Effective moments and transition operators in the *ab initio* No-Core Shell Model

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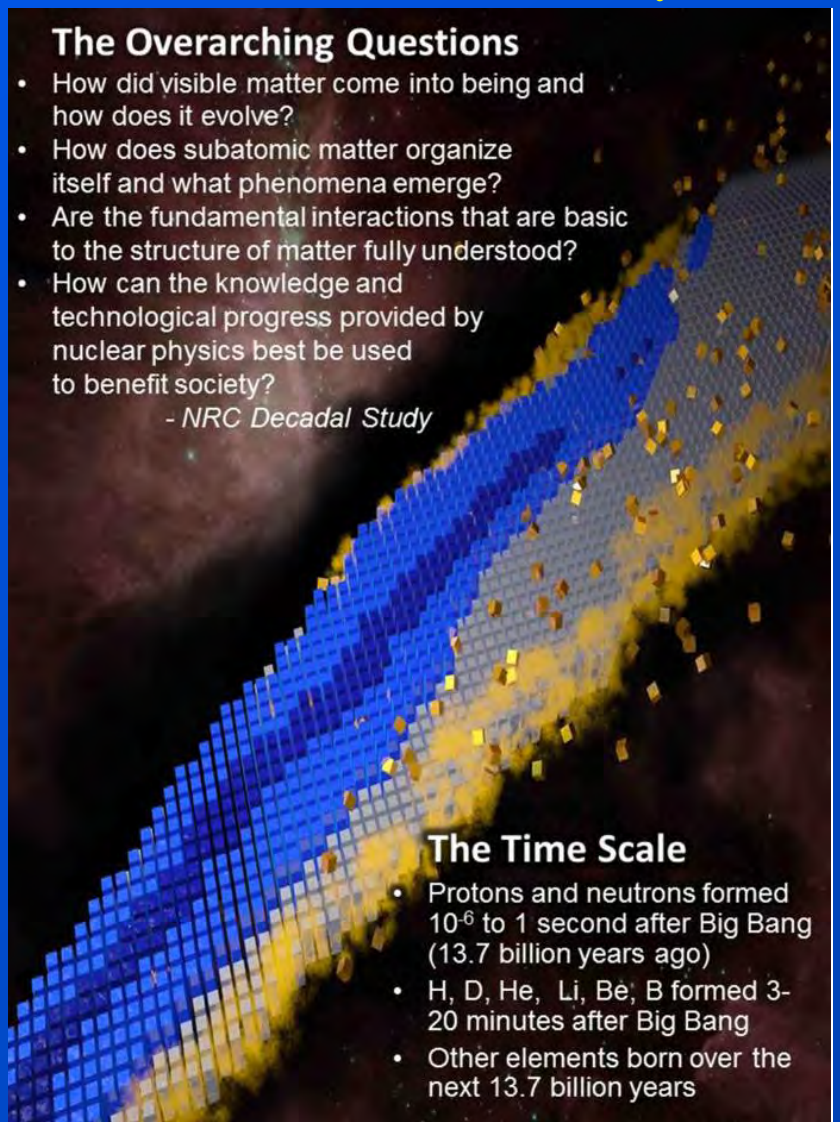
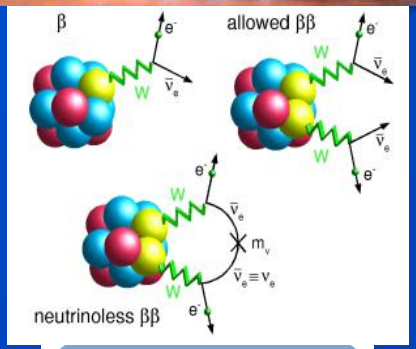
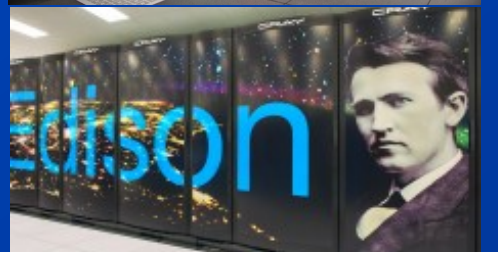




LENPIC



Main Message

Use light nuclei and precision calculations
to understand effective operators' (e.g. g_A)
dependences on Hamiltonians and basis spaces

Overview

Review of selected published results
and present some new "test" problems

Conclusion

Major efforts needed to quantify all theoretical uncertainties:
Effective Hamiltonians, Effective electroweak operators,
Many-body methods, ...

No-Core Configuration Interaction calculations

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

Given a Hamiltonian operator

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

solve the eigenvalue problem for wavefunction of A nucleons

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

- 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:

$\lambda \leq$ all relevant IR scale limits

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

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

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

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

A.M. Shirokov [a,b,*], J.P. Vary [b,c,d], A.I. Mazur [e], T.A. Weber [b]

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[b] *Department of Physics and Astronomy, Iowa State University, Ames, IA 50011-3160, USA*
[c] *Lawrence Livermore National Laboratory, L-414, 7000 East Avenue, Livermore, CA 94551, USA*
[d] *Stanford Linear Accelerator Center, MS81, 2575 Sand Hill Road, Menlo Park, CA 94025, USA*
[e] *Pacific National University, Tikhookeanskaya 136, Khabarovsk 680035, Russia*

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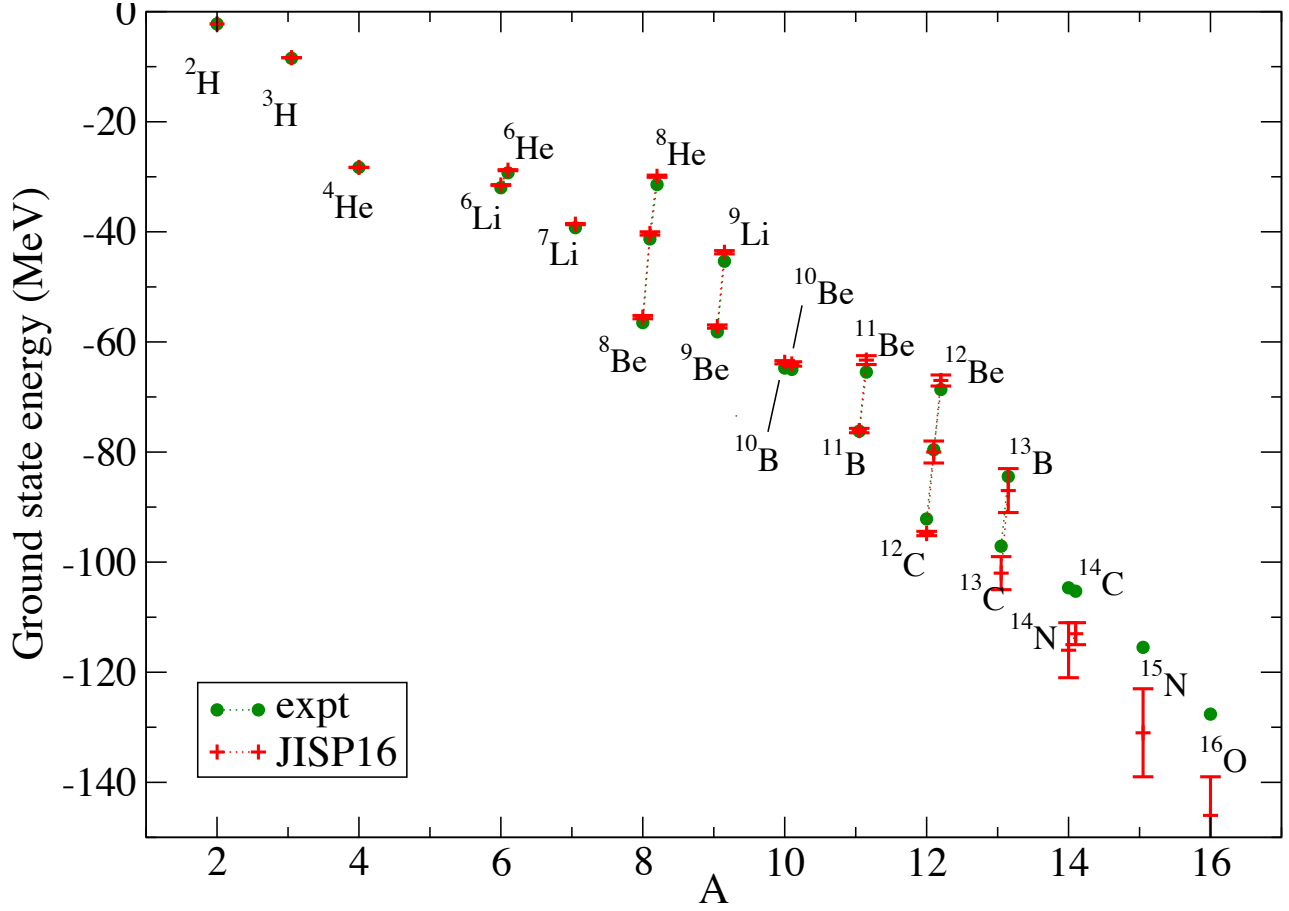
Ground state energy of p-shell nuclei with JISP16

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

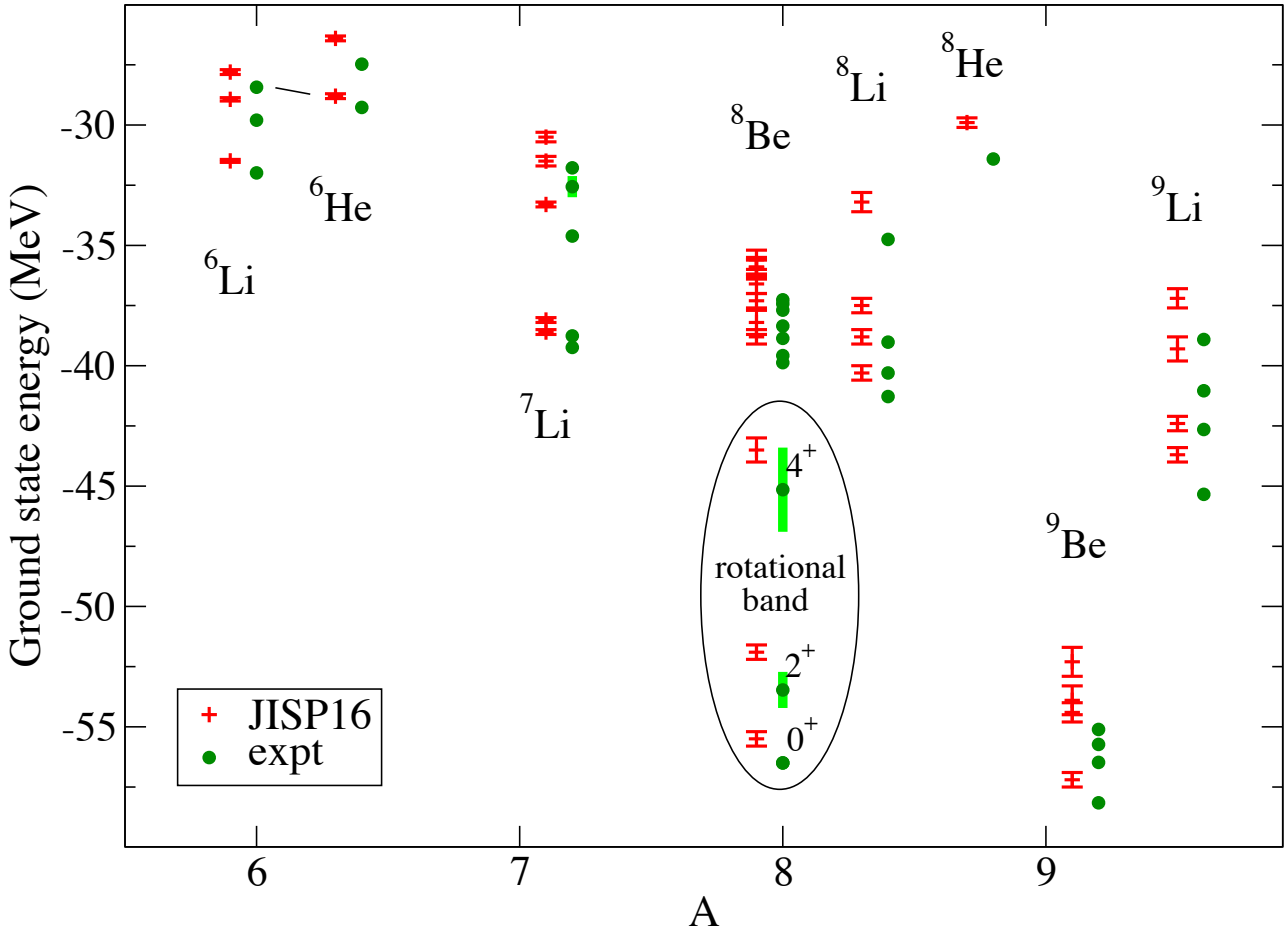


- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$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

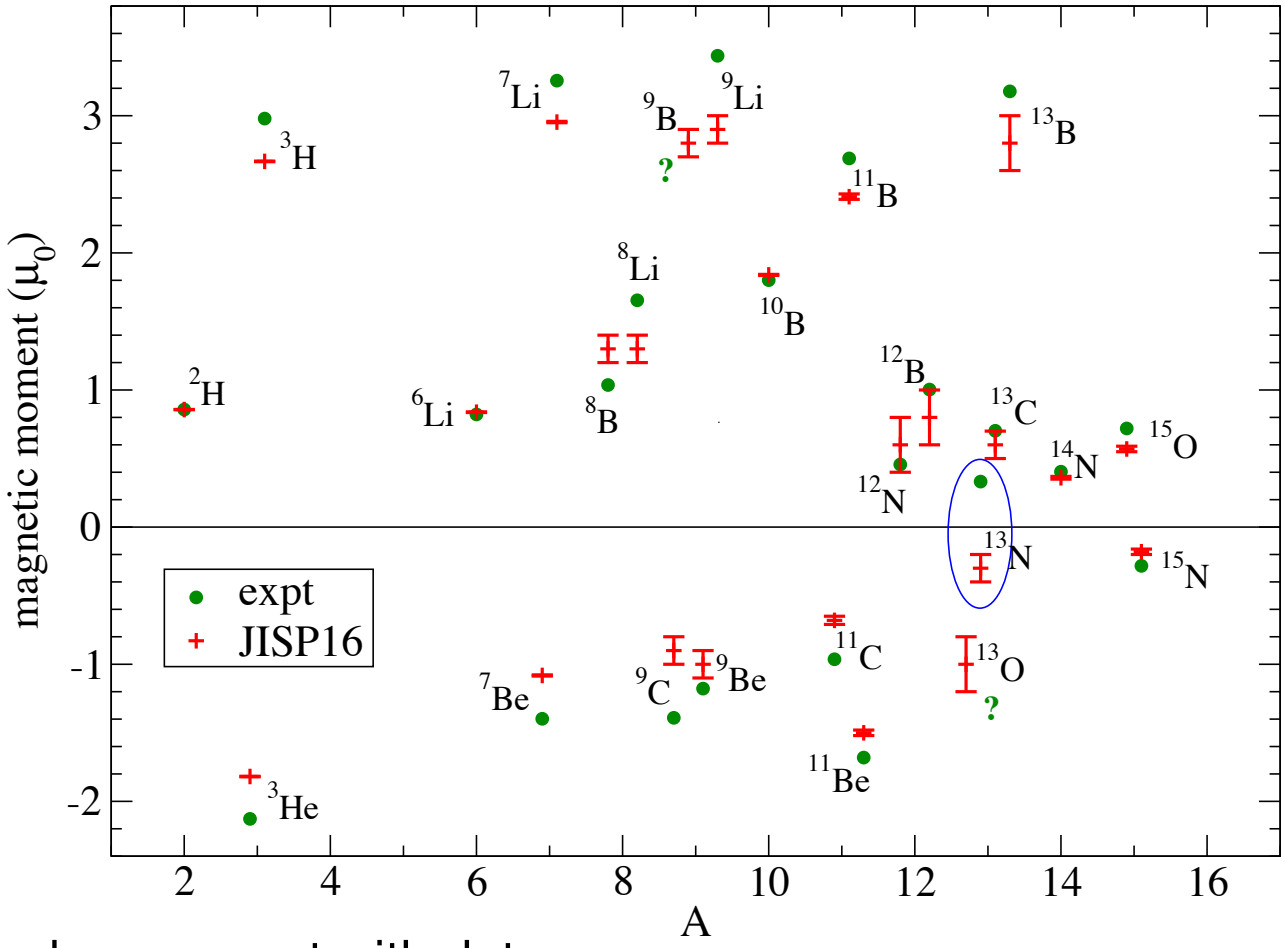


- Excitation spectrum narrow states in good agreement with data

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:

S.A. Coon, M.I. Avetian, M.K.G. Kruse, U. van Kolck, P. Maris, and J.P. Vary,
Phys. Rev. C 86, 054002 (2012); arXiv: 1205.3230

R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301

E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary,
Phys. Rev. C 87, 054312(2013); arXiv 1302.5473

S.N. More, A. Ekstroem, R.J. Furnstahl, G. Hagen and T. Papenbrock,
Phys. Rev. C87, 044326 (2013); arXiv 1302.3815

R.J. Furnstahl, S.N. More and T. Papenbrock,
Phys. Rev. C89, 044301 (2014); arXiv 1312.6876

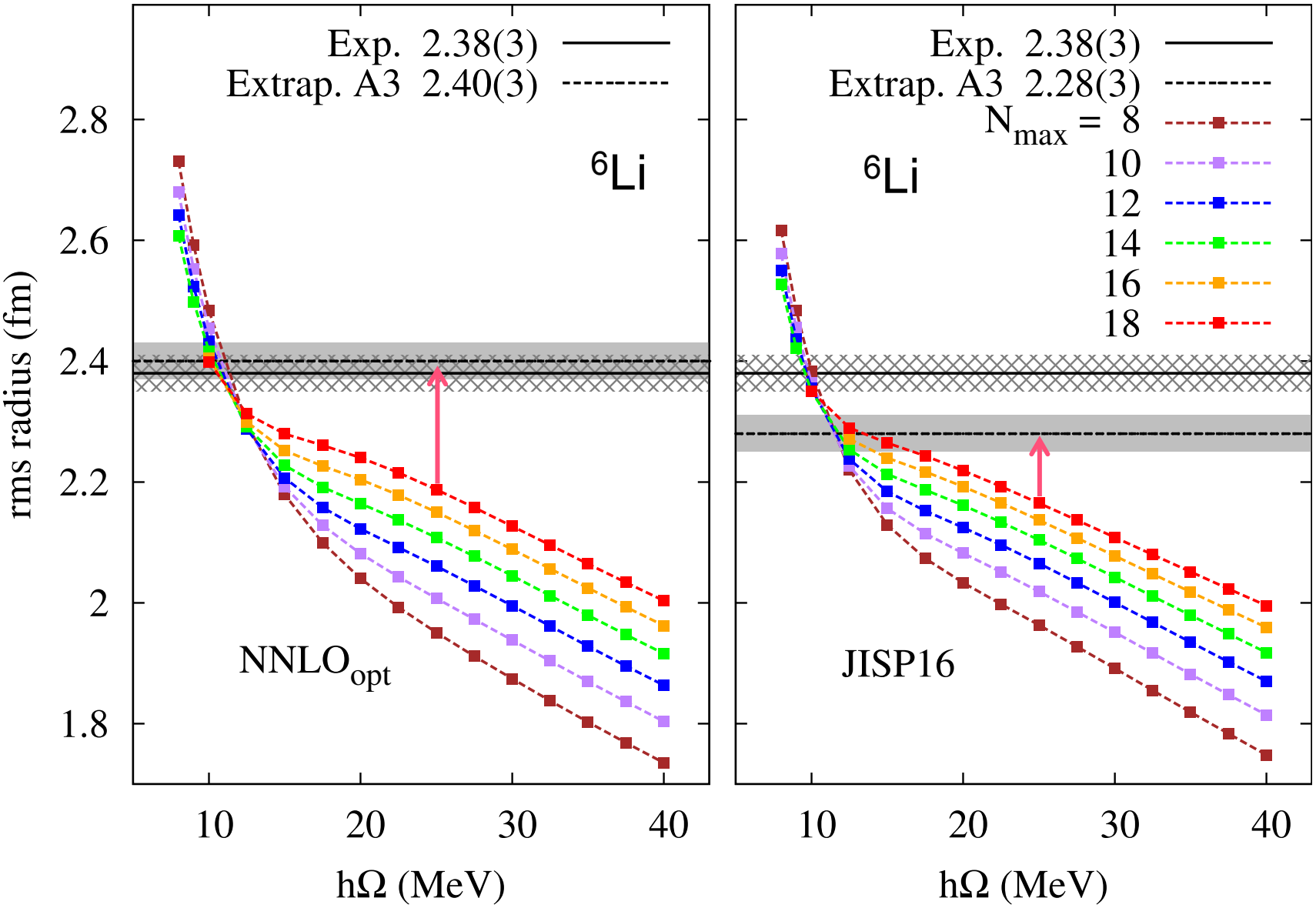
S. Koenig, S.K. Bogner, R.J. Furnstahl, S.N. More and T. Papenbrock,
Phys. Rev. C90, 064007 (2014); arXiv 1409.5997

R.J. Furnstahl, G. Hagen, T. Papenbrock and K.A. Wendt,
J. Phys. G: Nucl. Part. Phys. 42 034032 (2015): arXiv 1408.0252

K.A. Wendt, C. Forssen, T. Papenbrock, D. Saaf, Phys. Rev. C91, 061301 (2015)

D. Odell, T. Papenbrock and L. Platter, Phys. Rev. C93, 04851 (2016);arXiv 1512.04851

=> Uncertainty Quantification

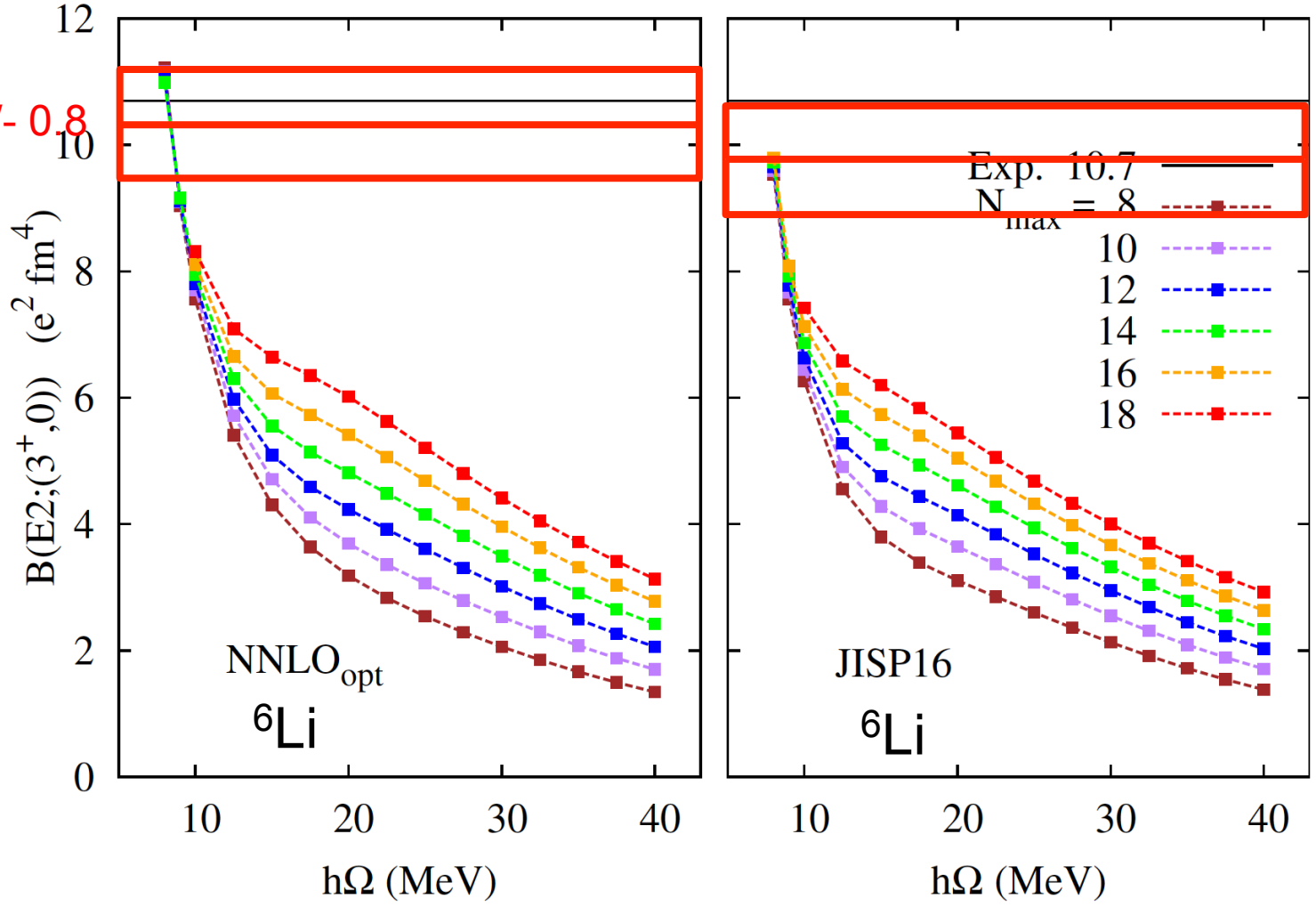


Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, arXiv:1605.02819

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

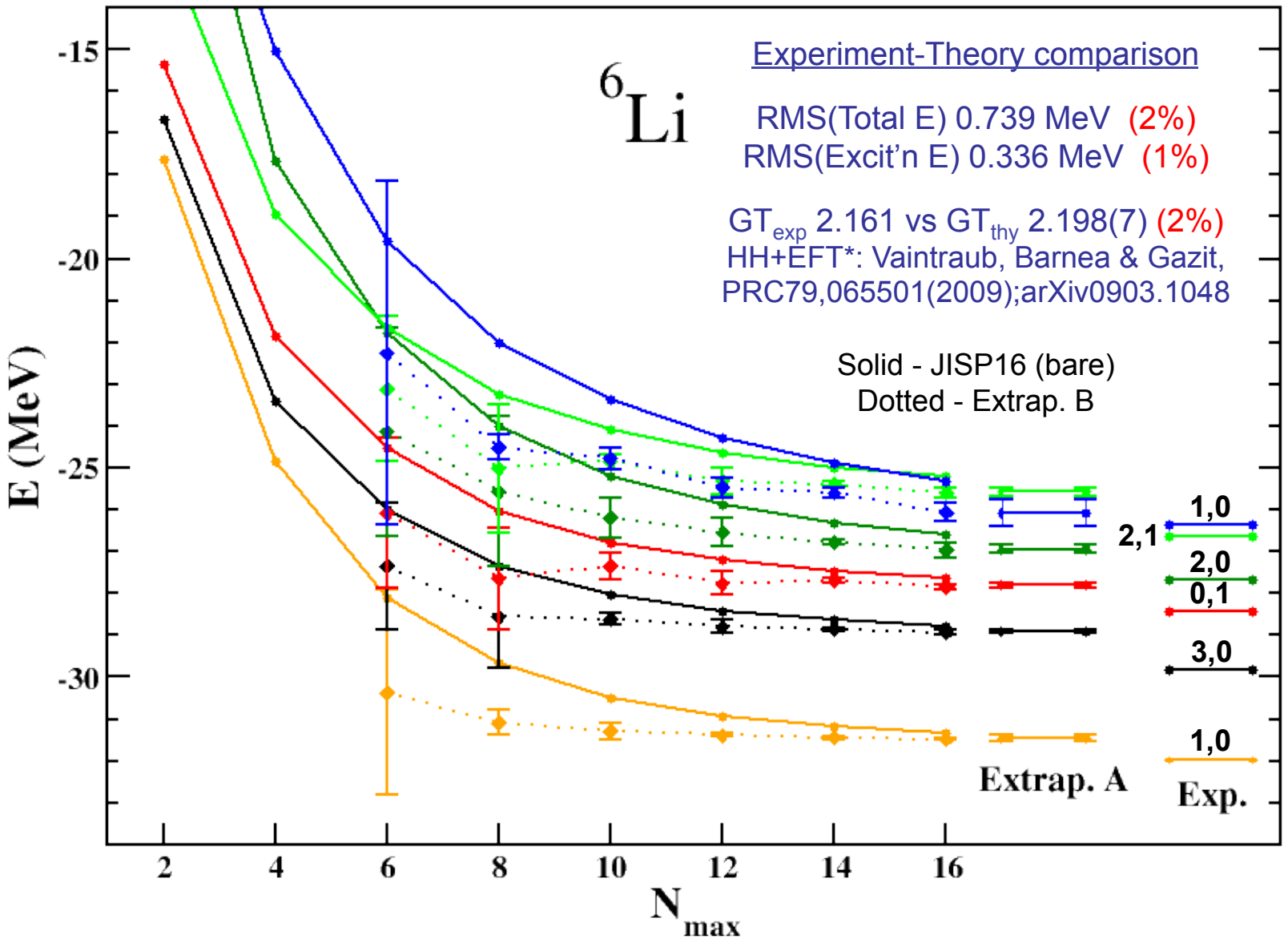
10.2 +/- 0.8

9.8 +/- 0.7

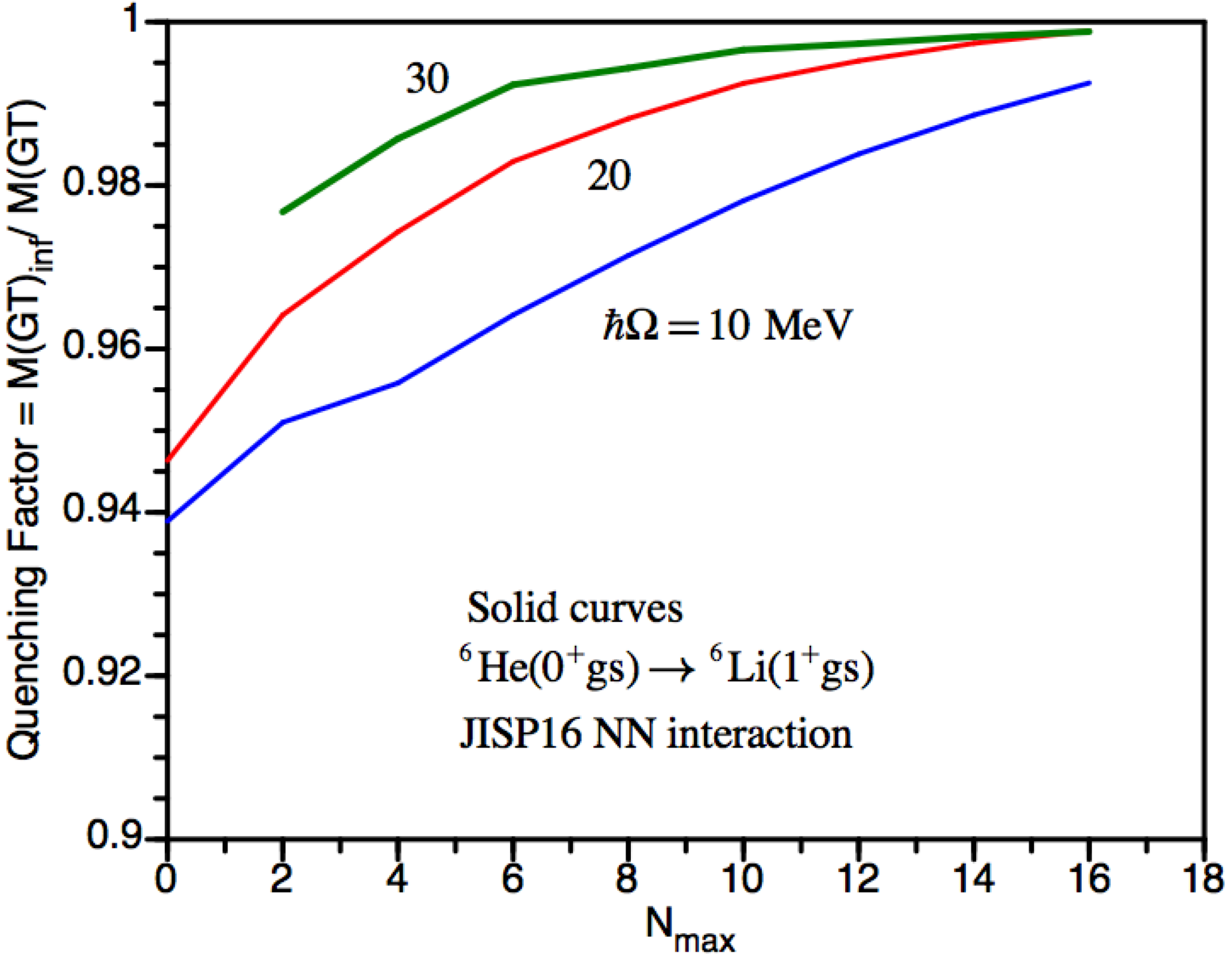


Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, arXiv:1605.02819

NCFC results (does not adopt a renormalization)



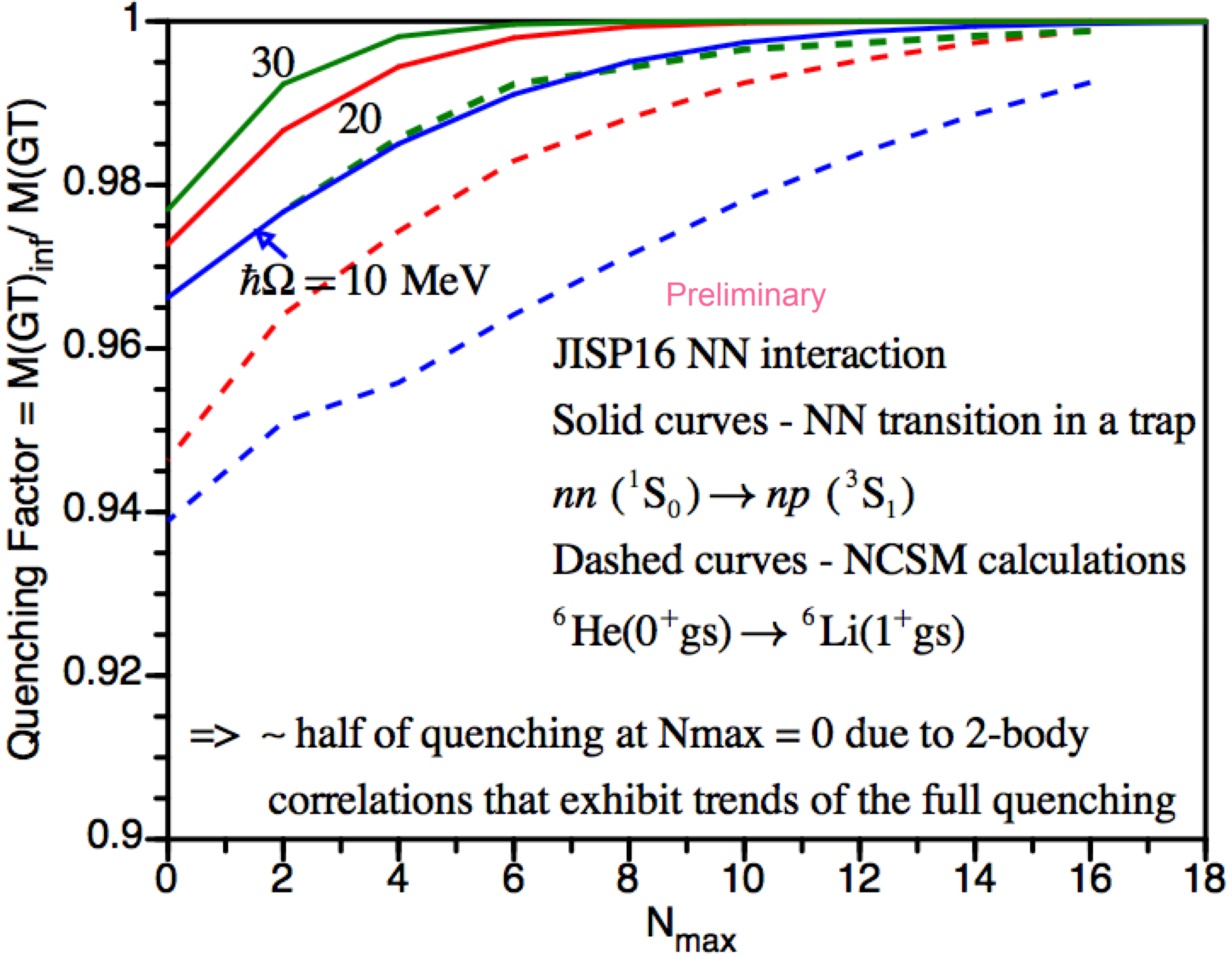
P. Maris, A. Shirokov and J.P. Vary, Phys. Rev. C 81, 021301(R) (2010). ArXiv 0911.2281
C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C 86, 034325 (2012); arXiv:1201.0724


1
0.98
0.96
0.94
0.92
0.9
Quenching Factor = M(GT)$_{inf}$/ M(GT)
30
20
$\hbar\Omega = 10$ MeV
Solid curves
^{6}He(0^+gs) $\rightarrow$ ^{6}Li(1^+gs)
JISP16 NN interaction
0
2
4
6
8
10
12
14
16
18
N$_{max}$

Now compare decay of ^{6}He with GT decay of two neutrons in a HO trap to a neutron-proton pair in the same trap.

In other words, take away all the many-body correlations but keep mean field effects on the NN correlations.

Examine that quenching as a function of the HO trap and the N_{max} of the HO basis and compare with the full quenching in ^{6}He.


Quenching Factor = M(GT)$_{inf}$/ M(GT)
1
0.98
0.96
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0.92
0.9
0
2
4
6
8
10
12
14
16
18
N$_{max}$
30
20
$\hbar\Omega = 10$ MeV
Preliminary
JISP16 NN interaction
Solid curves - NN transition in a trap
$nn\ (^1S_0) \rightarrow np\ (^3S_1)$
Dashed curves - NCSM calculations
$^6He(0^+gs) \rightarrow\ ^6Li(1^+gs)$
=> ~ half of quenching at Nmax = 0 due to 2-body
correlations that exhibit trends of the full quenching

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

1. Select basis regulators:

$\lambda \leq$ all relevant IR scale limits

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

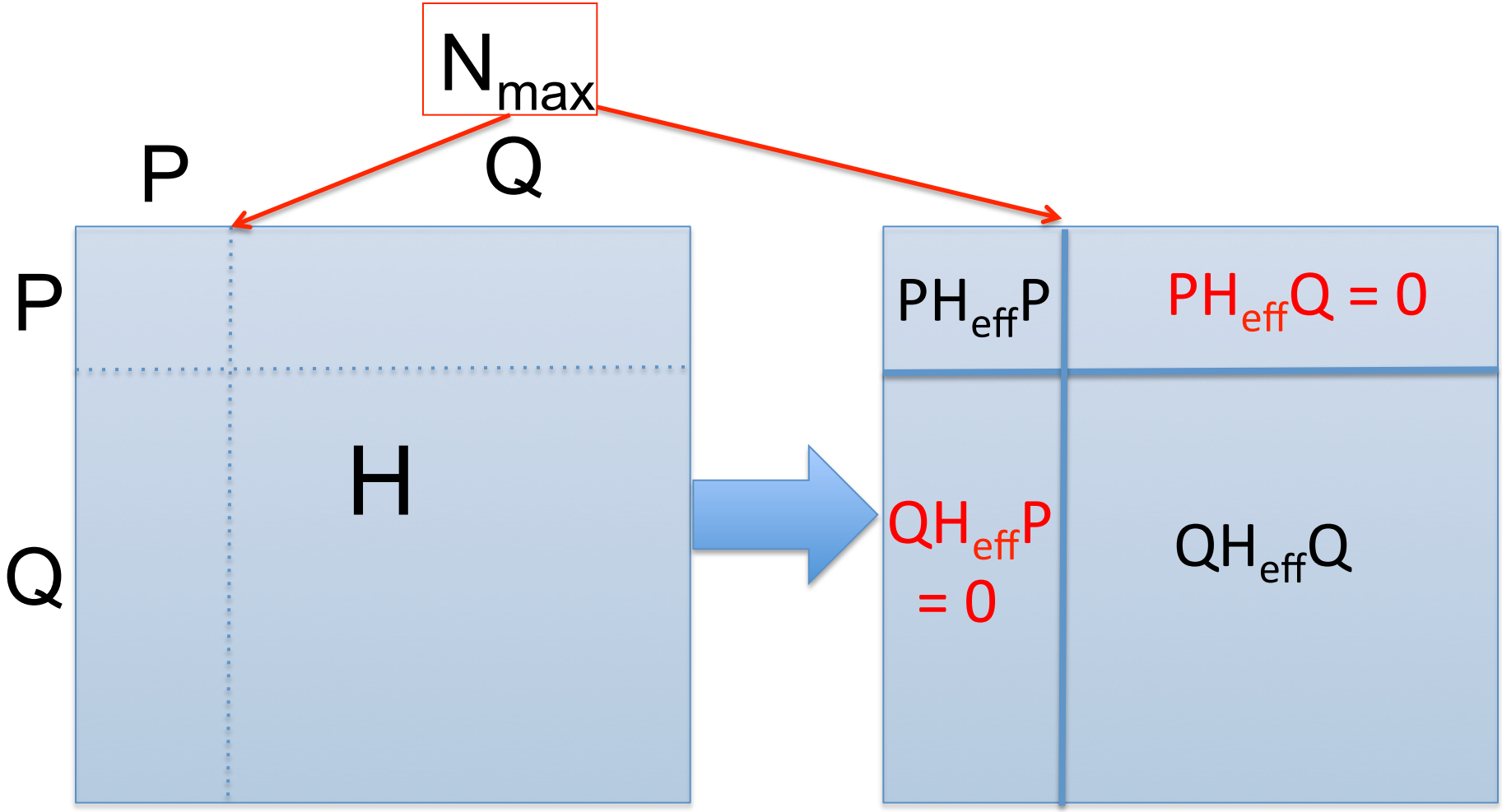
2. Since T_{rel} has simple IR and UV asymptotics, extrapolation is feasible for observables where T_{rel} dominates

✧ 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.

The cost: induced many-body operators need to be assessed.
The benefit: extrapolation may be avoided

OLS Transform on H



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

Outline of the OLS process

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

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

$$U^P = PUP$$

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

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

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

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

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

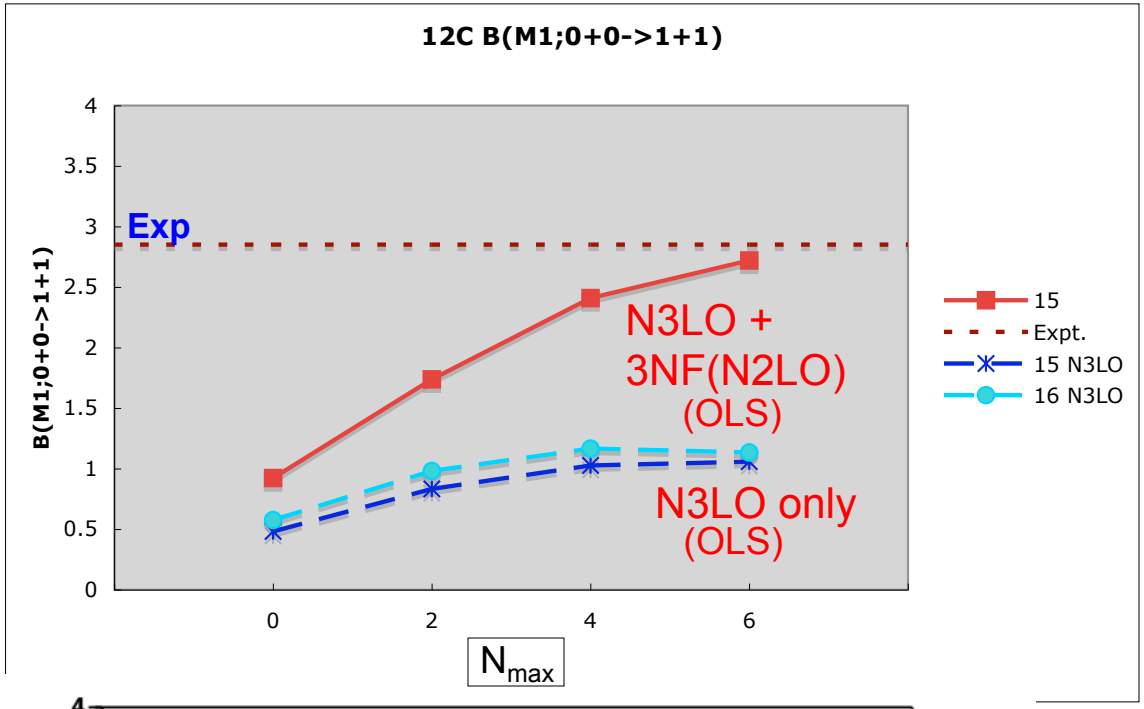
A.C.Hayes, P. Navratil, J.P. Vary, PRL 91, 012502 (2003); nucl-th/0305072

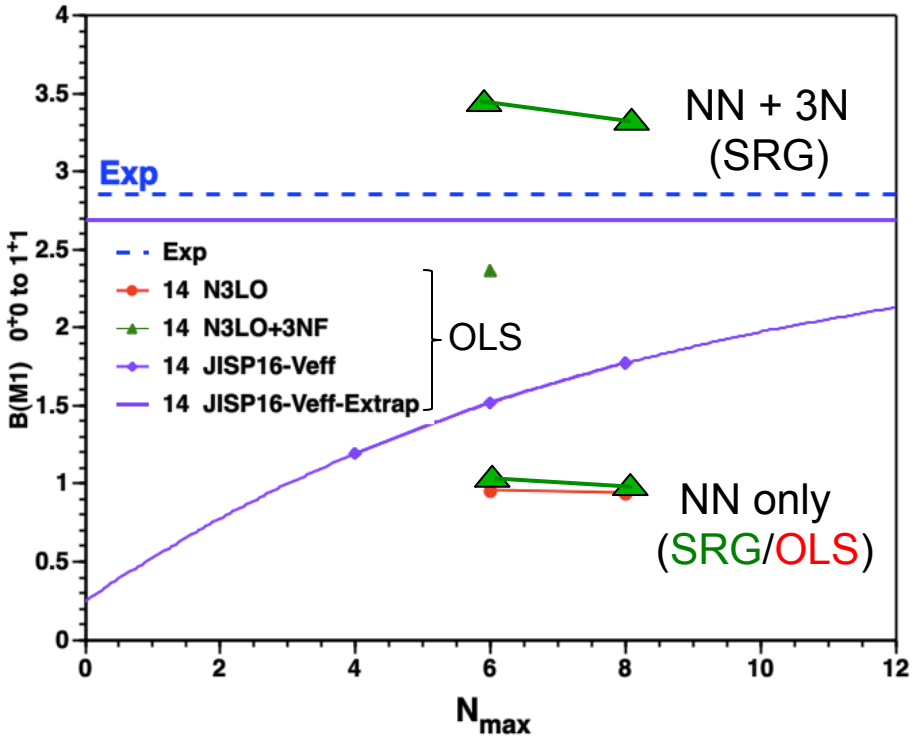
First successful description of the GT data required 3NF. Both CDBonn + TM' or AV8' + TM' => large enhancement

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

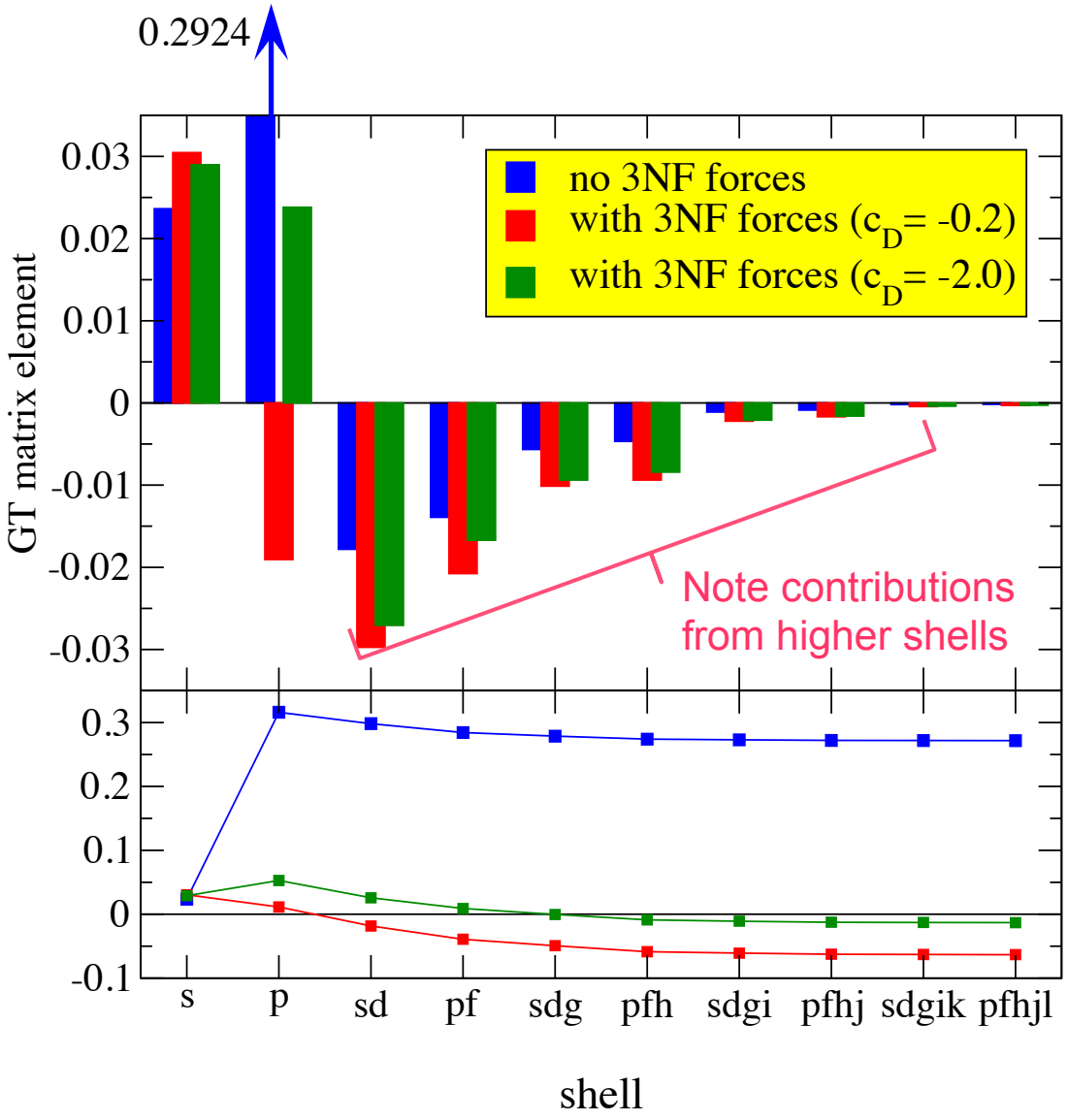
N_{max} = 6, 8 results with SRG on N3LO+3NF (N2LO); P. Maris, et al, PRC 90, 014314 (2014) [▲]

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





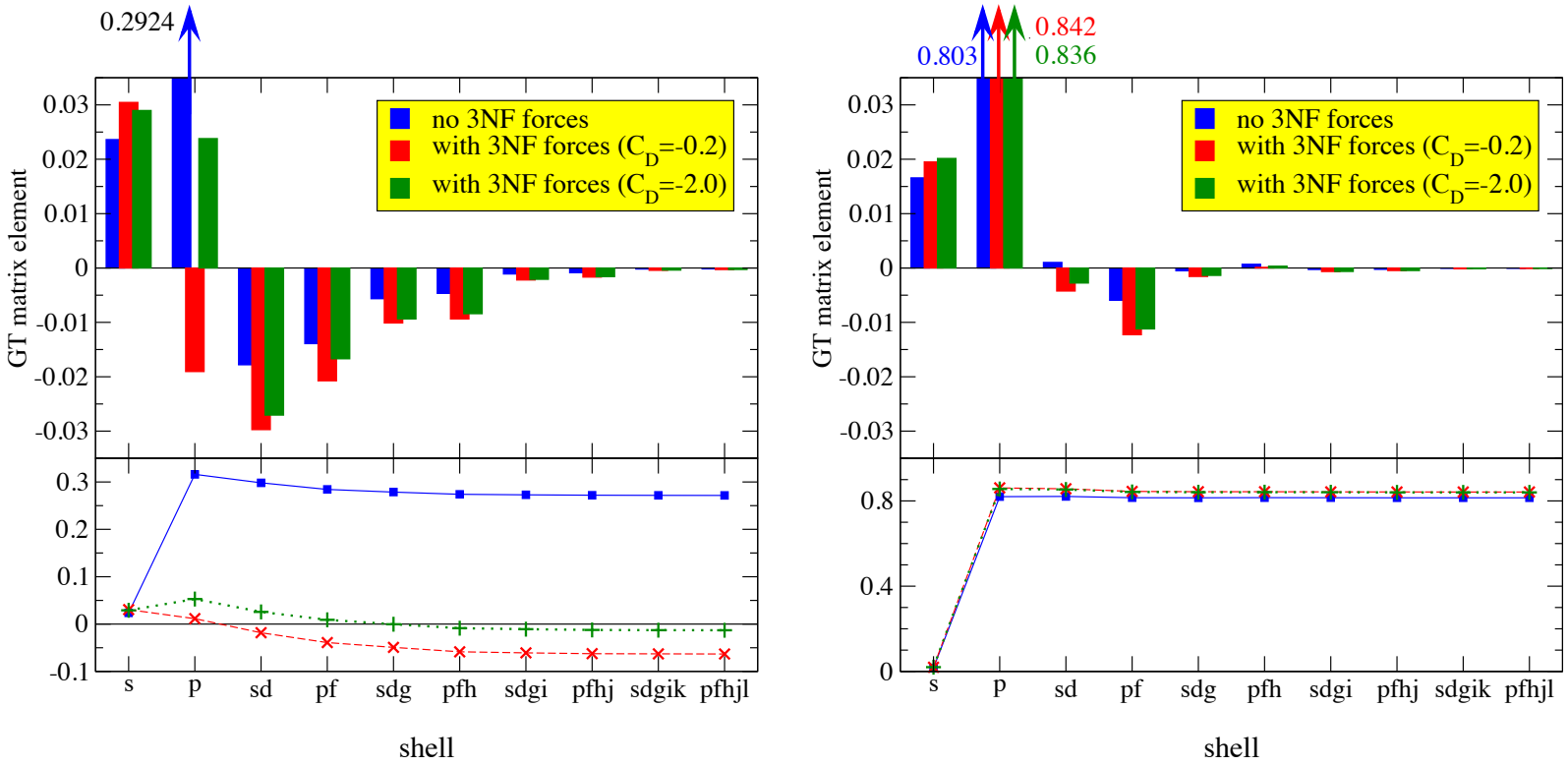
Origin of the anomalously long life-time of ^{14}C



- near-complete cancellations between dominant contributions within p-shell
- very sensitive to details

Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

Comparison GT transitions in A = 14



- Chiral 3-body interactions leads to suppression of GT transition for $^{14}\mathrm{C}(0^+, 0)$ state, but not for $^{14}\mathrm{C}^*(0^+, 2)$ state

Left panel: P. Maris, et al., Phys. Rev. Lett. 106, 202502 (2011).
Right panel: P. Maris, Journal of Physics: Conference Series 402, 012031 (2012)

Consider two nucleons as a model problem with V = JISP16
λ(JISP16) ~ 50 MeV/c & Λ(JISP16) ~ 500 MeV/c solved in the
harmonic oscillator basis with ħΩ = 10, 20 and 30 MeV.
Also, consider the role of an added harmonic oscillator quasipotential

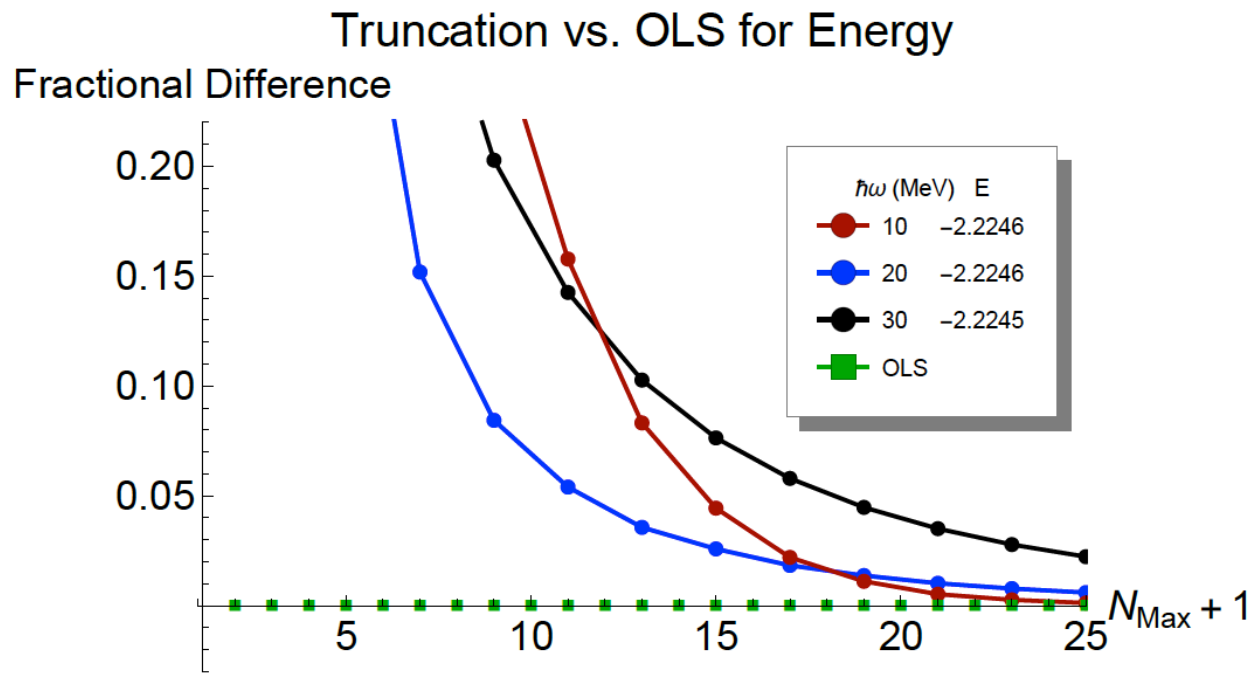
Hamiltonian #1 $H = T + V$

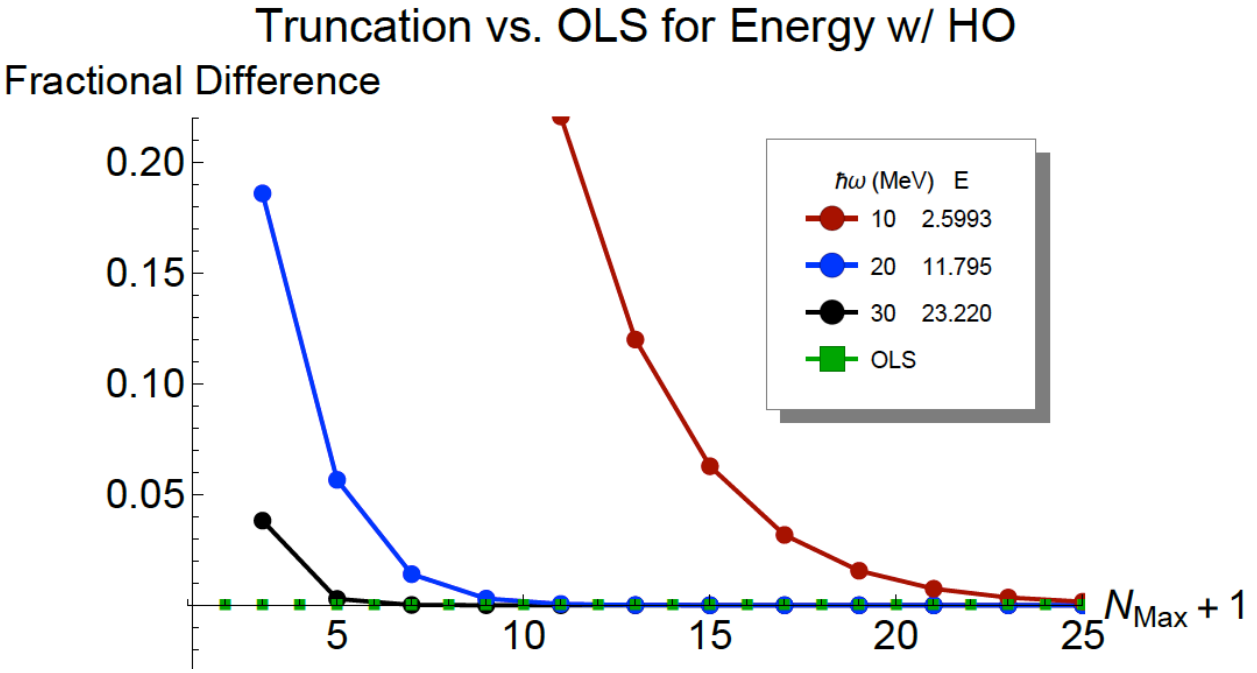
Hamiltonian #2 $H = T + U_{\mathrm{osc}}(\hbar\Omega_{\mathrm{basis}}) + V$

Other observables:

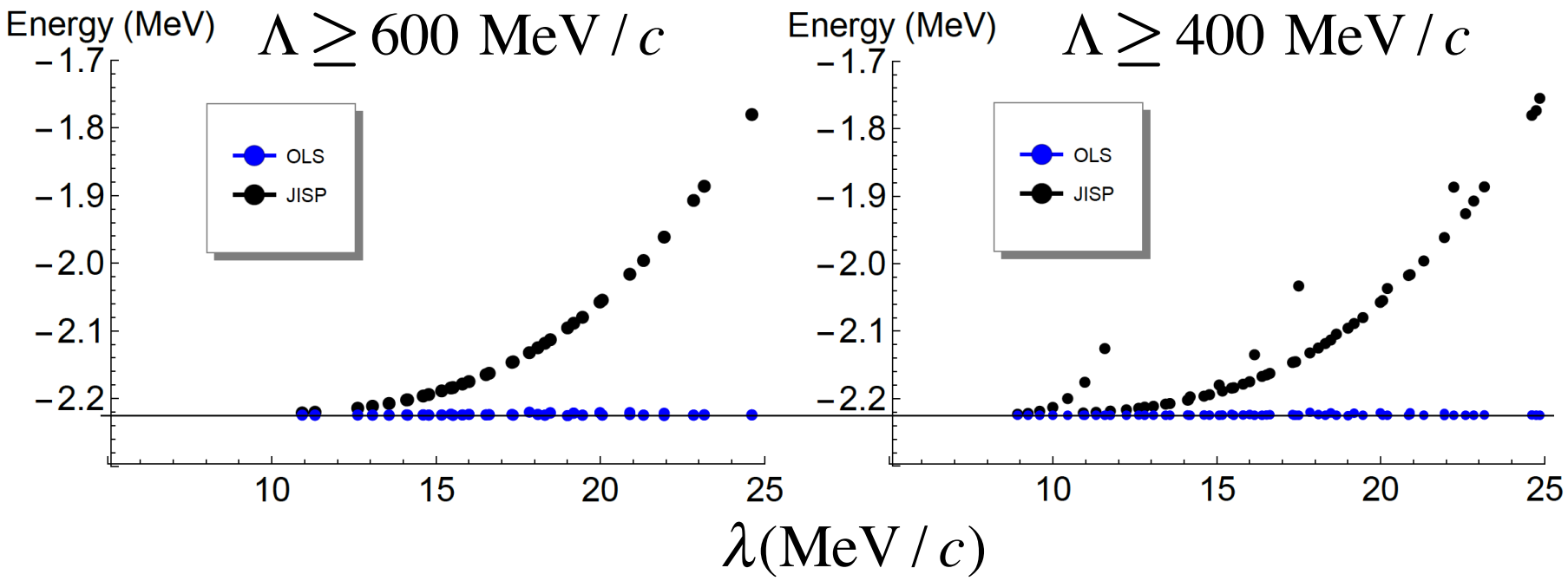
Magnetic dipole moment	M1
Root mean square radius	R
Electric quadrupole moment	Q
Gamow-Teller	GT

Dimension of the “full space” is 120 for all results depicted here

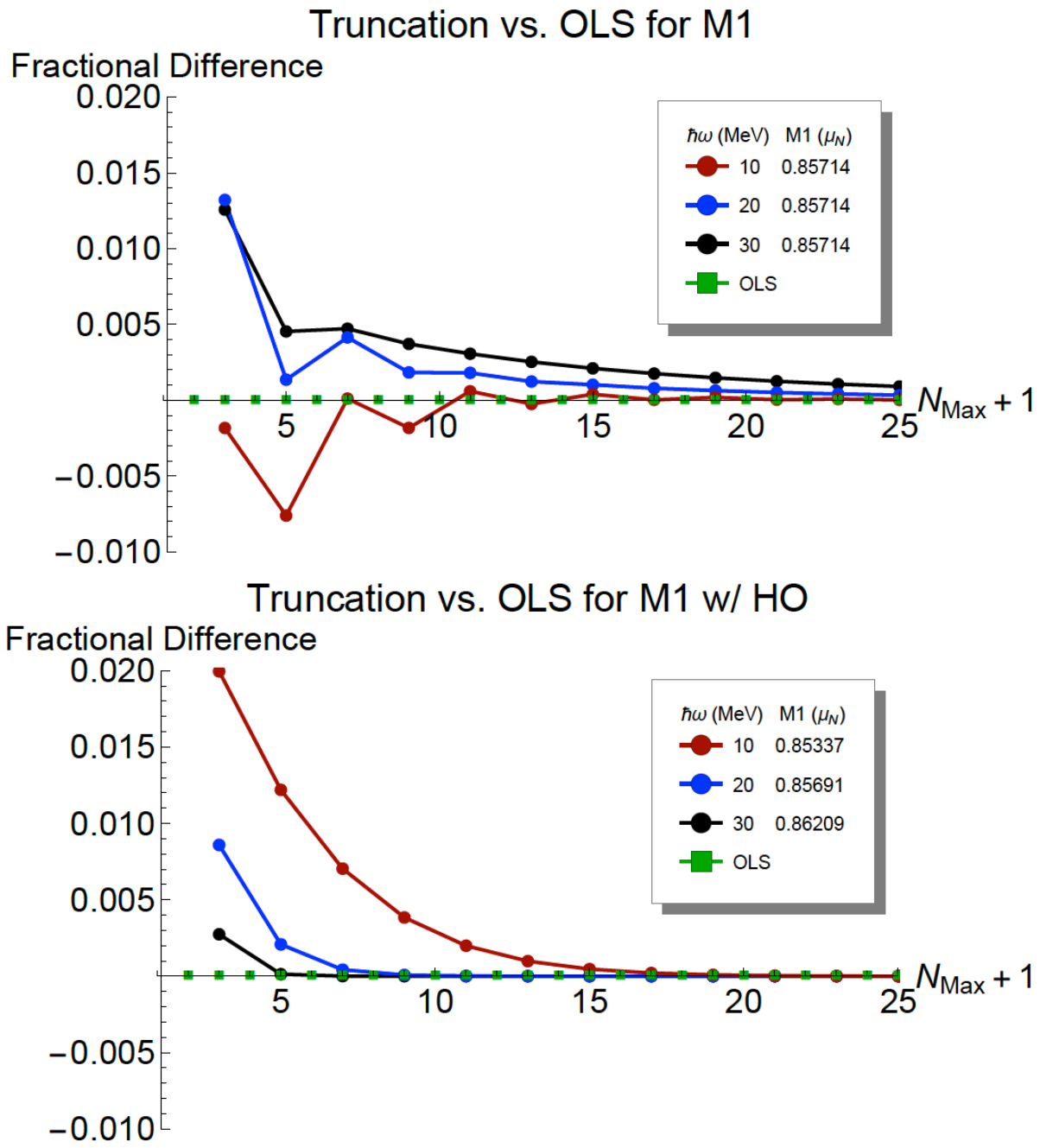

Truncation vs. OLS for Energy
Fractional Difference
0.20
0.15
0.10
0.05
5
10
15
20
25
$N_{Max} + 1$
ħω (MeV) E
10 −2.2246
20 −2.2246
30 −2.2245
OLS

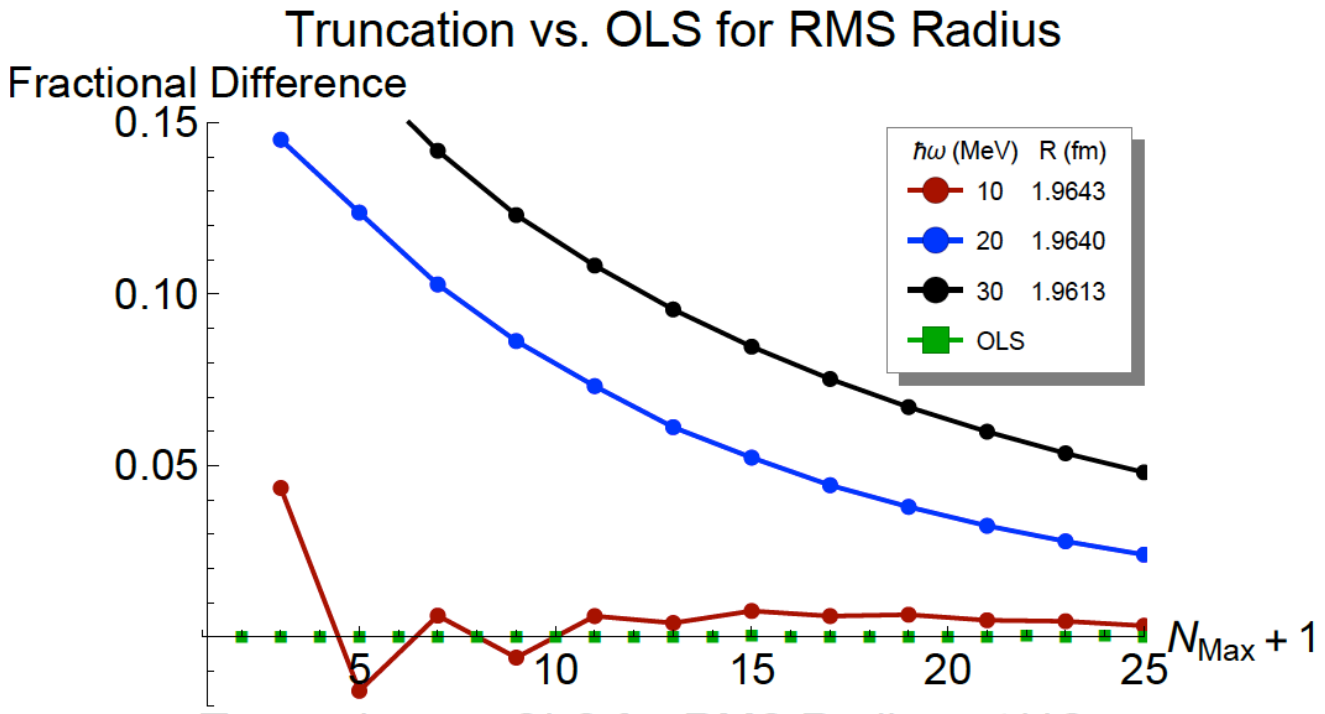

Truncation vs. OLS for Energy w/ HO
Fractional Difference
0.20
0.15
0.10
0.05
5
10
15
20
25
$N_{Max} + 1$
ħω (MeV) E
10 2.5993
20 11.795
30 23.220
OLS

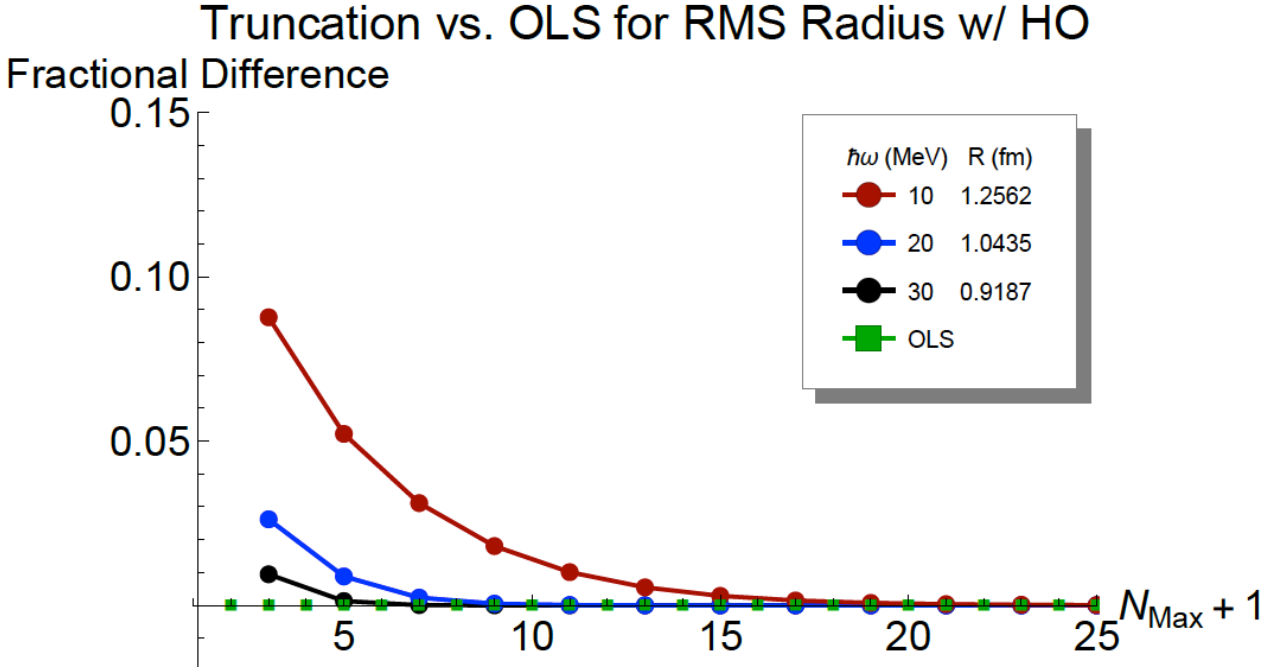
OLS manages the IR and UV regions of the interaction
Note that Λ_{NN}(JISP16) ~ 500 MeV/c

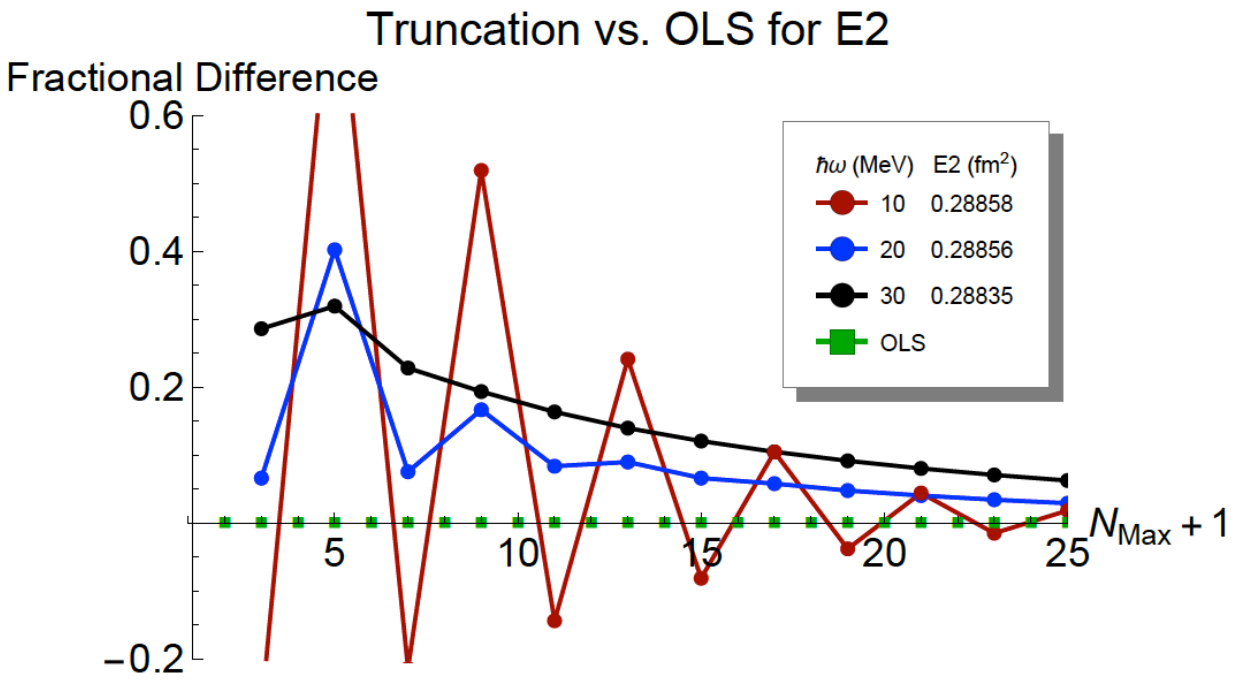


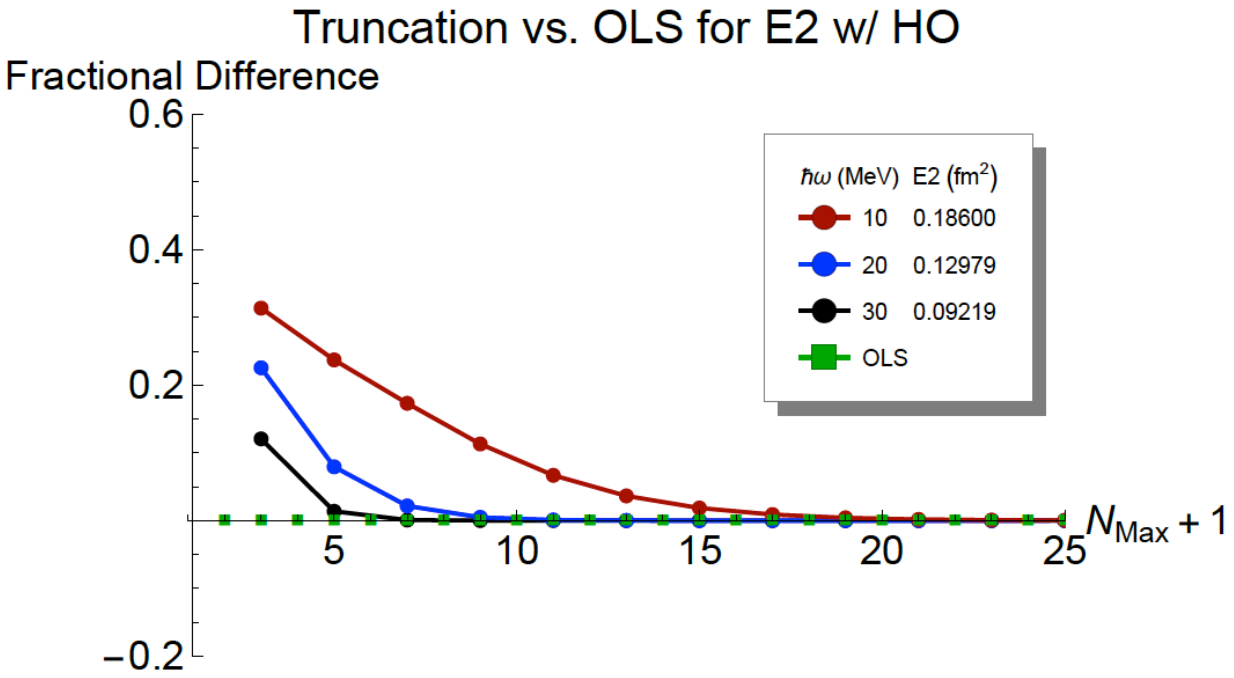
OLS results are independent of IR and UV basis regulators

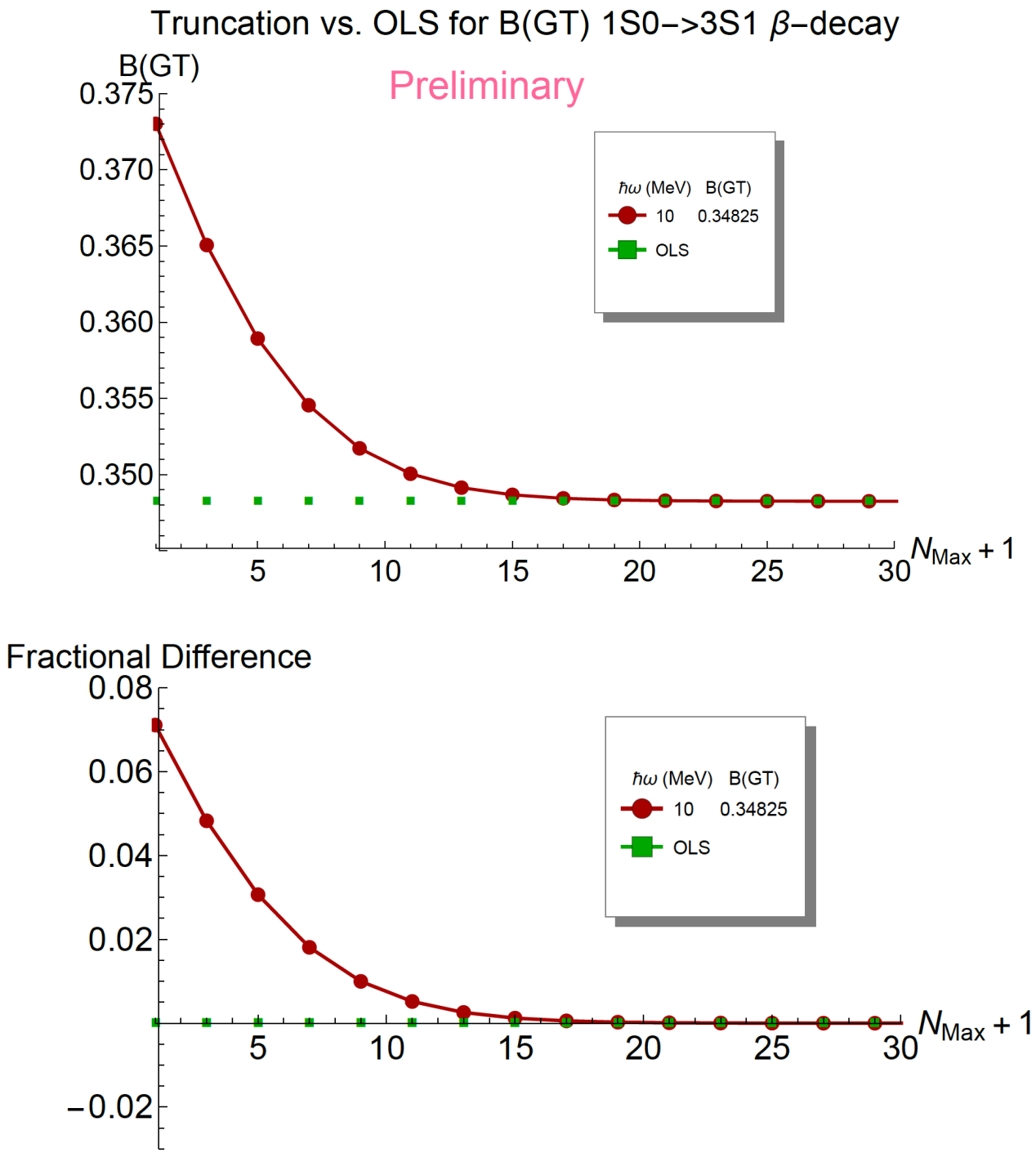

Truncation vs. OLS for M1
Fractional Difference
0.020
0.015
0.010
0.005
−0.005
−0.010
5
10
15
20
25
$N_{Max}+1$
ħω (MeV) M1 (μ_N)
10 0.85714
20 0.85714
30 0.85714
OLS
Truncation vs. OLS for M1 w/ HO
Fractional Difference
0.020
0.015
0.010
0.005
−0.005
−0.010
5
10
15
20
25
$N_{Max}+1$
ħω (MeV) M1 (μ_N)
10 0.85337
20 0.85691
30 0.86209
OLS


Truncation vs. OLS for RMS Radius
Fractional Difference
0.15
0.10
0.05
5
10
15
20
25
$N_{Max} + 1$
ħω (MeV) R (fm)
10 1.9643
20 1.9640
30 1.9613
OLS


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

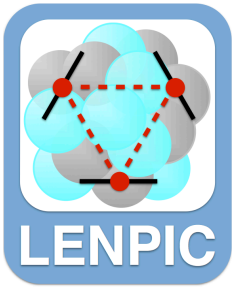

Truncation vs. OLS for E2
Fractional Difference
0.6
0.4
0.2
−0.2
5
10
15
20
25
$N_{Max} + 1$
ħω (MeV) E2 (fm²)
10 0.28858
20 0.28856
30 0.28835
OLS


Truncation vs. OLS for E2 w/ HO
Fractional Difference
0.6
0.4
0.2
−0.2
5
10
15
20
25
$N_{Max} + 1$
ħω (MeV) E2 (fm²)
10 0.18600
20 0.12979
30 0.09219
OLS


Truncation vs. OLS for B(GT) 1S0−>3S1 β−decay
B(GT)
Preliminary
0.375
0.370
0.365
0.360
0.355
0.350
ħω (MeV) B(GT)
10 0.34825
OLS
5
10
15
20
25
30
N_Max + 1
Fractional Difference
0.08
0.06
0.04
0.02
−0.02
ħω (MeV) B(GT)
10 0.34825
OLS
5
10
15
20
25
30
N_Max + 1

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

Low
Energy
Nuclear
Physics
International
Collaboration



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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)

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Main Message

Use light nuclei and precision calculations
to understand effective operators' (e.g. g_A)
dependences on Hamiltonians and basis spaces

Overview

Review of selected published results
and present some new "test" problems

Conclusion

Major efforts needed to quantify all theoretical uncertainties:
Effective Hamiltonians, Effective electroweak operators,
Many-body methods, ...