Daejeon16:
NN interaction for *ab initio* description of light nuclei

Andrey Shirokov
Skobeltsyn Institute of Nuclear Physics,
Moscow State University

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Collaborators:

- James Vary, Peter Maris, Iowa State University (Ames, IA, USA)
- Youngman Kim, Ik Jae Shin, Institute for Basic Science, RISP Project (Daejeon, South Korea)
- A. Mazur, I. Mazur, Pacific National University (Khabarovsk, Russia)
- M. Sosonkina, Old Dominion University (Norfolk, VA, USA)

Nuclear structure

- History of nuclear structure theory is a history of nuclear models (liquid drop model, Hartree–Fock, shell model, collective vibrations and rotations, cluster models, interacting boson model, etc.)
- Modern trend: switching to a model-free (*ab initio*) description of nuclear structure
- This modern trend is based on availability of new modern supercomputers and still restricted to light enough nuclei though extending to heavier systems…

Ab initio structure & *NN* interaction

- Various *effective NN* interactions (Cohen–Kurath, Volkov, etc.) were used historically in nuclear structure. These interactions were fitted to describe a restricted set of nuclei (e.g., *p*-shell nuclei) in a particular model (e.g., shell model) in a very restricted (e.g., $0\hbar\Omega$) model space. Such interactions have nothing to do with *NN* scattering data and deuteron properties
- *Ab initio* theory requires, of course, a realistic *NN* interaction accurately describing *NN* scattering data and deuteron properties

NN interaction

- New history of realistic *NN* interaction starts from 1993: Nijmegen *NN* database and phase shift analysis
- After 1993 various *NN* interactions describing *NN* data with $\chi^2/\text{datum} \approx 1$ have been suggested, in particular:

Meson exchange: Nijmegen I, II; Reid soft core; Argonne AV$_{18}$; CD-Bonn$_{2000}$; INOY (inside non-local, outside Yukawa)

Chiral EFT: N2LO(next-to-next-to-leading-order), N3LO, …

Inverse scattering: JISP6, JISP16, JISP16$_{2010}$

Daejeon16 combines ideas of Chiral EFT and inverse scattering approaches

($\chi^2/\text{datum} > 2$ for pre-1993 *NN* interactions)

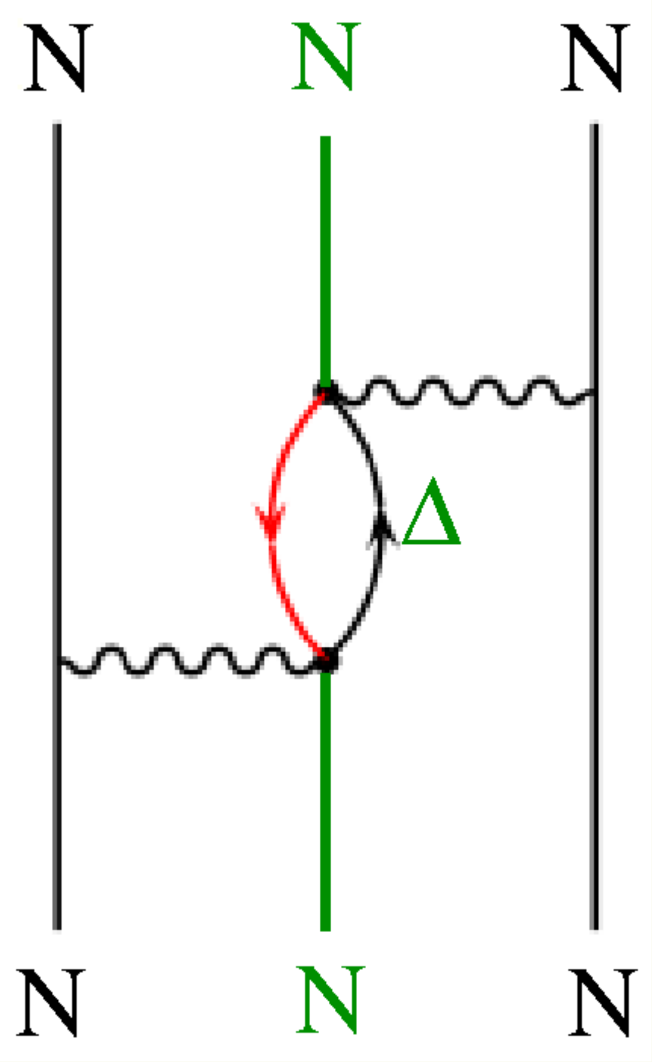
Constructing *NN* interaction

- Two possible ideas:
- (i) Derive ``real'' *NN* interaction from ``first principles'' (from underlying theory)
- (ii) Derive phenomenological *NN* interaction describing various observables including many-body ones
- Usually we have combination of (i) and (ii) (e.g., AV18, fitted parameters, fitted 3-body forces, etc.)

JISP16 & Daejeon16

- Our idea is to construct a *NN* interaction providing a fast convergence of shell model calculations and to get rid from *NNN* force
- We followed the phenomenological route with JISP16 and ``first principle” route with Daejeon16

NNN force



NNN contribution to nuclear observables is small but can be essential.

4*N* and higher forces are usually supposed to be inessential for description of nuclei.

Table of storage requirements for the nonzero matrix elements of the many-body Hamiltonian for a range of applications. The notation TB, PB and EB represent Terabytes (10^{12} bytes), Petabytes (10^{15} bytes) and Exabytes (10^{18} bytes), respectively. Roughly speaking, entries up to 400 TB imply Petascale computational facilities, while entries above 1PB imply Exascale computational facilities will likely be required.

Nucleus	N_{max}	Dimension	2-body	3-body	4-body
^{6}Li	12	$4.9 \cdot 10^6$	0.6 GB	33 TB	590 TB
^{12}C	8	$6.0 \cdot 10^8$	4 TB	180 TB	4 PB
^{12}C	10	$7.8 \cdot 10^9$	80 TB	5 PB	140 PB
^{16}O	8	$9.9 \cdot 10^8$	5 TB	300 TB	5 PB
^{16}O	10	$2.4 \cdot 10^{10}$	230 TB	12 PB	350 PB
^{8}He	12	$4.3 \cdot 10^8$	7 TB	300 TB	7 PB
^{11}Li	10	$9.3 \cdot 10^8$	11 TB	390 TB	10 PB
^{14}Be	8	$2.8 \cdot 10^9$	32 TB	1100 TB	28 PB
^{20}C	8	$2 \cdot 10^{11}$	2 PB	150 PB	6 EB
^{28}O	8	$1 \cdot 10^{11}$	1 PB	56 PB	2 EB

Role of *NNN* force?

- W. Polyzou and W. Glöckle theorem (Few-body Syst. **9**, 97 1990)):

  $H=T+V_{ij} \rightarrow H'=T+V'_{ij}+V_{ijk}$,

  where V_{ij} and V'_{ij} are phase-equivalent, H and H' are isospectral.

  Hope:

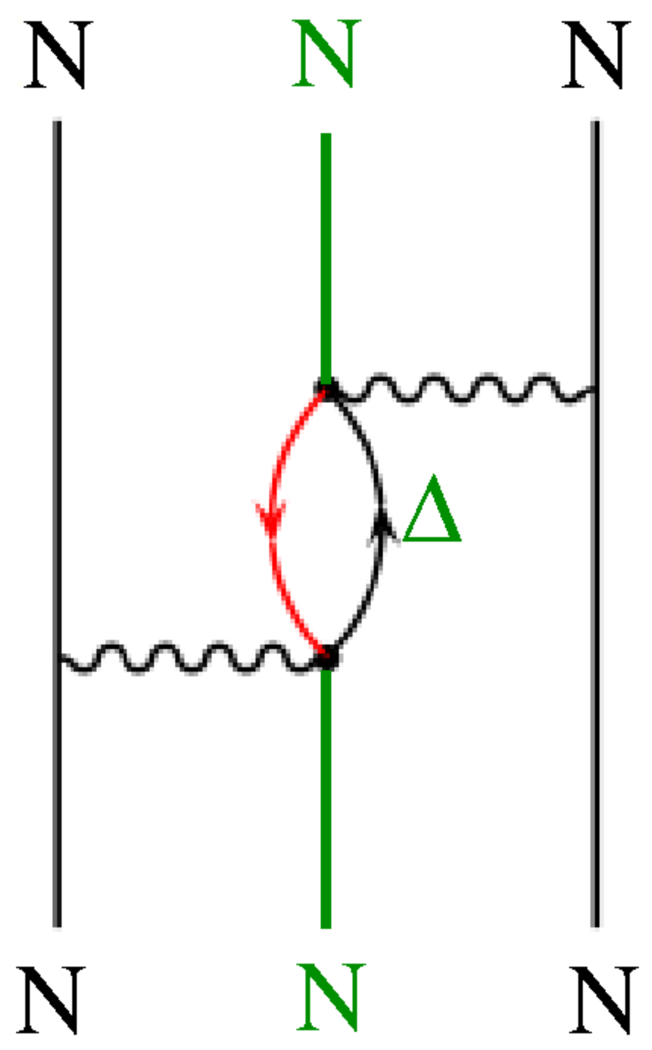
  $H'=T+V'_{ij}+V_{ijk} \rightarrow H=T+V_{ij}$

  with (approximately) isospectral H and H' .

JISP type interaction seems to be *NN* interaction minimizing *NNN* force.

Without *NNN* force calculations are simpler, calculations are faster, larger model spaces become available; hence predictions are more reliable.

NNN force



Peter Sauer: ``*NNN* force is only a baby of theoreticians who would like to work in a restricted Hilbert space", i.e., avoiding Δ isobar and other excited nucleon degrees of freedom

From this point of view, JISP and Daejeon16 *NN* interactions are an attempt to describe nuclei with nucleon degrees of freedom only

Historical evolution

- End of 1990th: ^{6}He = $\alpha+n+n$; PET for $n\alpha$ interaction to fit ^{6}He binding
- 2000th: why not to do the same with *NN* interaction?
- Use of inverse *J*-matrix theory to construct *NN* interaction providing fast convergence of many-body calculations
- Fitting deuteron rms radius and quadrupole moment by PET: good ^{3}H and ^{4}He bindings
- Fitting *p* waves to ^{6}Li spectrum: JISP6 manually
- Additional fitting *p* waves to ^{16}O binding: JISP16 manually
- More accurate fit to light nuclei (extrapolations, larger model spaces): JISP16$_{2010}$ newuoa
- Daejeon16 from SRG-evolved N3LO (extrapolations, large model spaces) pounders

Daejeon16:

- PETting SRG-evolved N3LO to obtain description of *p*-shell nuclei without *NNN*
- Idea: SRG induces *NNN*; let us search for PETs which induce additional *NNN* cancelling SRG-induced and intrinsic *NNN*s

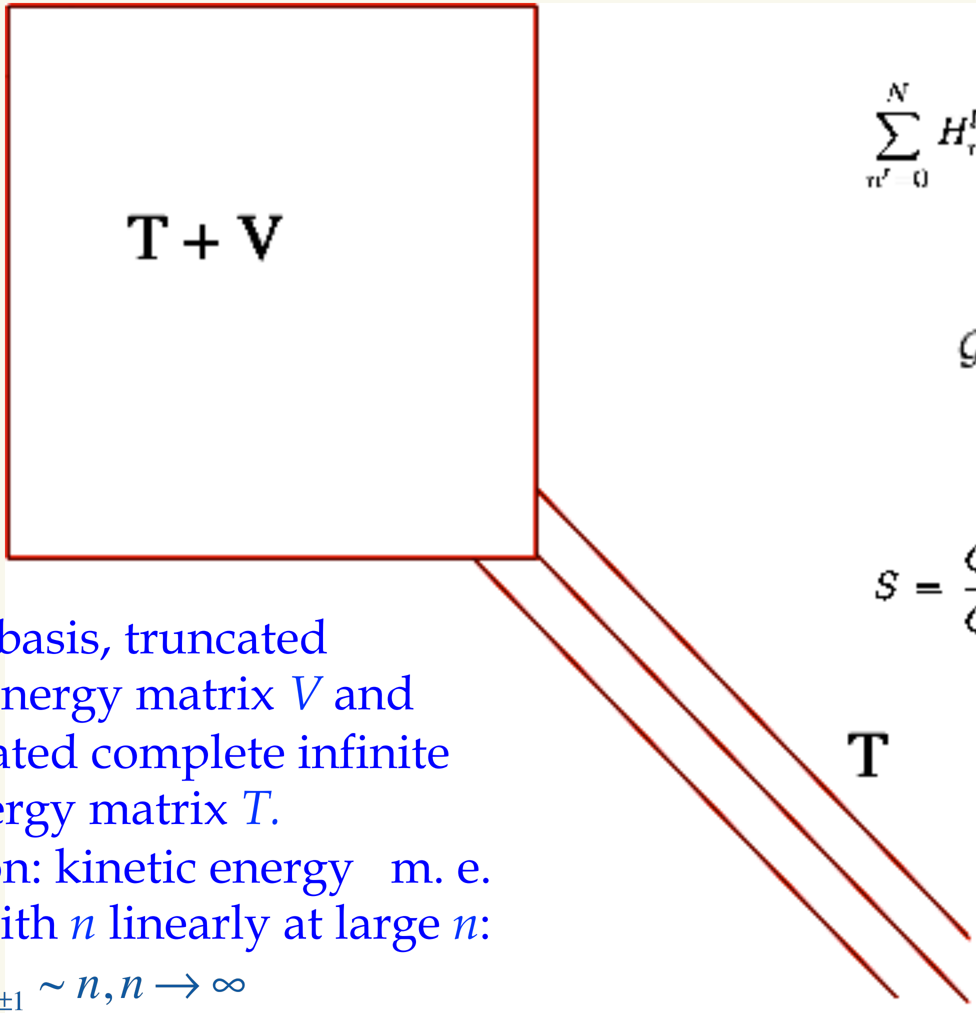
pounders

NN interaction: JISP summary

- JISP is *J*-matrix inverse scattering potential
- JISP interaction is completely phenomenological
- JISP provides a high-quality description of *NN* data: χ^2/datum = 1.03 up to E_{lab} = 350 MeV for the 1992 np data base
- JISP provides a good convergence of many-body calculations, eff. interaction is not needed
- No need of *NNN*
- JIPS interactions were fitted to describe light nuclei: JISP6 up to $A = 6$, JISP16 up to $A = 16$

J-matrix formalism:

scattering in the oscillator basis



$$\sum_{n'=0}^{N} H^{l}_{nn'}\langle n'|\lambda\rangle = E_\lambda\langle n|\lambda\rangle, \qquad n \le N.$$

$$\mathcal{G}_{NN}(E) = -\sum_{\lambda=0}^{N} \frac{\langle N|\lambda\rangle^2}{E_\lambda - E},$$

$$S = \frac{C^{(-)}_{Nl}(q) - \mathcal{G}_{NN}(E)\,T^{l}_{N,\,N+1}\,C^{(-)}_{N+1,\,l}(q)}{C^{(+)}_{Nl}(q) - \mathcal{G}_{NN}(E)\,T^{l}_{N,\,N+1}\,C^{(+)}_{N+1,\,l}(q)},$$

Oscillator basis, truncated potential energy matrix *V* and non-truncated complete infinite kinetic energy matrix *T*.
Justification: kinetic energy m. e. increase with *n* linearly at large *n*:
$T_{nn} \sim n, T_{n,n\pm1} \sim n, n \to \infty$
while potential energy m. e. V_{nm} decrease with *n* and *m*.

Both direct and inverse scattering *J*-matrix solutions are possible.

JISP *NN* interaction

- *NN* interaction is a small matrix of the in the oscillator basis with $\hbar\Omega = 40$ MeV:

  $9\hbar\Omega$ truncation, i.e. in each partial wave oscillator quanta $2n+l \leq 9$: 5×5 matrix in *s* (l=0) and *p* (l=1) waves; 4×4 matrix in *d* (l=2) and *f* (l=3) waves; etc.; in coupled waves dimensionalities are summed, e.g., 9×9 matrix in coupled *sd* waves, etc.
- This structure provides a good description of *NN* data and fast convergence of shell model calculations

JISP16 properties

- 1992 *np* data base (2514 data): χ^2/datum = 1.03
- 1999 *np* data base (3058 data): χ^2/datum = 1.05

Thanks to
R. Machleidt for
these numbers!

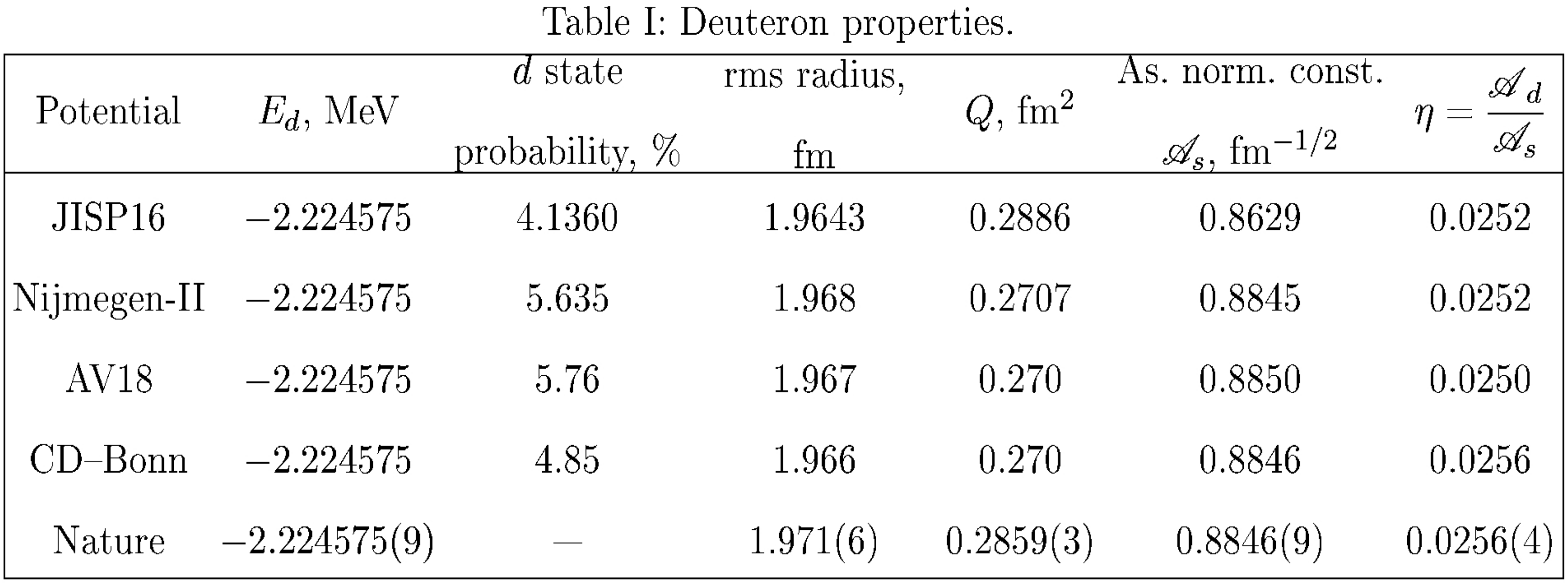
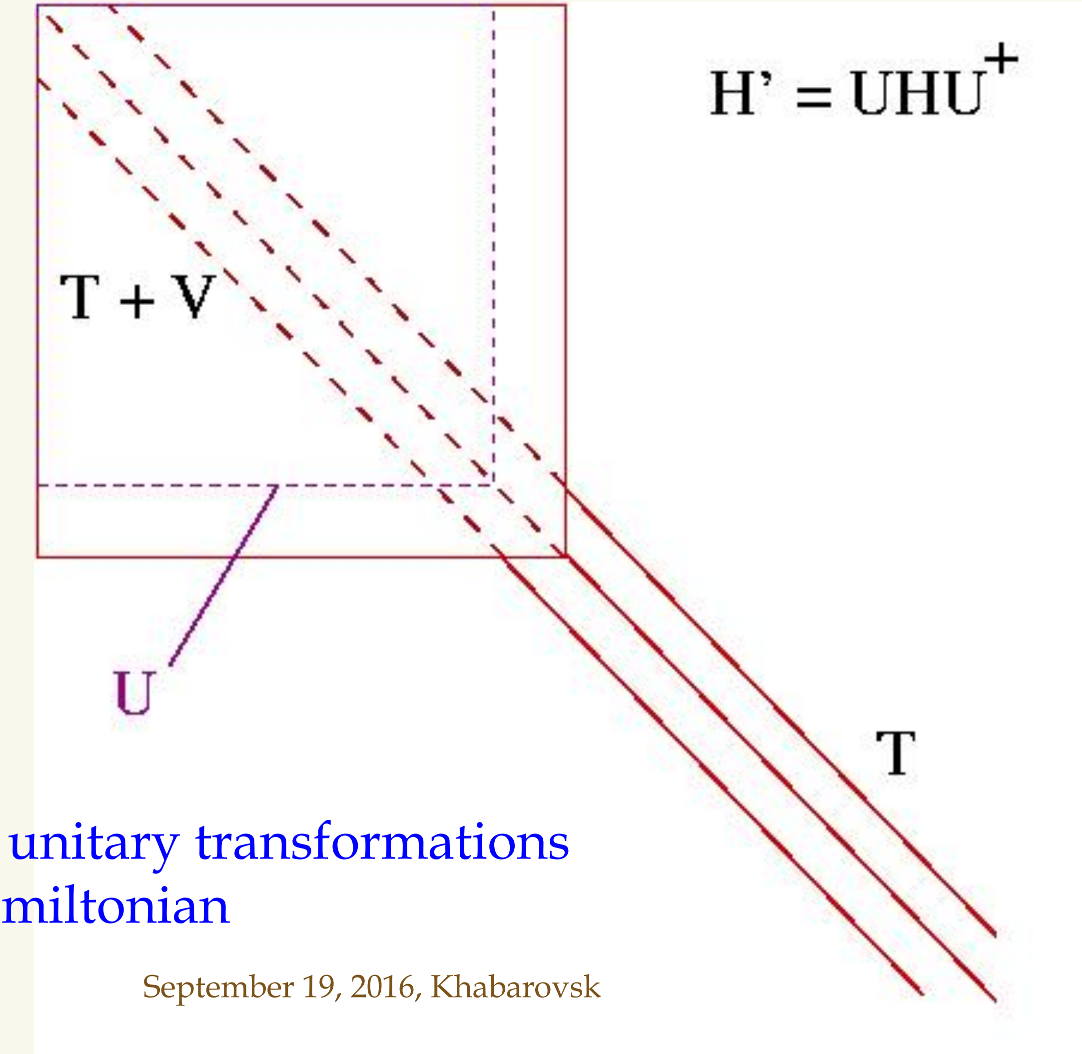


Table I: Deuteron properties.

Potential	E_d, MeV	d state probability, %	rms radius, fm	Q, fm^2	As. norm. const. $\mathscr{A}_s$, fm$^{-1/2}$	$\eta = \frac{\mathscr{A}_d}{\mathscr{A}_s}$
JISP16	-2.224575	4.1360	1.9643	0.2886	0.8629	0.0252
Nijmegen-II	-2.224575	5.635	1.968	0.2707	0.8845	0.0252
AV18	-2.224575	5.76	1.967	0.270	0.8850	0.0250
CD–Bonn	-2.224575	4.85	1.966	0.270	0.8846	0.0256
Nature	$-2.224575(9)$	—	1.971(6)	0.2859(3)	0.8846(9)	0.0256(4)

Phase-equivalent transformations (PETs)



PETs are generated by unitary transformations of the two-nucleon Hamiltonian

Ambiguity of JISP interaction

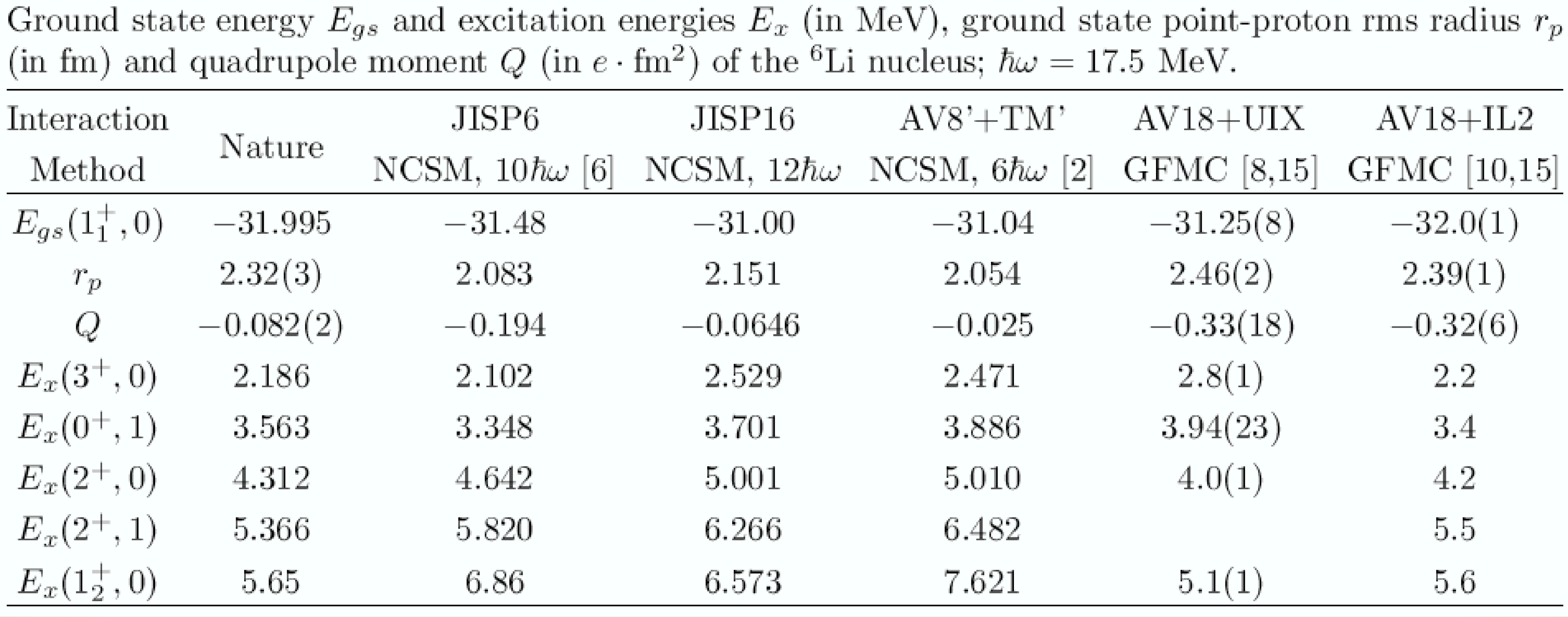
- Any unitary transformation of *NN* Hamiltonian *H* generates a phase-equivalent transformation (PET). Hence the *NN* interaction obtained by *J*-matrix inverse scattering technique is ambiguous.
- This ambiguity is used to fit JISP *NN* interaction to the properties of light nuclei in No-core Shell Model (NCSM) calculations.
- First, the simplest tridiagonal *NN* interaction is constructed fitting *NN* scattering. Next, the simplest PETs with continuous parameters are used in NCSM fit of light nuclei. These PETs are generated by the unitary transformations of the type of rotations mixing the lowest oscillator states in each partial wave:

$$\widetilde{[H]}=[U][H][U^{\dagger}]$$

$$[U]=[U_0]\oplus[I]=\begin{bmatrix} [U_0] & 0 \\ 0 & [I] \end{bmatrix}$$

$$[U_0]=\begin{bmatrix} \cos\beta & +\sin\beta \\ -\sin\beta & \cos\beta \end{bmatrix}$$

JISP16 results



Ground state energy E_{gs} and excitation energies E_x (in MeV), ground state point-proton rms radius r_p (in fm) and quadrupole moment Q (in $e \cdot \mathrm{fm}^2$) of the ^{6}Li nucleus; $\hbar\omega = 17.5$ MeV.

Interaction Method	Nature	JISP6 NCSM, $10\hbar\omega$ [6]	JISP16 NCSM, $12\hbar\omega$	AV8'+TM' NCSM, $6\hbar\omega$ [2]	AV18+UIX GFMC [8,15]	AV18+IL2 GFMC [10,15]
$E_{gs}(1_1^+,0)$	-31.995	-31.48	-31.00	-31.04	$-31.25(8)$	$-32.0(1)$
r_p	2.32(3)	2.083	2.151	2.054	2.46(2)	2.39(1)
Q	$-0.082(2)$	-0.194	-0.0646	-0.025	$-0.33(18)$	$-0.32(6)$
$E_x(3^+,0)$	2.186	2.102	2.529	2.471	2.8(1)	2.2
$E_x(0^+,1)$	3.563	3.348	3.701	3.886	3.94(23)	3.4
$E_x(2^+,0)$	4.312	4.642	5.001	5.010	4.0(1)	4.2
$E_x(2^+,1)$	5.366	5.820	6.266	6.482		5.5
$E_x(1_2^+,0)$	5.65	6.86	6.573	7.621	5.1(1)	5.6

^{10}B

Potential	Nature	JISP16	AV8'+TM'	AV18+IL2	ChPT
Approach		NCSM, $8\hbar\omega$[a]	NCSM, $4\hbar\omega$[b]	GFMC[c]	NCSM, $6\hbar\omega$[d]
$E_{gs}(3_1^+,0)$	-64.751	-60.14	-60.57	$-65.6(5)$	-64.78
r_p	2.30(12)	2.168	2.168	2.33(1)	2.197
Q	+8.472(56)	6.484	+5.682	+9.5(2)	+6.327
$E_x(1_1^+,0)$	0.718	0.555	0.340	0.9	0.523
$E_x(0^+,1)$	1.740	1.202	1.259		1.279
$E_x(1_2^+,0)$	2.154	2.379	1.216		1.432
$E_x(2_1^+,0)$	3.587	3.721	2.775	3.9	3.178
$E_x(3_2^+,0)$	4.774	6.162	5.971		6.729
$E_x(2_1^+,1)$	5.164	5.049	5.182		5.315
$E_x(2_2^+,0)$	5.92	5.548	3.987		4.835
$E_x(4^+,0)$	6.025	5.775	5.229	5.6	5.960
$E_x(2_2^+,1)$	7.478	7.776	7.491		7.823
$B(E2;1_1^+0 \to 3_1^+0)$	4.13(6)	3.317	1.959		3.05
$B(E2;1_2^+0 \to 3_1^+0)$	1.71(26)	0.627	1.010		0.50
$B(\mathrm{GT};3_1^+0 \to 2_1^+1)$	0.083(3)	0.042	0.066		0.07
$B(\mathrm{GT};3_1^+0 \to 2_2^+1)$	0.95(13)	1.652	1.291		1.22

[a] A.M.Shirokov, J.P.Vary, A.I.Mazur, T.A.Weber, Phys. Lett. **B644**, 33 (2007).

[b] P. Navrátil, W. E. Ormand, Phys. Rev. **C 68**, 034305 (2003).

[c] S. C. Pieper, K. Varga, R. B. Wiringa, Phys. Rev. **C 66**, 044310 (2002).

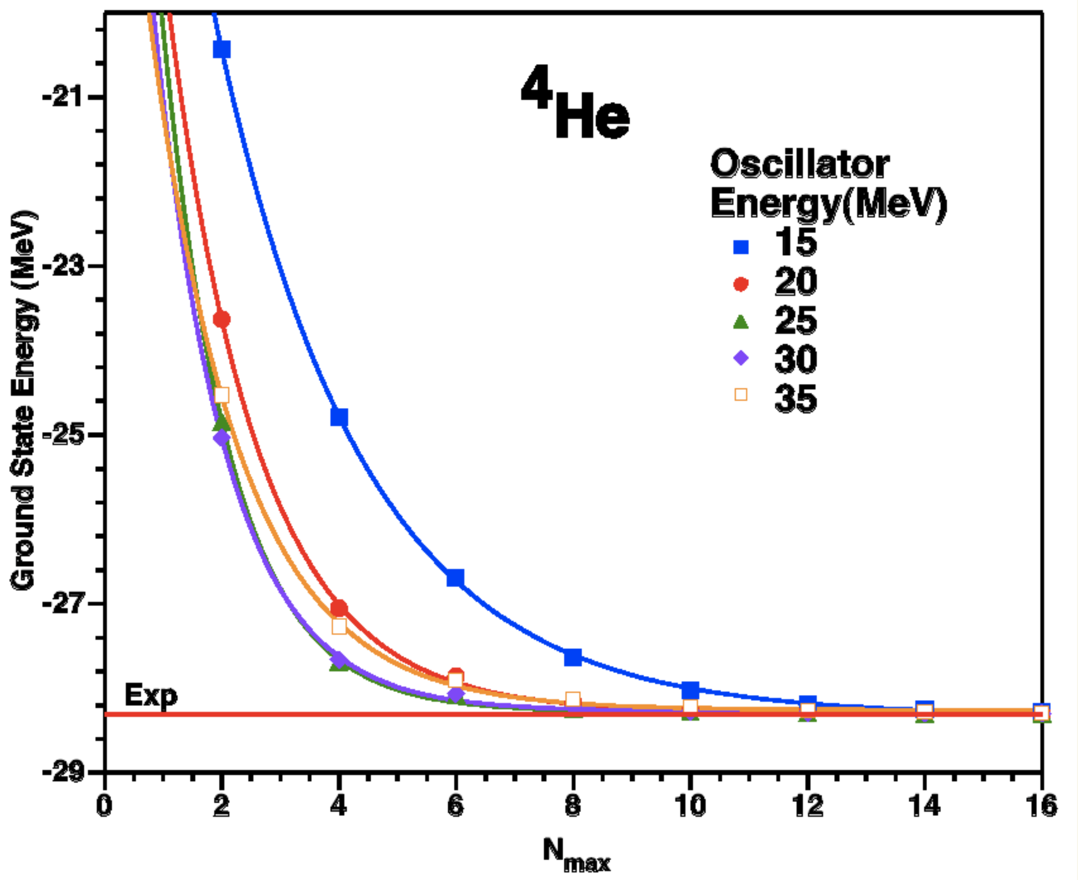
[d] P. Navrátil, V. G. Gueorguiev, J. P. Vary, W. E. Ormand, A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007).

Extrapolations

- Extrapolation:

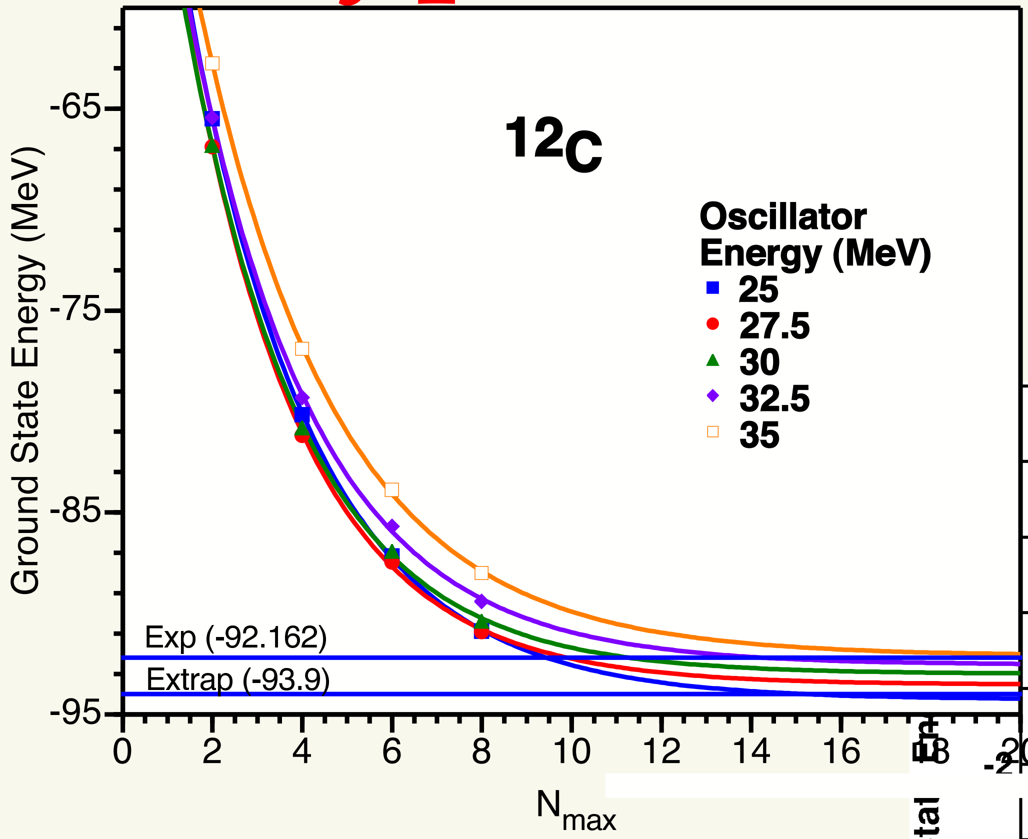
$$E_{gs}(N_{max}) = ae^{-bN\text{max}} + E_{gs}(\infty)$$

- Works with bare interaction only (e.g., JISP16)
- Example:



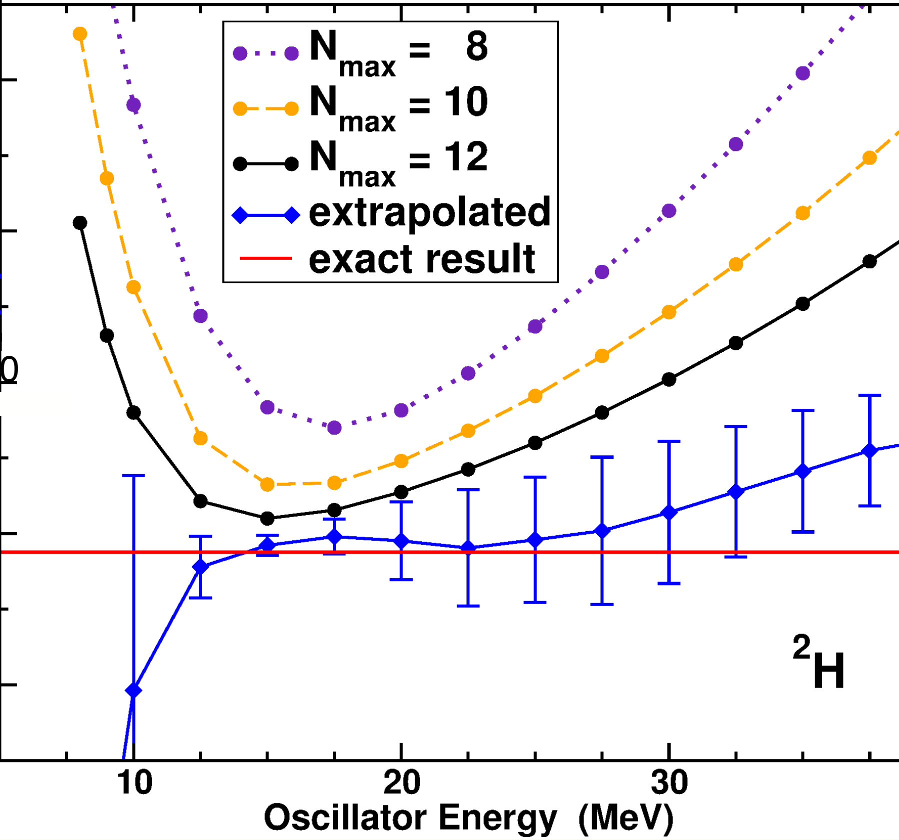
P. Maris, J. P. Vary, A. M. Shirokov, Phys. Rev. C 79, 014308 (2009)

2 types of extrapolations



Global (A)

Local (B)

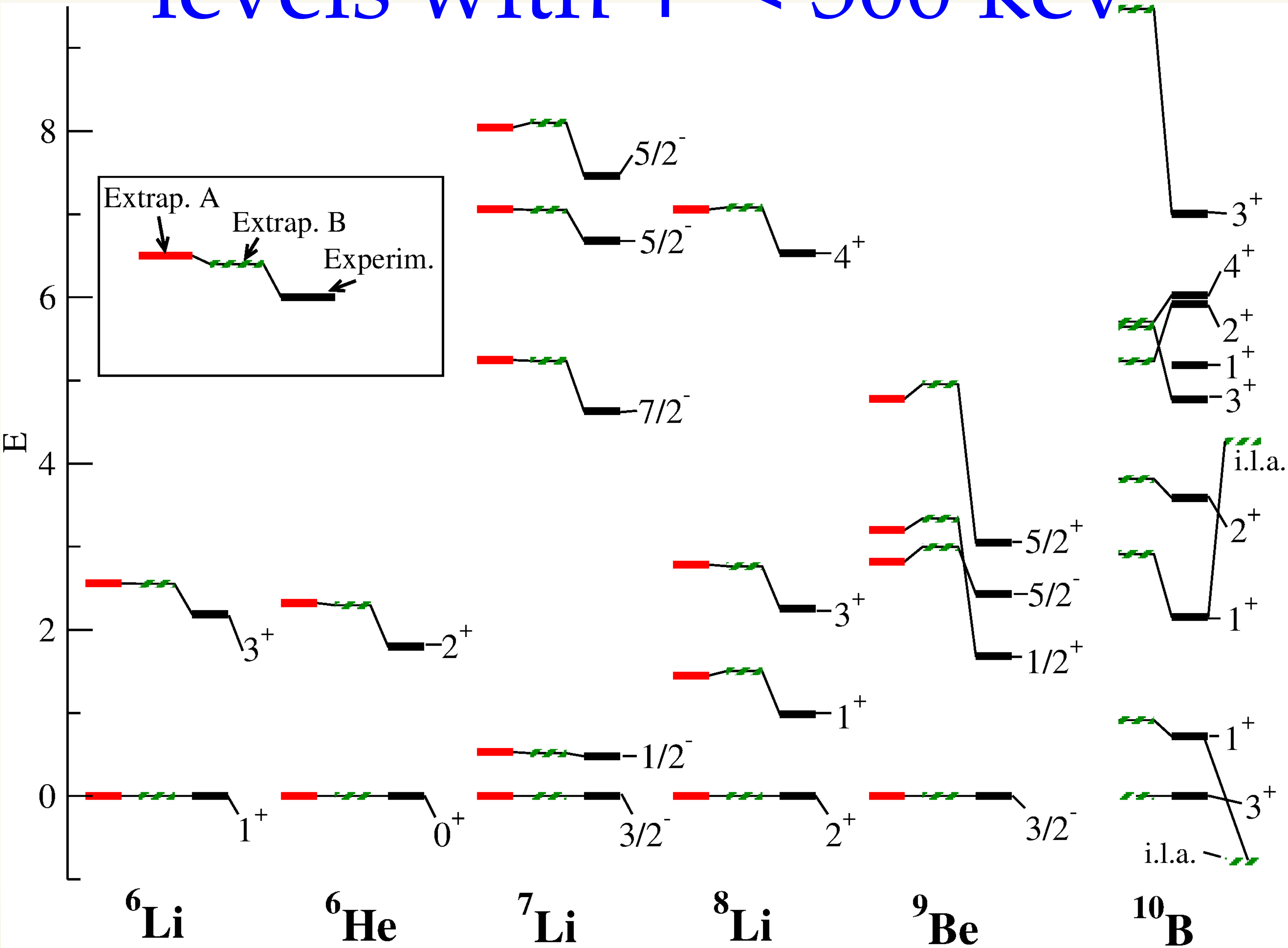


Uncertainties of extrapolations!

Other extrapolations

- Other extrapolation techniques were suggested recently:
- 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)
- R. J. Furnstahl, G. Hagen, and T. Papenbrock, Phys. Rev. C 86, 031301(R) (2012)
- ………………..
- These extrapolations does not seem to work better according to our analysis of 135 states in 26 *s*- and *p*-shell nuclei obtained in NCSM with JISP16 (A. M. Shirokov, V. A. Kulikov, P. Maris, and J. P. Vary, in *NN and 3N interactions*, eds. L. Blokhintsev and I. Strakovsky, Nova Science Publishers, 2014, p. 231).

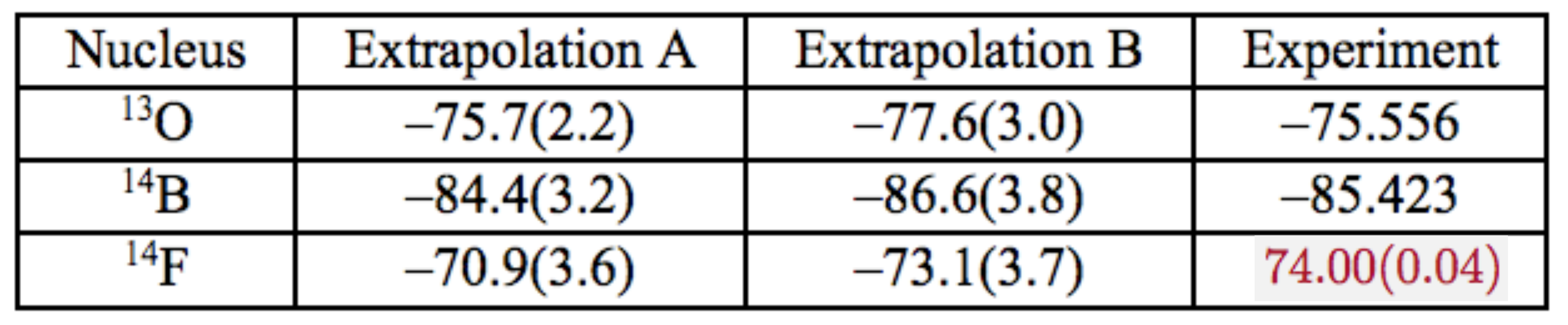
Extrapolations & JISP16: levels with Γ < 300 kev



Success of NCSM calculations with JISP16 interaction and extrapolations: Predictions of ^{14}F properties (2009)

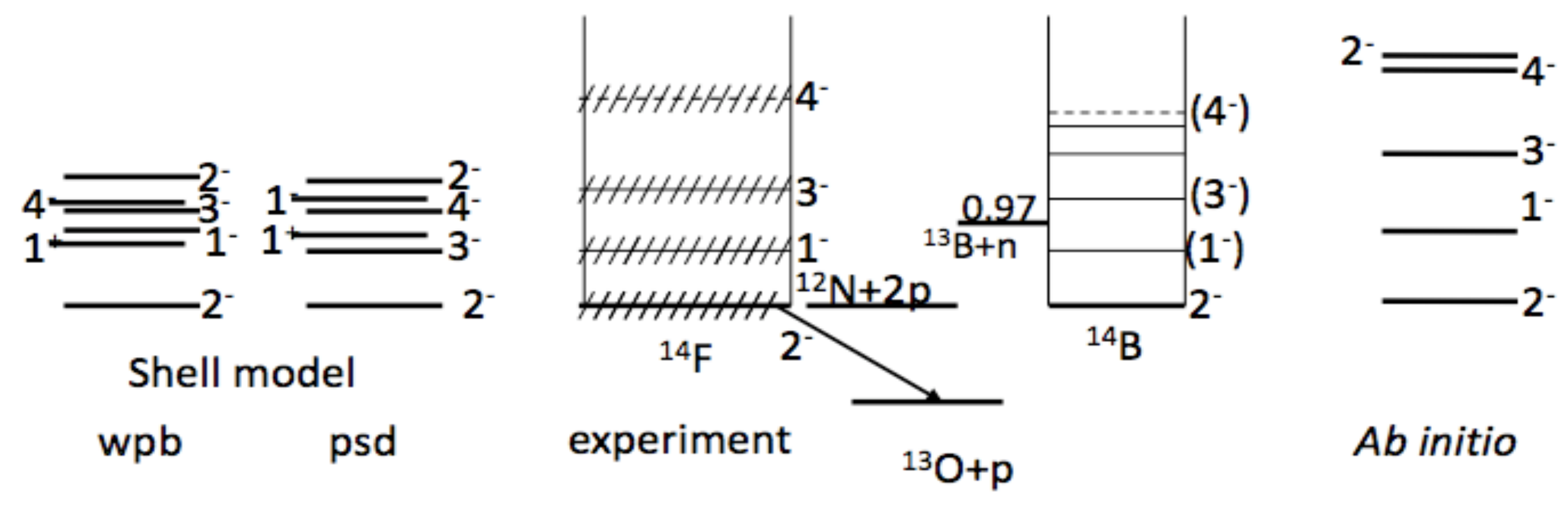
^{14}F

- 1,990,061,078 basis states in $N_{max} = 8$ model space
- each $\hbar\Omega$ point requires 2 to 3 hours on 7,626 quad-core compute nodes (30,504 processors in total) at the Jaguar supercomputer at ORNL



Nucleus	Extrapolation A	Extrapolation B	Experiment
^{13}O	–75.7(2.2)	–77.6(3.0)	–75.556
^{14}B	–84.4(3.2)	–86.6(3.8)	–85.423
^{14}F	–70.9(3.6)	–73.1(3.7)	74.00(0.04)

^{14}F spectrum



Summary of JISP16 results

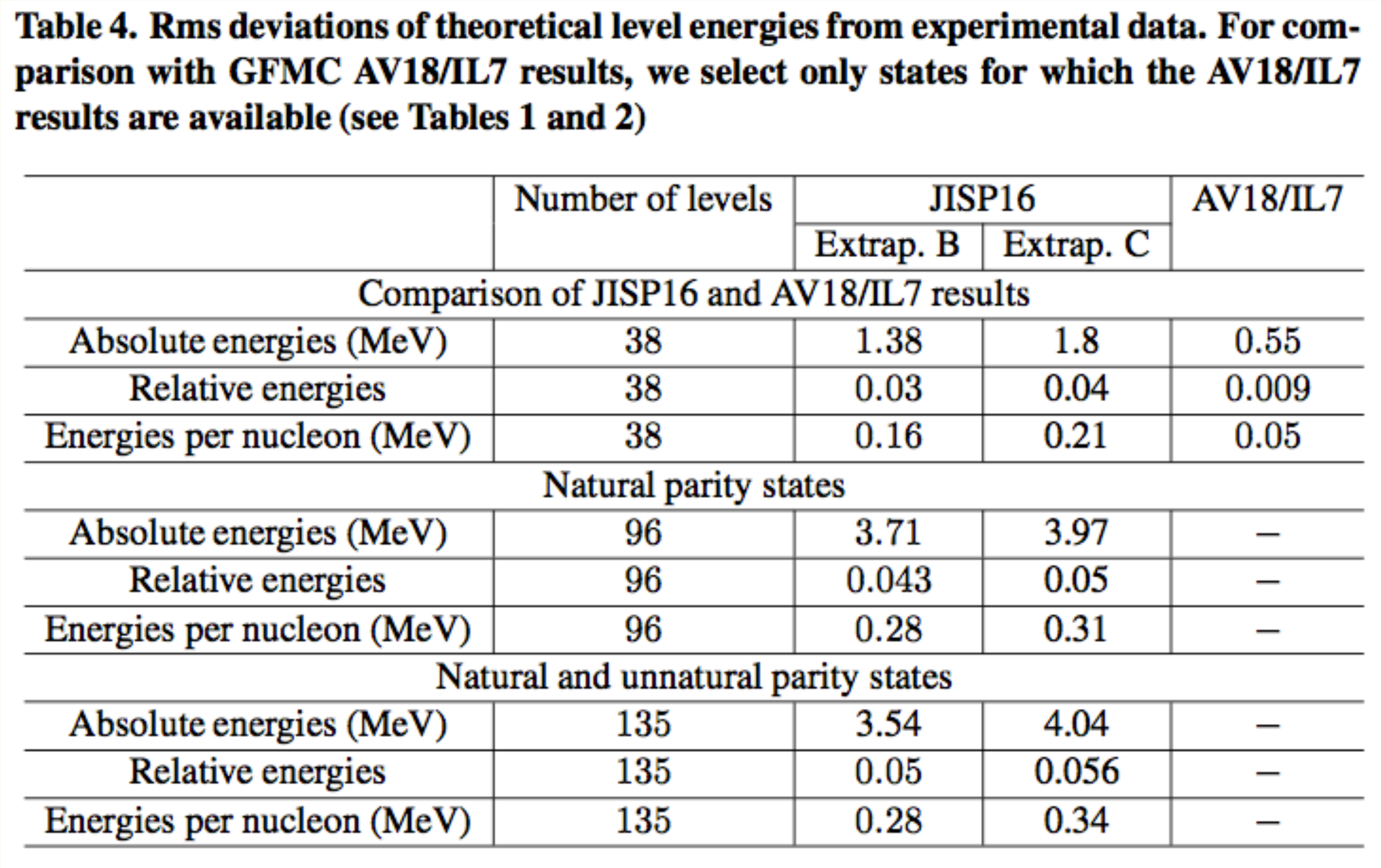
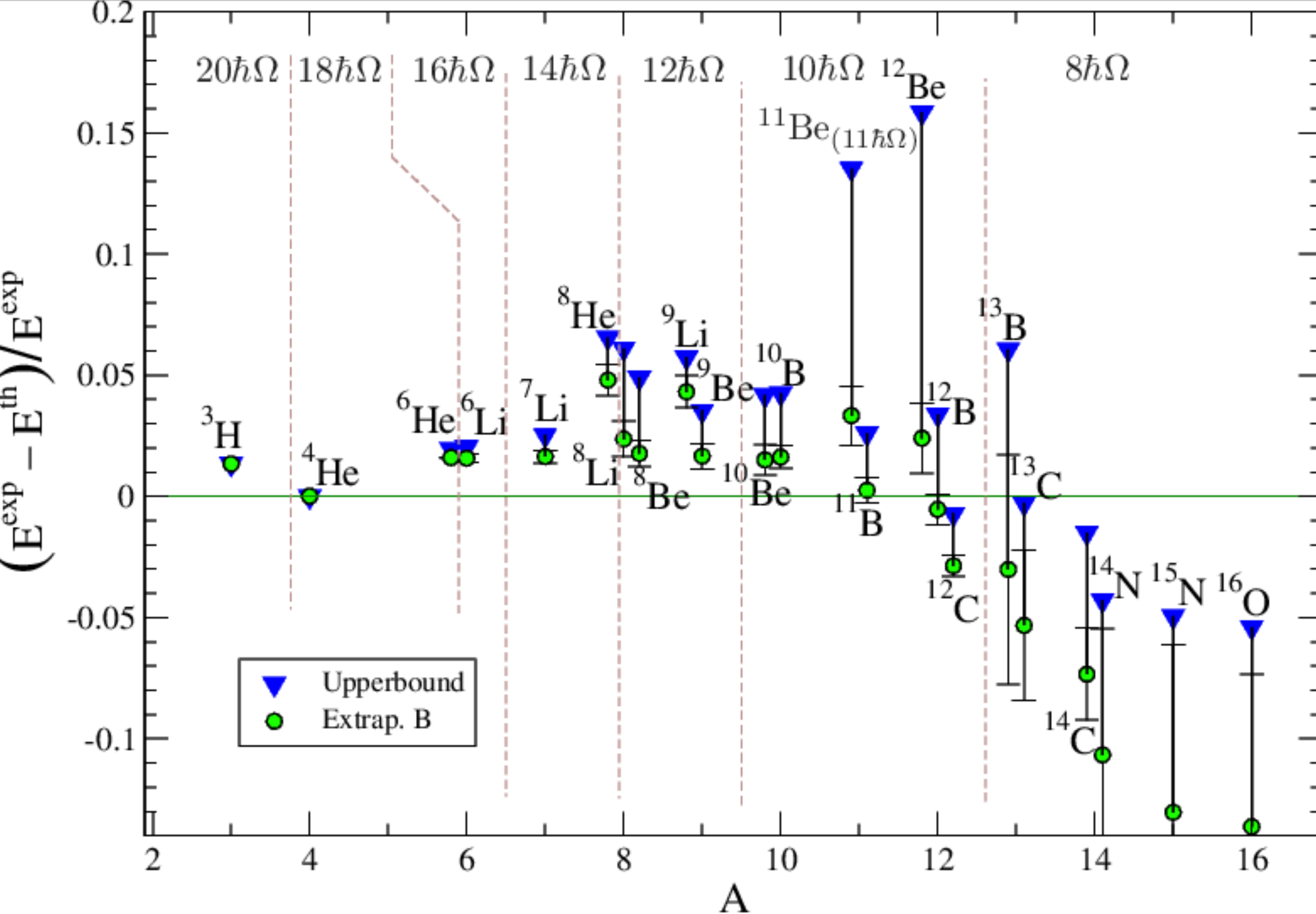


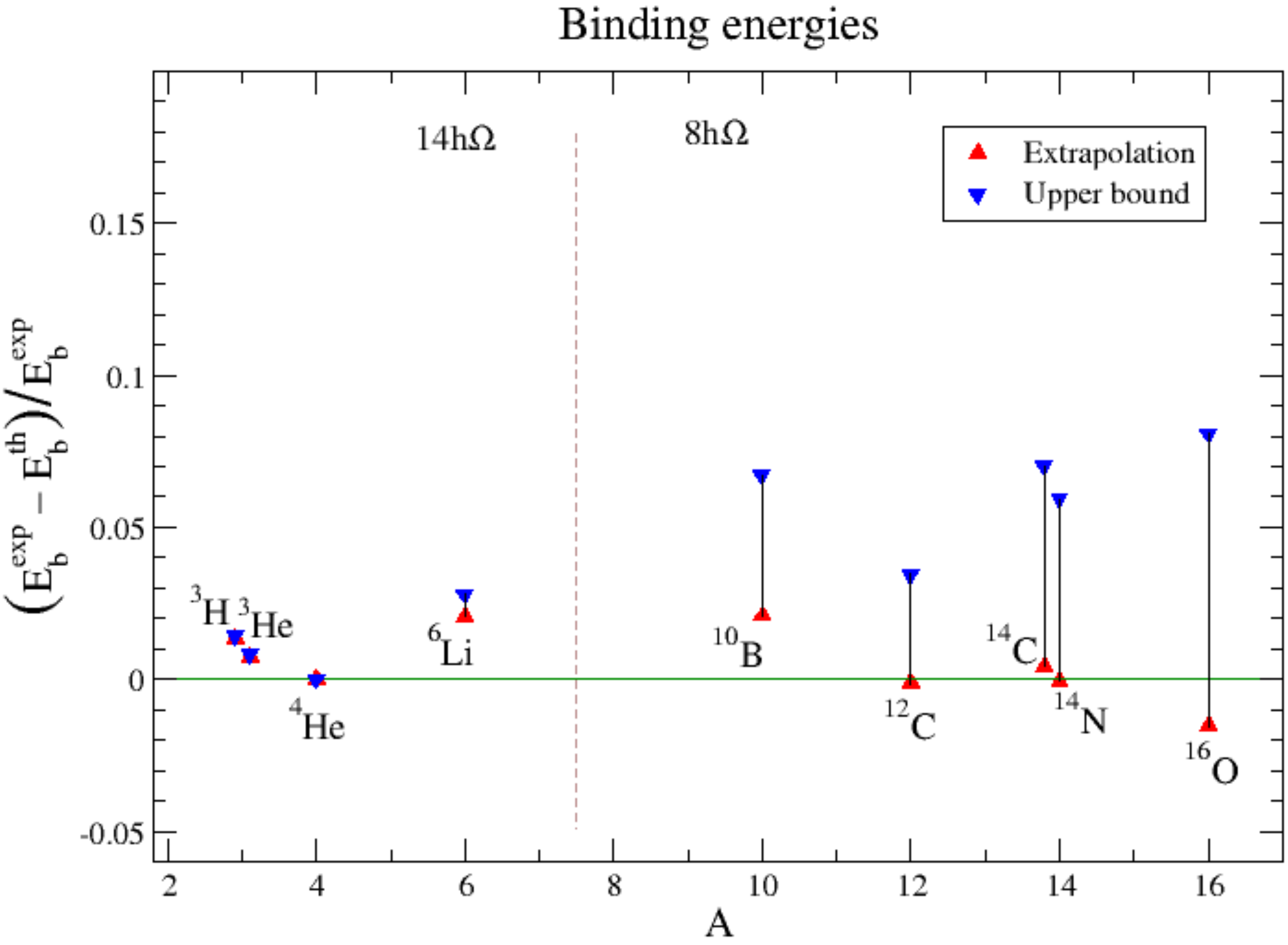
Table 4. **Rms deviations of theoretical level energies from experimental data. For comparison with GFMC AV18/IL7 results, we select only states for which the AV18/IL7 results are available (see Tables 1 and 2)**

	Number of levels	JISP16		AV18/IL7
		Extrap. B	Extrap. C	
Comparison of JISP16 and AV18/IL7 results				
Absolute energies (MeV)	38	1.38	1.8	0.55
Relative energies	38	0.03	0.04	0.009
Energies per nucleon (MeV)	38	0.16	0.21	0.05
Natural parity states				
Absolute energies (MeV)	96	3.71	3.97	–
Relative energies	96	0.043	0.05	–
Energies per nucleon (MeV)	96	0.28	0.31	–
Natural and unnatural parity states				
Absolute energies (MeV)	135	3.54	4.04	–
Relative energies	135	0.05	0.056	–
Energies per nucleon (MeV)	135	0.28	0.34	–

JISP16:drawbacks

- Deficiency of JISP16 revealed by the extrapolations and by the use of larger model spaces attainable due to new supercomputers


$(E^{exp}-E^{th})/E^{exp}$
0.2
0.15
0.1
0.05
0
-0.05
-0.1
$20\hbar\Omega$
$18\hbar\Omega$
$16\hbar\Omega$
$14\hbar\Omega$
$12\hbar\Omega$
$10\hbar\Omega$
$8\hbar\Omega$
^{3}H
^{4}He
^{6}He
^{6}Li
^{7}Li
^{8}He
^{8}Li
^{8}Be
^{9}Li
^{9}Be
^{10}B
^{10}Be
^{11}Be$_{(11\hbar\Omega)}$
^{11}B
^{12}Be
^{12}B
^{12}C
^{13}B
^{13}C
^{14}C
^{14}N
^{15}N
^{16}O
Upperbound
Extrap. B
2
4
6
8
10
12
14
16
A


Binding energies
14hΩ
8hΩ
Extrapolation
Upper bound
$\left(E_b^{exp} - E_b^{th}\right)/E_b^{exp}$
0.15
0.1
0.05
0
-0.05
^{3}H
^{3}He
^{4}He
^{6}Li
^{10}B
^{12}C
^{14}C
^{14}N
^{16}O
2
4
6
8
10
12
14
16
A

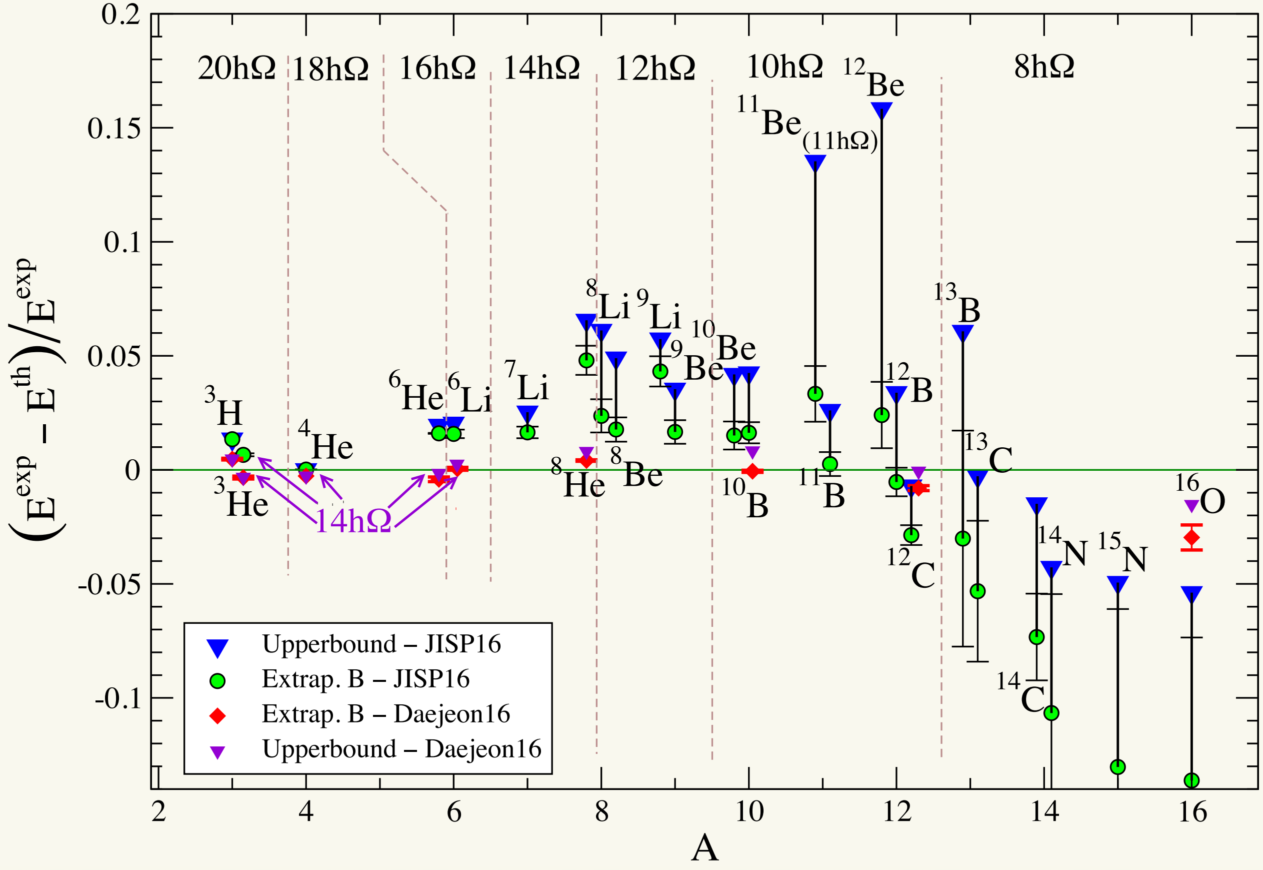
JISP16$_{2010}$ spectra

- Generally, a good description of excitation energies. The rms deviation from experiment of excitation energies of calculated nuclei is approximately 2 times smaller than for JISP16

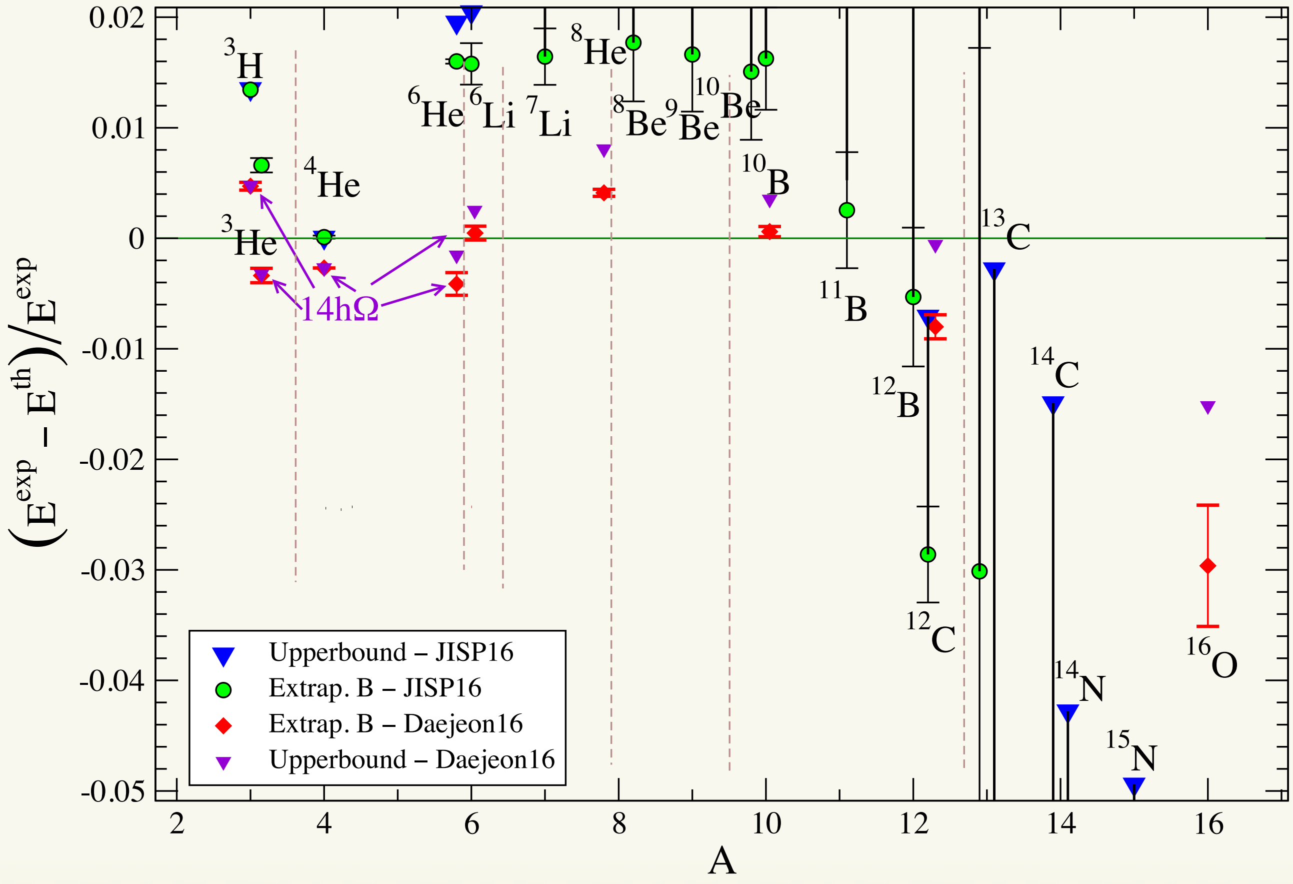
Daejeon16:

PETted SRG-evolved ($\lambda = 1.5\ \mathrm{fm}^{-1}$) N3LO for use without *NNN*

JISP16 vs Daejeon16



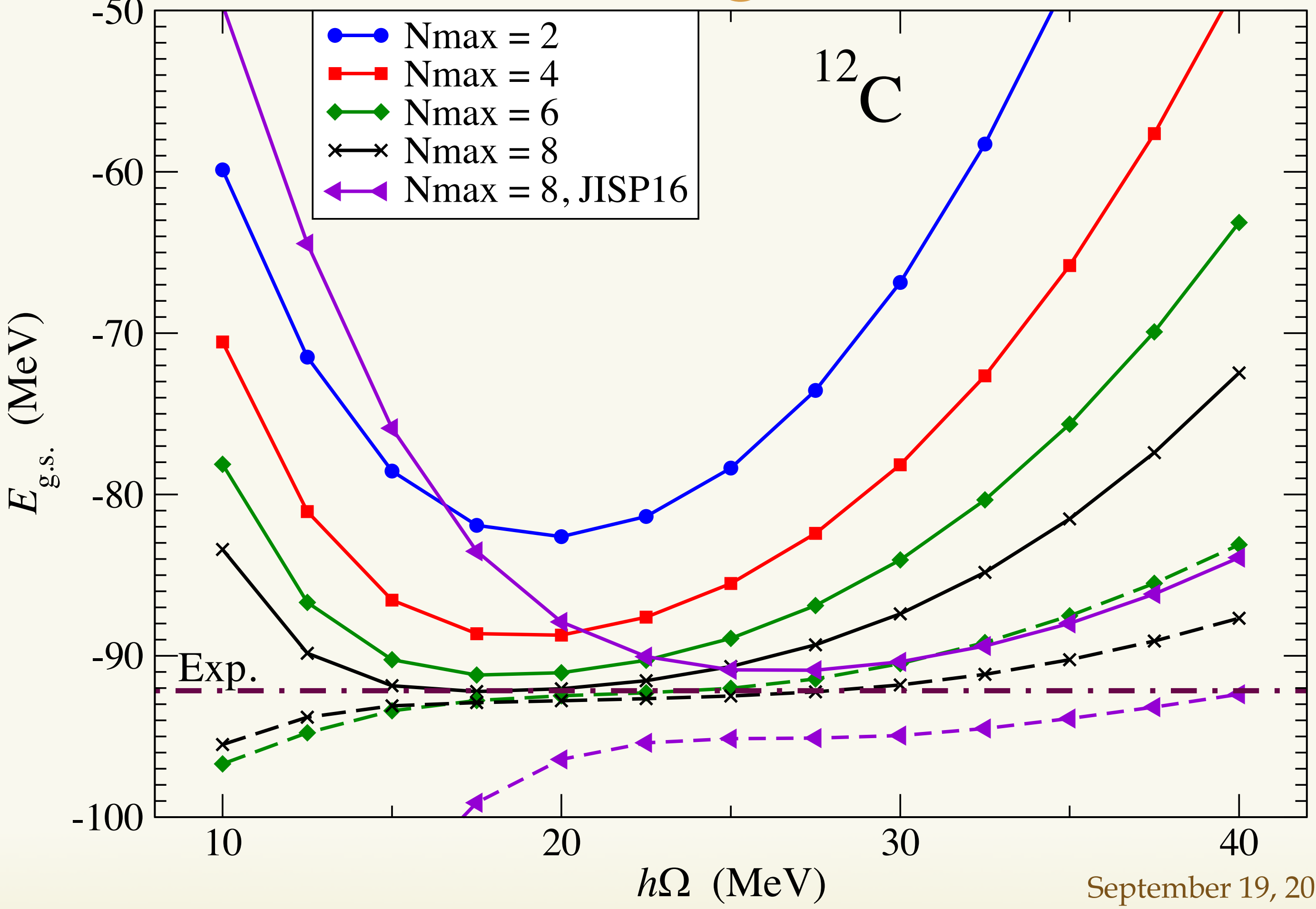
A larger scale is needed to see details



Daejeon16

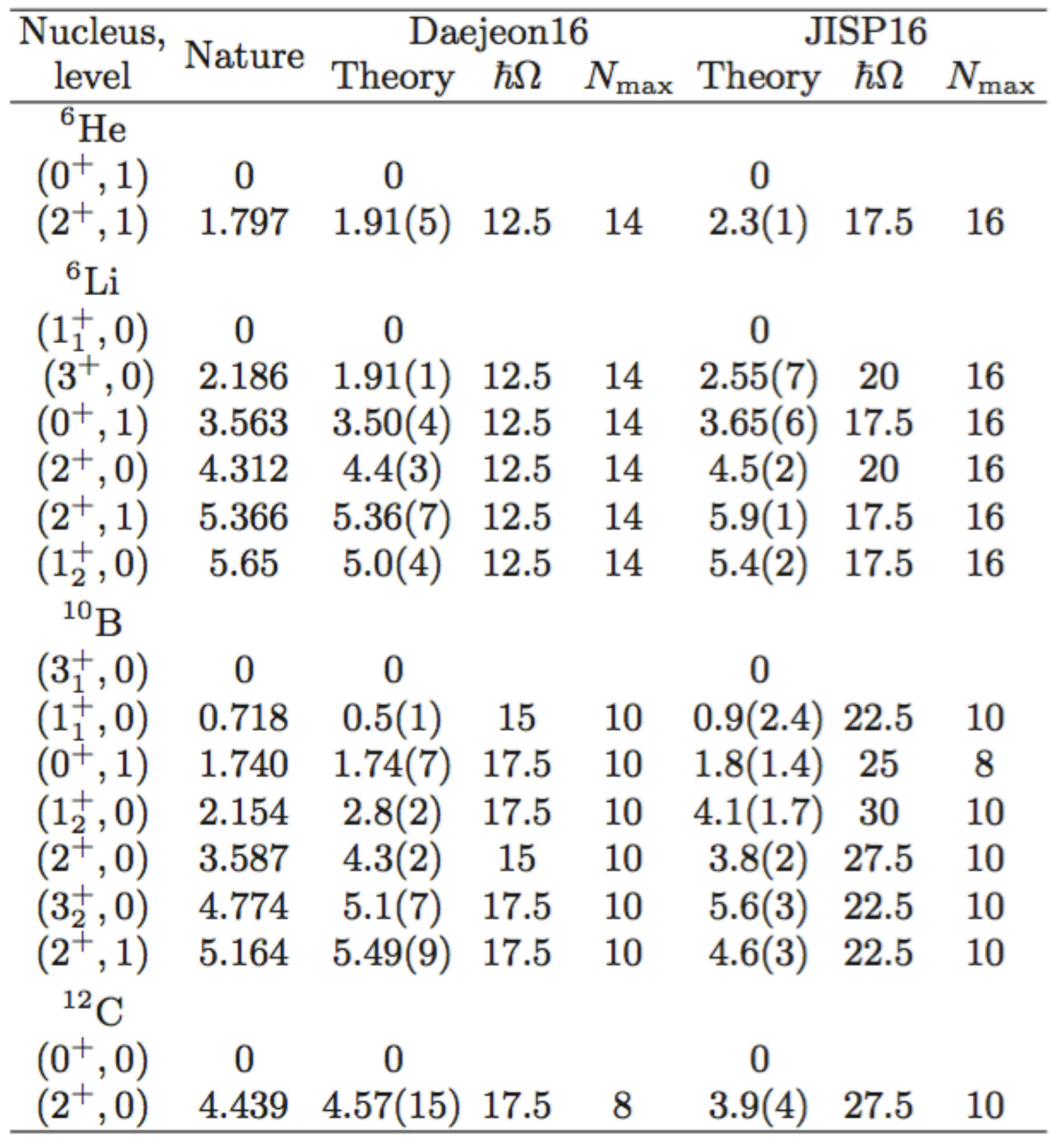
- Good convergence of NCSM calculations (better than with JISP16)
- Good descriptions of binding energies and spectra
- Improved description of other observables, e. g., rms radii

Daejeon16



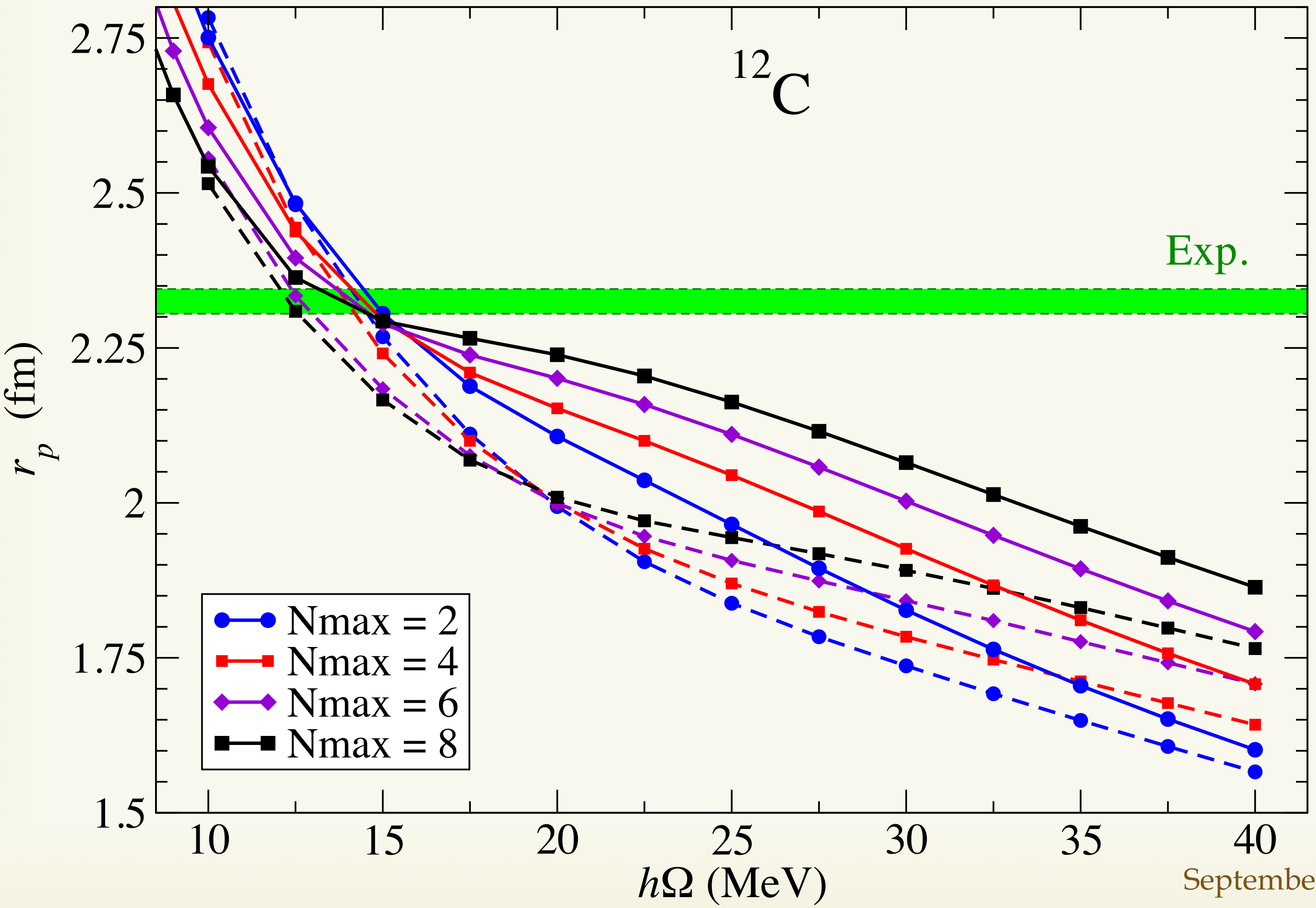
Nmax = 2
Nmax = 4
Nmax = 6
Nmax = 8
Nmax = 8, JISP16
^{12}C
Exp.
-50
-60
-70
-80
-90
-100
10
20
30
40
$E_{g.s.}$ (MeV)
$\hbar\Omega$ (MeV)

Daejeon16



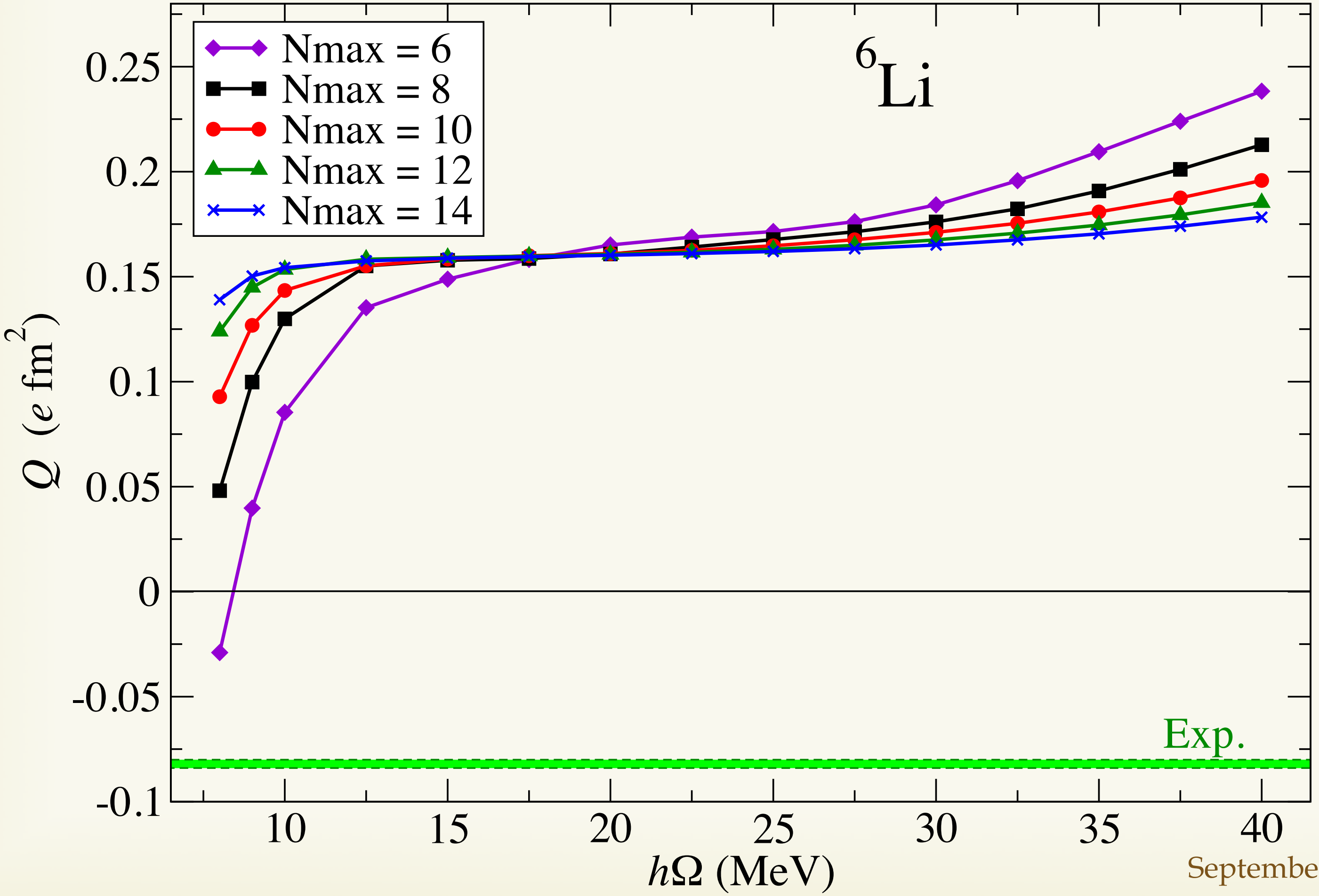
Nucleus, level	Nature	Daejeon16 Theory	$\hbar\Omega$	$N_{\max}$	JISP16 Theory	$\hbar\Omega$	$N_{\max}$
^{6}He							
$(0^+,1)$	0	0			0		
$(2^+,1)$	1.797	1.91(5)	12.5	14	2.3(1)	17.5	16
^{6}Li							
$(1^+_1,0)$	0	0			0		
$(3^+,0)$	2.186	1.91(1)	12.5	14	2.55(7)	20	16
$(0^+,1)$	3.563	3.50(4)	12.5	14	3.65(6)	17.5	16
$(2^+,0)$	4.312	4.4(3)	12.5	14	4.5(2)	20	16
$(2^+,1)$	5.366	5.36(7)	12.5	14	5.9(1)	17.5	16
$(1^+_2,0)$	5.65	5.0(4)	12.5	14	5.4(2)	17.5	16
^{10}B							
$(3^+_1,0)$	0	0			0		
$(1^+_1,0)$	0.718	0.5(1)	15	10	0.9(2.4)	22.5	10
$(0^+,1)$	1.740	1.74(7)	17.5	10	1.8(1.4)	25	8
$(1^+_2,0)$	2.154	2.8(2)	17.5	10	4.1(1.7)	30	10
$(2^+,0)$	3.587	4.3(2)	15	10	3.8(2)	27.5	10
$(3^+_2,0)$	4.774	5.1(7)	17.5	10	5.6(3)	22.5	10
$(2^+,1)$	5.164	5.49(9)	17.5	10	4.6(3)	22.5	10
^{12}C							
$(0^+,0)$	0	0			0		
$(2^+,0)$	4.439	4.57(15)	17.5	8	3.9(4)	27.5	10

Daejeon16



September 19, 2016, Khabarovsk

Daejeon16


Nmax = 6
Nmax = 8
Nmax = 10
Nmax = 12
Nmax = 14
^{6}Li
Exp.
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
Q (e fm^2)
10
15
20
25
30
35
40
$h\Omega$ (MeV)

^{11}Be: parity inversion

- Experimentally: $1/2^+$ -65.483(6) MeV
  $1/2^-$ -65.165(7) MeV, Exc. energy 0.318(7) MeV
- JISP16: $1/2^+$ -63.3(8) MeV, $N_{max}=11$
  $1/2^-$ -64.0(6) MeV, $N_{max}=10$
- Seems to be incorrect, however the uncertainties are too large
- Daejeon16: $1/2^+$ -64.9(3) MeV, $N_{max}=9$
  $1/2^-$ -64.62(2) MeV, $N_{max}=10$
- Parity inversion seems to be reproduced!
  $N_{max}=10$ results will be available soon

^{5}He resonances

- SS-HORSE approach, details in Alexander Mazur talk on Wednesday
- Experimentally: $3/2^-$ E_r=0.80 MeV, Γ=0.65 MeV
  $1/2^-$ E_r=2.07 MeV, Γ=5.57 MeV
- JISP16: $3/2^-$ E_r=0.89 MeV, Γ=0.99 MeV
  $1/2^-$ E_r=1.86 MeV, Γ=5.46 MeV
- Daejeon16: similar results

Tetraneutron resonance

- SS-HORSE + HH approach, details in Igor Mazur talk on Friday
- Experimentally: E_r=0.83 ± 0.65(stat.) ± 1.25(syst.) MeV, $\Gamma \leq$ 2.6 MeV
- JISP16: E_r=0.84 MeV, Γ=1.38 MeV
- Daejeon16: : E_r=1.48 MeV, Γ=2.72 MeV

Conclusions

Thank you!