Convergence properties of no-core nuclear calculations

Subthemes: Extrapolation and Uncertainty Quantification (UQ)

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Perspectives of the Ab Initio No-Core Shell Model
TRIUMF
February 23-25, 2012

- Some definitions and Scope
- Constrained extrapolation method & UQ – "Extrapolation A"
- Quasi hw-independent extrapolation & UQ – "Extrapolation B"
- A = 6 Benchmarks of NCFC with Hyperspherical Harmonics
- IR and UV properties of the Harmonic Oscillator (HO) & NN interactions
- New extrapolation method of Coon, Avetian, Kruse, van Kolck, Maris, Vary [Preliminary results]

Definitions:

No-Core Shell Model (NCSM)

Nmax truncation (P-space) of the infinite matrix problem with Hamiltonian renormalization (P-space dependent and A-dependent in the case of Lee-Suzuki)

No-Core Full Configuration (NCFC)

Exact result of the infinite basis calculation obtained by a sequence of Nmax truncations that, for the gs energy, converges uniformly from above since it retains the variational principle

Full Configuration Interaction (FCI)

Nshell truncation (sps cutoff) of the infinite matrix problem (CC, MCSM, HF & HFB approxs, . . .)

Uncertainty Quantification (UQ)

Tested methods employed to quote a mean deviation for a result with defined set of sources of that uncertainty (numerical, systematic, statistical,…)

Note: If one performs an Nmax-truncated calculation without a renormalization fixed by that truncation (e.g. Lee-Suzuki) and without an extrapolation, one may call it either an "NCSM basis" calculation or a "truncated NCFC" calculation with the above definitions.

PHYSICAL REVIEW C **79**, 014308 (2009)

Ab initio no-core full configuration calculations of light nuclei

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(Received 28 August 2008; published 22 January 2009)

$$E_{gs}(N_{max}) = a \exp(-c\, N_{max}) + E_{gs}(\infty).$$

Extrapolation A

- Locate the minimum of the highest Nmax vs hw curve employed
- Take hw 2.5 MeV below the min. and 3 hw values at increments of 2.5 MeV above min.
- For these 5 sets of hw values use 4 increments in Nmax leading to the highest value (we exclude Nmax = 0)
- Weight each point using the finite difference from the previous point (1^{st} wt = $3x2^{nd}$ wt)
- Perform a constrained chisquare fit to these 20 points – extract Egs(infty)
- Assigned uncertainty is ½ the spread in the extrapolants from independent fits to the 5 sets

P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

Extrapolation B: P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

- plot all data as function of $\hbar\omega$ at fixed $N_{\rm max}$
- use an exponential fit to extrapolate the results at fixed $\hbar\omega$ from three consecutive $N_{\rm max}$ values to $N_{\rm max} = \infty$
- for $N_{\rm max} \geq 8$, use the difference with the extrapolation from the next-smaller basis space (at fixed $\hbar\omega$) as a (tentative) estimate of the numerical uncertainty in extrapolation
- plot the extrapolated data, plus their numerical error estimates, as function of $\hbar\omega$
- validate the extrapolation by checking that
  1. error estimates decrease for increasing $N_{\rm max}$
  2. central values are within error estimates of extrapolations in smaller basis spaces
  3. $\hbar\omega$ dependence decreases with increasing $N_{\rm max}$
  4. over a reasonable range of $\hbar\omega$ the central values are within each others error estimates

See P. Maris talk at this meeting for NCFC application with Chiral N3LO results (Benchmark)

PHYSICAL REVIEW C 77, 024301 (2008)

Converging sequences in the *ab initio* no-core shell model

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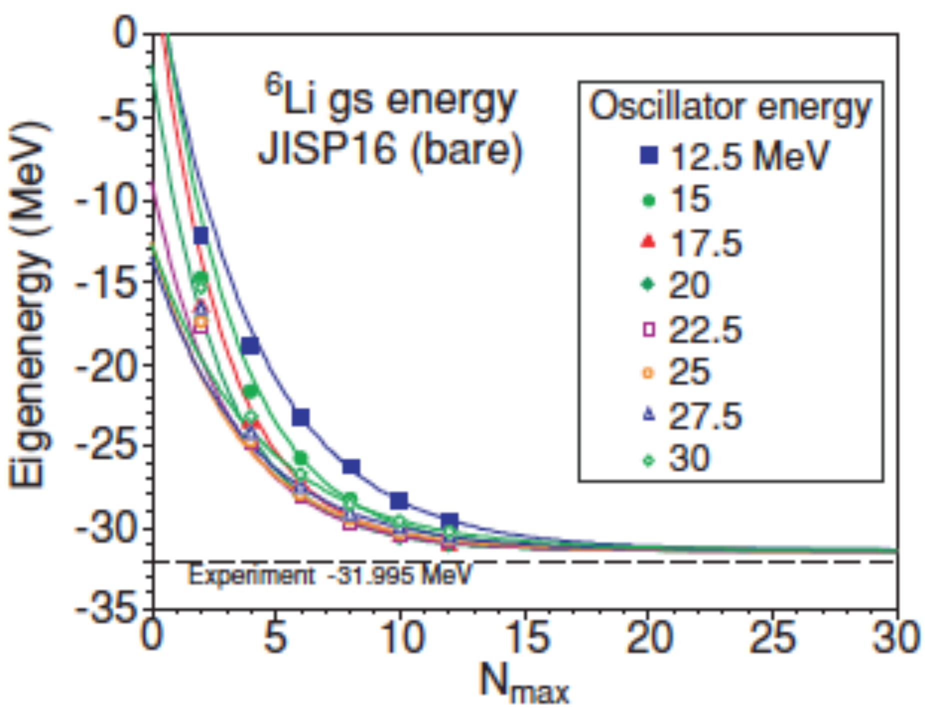
(Received 18 September 2007; published 4 February 2008)



First stage in the development of Extrapolation A

FIG. 6. (Color online) Ground-state binding energy of ^{6}Li calculated with the JISP16 Hamiltonian for different HO frequencies ($\hbar\Omega = 12.5$–30 MeV). The curves are extrapolated using a constrained exponential fit as described in the text.

2008: $N_{max} \leq 12$ used

JISP16: $E_{th} = -31.33(10)$ MeV

Pedagogical example – focus on infrared properties of NCFC

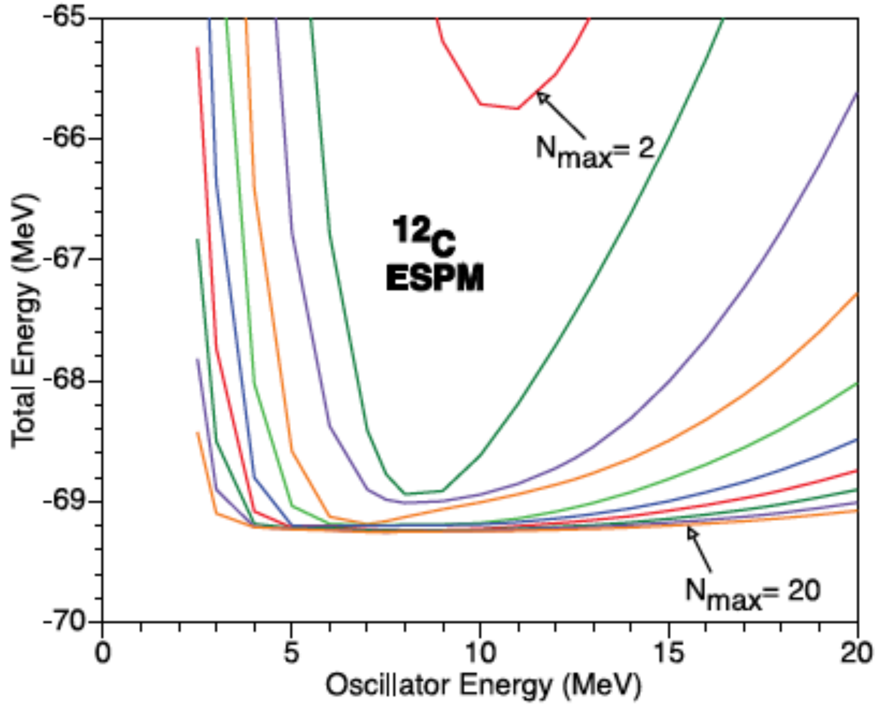


FIG. 4. (Color online) Calculated ground-state energy of ^{12}C in the ESPM as a function of $\hbar\Omega$ and $N_{\rm max}$, the maximum value of the HO states' quanta, $2n + l$, used in expanding the Saxon-Woods single-particle states. The curve closest to convergence corresponds to the value $N_{\rm max} = 20$ and successively higher curves are obtained with $N_{\rm max}$ decreased by 2 units for each curve.

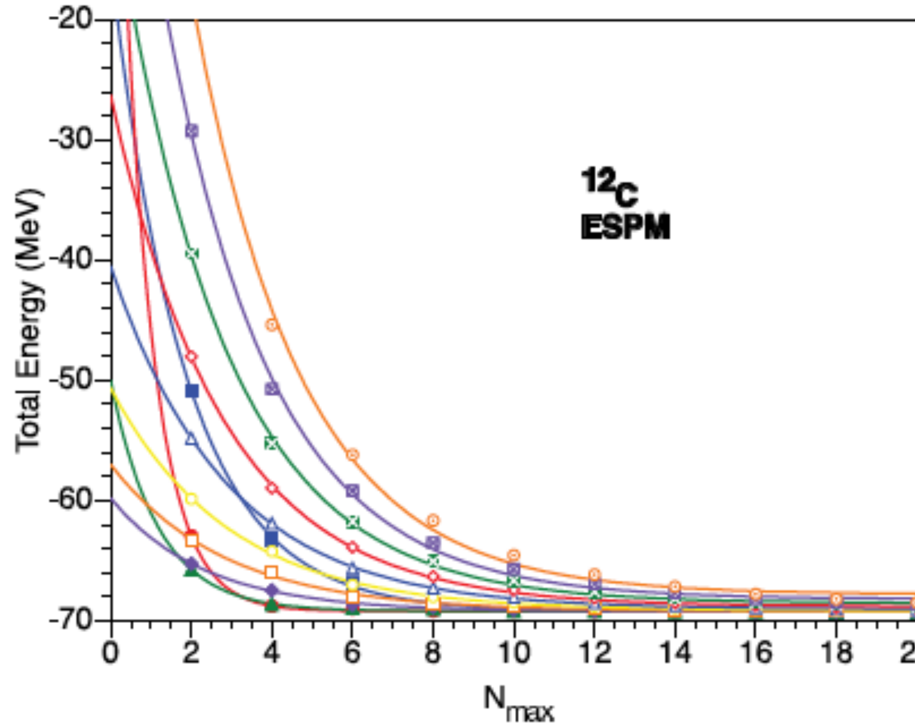


FIG. 5. (Color online) Calculated ground-state energy of ^{12}C in the ESPM as a function of $N_{\rm max}$ for selected values of $\hbar\Omega$ used in defining the basis states. The points correspond to $\hbar\Omega$ values ranging from 5 to 30 MeV in 2.5-MeV increments. The curves represent an exponential plus a constant fit to each set of results at fixed $\hbar\Omega$, excluding the $N_{\rm max} = 0$ result. Each point carries equal weight.

Conclusions: Exponential in N_{max} is very good for IR extrapolation
Alternating points are above/below the fit curve ("odd-even" effect)

P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

Pedagogical example #2 – focus on ultraviolet properties of NCFC

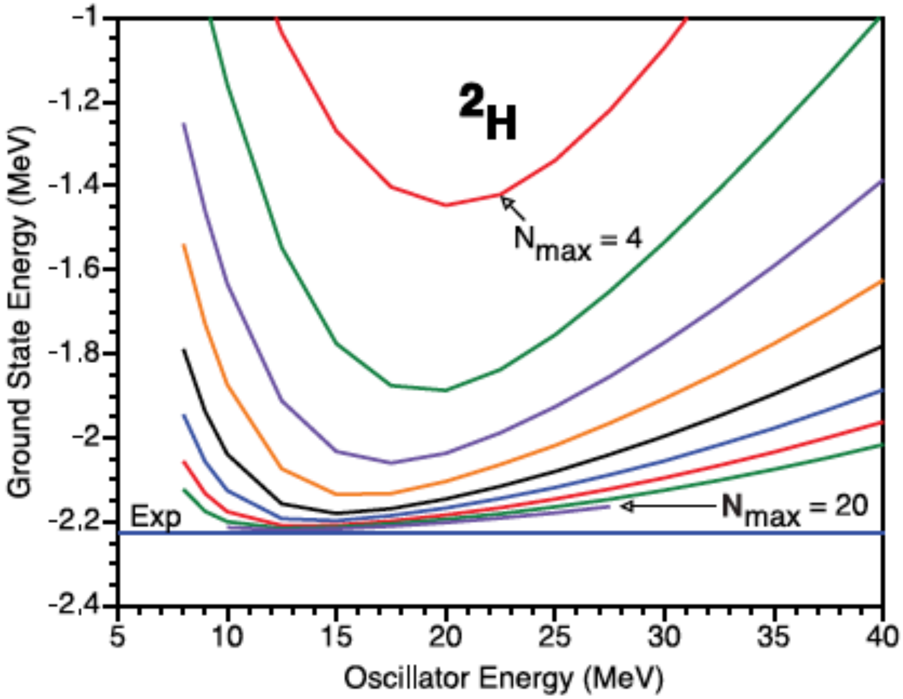


FIG. 6. (Color online) Calculated ground-state energy of ^{2}H as a function of the oscillator energy, $\hbar\Omega$, for selected values of N_{max} used in defining the basis states. The curve closest to experiment corresponds to the value $N_{max} = 20$ and successively higher curves are obtained with N_{max} decreased by two units for each curve. The curves are formed by straight-line segments joining calculated results.

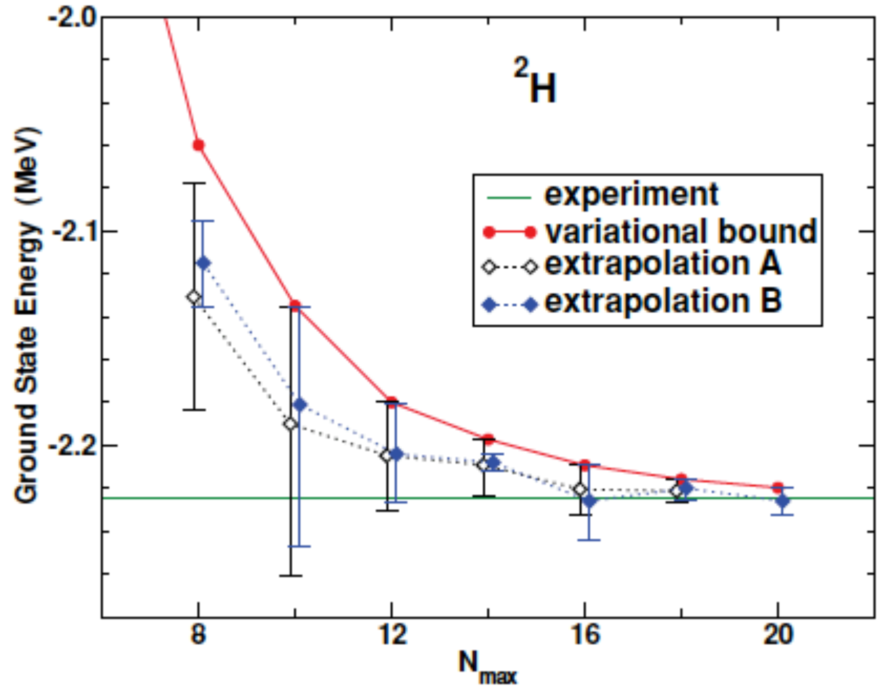


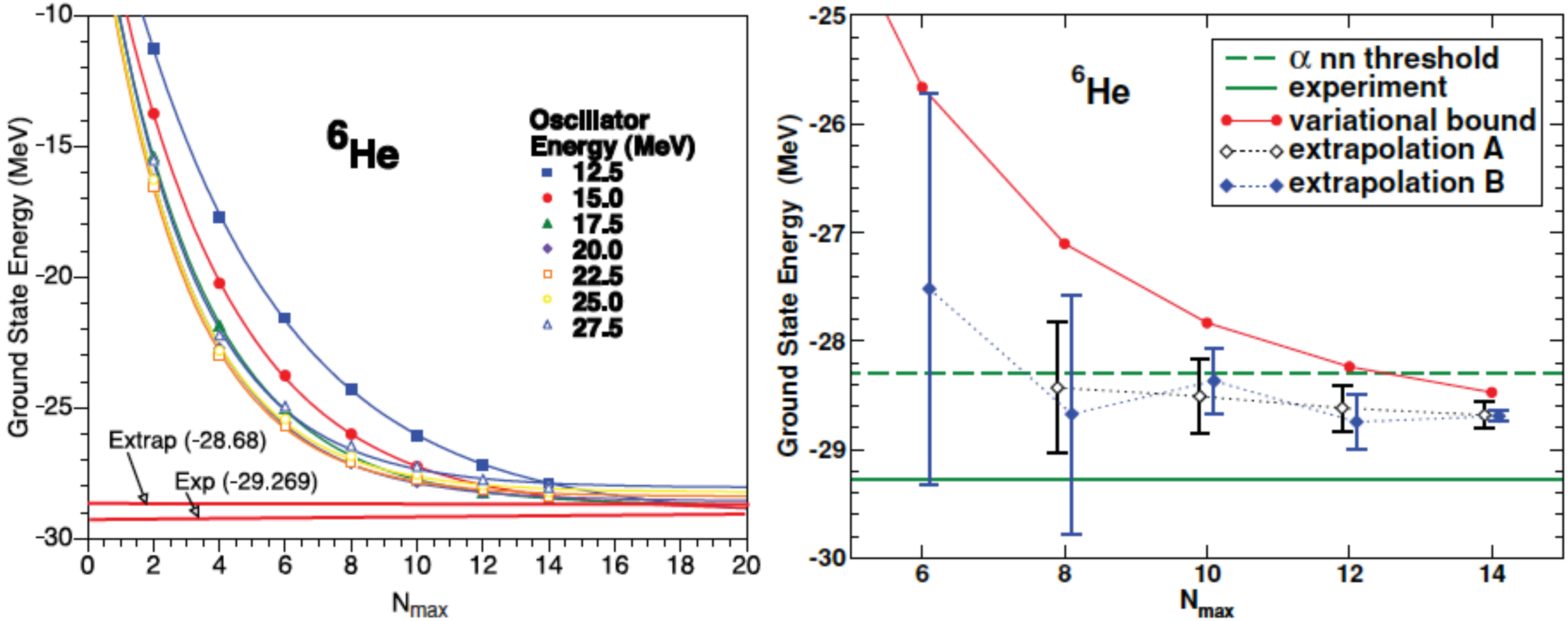
FIG. 8. (Color online) Extrapolated ground-state energies and variational upper bounds from each set of four (extrapolation A) or three (extrapolation B) successive N_{max} values as a function of the largest value of N_{max} in each set. Error bars are dominated by the uncertainties in the extrapolations and are obtained as described in the text. Note the expanded scale and the reasonable consistency of the extrapolated results: for $N_{max} \geqslant 10$ all but one are within their uncertainty range of the exact answer.

Conclusions: Exponential in N_{max} can be improved for UV extrapolation

Note the drift in the extrapolants – though covered by quoted uncertainty

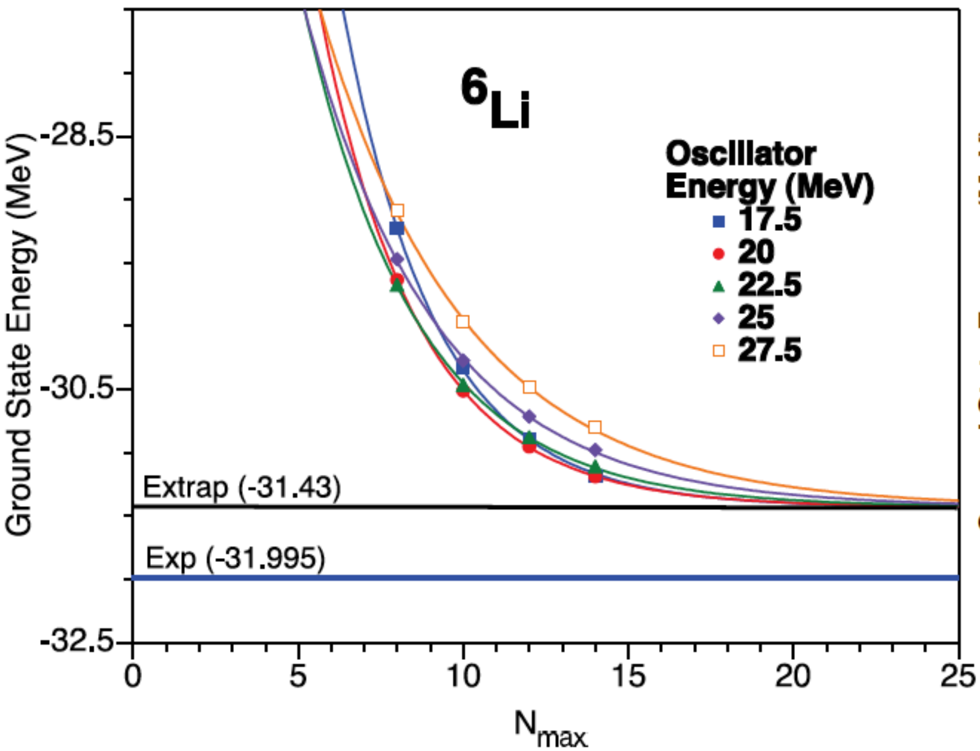
P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

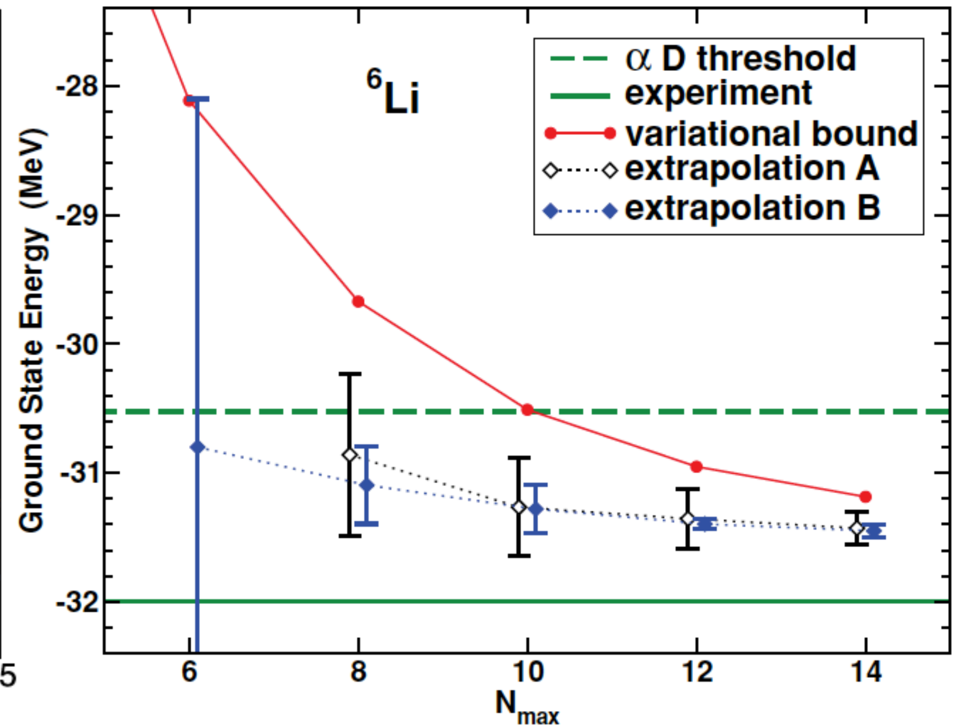
JISP16 NN interaction



P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

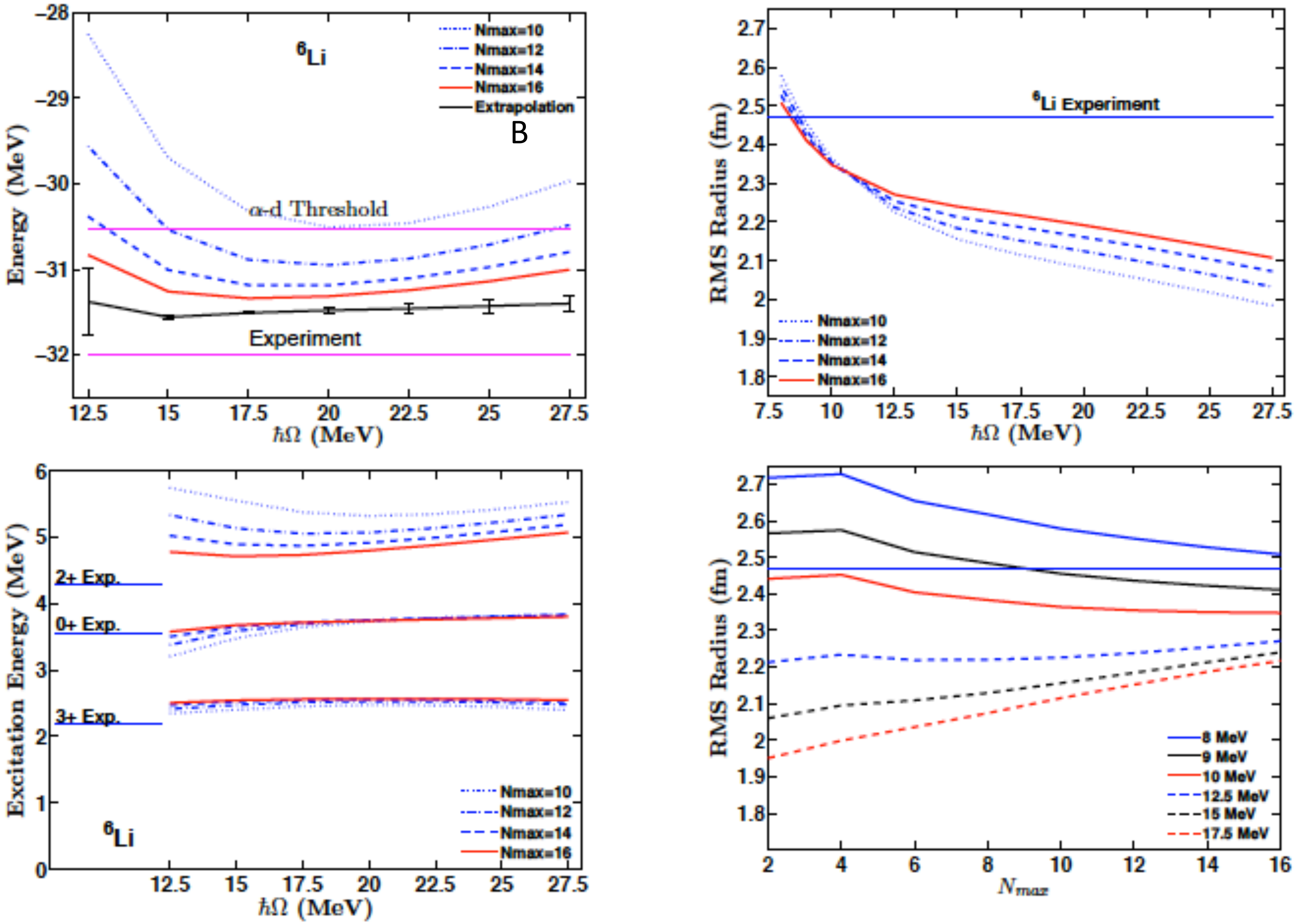
JISP16 NN interaction





Conclude: Extrapolations A and B are each internally consistent (each shows a systematic reduction in uncertainties and consistency with increasing Nmax) and are consistent with each other (A & B consistently overlap at each Nmax)

P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)



C. Cockrell, J.P. Vary and P. Maris, arXiv 1201.0724

No-Core Full Configuration (NCFC) Benchmarks with Hyperspherical Harmonics (HH) JISP16 NN interaction

	NCFC	HH
^{6}Li	-31.47(9)[a] -31.51(1)[b]	-31.46(5)[e]
^{6}He	-28.68(12)[c] -28.69(5)[d]	-28.70(13)[e]

NB: Each is within the quoted uncertainties of the others

[a] Extrap A [Nmax = 16]: P. Maris, A.M. Shirokov and J.P. Vary, Phys. Rev. C81, 021301(R) (2010)

[b] Extrap B [Nmax = 16]: C. Cockrell, J.P. Vary and P. Maris, arXiv:1201.0724

[c] Extrap A [Nmax = 14]: P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

[d] Extrap B [Nmax = 14]: P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C79, 014308 (2009)

[e] Exp Extrap [Kmax = 14]: S. Vaintraub, N. Barnea, D. Gazit, Phys. Rev. C79, 065501 (2009)

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Convergence in the no-core shell model with low-momentum two-nucleon interactions

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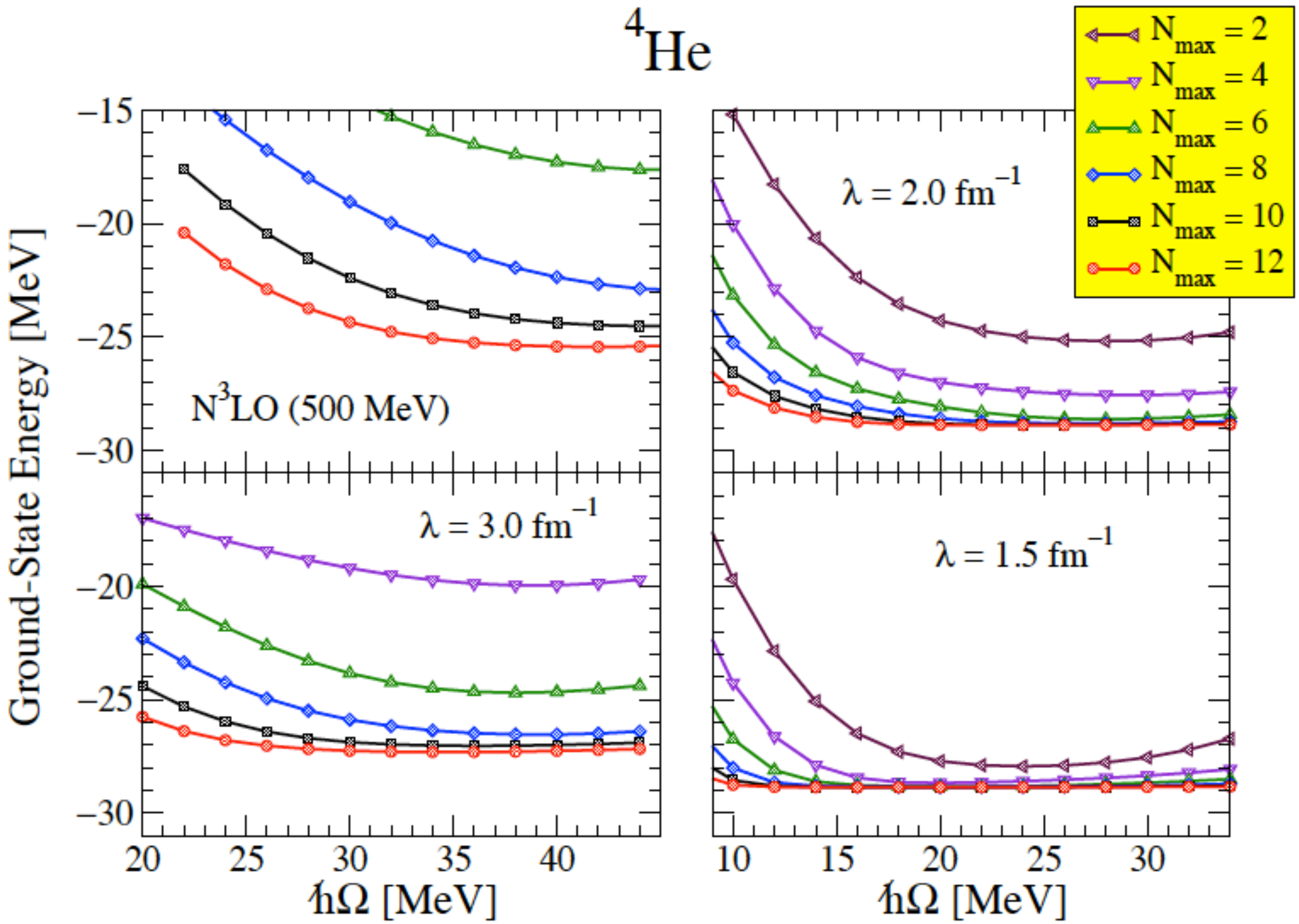
Employs a hybrid of extrapolations A & B

Table 1

Ground-state energies and optimal $\hbar\Omega$ (in MeV) of light nuclei for SRG-evolved potentials. When an uncertainty is given it represents a confidence interval derived from an extrapolation to $N_{\max} = \infty$. Otherwise the energy is converged to the digits shown

λ	^{3}H		^{4}He		^{6}He		^{6}Li		^{7}Li	
	$\hbar\Omega$	E_{gs}	$\hbar\Omega$	E_{gs}	$\hbar\Omega$	E_{gs}	$\hbar\Omega$	E_{gs}	$\hbar\Omega$	E_{gs}
∞	–	−7.85	42	−26.1(8)						
3.0	28	−8.29	34	−27.5(3)	28	−28(1)	28	−31.5(8)	24	−38.7(30)
2.5	24	−8.41	28	−28.2(2)	24	−28.9(3)	24	−32.1(3)	24	−38.7(20)
2.25	22	−8.47	24	−28.6(1)	22	−29.4(2)	22	−32.5(2)	22	−40.3(10)
2.0	18	−8.53	24	−28.90	20	−30.0(1)	20	−33.1(1)	20	−41.2(5)
1.75	16	−8.55	20	−29.13	16	−30.6	18	−33.6	18	−41.7(4)
1.5	12	−8.48	18	−28.86	14	−30.7	16	−33.7	16	−42.0(3)
1.25	10	−8.21	14	−27.58	12	−29.9	12	−32.9	12	−41.1(2)
1.0	8	−7.63	14	−24.80	10	−27.4	10	−30.4	12	−37.8(2)

Improve convergence rate by applying SRG to N3LO



(Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008), arXiv:0708.3754)

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Experiment published: Aug. 3, 2010

Contents lists available at ScienceDirect

Physics Letters B

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First observation of ^{14}F

V.Z. Goldberg [a,*], B.T. Roeder [a], G.V. Rogachev [b], G.G. Chubarian [a], E.D. Johnson [b], C. Fu [c], A.A. Alharbi [a,1], M.L. Avila [b], A. Banu [a], M. McCleskey [a], J.P. Mitchell [b], E. Simmons [a], G. Tabacaru [a], L. Trache [a], R.E. Tribble [a]

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ab initio predictions in close agreement with experiment

TAMU Cyclotron Institute

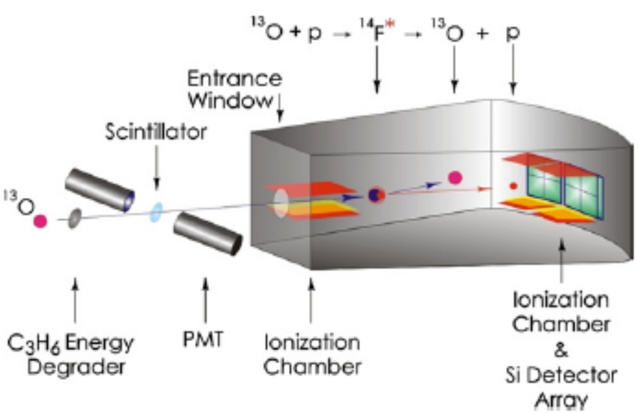

Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

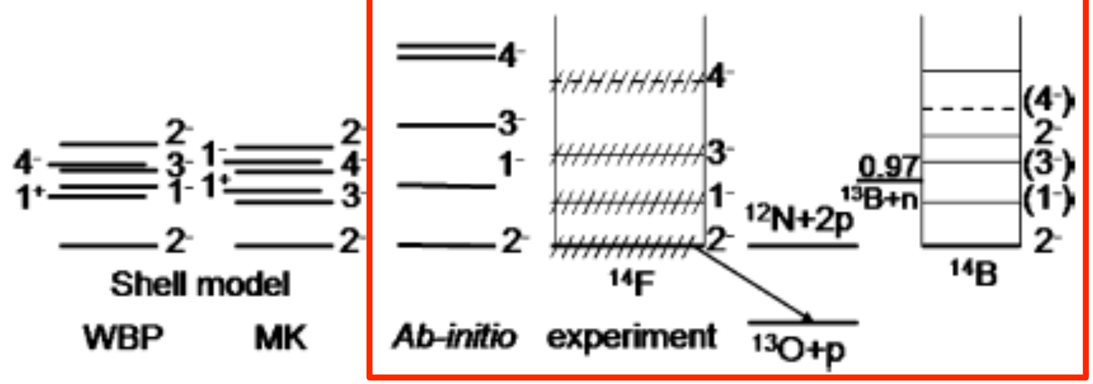

Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Can we do better?

Yes, we can!

Convergence properties of *ab initio* calculations of light nuclei in a harmonic oscillator basis

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PRELIMINARY

Definition of IR and UV parameters characterizing
the harmonic oscillator basis space (note that other definitions are possible)

$$\lambda \equiv \sqrt{\frac{m\omega}{\left(N+3/2\right)\hbar}}$$

= inverse rms radius of state in N+1 HO shell, the adopted IR regulator implicit in the basis

$$\Lambda \equiv \sqrt{\left(N+3/2\right) m\omega/\hbar}$$

= rms momentum of state in N+1 HO shell, a typical UV regulator implicit in the basis

Where N = max(2n+l); n = radial q. #, l = orbital q. #

Conclusion: New extrapolation techniques may prove more robust

Future: additional research needed

- Each observable requires separate analysis for its convergence properties
- Dependence on the Hamiltonian & renormalization (e.g. NN vs NN+NNN)
- Dependence on the adopted basis space cutoff (N_{max} vs N_{shell})

Watch this space for new developments

Thank You!