac{1}{E_{\text{gs}} - E_j} \langle \psi_j I^{-\pi} | V_{\text{NN}}^{\text{PNC}} | \psi_{\text{gs}} I^\pi \rangle$$

Recent high-precision measurements of the **molecular electric dipole moment of  $^{180}\text{Hf}^{19}\text{F}^+$**  in combination with **quantum-chemistry calculations** to evaluate the sensitivity of the hafnium monofluoride cation,  **$\text{HfF}^+$ , to the NSM of  $^{19}\text{F}$**  and with ***ab initio* calculations of the  $^{19}\text{F}$  NSM** allows to set an **experimental limit on the PTV pion-nucleon couplings**.

■ NN N<sup>4</sup>LO + 3N<sub>lnl</sub>E7  
▤ 1/2<sub>gs</sub><sup>+</sup> - 1/2<sub>1</sub><sup>-</sup>  
■ NN N<sup>3</sup>LO + 3N<sub>lnl</sub>

$$\bar{G}_t^\pi = g \bar{g}_t \quad (g \sim 13.5)$$

$$S(^{19}\text{F}) = (-4.3 g \bar{g}_0 - 3.1 g \bar{g}_1 - 1.4 g \bar{g}_2) \times 10^{-2} e \text{ fm}^3$$

Quantity	Limit
$ \bar{g}_0 $	$1.6 \times 10^{-8}$
$ \bar{g}_1 $	$2.2 \times 10^{-8}$
$ \bar{g}_2 $	$4.8 \times 10^{-8}$

## Nuclear Schiff moment of the fluorine isotope $^{19}\text{F}$

Kia Boon Ng,<sup>1,\*</sup> Stephan Foster,<sup>1,2</sup> Lan Cheng,<sup>3</sup> Petr Navrátil,<sup>1</sup> and Stephan Malbrunot-Ettenauer<sup>1,4</sup>

arXiv:2507.19811

## Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao<sup>1</sup>, Petr Navrátil<sup>2</sup>, Eric B. Norrgard<sup>3</sup>, Miroslav Iliaš<sup>4</sup>, Ephraim Eliav<sup>5</sup>, Rob G. E. Timmermans<sup>1</sup>, Victor V. Flambaum<sup>6</sup>, and Anastasia Borschevsky<sup>1,\*</sup>

38

## Nuclear spin-dependent parity-violating effects from NCSM

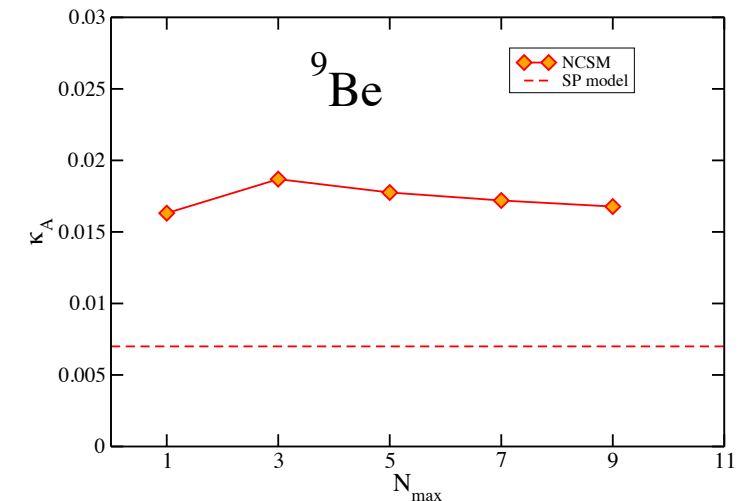
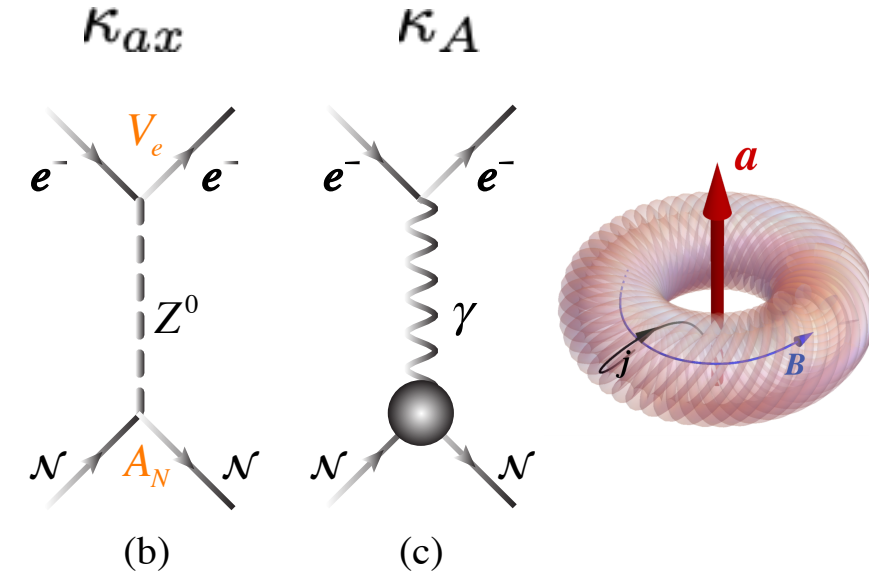
- Contributions from nucleon axial-vector and the anapole moment

	<sup>9</sup> Be	<sup>13</sup> C	<sup>14</sup> N	<sup>15</sup> N	<sup>25</sup> Mg
$I^\pi$	$3/2^-$	$1/2^-$	$1^+$	$1/2^-$	$5/2^+$
$\mu^{\text{exp.}}$	$-1.177^{\text{a}}$	$0.702^{\text{b}}$	$0.404^{\text{c}}$	$-0.283^{\text{d}}$	$-0.855^{\text{e}}$
NCSM calculations					
$\mu$	$-1.05$	$0.44$	$0.37$	$-0.25$	$-0.50$
$\kappa_A$	$0.016$	$-0.028$	$0.036$	$0.088$	$0.035$
$\langle s_{p,z} \rangle$	$0.009$	$-0.049$	$-0.183$	$-0.148$	$0.06$
$\langle s_{n,z} \rangle$	$0.360$	$-0.141$	$-0.1815$	$0.004$	$0.30$
$\kappa_{ax}$	$0.035$	$-0.009$	$0.0002$	$0.015$	$0.024$
$\kappa$	$0.050$	$-0.037$	$0.037$	$0.103$	$0.057$

$$\kappa_{ax} \simeq -2C_{2p}\langle s_{p,z} \rangle - 2C_{2n}\langle s_{n,z} \rangle \simeq -0.1\langle s_{p,z} \rangle + 0.1\langle s_{n,z} \rangle$$

$$\langle s_{\nu,z} \rangle \equiv \langle \psi_{\text{gs}} | I^\pi I_z = I | \hat{s}_{\nu,z} | \psi_{\text{gs}} | I^\pi I_z = I \rangle$$

$$C_{2p} = -C_{2n} = g_A(1 - 4\sin^2 \theta_W)/2 \simeq 0.05$$



## Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao<sup>1</sup>, Petr Navrátil<sup>2</sup>, Eric B. Norrgard<sup>3</sup>, Miroslav Iliaš<sup>4</sup>, Ephraim Eliav<sup>5</sup>, Rob G. E. Timmermans<sup>1</sup>, Victor V. Flambaum<sup>6</sup>, and Anastasia Borschevsky<sup>1,\*</sup>

39

## Nuclear spin-dependent parity-violating effects from NCSM

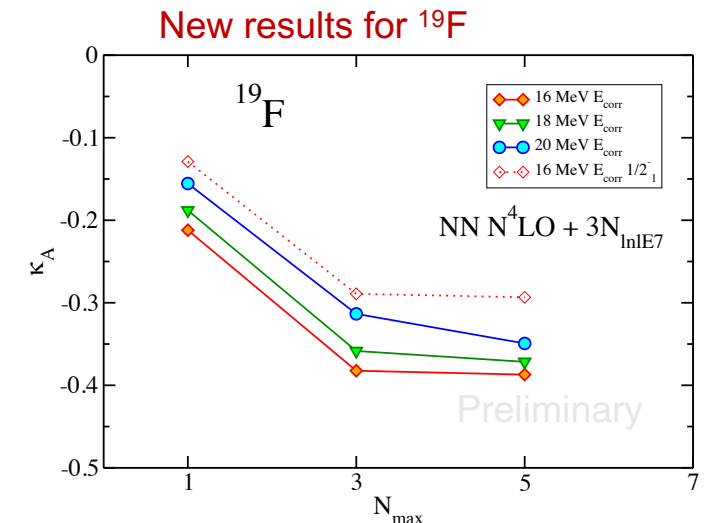
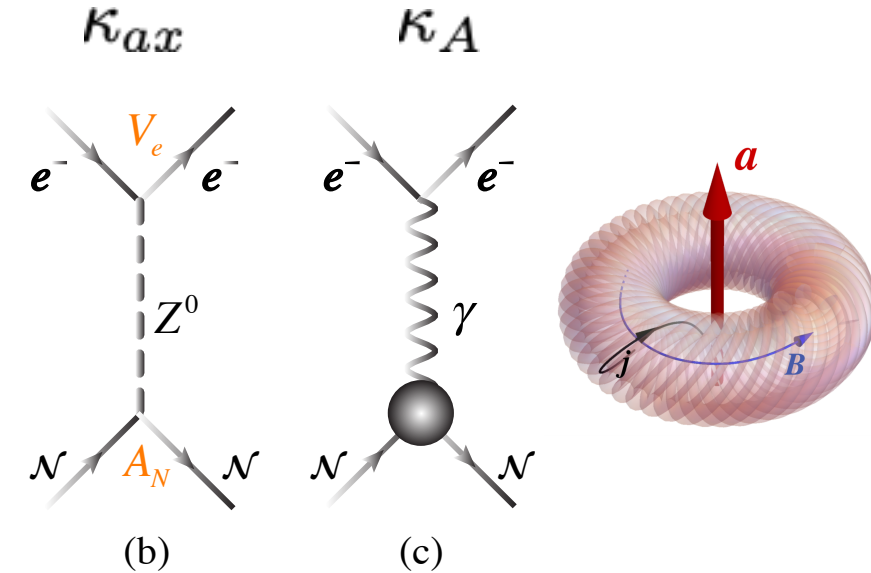
- Contributions from nucleon axial-vector and the anapole moment

	<sup>9</sup> Be	<sup>13</sup> C	<sup>14</sup> N	<sup>15</sup> N	<sup>25</sup> Mg
$I^\pi$	$3/2^-$	$1/2^-$	$1^+$	$1/2^-$	$5/2^+$
$\mu^{\text{exp.}}$	$-1.177^{\text{a}}$	$0.702^{\text{b}}$	$0.404^{\text{c}}$	$-0.283^{\text{d}}$	$-0.855^{\text{e}}$
NCSM calculations					
$\mu$	$-1.05$	$0.44$	$0.37$	$-0.25$	$-0.50$
$\kappa_A$	$0.016$	$-0.028$	$0.036$	$0.088$	$0.035$
$\langle s_{p,z} \rangle$	$0.009$	$-0.049$	$-0.183$	$-0.148$	$0.06$
$\langle s_{n,z} \rangle$	$0.360$	$-0.141$	$-0.1815$	$0.004$	$0.30$
$\kappa_{ax}$	$0.035$	$-0.009$	$0.0002$	$0.015$	$0.024$
$\kappa$	$0.050$	$-0.037$	$0.037$	$0.103$	$0.057$

$$\kappa_{ax} \simeq -2C_{2p}\langle s_{p,z} \rangle - 2C_{2n}\langle s_{n,z} \rangle \simeq -0.1\langle s_{p,z} \rangle + 0.1\langle s_{n,z} \rangle$$

$$\langle s_{\nu,z} \rangle \equiv \langle \psi_{\text{gs}} | I^\pi I_z = I | \hat{s}_{\nu,z} | \psi_{\text{gs}} | I^\pi I_z = I \rangle$$

$$C_{2p} = -C_{2n} = g_A(1 - 4\sin^2 \theta_W)/2 \simeq 0.05$$



## Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao<sup>1</sup>, Petr Navrátil<sup>2</sup>, Eric B. Norrgard<sup>3</sup>, Miroslav Iliaš<sup>4</sup>, Ephraim Eliav<sup>5</sup>, Rob G. E. Timmermans<sup>1</sup>, Victor V. Flambaum<sup>6</sup>, and Anastasia Borschevsky<sup>1,\*</sup>

40

## Nuclear spin-dependent parity-violating effects from NCSM

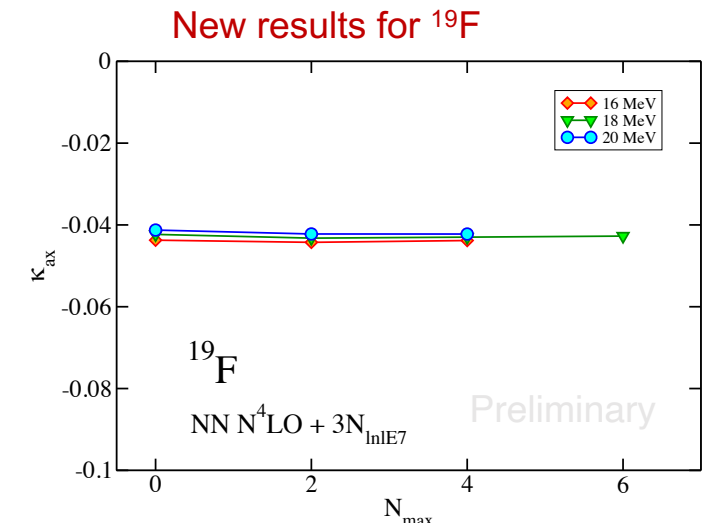
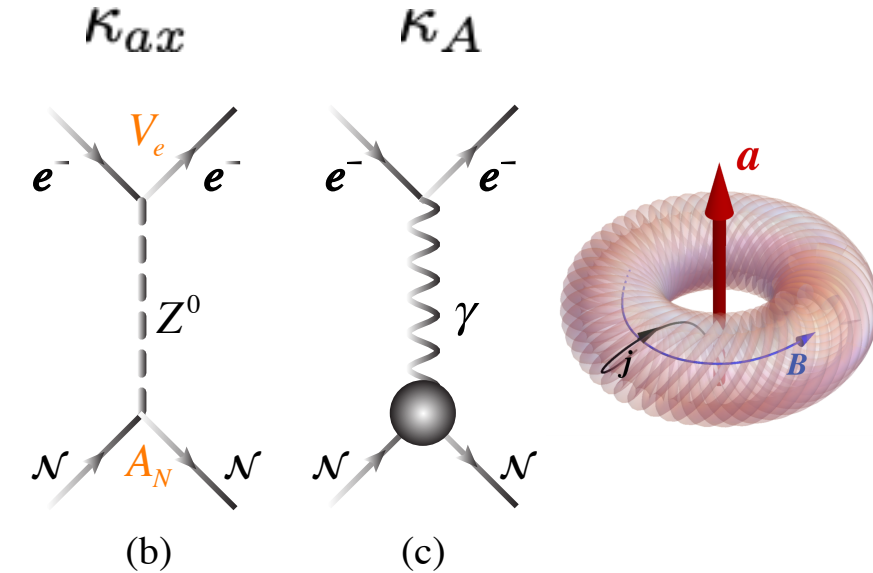
- Contributions from nucleon axial-vector and the anapole moment

	<sup>9</sup> Be	<sup>13</sup> C	<sup>14</sup> N	<sup>15</sup> N	<sup>25</sup> Mg
$I^\pi$	$3/2^-$	$1/2^-$	$1^+$	$1/2^-$	$5/2^+$
$\mu^{\text{exp.}}$	$-1.177^{\text{a}}$	$0.702^{\text{b}}$	$0.404^{\text{c}}$	$-0.283^{\text{d}}$	$-0.855^{\text{e}}$
NCSM calculations					
$\mu$	$-1.05$	$0.44$	$0.37$	$-0.25$	$-0.50$
$\kappa_A$	$0.016$	$-0.028$	$0.036$	$0.088$	$0.035$
$\langle s_{p,z} \rangle$	$0.009$	$-0.049$	$-0.183$	$-0.148$	$0.06$
$\langle s_{n,z} \rangle$	$0.360$	$-0.141$	$-0.1815$	$0.004$	$0.30$
$\kappa_{ax}$	$0.035$	$-0.009$	$0.0002$	$0.015$	$0.024$
$\kappa$	$0.050$	$-0.037$	$0.037$	$0.103$	$0.057$

$$\kappa_{ax} \simeq -2C_{2p}\langle s_{p,z} \rangle - 2C_{2n}\langle s_{n,z} \rangle \simeq -0.1\langle s_{p,z} \rangle + 0.1\langle s_{n,z} \rangle$$

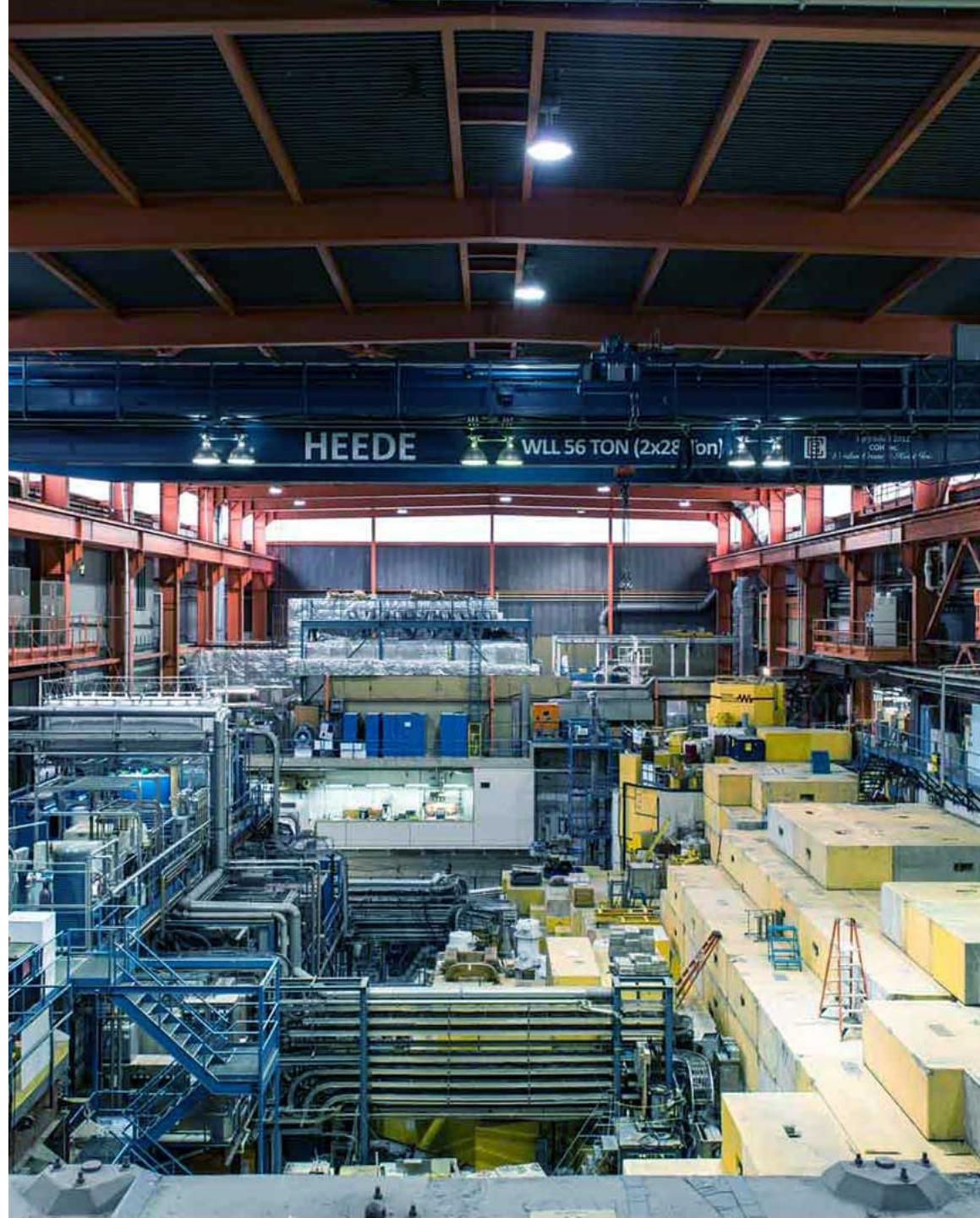
$$\langle s_{\nu,z} \rangle \equiv \langle \psi_{\text{gs}} | I^\pi I_z = I | \hat{s}_{\nu,z} | \psi_{\text{gs}} | I^\pi I_z = I \rangle$$

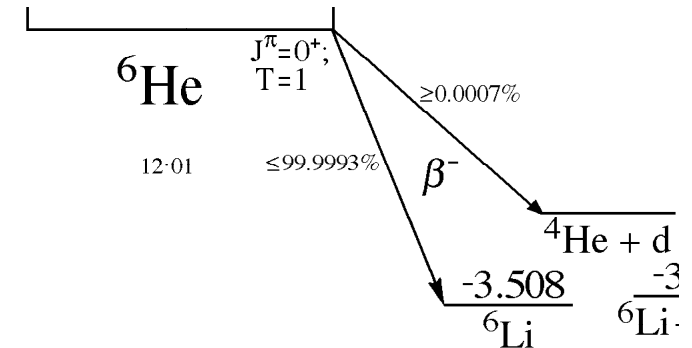
$$C_{2p} = -C_{2n} = g_A(1 - 4\sin^2 \theta_W)/2 \simeq 0.05$$



# Search for beyond the standard model physics in ${}^6\text{He}$ $\beta$ decay

2025-09-30





# Precise measurements of $\beta$ decays to search for Physics Beyond the Standard Model

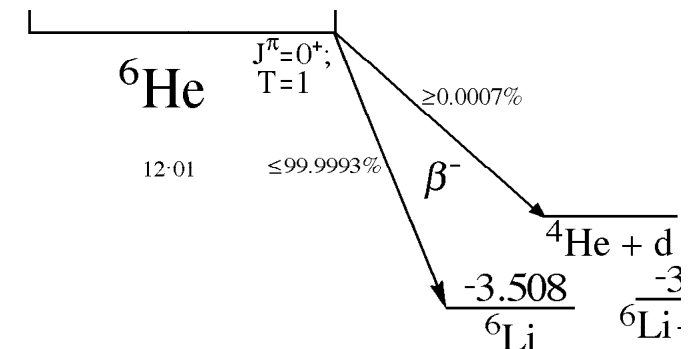
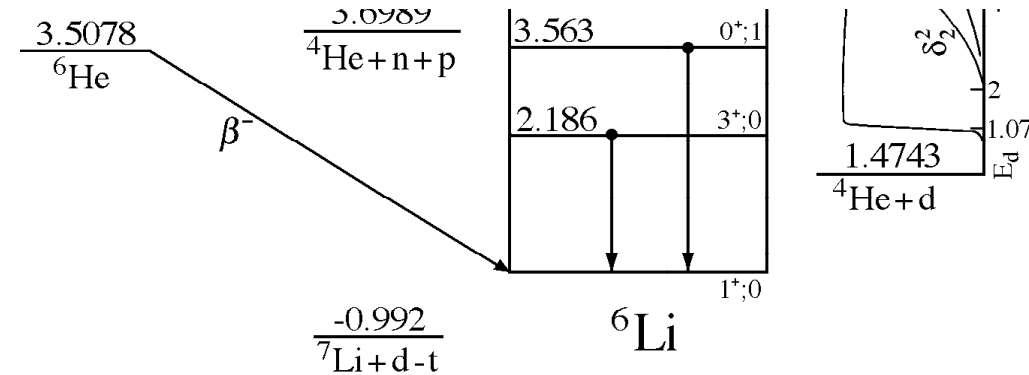
43

- In the presence of Beyond the Standard Model interactions

$$a_{\beta\nu}^{\text{BSM}} = -\frac{1}{3} \left( 1 - \frac{|C_T|^2 + |C'_T|^2}{2|C_A|^2} \right)$$

$$b_{\text{Fierz}}^{\text{BSM}} = \frac{C_T + C'_T}{C_A}$$

- with tensor and pseudo-tensor contributions
- However, deviations also within the Standard Model caused by the finite momentum transfer, higher-order transition operators, and nuclear structure effects
  - Detailed, accurate, and precise calculations required



# Precise measurements of $\beta$ decays to search for Physics Beyond the Standard Model

44

- Higher-order Standard Model recoil and shape corrections

$$a_{\beta\nu}^{1+\beta^-} = -\frac{1}{3} \left( 1 + \tilde{\delta}_a^{1+\beta^-} \right)$$

$$b_F^{1+\beta^-} = \delta_b^{1+\beta^-}$$

$$\delta_1^{1+\beta^-} \equiv \frac{2}{3} \Re \left[ -E_0 \frac{\langle \|\hat{C}_1^A/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} + \sqrt{2} (E_0 - 2E) \frac{\langle \|\hat{M}_1^V/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} \right] - \frac{4}{7} ER\alpha Z_f - \frac{233}{630} (\alpha Z_f)^2,$$

$$\tilde{\delta}_a^{1+\beta^-} \equiv \frac{4}{3} \Re \left[ 2E_0 \frac{\langle \|\hat{C}_1^A/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} + \sqrt{2} (E_0 - 2E) \frac{\langle \|\hat{M}_1^V/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} \right] + \frac{4}{7} ER\alpha Z_f - \frac{2}{5} E_0 R\alpha Z_f,$$

$$\delta_b^{1+\beta^-} \equiv \frac{2}{3} m_e \Re \left[ \frac{\langle \|\hat{C}_1^A/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} + \sqrt{2} \frac{\langle \|\hat{M}_1^V/q\| \rangle}{\langle \|\hat{L}_1^A\| \rangle} \right],$$

$$\vec{q} = \vec{k} + \vec{\nu} \quad \text{momentum transfer}$$

$$\hat{C}_1^A \quad \text{axial charge}$$

$$\hat{M}_1^V \quad \text{vector magnetic or weak magnetism}$$

$$\hat{L}_1^A \propto 1 \quad \text{Gamow-Teller leading order}$$

$$\hat{C}_1^A \quad \hat{M}_1^V \quad \text{NLO recoil corrections, order } q/m_N$$

Apply *ab initio* No-Core Shell Model to calculate the  ${}^6\text{Li}$  and  ${}^6\text{He}$  wave functions and the operator matrix elements

# Precise measurements of $\beta$ decays to search for Physics Beyond the Standard Model

45

- Higher-order Standard Model recoil and shape corrections

$$\begin{aligned}\frac{\hat{C}_{JM_J}^A}{q} &= \sum_{j=1}^A \frac{i}{m_N} \left[ g_A \hat{\Omega}'_{JM_J}(q\vec{r}_j) \right. \\ &\quad \left. - \frac{1}{2} \frac{\tilde{g}_P}{2m_N} (E_0 + \Delta E_c) \hat{\Sigma}''_{JM_J}(q\vec{r}_j) \right] \tau_j^+, \\ \hat{L}_{JM_J}^A &= \sum_{j=1}^A i \left( g_A + \frac{\tilde{g}_P}{(2m_N)^2} q^2 \right) \hat{\Sigma}''_{JM_J}(q\vec{r}_j) \tau_j^+, \\ \frac{\hat{M}_{JM_J}^V}{q} &= \sum_{j=1}^A \frac{-i}{m_N} \left[ g_V \hat{\Delta}_{JM_J}(q\vec{r}_j) - \frac{1}{2} \mu \hat{\Sigma}'_{JM_J}(q\vec{r}_j) \right] \tau_j^+\end{aligned}$$

Hadronic vector, axial vector and pseudo-scalar charges

$$g_V = 1 \quad g_A = -1.2756(13) \quad \tilde{g}_P = -\frac{(2m_N)^2}{m_\pi^2 - q^2} g_A$$

$\mu \approx 4.706$  is the nucleon isovector magnetic moment

$$\Delta E_c \equiv \langle {}^6\text{Li } 1_{\text{gs}}^+ | V_c | {}^6\text{Li } 1_{\text{gs}}^+ \rangle - \langle {}^6\text{He } 0_{\text{gs}}^+ | V_c | {}^6\text{He } 0_{\text{gs}}^+ \rangle$$

$$\begin{aligned}\hat{\Sigma}''_{JM_J}(q\vec{r}_j) &= \left[ \frac{1}{q} \vec{\nabla}_{\vec{r}_j} M_{JM_J}(q\vec{r}_j) \right] \cdot \vec{\sigma}(j), \\ \hat{\Omega}'_{JM_J}(q\vec{r}_j) &= M_{JM_J}(q\vec{r}_j) \vec{\sigma}(j) \cdot \vec{\nabla}_{\vec{r}_j} + \frac{1}{2} \hat{\Sigma}''_{JM_J}(q\vec{r}_j), \\ \hat{\Delta}_{JM_J}(q\vec{r}_j) &= \vec{M}_{J JM_J}(q\vec{r}_j) \cdot \frac{1}{q} \vec{\nabla}_{\vec{r}_j}, \\ \hat{\Sigma}'_{JM_J}(q\vec{r}_j) &= -i \left[ \frac{1}{q} \vec{\nabla}_{\vec{r}_j} \times \vec{M}_{J JM_J}(q\vec{r}_j) \right] \cdot \vec{\sigma}(j),\end{aligned}$$

$$\begin{aligned}M_{JM_J}(q\vec{r}_j) &= j_J(qr_j) Y_{JM_J}(\hat{r}_j) \\ \vec{M}_{J LM_J}(q\vec{r}_j) &= j_L(qr_j) \vec{Y}_{J LM_J}(\hat{r}_j)\end{aligned}$$

Ultimately, we need to calculate  
 ${}^6\text{He}(0^+ 1) \rightarrow {}^6\text{Li}(1^+ 0)$  matrix elements  
of these “one-body” operators

## Apply *ab initio* No-Core Shell Model to calculate the ${}^6\text{Li}$ and ${}^6\text{He}$ wave functions and the operator matrix elements

- Matrix elements of the relevant operators

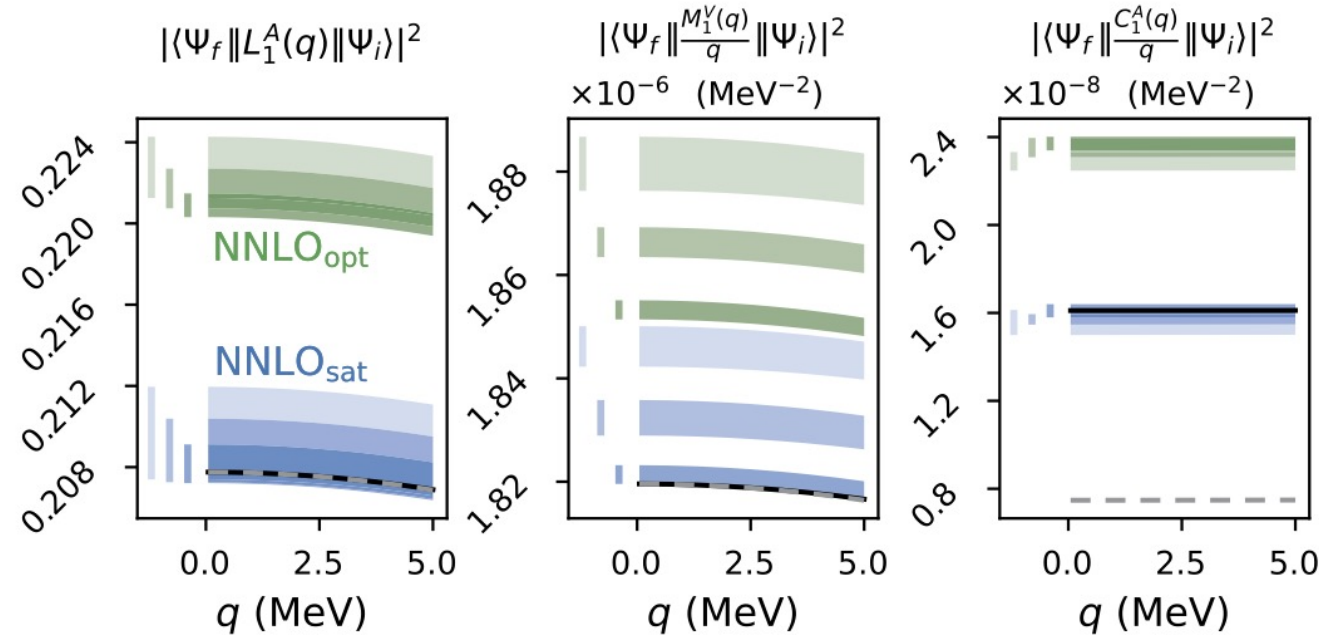
$$\frac{\hat{C}_{JM_J}^A}{q} = \sum_{j=1}^A \frac{i}{m_N} \left[ g_A \hat{\Omega}'_{JM_J}(q\vec{r}_j) - \frac{1}{2} \frac{\tilde{g}_P}{2m_N} (E_0 + \Delta E_c) \hat{\Sigma}''_{JM_J}(q\vec{r}_j) \right] \tau_j^+,$$

$$\hat{L}_{JM_J}^A = \sum_{j=1}^A i \left( g_A + \frac{\tilde{g}_P}{(2m_N)^2} q^2 \right) \hat{\Sigma}''_{JM_J}(q\vec{r}_j) \tau_j^+,$$

$$\frac{\hat{M}_{JM_J}^V}{q} = \sum_{j=1}^A \frac{-i}{m_N} \left[ g_V \hat{\Delta}_{JM_J}(q\vec{r}_j) - \frac{1}{2} \mu \hat{\Sigma}'_{JM_J}(q\vec{r}_j) \right] \tau_j^+$$

- Convergence investigation

- Variation of HO frequency
  - $\hbar\Omega = 16 - 24$  MeV
- Variation of basis size
  - $N_{\max} = 0 - 14$  for NNLO<sub>opt</sub>
  - $N_{\max} = 0 - 12$  for NNLO<sub>sat</sub>



- Impact of the CM correction

$$\langle \Psi_f || \sum_{j=1}^A \hat{O}_J(\vec{r}_j) || \Psi_i \rangle \longleftrightarrow \langle \Psi_f || \sum_{j=1}^A \hat{O}_J(\vec{r}_j - \vec{R}_{\text{CM}}) || \Psi_i \rangle$$

Almost no difference for  $\hat{L}_{JM_J}^{A\pm}$  and  $\hat{M}_{JM_J}^{V\pm}$

Change of ~40% for  $\hat{C}_{JM_J}^{A\pm}$

## Overall results for ${}^6\text{He}(0^+ 1) \rightarrow {}^6\text{Li}(1^+ 0) + e^- + \bar{\nu}$

- We find up to 1% correction for the  $\beta$  spectrum and up to 2% correction for the angular correlation
- Propagating nuclear structure and  $\chi\text{EFT}$  uncertainties results in an overall uncertainty of  $10^{-4}$ 
  - Comparable to the precision of current experiments

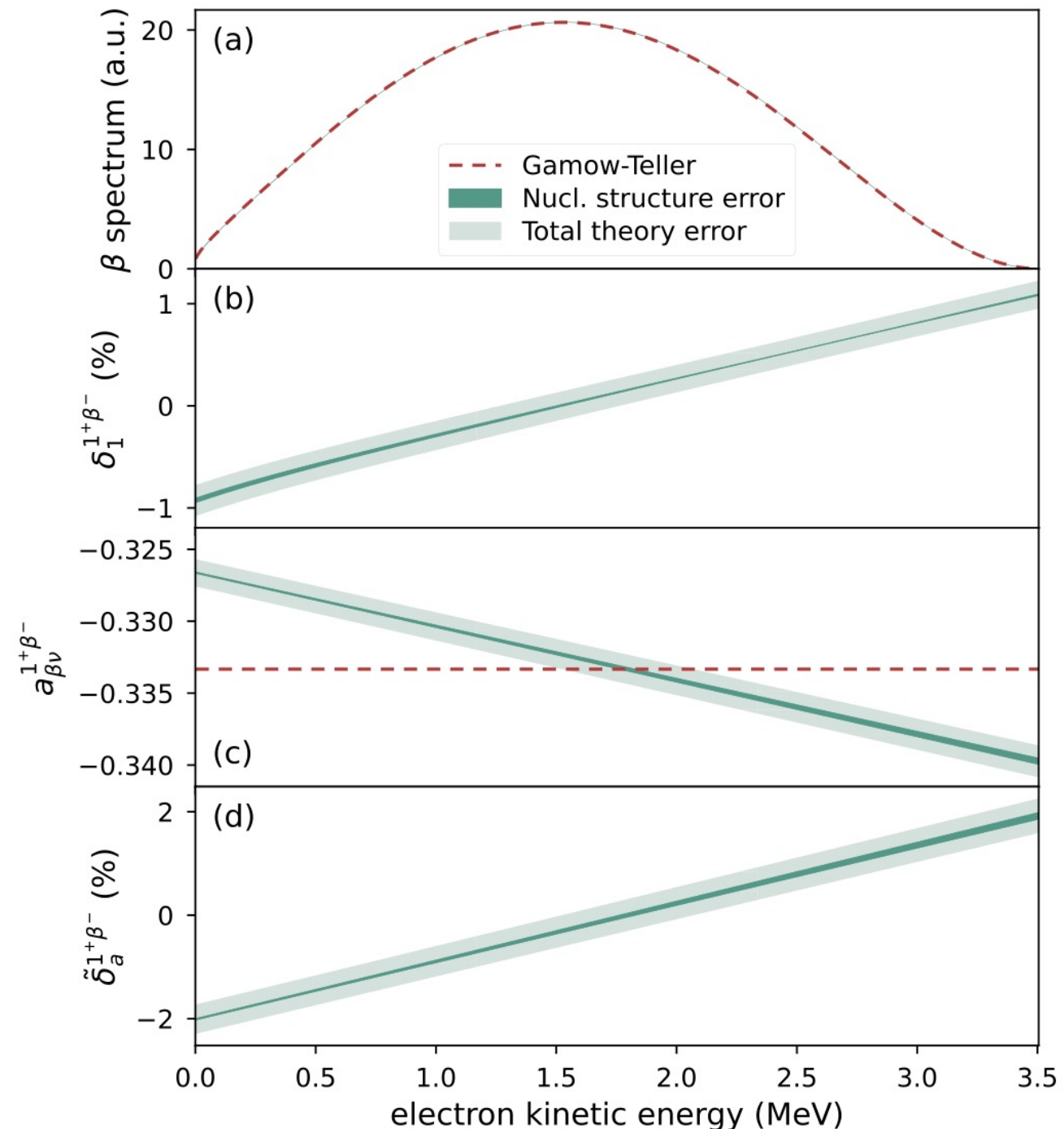
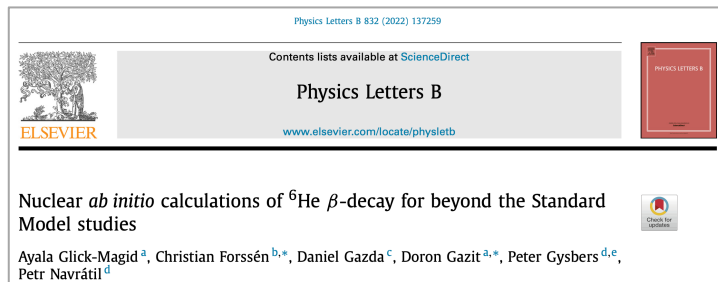
$$b_F^{1^+\beta^-} = \delta_b^{1^+\beta^-} = -1.52(18) \cdot 10^{-3}$$

$$\langle \tilde{\delta}_a^{1^+\beta^-} \rangle = -2.54(68) \cdot 10^{-3}$$

Non-zero Fierz interference term due to nuclear structure corrections

Note that new physics at TeV scale implies

$$b_{\text{Fierz}}^{\text{BSM}} = \frac{C_T + C'_T}{C_A} \sim 10^{-3}$$



# Conclusions

- *Ab initio* nuclear theory
  - Makes connections between the low-energy QCD and many-nucleon systems
- No-core shell model is an *ab initio* configuration interaction method
  - Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries
  - In combination with the Lanczos strength method provides robust results for electroweak observables and nuclear structure dependent corrections