Effective electroweak operators for the No-Core Shell Model – an update

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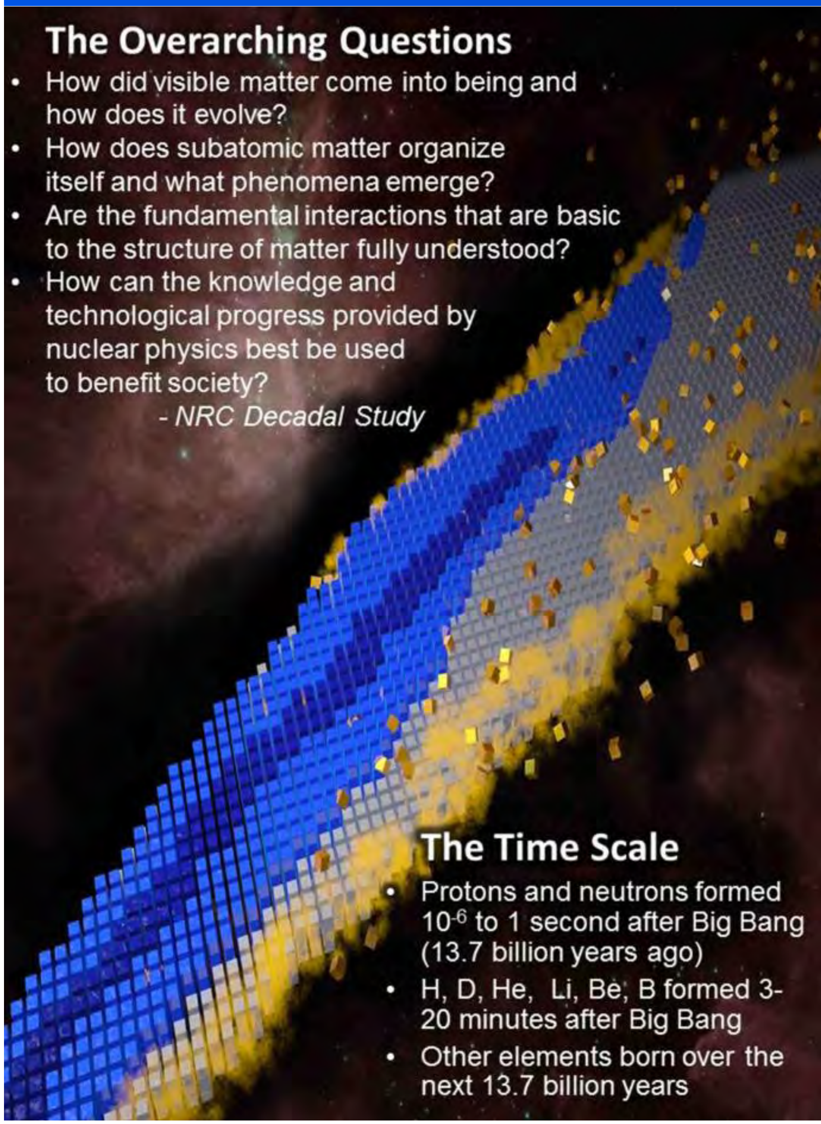
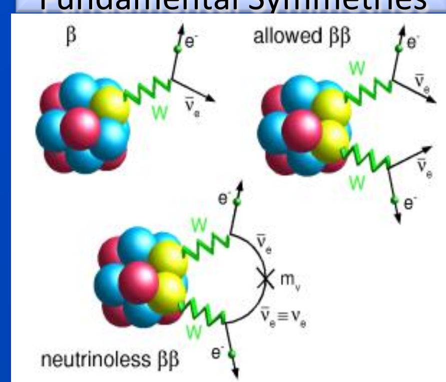
TRIUMF Workshop on Progress in Ab Initio Techniques in Nuclear Physics, Vancouver February 27 – March 2, 2018



LENPIC

Topical Collaboration on Neutrinos and Fundamental Symmetries



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NUCLEI Nuclear Computational Low-Energy Initiative

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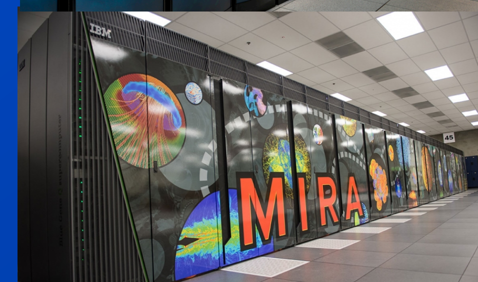


No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

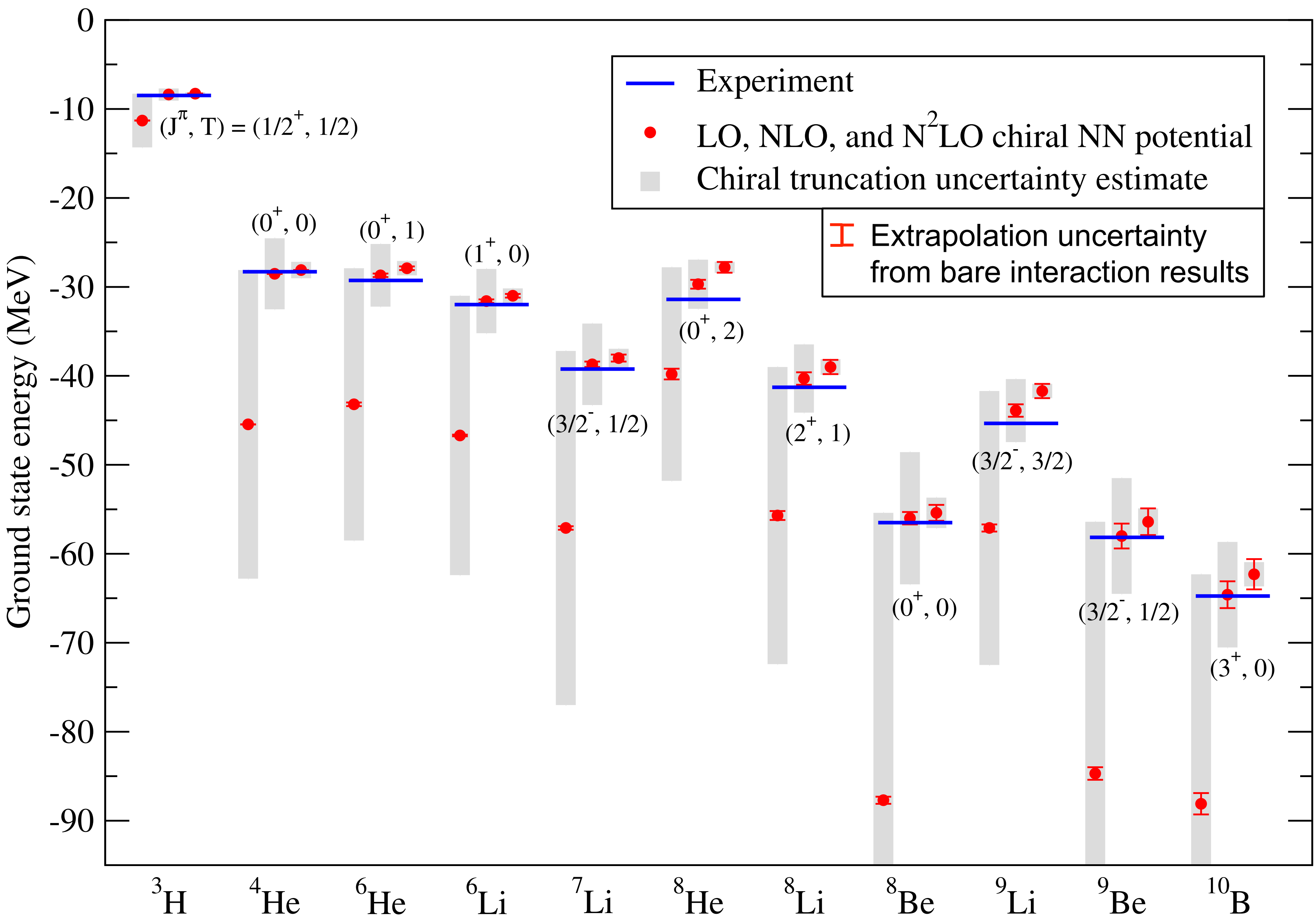
Given a Hamiltonian operator

$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wavefunction of A nucleons

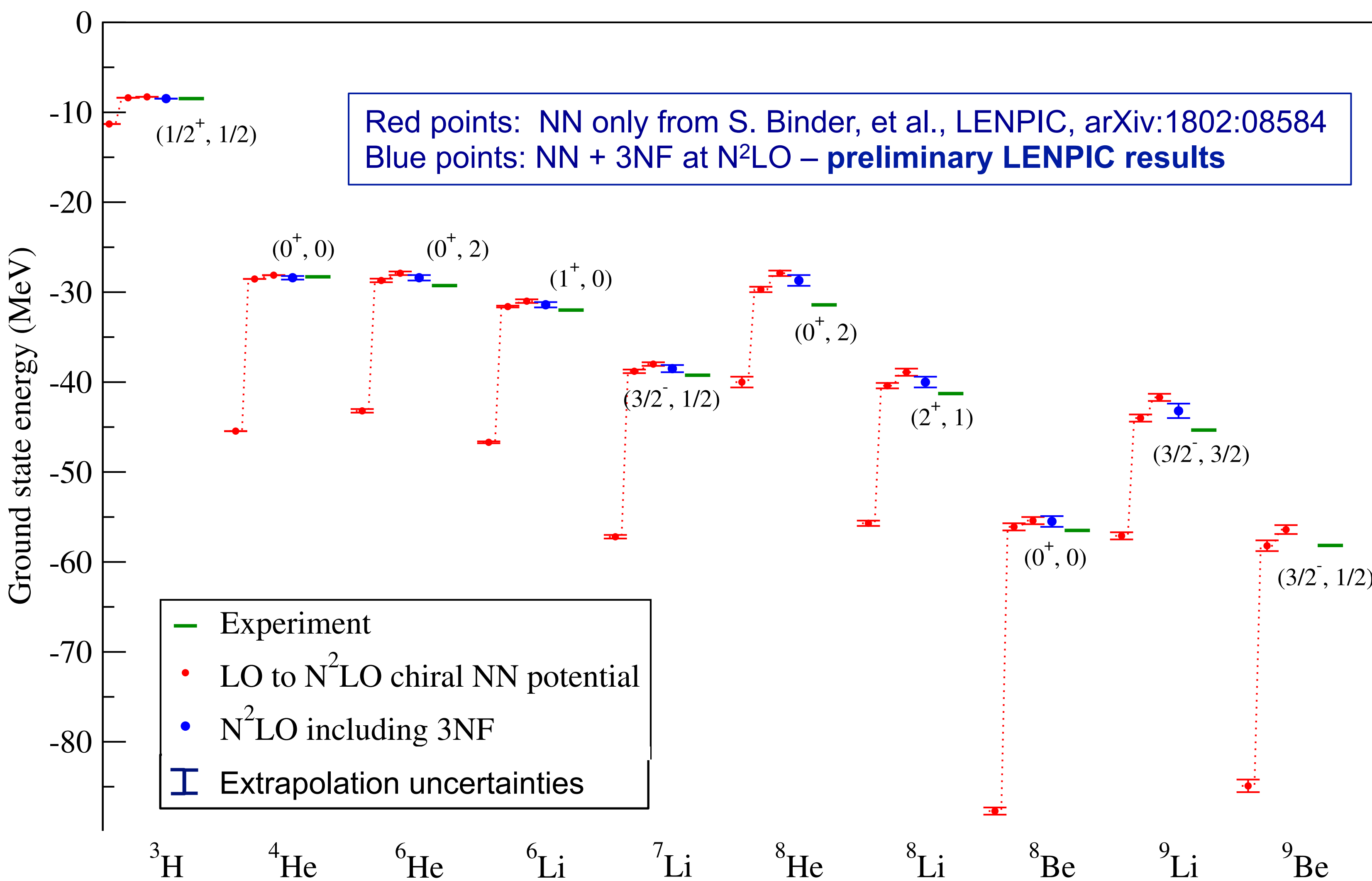
$$\hat{\mathbf{H}}\,\Psi(r_1, \ldots, r_A) = \lambda\,\Psi(r_1, \ldots, r_A)$$

- Expand eigenstates in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle$
- No Core Full Configuration (NCFC) – All A nucleons treated equally
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation



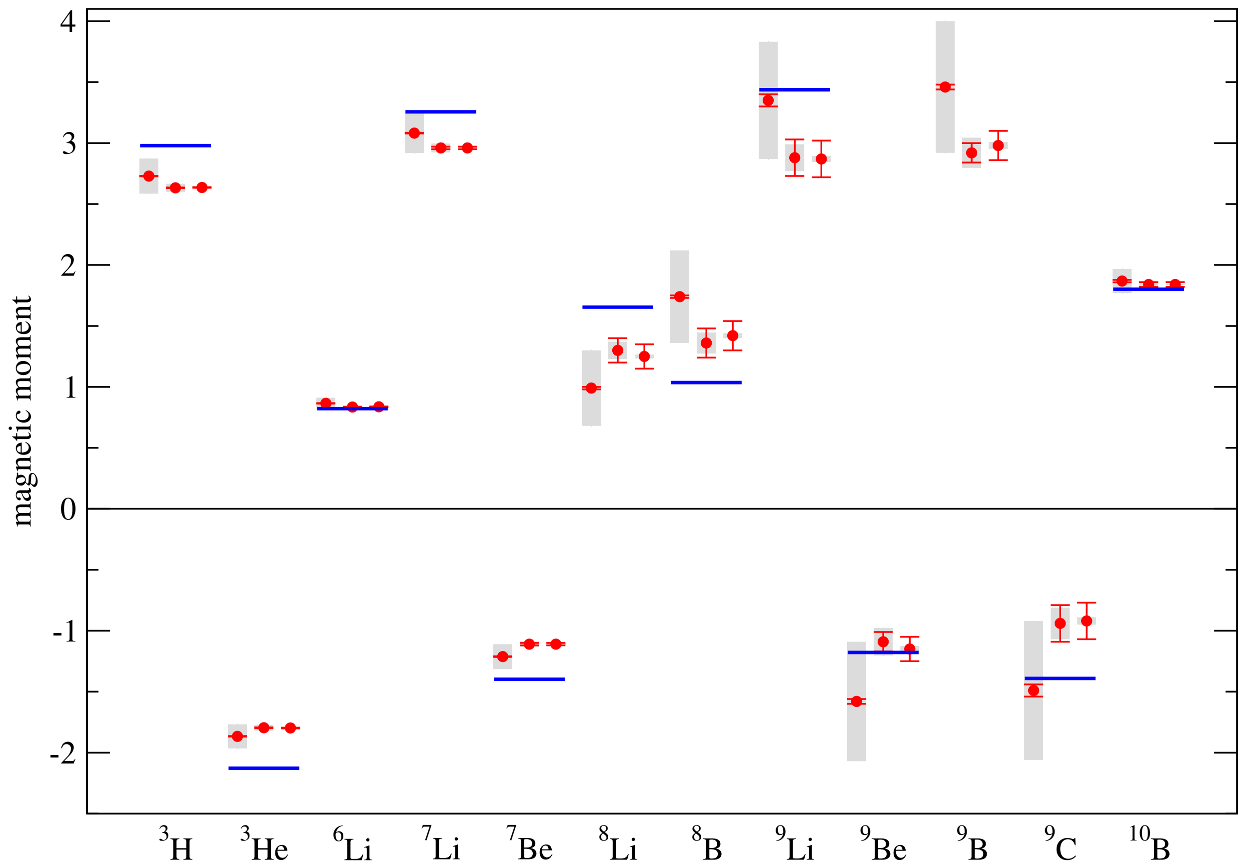
S. Binder, et al., LENPIC Collaboration, arXiv: 1802:08584

Ground state energies up to N²LO including 3NF



Results for magnetic moments with EKM interaction

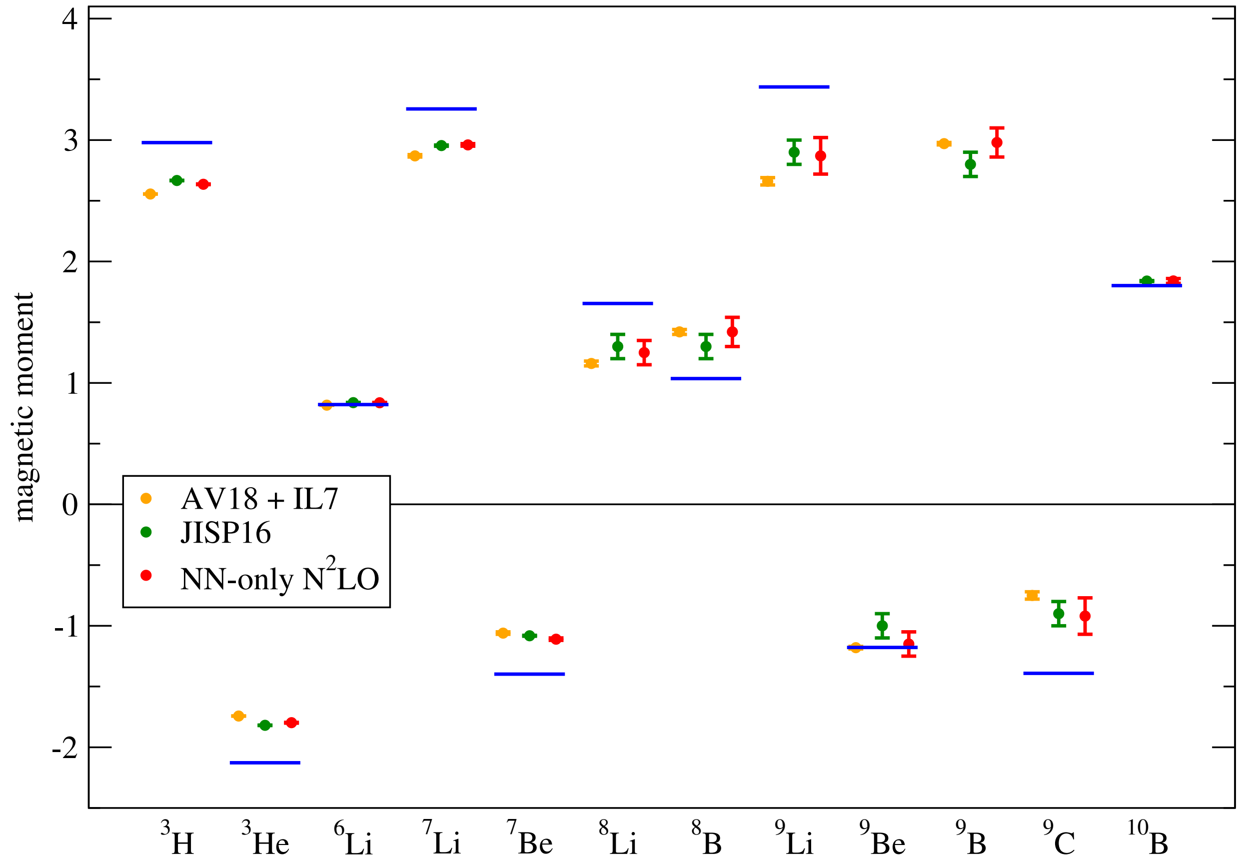
$$\mu = \frac{1}{J+1}\Big(\langle\vec{J}\cdot\vec{L}_p\rangle + 5.586\langle\vec{J}\cdot\vec{S}_p\rangle - 3.826\langle\vec{J}\cdot\vec{S}_n\rangle\Big)\,\mu_0$$



- NN-only potential up to N^{2}LO, but no current corrections

S. Binder, et al., LENPIC, arXiv:1802:08584

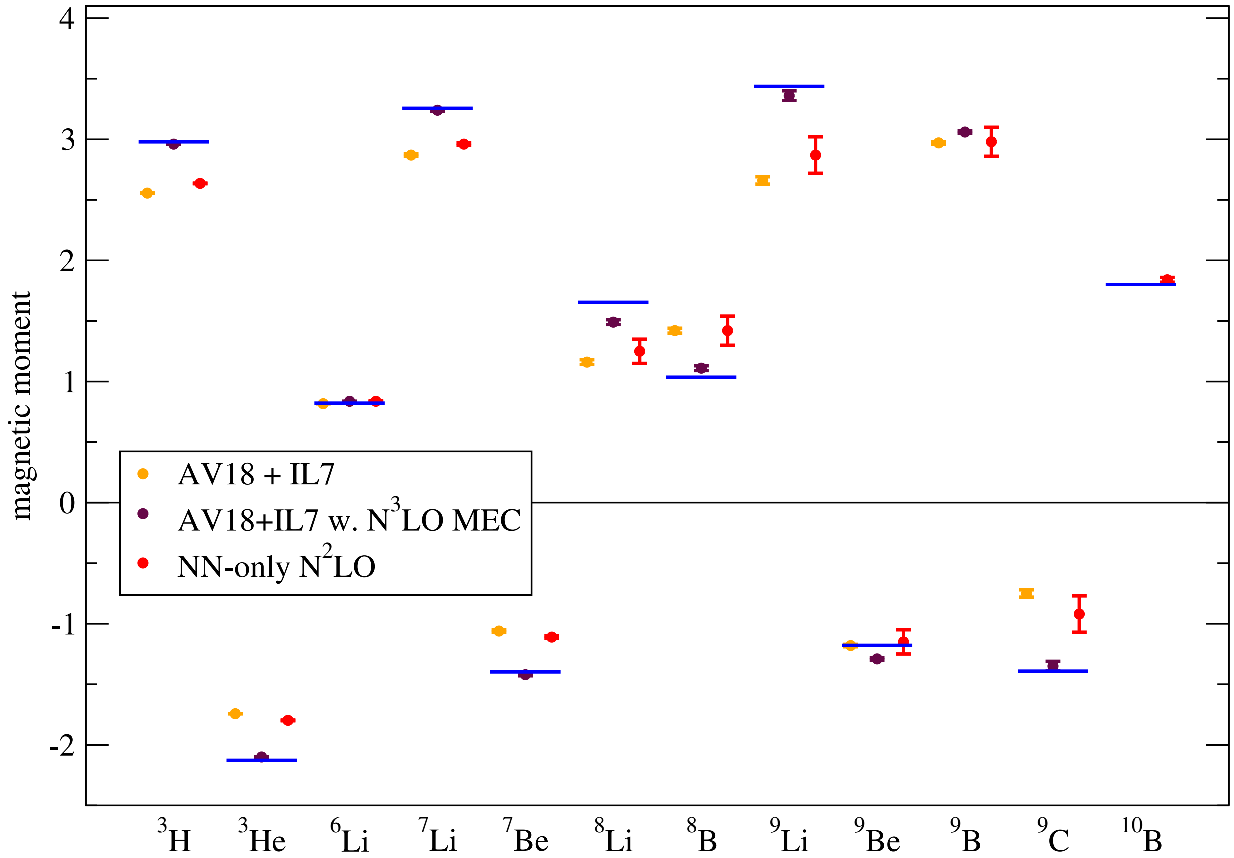
Magnetic moments not very sensitive to interaction



Similar results with very different interactions and many-body methods

- AV18 + IL7 Pastore, Pieper, Schiavilla, Wiringa, PRC87, 035503 (2013)
- JISP16 Maris and Vary, IJMPE22, 1330016 (2013)
- NN-only N^{2}LO S. Binder, et al., LENPIC, arXiv: 1802:08584

but do need 'meson-exchange currents'



- Chiral EFT current corrections up to N^{3}LO improve agreement with data significantly for AV18 + IL7
- Similar current corrections would also improve the LENPIC N^{2}LO results from S. Binder, et al., LENPIC, arXiv:1802:08584

Motivation for 2-body currents: B(M1; $0^+0 \rightarrow 1^+1$) in ^{12}C without 2-body currents

v-^{12}C cross section
and the 0^+ 0 -> 1^+ 1
Gamow-Teller transition

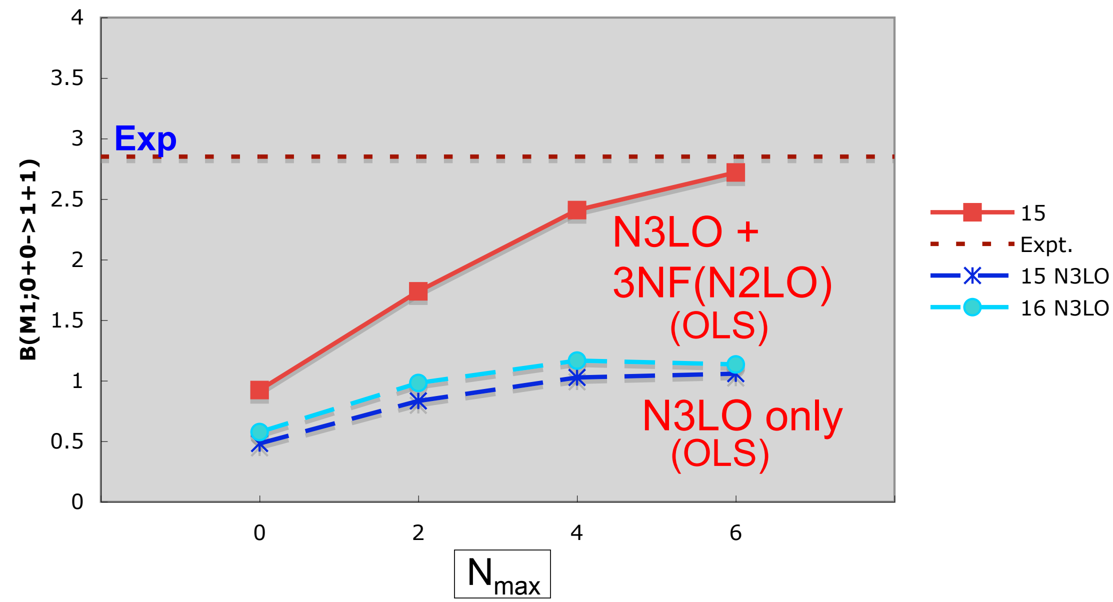
A.C.Hayes, P. Navratil, J.P. Vary, PRL 91, 012502 (2003); nucl-th/0305072

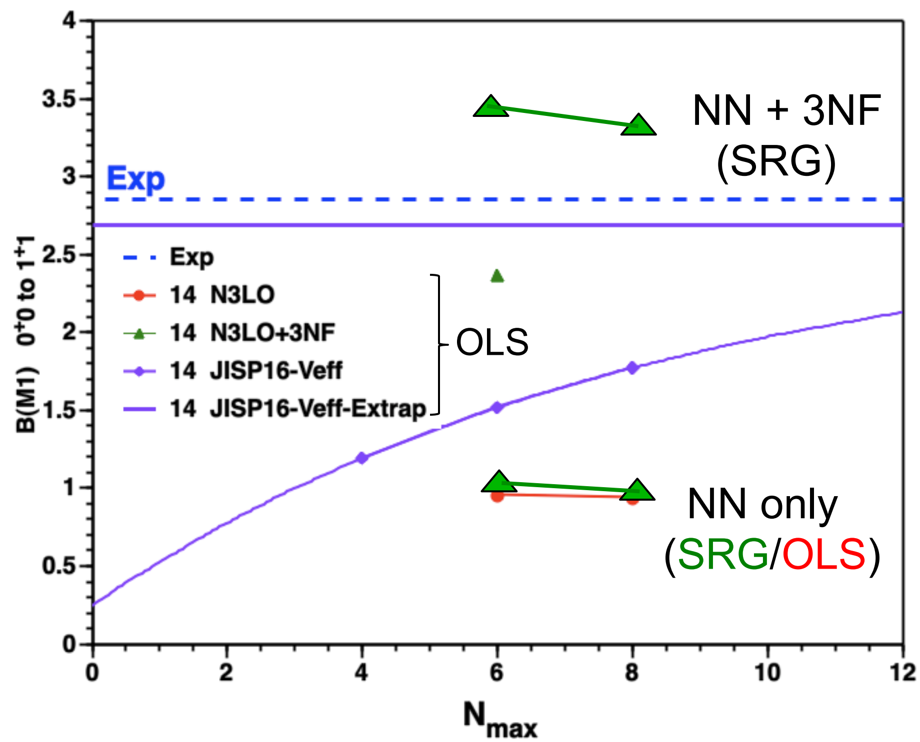
First successful description of the GT data required 3NF. Both CDBonn + TM' or AV8' + TM' => large enhancement

N3LO+3NF (OLS) results from: P. Navartil, V.G. Gueorguiev, J.P. Vary, W.E. Ormand and A. Nogga, PRL 99, 042501 (2007).

N_{max} = 6, 8 results with SRG on N3LO+3NF (N2LO); P. Maris, et al, PRC 90, 014314 (2014) [▲]

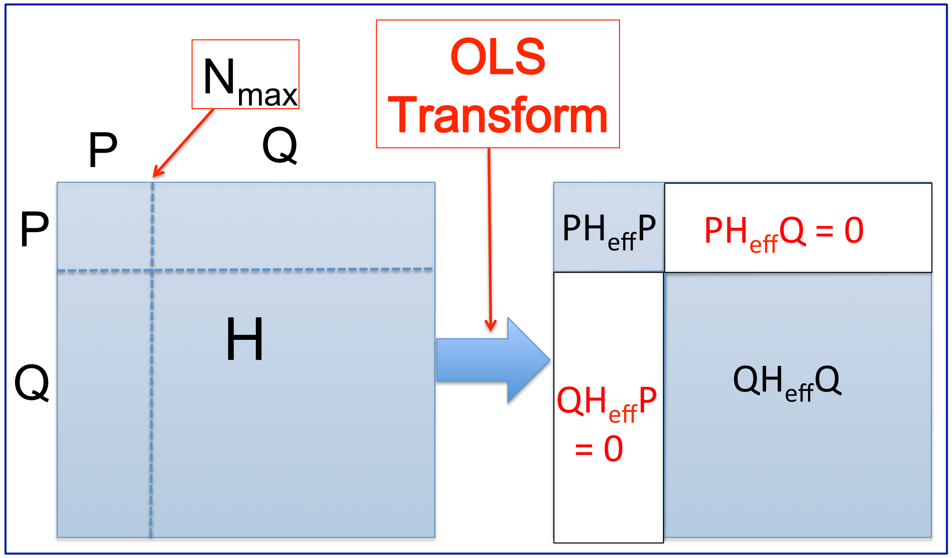
Non-local NN interaction from inverse scattering (JISP16) also successful





OLS Transform:

Unitary transformation that block-diagonalizes the Hamiltonian



$$UHU^{\dagger} = U[T+V]U^{\dagger} = H_d$$

$$H_{\text{eff}} = U_{OLS} H U_{OLS}^{\dagger} = PH_{\text{eff}}P = P[T+V_{\text{eff}}]P$$

$$U^P = PUP$$

$$\tilde{U}^P = P\tilde{U}^P P = \frac{U^P}{\sqrt{U^{P\dagger}U^P}}$$

$$H_{\text{eff}} = \tilde{U}^{P\dagger} H_d \tilde{U}^P = \tilde{U}^{P\dagger} UHU^{\dagger} \tilde{U}^P = P[T+V_{\text{eff}}]P$$

$$O_{\text{eff}} = \tilde{U}^{P\dagger} UOU^{\dagger} \tilde{U}^P = P[O_{\text{eff}}]P$$

Consistent observables

$$U_{OLS} = \tilde{U}^{P\dagger} U$$

Consider two nucleons as a model problem with V = LENPIC chiral NN solved in the harmonic oscillator basis with $\hbar\Omega$ = 5, 10 and 20 MeV. Also, consider the role of an added harmonic oscillator quasipotential

Hamiltonian #1 $H = T + V$

Hamiltonian #2 $H = T + U_{\text{osc}}(\hbar\Omega_{\text{basis}}) + V$

Other observables:

Root mean square radius	R
Magnetic dipole operator	M1
Electric dipole operator	E1
Electric quadrupole moment	Q
Electric quadrupole transition	E2
Gamow-Teller	GT
Neutrinoless double-beta decay	M(0v2β)

Dimension of the “full space” is 400 for all results depicted here

Deuteron gs energy: "models" are N_{max} truncation & OLS

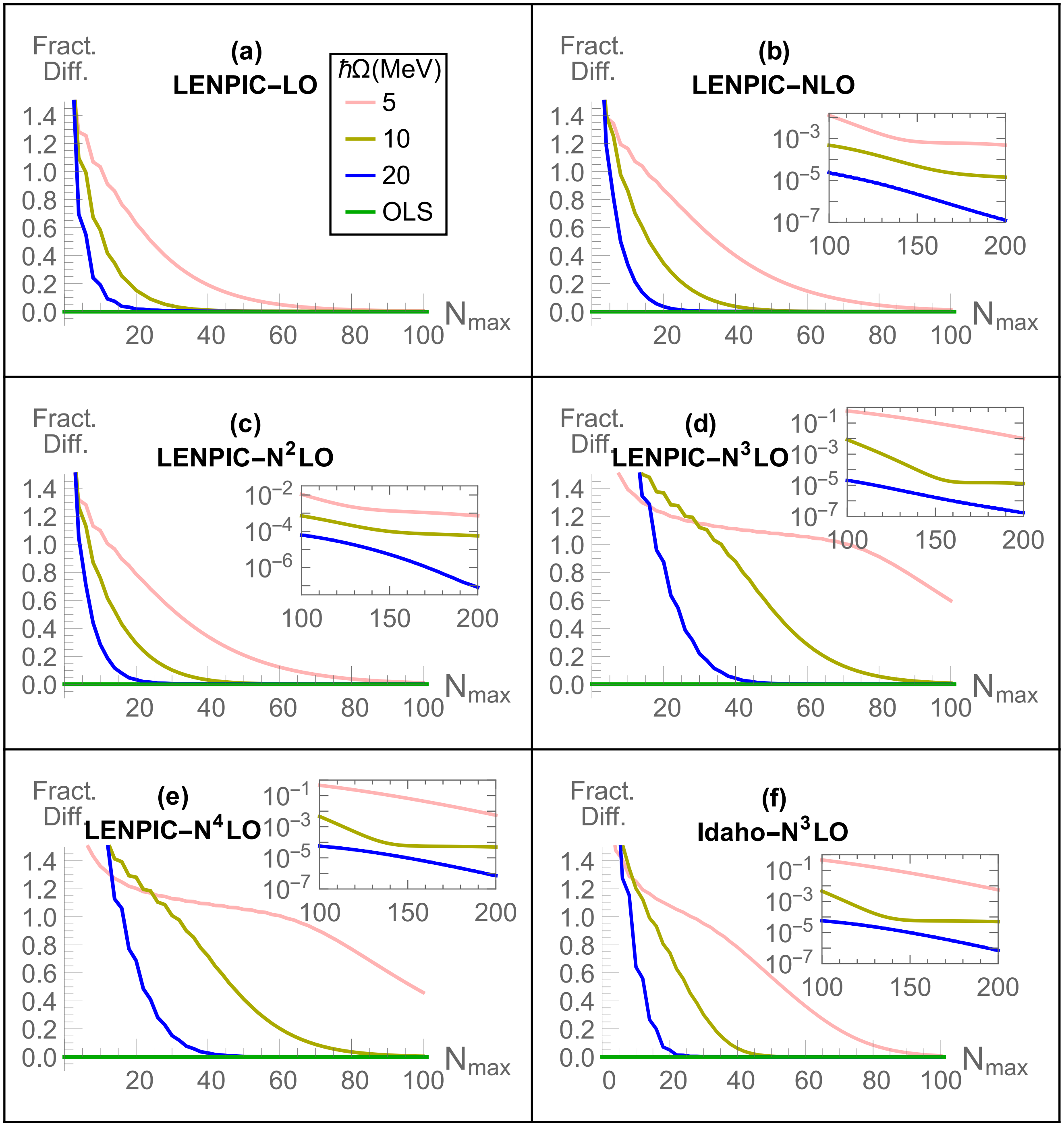
Fract. Diff. = $(E_{model} - E_{exact})/|E_{exact}|$

Insets: Semilog plots of high N_{max} region

OLS gives exact results for all cases (green lines at Fract. Diff. = 0)

Convergence patterns sensitive to chiral order

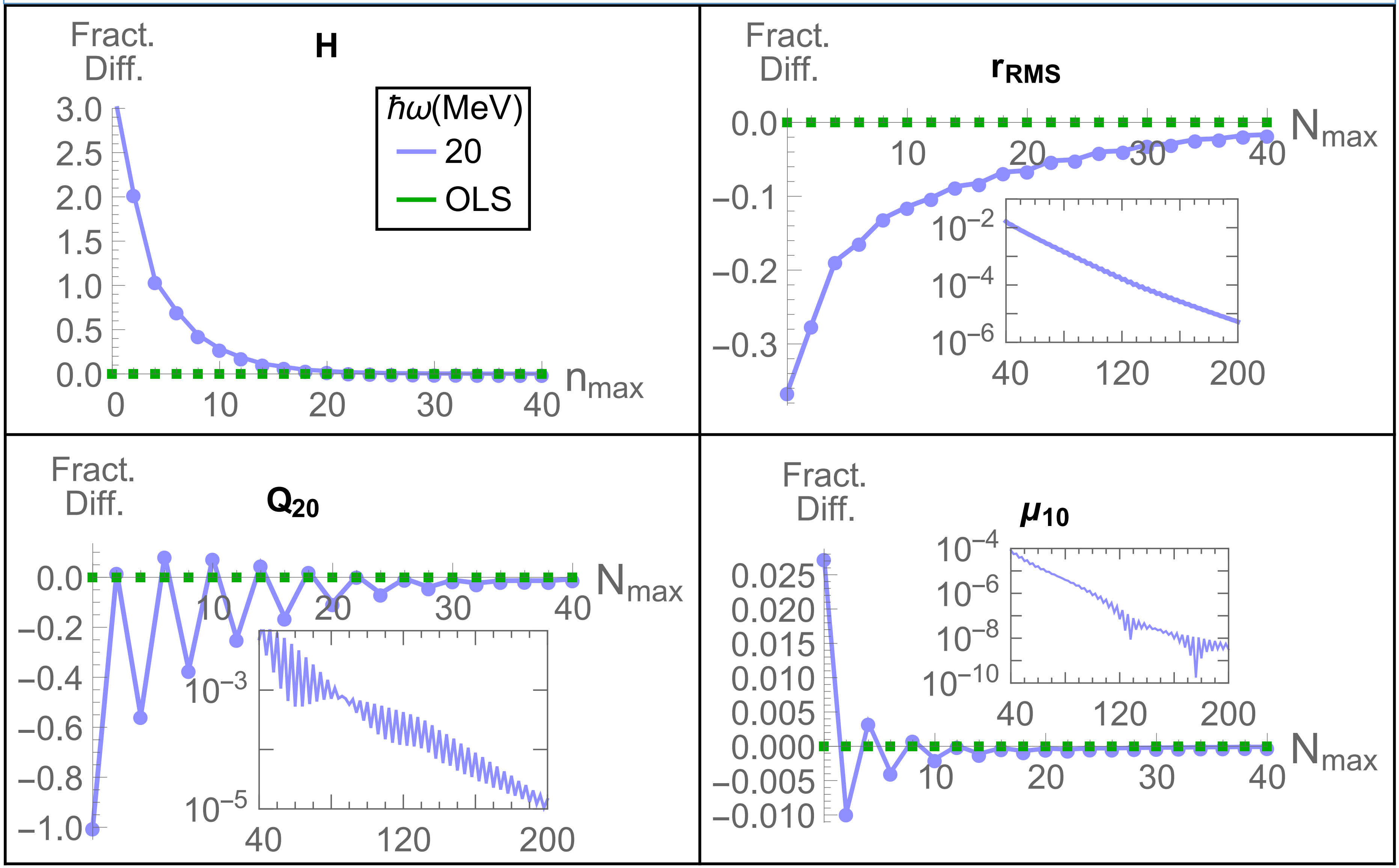
Even unbound cases (Fract. Diff. > 1.0) are accurately treated with OLS



Preliminary

LENPIC NN interaction at N^2LO and electroweak operators – truncation vs OLS

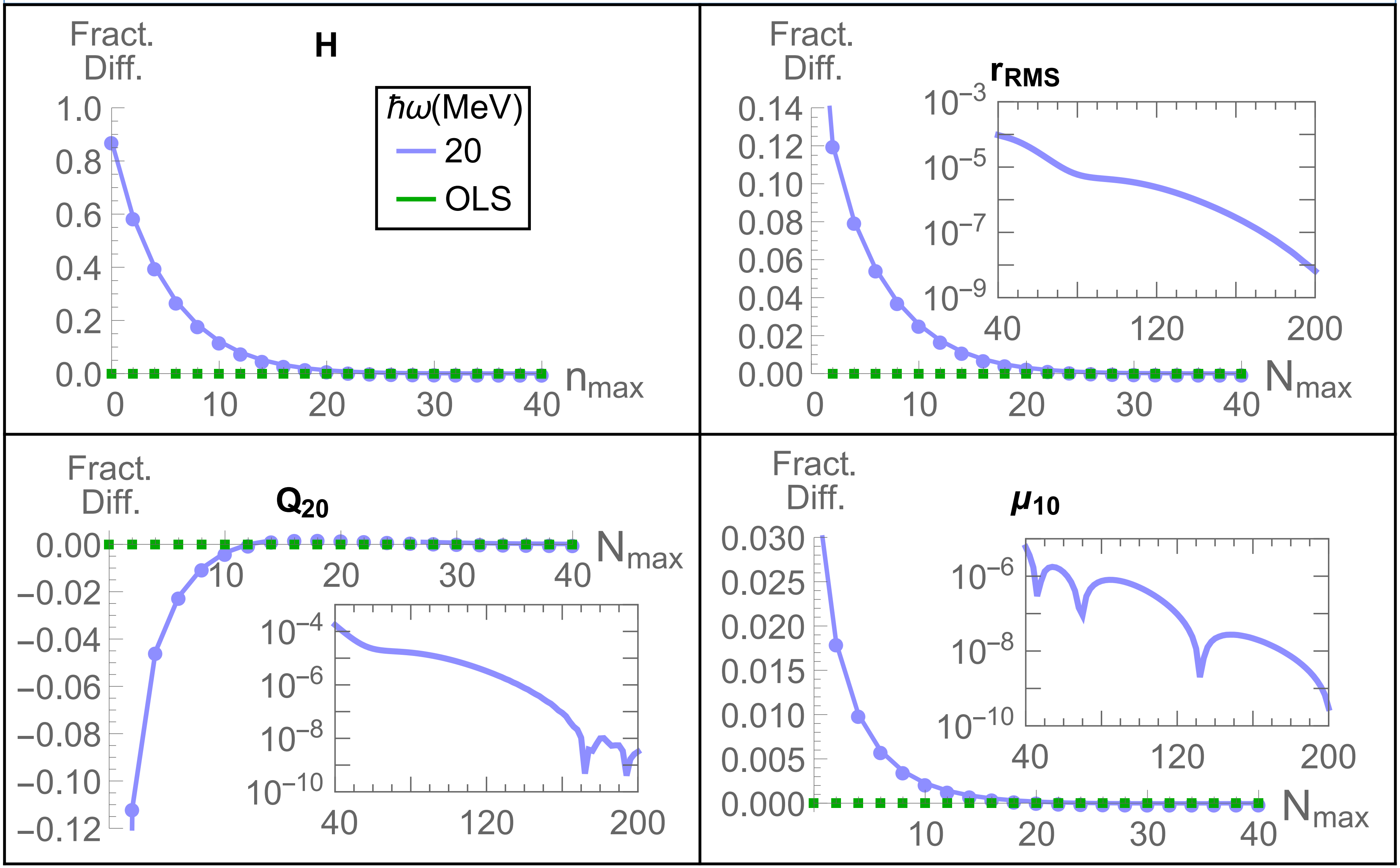
Deuteron properties with "Fract. Diff." = (Model-Exact)/|Exact|; inset=log(|Fract. Diff.|)



Preliminary

LENPIC NN interaction at N^{2}LO and electroweak operators – truncation vs OLS

Deuteron properties in 20 MeV trap with "Fract. Diff." = (Model-Exact)/|Exact|; inset=log(|Fract. Diff.|)

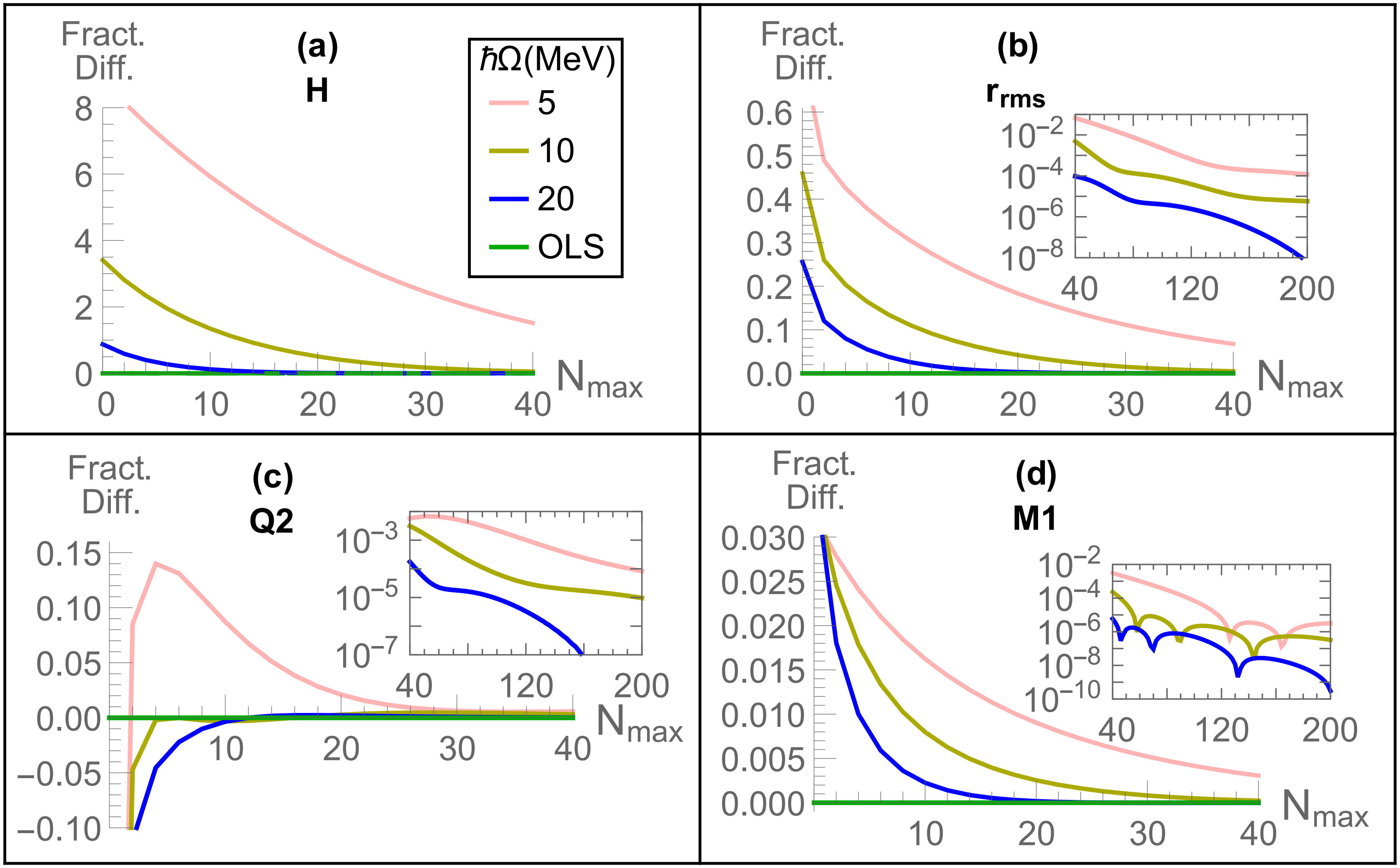


Deuteron in a Harmonic Oscillator trap with trap ħΩ = basis ħΩ

LENPIC Chiral NN interaction at N^{2}LO with R = 1.0 fm

Comparison of results from truncation with OLS results

"Fract. Diff." = (Model-Exact)/|Exact|



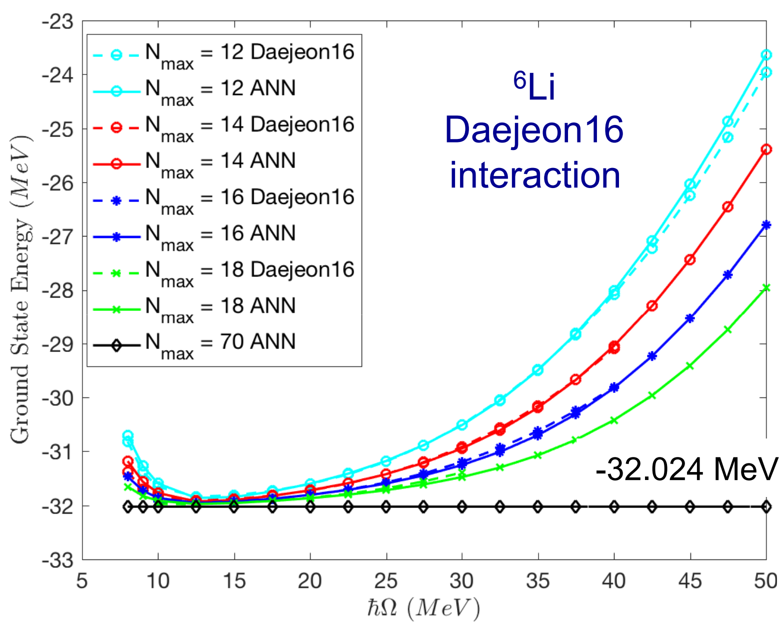
Demonstrates OLS is accurate for EM observables with trap simulating the nuclear environment

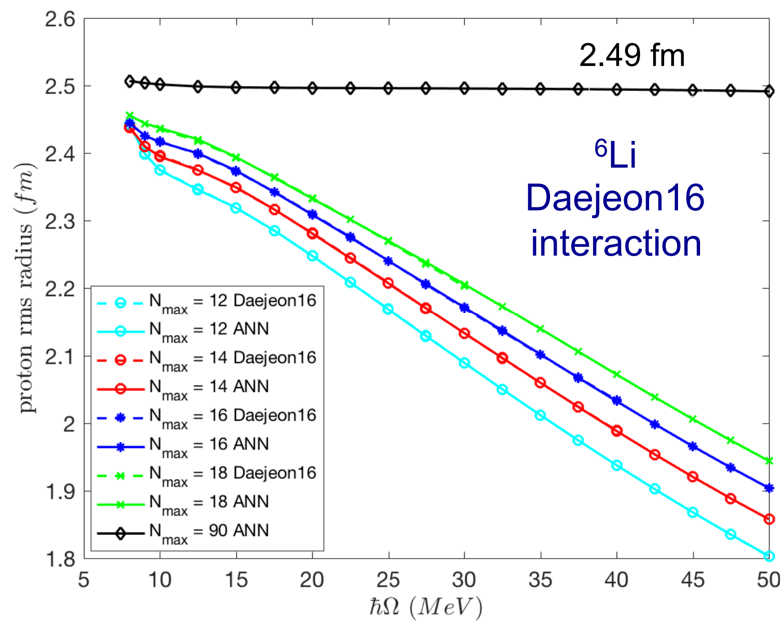
Extrapolating to complete basis

- Perform a series of calculations with increasing N_{max} truncation
- Empirical extrapolation binding energy

$$E^{N}_{\text{binding}} = E^{\infty}_{\text{binding}} + a \exp(-bN_{\text{max}})$$

- Artificial Neural Networks trained with Nmax ≤ 10 NCSM results





Negoita, et al., Computation Tools 2018, Barcelona, Feb. 19, 2018: Published online:
http://www.thinkmind.org/index.php?view=article&articleid=computation_tools_2018_1_40_80017
Also to appear shortly on the arXiv

Compare traditional methods with Artificial Neural Networks (ANN) which use Nmax ≤ 10 NCSM results for training

^{6}Li
Daejeon16 interaction

Observable	Upper Bound $N_{\max} = 10$	Upper Bound $N_{\max} = 18$	Estimation[a] $N_{\max} \leq 10$	ANN $N_{\max} \leq 10$
gs energy (MeV)	-31.688	-31.977	-31.892	-32.024
gs rms radius (fm)	–	–	2.40	2.49

[a]Exponential extrapolation for gs energy and crossover method for gs rms radius

Negoita, et al., Computation Tools 2018, Barcelona, Feb. 19, 2018: Published online:
http://www.thinkmind.org/index.php?view=article&articleid=computation_tools_2018_1_40_80017
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Outlook

Extend the regulator sensitivity study => uncertainty quantification

Implement new generation of LENPIC chiral EFT interactions & EW operators

Perform benchmark 0n2b-decay calculations with UNC group (underway)

Streamline workflow and extend applications in light nuclei with Notre Dame group (underway)

Evaluate/save density matrices (static and transition) and use them to evaluate consistent OLS'd or SRG'd observables

Extend to medium weight nuclei with "Double OLS" approach - underway

Improve convergence: natural orbitals - **see Patrick Fasano's poster**, neural network developments, . . .

Reactions – HORSE, time-dependent Basis Function (tBF), . . .

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Weijie Du (grad student)
Matthew Lockner (grad student)
Pieter Maris
Soham Pal (grad student)
Shiplu Sarker (grad student)

New faculty position at Iowa State in Nuclear Theory
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