Full Configuration Interaction (FCI) studies of light nuclei - opportunities and challenges

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- FCI - defined & difference from NCSM
- N3LO & JISP16 Comparisons
- Energy Extrapolations for N_{max} -> inf
- Conclusions/Opportunities/Challenges

Foundations (depending on renormalization of H [RN])

1. *ab-initio* No-Core Shell Model (NCSM): RN = Lee-Suzuki-Okamoto
2. Full Configuration Interaction (FCI): Bare H, RN = Vlowk, SRG

Common features:

- Both are *ab-initio*
- Both use a many-body basis constructed from harmonic oscillator single-particle states
  => basis space depends on (N_{max}, $\hbar\Omega$)

Major distinction:

NCSM uses Heff calculated for each N_{max}
FCI uses H independent of N_{max}

FCI Problem Statement

Solve eigenvalue problem in large enough basis to converge

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H\left|\Psi_i\right\rangle = E_i\left|\Psi_i\right\rangle$$

$$\left|\Psi_i\right\rangle = \sum_{n=0}^{\infty} A_n^i \left|\Phi_n\right\rangle$$

$$\text{Diagonalize } \left\{\left\langle \Phi_m \middle| H \middle| \Phi_n \right\rangle\right\}$$

Employ eigenvectors to calculate experimental observables

$$\text{Transition Rate } (i \rightarrow k) \propto \left|\left\langle \Psi_k \middle| \hat{O} \middle| \Psi_i \right\rangle\right|^2$$

Test fundamental strong interaction forces in nature

Test fundamental symmetries - standard model and beyond

What is the FCI approach to solving the problem?

- Adopt a realistic NN (and 3N) interaction & renormalize via SRG or Vlowk as needed
- Adopt the 3-D Harmonic Oscillator (HO) for the single nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)

$$\left|\Phi_n\right\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n \left|0\right\rangle$$

- Diagonalize H in sufficiently large basis to achieve converged results

$$n = 1, 2, \ldots, 10^9 \text{ or more!}$$

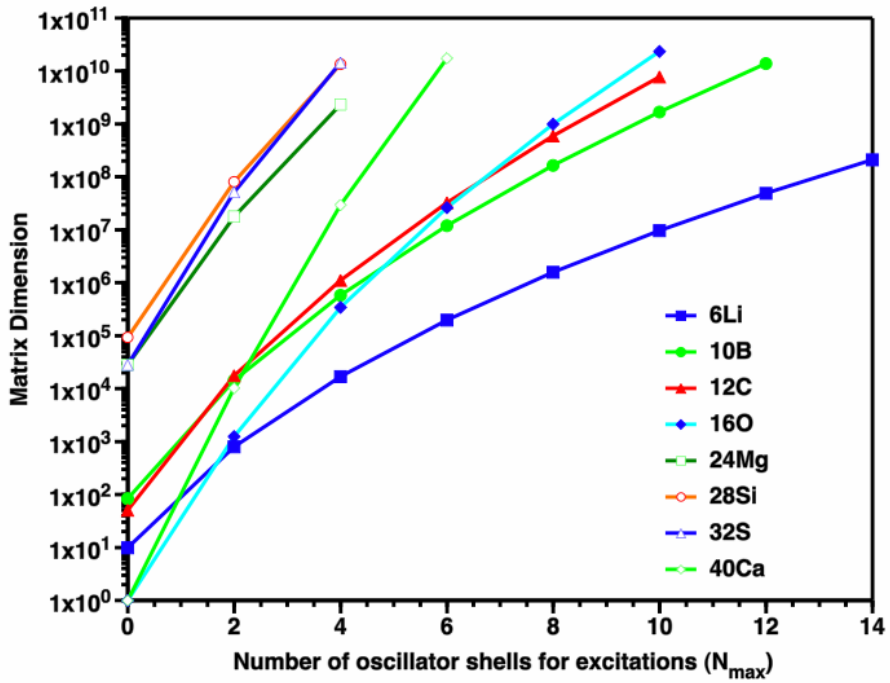
- Evaluate observables and compare with experiment

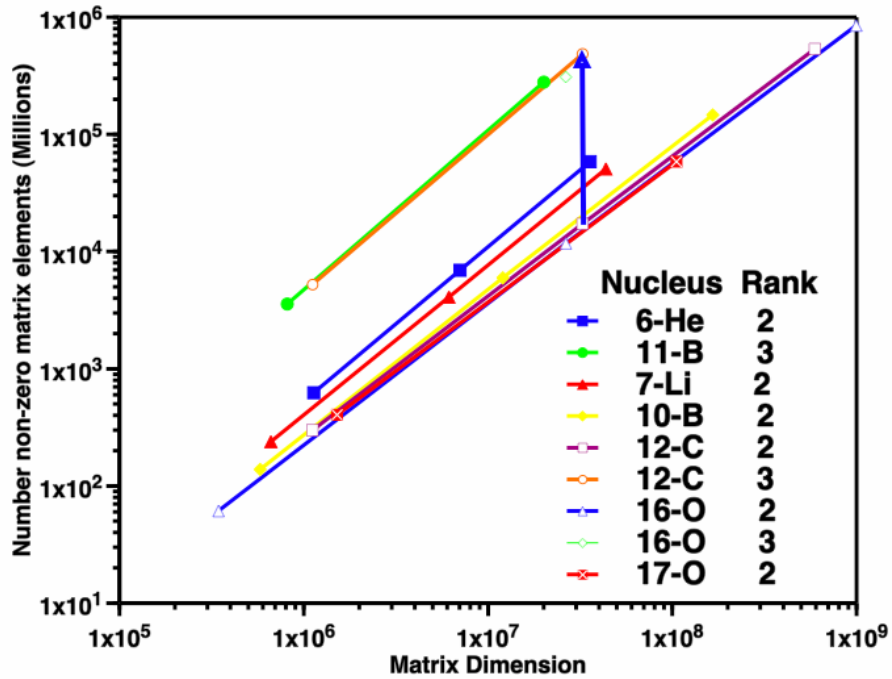
Comments:

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments
- Achievable for nuclei up to A=16 (40) today with largest computers available

Challenge

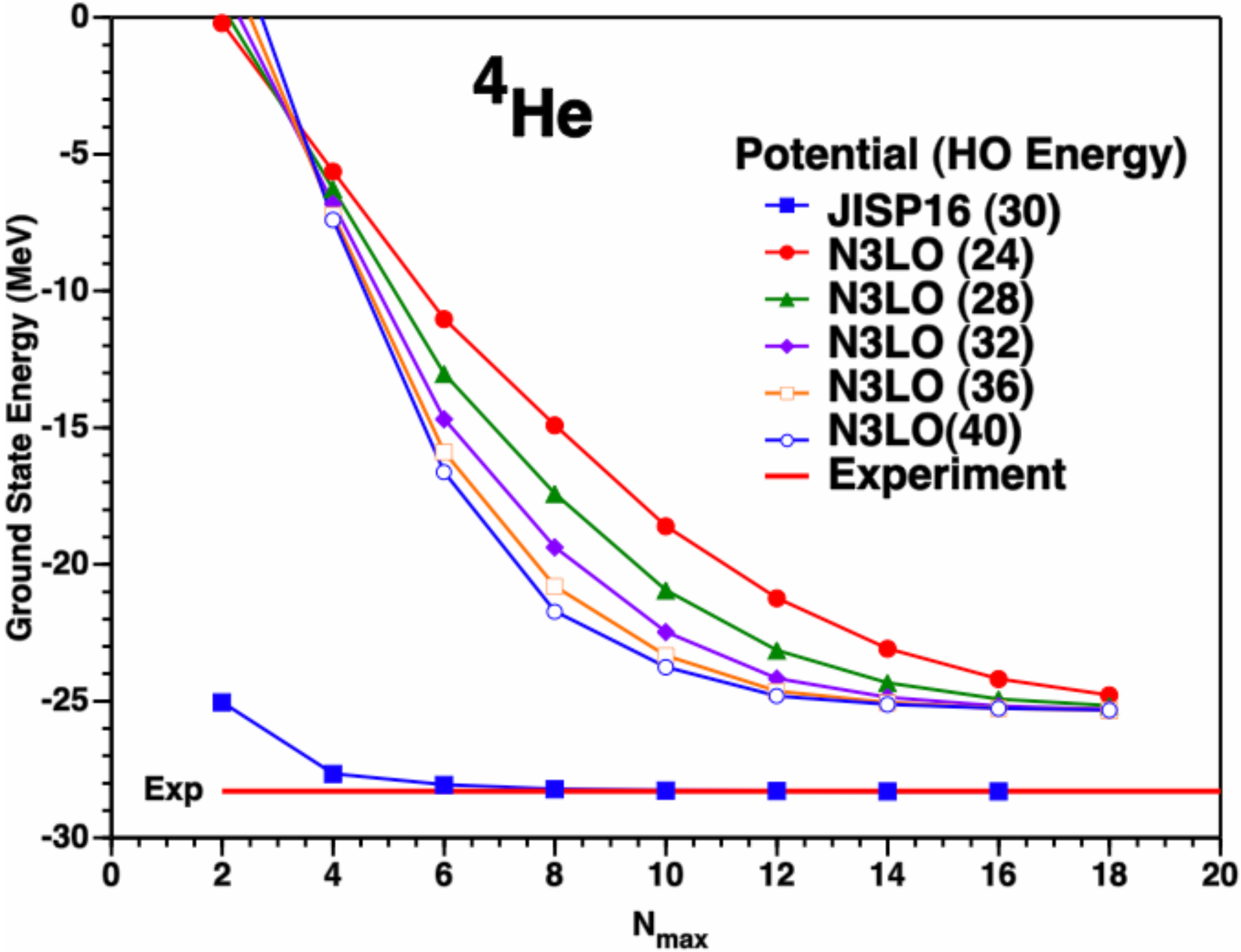
Exponential increase in dimension (D)

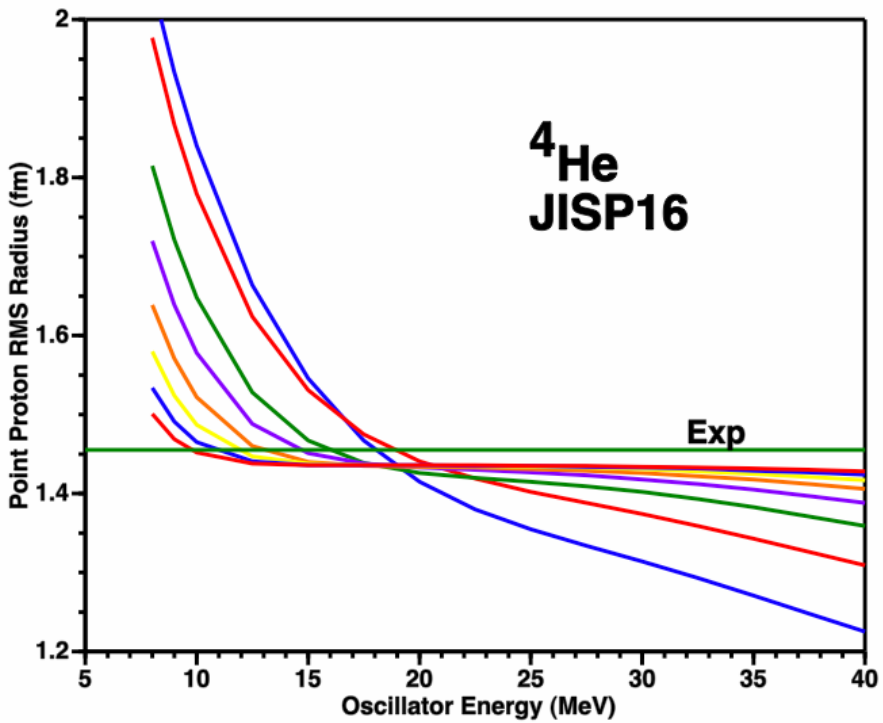


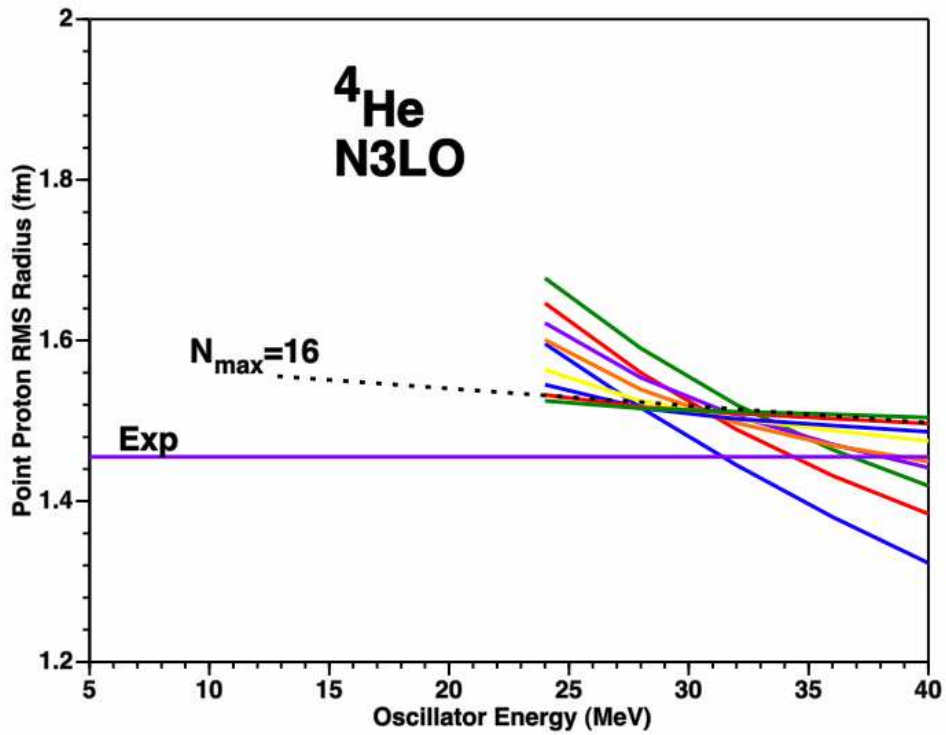


Opportunities

- Memory/cpu time grows only as $D^{3/2}$
- Algorithm development (UNEDF/SciDAC funding)
- Petaflop machines on order (Japan, US-NSF, US-DOE, …)
- Improved understanding of H & RN (Chiral EFT, others)
- Developing methods for extrapolating D->inf


^{4}He
Potential (HO Energy)
JISP16 (30)
N3LO (24)
N3LO (28)
N3LO (32)
N3LO (36)
N3LO(40)
Experiment
Exp
Ground State Energy (MeV)
N_{max}
0
-5
-10
-15
-20
-25
-30
0
2
4
6
8
10
12
14
16
18
20


^{4}He
JISP16
Exp
Point Proton RMS Radius (fm)
Oscillator Energy (MeV)
2
1.8
1.6
1.4
1.2
5
10
15
20
25
30
35
40


^{4}He
N3LO
N_{max}=16
Exp
Point Proton RMS Radius (fm)
Oscillator Energy (MeV)
2
1.8
1.6
1.4
1.2
5
10
15
20
25
30
35
40

Reflect on successes of the *ab-initio* NCSM

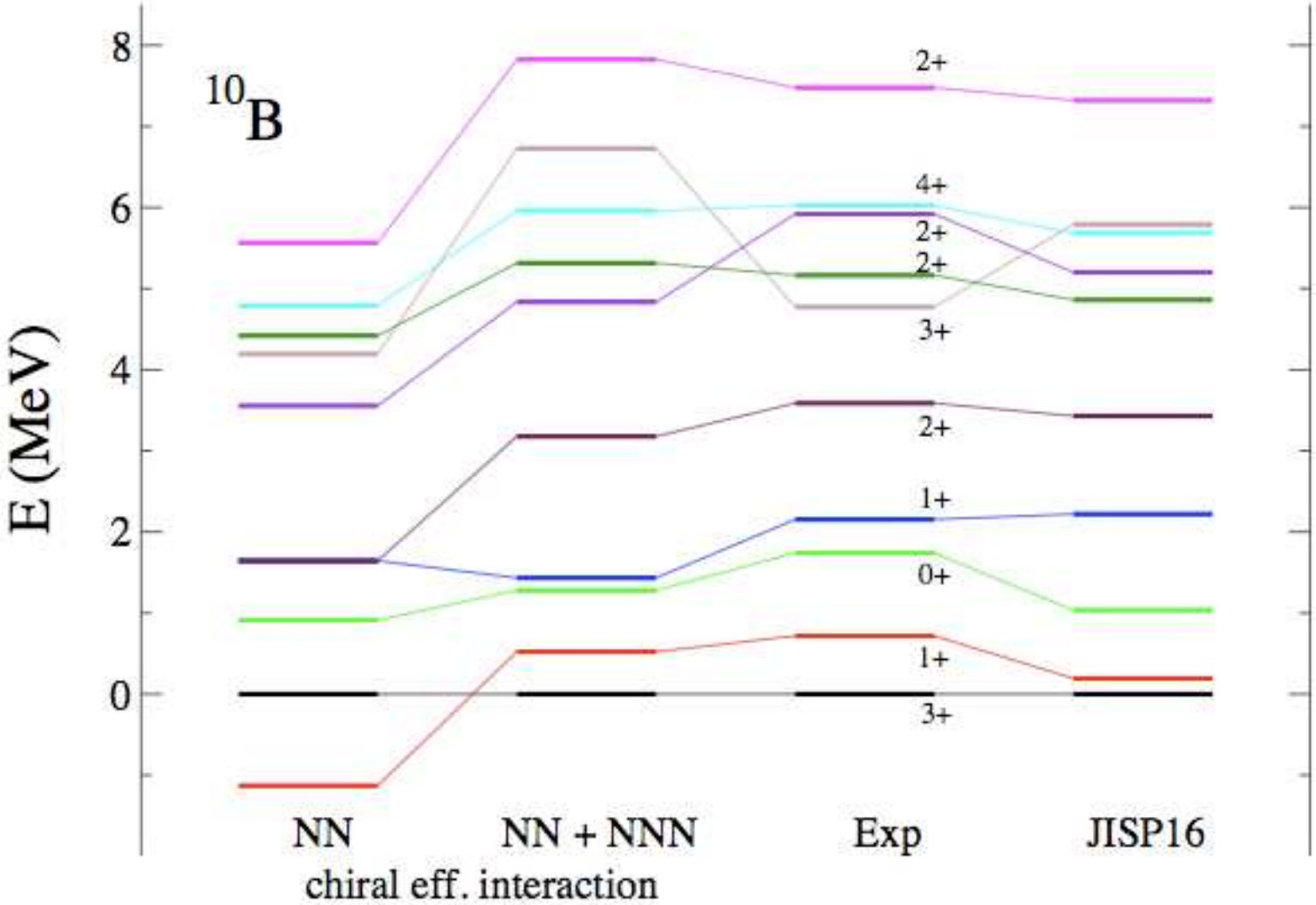
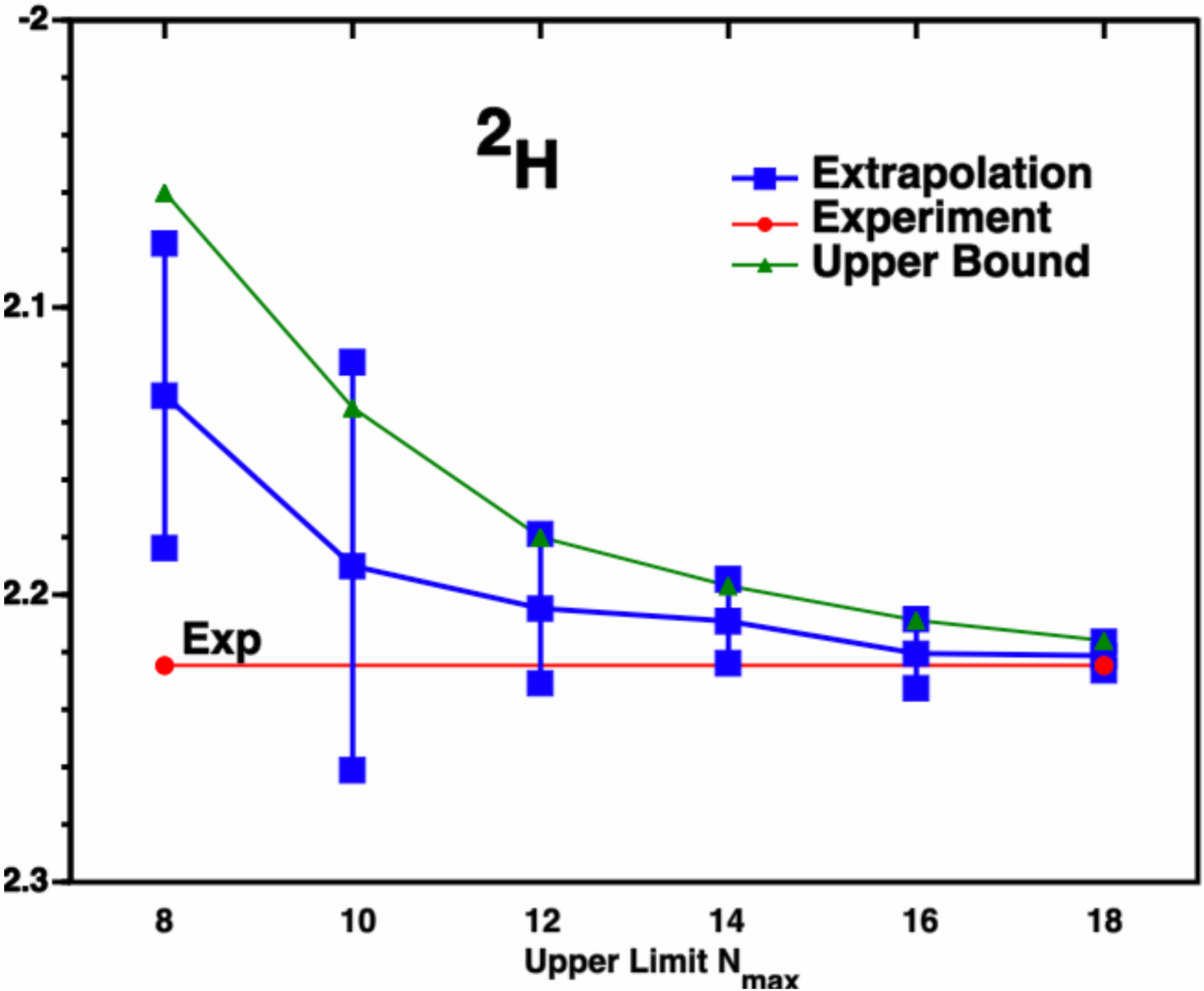
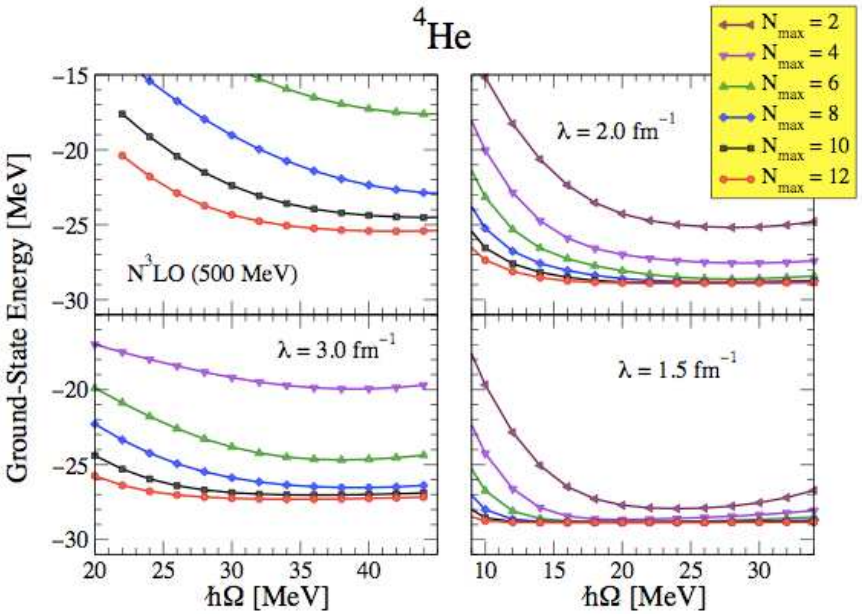


FIGURE 2. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state at an oscillator energy $\hbar\Omega = 14\ MeV$. The chiral effective interaction results are obtained at $N_{max} = 6$ while the JISP16 results are obtained at $N_{max} = 8$.


^{2}H
Extrapolation
Experiment
Upper Bound
Exp
-2
2.1
2.2
2.3
8
10
12
14
16
18
Upper Limit N_{max}

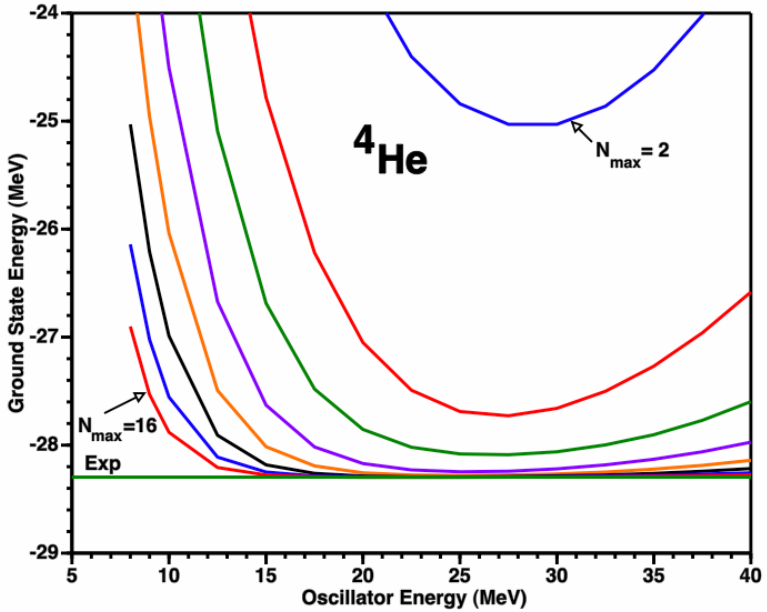
Sample of FCI results

Chiral N3LO & SRG



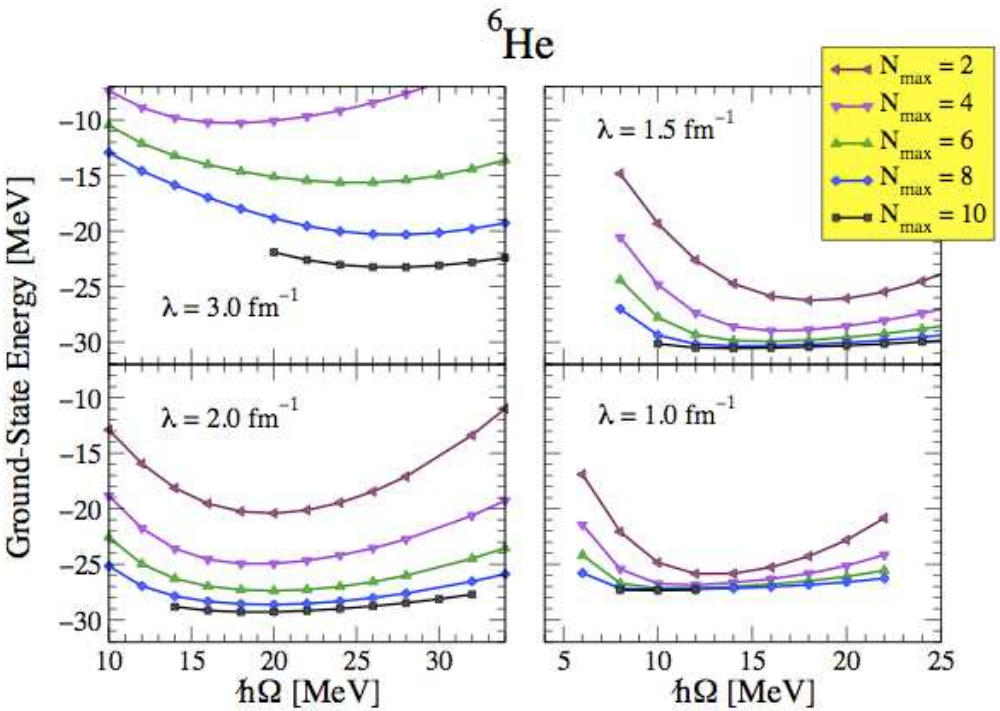
(Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, arXiv:0708.3754)

JISP16

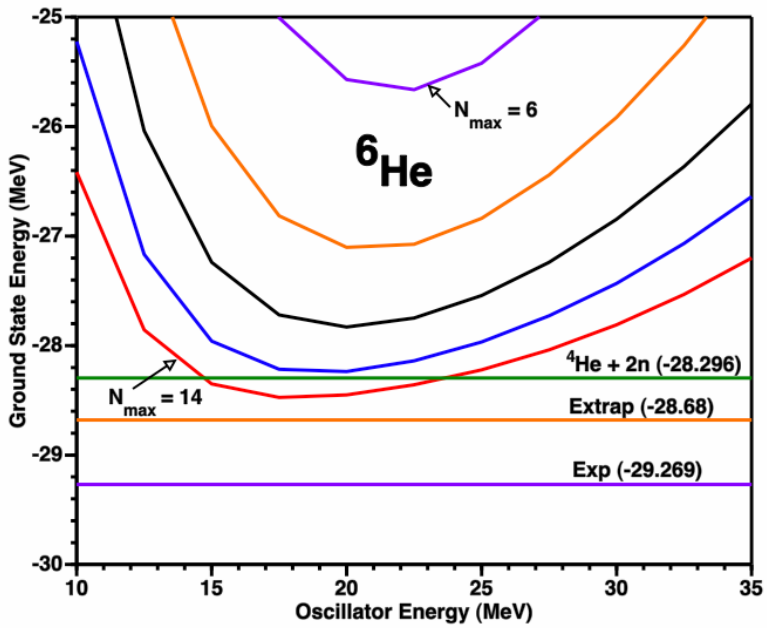


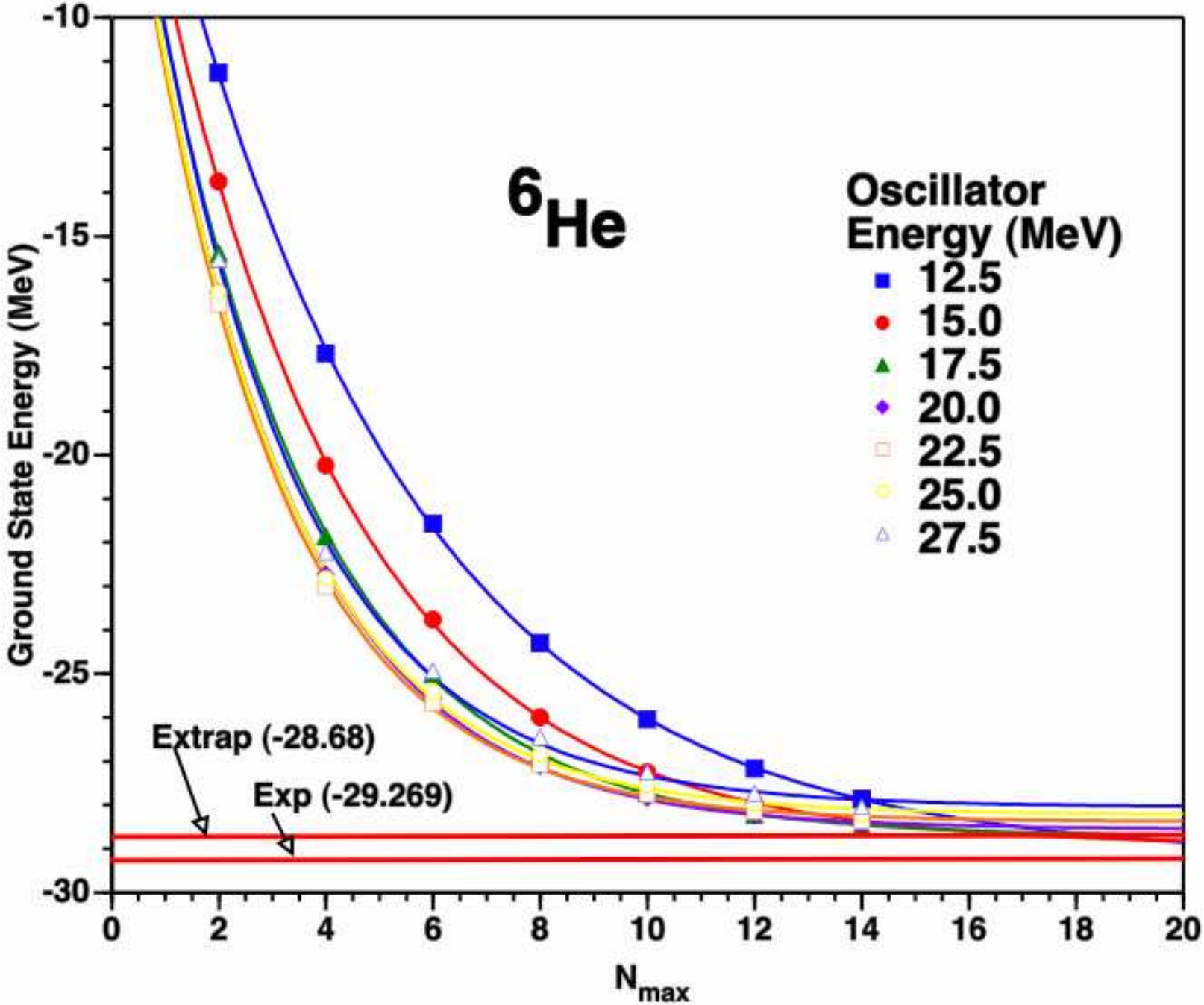
(Maris, Vary and Shirokov, in preparation)

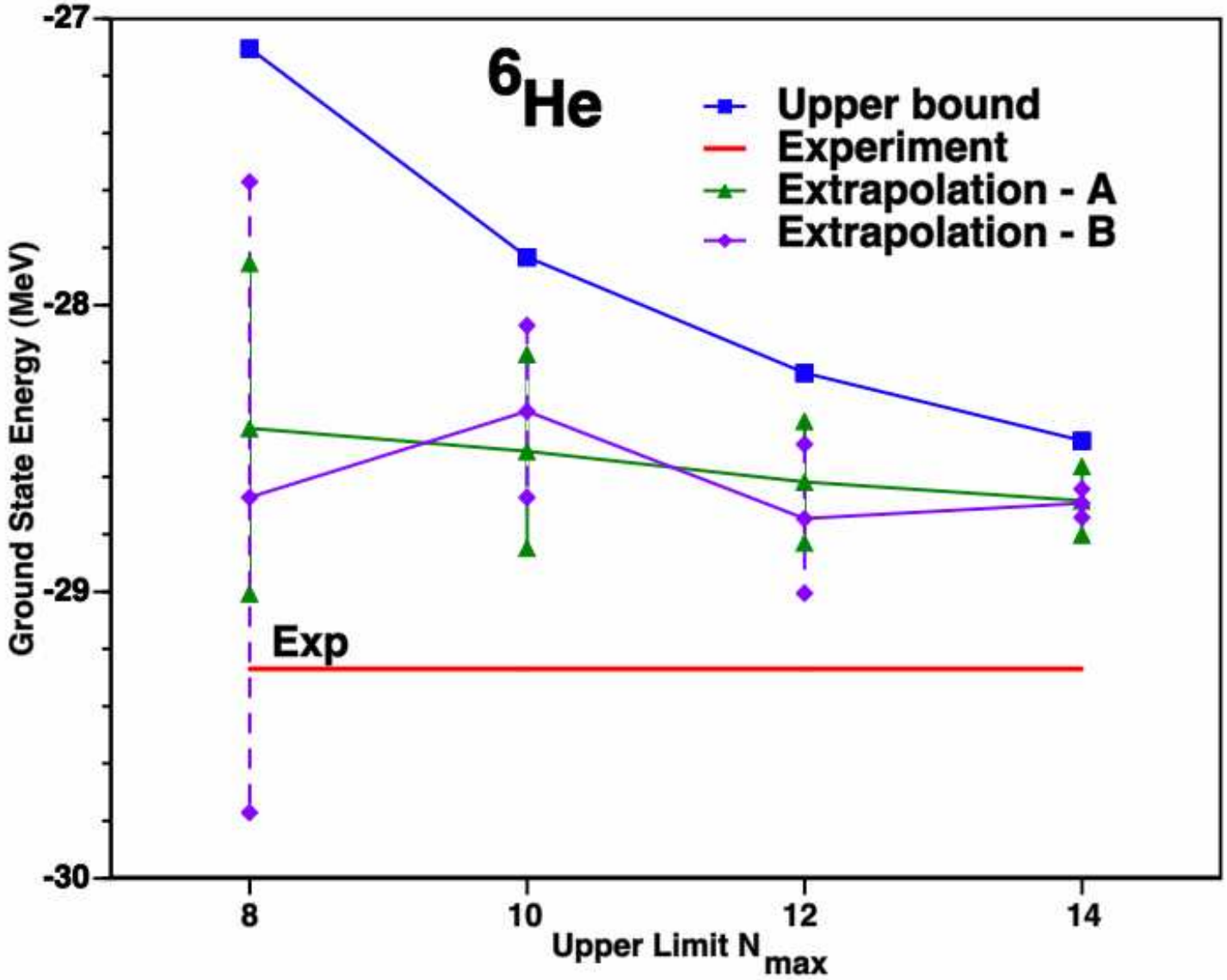
Chiral N3LO & SRG



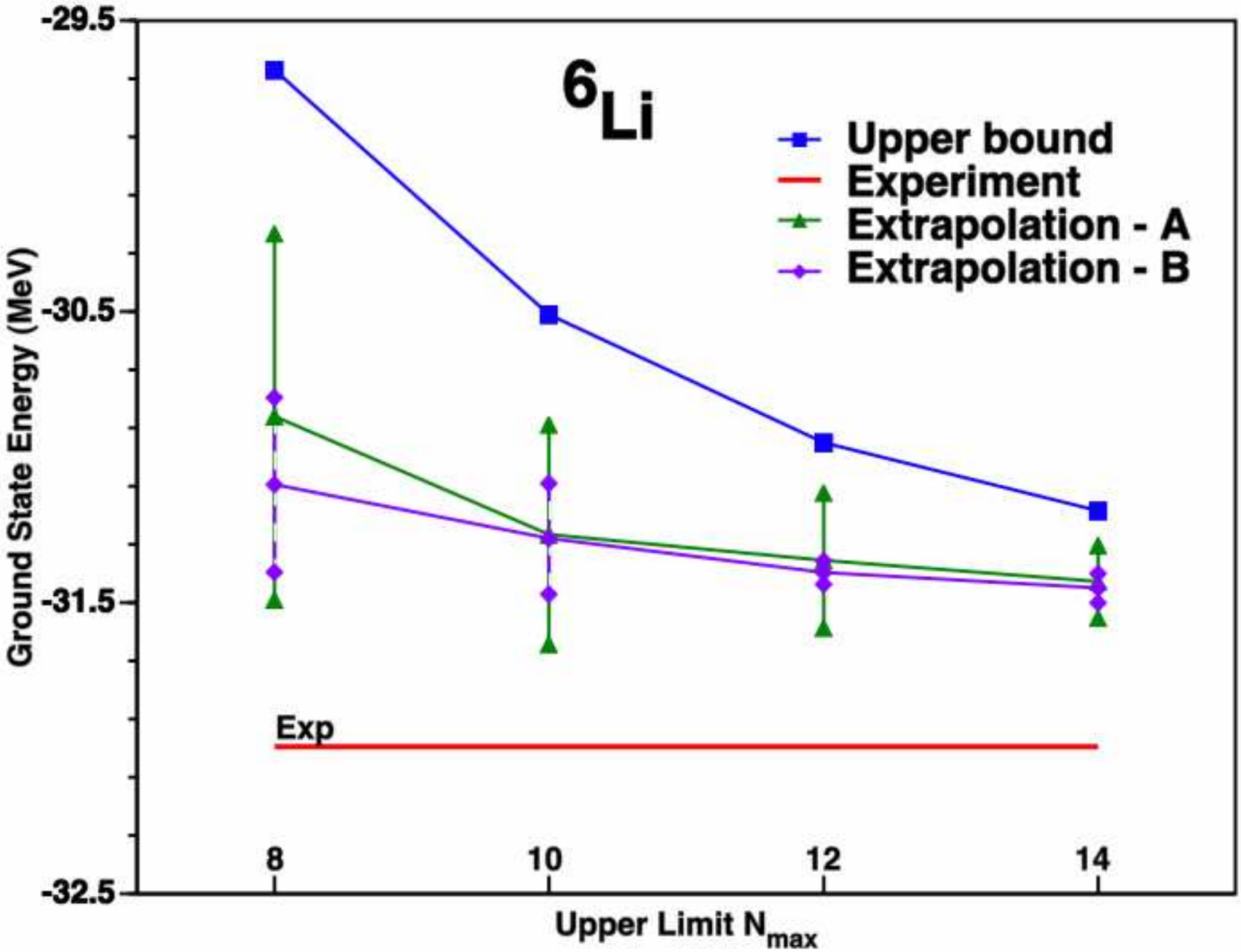
JISP16

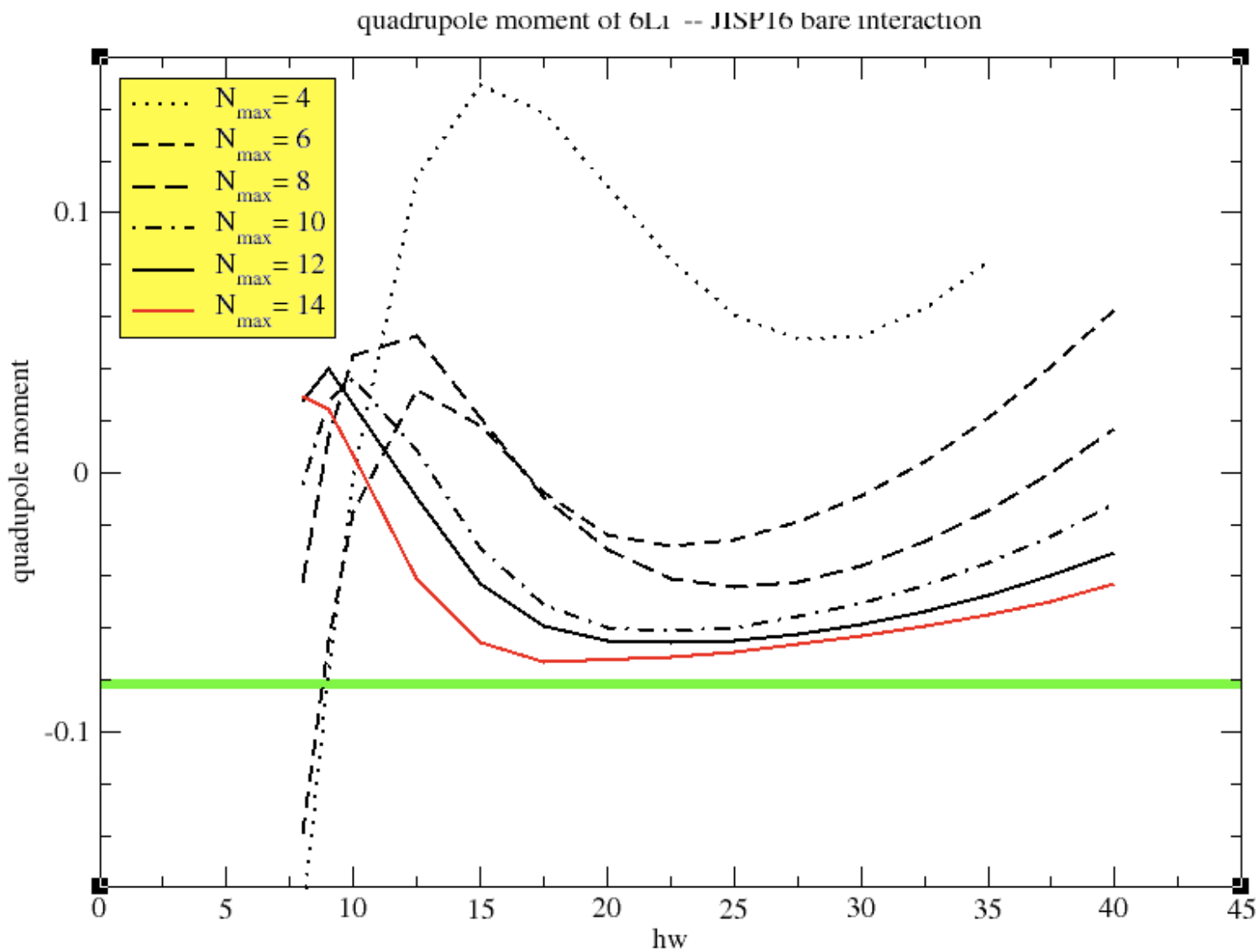


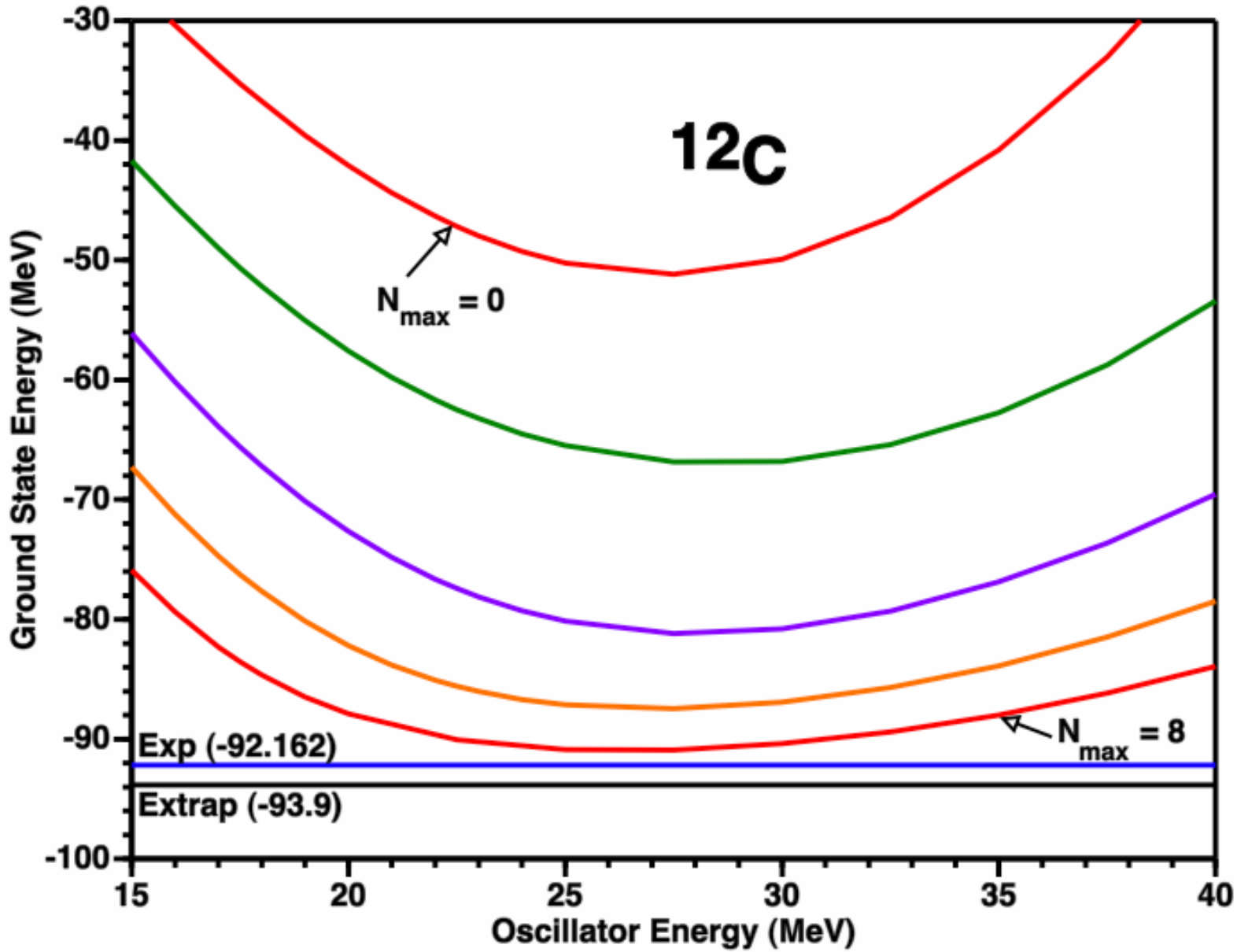

^{6}He
Oscillator Energy (MeV)
12.5
15.0
17.5
20.0
22.5
25.0
27.5
Extrap (-28.68)
Exp (-29.269)
Ground State Energy (MeV)
-10
-15
-20
-25
-30
0
2
4
6
8
10
12
14
16
18
20
N_{max}

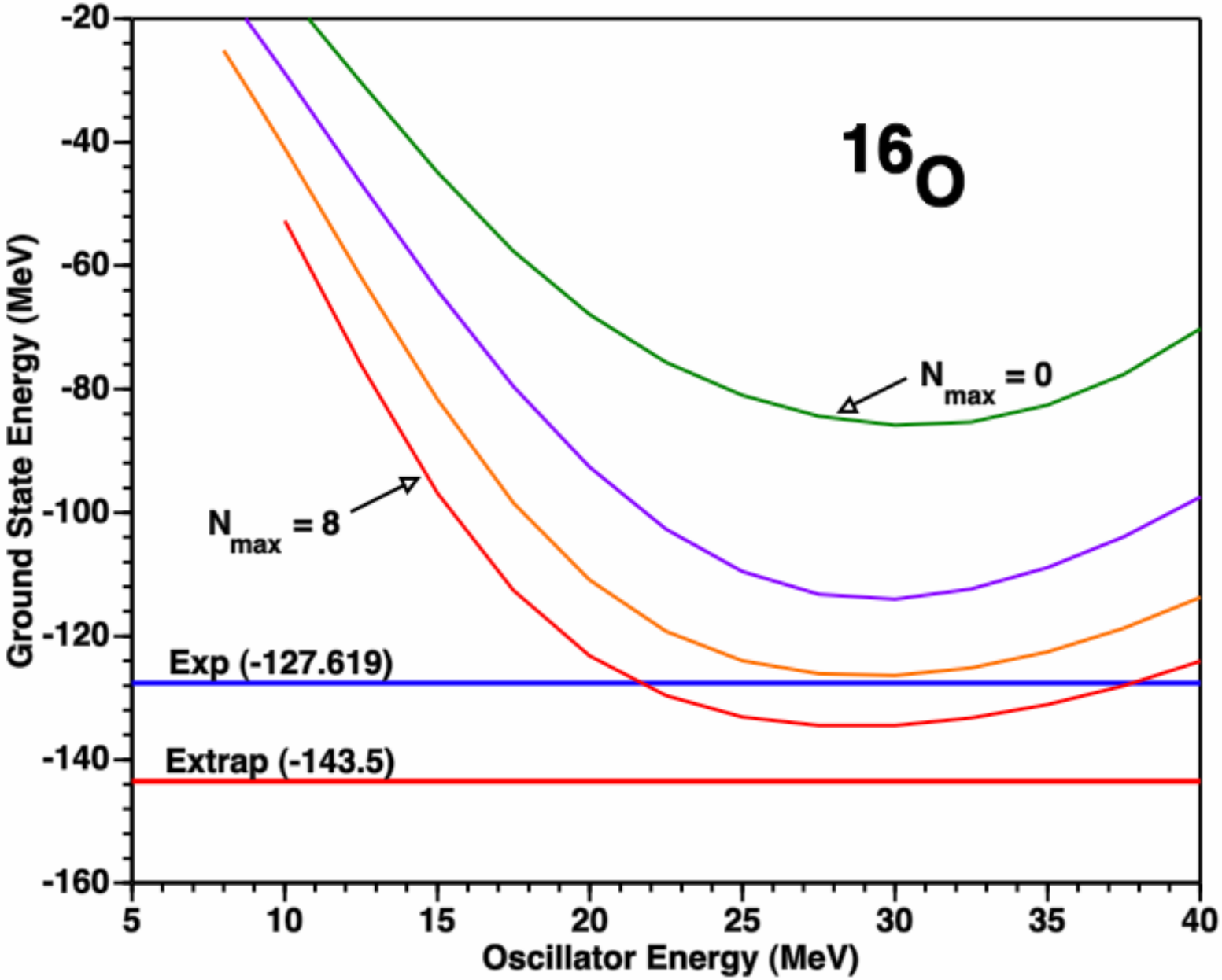


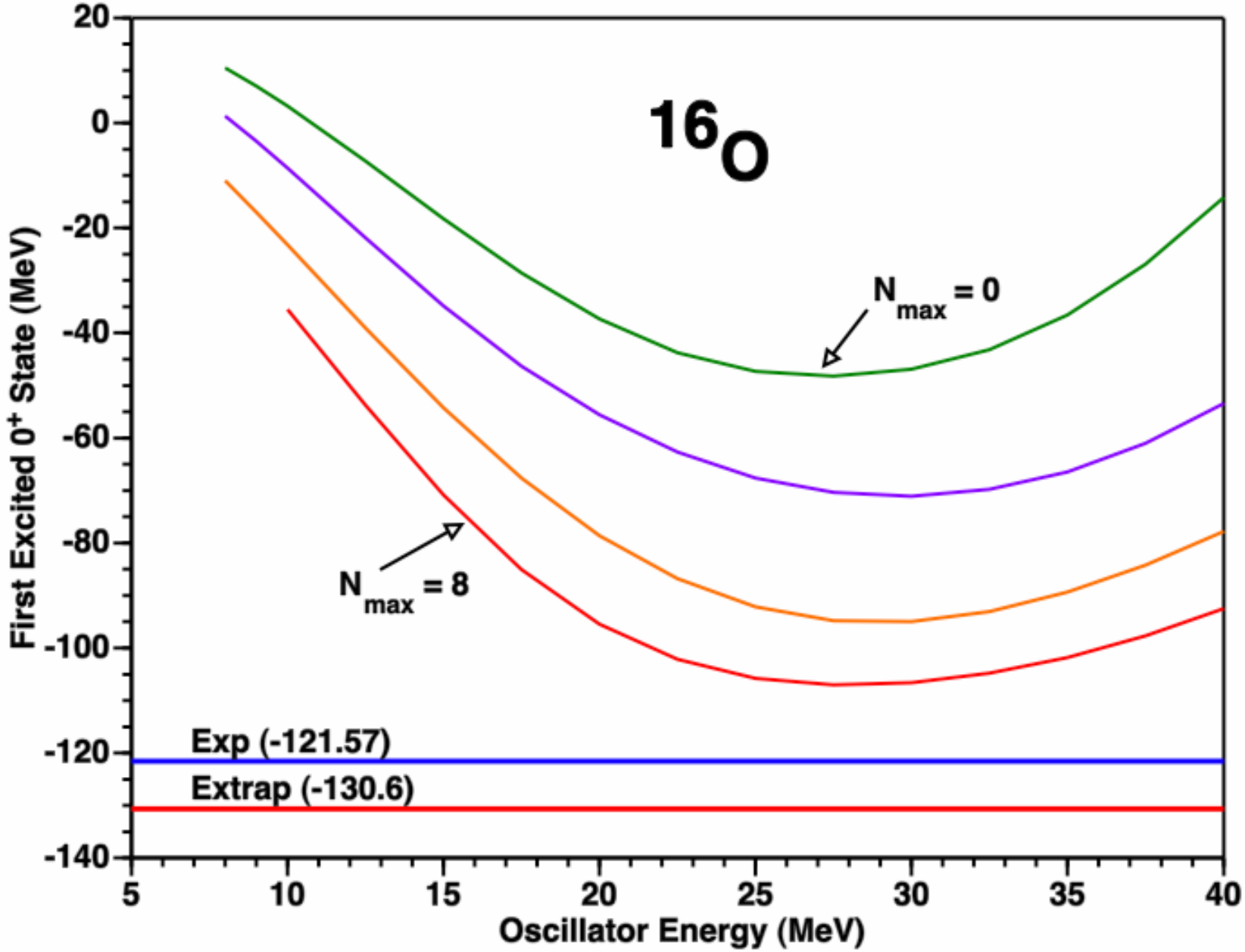
A-uses 4 successive Nmax points
B-uses 3 successive Nmax points


^{6}Li
Upper bound
Experiment
Extrapolation - A
Extrapolation - B
Exp
-29.5
-30.5
-31.5
-32.5
Ground State Energy (MeV)
8
10
12
14
Upper Limit N_{max}

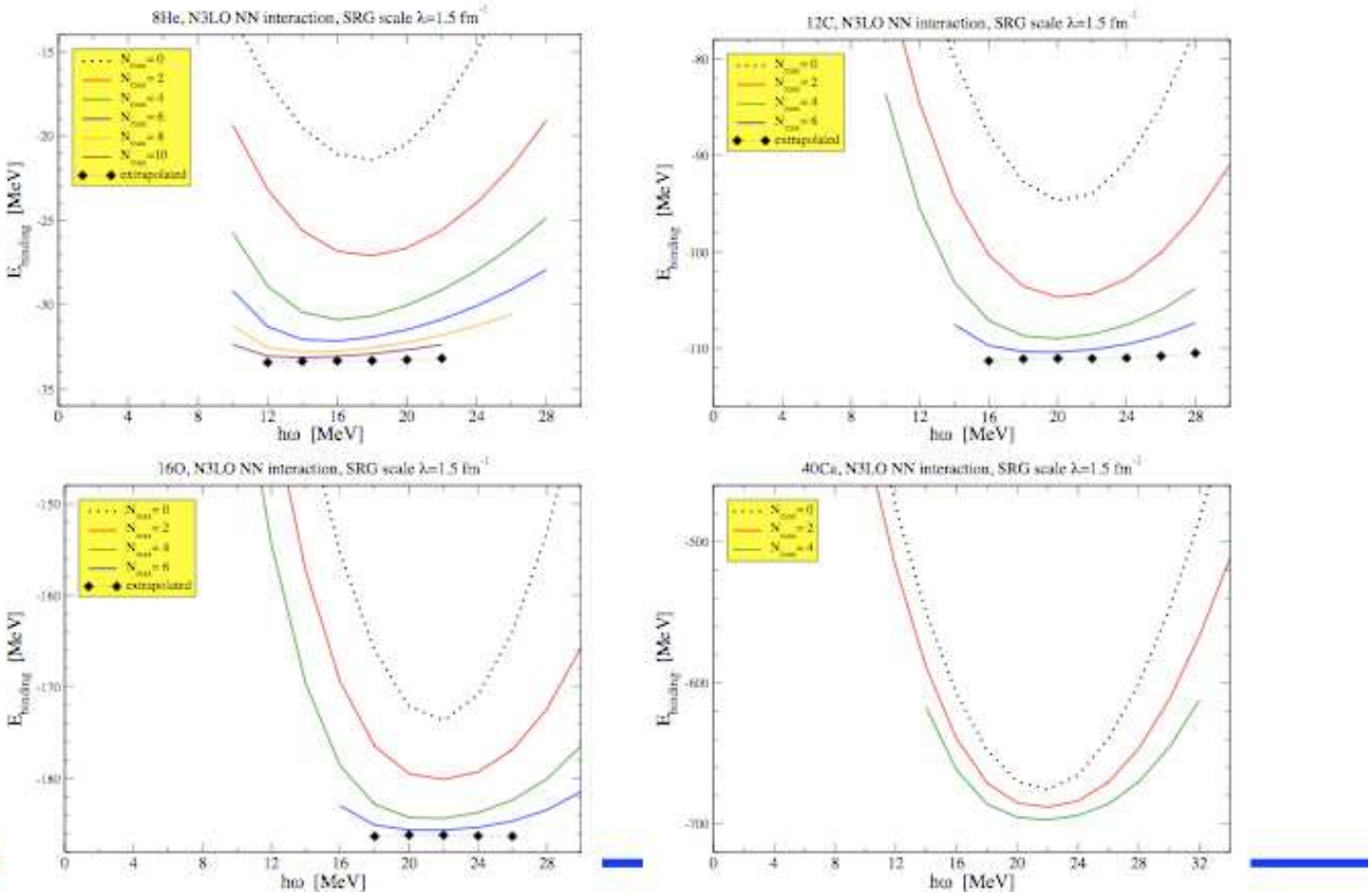

quadrupole moment of 6Li -- JISP16 bare interaction
N max = 4
N max = 6
N max = 8
N max = 10
N max = 12
N max = 14
quadupole moment
0.1
0
-0.1
0
5
10
15
20
25
30
35
40
45
hw


12C
Ground State Energy (MeV)
Oscillator Energy (MeV)
-30
-40
-50
-60
-70
-80
-90
-100
15
20
25
30
35
40
N max = 0
N max = 8
Exp (-92.162)
Extrap (-93.9)


16O
Ground State Energy (MeV)
Oscillator Energy (MeV)
-20
-40
-60
-80
-100
-120
-140
-160
5
10
15
20
25
30
35
40
N max = 0
N max = 8
Exp (-127.619)
Extrap (-143.5)


16O
N max = 0
N max = 8
Exp (-121.57)
Extrap (-130.6)
First Excited 0+ State (MeV)
Oscillator Energy (MeV)
20
0
-20
-40
-60
-80
-100
-120
-140
5
10
15
20
25
30
35
40

rapid convergence 8He, 12C, 16O, 40Ca; all overbound at $\lambda = 1.5$



Conclude: Need consistent Chiral 3N potentials

Opportunities and Challenges

- Full CI with realistic NN interactions can be extrapolated to obtain converged gs energies & uncertainties
- JISP16 & N3LO+SRG are suitable NN interactions for light nuclei up through 16-O (40-Ca under investigation)
- Established need for 3N potentials
- Additional observables under investigation
- Examine properties with tunable external fields
- Race to explore exotic nuclei with these new frameworks

Additional New Developments/Collaborators & Other talks at this meeting!

- Renormalization with a core - Lisetskiy, Barrett, Navratil
- Chiral V_{NN} + V_{3N} in light nuclei with NCSM - Navratil, Ormand
- Trapped fermion systems - Stetcu, Barrett, van Kolck
- Symplectic basis spaces - Draayer, Sviratcheva, Dytrych, Bahri
- V_{NN} + V_{3N} /SRG/Vlowk - Schwenk, Bogner, Furnstahl, Maris
- Comparison of CC with FCI - Maris, Hagen, Papenbrock, Dean
- UNEDF/SciDAC external fields - Maris, Furnstahl, Bogner
- UNEDF/SciDAC realistic basis - Maris, Negoita, Shirokov
- UNEDF/SciDAC *ab-initio* scattering - Mazur, Shirokov