

Recent results obtained with JISP16

Andrey Shirokov

M. V. Lomonosov Moscow State University

*** Collaborators:**

- **V. Kulikov (Moscow State University)**
- **J. Vary and P. Maris (Iowa State University)**
- **A. Mazur, I. Mazur, E. Mazur (Pacific National University, Khabarovsk)**

Plan

- * Motivation
- * Structure of JISP interaction
- * Bindings and spectra of light nuclei with JISP16
- * Nuclear matter
- * Future prospect

NN interaction

- * Modern 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-Bonn₂₀₀₀; INOY (inside non-local, outside Yukawa)

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

Inverse scattering: JISP6, JISP16, JISP16₂₀₁₀

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

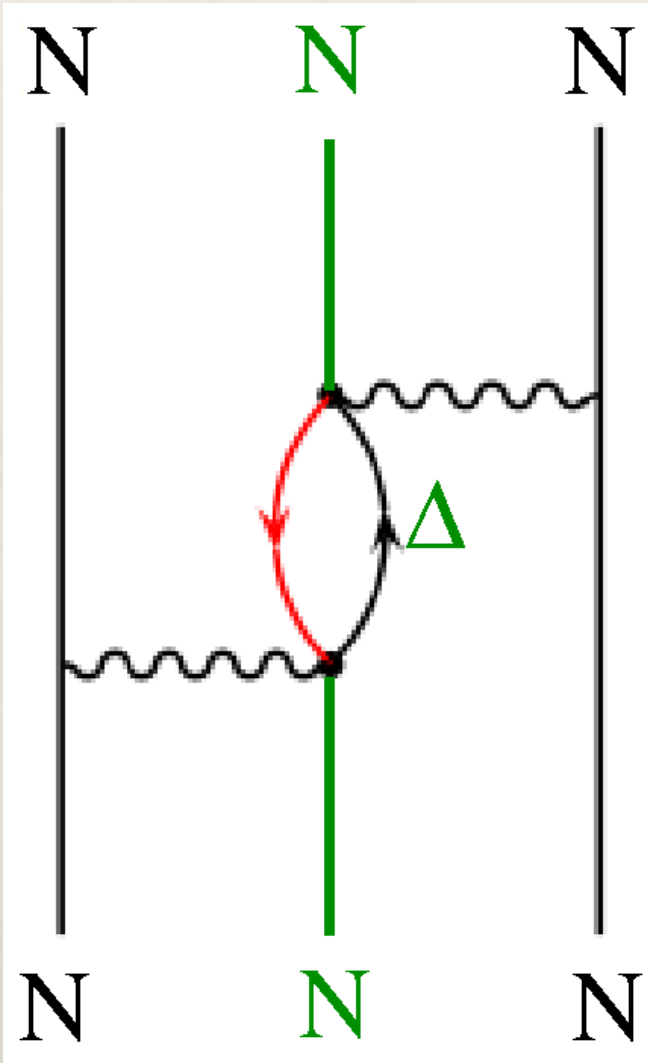
Ideal NN interaction from nuclear theorist viewpoint

- * Derived from QCD without model approximations and assumptions
- * Perfectly describing NN data at low energies
- * Perfectly describing bindings, spectra and other observables in light nuclei
- * Describing heavier nuclei, nuclear matter, etc.
- * Describing other experimental data ($p+d$ scattering, etc.)
- * Providing fast convergence of shell model and other calculations
- * No need of NNN forces

Ideal NN interaction from nuclear theorist viewpoint

- * Derived from QCD without model approximations and assumptions
- * Perfectly describing pn data at low energies
- * Reasonably describing bindings, spectra and other observables in light nuclei
- * Describing heavier nuclei, nuclear matter, etc.
- * Describing other experimental data ($p+d$ scattering, etc.)
- * Providing fast convergence of shell model and other calculations
- * No need of NNN forces
- * JISP16

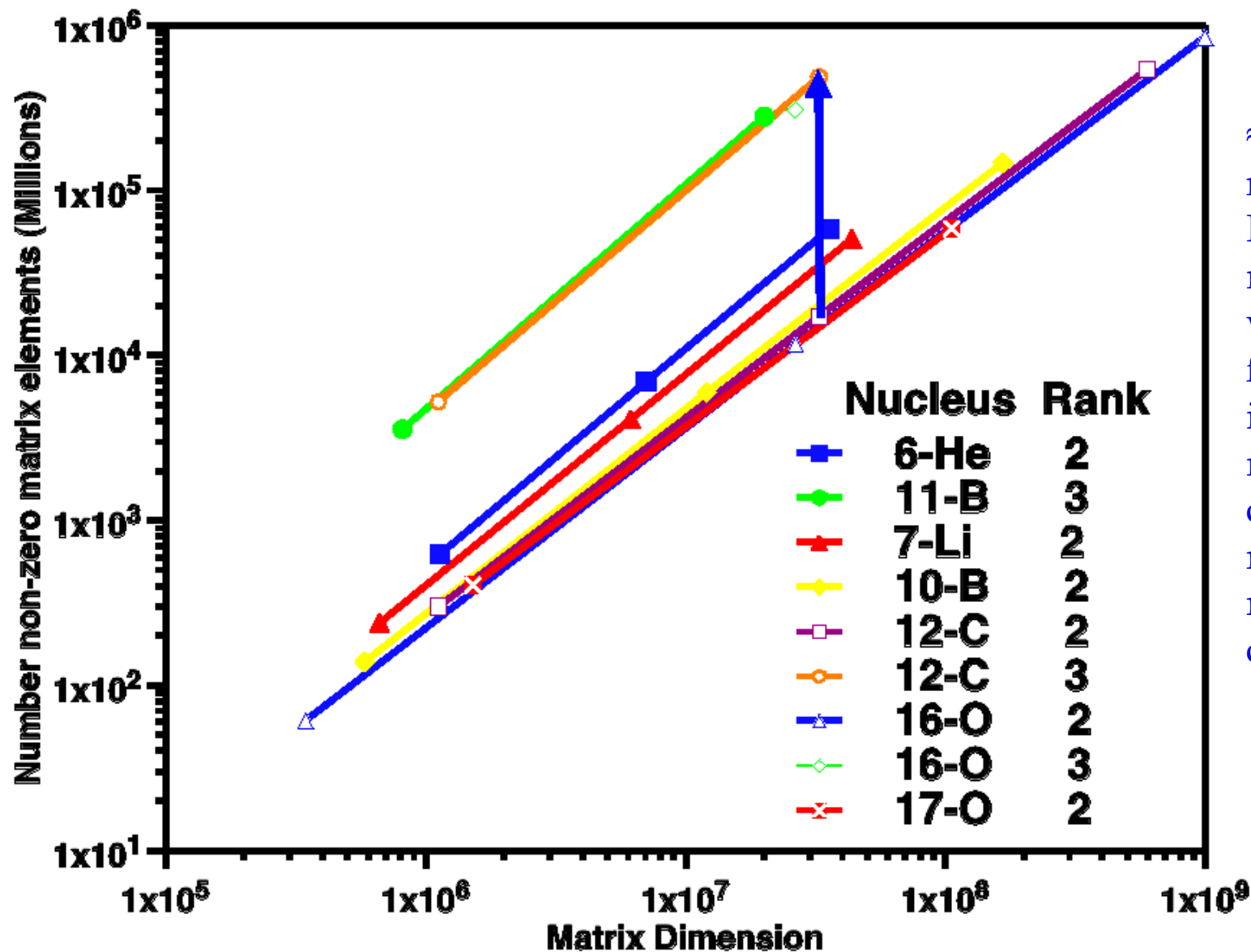
NNN force



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

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

Why would be nice to avoid *NNN* forces?



≈30 times more non-zero Hamiltonian matrix elements when *NNN* forces are involved; hence much more computer resources are required for calculations

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:

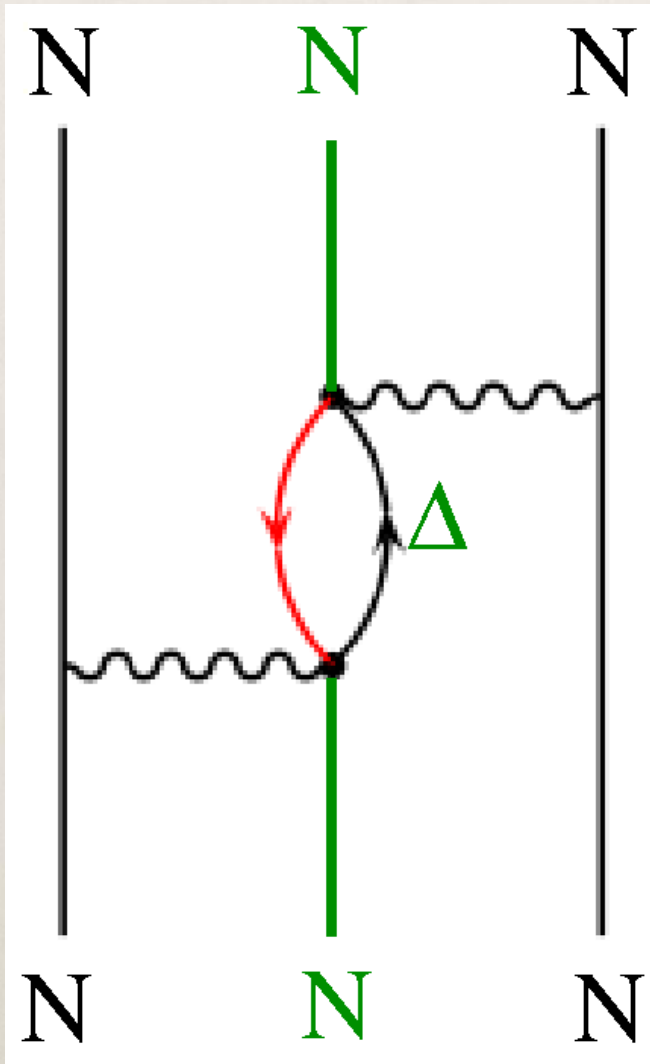
$$H'=T+V'_{ij}+V_{ijk} \rightarrow H=T+V_{ij}$$

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 NN interaction is an attempt to describe nuclei with nucleon degrees of freedom only

Modern NN interactions: need of NNN

- * Meson exchange: Nijmegen I, II; Reid soft core; Argonne AV_{18} ; CD-Bonn₂₀₀₀: require NNN potentials (U, IL, TM, ...) which are usually inconsistent with NN interaction
 - * Chiral EFT: N3LO requires NNN potential – N2LO at the moment, consistent with NN at the N2LO level
 - * Inverse scattering: JISP6, JISP16, JISP16₂₀₁₀: no need of NNN ; fitted to light nuclei
- + INOY (inside non-local, outside Yukawa)

NN interaction: convergence

- * To improve convergence of *ab initio* nuclear structure, usually (exception: GFMC) an effective interaction based on intrinsic *NN* (and, generally, *NNN*) interaction is constructed
- * Modern approaches to eff. interaction:
- * Lee–Suzuki–Okamoto (LSO): popular up to 2010, less popular now. Idea is to reproduce in a given small model space the results in the infinite model space (of course, approximately). New interaction for each model space. No variational principle, non-monotonic convergence in many-body nuclei, no way to extrapolate results to infinite model space. Induced *NNN* to improve convergence.
- * Similarity renormalization group (SRG): a modern trend. Idea is to reduce matrix elements coupling low- and high-momentum components of interaction by unitary transformation. The variational principle works, results can be extrapolated. Induced *NNN* to restore ‘bare’ interaction results in many-body nuclei.

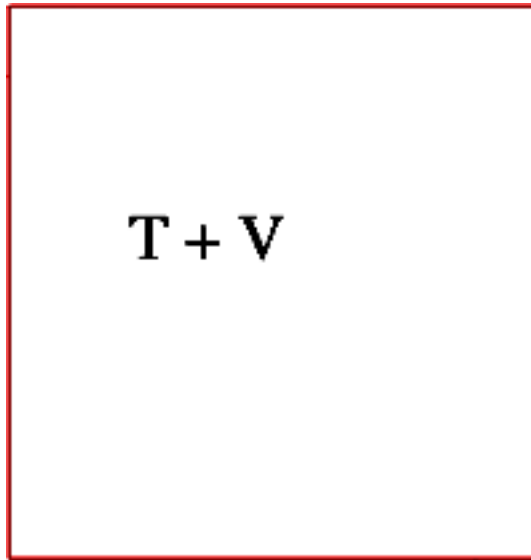
Modern NN interactions

- * Meson exchange NN (Argonne AV_{18} ; CD-Bonn₂₀₀₀; INOY, ...): high-quality description of NN data: $\chi^2/\text{datum} \approx 1$ up to $E_{\text{lab}} = 350$ MeV. Somewhat phenomenological: no ties to QCD, phenomenological terms, inconsistent parameters. Should be combined with (usually inconsistent)(semi)phenomenological NNN (IL, U, TM, ...). Bad convergence, eff. interaction needed. (*R. Machleidt*: “If you want more more accuracy, you have to use less theory”)
- * Chiral EFT NN (N3LO): A modern trend. Less accurate (at the moment) description of NN data: np : $\chi^2/\text{datum} = 1.10$ up to $E_{\text{lab}} = 290$ MeV; pp : $\chi^2/\text{datum} = 1.50$ up to $E_{\text{lab}} = 290$ MeV. Tied to QCD through expansion in p/p_χ , p_χ is a chiral symmetry breaking momentum. Should be combined with Chiral EFT NNN (N2LO now). Bad convergence, eff. interaction needed. (*R. Machleidt*: “If you want more more accuracy, you have to use more theory”)
- * Inverse scattering NN (JISP16, JISP16₂₀₁₀): high-quality description of np data: $\chi^2/\text{datum} \approx 1$ up to $E_{\text{lab}} = 350$ MeV. Completely phenomenological. No need of NNN

Construction of JISP *NN* interaction

- * JISP = *J*-matrix inverse scattering potential

J-matrix formalism: scattering in the oscillator basis



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 :

$$T_{nn} \sim n, T_{n,n\pm 1} \sim n, n \rightarrow \infty$$

while potential energy m. e. V_{nm} decrease with n and m .

$$\sum_{n'=0}^N H_{nn'}^l \langle n' | \lambda \rangle - E_\lambda \langle n | \lambda \rangle, \quad n \leq N.$$

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

$$S = \frac{C_{NI}^{(-)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^l C_{N+1,I}^{(-)}(q)}{C_{NI}^{(+)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^l C_{N+1,I}^{(+)}(q)},$$

T

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

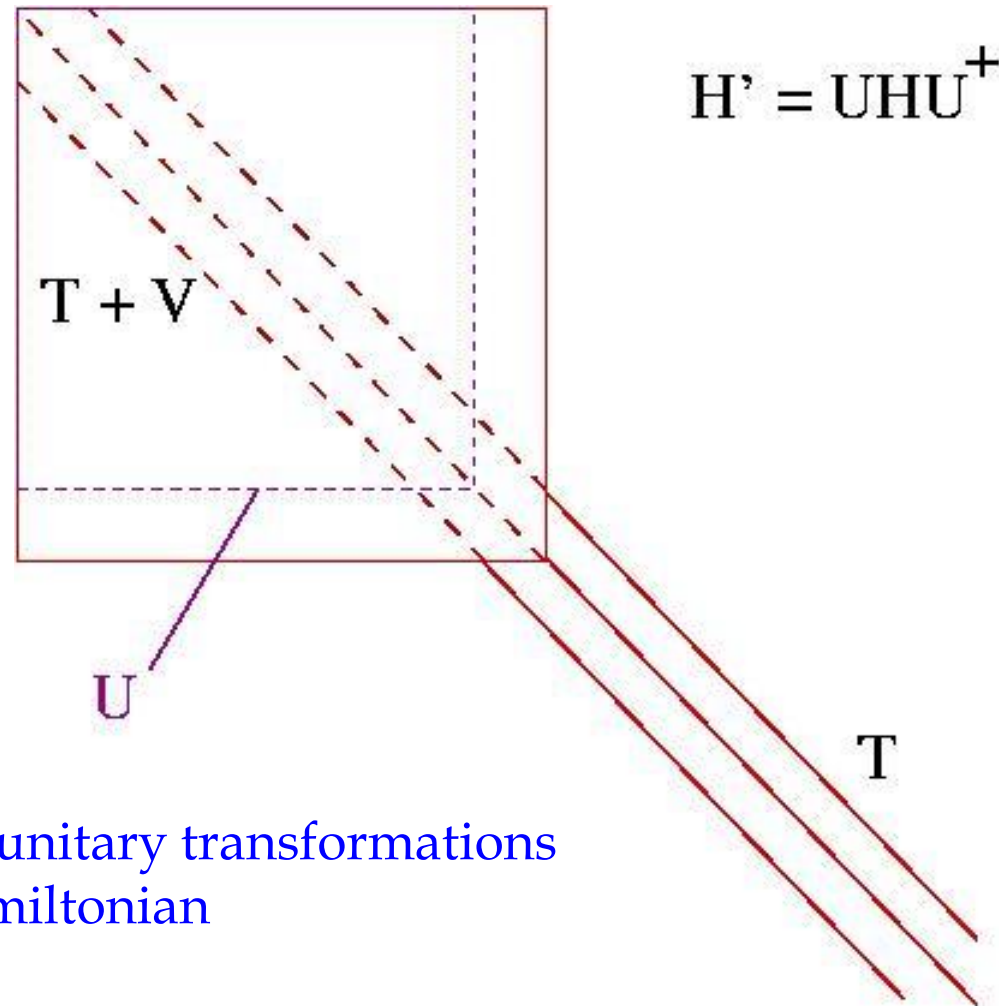
JISP16 properties

- * 1992 *np* data base (2514 data): $\chi^2/\text{datum} = 1.03$
- * 1999 *np* data base (3058 data): $\chi^2/\text{datum} = 1.05$

Table I: Deuteron properties.

Potential	E_d , MeV	<i>d</i> state probability, %	rms radius, fm	Q , fm ²	As. norm. const. \mathcal{A}_s , fm ^{-1/2}	$\eta = \frac{\mathcal{A}_d}{\mathcal{A}_s}$
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:

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

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

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

JISP *NN* interactions

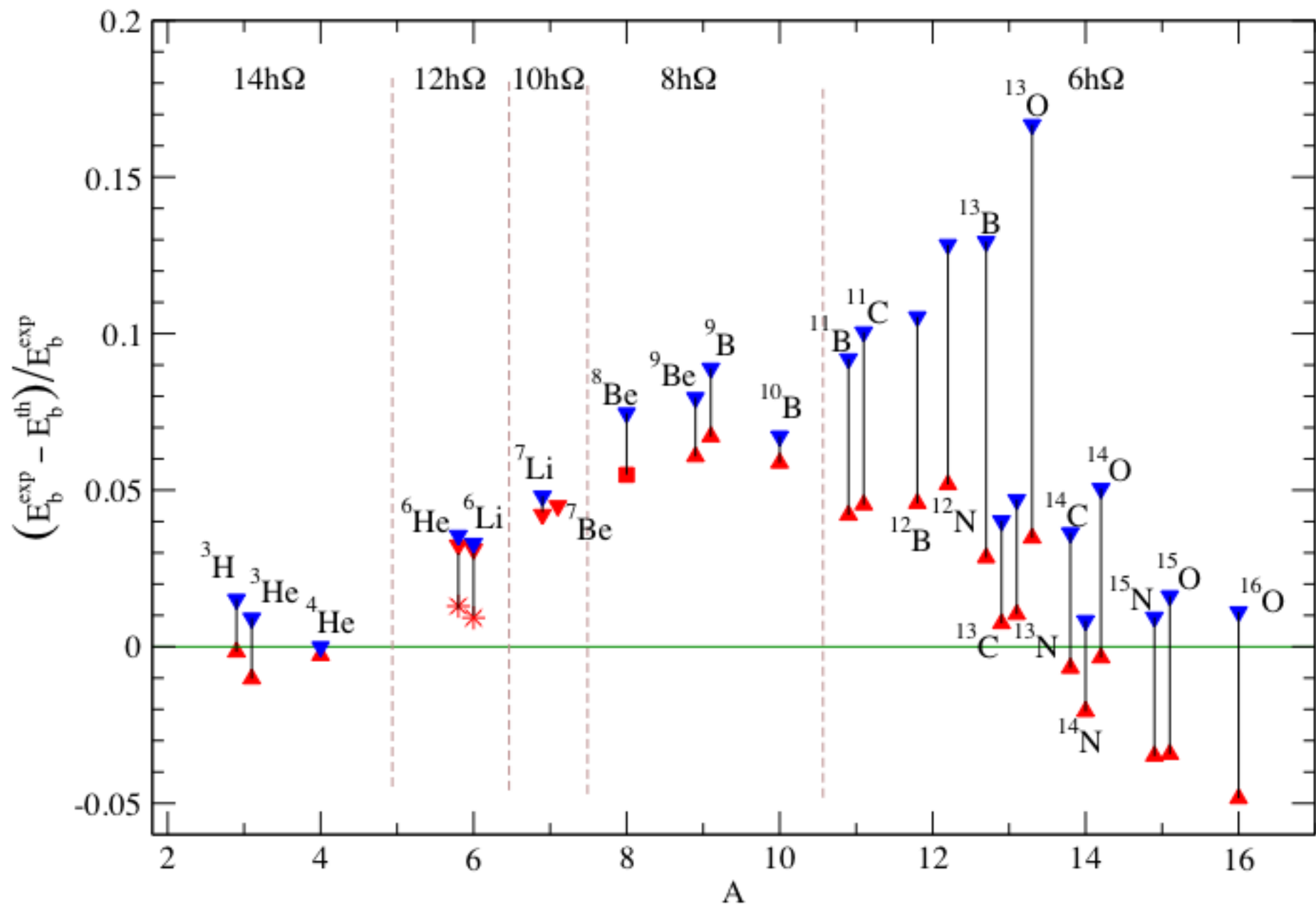
- * A. M. Shirokov, A. I. Mazur, S. A. Zaytsev, J. P. Vary, T. A. Weber, Phys. Rev. C 70, 044005 (2004): $A \leq 4$
- * A. M. Shirokov, J. P. Vary, A. I. Mazur, S. A. Zaytsev, T. A. Weber, Phys. Lett. B 621, 96 (2005): $A \leq 6$ – JISP6
- * A. M. Shirokov, J. P. Vary, A. I. Mazur, T. A. Weber, Phys. Lett. B 644, 33 (2007): $A \leq 16$ – JISP16

JISP16 initial fit

- * Fitted manually to binding energies of (^2H), ^3H , ^4He , ^6Li , ^{12}C , ^{16}O
- * Spectrum: ^6Li
- * Lee–Suzuki–Okamoto effective interaction was used
- * This fit appeared to be surprisingly successful

Typical NCSM results
obtained with bare
NN interaction and
Lee–Suzuki–Okamoto
effective interaction

Binding energies



JISP16 results

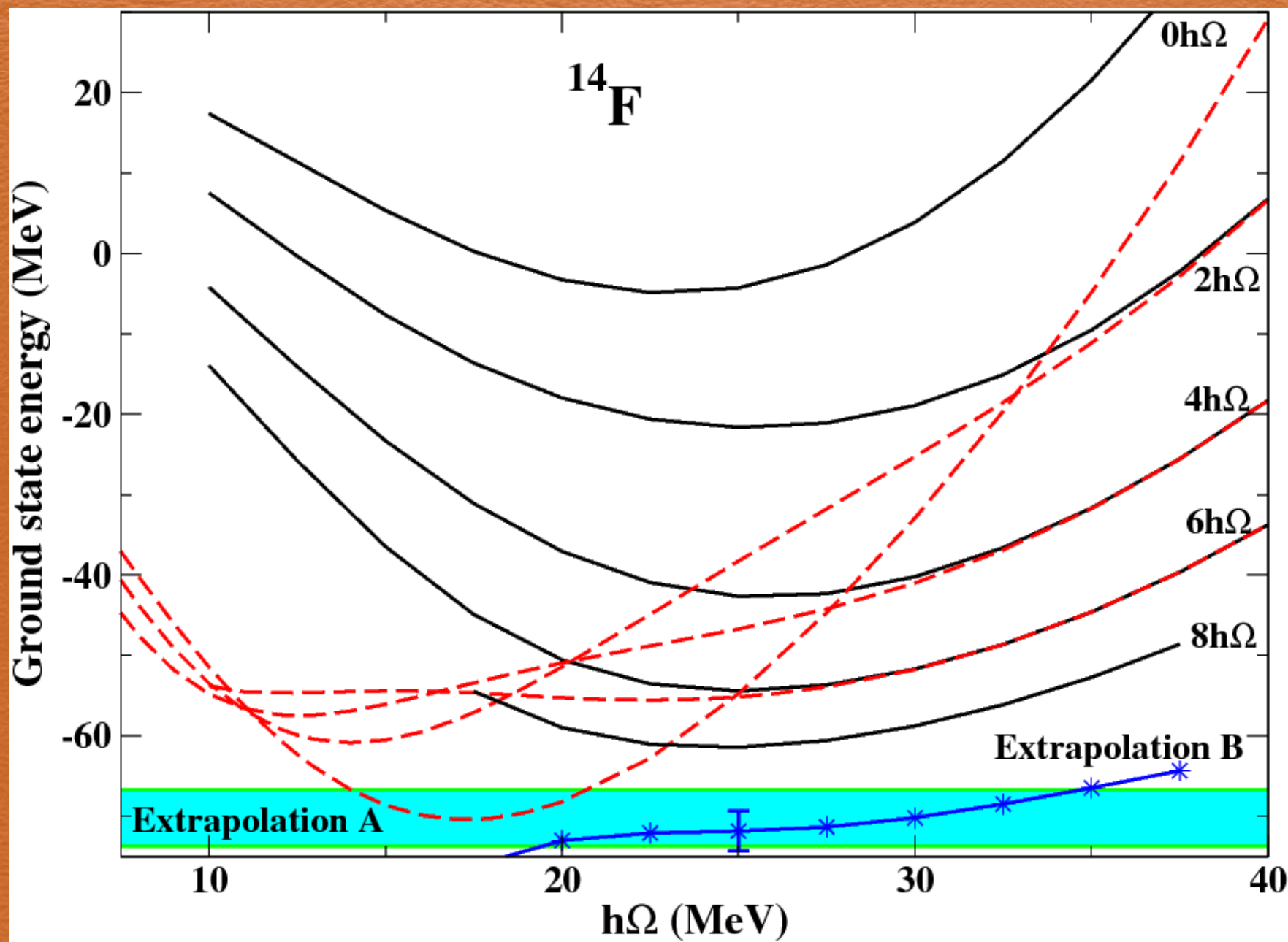
Ground state energy E_{gs} and excitation energies E_x (in MeV), ground state point-proton rms radius r_p (in fm) and quadrupole moment Q (in $e \cdot \text{fm}^2$) of the ${}^6\text{Li}$ nucleus; $\hbar\omega = 17.5$ MeV.

Interaction	Nature	JISP6	JISP16	AV8'+TM'	AV18+UIX	AV18+IL2
Method		NCSM, $10\hbar\omega$ [6]	NCSM, $12\hbar\omega$	NCSM, $6\hbar\omega$ [2]	GFMC [8,15]	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

Potential Approach	Nature	JISP16 NCSM, $8\hbar\omega^a$	AV8'+TM' NCSM, $4\hbar\omega^b$	AV18+IL2 GFMC ^c	ChPT 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
$B(E2; 1_1^+0 \rightarrow 3_1^+0)$	4.13(6)	3.317	1.959		3.05
$B(E2; 1_2^+0 \rightarrow 3_1^+0)$	1.71(26)	0.627	1.010		0.50
$B(\text{GT}; 3_1^+0 \rightarrow 2_1^+1)$	0.083(3)	0.042	0.066		0.07
$B(\text{GT}; 3_1^+0 \rightarrow 2_2^+1)$	0.95(13)	1.652	1.291		1.22

^aA.M.Shirokov, J.P.Vary, A.I.Mazur, T.A.Weber, Phys. Lett. **B644**, 33 (2007).^bP. Navrátil, W. E. Ormand, Phys. Rev. **C 68**, 034305 (2003).^cS. C. Pieper, K. Varga, R. B. Wiringa, Phys. Rev. **C 66**, 044310 (2002).^dP. Navrátil, V. G. Gueorguiev, J. P. Vary, W. E. Ormand, A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007).

Is LSO effective interaction reliable?



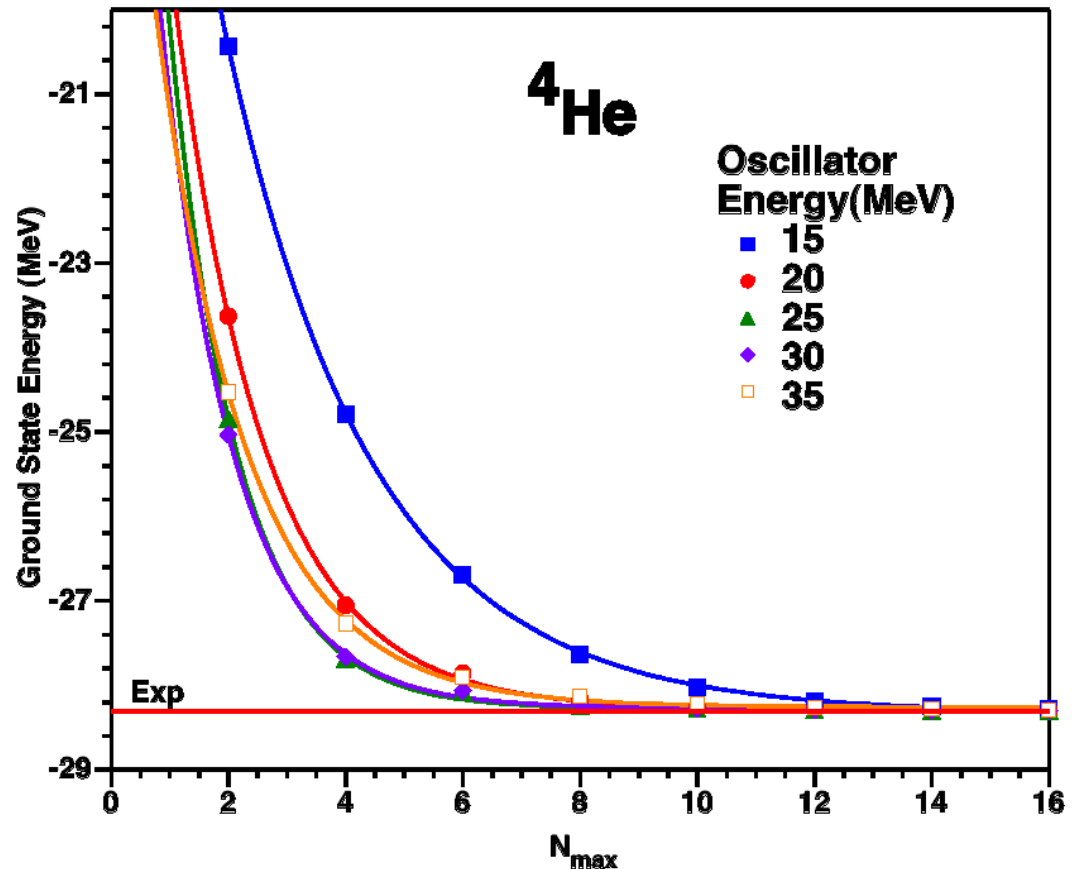
From effective interactions to no-core full configuration (NCFC) calculations

- ★ Extrapolation:

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

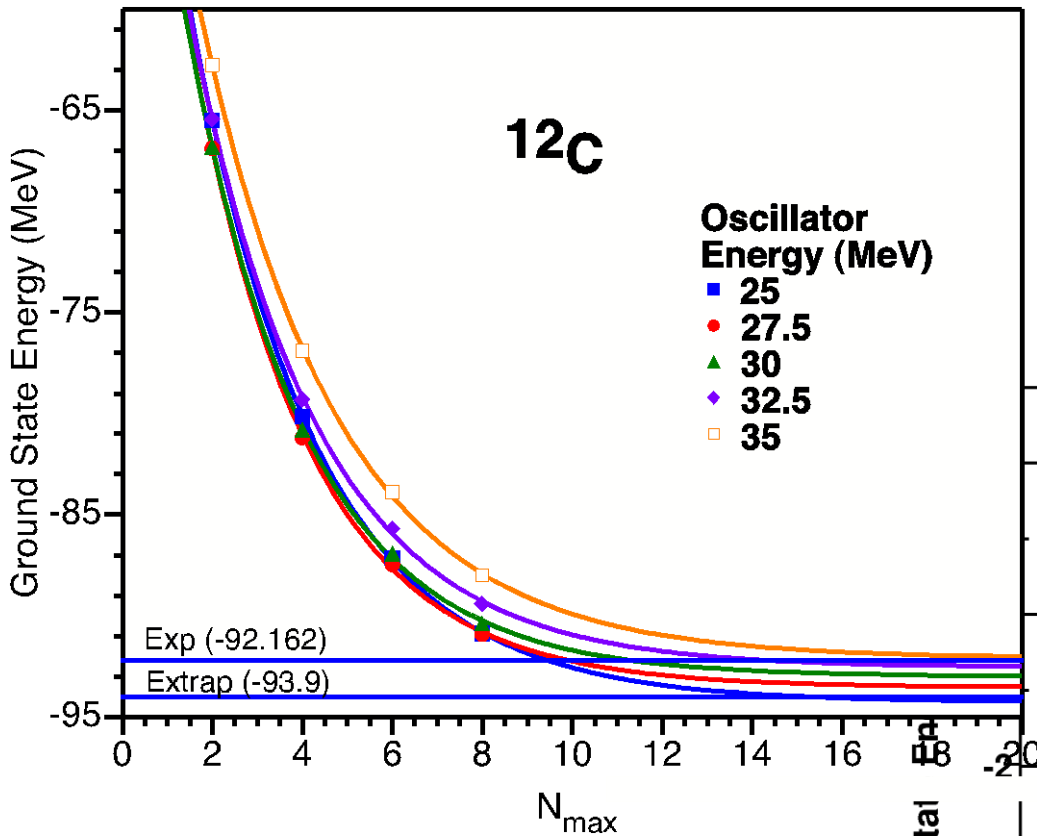
- ★ Works with bare interaction only (e.g., JISP16)

- ★ Example:

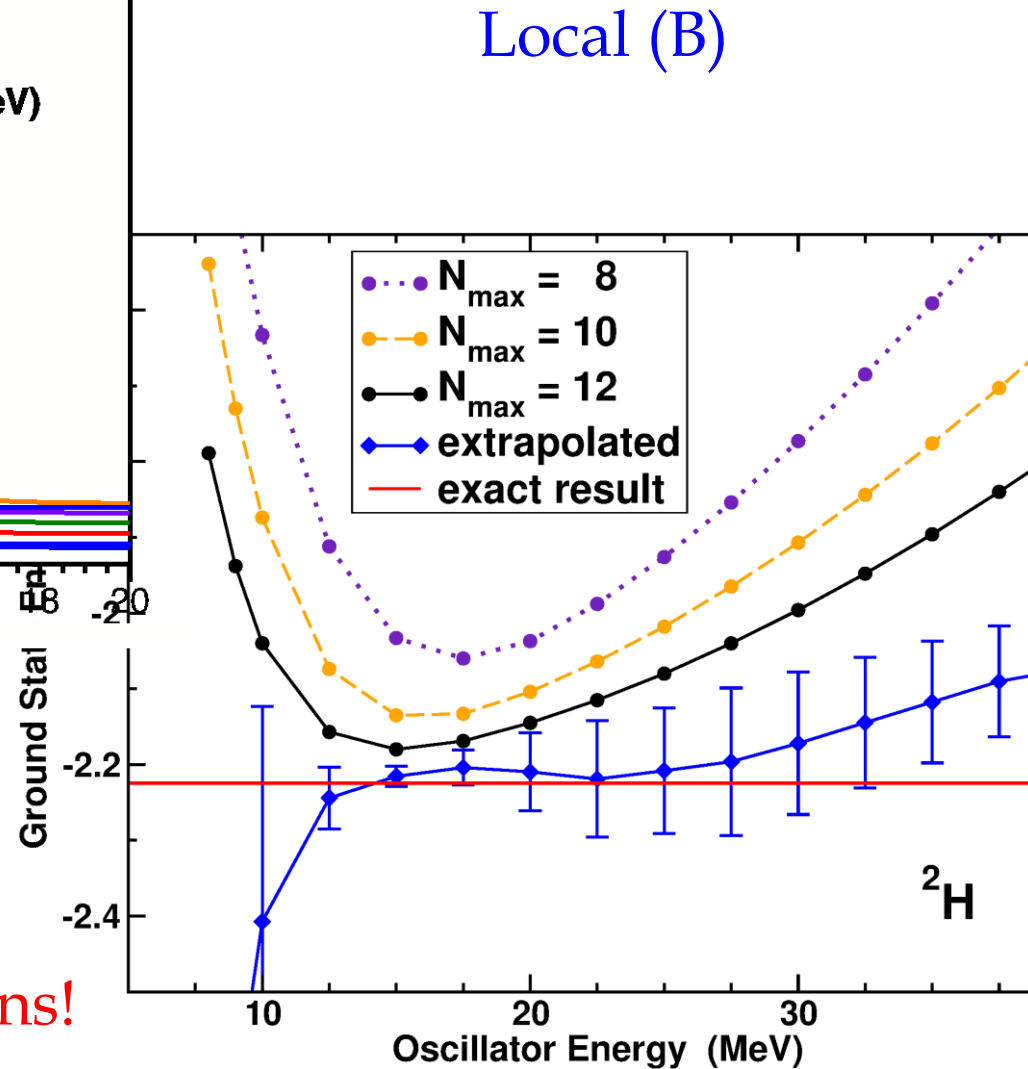


P. Maris, J. P. Vary, A. M. Shirokov,
Phys. Rev. C **79**, 014308 (2009)

2 types of extrapolations



Global (A)



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 are better theoretically grounded. However, from our recent analysis of large number of nuclei, they seem to be less accurate than our phenomenological extrapolations

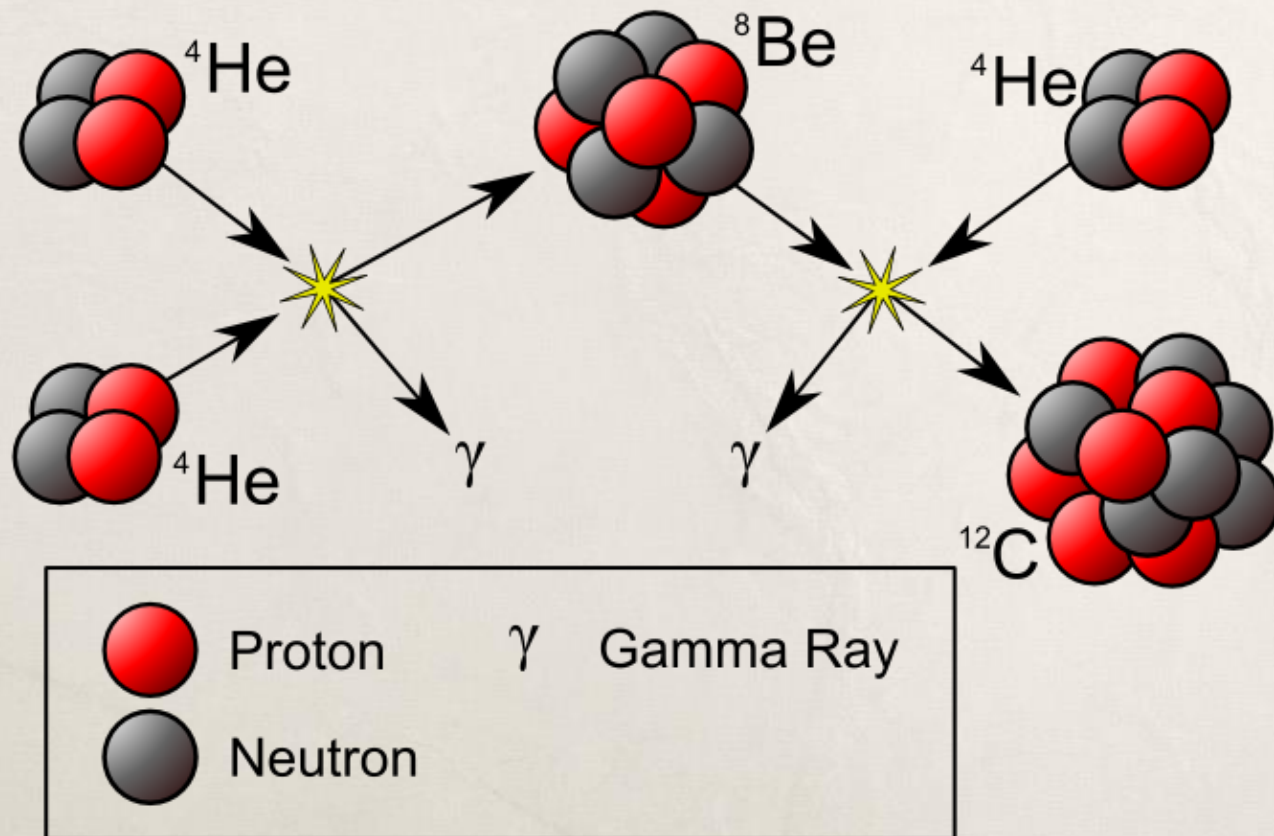
NCSM-NCFC approach: Some problems

Temporary problems

- * We can extrapolate energies but still cannot extrapolate other observables: rms radii, EM moments, EM transition probabilities, etc.
- * We calculate these observables but they have an $\hbar\Omega$ dependence, so, we cannot estimate the uncertainties that are large.
- * **Note:** extrapolation technique for rms radii was suggested: R. J. Furnstahl, G. Hagen, and T. Papenbrock, Phys. Rev. C 86, 031301(R) (2012). However it has not been carefully tested yet

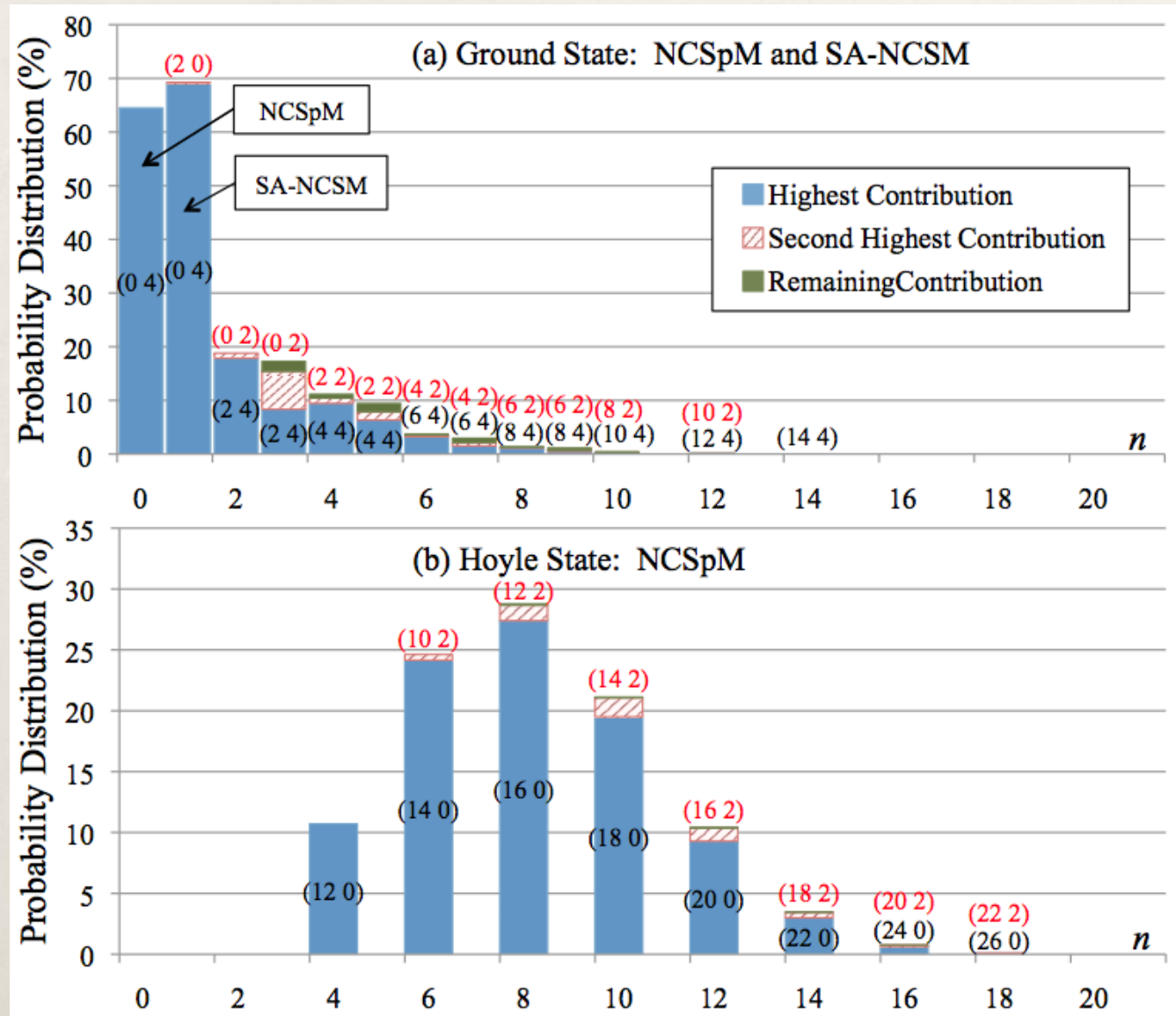
Problems

- * We cannot obtain some levels, e.g., the Hoyle state predicted by Fred Hoyle in the 1950s and later confirmed experimentally. This state is essential for the production of the ^{12}C isotope in stars via the triple- α process, i.e., for the origin of life on Earth.

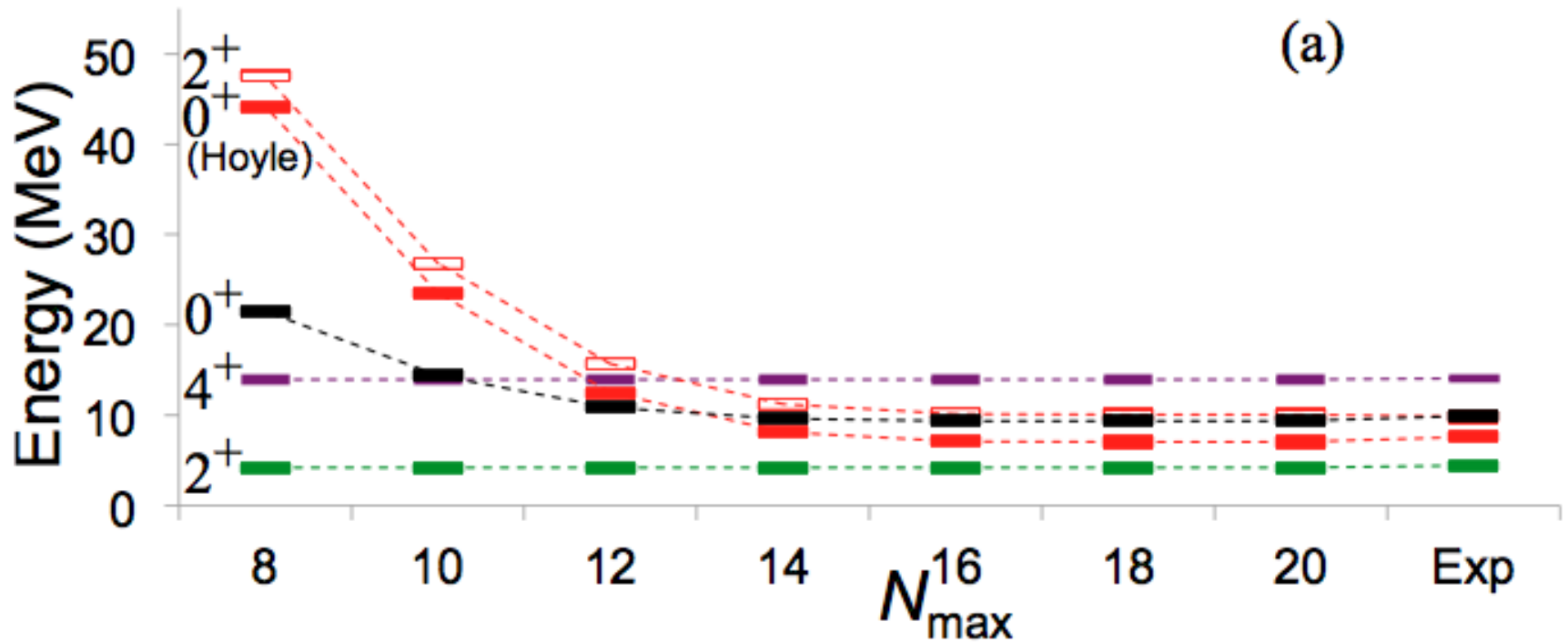


Hoyle state

Too large
 N_{\max} required
 for Hoyle



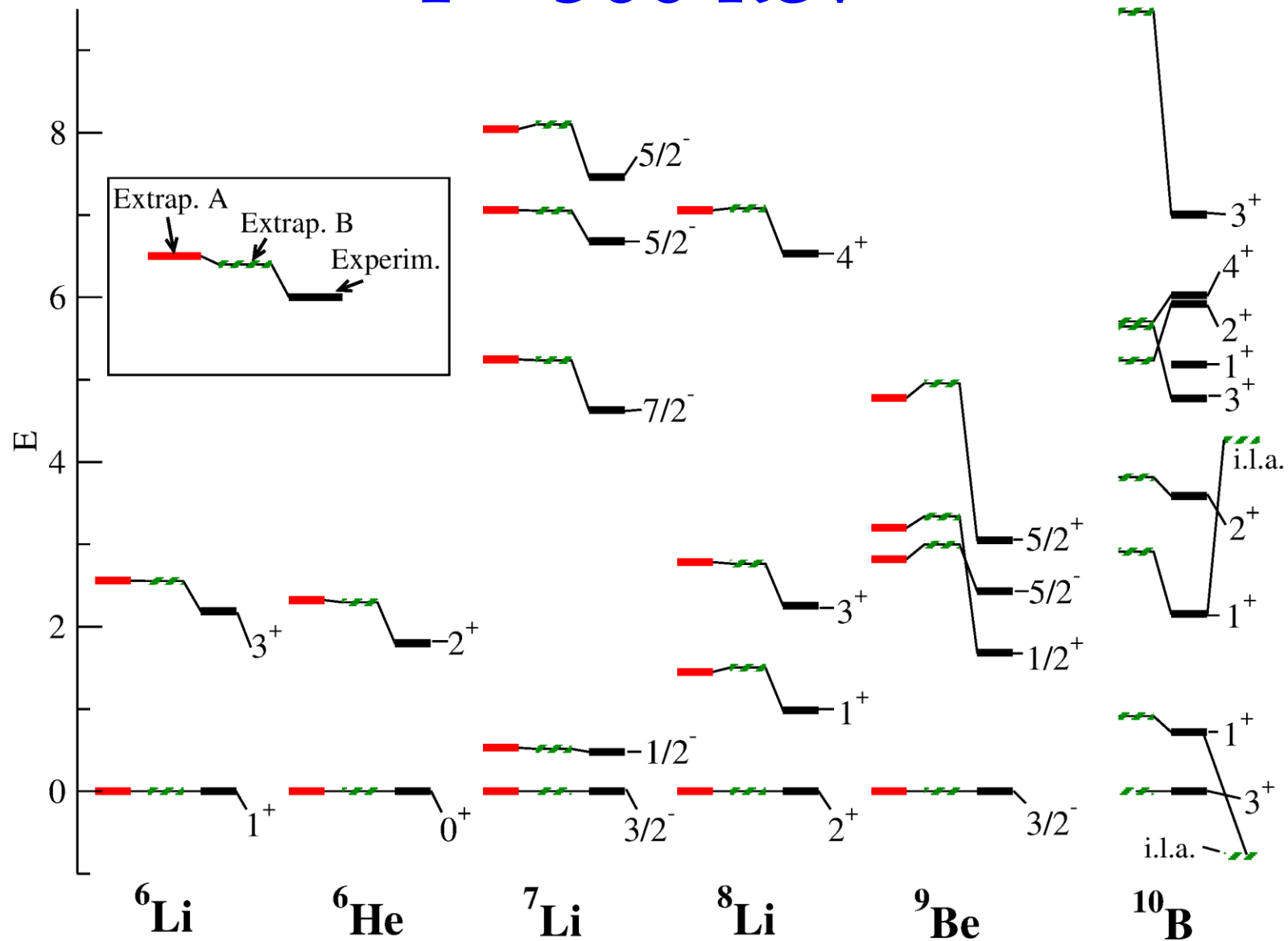
Hoyle state



Taken from A. C. Dreyfuss, K. D. Launey, T. Dytrych, J. P. Draayer, C. Bahri, arXiv:212.2255 (2012).

Obtained in symplectic NCSM

NCFC & JISP16: levels with $\Gamma < 300$ keV



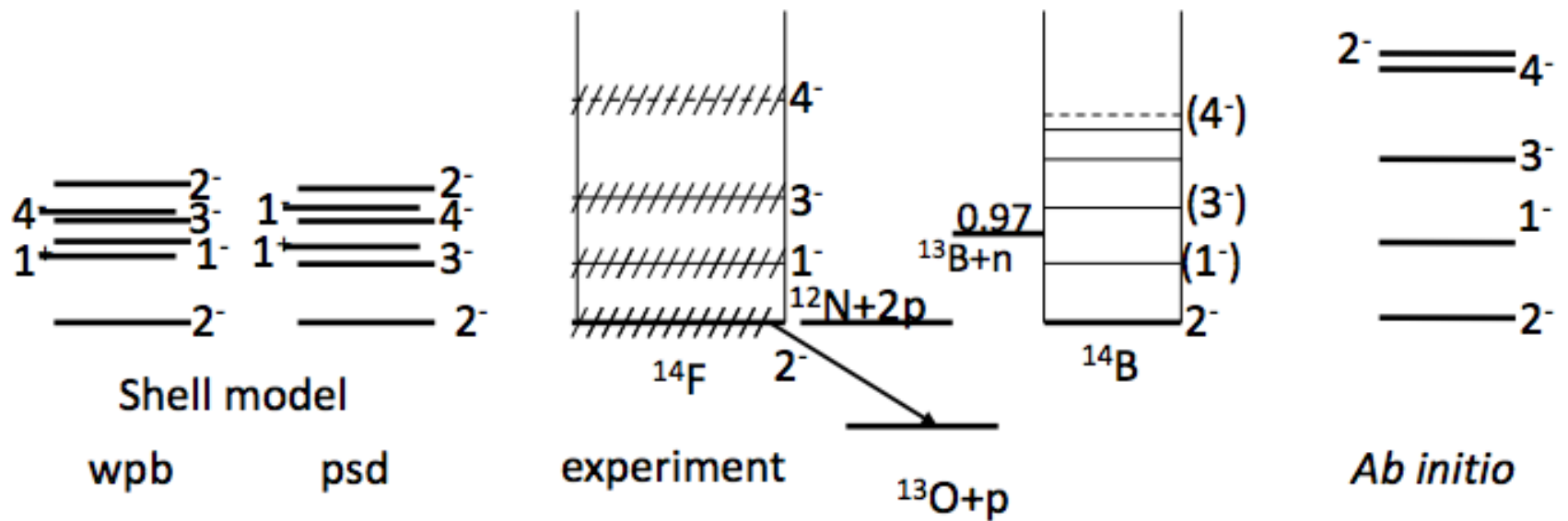
Success of NCSM
calculations with JISP16
interaction and NCFC
extrapolations:
Predictions of ^{14}F properties
(2009)

^{14}F

- * 1,990,061,078 basis states in $N_{\text{max}} = 8$ 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

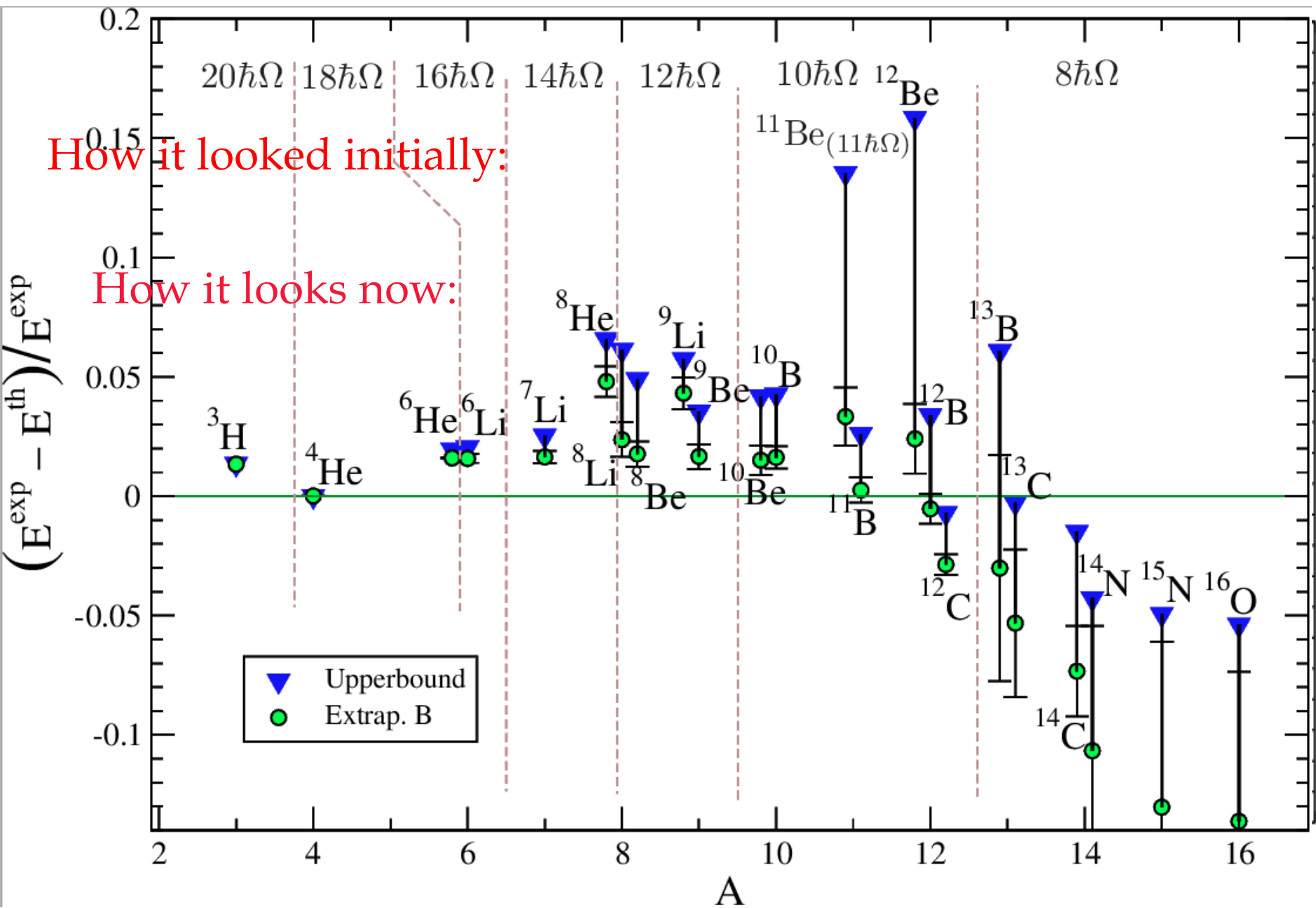
Nucleus	Extrapolation A	Extrapolation B	Experiment
^{13}O	-75.7(2.2)	-77.6(3.0)	-75.556
^{14}B	-84.4(3.2)	-86.6(3.8)	-85.423
^{14}F	-70.9(3.6)	-73.1(3.7)	74.00(0.04)

^{14}F spectrum



Back to JISP16: drawbacks

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



Light nuclei with JISP16: comprehensive analysis

- * 26 nuclei, 135 natural and unnatural parity states
- * Analyzed rms deviations from experiment for absolute energies E_i^{th} , for energies per nucleon E_i^{th}/A , and rms for relative energies $(E_i^{th} - E_i^{exp})/E_i^{exp}$.

Light nuclei with JISP16: comprehensive analysis

rms for binding energies

	Number of nuclei	JISP16		AV18/IL7
		Extrap. B	Extrap. C	
Comparison of JISP16 and AV18/IL7 results				
Absolute energies (MeV)	13	1.16	1.44	0.43
Relative energies	13	0.023	0.029	0.007
Energies per nucleon (MeV)	13	0.12	0.16	0.04
$A \leq 12$ ground states				
Absolute energies (MeV)	19	1.68	2.33	–
Relative energies	19	0.033	0.047	–
Energies per nucleon (MeV)	19	0.16	0.22	–
All ground states				
Absolute energies (MeV)	26	5.63	5.49	–
Relative energies	26	0.055	0.059	–
Energies per nucleon (MeV)	26	0.39	0.39	–

Light nuclei with JISP16: comprehensive analysis

rms for level energies

	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	—

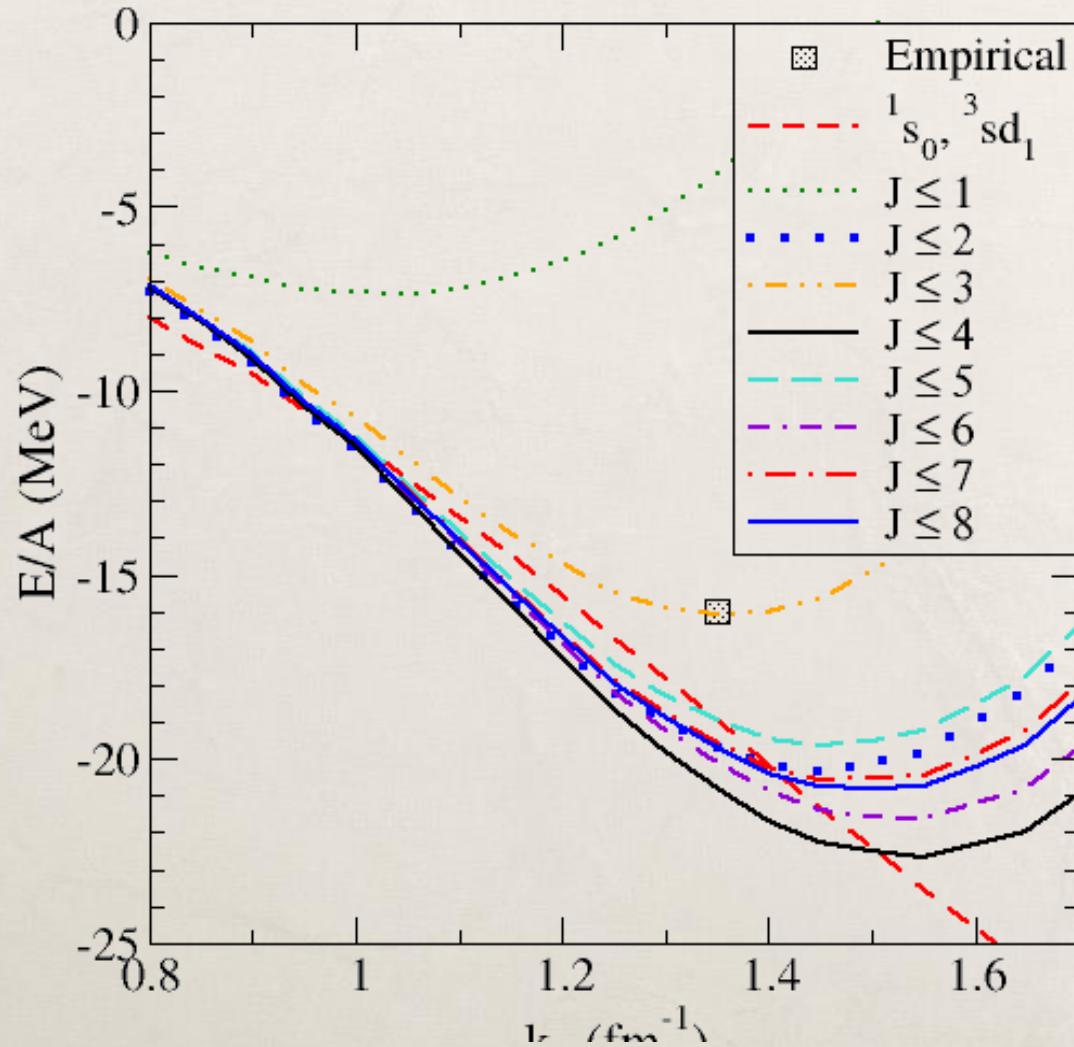
Light nuclei with JISP16: comprehensive analysis

rms for excitation energies

	Number of levels	JISP16				AV18/IL7
		Extrap. B	Extrap. C	Av. $\hbar\Omega$	Av. N_{max}	
Natural parity states						
Excitation energies (MeV)	25	0.61	0.74	0.96	1.60	0.42
Excitation energies (MeV)	70	1.62	2.88	3.49	4.43	–
Unnatural parity states						
Excitation energy (MeV)	31	2.25	1.57	2.05	2.32	–

Nuclear matter with JISP16

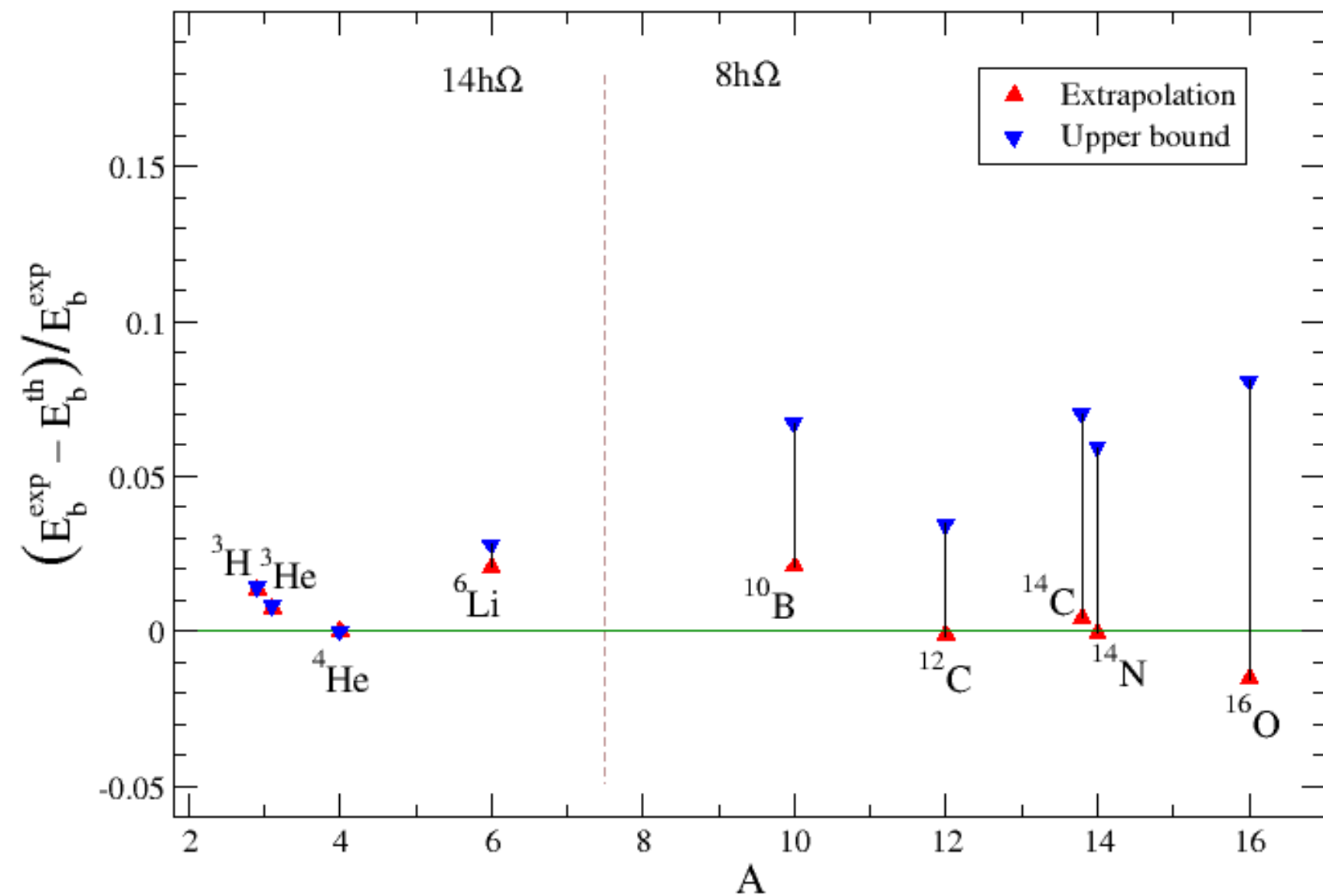
Nuclear Matter from JISP16
with various J truncations



Nuclear matter with JISP16

- * Nuclear matter is a model that somehow simulates bulk properties of heavy nuclei.
- * Surprisingly strong J dependence of nuclear matter equation of state even for high J in case of JISP16 NN interaction.
- * Light nuclei are insensitive to high- J components of the NN interaction. Hence it will be possible to fit JISP16 to nuclear matter properties by PETs in high- J partial waves. This will be interesting!

Binding energies



JISP16₂₀₁₀

- * JISP16₂₀₁₀ is still somewhat preliminary version of the interaction: it is needed to calculate more nuclei and to check it in more detail. However it is clear that it improves JISP16 essentially

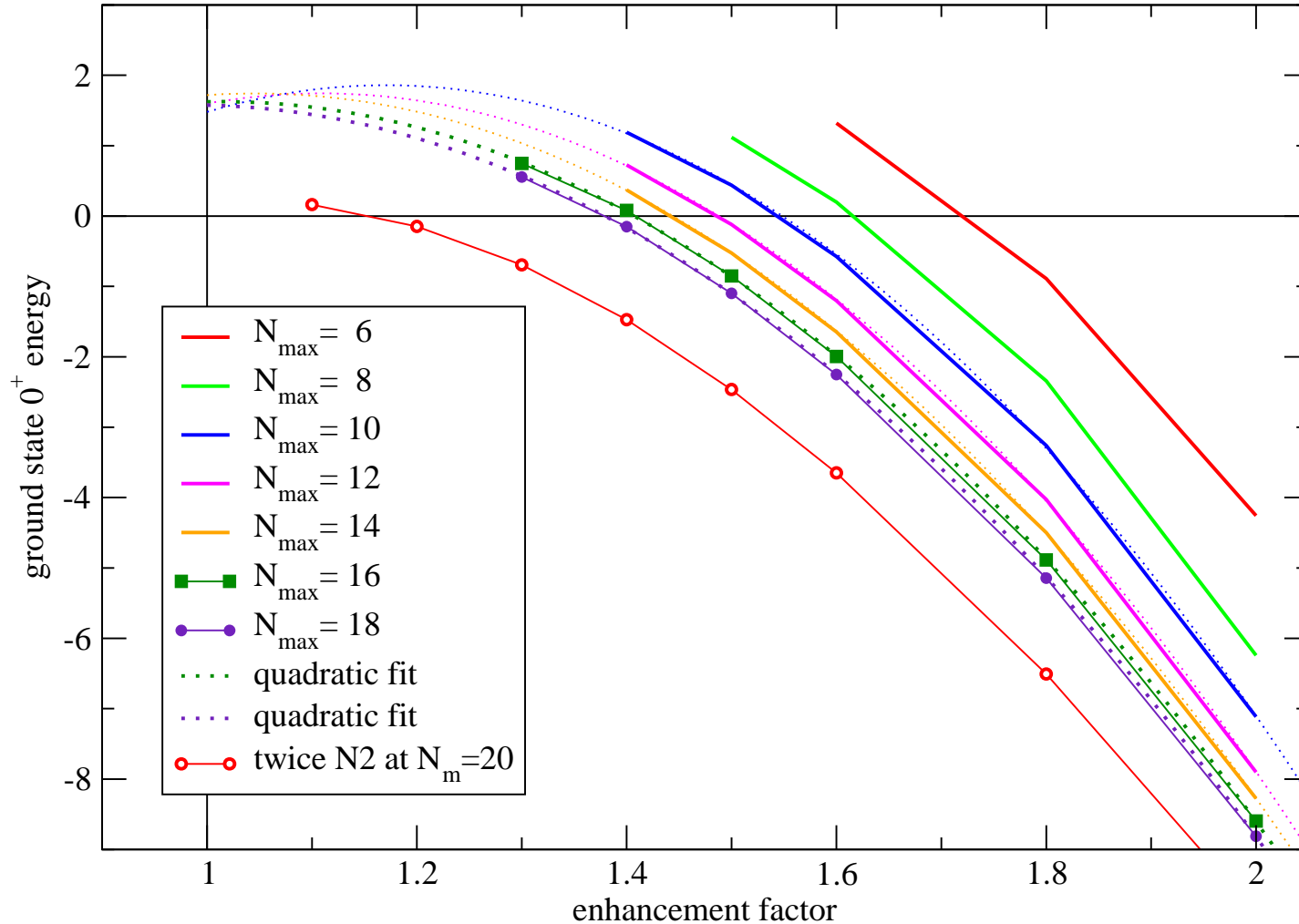
Tetraneutron

- * Interest from experimentalists
- * How to evaluate the energy of unbound $4n$ system?
- * Increase JISP16 to obtain bound 4 neutron state
- * Use NCSM to obtain ground state energy
- * Extrapolate to NN interaction without enhancement

Tetraneutron

4 neutrons with enhanced JISP16

variational min. (if there is a local var. min...) on available hw grid



Tetraneutron

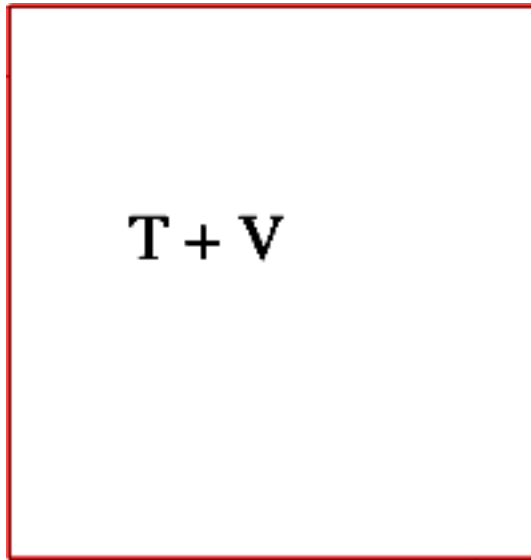
- * How to evaluate the energy of unbound $4n$ system?
- * Why not to try to do the same with PETs?
- * I. e. to bind $4n$ by PETs
- * and to leave unchanged ${}^4\text{He}$ binding...

Tetraneutron:

The power of PETs

- * It is possible!
- * Fits in small model spaces, hence not very accurate.
- * The PETted JISP16 provides the following NCFC extrapolated results:
- * ${}^4\text{He}$ energy: -29.634 MeV (exp. -28.296 MeV) + low-lying state $(J,T)=(3,1)$
- * ${}^3\text{H}$ energy: -8.231 MeV (exp. -8.482 MeV)
- * $3n$ unbound
- * $4n$: two bound states: $(J,T)=(2,2)$ at -14.1 MeV and $(J,T)=(0,2)$ at -6 MeV

J-matrix formalism: scattering in the oscillator basis



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 :

$$T_{nn} \sim n, T_{n,n\pm 1} \sim n, n \rightarrow \infty$$

while potential energy m. e. V_{nm} decrease with n and m .

$$\sum_{n'=0}^N H_{nn'}^l \langle n' | \lambda \rangle - E_\lambda \langle n | \lambda \rangle, \quad n \leq N.$$

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

$$S = \frac{C_{NI}^{(-)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^l C_{N+1,I}^{(-)}(q)}{C_{NI}^{(+)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^l C_{N+1,I}^{(+)}(q)},$$

T

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

Tetraneutron: J -matrix formalism

* Impossible to calculate all E_λ

$$\text{At } E = E_\lambda : S(E_\lambda) = \frac{C_{N+1,K}^{(-)}(E_\lambda)}{C_{N+1,K}^{(+)}(E_\lambda)}$$

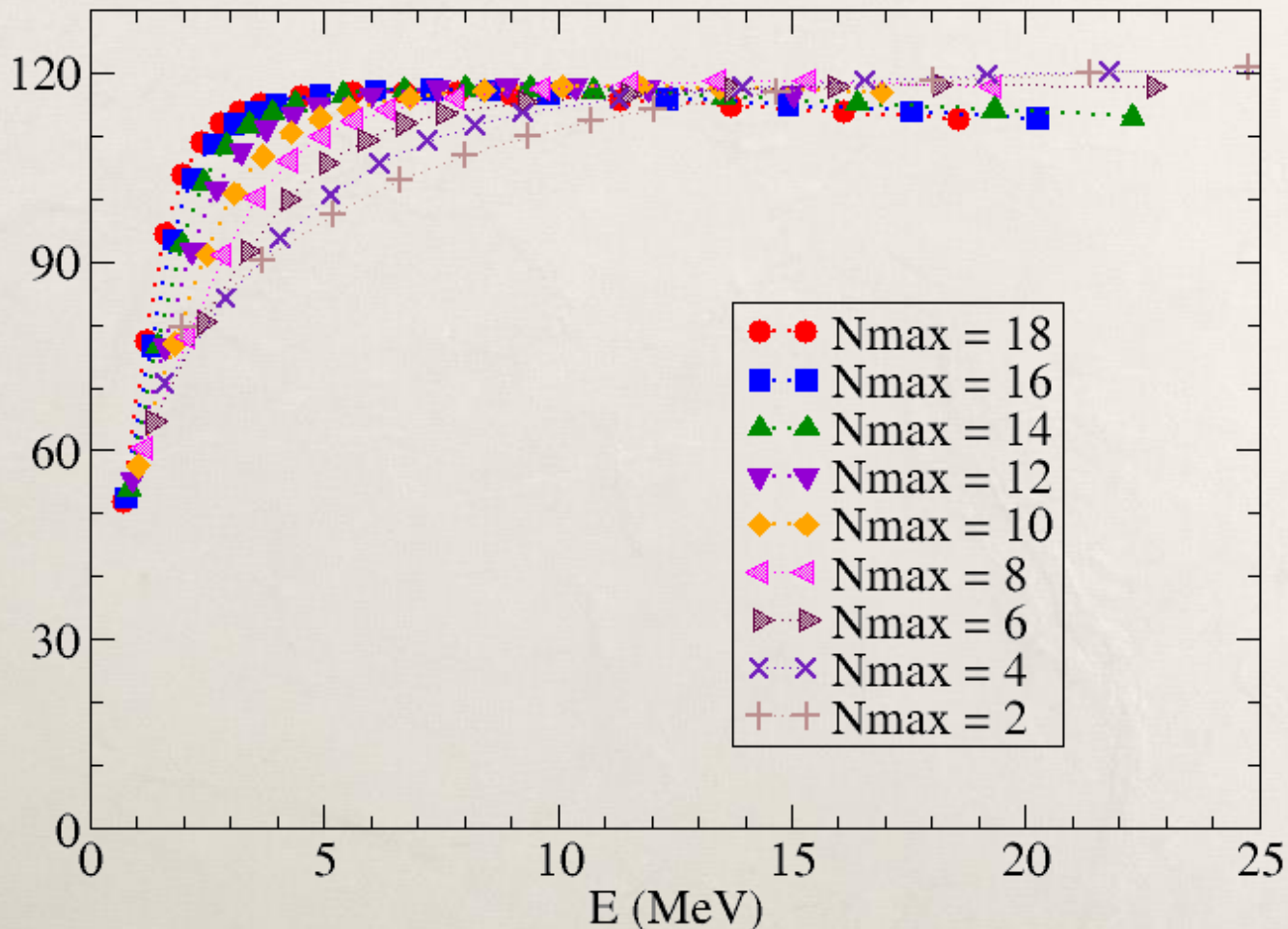
4-body decay, hyperspherical formalism, lowest possible hypermomentum K

In the vicinity of the resonance

$$S(E) = e^{2i\delta}$$
$$\delta(E) = \frac{\pi}{2} + \arctan \frac{E-b}{a\sqrt{E}} + c\sqrt{E}$$

a, b, c - fitting parameters

Tetraneutron: *J*-matrix formalism



$$E_r = 0.56 \text{ MeV}$$

$$\Gamma_r = 2.98 \text{ MeV}$$

Future

- * Involving more observables including resonance energies and widths
- * Improved JISP16₂₀₁₀ fitted also to nuclear matter
- * PETted N3LO to avoid use *NNN* forces
- * ...

Present

Thank you!