TRIUMF

Ab initio calculations of electric dipole, Schiff, and anapole moments in atomic nuclei

Espace de Structure et de réactions Nucléaires Théorique

Theoretical and experimental developments for symmetry-violating nuclear properties

CEA Saclay, June 23-27, 2025

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TRIUMF

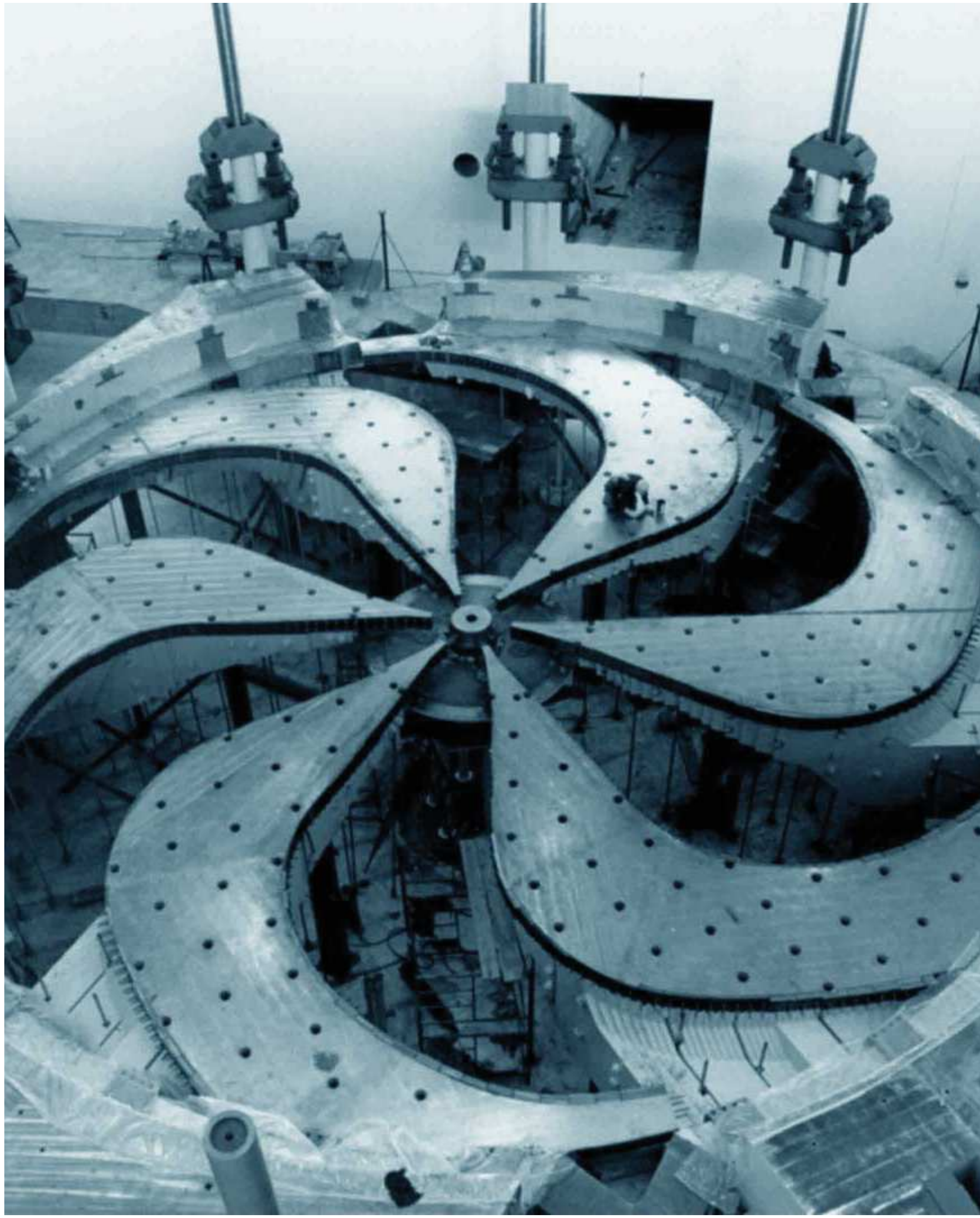
Collaborator:

Stephan Foster (TRIUMF, McMaster U)

2025-06-24

NRC·CNRC Canada

NSERC CRSNG



Discovery, accelerated

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
        - Schiff moment of ^{19}F
- Conclusions

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

2025-06-24

Discovery, accelerated

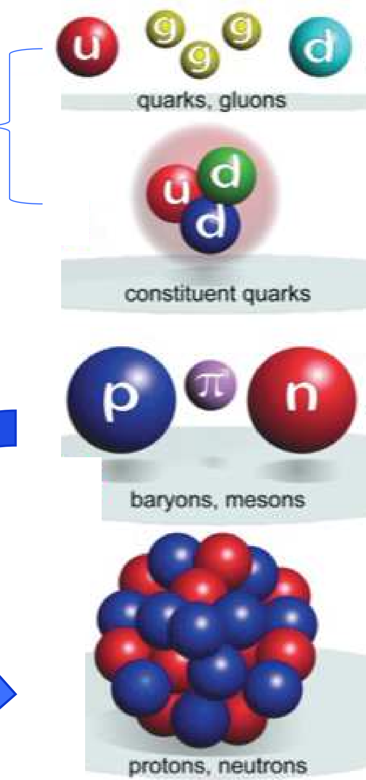
First principles or *ab initio* nuclear theory

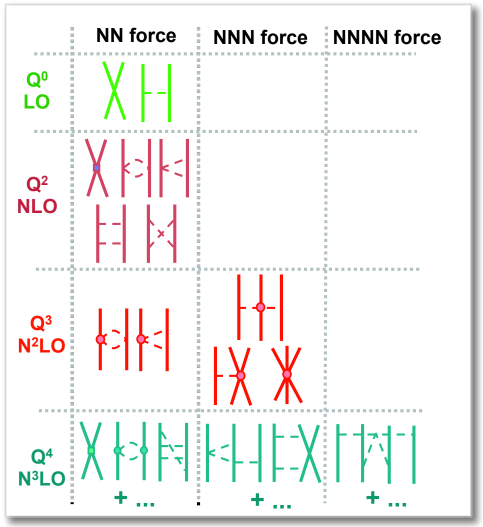
Quantum Chromodynamics (QCD)

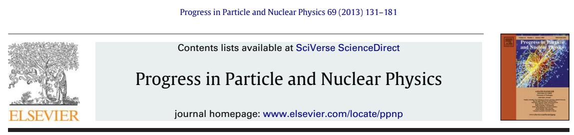
Chiral Effective Field Theory (parameters fitted to NN data)

Many-body *ab initio* nuclear theory

$$H\,\Psi^{(A)} = E\,\Psi^{(A)}$$

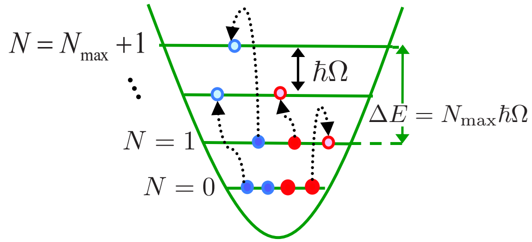




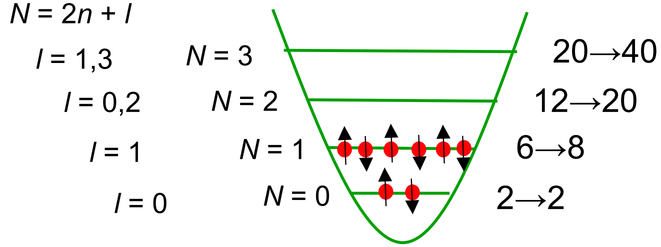

Progress in Particle and Nuclear Physics 69 (2013) 131–181
Contents lists available at SciVerse ScienceDirect
Progress in Particle and Nuclear Physics
journal homepage: www.elsevier.com/locate/ppnp
ELSEVIER
Review
Ab initio no core shell model
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

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}He, ^{16}O, ^{40}Ca)
    - Equivalent description in relative(Jacobi)-coordinate and Slater determinant basis – nuclei self-bound, $[H,P_{CM}]=0$
      - Exact factorization of CM and intrinsic eigenfunctions at each N_{max}

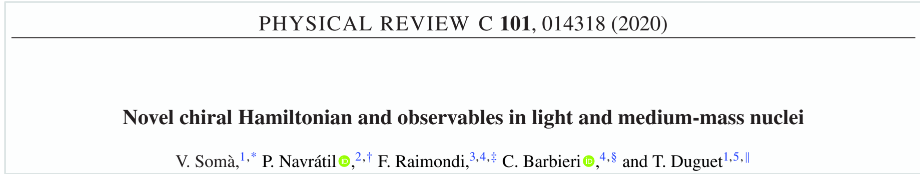


$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni}\, \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \ldots, \vec{\eta}_{A-1})$$



$$E = (2n + l + \tfrac{3}{2})\hbar\Omega$$

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


PHYSICAL REVIEW C **101**, 014318 (2020)

Novel chiral Hamiltonian and observables in light and medium-mass nuclei

V. Somà,[1,*] P. Navrátil,[2,†] F. Raimondi,[3,4,‡] C. Barbieri,[4,§] and T. Duguet[1,5,‖]

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
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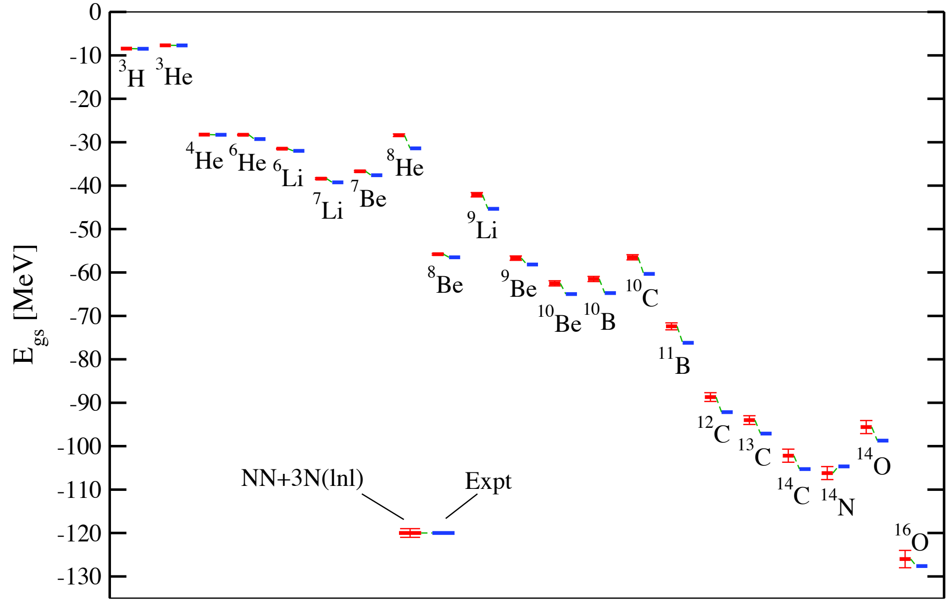
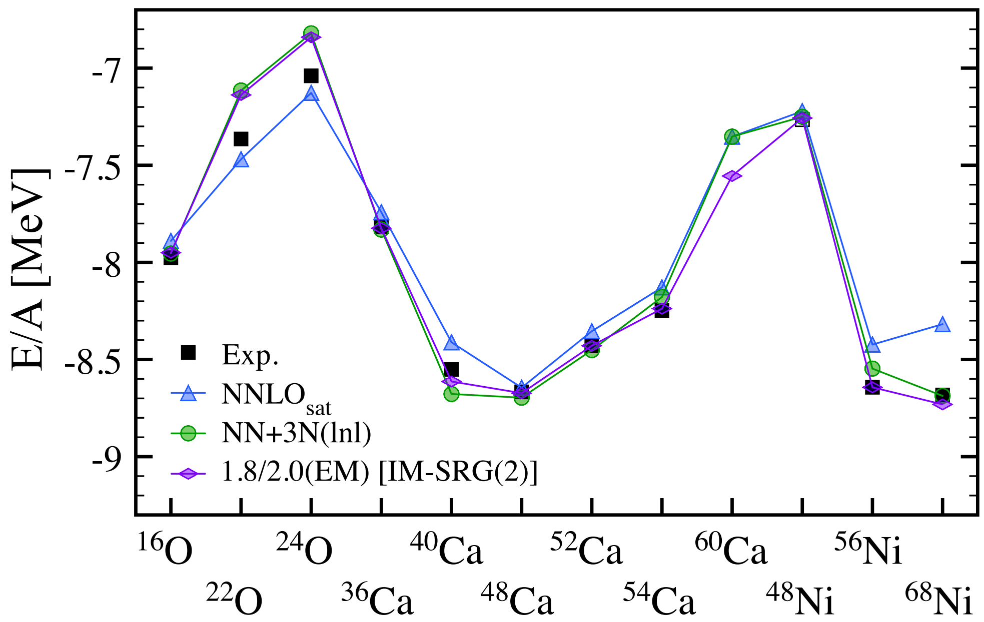
    - Nucleon–nucleon scattering, deuteron properties, ^{3}H and ^{4}He binding energy, ^{3}H half life
  - Light nuclei – NCSM
  - Medium mass nuclei – Self-Consistent Green's Function method

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





1.8/2.0 (EM) results: J. Simonis, S. R. Stroberg, K. Hebeler, J. D. Holt, and A. Schwenk, Phys. Rev. C 96, 014303 (2017).

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  - Light nuclei – NCSM
  - Heavy nuclei – HF-MBPT(3)

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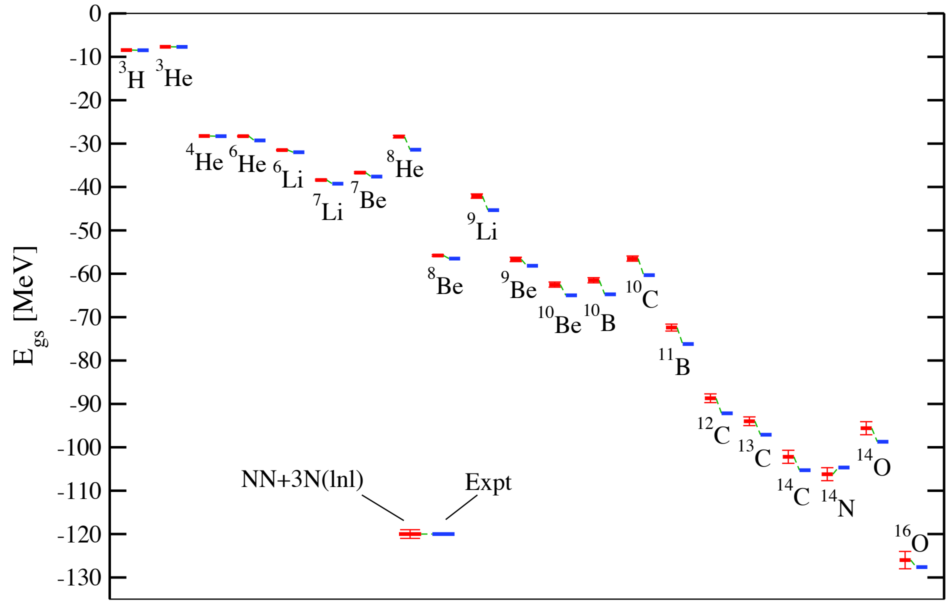
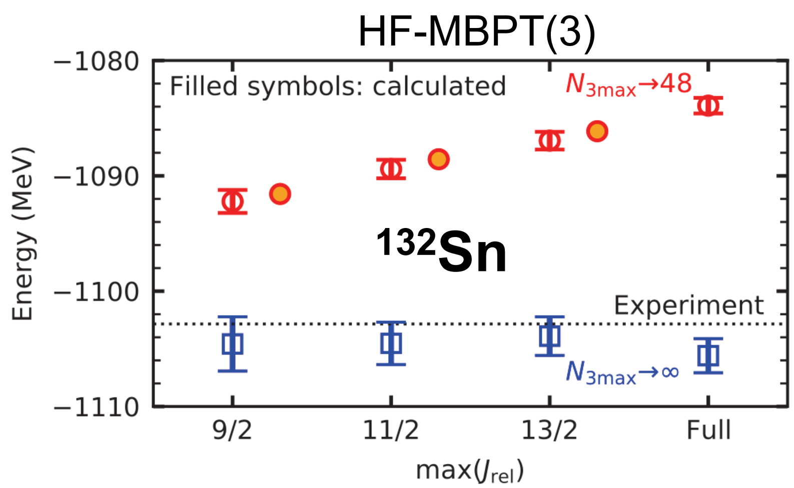
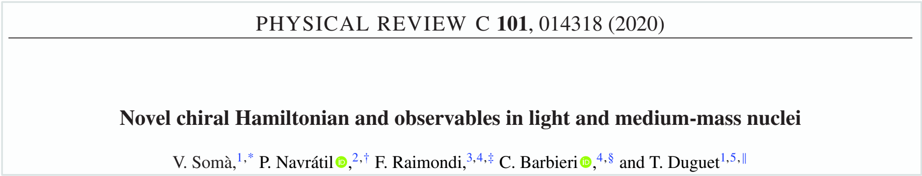




PHYSICAL REVIEW C **105**, 014302 (2022)

Converged *ab initio* calculations of heavy nuclei

T. Miyagi,[1,*] S. R. Stroberg,[2,†] P. Navrátil,[1,‡] K. Hebeler,[3,4,5,§] and J. D. Holt[1,6,‖]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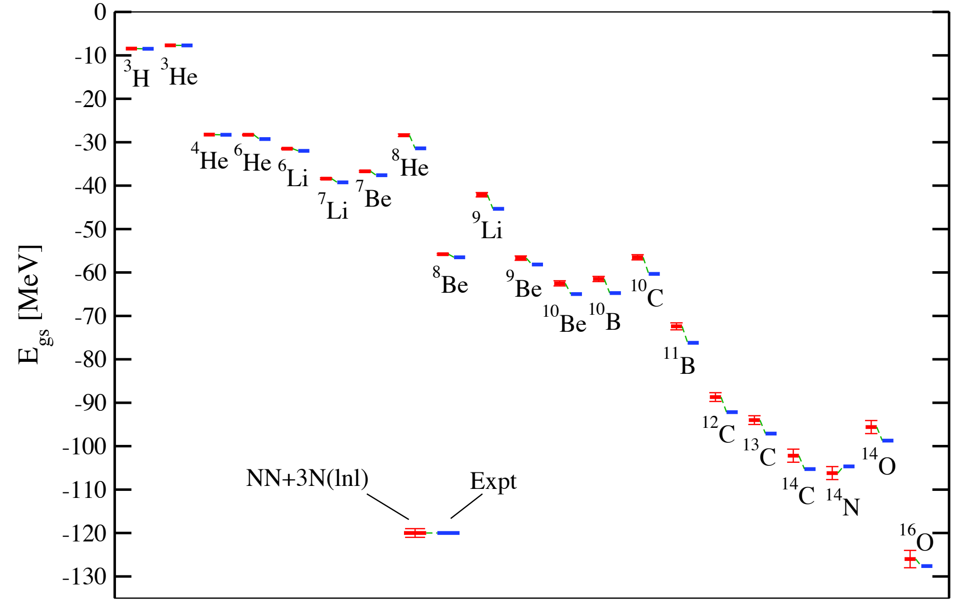

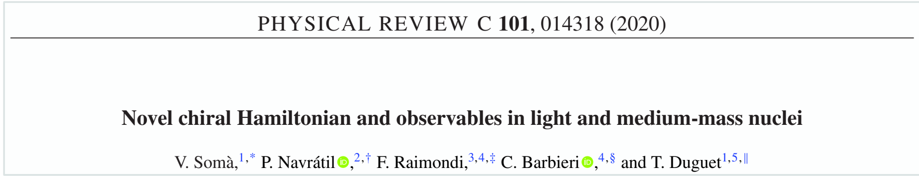
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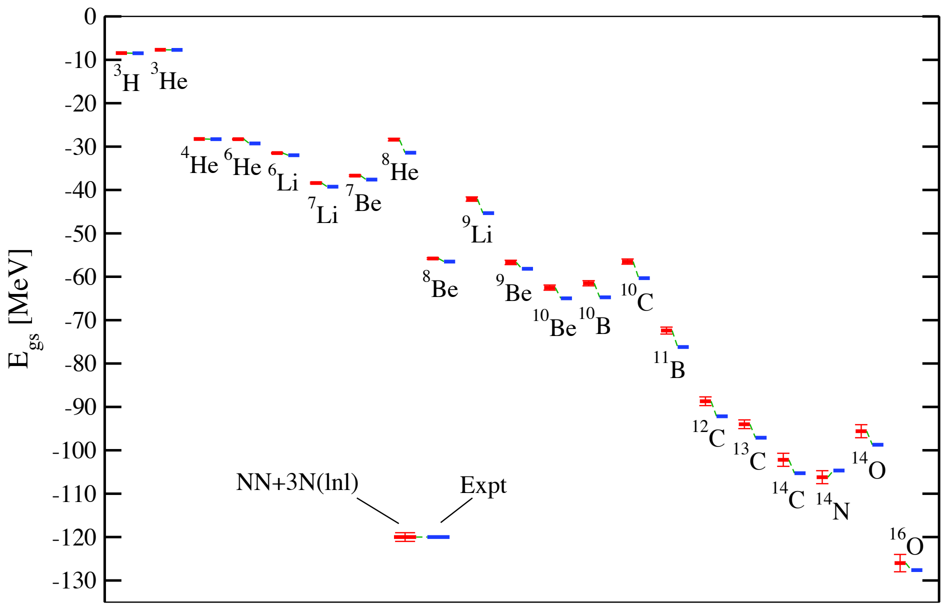

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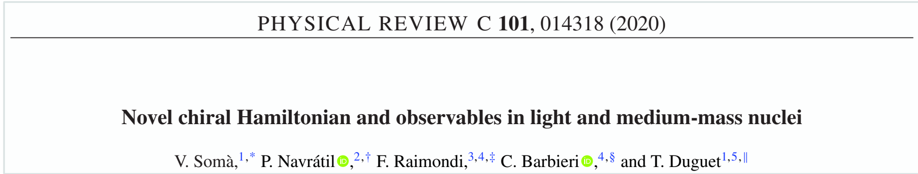
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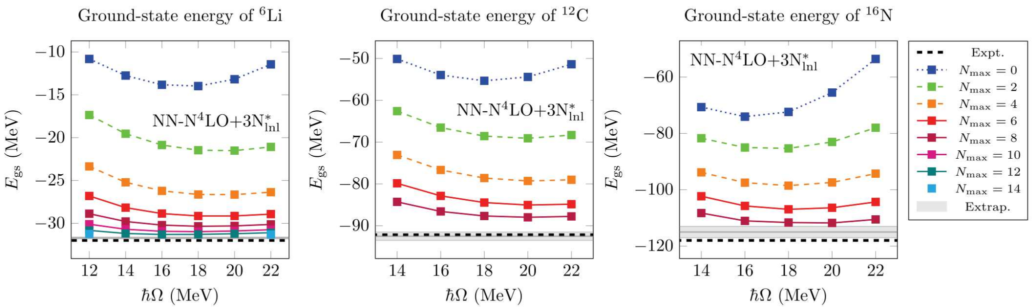

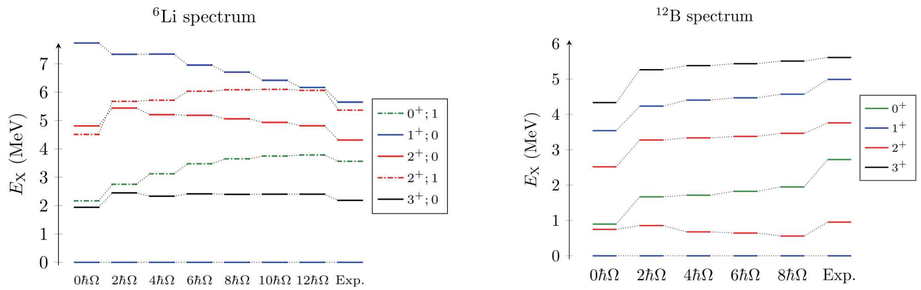

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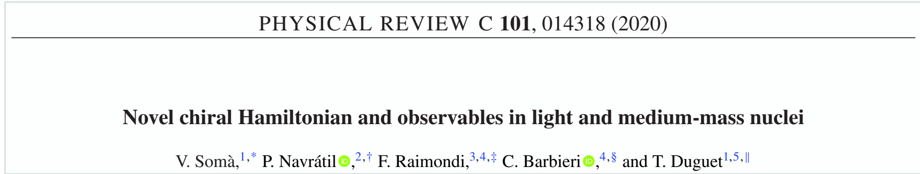
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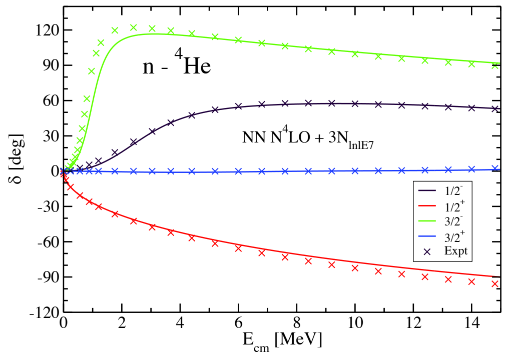

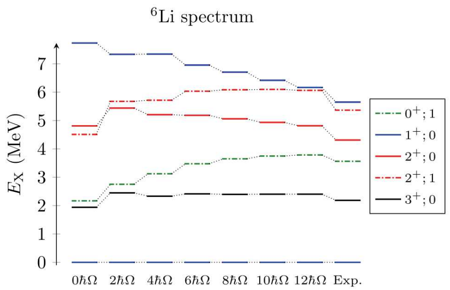

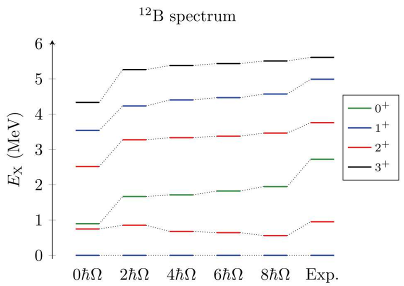

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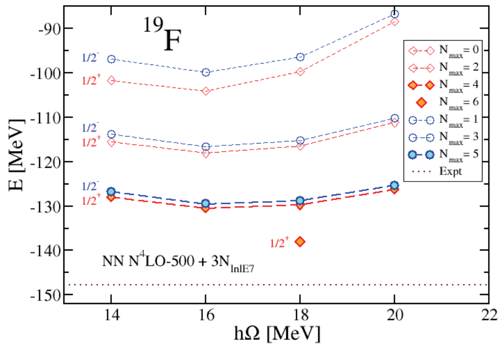

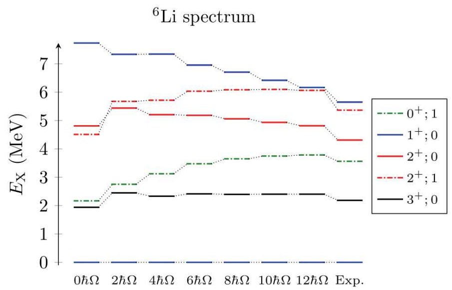

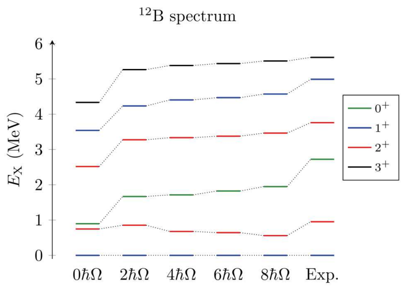

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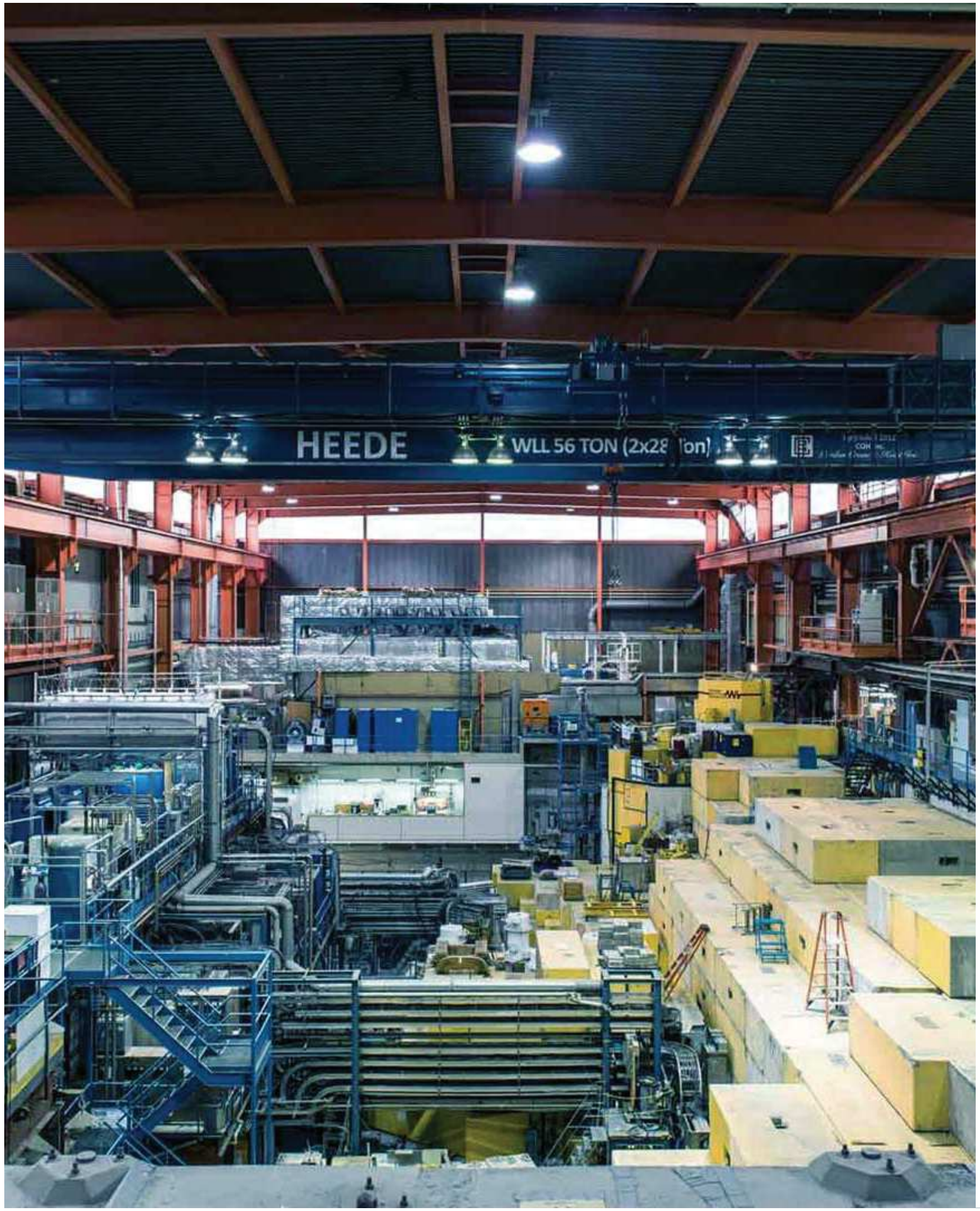
TRIUMF

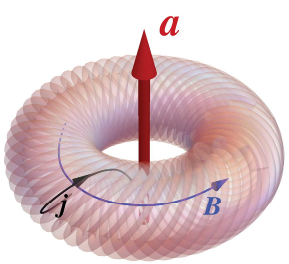
Ab initio calculations of parity-violating moments - anapole moment electric dipole moment (EDM) Schiff moment



Discovery, accelerated

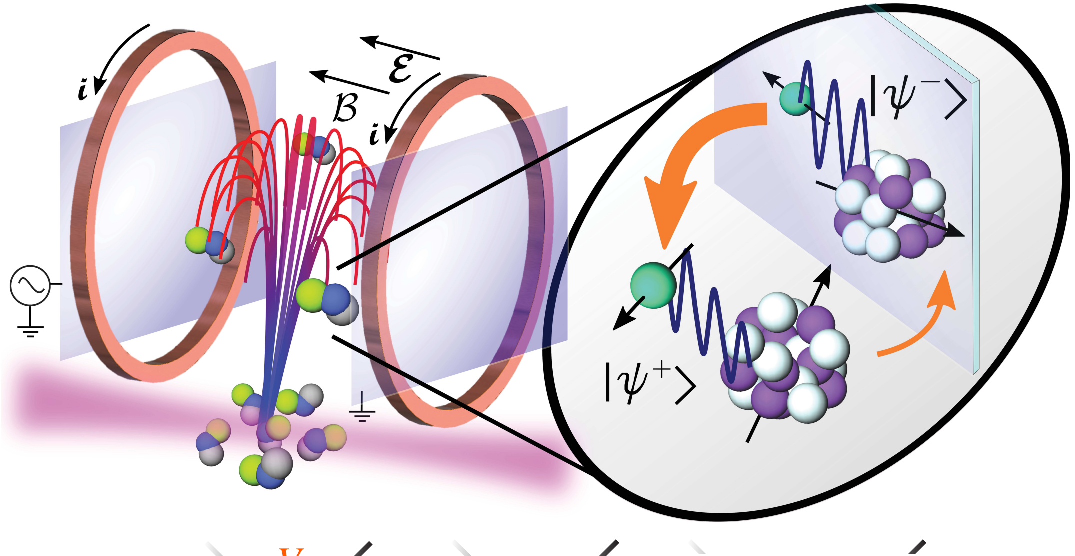
Why investigate parity violation in atomic and molecular systems and the nuclear anapole moment?

- 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



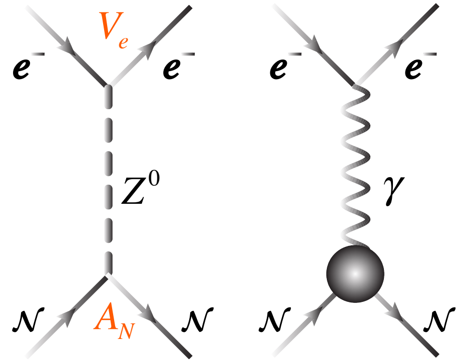
Nuclear spin dependent parity violating effects in light polyatomic molecules

- Experiments proposed for ^{9}BeNC, ^{25}MgNC



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

- 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)



(b) (c)

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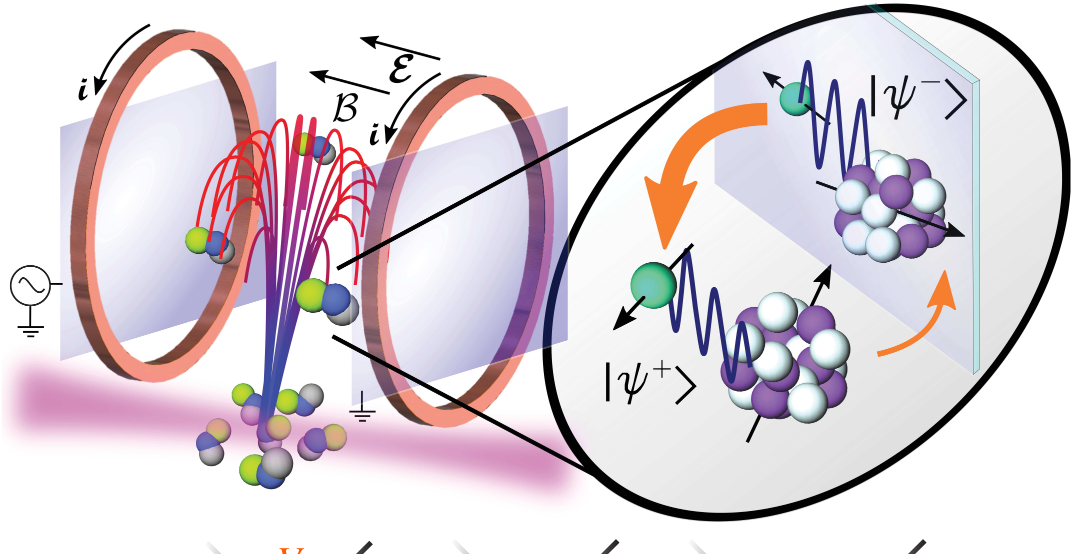

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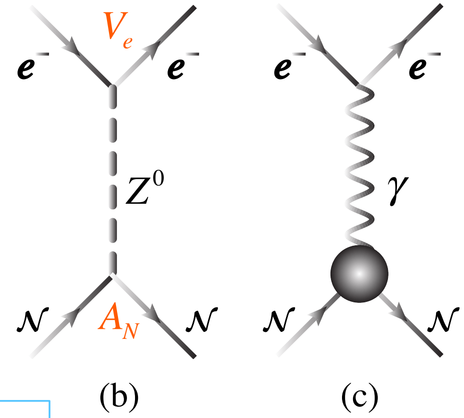


Anapole moment measurements also planned in ^{137}BaF molecule

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

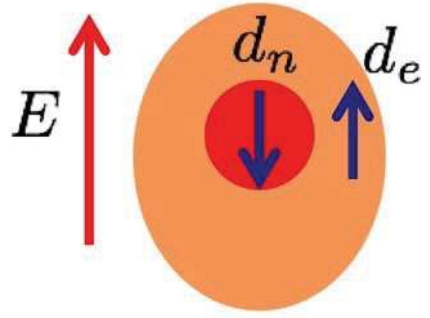
- Unsolved problem in physics: matter-antimatter asymmetry of the universe
- Standard model predicts some CP violation, not enough to explain this asymmetry
- The EDM and nuclear Schiff moment is a promising probe for CP violation beyond the standard model, as well as CP violating QCD $\bar{\theta}$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

- 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 $^{227}ThF^{+}$, RaF, and FrAg molecules

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

What is the nuclear Schiff moment?



Schiff Moment

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

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!

Slide by Matthew R. Dietrich (ANL)

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}^{PNC} interaction
  - Conserves total angular momentum *I*
  - Mixes opposite parities
  - Has isoscalar, isovector and isotensor components

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

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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†

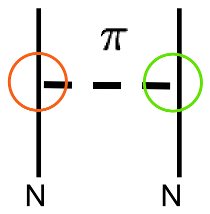
frontiers in Physics

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

Parity- and Time-Reversal-Violating Nuclear Forces

Jordy de Vries[1,2], Evgeny Epelbaum[3], Luca Girlanda[4,5], Alex Gnech[6], Emanuele Mereghetti[7] and Michele Viviani[8]

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



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

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

Include π, ρ, ω meson exchanges

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

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

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

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

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

ANNALS OF PHYSICS 124, 449–495 (1980)

Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES*

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JOHN F. DONOGHUE†

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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
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Jordy de Vries[1,2], Evgeny Epelbaum[3], Luca Girlanda[4,5], Alex Gnech[6], Emanuele Mereghetti[7] and Michele Viviani[8]*

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

C.-P. Liu* and R. G. E. Timmermans†

$$
\begin{aligned}
H_{PTV}(\boldsymbol{r}) = \frac{1}{2m_n} & \boldsymbol{\sigma}_- \cdot \boldsymbol{\nabla} \left(-\bar{G}_\omega^0 y_\omega(r)\right) \\
& + \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2}\, \boldsymbol{\sigma}_- \cdot \boldsymbol{\nabla} \left(\bar{G}_\pi^0 y_\pi(r) - \bar{G}_\rho^0 y_\rho(r)\right) \\
& + \frac{\tau_+^z}{2} \boldsymbol{\sigma}_- \cdot \boldsymbol{\nabla} \left(\bar{G}_\pi^1 y_\pi(r) - \bar{G}_\rho^1 y_\rho(r) - \bar{G}_\omega^1 y_\omega(r)\right) \\
& + \frac{\tau_-^z}{2} \boldsymbol{\sigma}_+ \cdot \boldsymbol{\nabla} \left(\bar{G}_\pi^1 y_\pi(r) + \bar{G}_\rho^1 y_\rho(r) - \bar{G}_\omega^1 y_\omega(r)\right) \\
& + (3\tau_1^z \tau_2^z - \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2}) \boldsymbol{\sigma}_- \cdot \boldsymbol{\nabla} \left(\bar{G}_\pi^2 y_\pi(r) - \bar{G}_\rho^2 y_\rho(r)\right)
\end{aligned}
$$

- Based on one meson exchange model
- $y_x(r) = e^{-m_x r}/(4\pi r)$

$$\sigma_\pm = \sigma_1 \pm \sigma_2$$

$$\tau_\pm^z = \tau_1^z \pm \tau_2^z$$

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\end{aligned}
$$

- Based on one meson exchange model
- $y_x(r) = e^{-m_x r}/(4\pi r)$
- Coupling constants $\boxed{\overline{G}_\pi^t = g_{\pi NN}\, \overline{g}_{\pi NN}^t \quad (g_{\pi NN} \sim 13.3)}$

$$\sigma_\pm = \sigma_1 \pm \sigma_2$$

$$\tau_\pm^z = \tau_1^z \pm \tau_2^z$$

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

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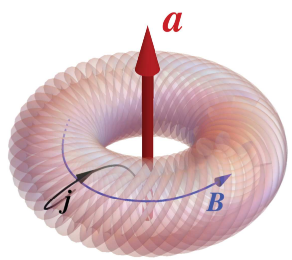
- Anapole moment operator dominated by spin contribution

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



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

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

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

- Anapole moment calculation:

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

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

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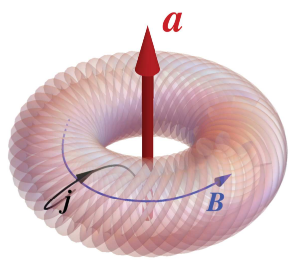

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- Anapole moment calculation:

Low lying states of opposite parity can lead to enhancement!

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

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- EDM and Schiff moment operators

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

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

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

$$D^{(pol)} = \left\langle\psi_{\text{gs}}\ I^{\pi}\middle|\hat{D}_z\middle|\psi_{\text{gs}}\ I\right\rangle + c.c. \qquad S = \left\langle\psi_{\text{gs}}\ I^{\pi}\middle|\boldsymbol{S}\middle|\psi_{\text{gs}}\ I\right\rangle + c.c.$$

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

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

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Sum over all possible intermediate states

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- Solving Schroedinger equation with inhomogeneous term

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

- To invert this equation, we apply the Lanczos algorithm

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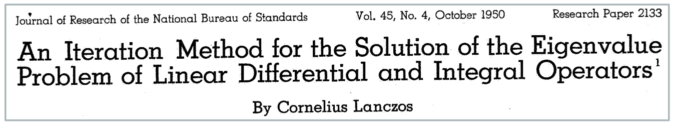
- To invert this equation, we apply the Lanczos algorithm
  - Bring matrix to tri-diagonal form ($\mathbf{v}_1$, $\mathbf{v}_2$ … orthonormal, H Hermitian)

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



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[1]

By Cornelius Lanczos

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

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

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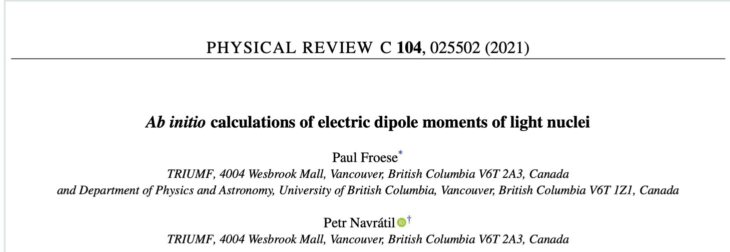
- To invert this equation, we apply the Lanczos algorithm

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

^{3}He EDM Benchmark Calculation


PHYSICAL REVIEW C **104**, 025502 (2021)

***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

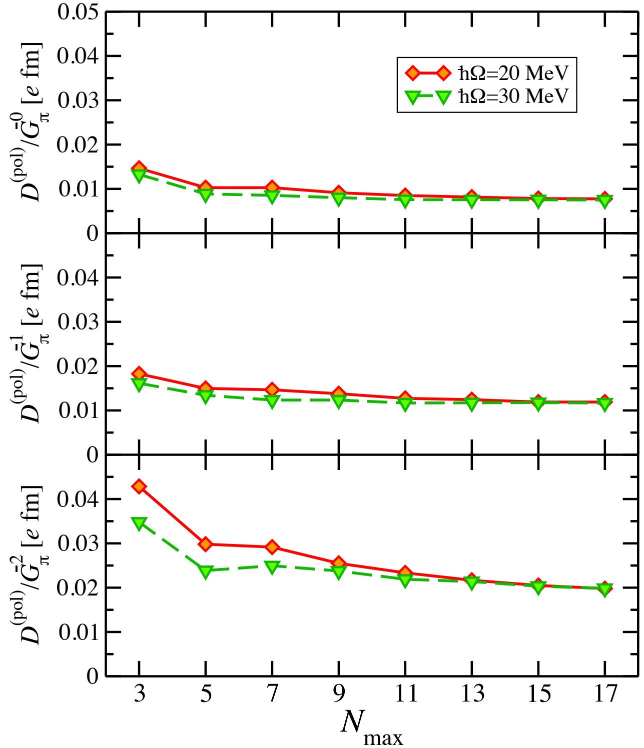
Petr Navrátil†
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

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 ^{3}He

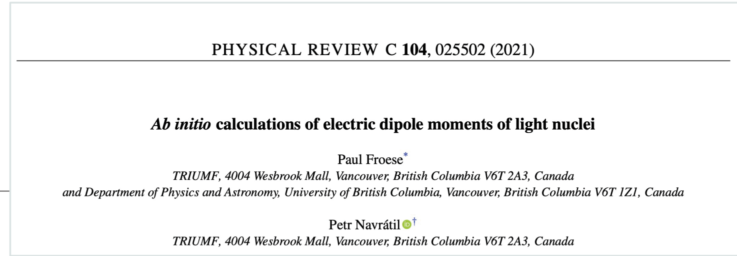
N^{3}LO NN



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

NCSM applications to parity-violating moments:

EDMs of light stable nuclei



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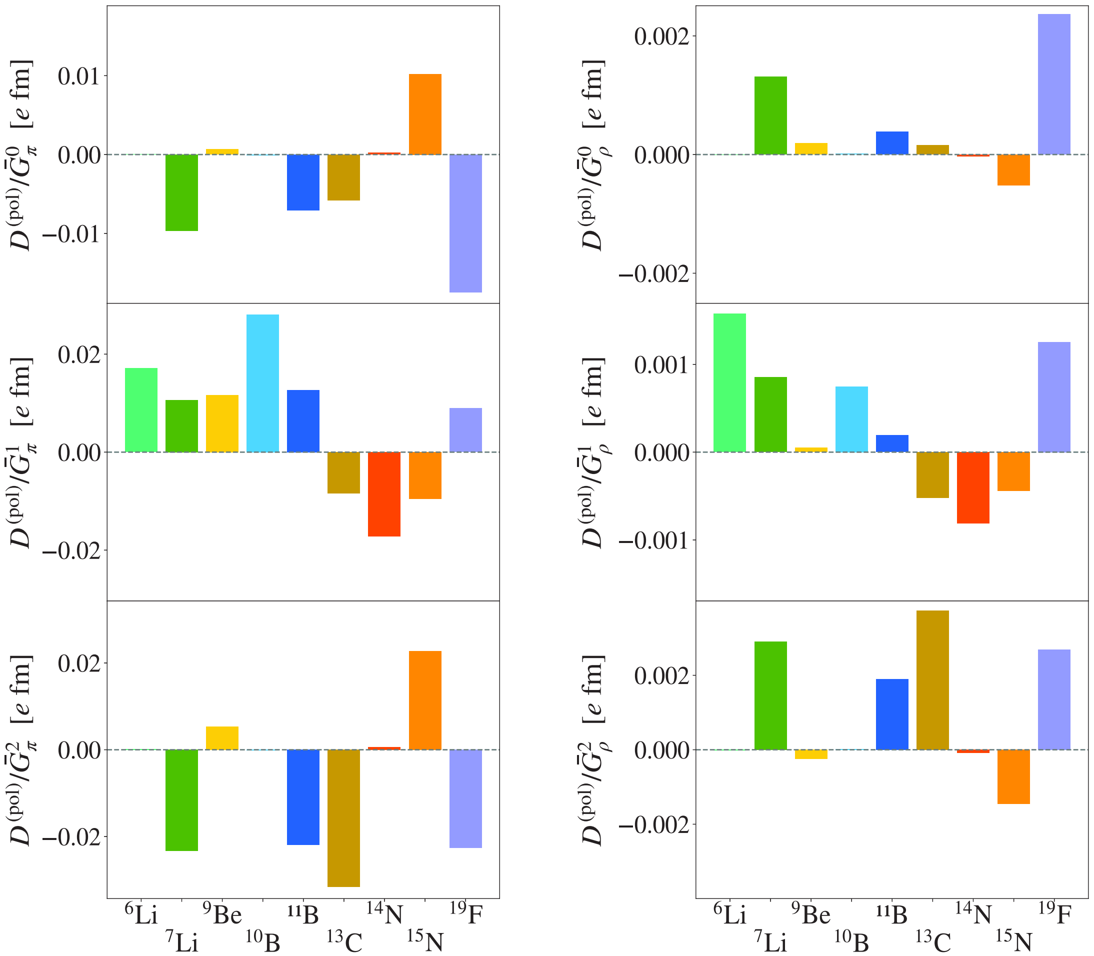
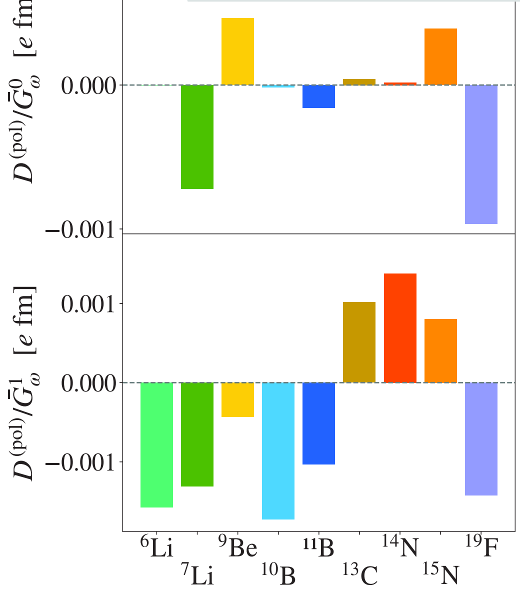
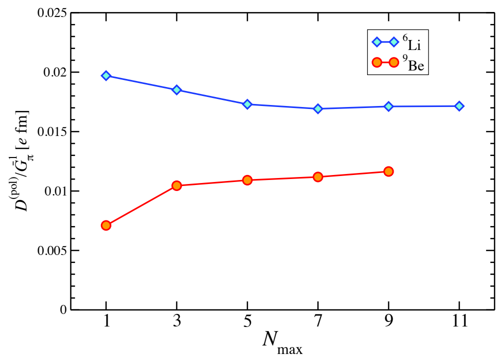



Examples of N_{max} convergence



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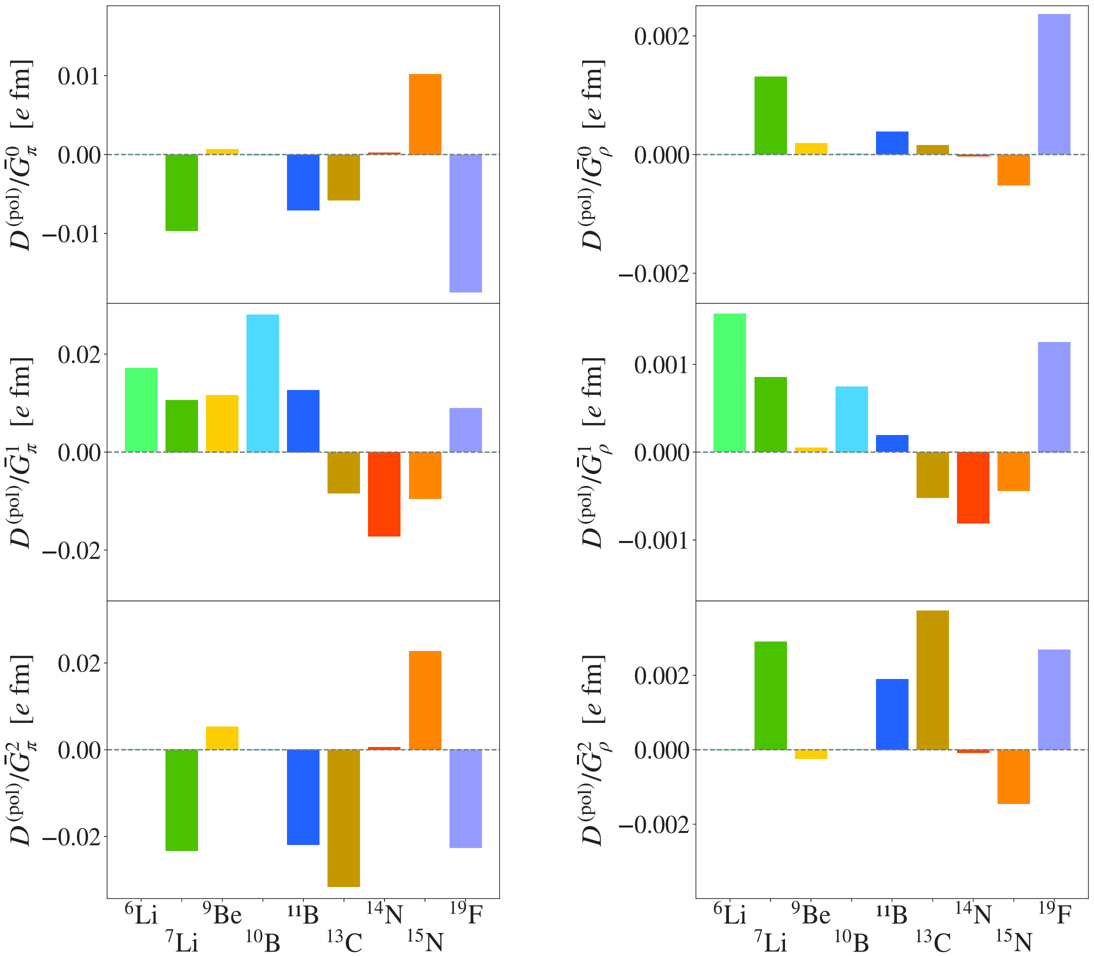
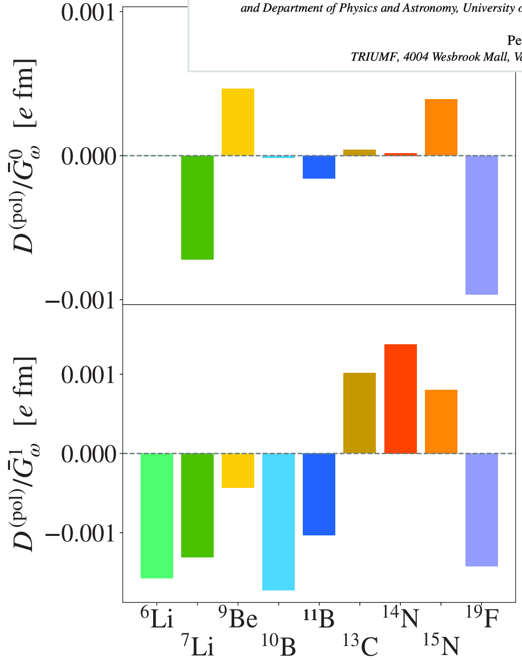

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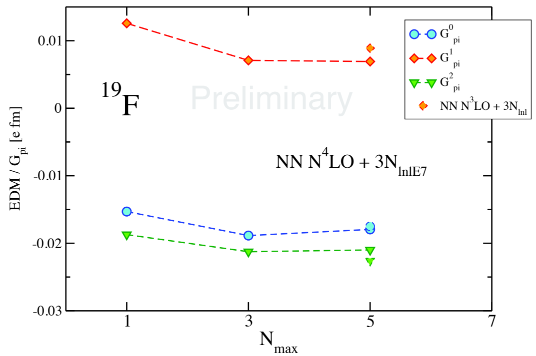
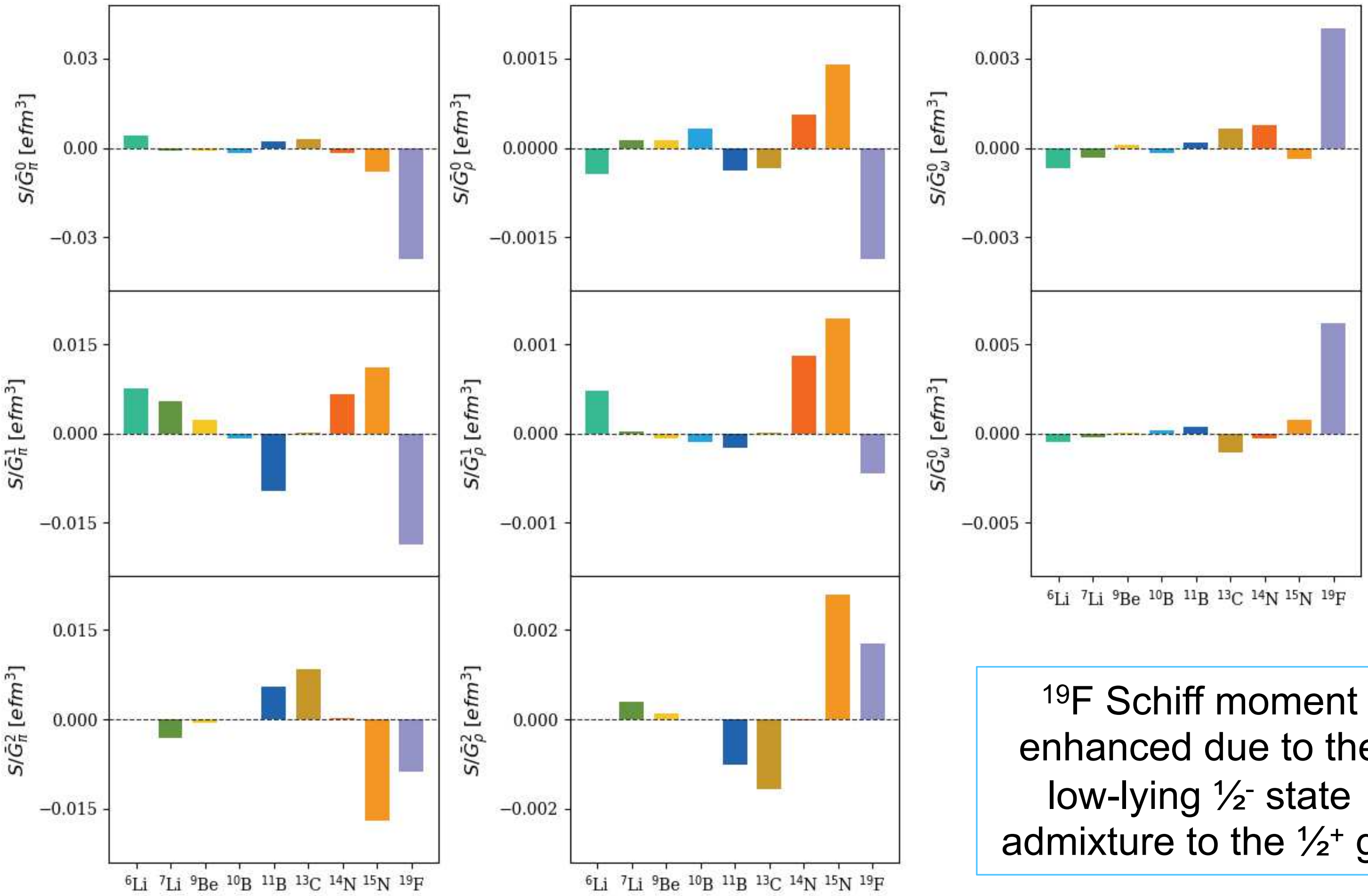


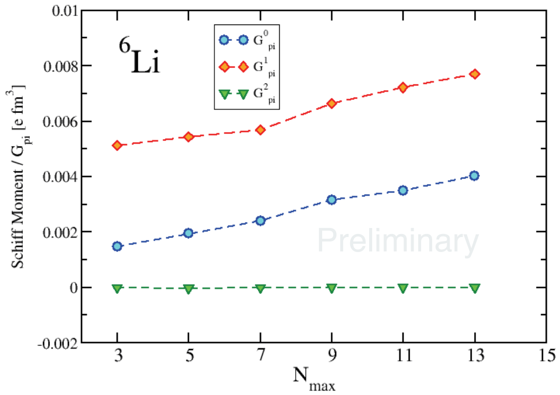
NCSM applications to parity-violating moments:
Schiff moments of light stable nuclei

Results preliminary



Work in progress with Stephan Foster, McMaster University undergraduate student

Examples of N_{max} convergence



^{19}F Schiff moment enhanced due to the low-lying ½⁻ state admixture to the ½⁺ gs

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

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

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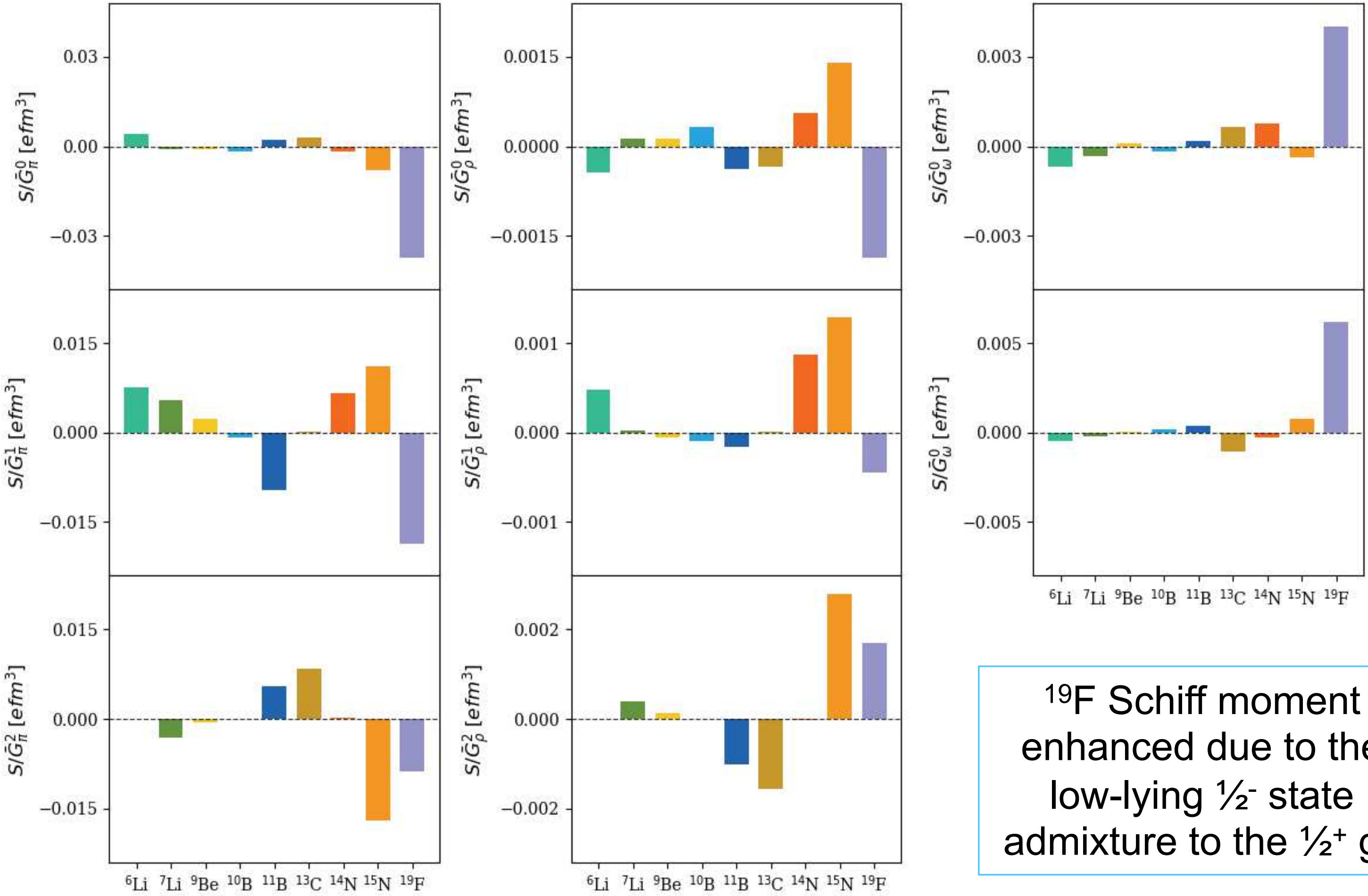


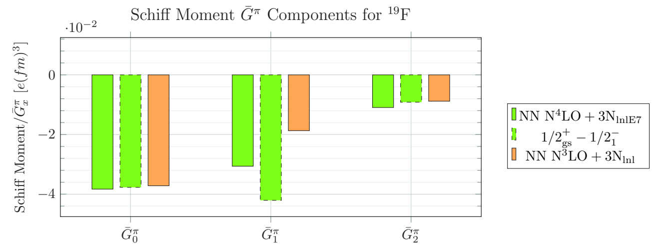


Figure 1: Comparison of ^{19}F $\bar{G}^\pi$ components for different interactions and included states.

^{19}F Schiff moment enhanced due to the low-lying ½⁻ state admixture to the ½⁺ gs

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

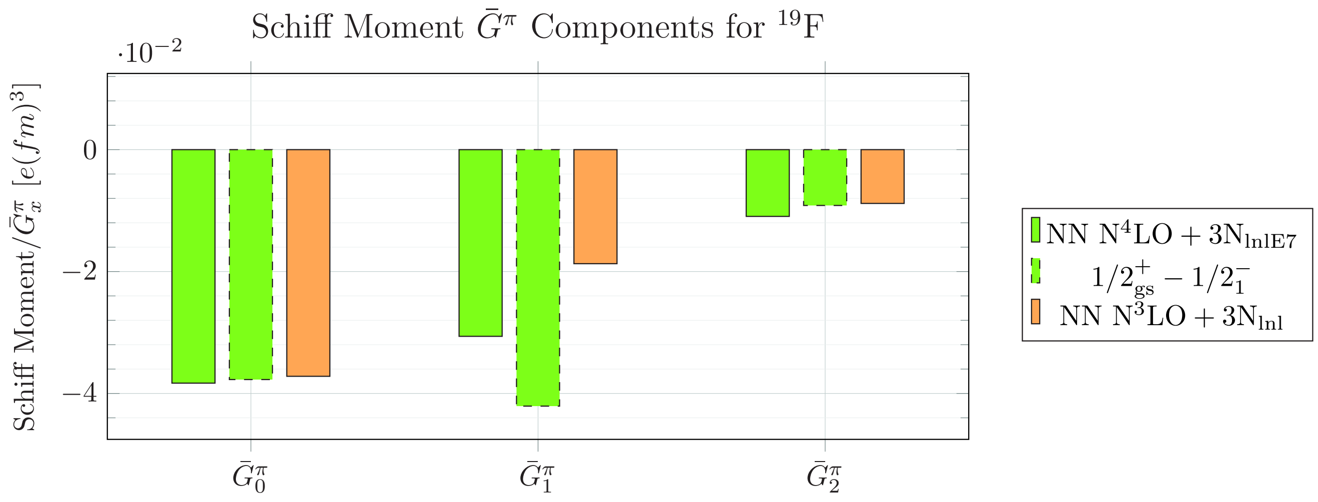
NCSM applications to parity-violating moments:
Schiff moments of light stable nuclei

Results preliminary

Calculated ½- state energies shifted to match the ½-₁ excitation energy

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

Work in progress with Stephan Foster, McMaster University undergraduate student



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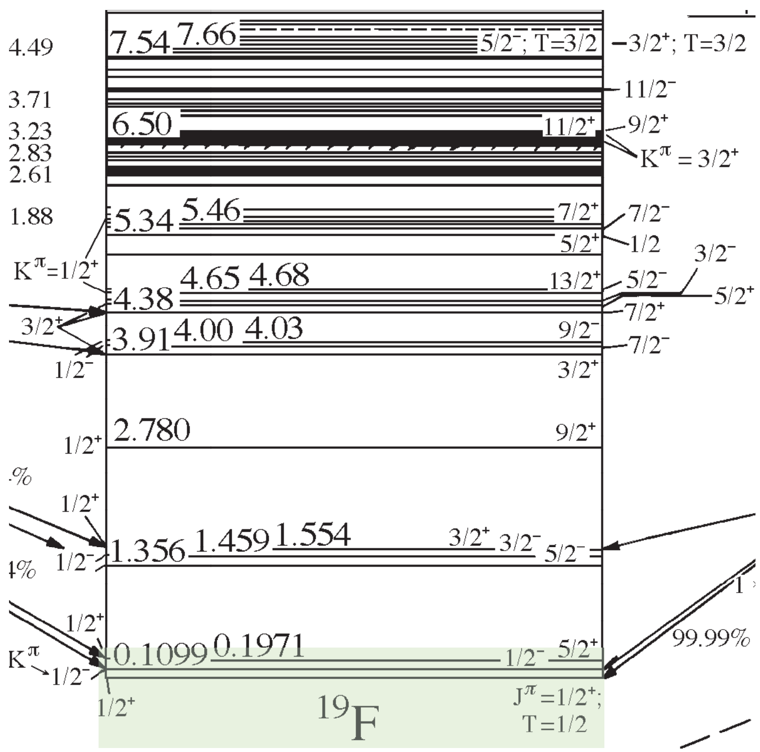

$$S = \langle \psi_{\text{gs}}\, I^{\pi} | \boldsymbol{S} | \psi_{\text{gs}}\, I \rangle + c.c.$$

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

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

^{19}F Schiff moment enhanced due to the low-lying ½- state admixture to the ½+ gs

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

NCSM applications to parity-violating moments:

Schiff moments of light stable nuclei

Results preliminary

Calculated ½- state energies shifted to match the ½-$_1$ excitation energy

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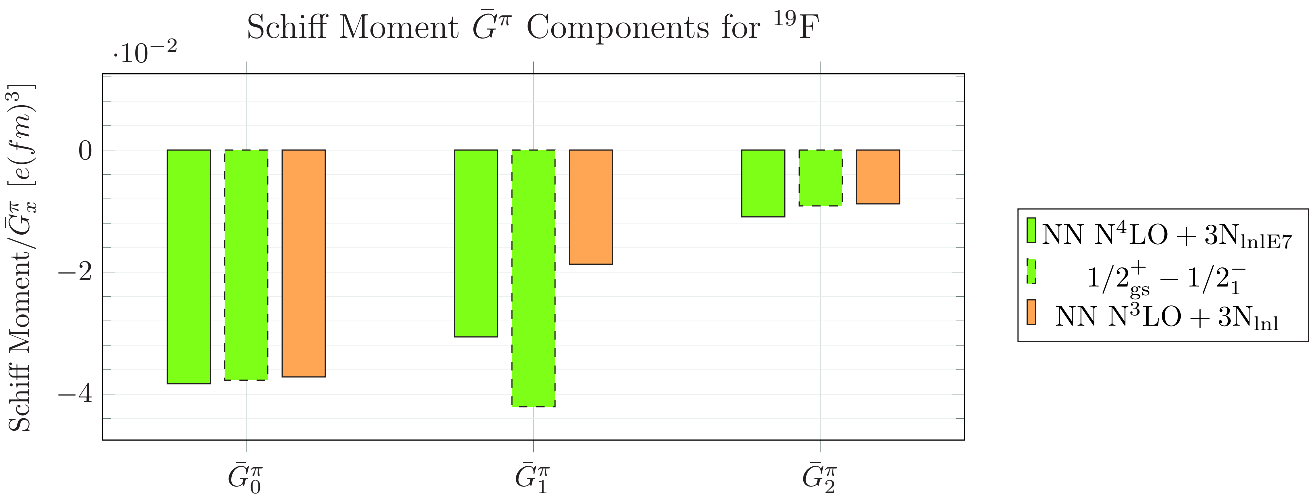

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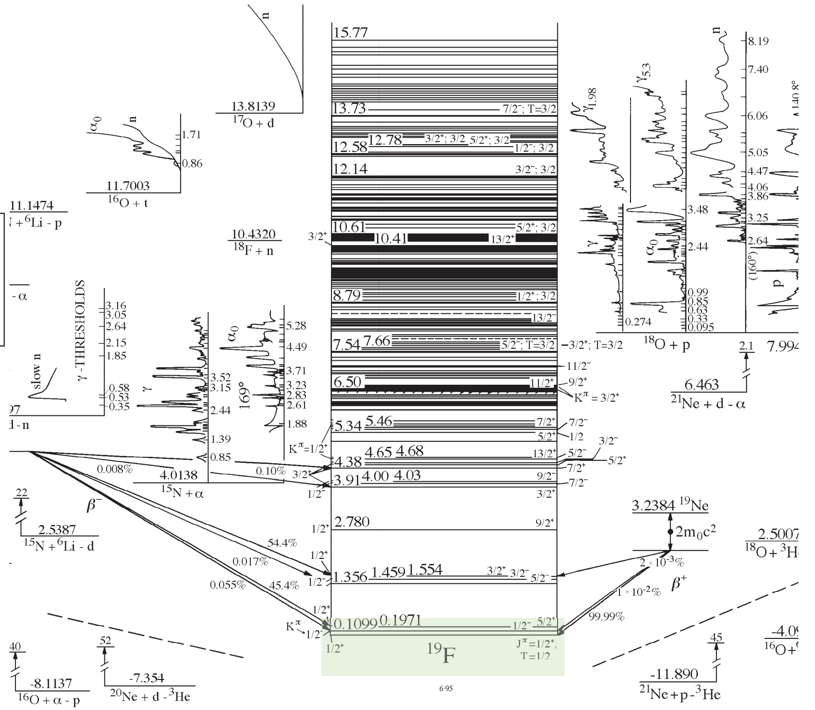

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^{19}F Schiff moment enhanced due to the low-lying ½$^-$ state admixture to the ½$^+$ gs

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

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Calculated ½- state energies shifted to match the $½^-_1$ excitation energy

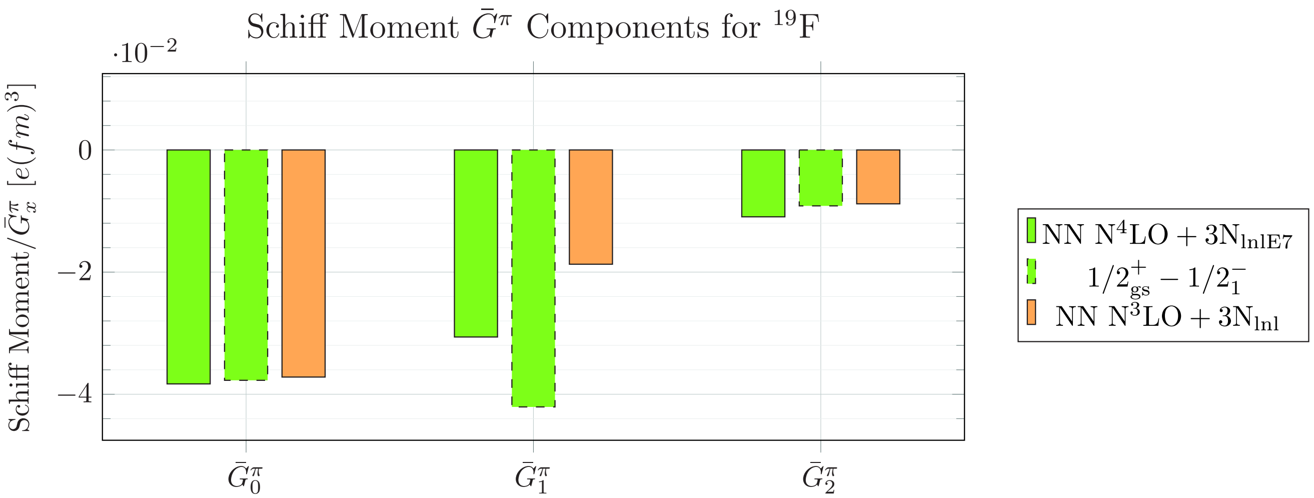

Figure 1: Comparison of ^{19}F $\bar{G}^\pi$ components for different interactions and included states.

^{19}F Schiff moment comparable to ^{129}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}Xe and ^{199}Hg

Kota Yanase* and Noritaka Shimizu†

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

	a_0	a_1	a_2
IPM ($m_\pi \to \infty$)	−9.9	−9.9	−19.8
IPM	−4.6	−4.6	−9.2
LSSM (SN100PN, $m_\pi \to \infty$)	−8.7	−8.2	−15.8
LSSM (SNV, $m_\pi \to \infty$)	−8.6	−8.3	−16.2
LSSM (SN100PN)	−3.7	−4.1	−8.0
LSSM (SNV)	**−3.8**	**−4.1**	**−8.1**
IPM ($m_\pi \to \infty$) [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

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

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

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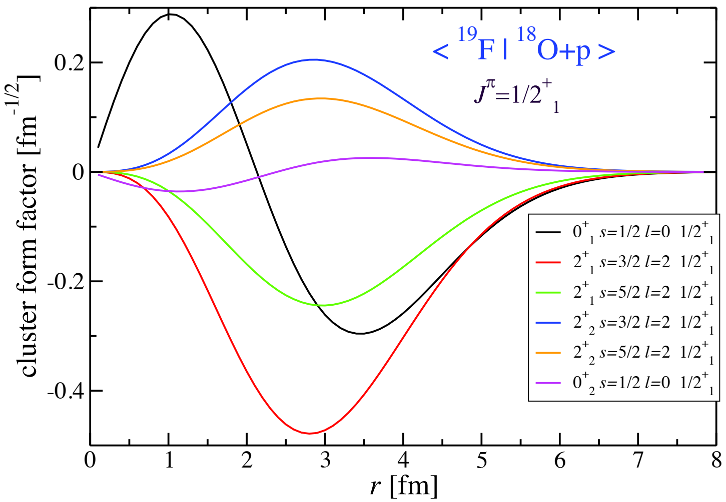
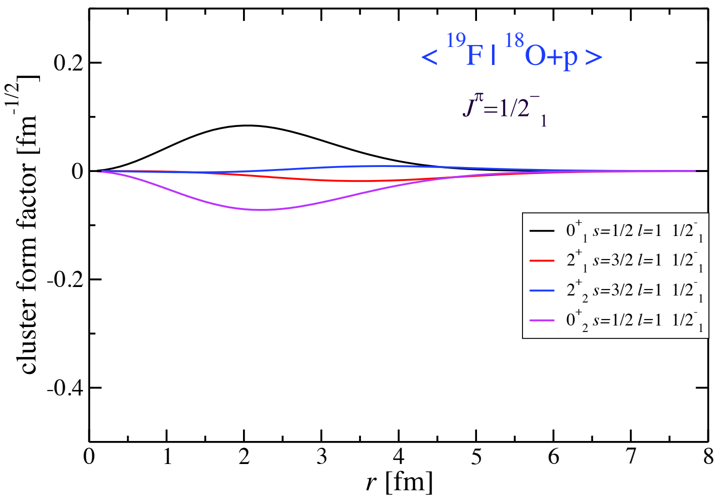
^{19}F Schiff moment dominated by the contribution of the lowest ½$^-$ state
However, its contribution to the EDM of ^{19}F is negligible.

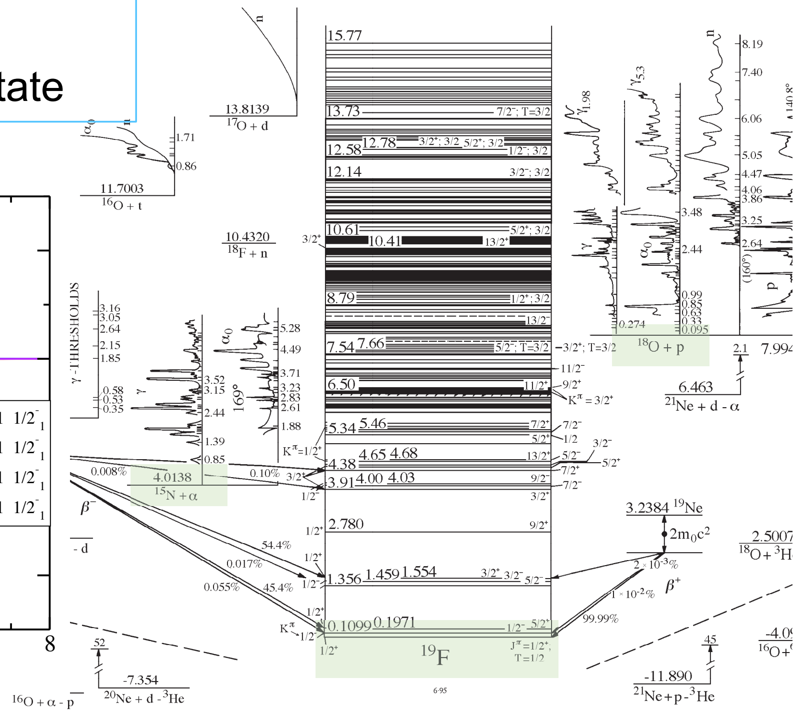
This is due to very different structure of the ½+ g.s. and the ½-$_1$ state



^{18}O+p (shell-model-like)



^{15}N+^{4}He – alpha-clustering



E1 matrix element small
S matrix element large due to the r^3 term

$$\hat{D}_z = \frac{e}{2}\sum_{i=1}^{A}(1+\tau_i^z)\, z_i \qquad \boldsymbol{S} = \frac{e}{10}\sum_{i=1}^{Z}\left(r_i^2\boldsymbol{r}_i - \frac{5}{3}\langle r^2\rangle_{\mathrm{ch}}\boldsymbol{r}_i\right)$$

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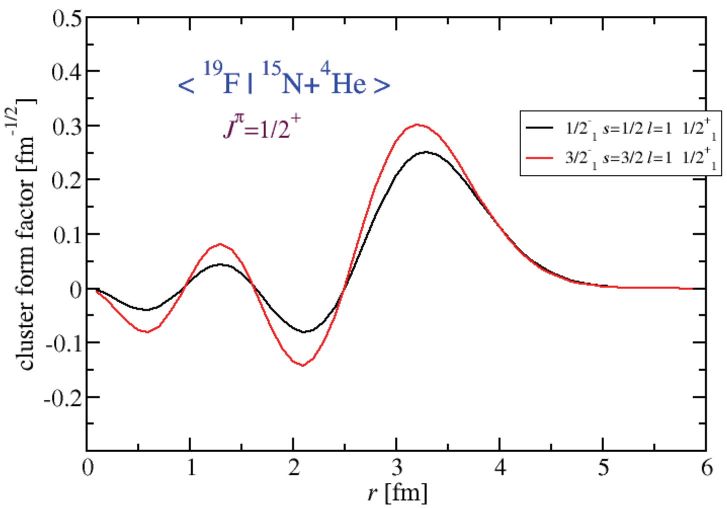

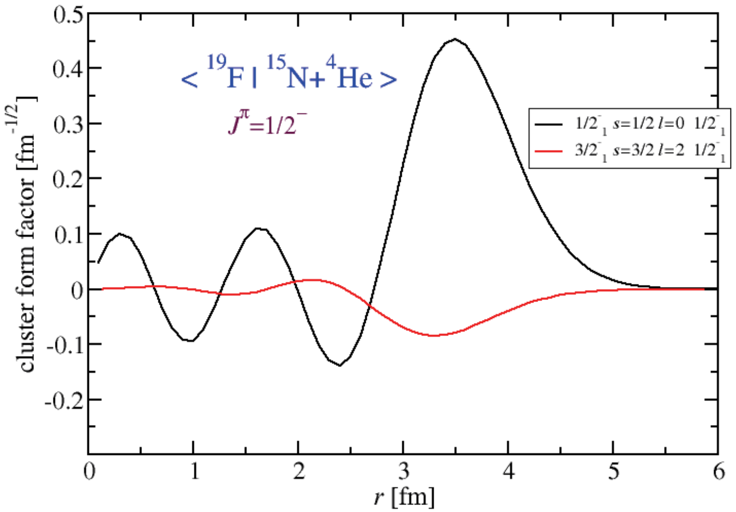

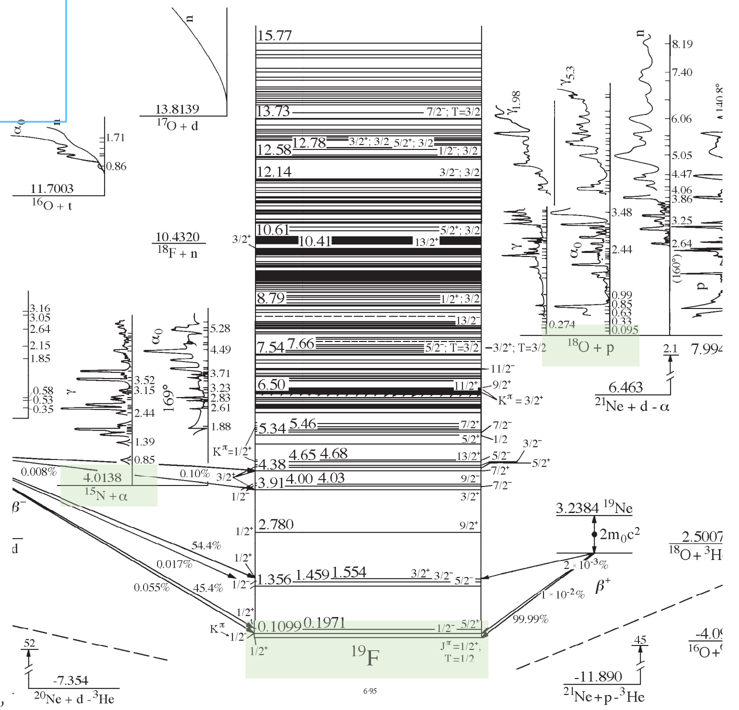

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Nuclear spin-dependent parity-violating effects from NCSM

- Contributions from nucleon axial-vector and the anapole moment

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

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

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

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