Daejeon16 NN interaction

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Nuclear Theory in the Supercomputing Era – 2018 (NTSE-2018)
IBS Headquarters, Daejeon, Korea
29 October – 2 November 2018

In collaboration with:
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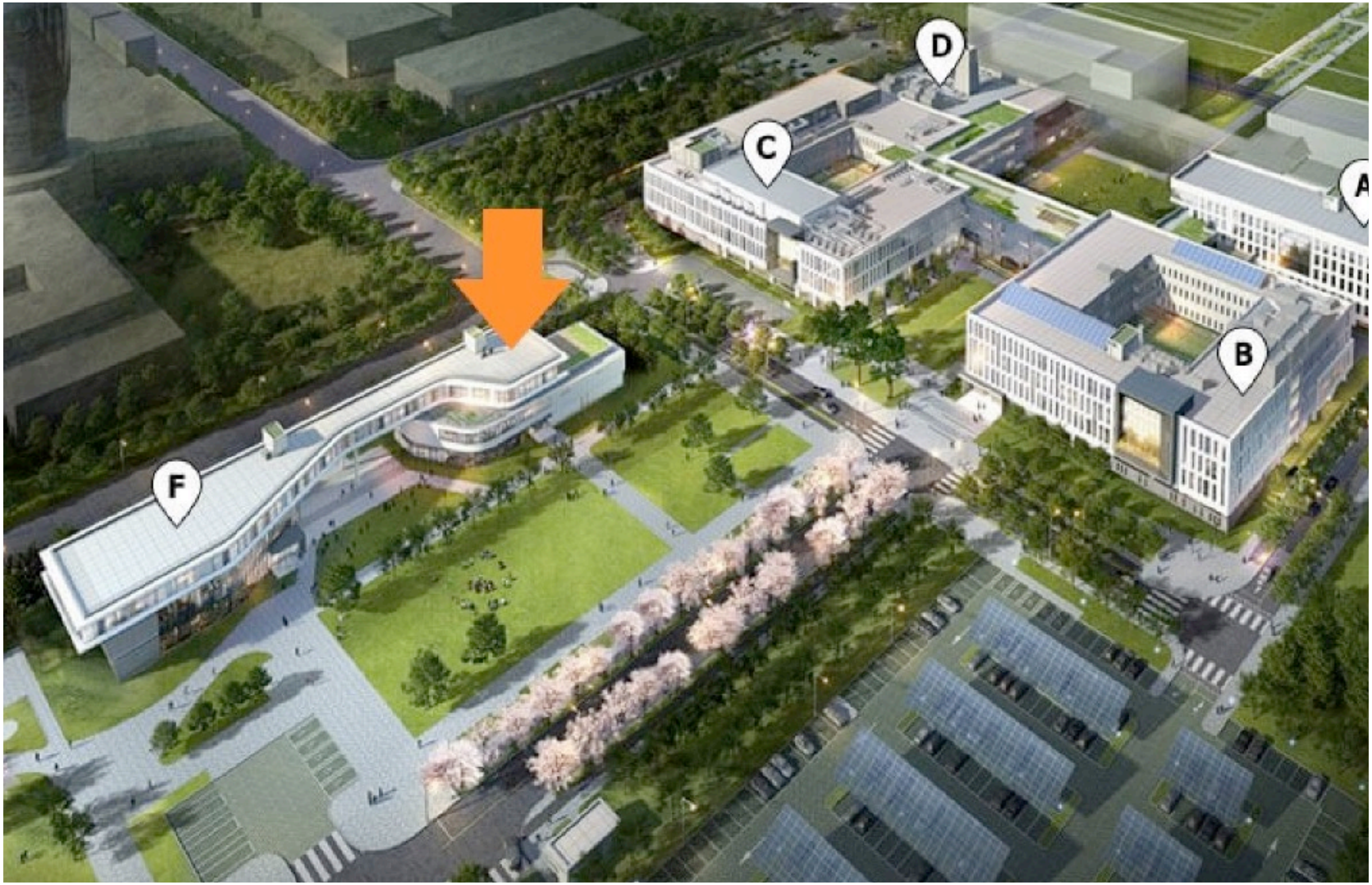
& more

Practical information on NTSE 2018

- Lunch at IBS cafeteria from 12:30. We may have to stick to the timetable, especially second morning sessions.
- Every participant (including your family) is cordially invited to the conference dinners : Today: simple Korean style dinner, from 7:00 pm the restaurant will provide transportation

  Wednesday: from 6:30pm after the excursion.
- Restaurant Guide is posted on the NTSE 2018 website
- Excursion to Gonju and RAON site we have enough seats for all of you (and also for your family).



B: theory building, IBS cafeteria

GongJu mountain fortress wall

무령왕릉 501-523

- **Please copy your talk files to the laptop before your session starts.**

Contents

- **Ab initio NCSM**

- **Daejeon 16**

  + some isotopes

  + parity inversion in ^{11}Be

  + tetra neutron

  + artificial neural network

  + nucleon-alpha scattering

  + microscopic effective shell-model interactions

Ab initio No Core Shell Model

- Ab initio: nuclei from first principles using fundamental interactions without uncontrolled approximations.
- No core: all nucleons are active, no inert core.
- Shell model: harmonic oscillator basis
- Point nucleons

- *A*-nucleon Schrödinger equation

$$\hat{H}\,\Psi(r_1,\cdots,r_A) = E\,\Psi(r_1,\cdots,r_A)$$

  - Hamiltonian with $NN(+NNN)$ interactions

$$\hat{H} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p_i}-\vec{p_j})^2}{2m} + \sum_{i<j}V_{ij} + \sum_{i<j<k}V_{ijk} + \cdots$$

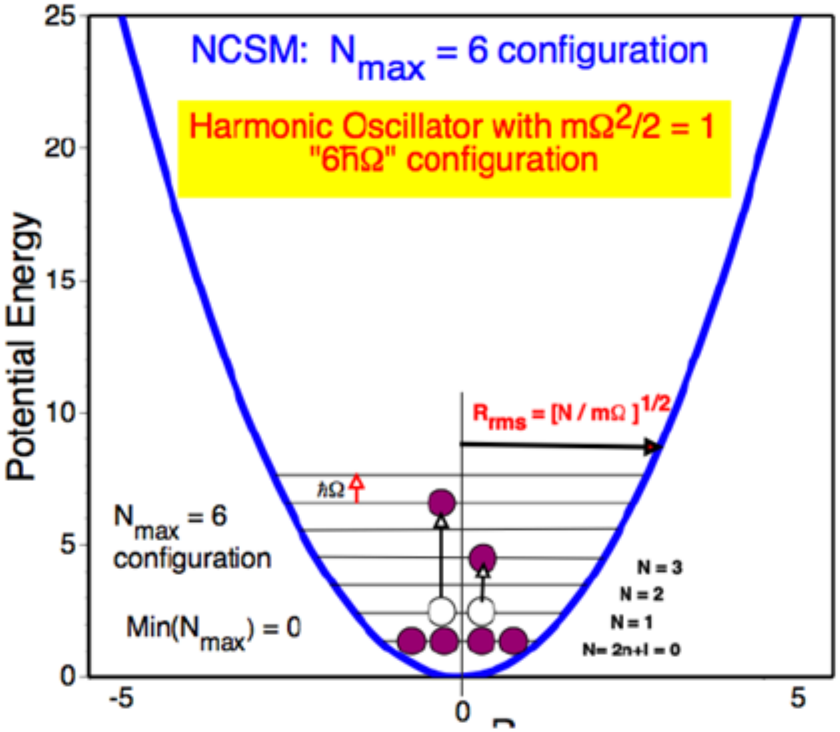
  - Wave functions are expanded in basis states

$$\Psi(r_1,\cdots,r_A) = \sum a_i\Phi_i(r_1,\cdots,r_A)$$

basis states Φ_i : Slater determinants of single particle states

- single particle states ϕ
  for radial wave functions, harmonic oscillators are used

$$\Rightarrow \Phi_i \sim \phi_1^{(i)} \times \phi_2^{(i)} \times \cdots \times \phi_A^{(i)}$$

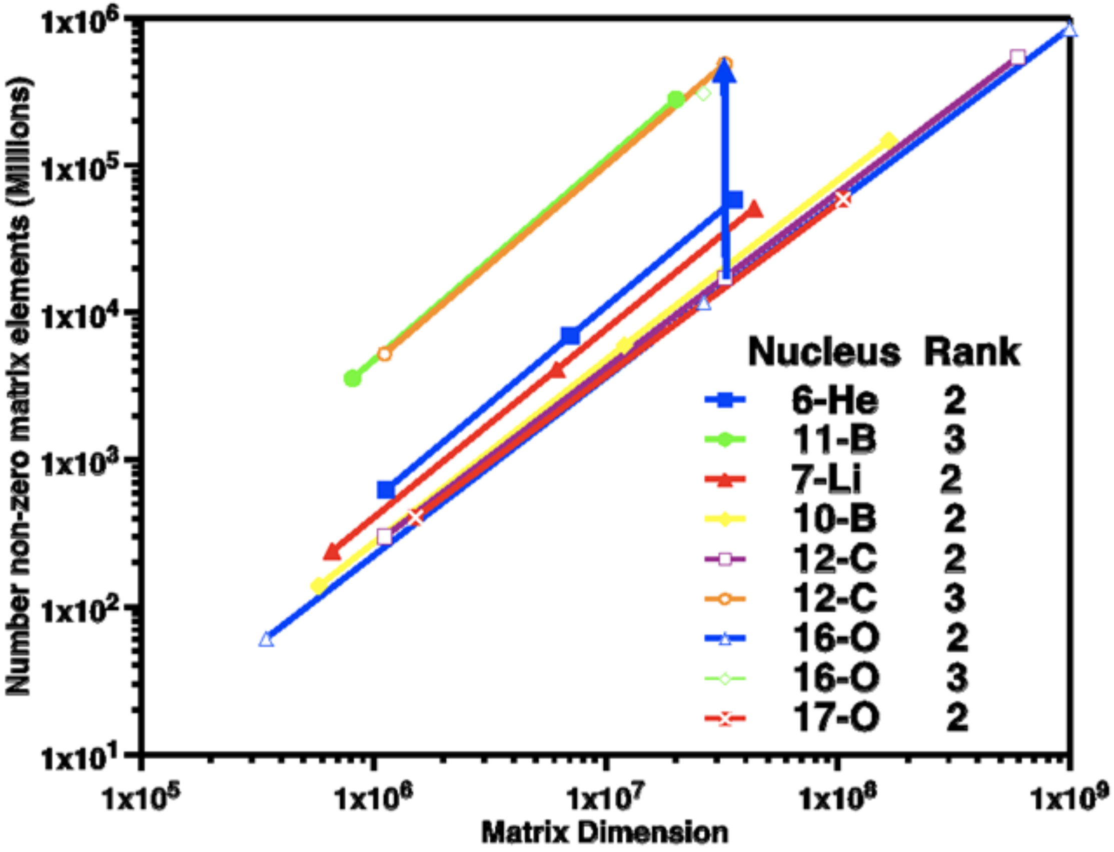


from the talk by J. Vary @ RISP, Mar. 2013

Ab initio structure and NN interaction

- Unfortunately, the NN interaction at low energies needed for nuclear physics applications cannot be directly derived from QCD at the moment
- Ab initio theory requires, of course, a realistic NN interaction accurately describing NN scattering data and deuteron properties
- Nice to avoid NNN forces? Yes

Why would be nice to avoid *NNN* forces?

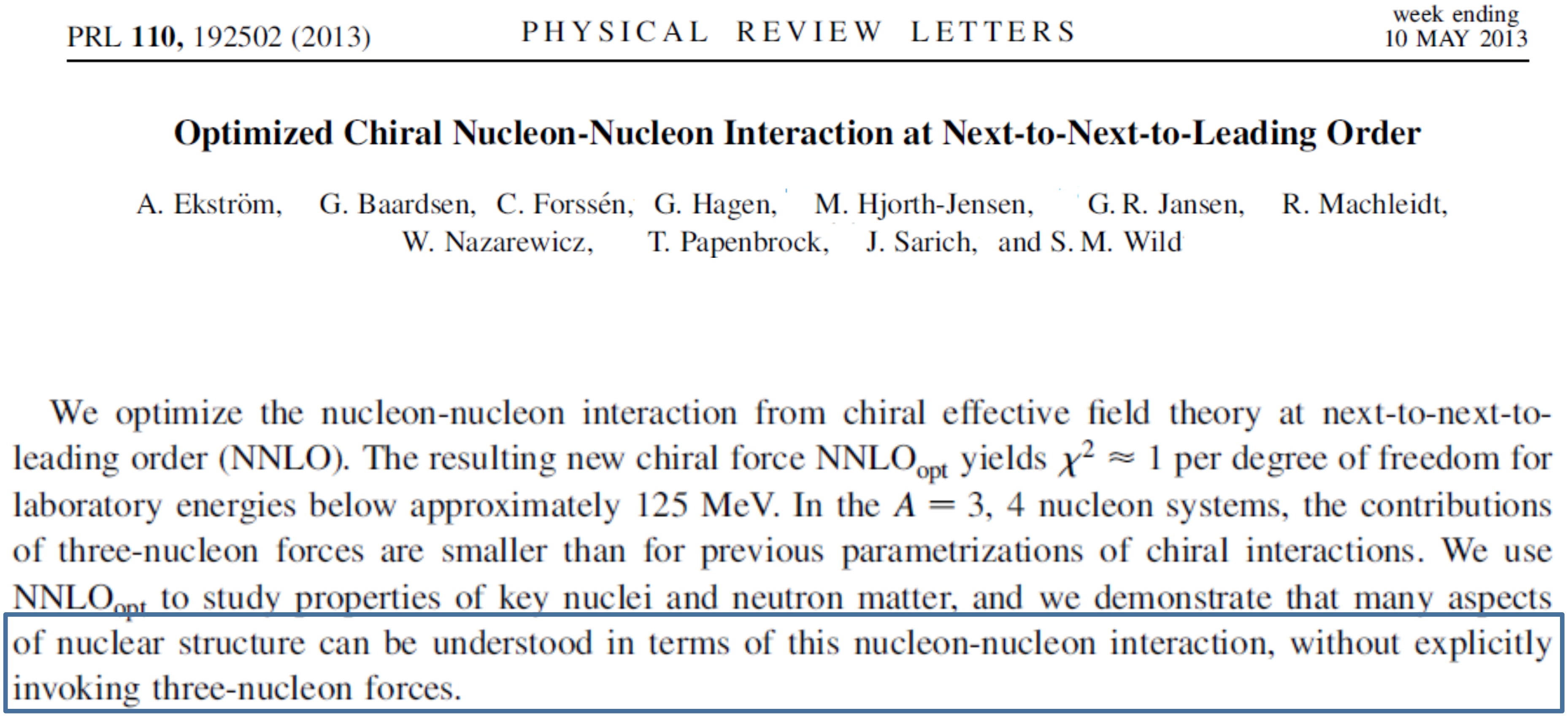


≈30 times more Hamiltonian matrix elements when *NNN* forces are involved; hence much more computer resources are required for calculations

(Andrey Shirokov)

^{6}Li

Ik Jae Shin, Y. Kim, P. Maris, J. P. Vary, C. Forssén, J. Rotureau, N. Michel,
J .Phys. G44, 075103 (2017)



PRL **110,** 192502 (2013) PHYSICAL REVIEW LETTERS week ending 10 MAY 2013

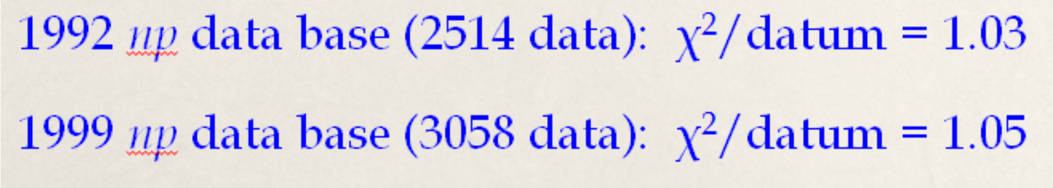
Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt,
W. Nazarewicz, T. Papenbrock, J. Sarich, and S. M. Wild

We optimize the nucleon-nucleon interaction from chiral effective field theory at next-to-next-to-leading order (NNLO). The resulting new chiral force $\mathrm{NNLO_{opt}}$ yields $\chi^2 \approx 1$ per degree of freedom for laboratory energies below approximately 125 MeV. In the $A = 3, 4$ nucleon systems, the contributions of three-nucleon forces are smaller than for previous parametrizations of chiral interactions. We use $\mathrm{NNLO_{opt}}$ to study properties of key nuclei and neutron matter, and we demonstrate that many aspects of nuclear structure can be understood in terms of this nucleon-nucleon interaction, without explicitly invoking three-nucleon forces.

JISP (J-matrix Inverse Scattering Potential)

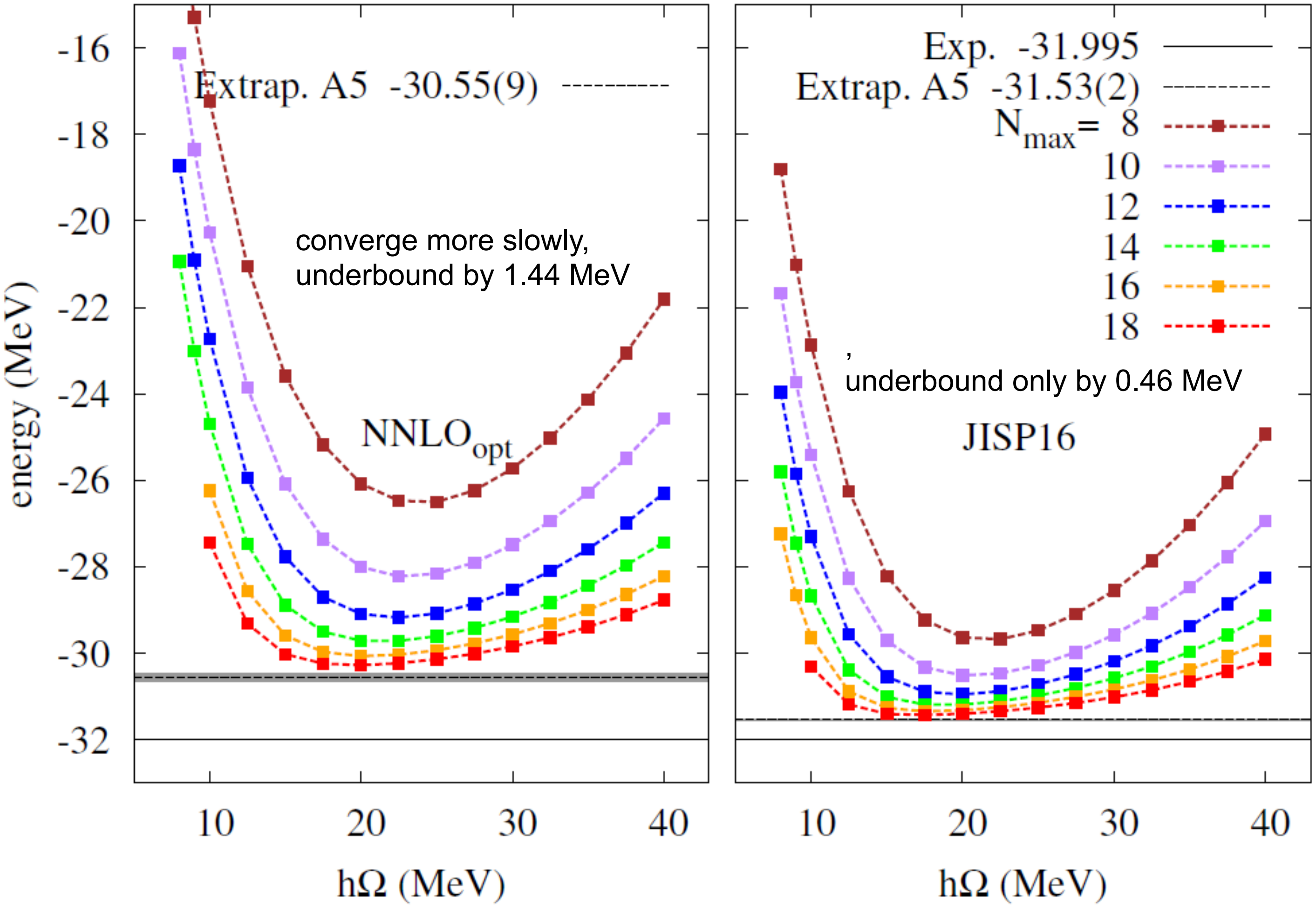
- completely phenomenological
- provides a good convergence of many-body calculations, eff. interaction is not needed
- fitted to describe light nuclei: JISP6 up to A = 6, JISP16 up to A = 16
- provides a high-quality description of NN data: chi^2/datum = 1.03 up to E_{lab} = 350 MeV for the 1992 np data base (Andrey Shirokov)



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

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

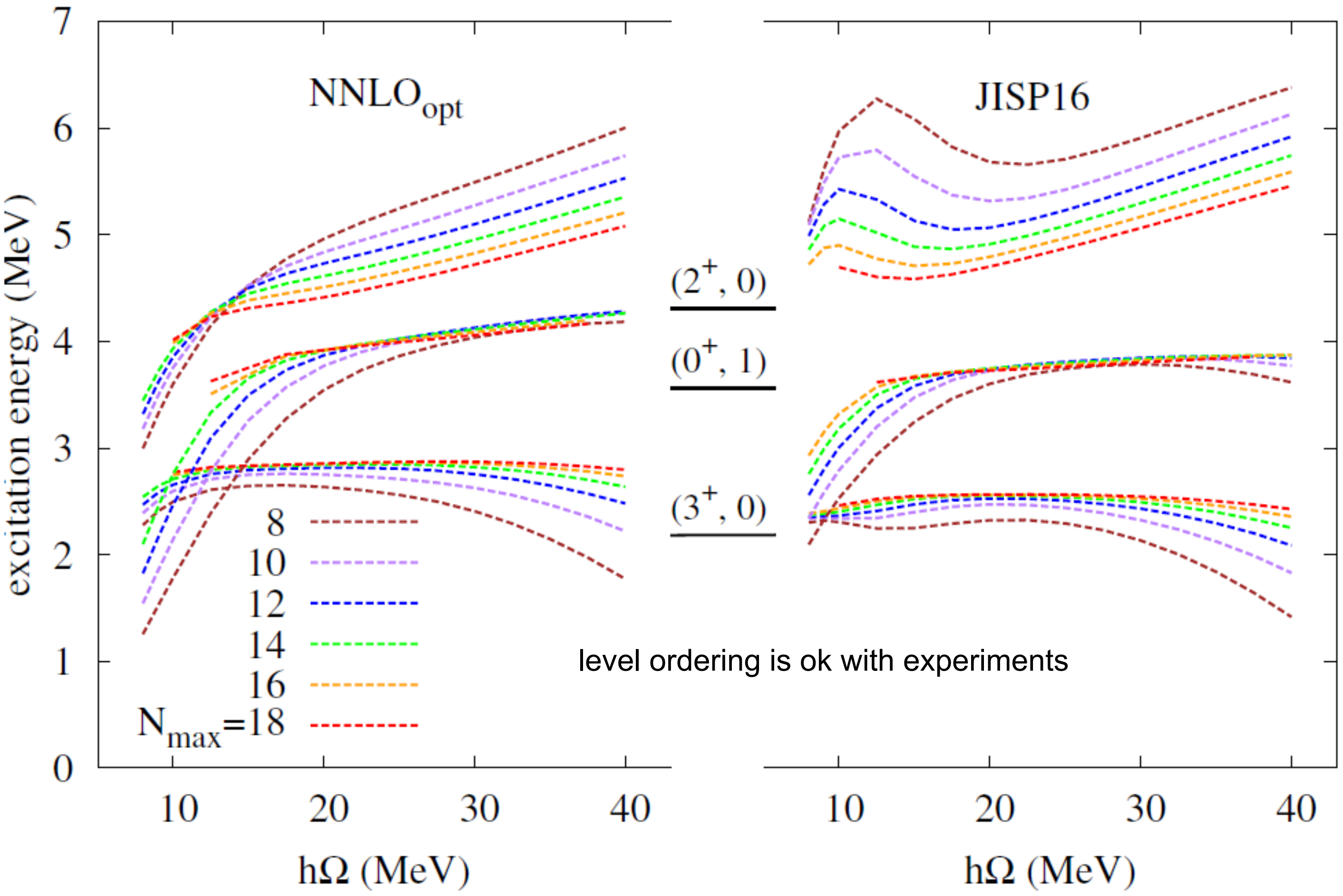
A. M. Shirokov, A. I. Mazur, S. A. Zaytsev, J. P. Vary, T. A. Weber, Phys. Rev. C 70, 044005 (2004)
A. M. Shirokov, J. P. Vary, A. I. Mazur, S. A. Zaytsev, T. A. Weber, Phys. Lett. B 621, 96 (2005)
A. M. Shirokov, J. P. Vary, A. I. Mazur, T. A. Weber, Phys. Lett. B 644, 33 (2007)



converge more slowly, underbound by 1.44 MeV

, underbound only by 0.46 MeV

The ground state energy of ^{6}Li calculated with NNLO$_{opt}$ and JISP16 as a function of the HO energy



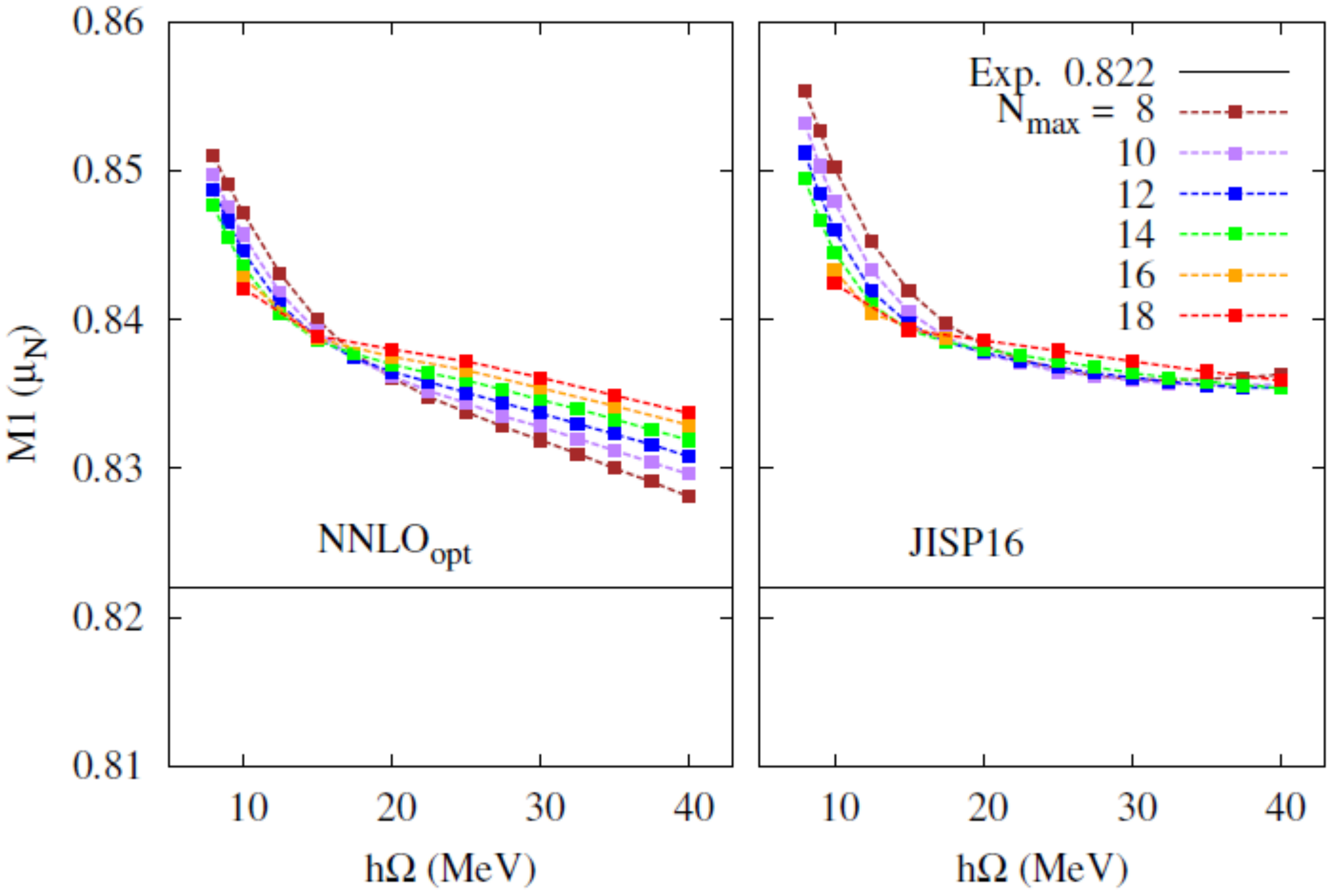
level ordering is ok with experiments

1.3 MeV

8.2 eV

24 keV

Excitation energies for the three lowest natural parity excited states of ^{6}Li



Magnetic dipole moment of the ground state of ^{6}Li as a function of the HO energy

Both are within 2% of the experimental value

^{6}Li	Exp.	NNLO$_{\mathrm{opt}}$	JISP16	JISP16*	AV18/IL2
$E_{\mathrm{gs}}(1^+,0)$	31.995	30.55(9)	31.53(2)	31.49(3)	32.0(1)
$\langle r_{pp}^2\rangle^{1/2}$	2.38(3)	2.40(3)	2.28(3)	2.3	2.39(1)
$E_{\mathrm{x}}(3^+,0)$	2.186(2)	2.843(1)	2.560(3)	2.56(2)	2.2(2)
$E_{\mathrm{x}}(0^+,1)$	3.56(1)	3.879(15)	3.708(6)	3.68(6)	3.4(2)
$E_{\mathrm{x}}(2^+,0)$	4.312(22)	4.36(9)	4.63(10)	4.5(3)	4.2(2)
$E_{\mathrm{x}}(2^+,1)$	5.366(15)	6.19(6)	6.07(6)	5.9(2)	5.5(2)
$Q(1^+,0)$	-0.082(2)	-0.032(7)	-0.078(3)	-0.077(5)	-0.32(6)
$Q(3^+,0)$	-	-5.1(3)	-4.8(2)	-4.9	
$\mu(1^+,0)$	0.822	$0.8380(5)^{\dagger}$	0.8389(2)	0.839(2)	0.800(1)
$\mu(3^+,0)$	-	$1.8607(1)^{\dagger}$	1.8654(1)	1.866(2)	
B(E2;$(3^+,0)$)	10.7(8)	6.4(6)	5.8(4)	6.1	11.65(13)
B(E2;$(2^+,0)$)	4.4(23)	$6.6(7)^{\dagger}$	6.7(7)	7.5	8.66(47)
B(M1;$(0^+,1)$)	15.43(32)	14.59(8)	14.25(4)	14.2(1)	15.02(11)
B(M1;$(2^+,1)$)	0.15	0.031(3)	0.042(3)	0.05(1)	
M_{GT}	2.170	2.260(4)	2.225(2)	2.227(2)	2.18(3)

Experimental results for ^{6}Li observables and corresponding theoretical results

Daejeon 16

"N3LO NN interaction adjusted to light nuclei in ab exitu approach,"
A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris, J.P. Vary, PLB761 (2016) 87

- Unfortunately, the NN interaction at low energies needed for nuclear physics applications cannot be directly derived from QCD at the moment
- Ab initio theory (NCSM in our case) requires, of course, a realistic NN interaction accurately describing NN scattering data and deuteron properties
- NNN requires a significant increase of computational resources, e.g. by a factor of 30 in the case of p-shell nuclei
- Nice to avoid NNN forces? Yes

Daejeon 16

- We use phase-equivalent transformations to adjust off-shell properties of similarity renormalization group evolved chiral effective field theory NN interaction (Idaho N3LO) to describe binding energies and spectra of light nuclei without NNN forces.

PET (phase equivalent transformation)

- Assume unitary matrix [U] has only a finite matrix mixing of a few selected basis function. Then H and H' have identical eigenvalues, and also asymptotic behavior of their eigenvector wave functions are same.

✓ do not change scattering phase shifts and bound state energies of two-body system

✓ but are supposed to modify two-body bound state observables such as the rms radius and electromagnetic moments

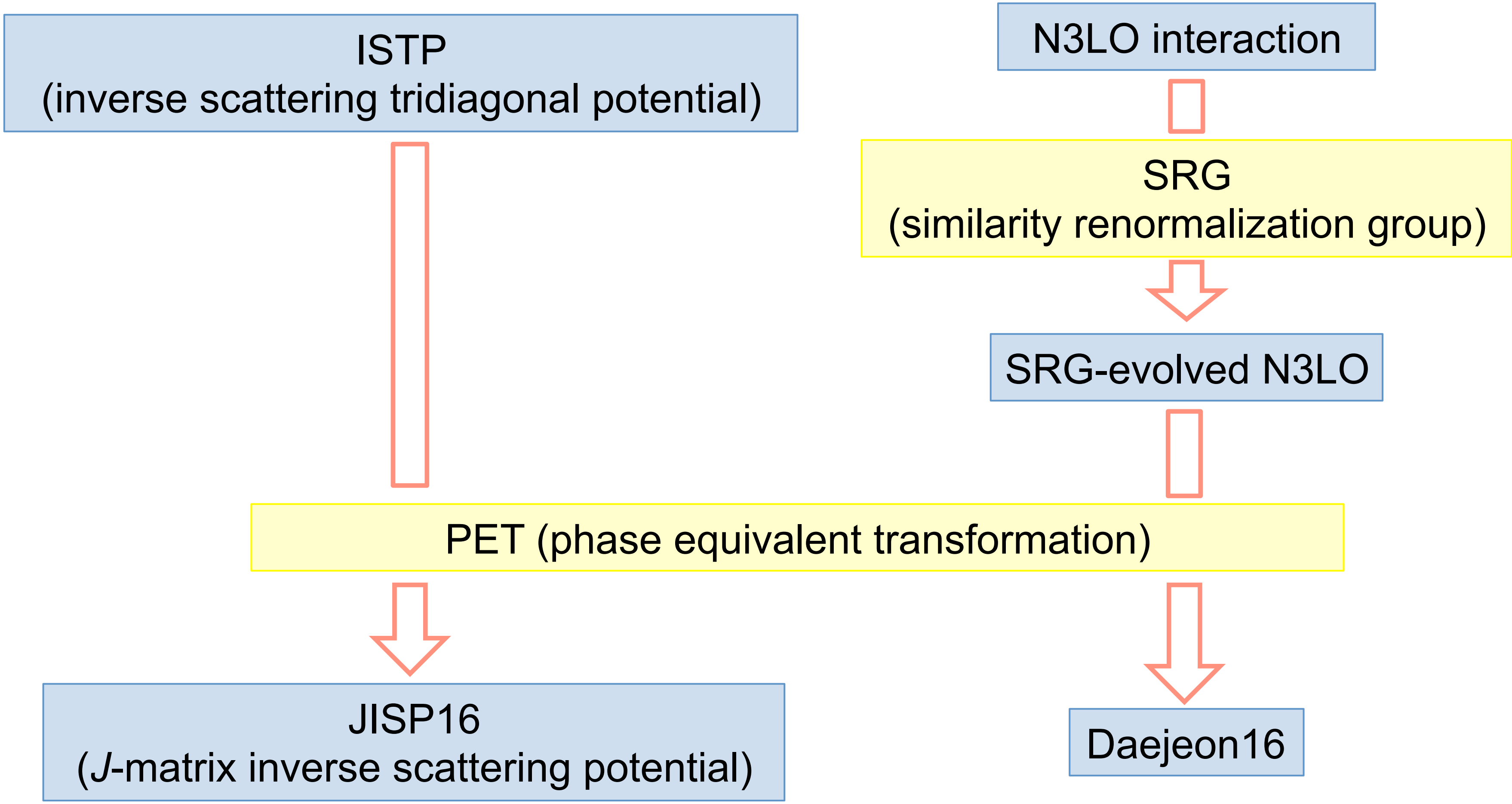
ex) JISP16 [A.M. Shirokov, J.P. Vary, A.I. Mazur and T.A. Weber, Phys. Lett. B 644 (2007) 33]

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

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

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

JISP16 vs Daejeon16



ISTP
(inverse scattering tridiagonal potential)

N3LO interaction

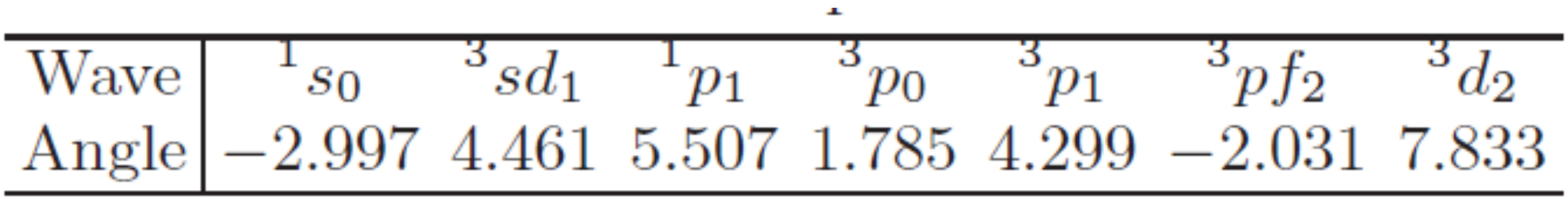
SRG
(similarity renormalization group)

SRG-evolved N3LO

PET (phase equivalent transformation)

JISP16
(*J*-matrix inverse scattering potential)

Daejeon16



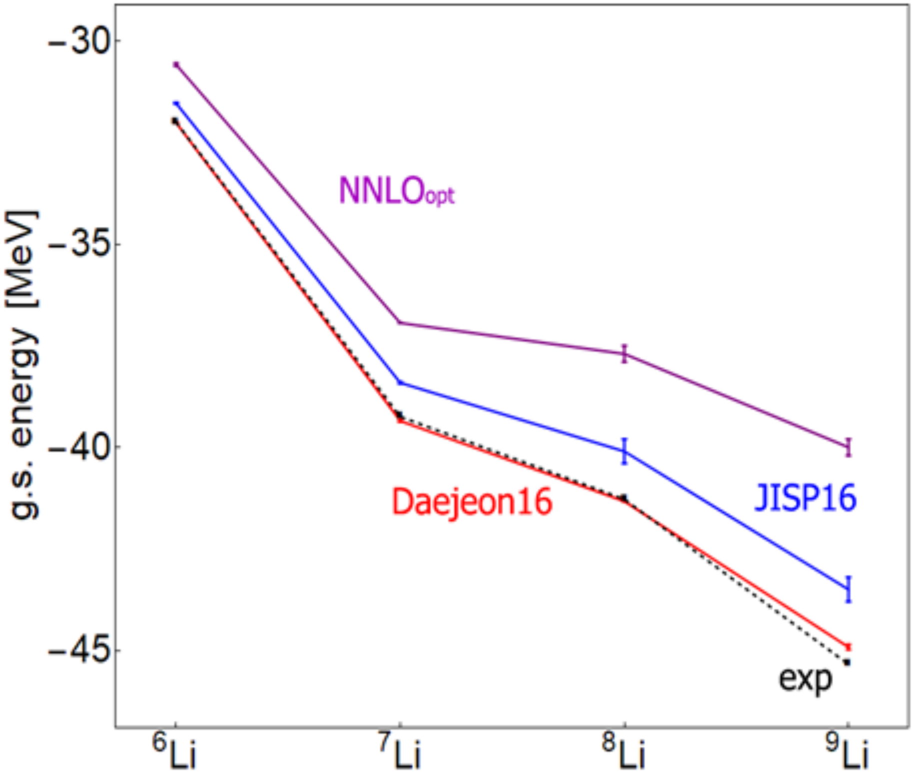
Wave	$^1s_0$	$^3sd_1$	$^1p_1$	$^3p_0$	$^3p_1$	$^3pf_2$	$^3d_2$
Angle	-2.997	4.461	5.507	1.785	4.299	-2.031	7.833

PET angles (in degrees) defining the Daejeon16 NN interaction in various NN partial waves.

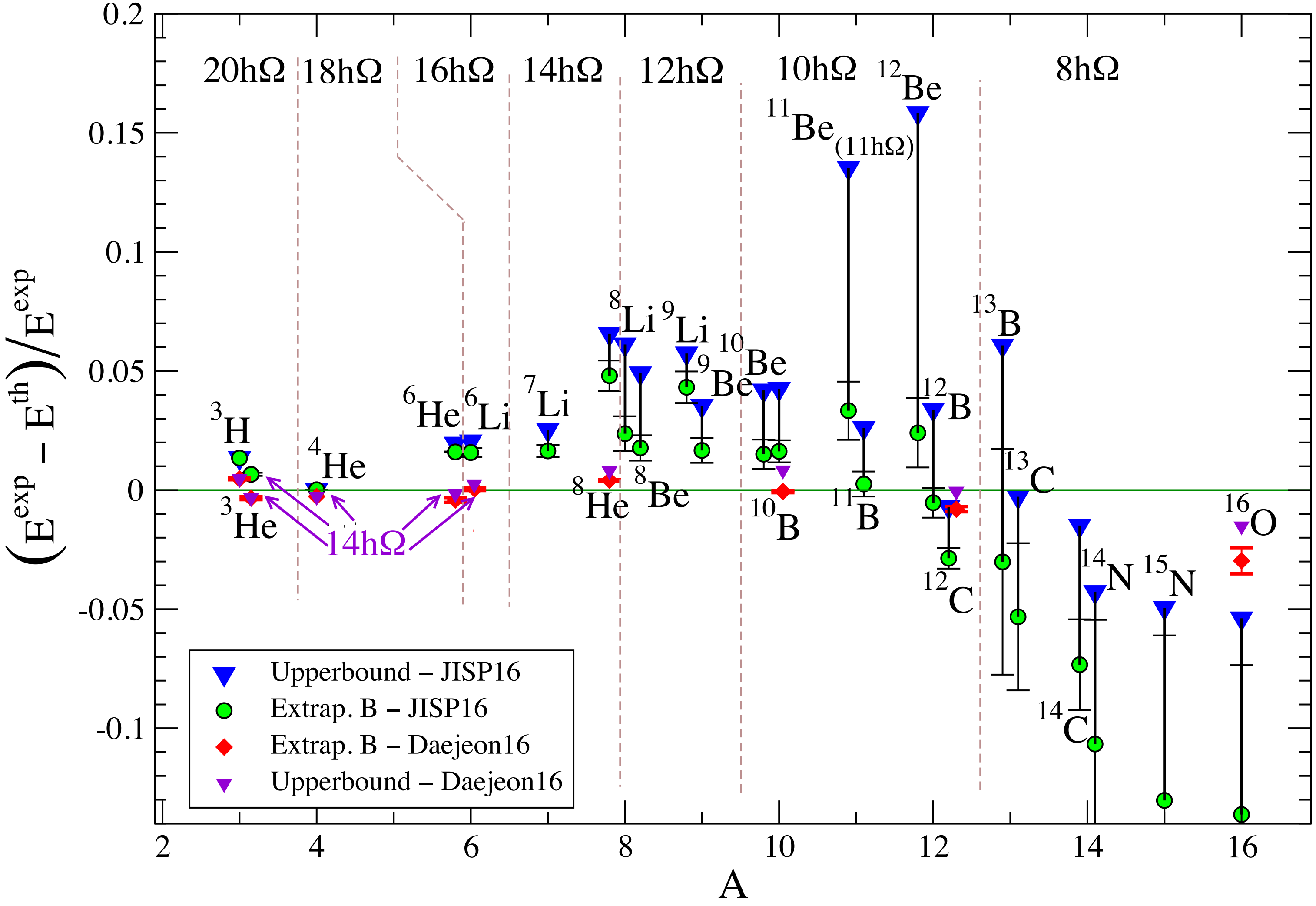
- binding energies of ^{3}H, ^{4}He, ^{6}Li, ^{8}He, ^{10}B, ^{12}C, ^{16}O
- excitation energies of ^{6}Li [$(3^+,0)$, $(0^+,1)$], ^{10}B[$(1^+,0)$], ^{12}C[$(2^+,0)$]

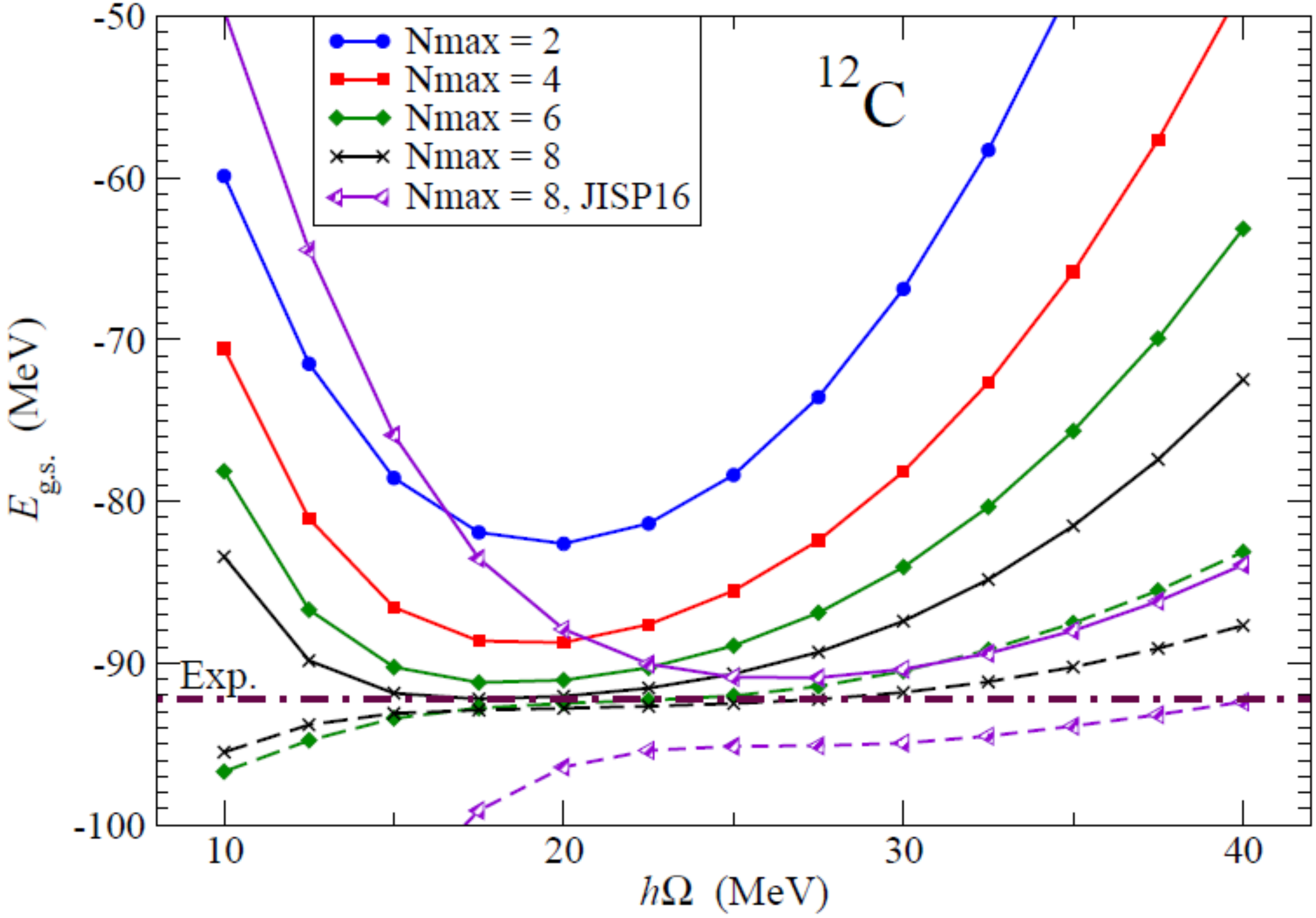
Ground state energies of Li isotopes

calculated w/ JISP16, $\mathrm{NNLO_{opt}}$ and Daejeon16 compared to experimental data.

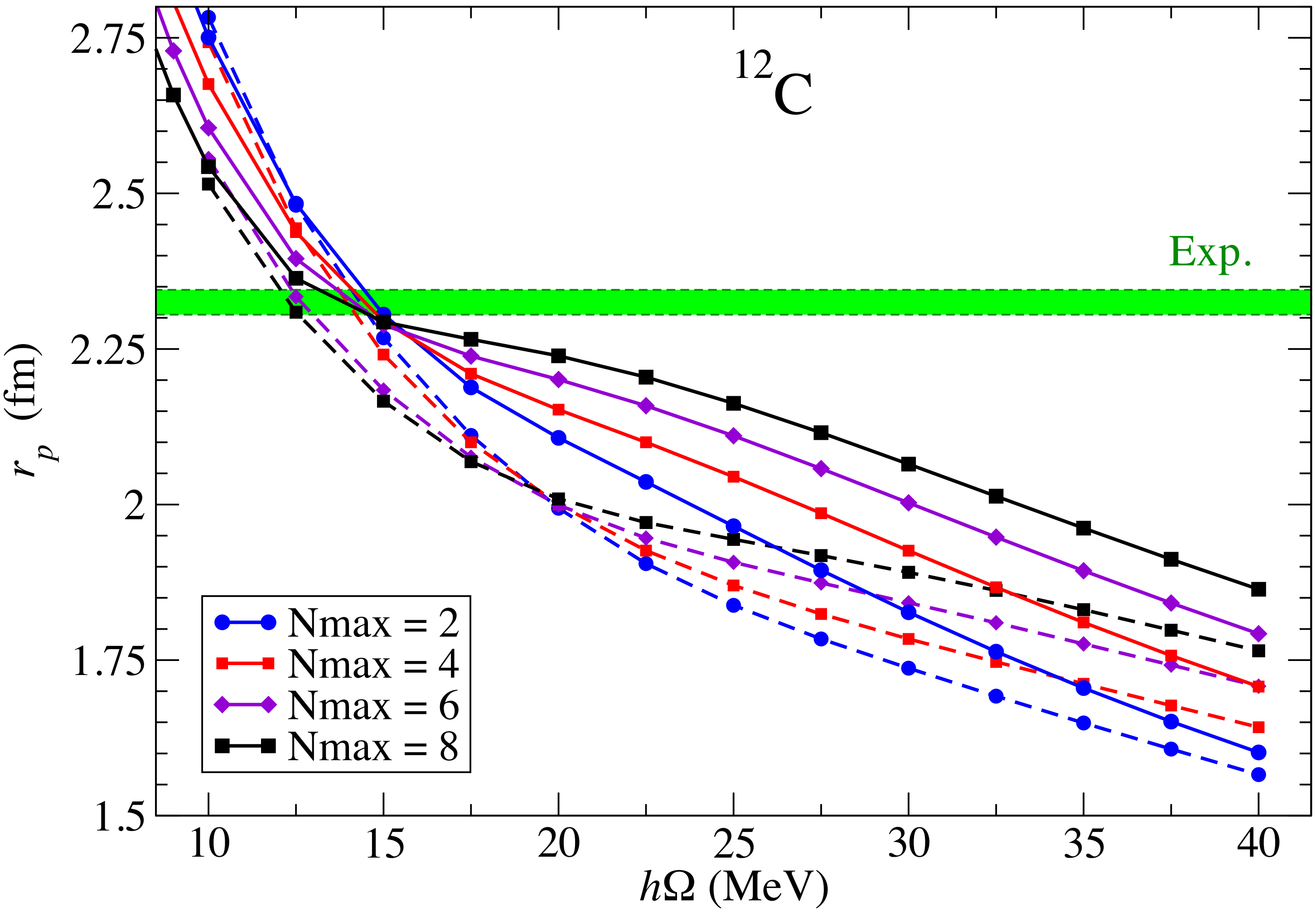


- Daejeon16 shows more excellent description for the binding energies of Lithium isotopes than $\mathrm{NNLO_{opt}}$ (from the first principle) and JISP16 (phenomenological.)
- For each result, extrapolation is adopted.
- ^{6}Li : ~N_{max}=18
  ^{7}Li ~ ^{9}Li : ~N_{max}=10

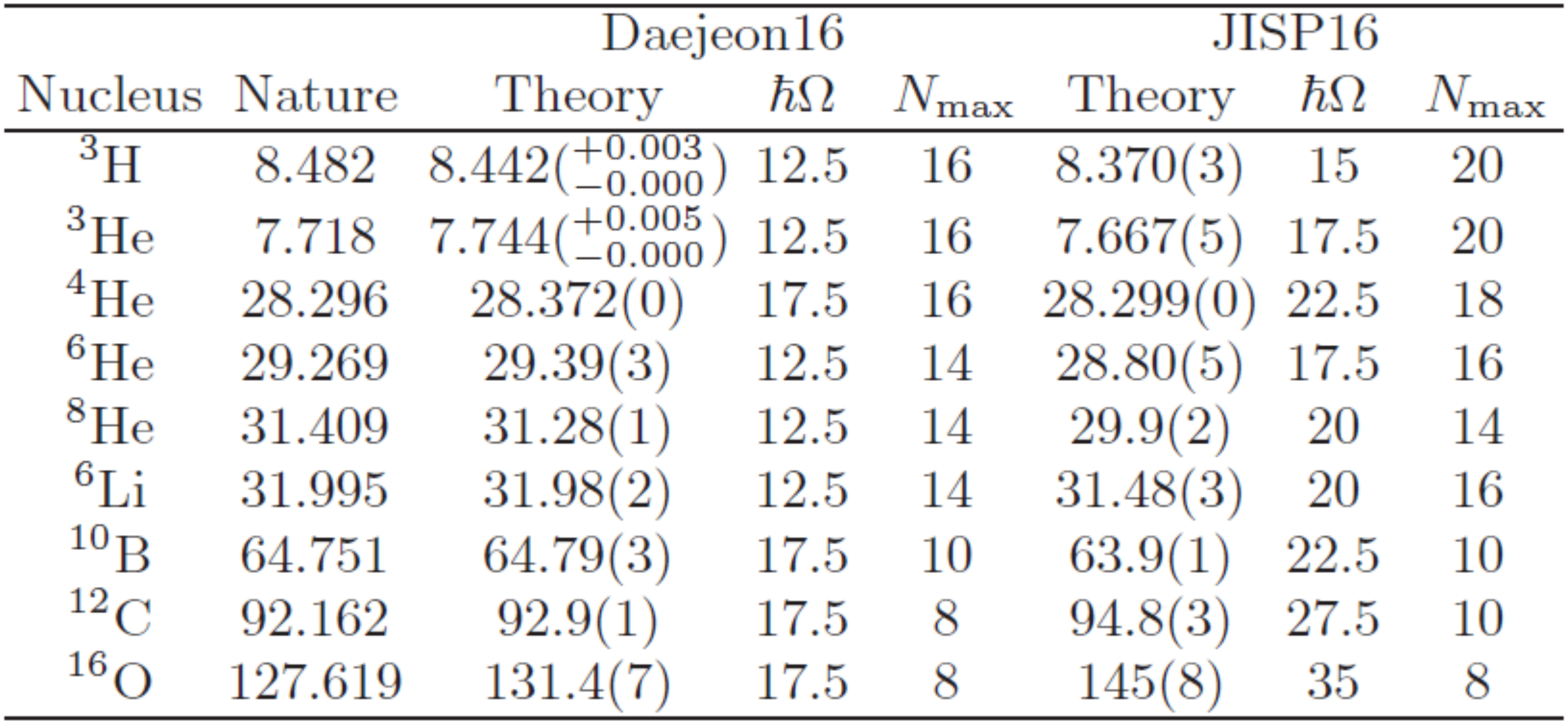

$(E^{exp} - E^{th})/E^{exp}$
A
0.2
0.15
0.1
0.05
0
-0.05
-0.1
2
4
6
8
10
12
14
16
20hΩ
18hΩ
16hΩ
14hΩ
12hΩ
10hΩ
8hΩ
14hΩ
11hΩ
^{3}H
^{3}He
^{4}He
^{6}He
^{6}Li
^{7}Li
^{8}He
^{8}Li
^{8}Be
^{9}Li
^{9}Be
^{10}Be
^{10}B
^{11}Be$_{(11h\Omega)}$
^{11}B
^{12}Be
^{12}B
^{12}C
^{13}B
^{13}C
^{14}C
^{14}N
^{15}N
^{16}O
Upperbound – JISP16
Extrap. B – JISP16
Extrap. B – Daejeon16
Upperbound – Daejeon16



^{12}C ground state energy in NCSM calculations obtained with Daejeon16 NN interaction



^{12}C
Exp.
r_p (fm)
$h\Omega$ (MeV)
Nmax = 2
Nmax = 4
Nmax = 6
Nmax = 8
2.75
2.5
2.25
2
1.75
1.5
10
15
20
25
30
35
40

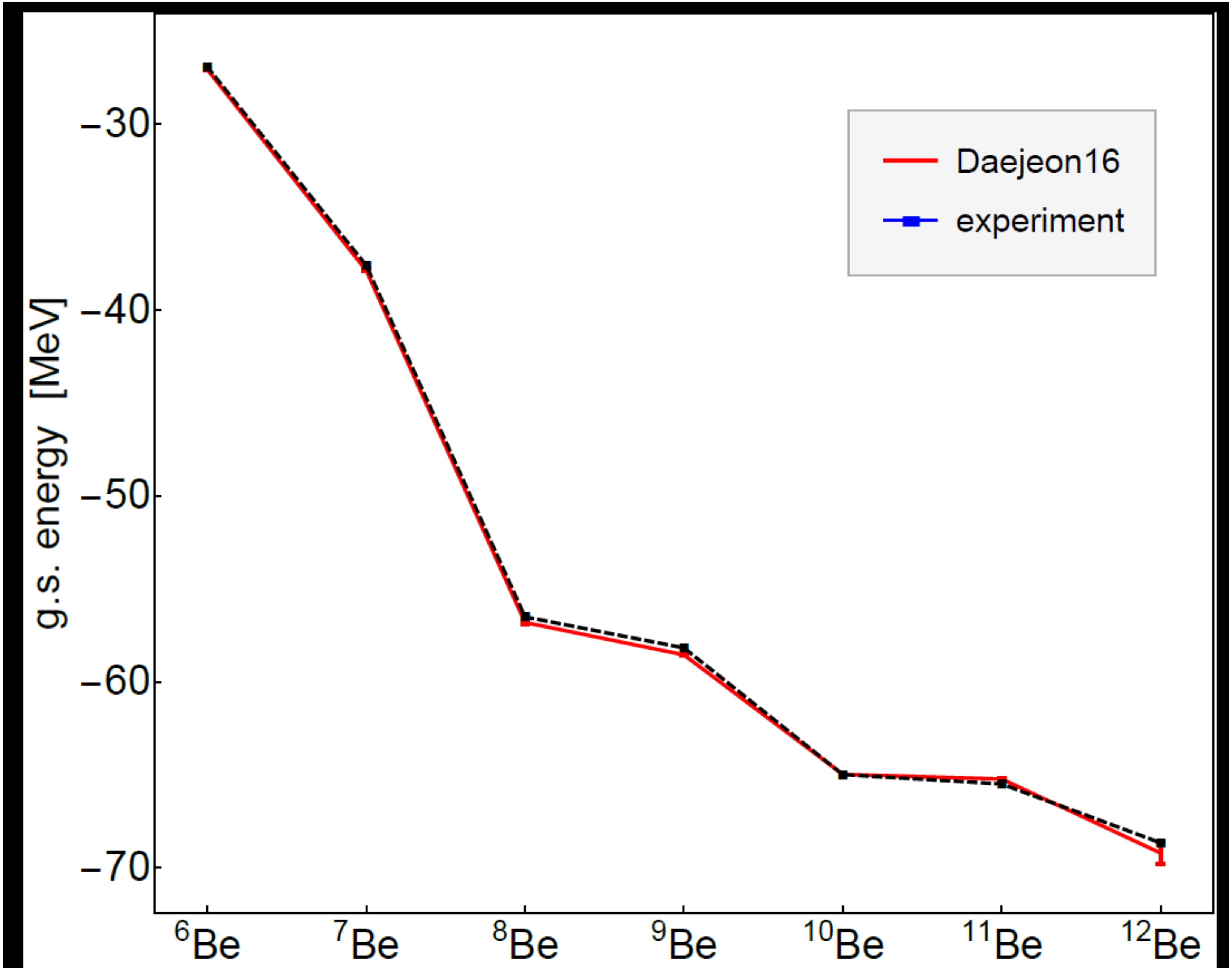


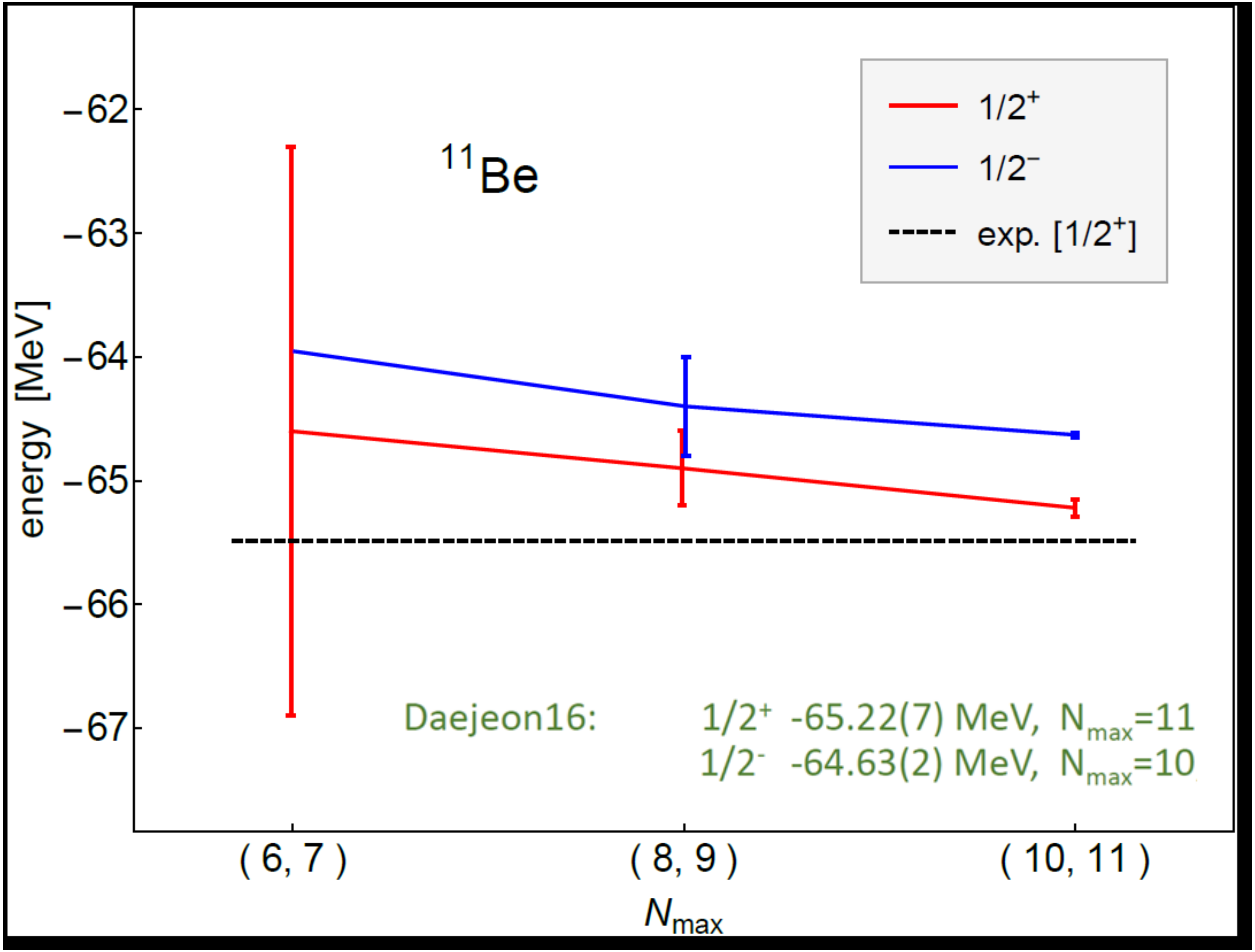
		Daejeon16			JISP16		
Nucleus	Nature	Theory	$\hbar\Omega$	$N_{\max}$	Theory	$\hbar\Omega$	$N_{\max}$
^{3}H	8.482	$8.442(^{+0.003}_{-0.000})$	12.5	16	8.370(3)	15	20
^{3}He	7.718	$7.744(^{+0.005}_{-0.000})$	12.5	16	7.667(5)	17.5	20
^{4}He	28.296	28.372(0)	17.5	16	28.299(0)	22.5	18
^{6}He	29.269	29.39(3)	12.5	14	28.80(5)	17.5	16
^{8}He	31.409	31.28(1)	12.5	14	29.9(2)	20	14
^{6}Li	31.995	31.98(2)	12.5	14	31.48(3)	20	16
^{10}B	64.751	64.79(3)	17.5	10	63.9(1)	22.5	10
^{12}C	92.162	92.9(1)	17.5	8	94.8(3)	27.5	10
^{16}O	127.619	131.4(7)	17.5	8	145(8)	35	8

Binding energies (in MeV) of nuclei obtained with Daejeon16 NN interaction using Extrapolation B with estimated uncertainty of the extrapolation.

Parity Inversion in ^{11}Be

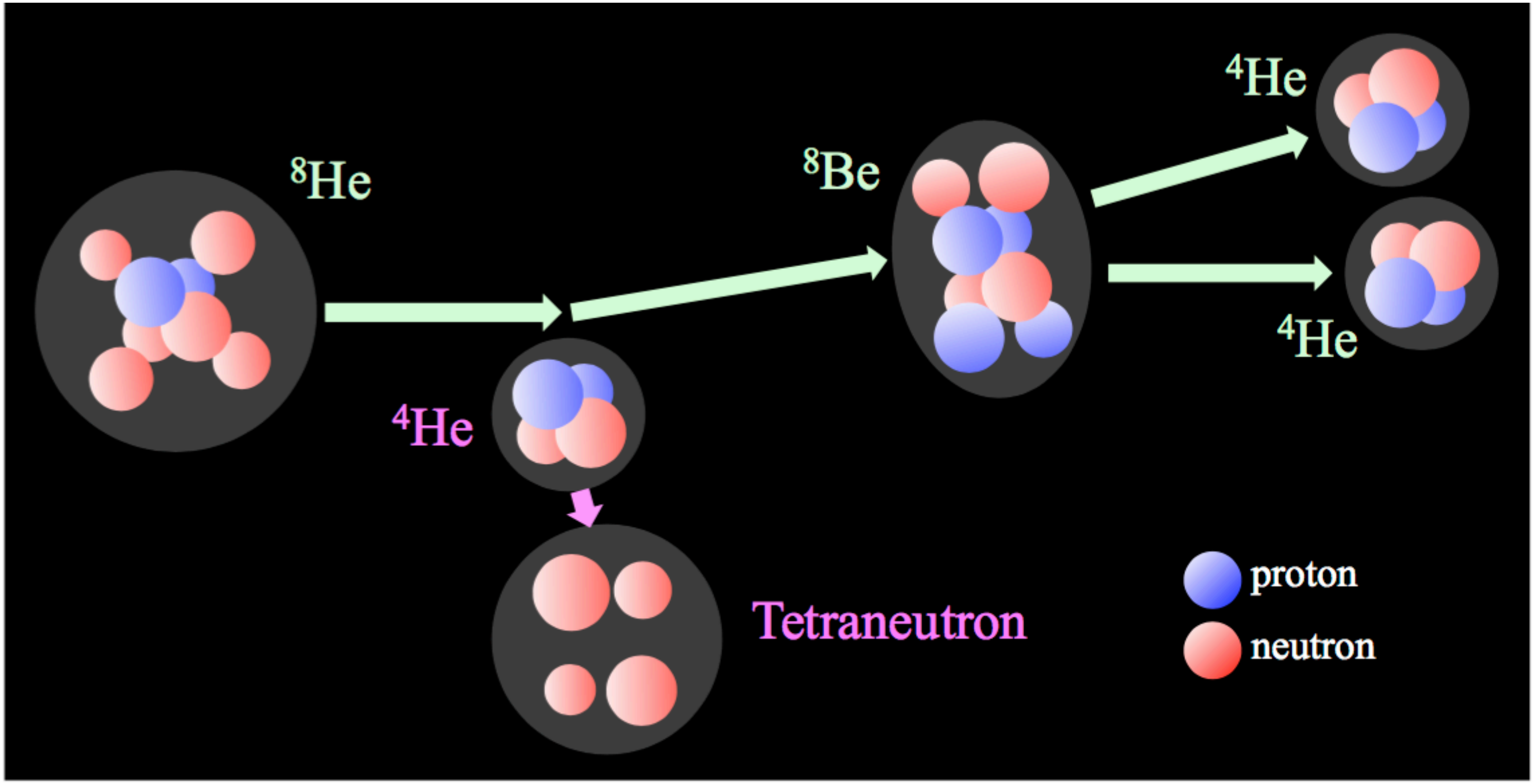
- Experimentally: $1/2^+$ -65.483(6) MeV
  $1/2^-$ -65.165(7) MeV, Exc. energy 0.318(7) MeV
- JISP16: $1/2^+$ -63.3(8) MeV, N_{max}=11
  $1/2^-$ -64.0(6) MeV, N_{max}=10


g.s. energy [MeV]
−30
−40
−50
−60
−70
^{6}Be
^{7}Be
^{8}Be
^{9}Be
^{10}Be
^{11}Be
^{12}Be
Daejeon16
experiment

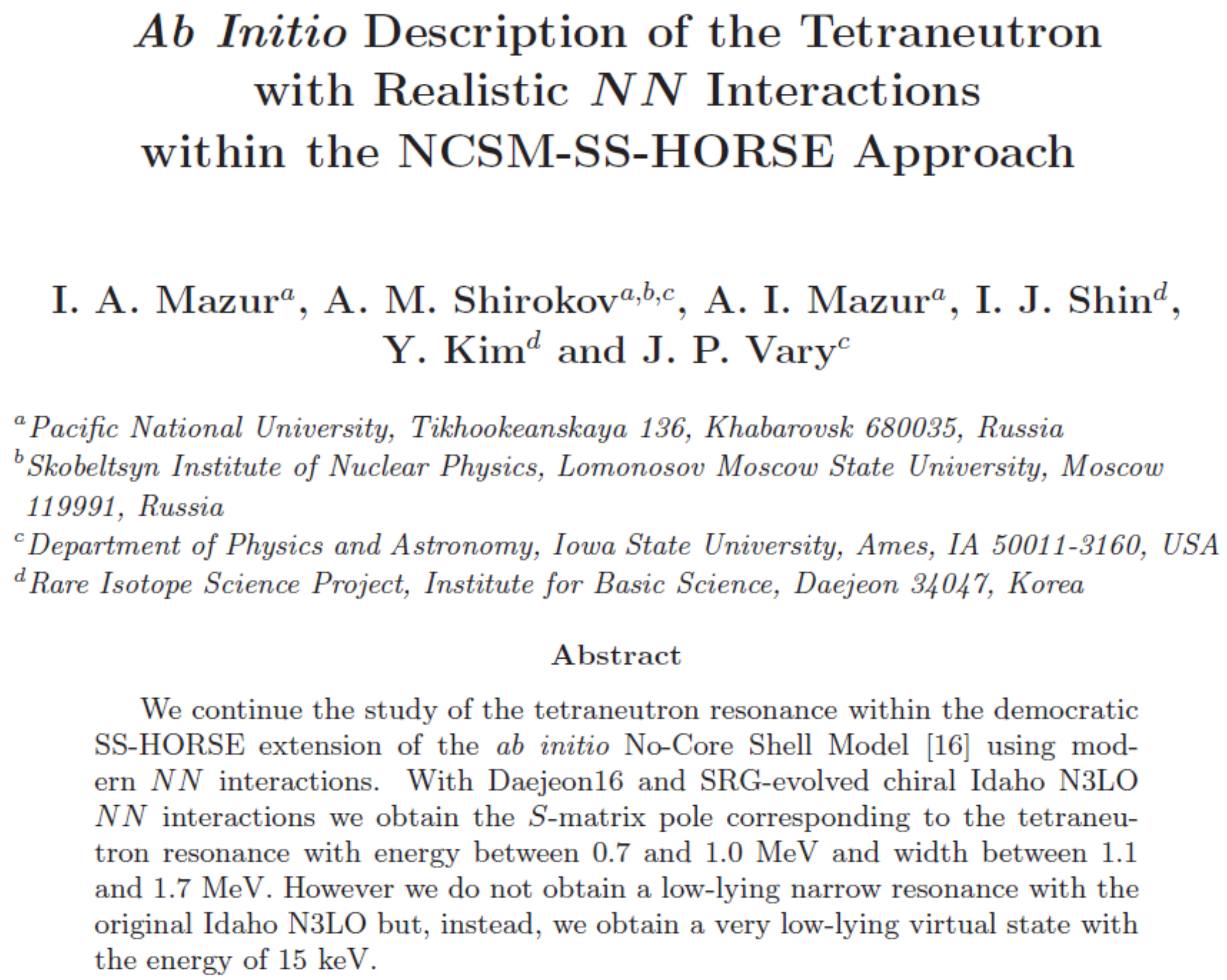


Daejeon16: 1/2^{+} -65.22(7) MeV, N_{max}=11
1/2^{-} -64.63(2) MeV, N_{max}=10

Tetra neutron



K. Kisamori et al., Phys. Rev. Lett. **116**, 052501 (2016):
E_R = 0.83 ± 0.63(statistical) ± 1.25(systematic) MeV; width $\Gamma \leq 2.6$ MeV



Ab Initio Description of the Tetraneutron with Realistic *NN* Interactions within the NCSM-SS-HORSE Approach

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Abstract

We continue the study of the tetraneutron resonance within the democratic SS-HORSE extension of the *ab initio* No-Core Shell Model [16] using modern *NN* interactions. With Daejeon16 and SRG-evolved chiral Idaho N3LO *NN* interactions we obtain the S-matrix pole corresponding to the tetraneutron resonance with energy between 0.7 and 1.0 MeV and width between 1.1 and 1.7 MeV. However we do not obtain a low-lying narrow resonance with the original Idaho N3LO but, instead, we obtain a very low-lying virtual state with the energy of 15 keV.

Proceedings of the International Conference ‘Nuclear Theory in the Supercomputing Era — 2016’ (NTSE-2016), Khabarovsk, Russia, September 19–23, 2016. Eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, Russia, 2018, p. 280.
http://ntse.khb.ru/files/uploads/2016/proceedings/IMazur.pdf

Deep Learning: A Tool for Computational Nuclear Physics

G. A. Negoita, et al., Proceedings of the Ninth International Conference
on Computational Logics, Algebras, Programming, Tools, and Benchmarking
COMPUTATION TOOLS 2018, [arXiv:1803.03215 [physics.comp-ph]].

Deep Learning: Extrapolation Tool for Ab Initio Nuclear Theory

Gianina Alina Negoita et al, e-Print: arXiv:1810.04009 [nucl-th]

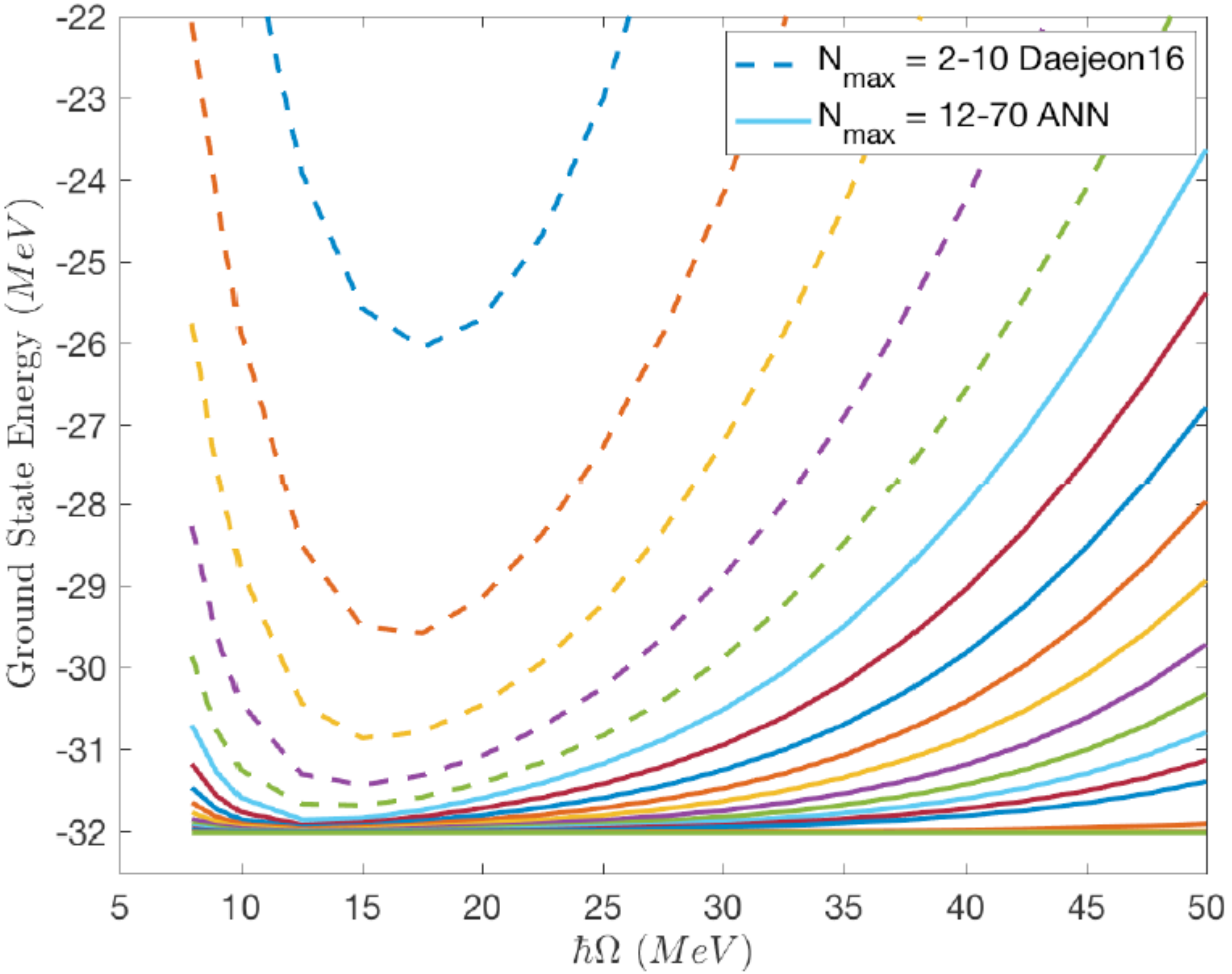

Figure 6. Calculated and predicted gs energy of ^{6}Li as a function of $\hbar\Omega$ at selected N_{max} values.

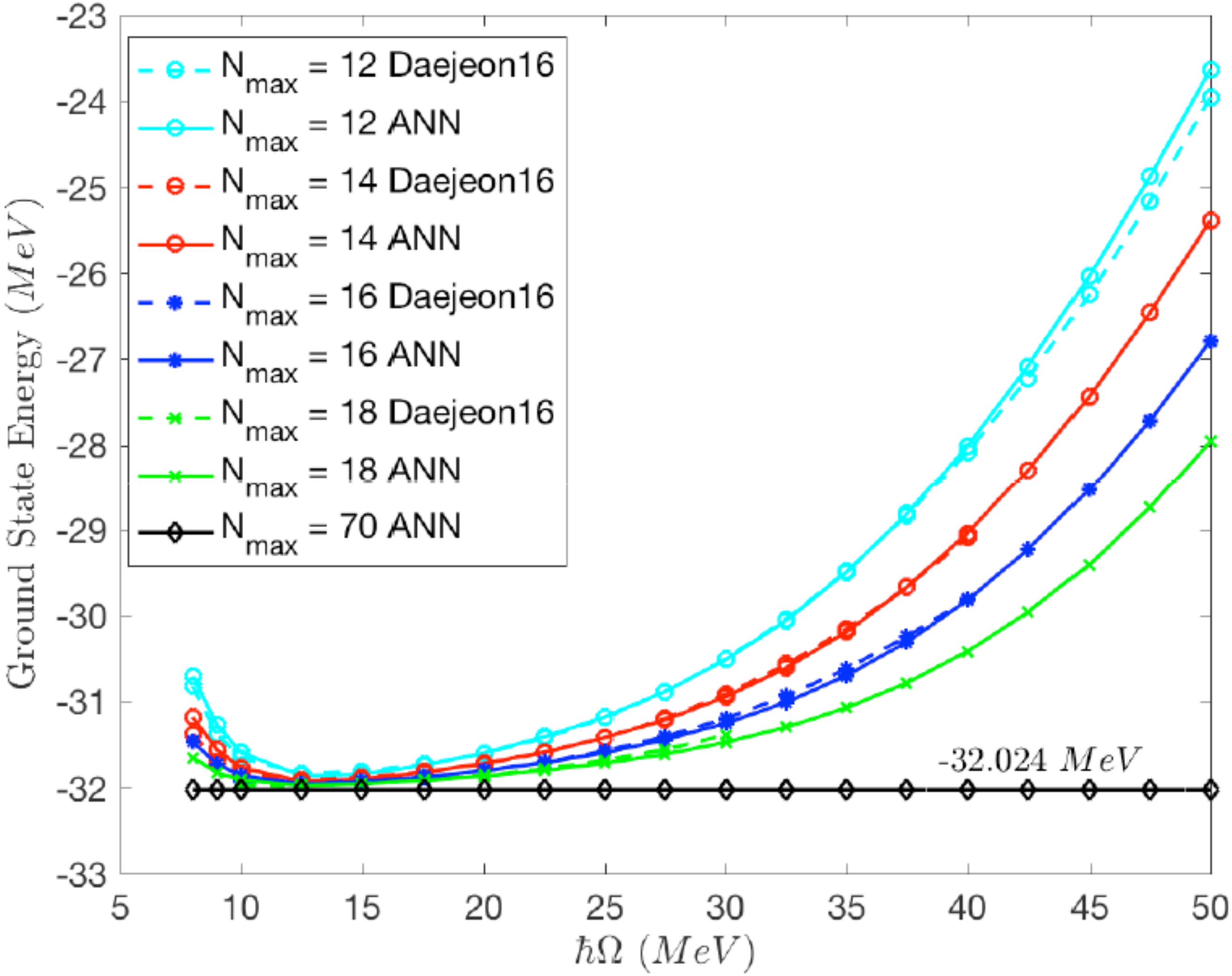

Figure 7. Comparison of the NCSM calculated and the corresponding ANN predicted gs energy values of ^{6}Li as a function of $\hbar\Omega$ at $N_{\max} = 12, 14, 16,$ and 18. The lowest horizontal line corresponds to the ANN nearly converged result at $N_{\max} = 70$.

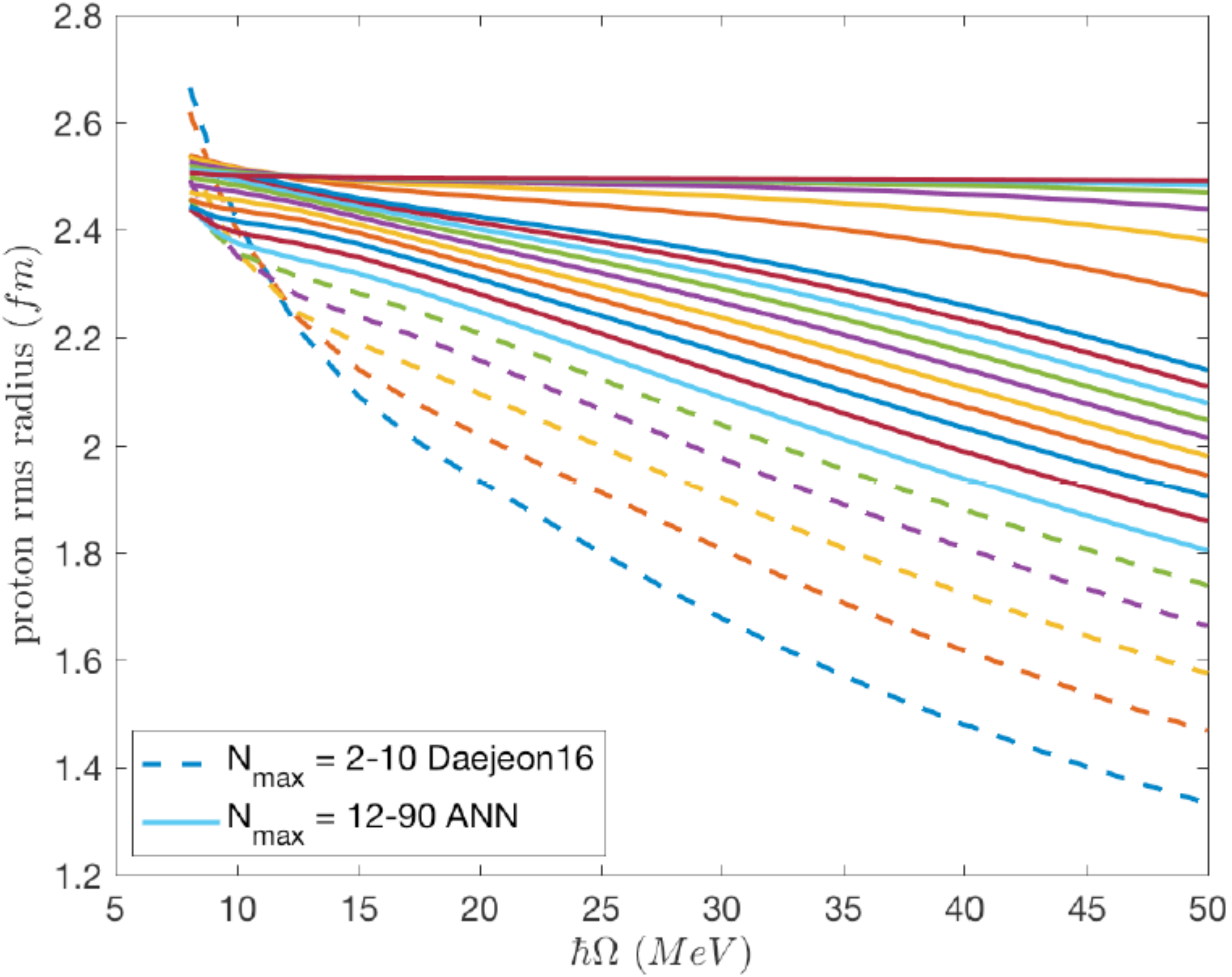

Figure 8. Calculated and predicted gs point proton rms radius of ^{6}Li as a function of $\hbar\Omega$ at selected $N_{\max}$ values.

Nucleon-α scattering and resonances in ^{5}He and ^{5}Li with JISP16 and Daejeon16 *NN* interactions

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The approach called the single-state harmonic oscillator representation of scattering equations (SS-HORSE) to analyze resonant states is generalized to the case of charged particle scattering by using the analytical properties of partial scattering amplitudes and is applied to the study of resonant states in the ^{5}Li nucleus and nonresonant *s*-wave proton-α scattering within the no-core shell model using the JISP16 and Daejeon16 *NN* interactions. We present also the results of calculations of neutron-α scattering and resonances in the ^{5}He nucleus with Daejeon16 and compare with results published previously using JISP16.

Effective interactions in the *sd* shell

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(Dated: September 25, 2018)

We perform a quantitative study of the microscopic effective shell-model interactions in the valence *sd* shell, obtained from modern nucleon-nucleon potentials, chiral N3LO, JISP16 and Daejeon16, using no-core shell-model wave functions and the Okubo-Lee-Suzuki transformation. We investigate the monopole properties of those interactions in comparison with the phenomenological universal *sd*-shell interaction, USDB. Theoretical binding energies and low-energy spectra of O-isotopes and of selected *sd*-shell nuclei, are presented. In general, we conclude that there is a noticeable improvement in the quality of the effective interaction derived from the Daejeon16 potential. We show that its proton-neutron centroids are consistent with those from USDB. We then propose monopole modifications of the centroids in order to provide an adjusted interaction yielding significantly improved agreement with the experiment. A spin-tensor decomposition of two-body effective interactions is applied in order to extract more information on the structure of the centroids and to understand the reason for deficiences arising from the present level of theoretical approximations. The issue of the possible role of the three-nucleon forces is addressed.

Summary

- Thanks to invaluable international collaborators, we have made so far wonderful progress in ab initio nuclear studies for RAON.