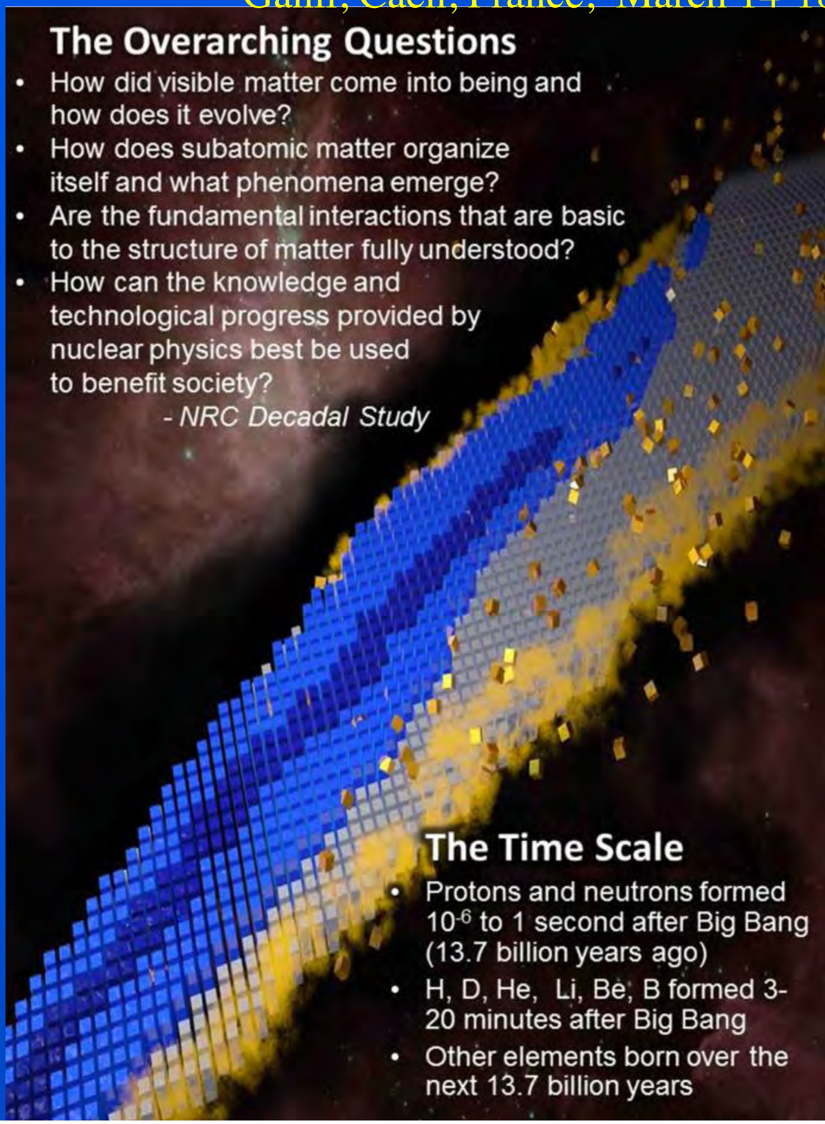
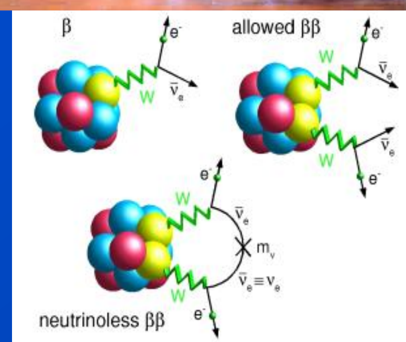
ab initio No-Core Shell Model with Consistent Electromagnetic Properties

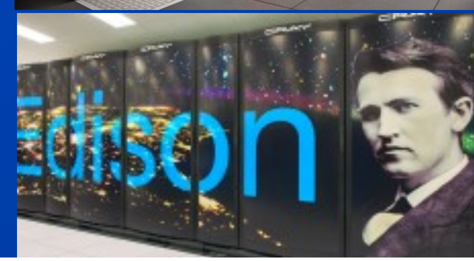
James P. Vary, Iowa State University

Future directions for nuclear structure and reaction theories: Ab initio approaches for 2020

Ganil, Caen, France, March 14-18, 2016







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SciDAC — Scientific Discovery through Advanced Computing

NUCLEI — Nuclear Computational Low-Energy Initiative

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LENPIC

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 CI: all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

Nuclei represent strongly interacting, self-bound, open systems with multiple scales – a computationally hard problem whose solution has potential impacts on other fields

Question: What controls convergence/uncertainties of observables?
Answer: Characteristic infrared (IR) and ultraviolet (UV) scales of the operators.

In a plane-wave basis:
- λ = lowest momentum scale - can be zero (e.g. T_{rel}, r^2, B(EL), . . .)
- Λ = highest momentum scale - can be infinity (e.g. T_{rel}, hard-core V_{NN})

In a harmonic-oscillator basis with N_{max} truncation:

$$\lambda \approx \sqrt{\hbar\Omega / N_{max}}$$

$$\Lambda \approx \sqrt{\hbar\Omega \, N_{max}}$$

What are examples of the other physically relevant scales in nuclear physics?
- Interaction scales (total binding, Fermi momentum, SRCs, one-pion exchange, . . .)
- Leading dissociation scale (halos, nucleon removal energy, . . .)
- Collective motion, clustering scales (Q, B(E2), giant modes, . . .)

Guidelines for many-body calculations to guarantee preserved predictive power:

1. Select basis regulators:

$$\lambda \leq \text{ all relevant IR scale limits}$$

$$\Lambda \geq \text{ all relevant UV scale limits except } T_{rel}$$

2. Since T_{rel} has simple IR and UV asymptotics, extrapolation is feasible.

✧ J-matrix for scattering – takes both IR and UV limits of HO basis
✧ IR extrapolation tools developed over past ~5 years

To follow guideline #1, the OLS method provides the advantage of transforming all operators to act only within the scale fixed by the basis regulators.

<u>The cost:</u> induced many-body operators need to be assessed
<u>The benefit:</u> extrapolation may be avoided

Phenomeological NN interaction: JISP16

JISP16 tuned up to ^{16}O

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

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Realistic nuclear Hamiltonian: Ab exitu approach

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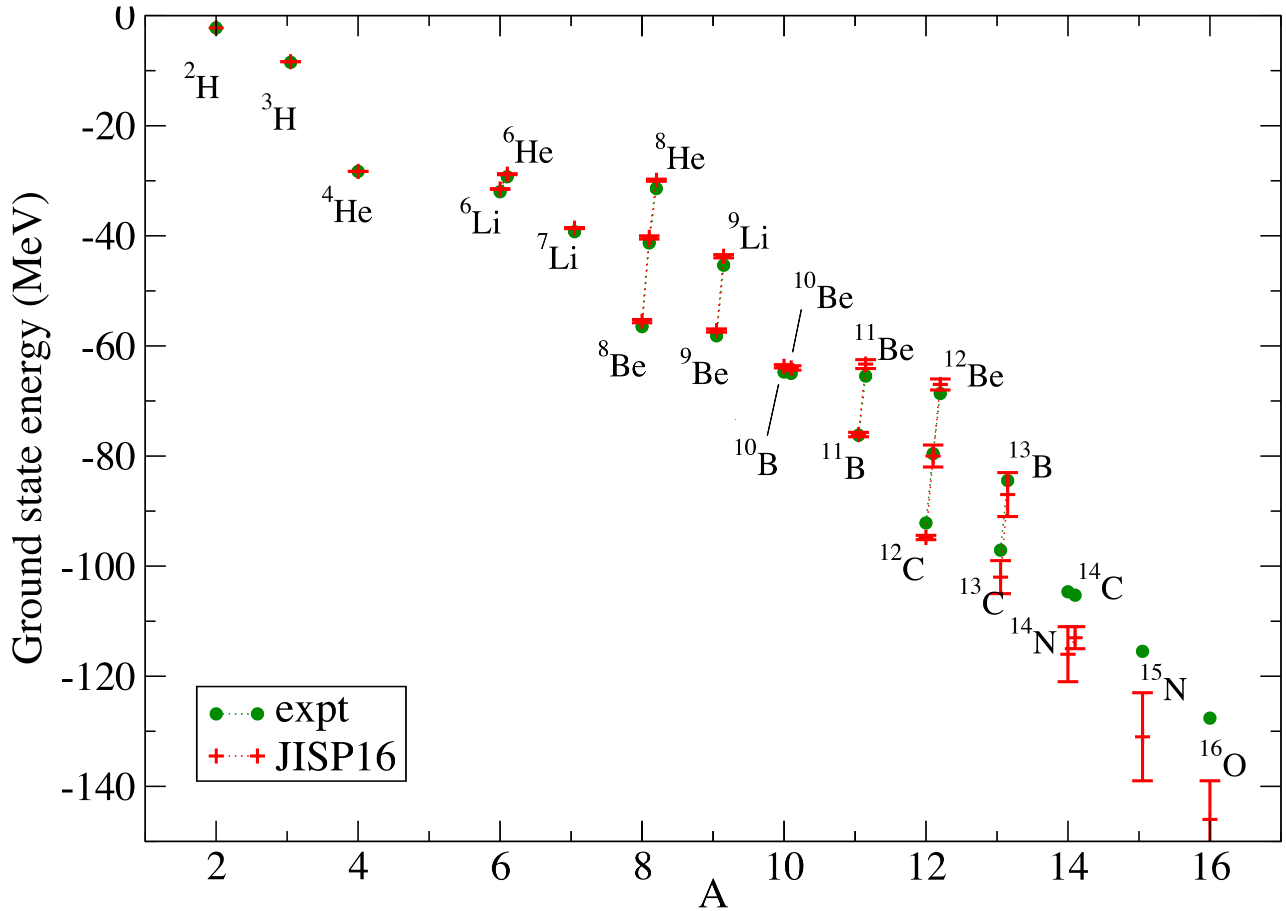
Ground state energy of p-shell nuclei with JISP16

Compare theory and experiment for 24 nuclei Maris, Vary, IJMPE22, 1330016 (2013)

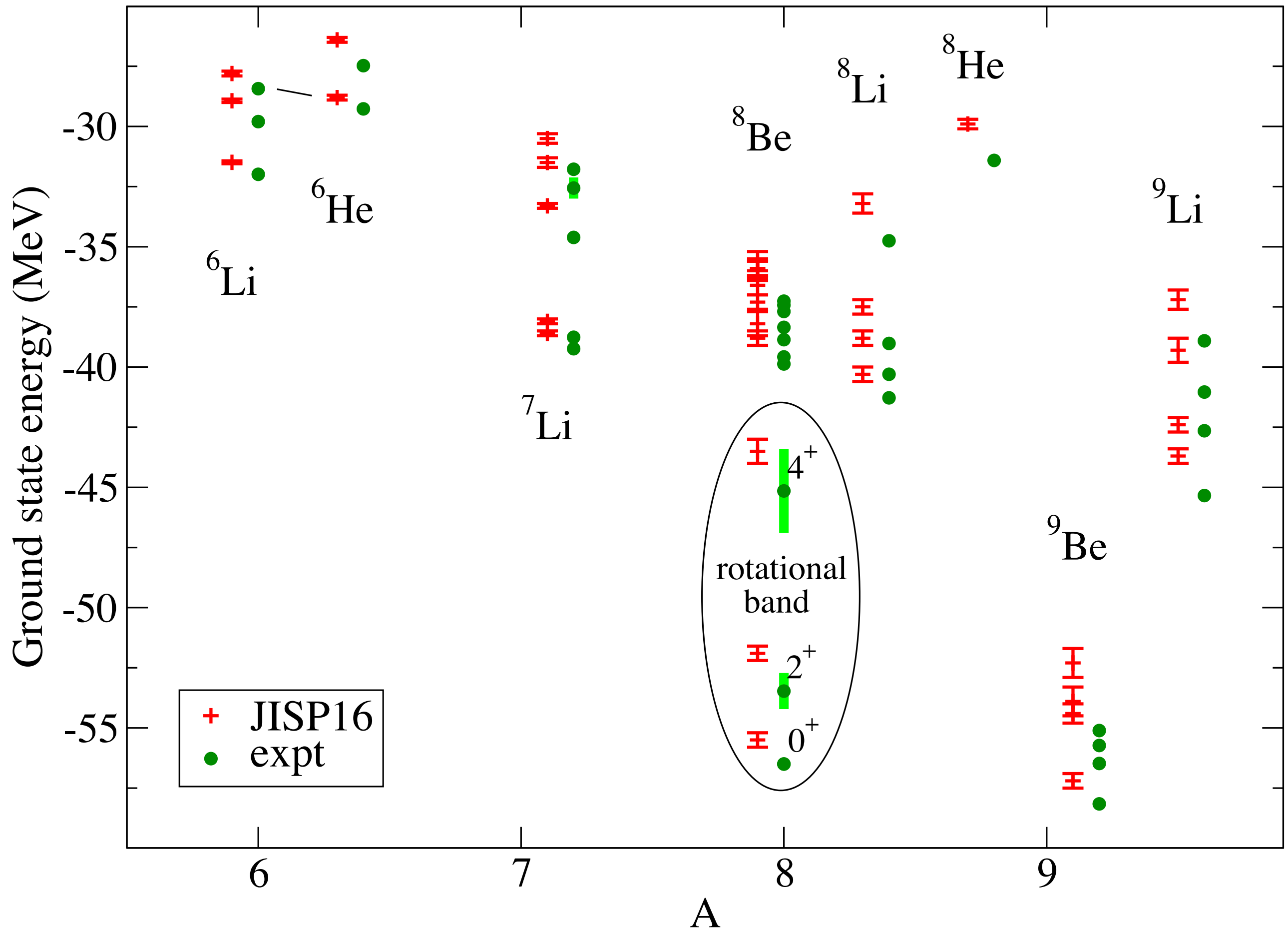


- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$ MeV) with JISP16

Energies of narrow A=6 to A=9 states with JISP16

Compare theory and experiment for 33 states

Maris, Vary, IJMPE22, 1330016 (2013)

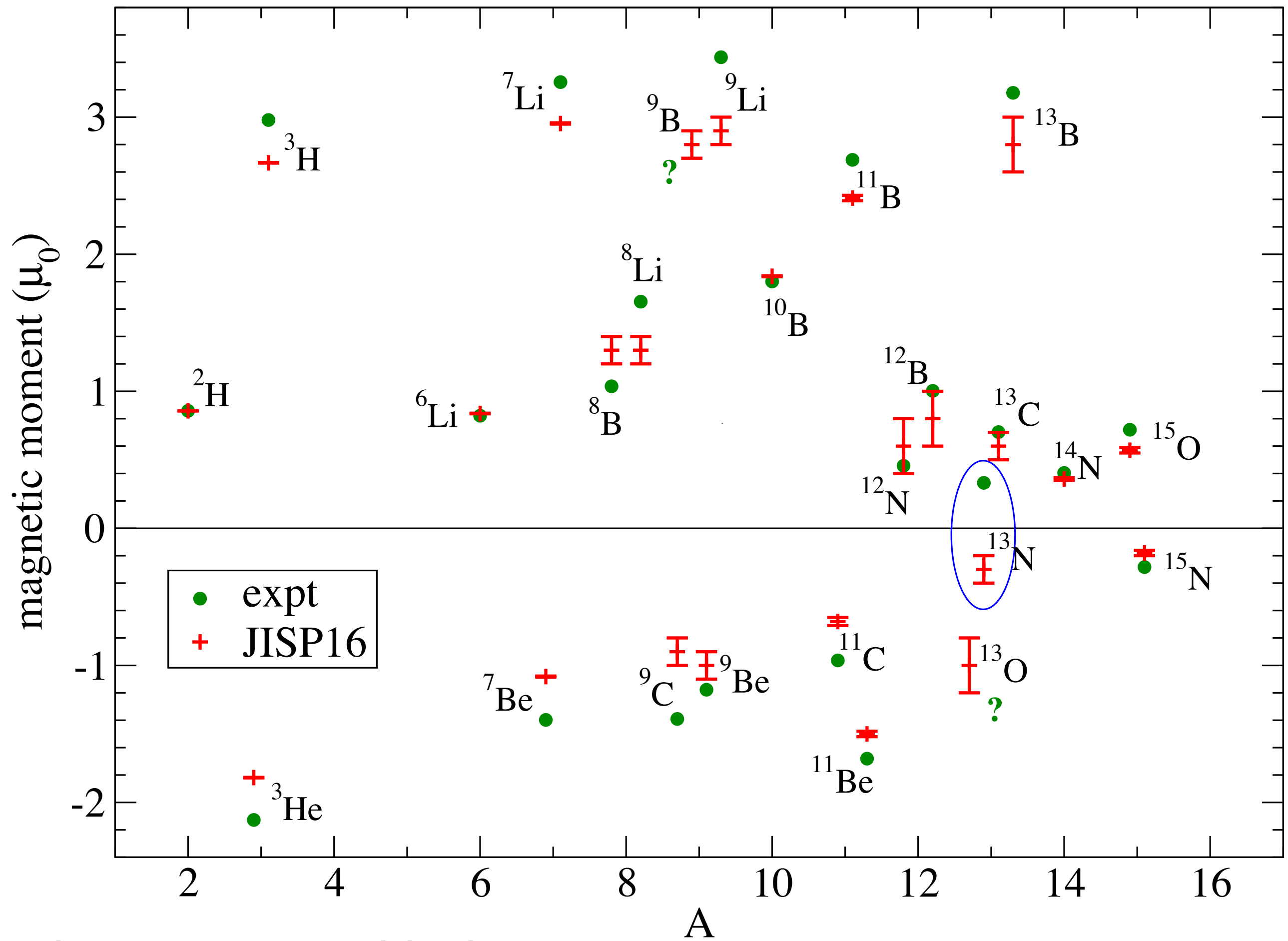


- Excitation spectrum narrow states in good agreement with data

Ground state magnetic moments with JISP16

Compare theory and experiment for 22 magnetic moments Maris, Vary, IJMPE22, 1330016 (2013)

$$\mu = \frac{1}{J+1}\left(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + 5.586\langle \mathbf{J}\cdot\mathbf{S}_p\rangle - 3.826\langle \mathbf{J}\cdot\mathbf{S}_n\rangle\right)\mu_0$$



- Good agreement with data,
  given that we do not have any meson-exchange currents

Extrapolating to the infinite matrix limit
i.e. to the "continuum limit"

Results with both IR and UV extrapolations

References:

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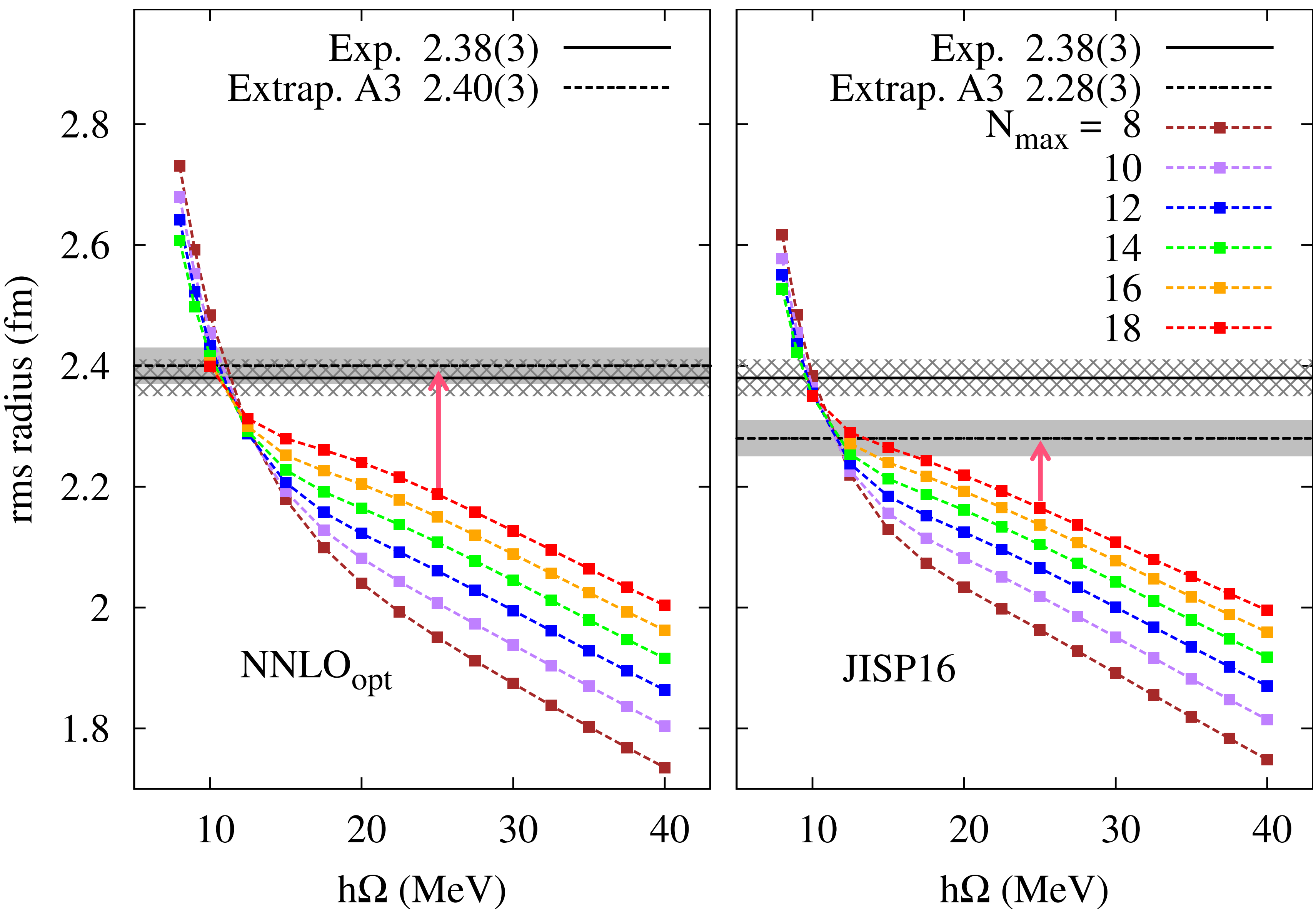
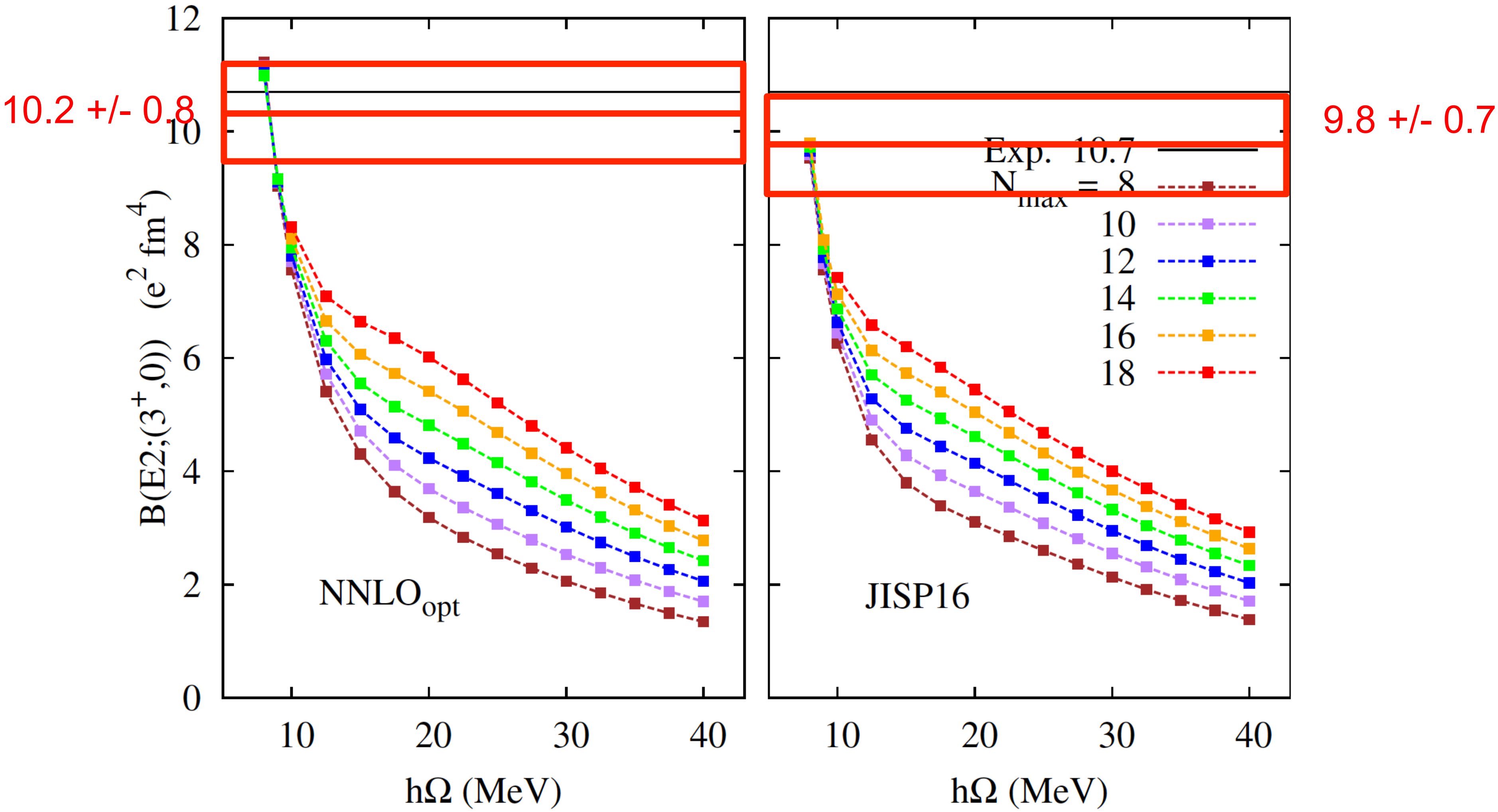
D. Odell, T. Papenbrock and L. Platter, arXiv 1512.04851

=> Uncertainty Quantification



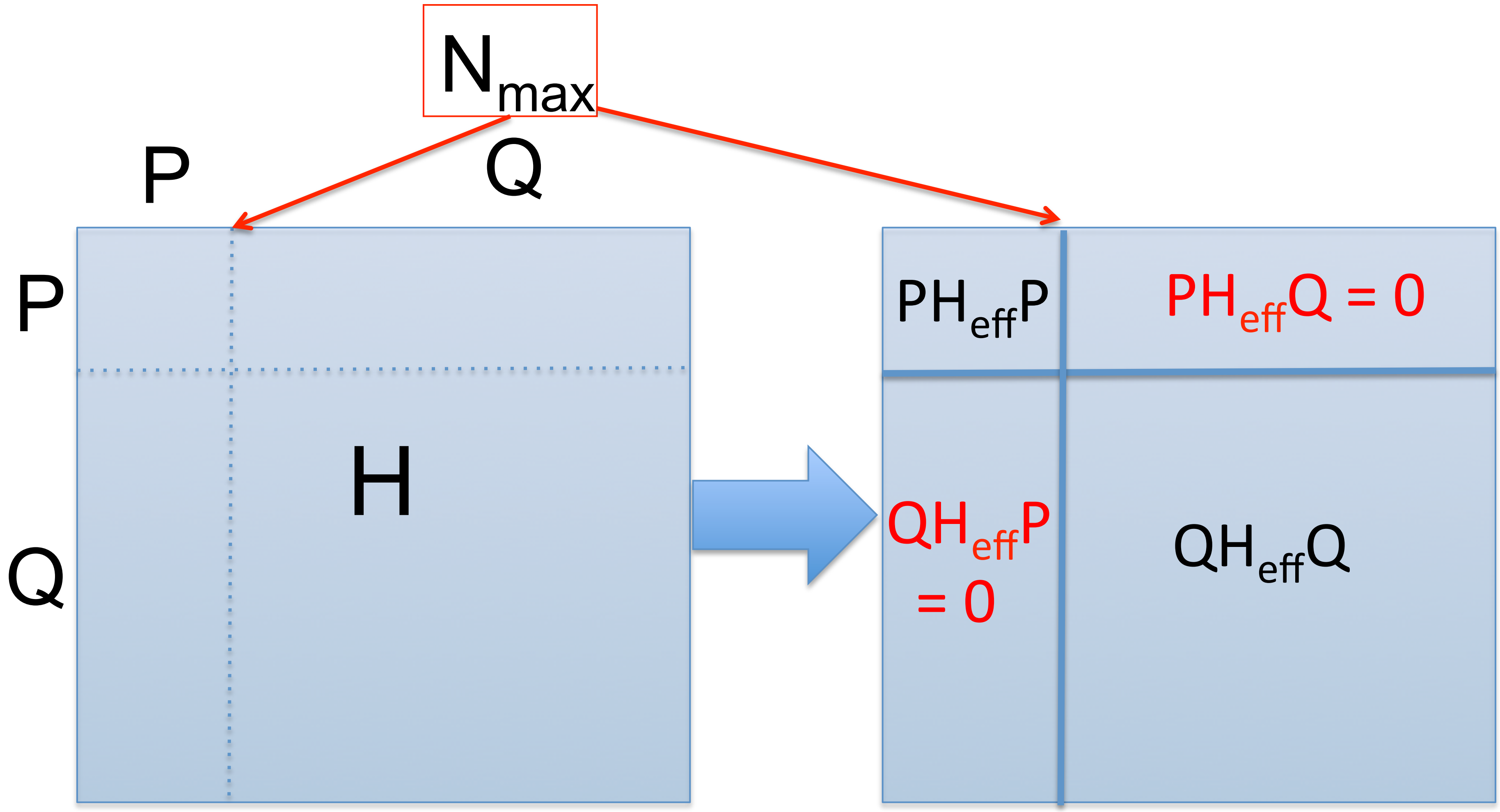
Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, in preparation

=> Apply new extrapolation method:
D. Odell, T. Papenbrock and L. Patter, arXiv 1512.04851
Extrapolations by Thomas Papenbrock



Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, in preparation

OLS Transform on H



With H defining the OLS transformation,
same picture applies to other Hermitian operators

Outline of the OLS process

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

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

$$U^P = PUP$$

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

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

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

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

Consider the Deuteron as a model problem with V = JISP16
λ(JISP16) ~ 50 MeV/c & Λ(JISP16) ~ 500 MeV/c solved in the harmonic oscillator basis with $\hbar\Omega_{basis}$ = 10, 20, 30 and 40 MeV.
Also, consider the role of an added harmonic oscillator quasipotential

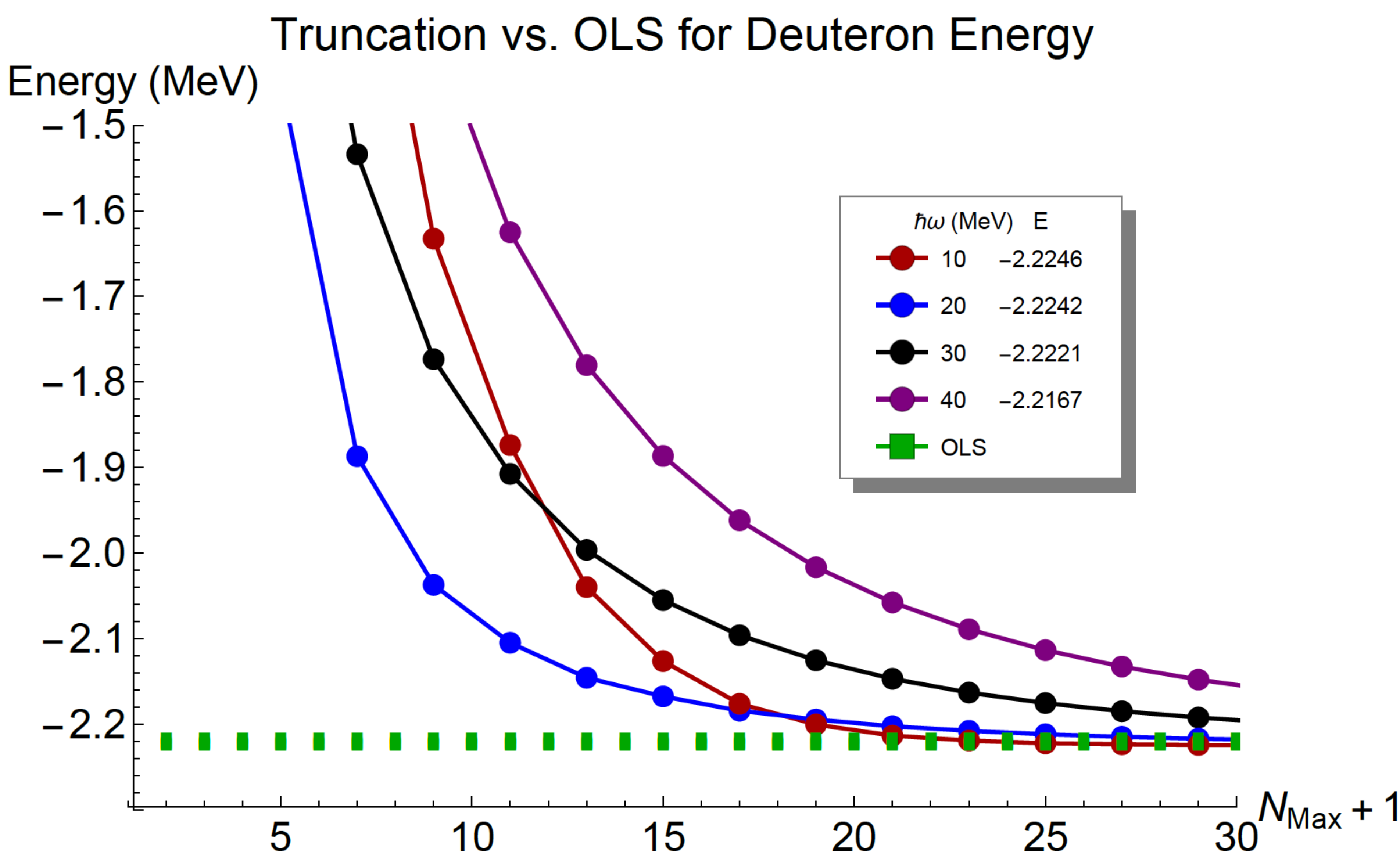
Hamiltonian #1 $$H = T + V$$

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

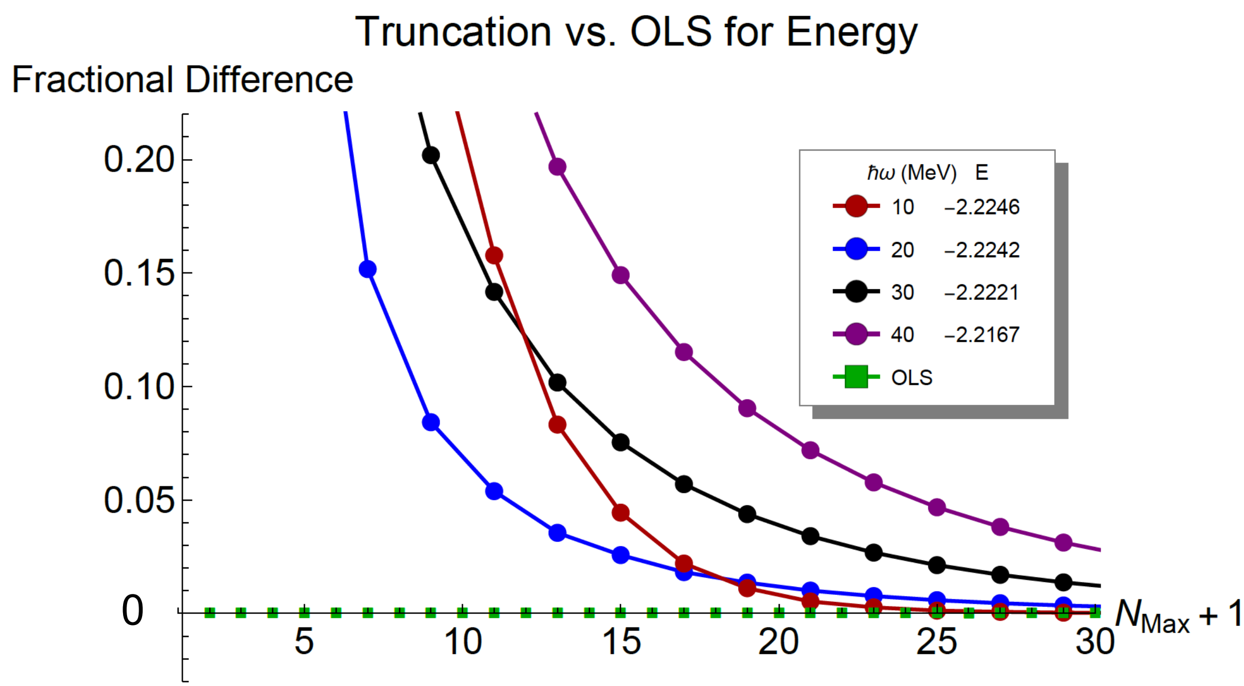
Other observables:

Magnetic dipole moment	M1
Root mean square radius	R
Electric quadrupole moment	Q2
E2 transition (J=2 to deuteron gs)	E2

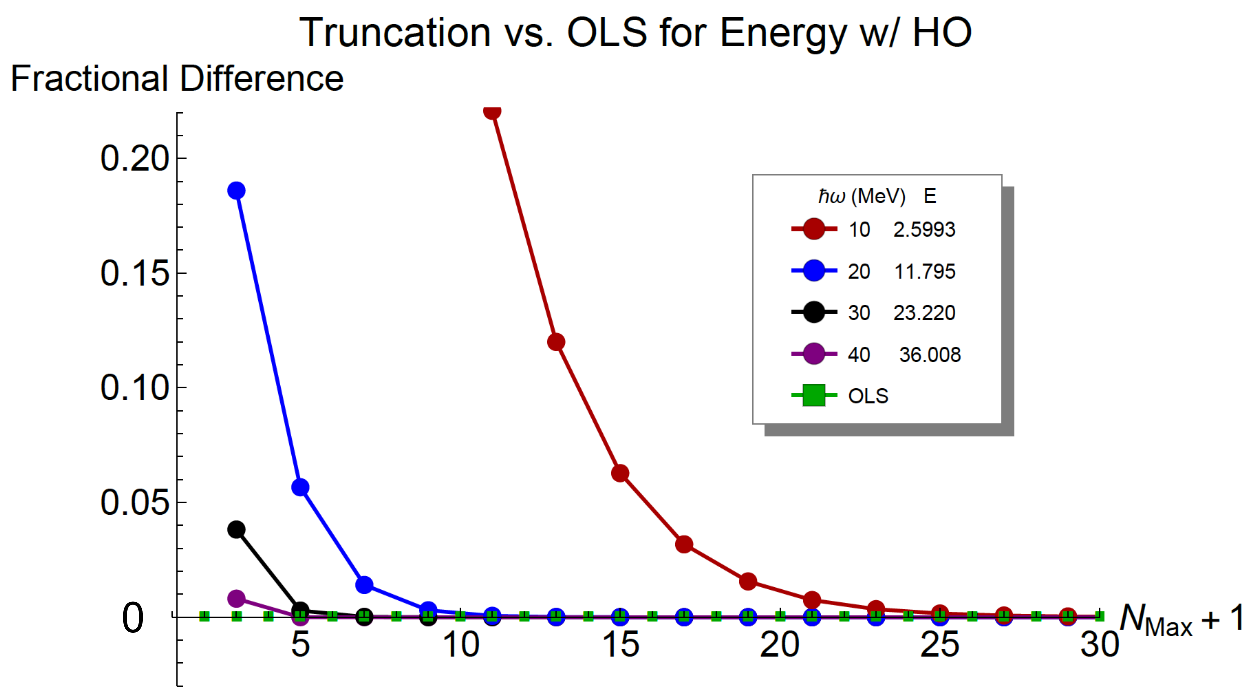
Dimension of the “full space” is 60 for the results depicted here



Truncation vs. OLS for Deuteron Energy
Energy (MeV)
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
−2.2
5
10
15
20
25
30
$N_{Max} + 1$
ħω (MeV) E
10 −2.2246
20 −2.2242
30 −2.2221
40 −2.2167
OLS

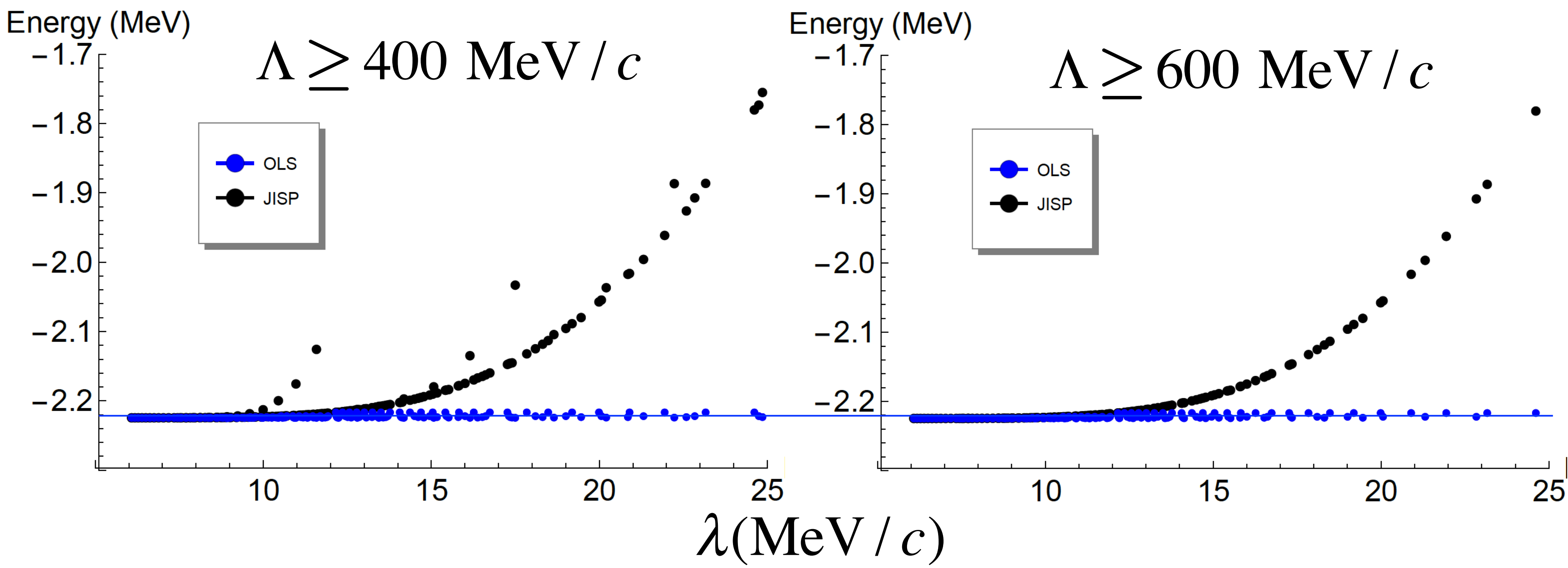


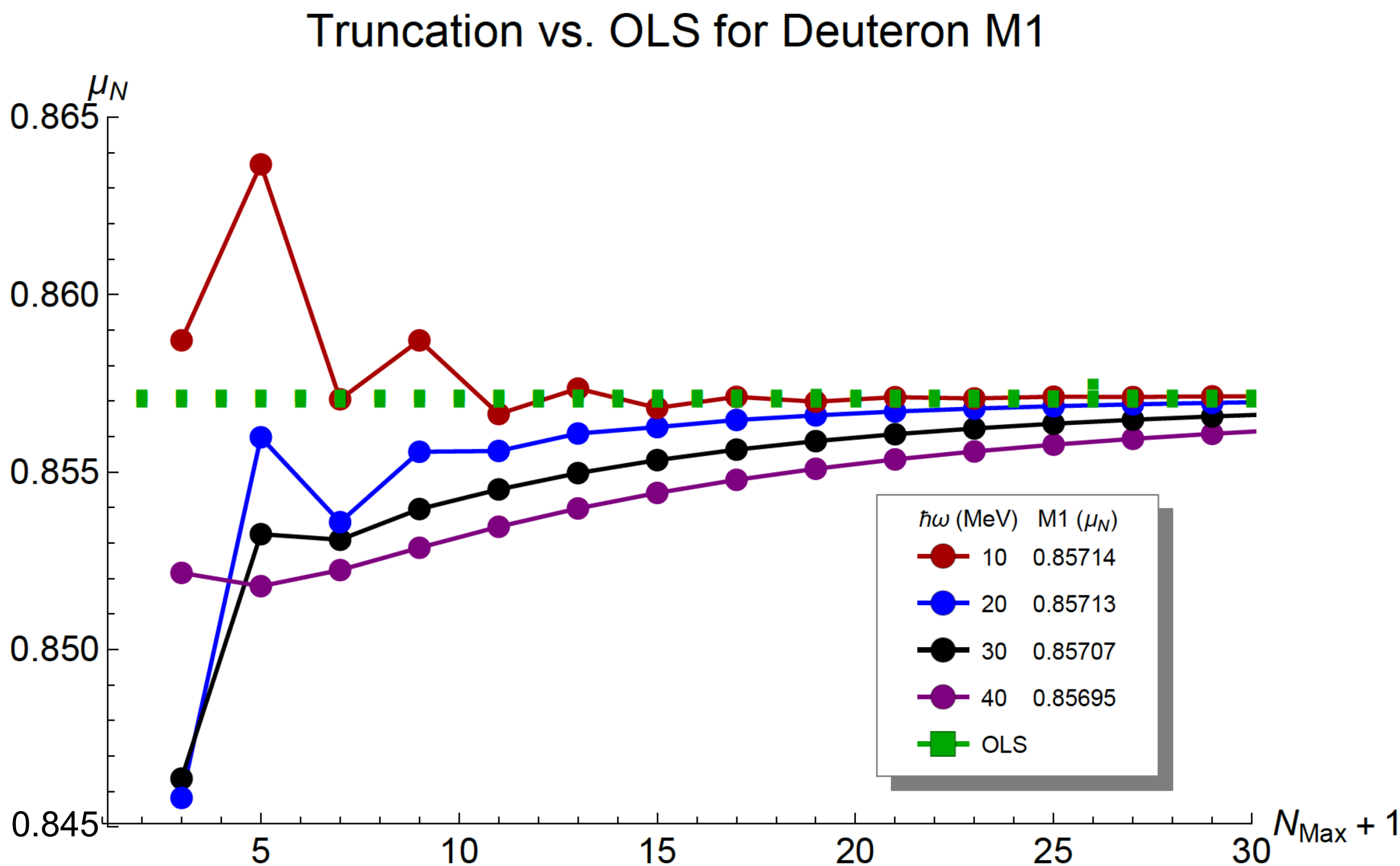
Truncation vs. OLS for Energy
Fractional Difference
0.20
0.15
0.10
0.05
0
5
10
15
20
25
30
$N_{Max}+1$
ℏω (MeV) E
10 −2.2246
20 −2.2242
30 −2.2221
40 −2.2167
OLS



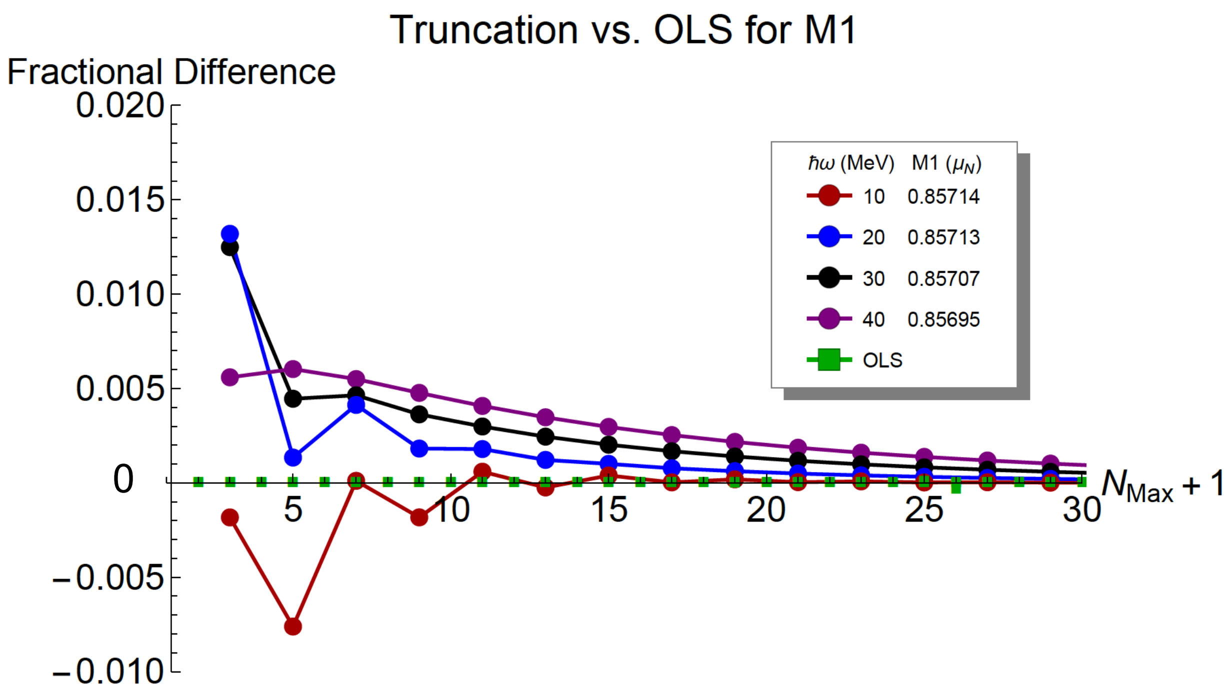
Truncation vs. OLS for Energy w/ HO
Fractional Difference
0.20
0.15
0.10
0.05
0
5
10
15
20
25
30
$N_{Max}+1$
ℏω (MeV) E
10 2.5993
20 11.795
30 23.220
40 36.008
OLS

Single function of λ emerges when $\Lambda_{basis} > \Lambda_{NN}$(JISP16) ~ 500 MeV/c
However, OLS results are independent of basis regulators λ and Λ

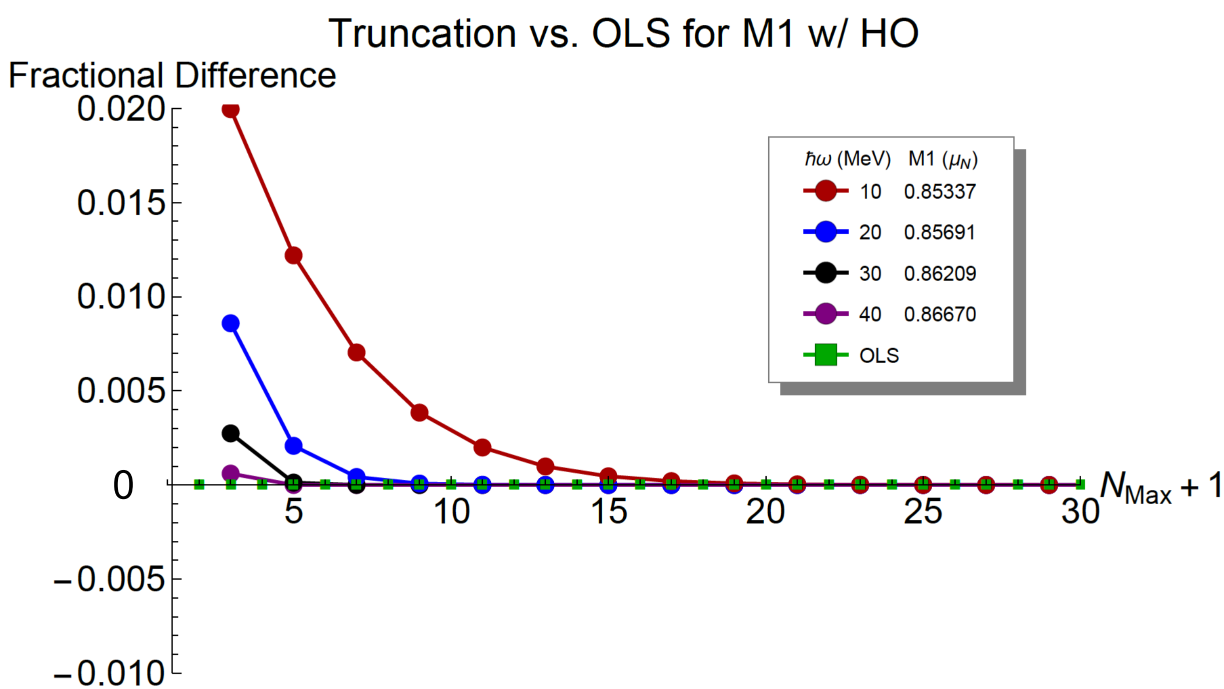




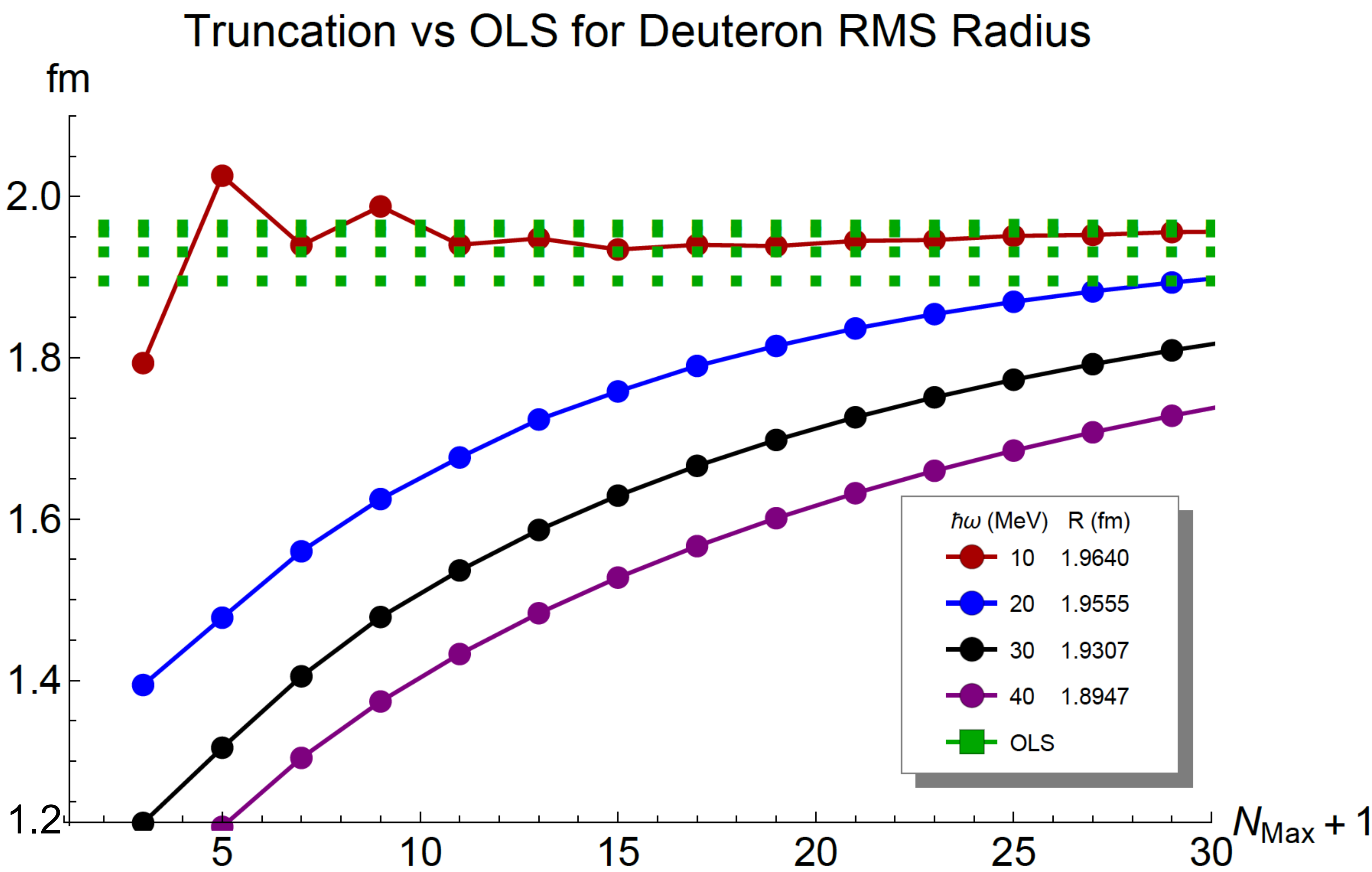
Truncation vs. OLS for Deuteron M1
μ_N
0.865
0.860
0.855
0.850
0.845
5
10
15
20
25
30
$N_{Max} + 1$
$\hbar\omega$ (MeV) M1 (μ_N)
10 0.85714
20 0.85713
30 0.85707
40 0.85695
OLS



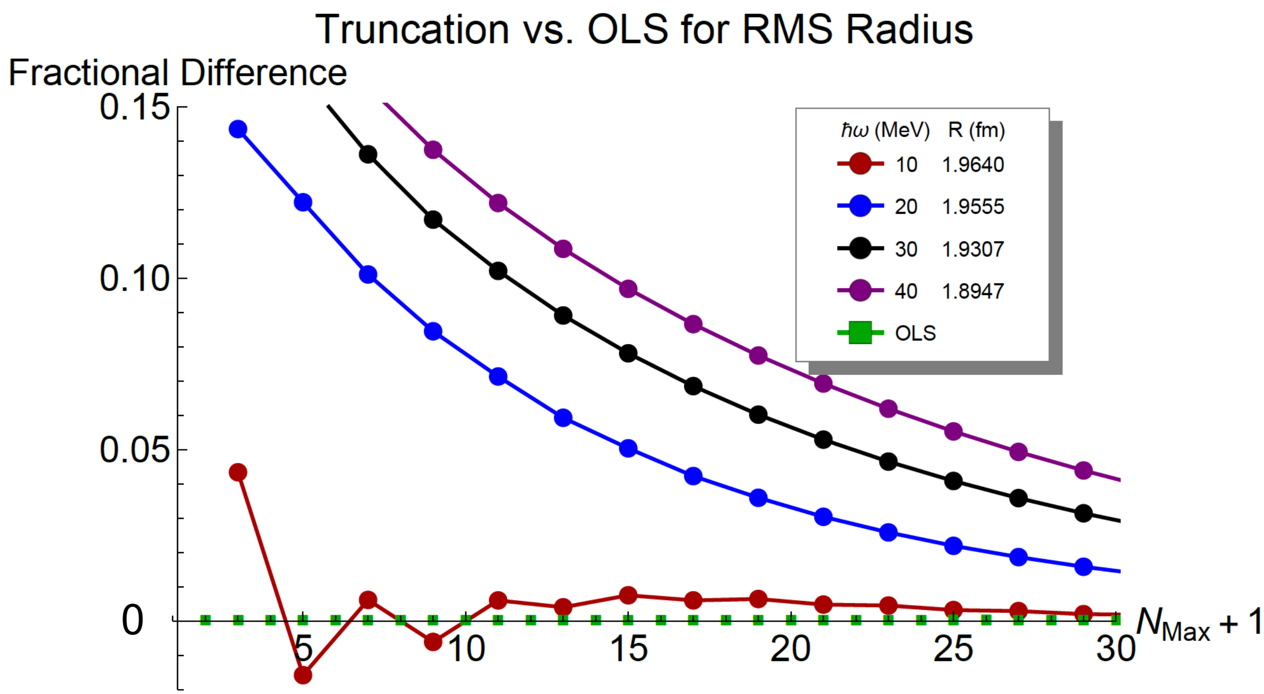
Truncation vs. OLS for M1
Fractional Difference
0.020
0.015
0.010
0.005
0
−0.005
−0.010
5
10
15
20
25
30
$N_{Max} + 1$
$\hbar\omega$ (MeV) M1 (μ_N)
10 0.85714
20 0.85713
30 0.85707
40 0.85695
OLS

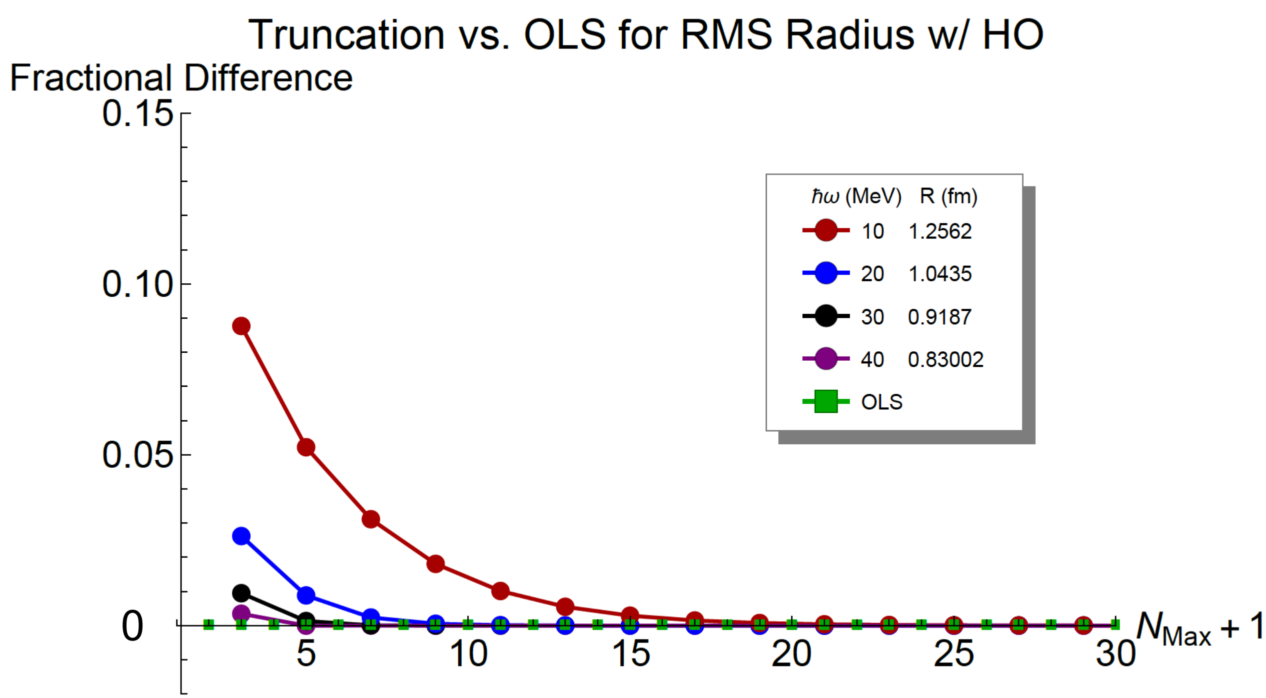


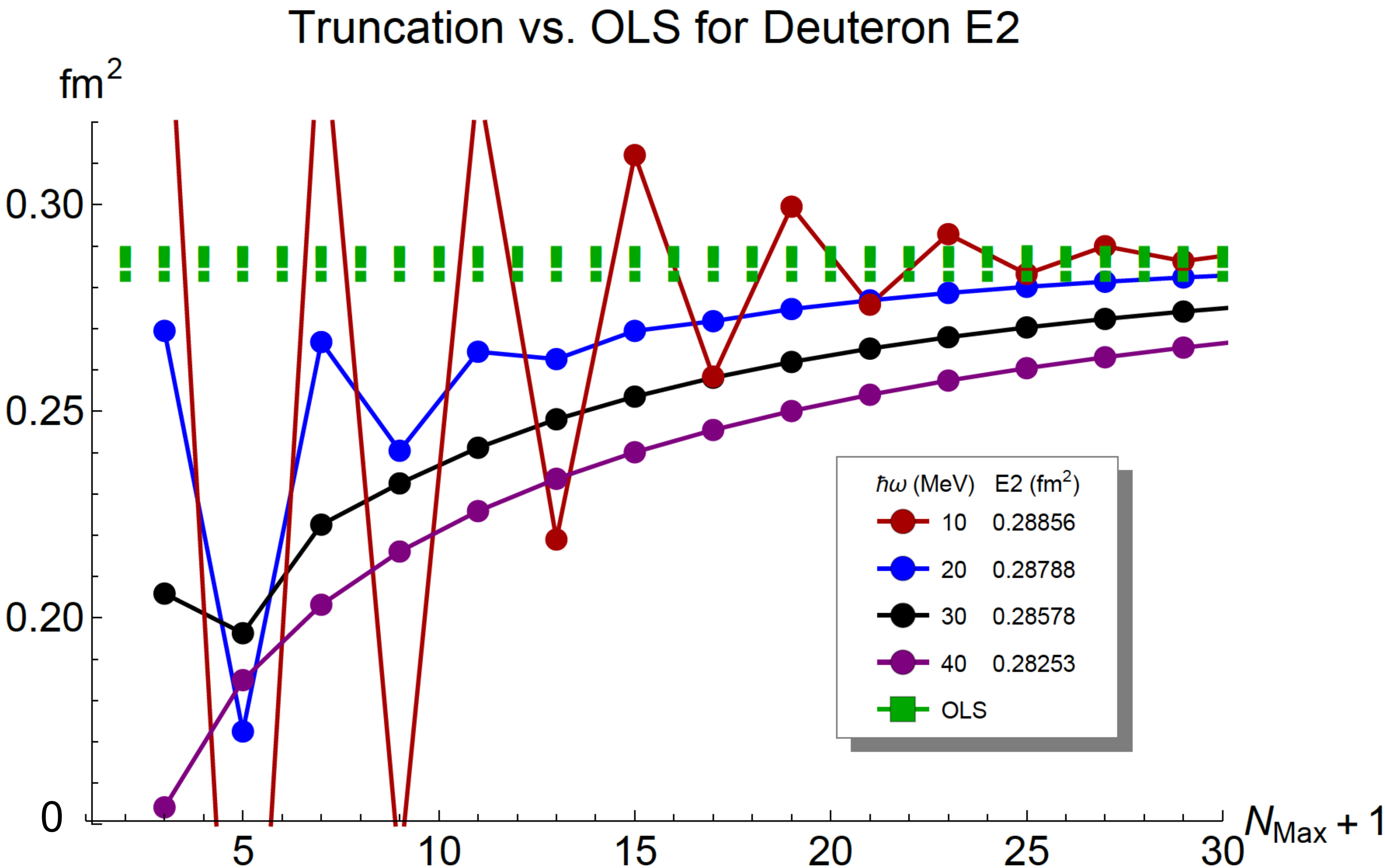
Truncation vs. OLS for M1 w/ HO
Fractional Difference
0.020
0.015
0.010
0.005
0
−0.005
−0.010
5
10
15
20
25
30
$N_{Max} + 1$
$\hbar\omega$ (MeV) M1 (μ_N)
10 0.85337
20 0.85691
30 0.86209
40 0.86670
OLS



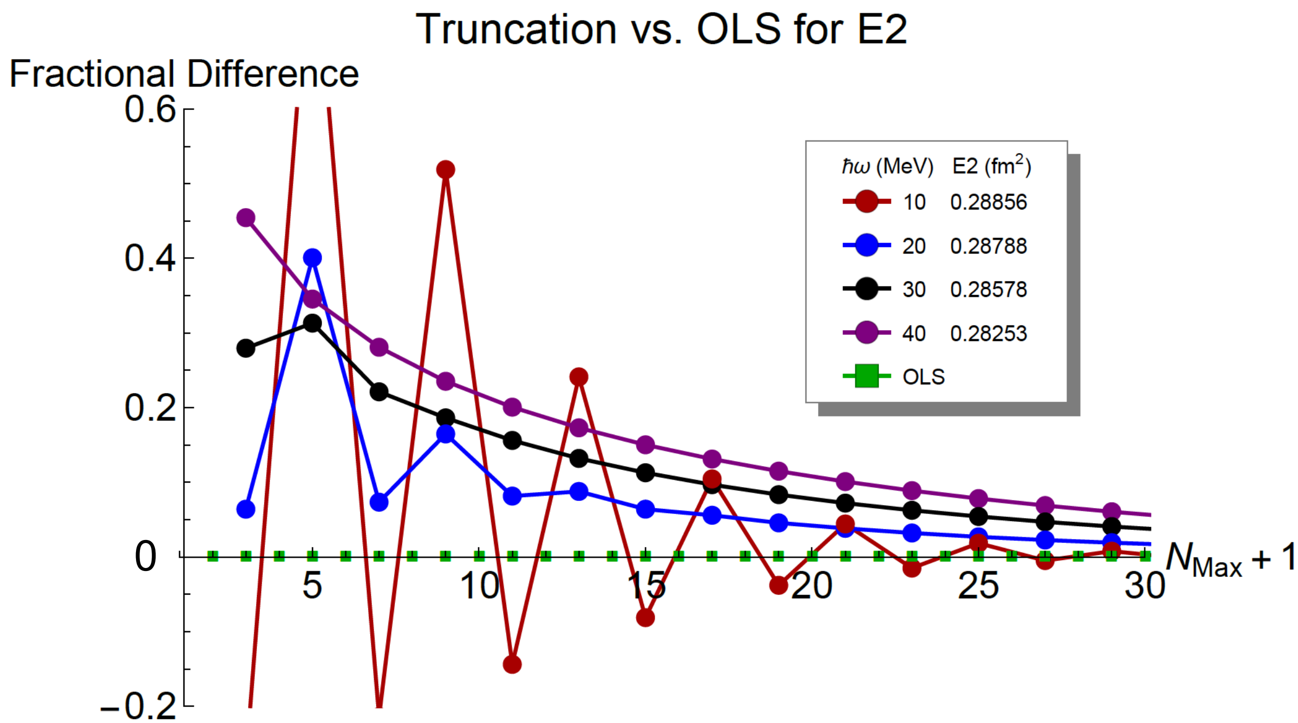
Truncation vs OLS for Deuteron RMS Radius
fm
2.0
1.8
1.6
1.4
1.2
5
10
15
20
25
30
$N_{Max}+1$
$\hbar\omega$ (MeV) R (fm)
10 1.9640
20 1.9555
30 1.9307
40 1.8947
OLS


Truncation vs. OLS for RMS Radius
Fractional Difference
0.15
0.10
0.05
0
5
10
15
20
25
30
$N_{\text{Max}} + 1$
ħω (MeV) R (fm)
10 1.9640
20 1.9555
30 1.9307
40 1.8947
OLS

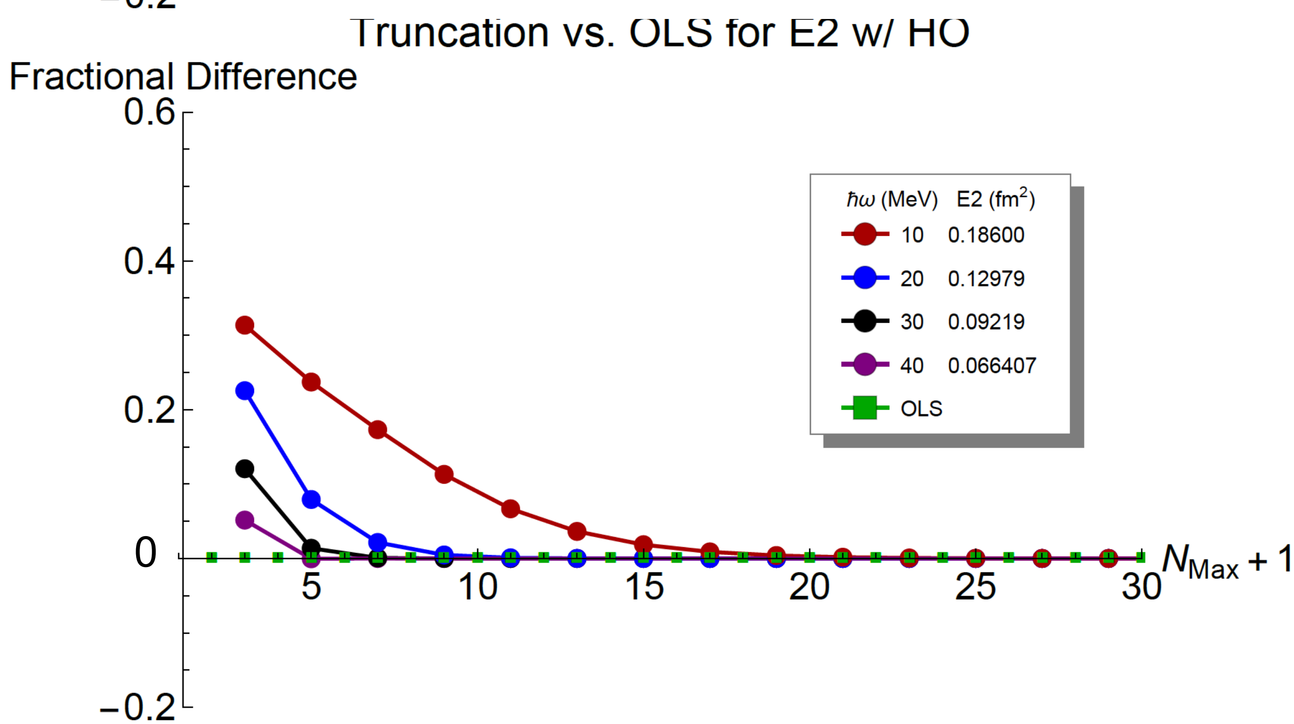

Truncation vs. OLS for RMS Radius w/ HO
Fractional Difference
0.15
0.10
0.05
0
5
10
15
20
25
30
$N_{\text{Max}} + 1$
ħω (MeV) R (fm)
10 1.2562
20 1.0435
30 0.9187
40 0.83002
OLS



Truncation vs. OLS for Deuteron E2
fm^2
0.30
0.25
0.20
0
5
10
15
20
25
30
$N_{Max}+1$
$\hbar\omega$ (MeV) E2 (fm^2)
10 0.28856
20 0.28788
30 0.28578
40 0.28253
OLS



Truncation vs. OLS for E2
Fractional Difference
0.6
0.4
0.2
0
−0.2
5
10
15
20
25
30
$N_{Max} + 1$
ħω (MeV) E2 (fm^2)
10 0.28856
20 0.28788
30 0.28578
40 0.28253
OLS



Truncation vs. OLS for E2 w/ HO
Fractional Difference
0.6
0.4
0.2
0
−0.2
5
10
15
20
25
30
$N_{Max} + 1$
ħω (MeV) E2 (fm^2)
10 0.18600
20 0.12979
30 0.09219
40 0.066407
OLS

Future Plans:

Expand treatment to larger set of EW operators

Include corrections (e.g. from Chiral EFT) to EW operators

Implement in finite nuclei:

- Input OLS'd operators as TBMEs
- Use TB density matrices (static and transition) to evaluate OLS'd observables and compare with results from bare observables

Extend to 3-body H with OLS at 3-body level

Calculation of three-body forces at N^{3}LO

Low
Energy
Nuclear
Physics
International
Collaboration

LENPIC

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Iowa State — P. Maris, J. Vary

Kyutech — H. Kamada

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

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Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

Conclusions/Outlook

- ✧ OLS procedure is well-suited for renormalizing the strong and the electroweak interactions to match the IR and UV scales of the many-body basis.

- ✧ Much work needs to be done to improve the inter-nucleon interactions, electroweak observables consistent with those interactions and the many-body methods to further increase predictive power and fully exploit the discovery potential.

Collaborators at Iowa State University

Weijie Du
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