Daejeon 16 interaction

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In collaboration with:

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N. A. Smirnova, CENBG (CNRS/IN2P3 – U. de Bordeaux) & more

Now RISP, the nest of RAON, has a new name: IRIS (Institute for Rare Isotope Sciences)

- **Ab initio NCSM**
  - 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
- **Daejeon 16 NN interaction**

- **Ab initio NCSM with Daejeon 16: a few selected works**

Ab initio no-core shell model

- A-nucleon Schrödinger equation

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

- Hamiltonian with $NN(+NNN)$ interactions

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

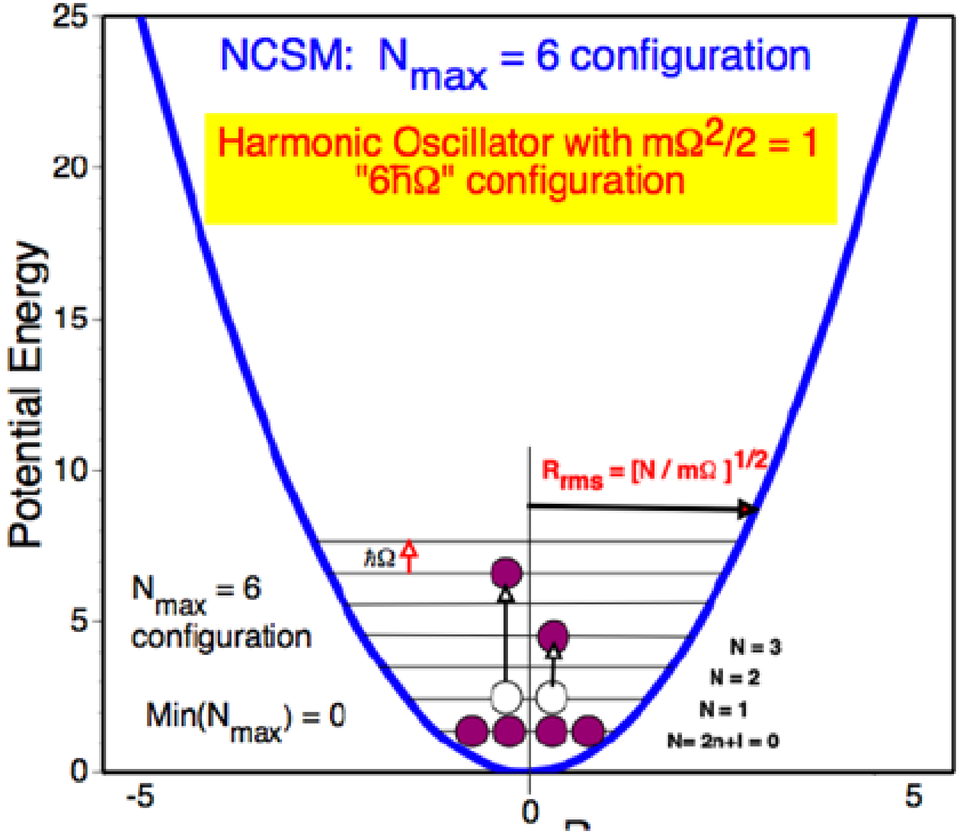
- Wave functions are expanded in basis states

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

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

June, 2012 (for a workshop)
March, 2013 (for collaboration), ...

Daejeon 16 NN interaction

Used in many ab initio nuclear studies and more are planned

"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

N3LO interaction

SRG
(similarity renormalization group)

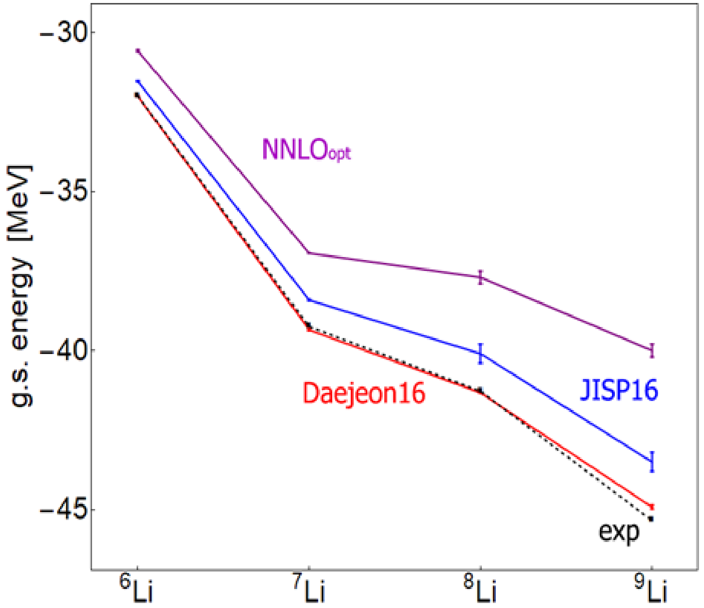
SRG-evolved N3LO

PET (phase equivalent transformation)

Daejeon16

Ground state energies of Li isotopes

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



- Daejeon16 shows more excellent description for the binding energies of Lithium isotopes than $NNLO_{opt}$ (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

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris, J.P. Vary, PLB761 (2016) 87

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.

✓ does 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]

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

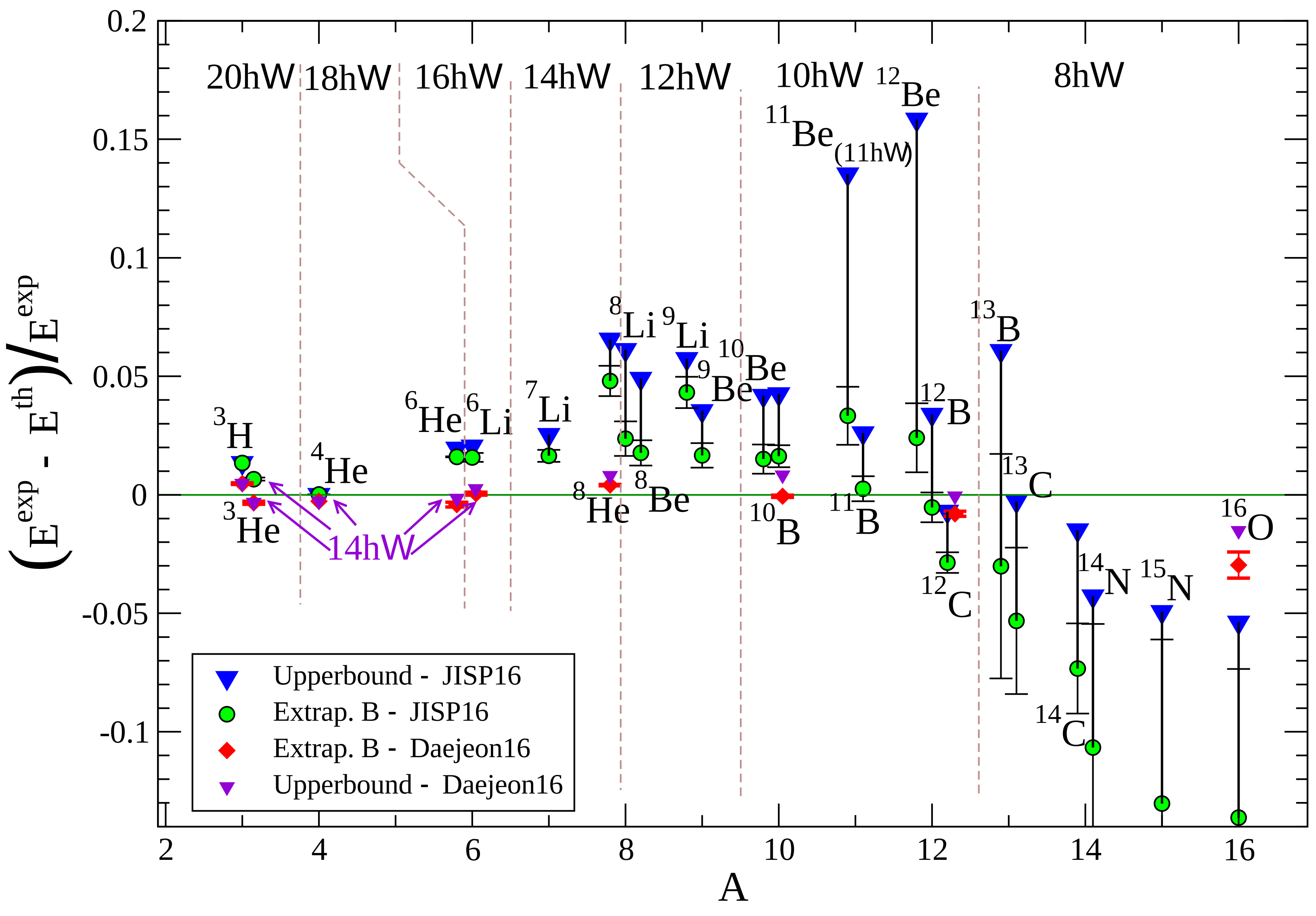
$$[U] = [U_0] \oplus [I] = \begin{bmatrix} [U_0] & 0 \\ 0 & [I] \end{bmatrix}$$

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

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[$(2^+,0)$]



20hW
18hW
16hW
14hW
12hW
10hW
8hW
3H
3He
4He
6He
6Li
7Li
8Li
9Li
8He
8Be
9Be
10Be
10B
11Be (11hW)
11B
12Be
12B
12C
13B
13C
14C
14N
15N
16O
14hW
Upperbound - JISP16
Extrap. B - JISP16
Extrap. B - Daejeon16
Upperbound - Daejeon16
(E^exp - E^th)/E^exp
A

		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.

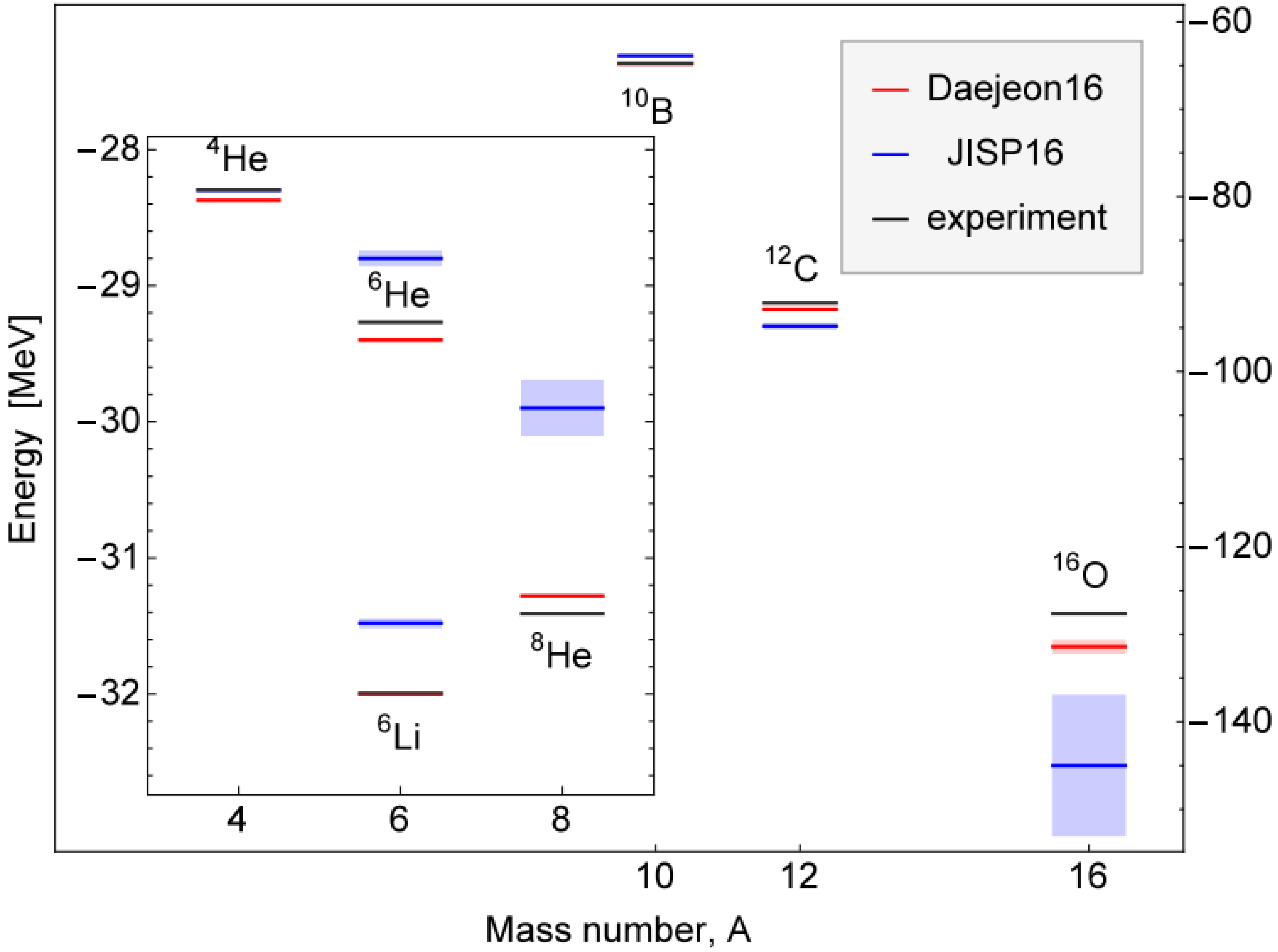
Ab initio NCSM with Daejeon 16: a few selected works

Parity Inversion in ^{11}Be

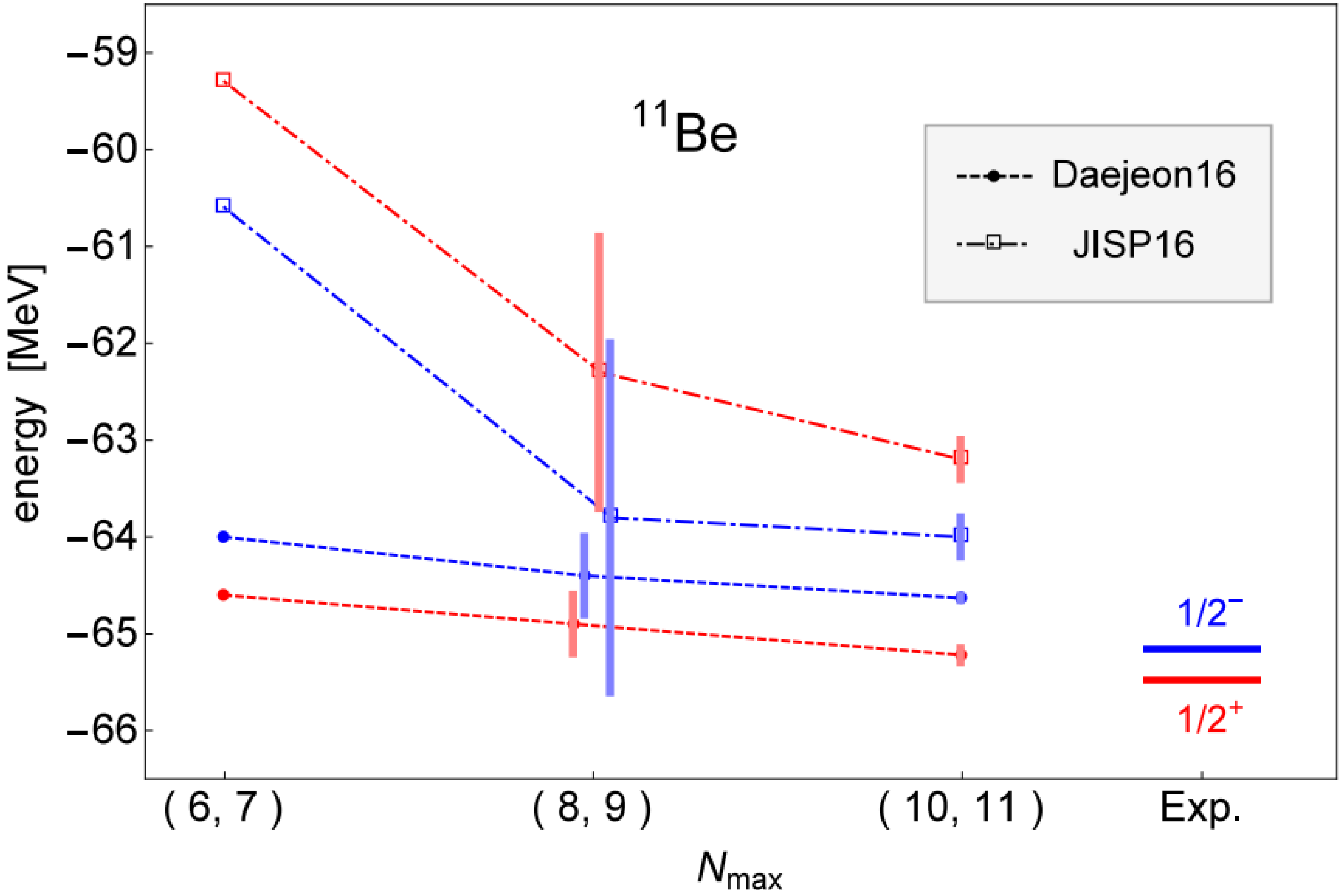
Y. Kim, I.J. Shin, A.M. Shirokov, M. Sosonkina, P. Maris and J. P. Vary, NTSE-2018 • e-Print: 1910.04367 [nucl-th]

- 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

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



The ground state energies of several p-shell nuclei using Daejeon16 and JISP16 compared with experiment.



Energies of the ground and first-excited states of 11Be calculated within the ab initio NCSM with Daejeon16 and JISP16.

Daejeon 16 for heavier nuclear systems

Many-body method:

- HF + perturbation theory (MBPT) for ground states and radii
- RPA for the centroid energy of the isoscalar giant monopole resonance (E_c) and the electric dipole polarizability (a_D)

..... since at the moment NCSM is not applicable to heavier systems

Our strategy:

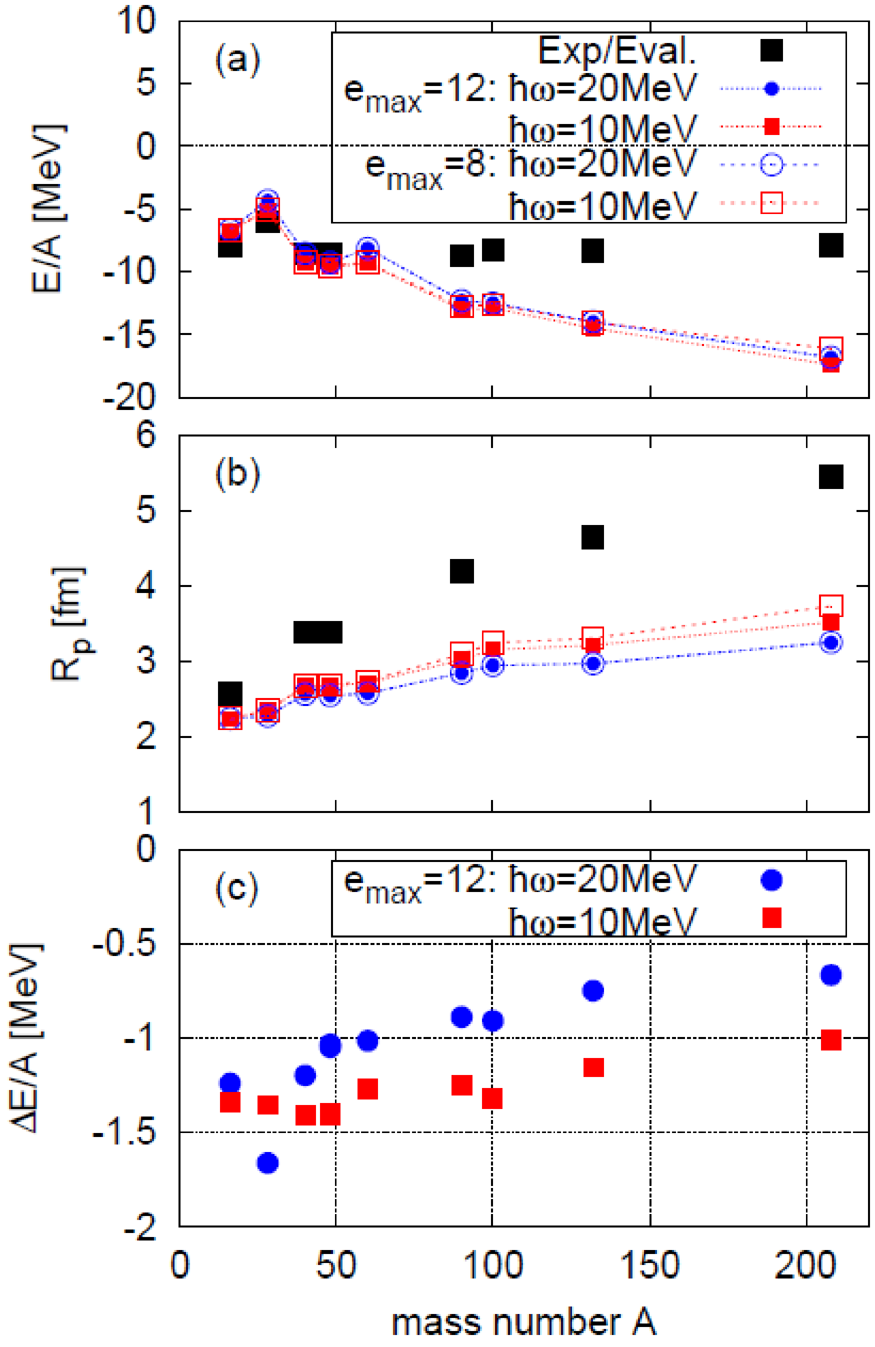
- We first discuss perturbative nature of Daejeon 16 in MBPT.
- We seek for a phenomenological corrections to Daejeon 16 to introduce density-dependent two nucleon interactions.

P. Papakonstantinou, J. P. Vary, Y. Kim, J. Phys. G 48 (2021) 085105

Experimental data referenced in our work

Property \ Nuclide	^{16}O	^{40}Ca	^{48}Ca	^{90}Zr	^{132}Sn	^{208}Pb
E/A [MeV]	7.976	8.551	8.667	8.710	8.355	7.867
R_{ch} [fm]	2.699	3.478	3.477	4.264	4.709	5.501
R_p [fm]	2.581	3.387	3.393	4.199	4.650	5.450
E_c(GMR) [MeV]$^{(*)}$	−−	19.88	19.18	18.13	−−	13.96
a_D [fm$^3/e^2$]	−−	−−	2.07(22)	−−	−−	20.1(6)

$^{(*)}$ Error bars for E_c(GMR) are of the order of 10^{-1}MeV.

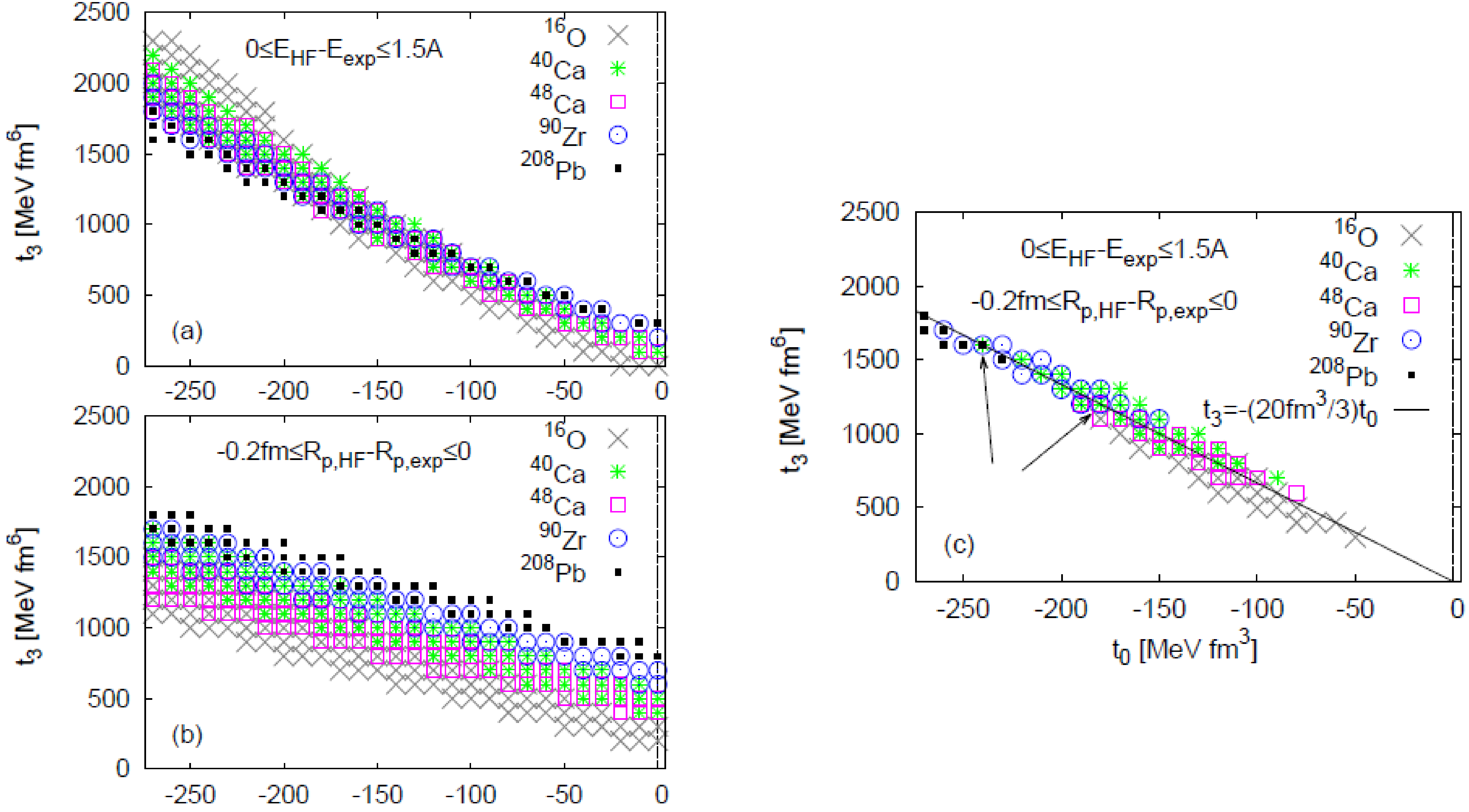


Results for closed-shell nuclei:
^{16}O, ^{28}O, ^{40}Ca, ^{48}Ca, ^{60}Ca, ^{90}Zr, ^{100}Sn, ^{132}Sn, ^{208}Pb.

Phenomenological corrections: density-dependent two nucleon interactions
(two-plus-three-nucleon contact interaction within the mean field approximation)

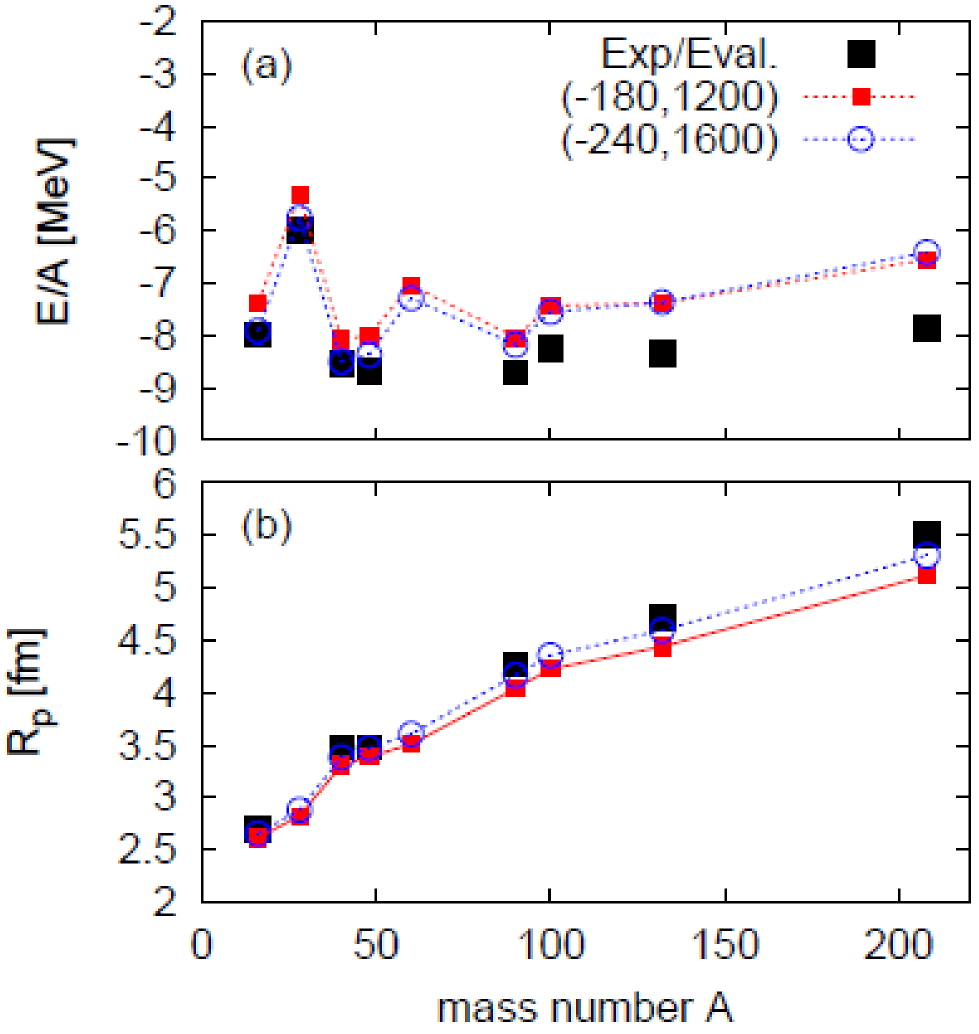
$$V_\rho = \frac{1}{6}(1+\hat{P}_\sigma)\{t_0 + t_3\rho([\vec{r}_i+\vec{r}_j]/2)\}\delta(\vec{r}_i-\vec{r}_j)$$

Shang-fang Tsai, Coordinate-space formalism of the random-phase approximation," Phys. Rev. C 17, 1862 (1978).



0≤E_HF-E_exp≤1.5A
-0.2fm≤R_p,HF-R_p,exp≤0
16O
40Ca
48Ca
90Zr
208Pb
t_3=-(20fm^3/3)t_0
t_3 [MeV fm^6]
t_0 [MeV fm^3]
(a)
(b)
(c)

Exemplary results with selected values of (t_0, t_3)

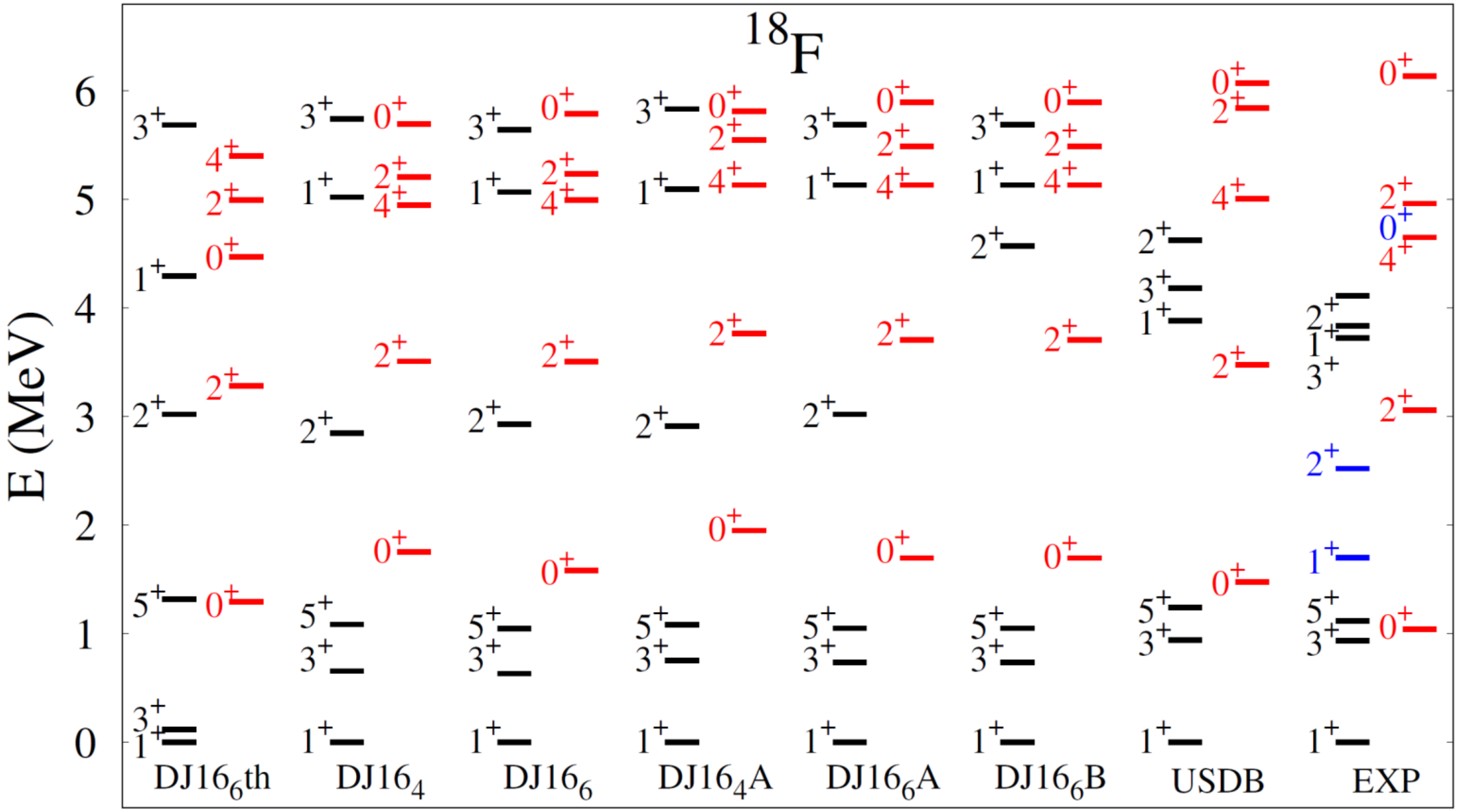


	E/A [MeV]		R_p [fm]	
	(-180,1200)	(-240,1600)	(-180,1200)	(-240,1600)
^{16}O	-7.367	-7.912	2.614	2.655
^{28}O	-5.322	-5.751	2.825	2.883
^{40}Ca	-8.082	-8.493	3.308	3.383
^{48}Ca	-7.999	-8.366	3.386	3.470
^{60}Ca	-7.036	-7.290	3.509	3.607
^{90}Zr	-8.038	-8.180	4.038	4.166
^{100}Sn	-7.432	-7.554	4.226	4.358
^{132}Sn	-7.382	-7.366	4.440	4.593
^{208}Pb	-6.556	-6.425	5.116	5.308

Effective shell-model interactions from Daejeon 16

A new microscopic effective shell-model interactions in the valence sd shell, obtained from the modern Daejeon16 nucleon-nucleon potential using no-core shell-model (NCSM) wave functions of ^{18}F at $N_{max} = 6$

Ik Jae Shin, Nadezda A. Smirnova, A. M. Shirokov, Zuxing Yang, B. R. Barrett, Zhen Li, Y. Kim, P. Maris, and J. P. Vary, Effective interactions in the sd shell from Daejeon16, *in preparation.*



$$\Delta\varepsilon_{jj'} = \frac{\sum_J (1-(-1)^{2j-J}\delta_{jj'})\,(2J+1)\langle jj'|V|jj'\rangle_J}{(2j+1)(2j'+1)}$$

[$N_{max} = 4$: Nadezda A. Smirnova, B. R. Barrett, Y. Kim, Ik Jae Shin, A. M. Shirokov, E. Dikmen, P. Maris and J. P. Vary, Phys. Rev. C 100 (2019) 054329]

Harmonic Oscillator Representation of Scattering Equations

- This is one of the reliable method for describing two particle scattering
  For example, see Ref: Annals of Physics 280, 299 (2000)
- One-channel, short range potential case:
  - Radial Schrödinger Eq: $H^\ell u_\ell(E,r) = E u_\ell(E,r)$
  - Expansion to oscillator functions: $u_\ell(E,r) = \sum_n a_{n\ell}(E) R_{n\ell}(r)$
  - Approximation of short range potential $\tilde{V}_{nn'} = \begin{cases} V_{nn'} & n,n' \le N \sim N_{\max} \quad (P \text{ space}) \\ 0 & n,n' > N \sim N_{\max} \quad (Q \text{ space}) \end{cases}$
  - Kinetic energy $T^\ell_{nn'}$ matrix stay full and infinite! (tri-diagonal, have explicit values)
  - Q space solution: $a_{n\ell}(E) = \#\text{norm}\left(S_{n\ell}(E) + \tan\delta_\ell\, C_{n\ell}(E)\right)$

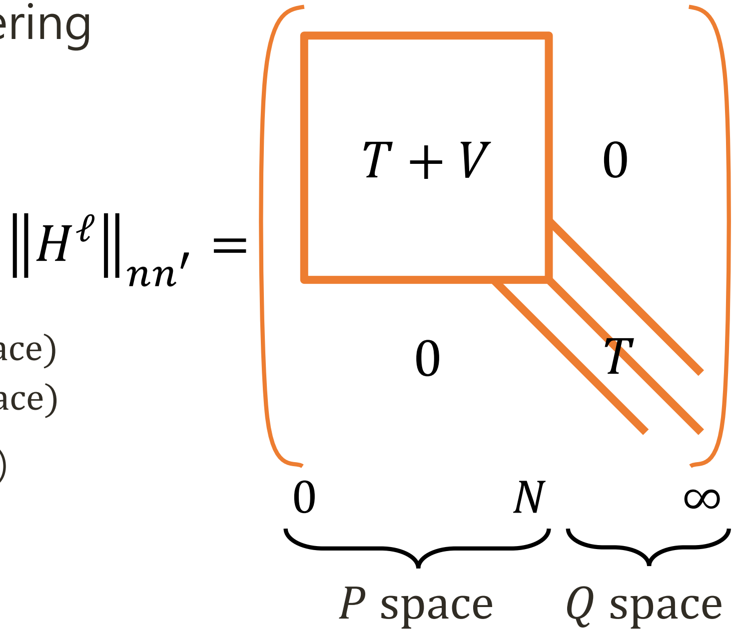
$$S_{n\ell}(E) = \#\text{norm}\left(\left(\frac{2E}{\hbar\Omega}\right)^{\frac{\ell+1}{2}} \exp\left(-\frac{E}{\hbar\Omega}\right) L_n^{\ell+\frac{1}{2}}\left(\frac{2E}{\hbar\Omega}\right)\right), \qquad \sum_{n=0}^{\infty} S_{n\ell}(E) R_{n\ell}(r) = j_\ell(r)$$

$$C_{n\ell}(E) = \#\text{norm}\left(\left(\frac{2E}{\hbar\Omega}\right)^{-\frac{\ell}{2}} \exp\left(-\frac{E}{\hbar\Omega}\right) {}_1F_1\left(-n+\ell-\frac{1}{2}, -\ell+\frac{1}{2}; \frac{2E}{\hbar\Omega}\right)\right), \qquad \sum_{n=0}^{\infty} C_{n\ell}(E) R_{n\ell}(r) \to n_\ell(r),\ r\to\infty.$$

  - After matching => phase shift: $\tan\delta_\ell = -\frac{S_{N\ell}(E) - G_{NN}(E) T_{NN+1} S_{N+1,\ell}(E)}{C_{N\ell}(E) - G_{NN}(E) T_{NN+1} C_{N+1,\ell}(E)}$

$$G_{nn'}(E) = -\sum_{\nu=1}^{\mathcal{N}} \frac{\langle\nu|n\ell\rangle\langle n'\ell|\nu\rangle}{E_\nu - E}, \qquad |\nu\rangle, E_\nu \text{ from: } \sum_{n'} H^\ell_{nn'} \langle n'\ell|\nu\rangle = E_\nu \langle n\ell|\nu\rangle \quad (\text{from } P \text{ space})$$

- Coulomb + short range, multi-channel scattering description: also exists



- $\tan\delta_\ell = -\frac{S_{N\ell}(E) - G_{NN}(E)T_{NN+1}S_{N+1,\ell}(E)}{C_{N\ell}(E) - G_{NN}(E)T_{NN+1}C_{N+1,\ell}(E)}$

  $G_{nn'}(E) = -\sum_{\nu=1}^{\mathcal{N}} \frac{\langle\nu|n\ell\rangle\langle n'\ell|\nu\rangle}{E_\nu - E}$, $\sum_{n'} H^{\ell}_{nn'}\langle n'\ell|\nu\rangle = E_\nu\langle n\ell|\nu\rangle$

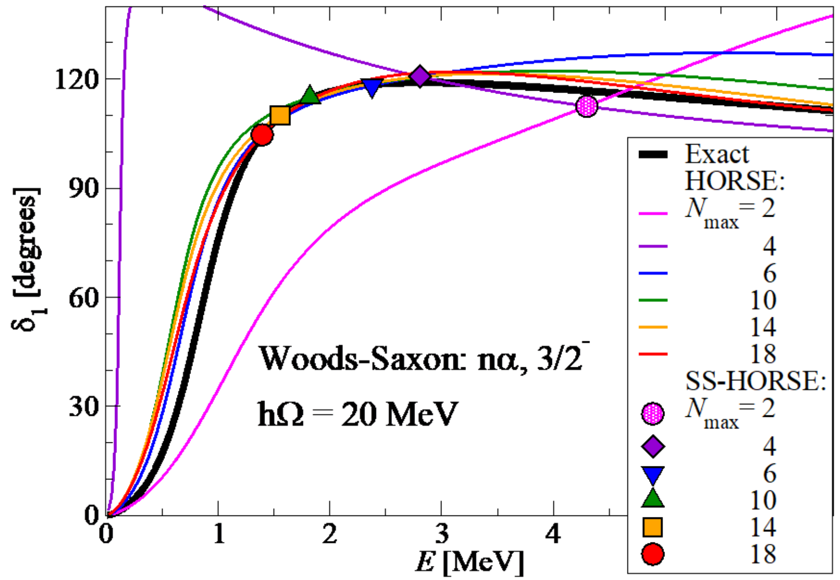
  In *P* space we may use various calculations with oscil lator basis, for example, *ab initio* No-Core Shell Mod el calculations

- Phase shifts require ALL eigenstates, number of them ($\mathcal{N} \sim \exp N_{\max}$) increase rapidly

- Special case $E = E_\nu$: $\tan\delta_\ell = -\frac{S_{N+1,\ell}(E_\nu)}{C_{N+1,\ell}(E_\nu)}$

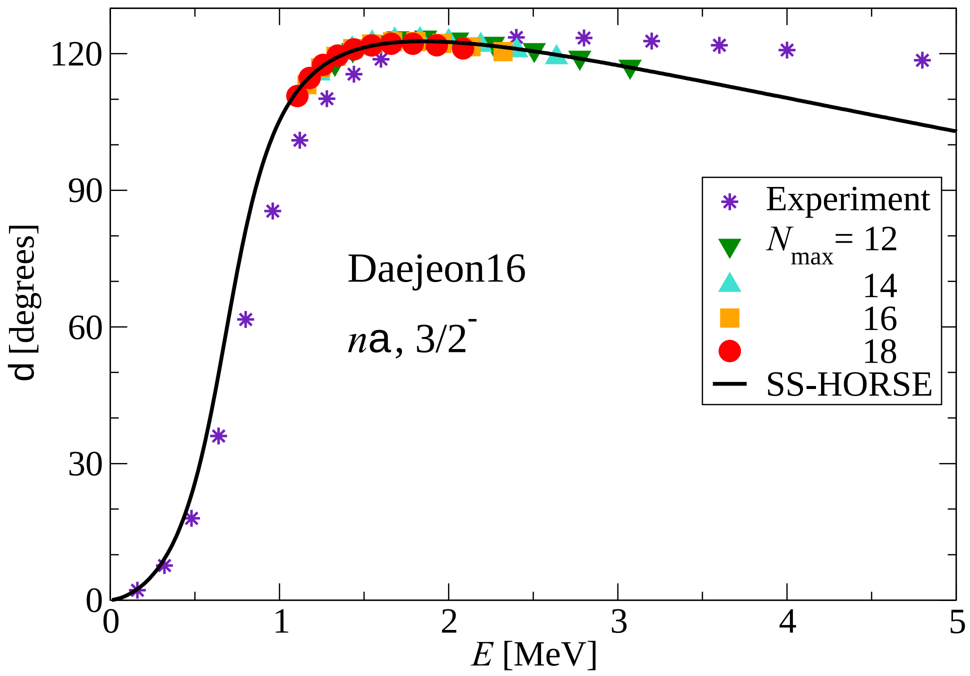
- Two body test problem: $\delta_\ell(E_\nu)$ are ``good" phases

- By varying N (or $N_{\max}$) and $\hbar\Omega$ we obtain E_ν and δ_ℓ i n some interval , parametrize and extract resonances from $\delta_\ell(E)$



Example: $n\alpha$ scattering

1. No Core Shell Model calculations:
   $E^{5He}(N_{max}, \hbar\Omega)$, $E^{4He}(N_{max}, \hbar\Omega)$
2. $E_{rel.n\alpha} = E = E^{5He} - E^{4He}$
   $\tan\delta = f(E)$: obtaining
   phases in points, f is known function
3. Selection criteria
   for N_{max} and $\hbar\Omega$:
   phases form smooth curve
4. Parameterization: $\delta = \delta_r$ + smooth function
5. Extracting E_r, Γ from δ_r



Resonance			This work				
J^π (^{7}He)	J^π (^{6}He)		JISP16	Daejeon16	Experiment		
$3/2^-_1$	0^+	E_r	0.665(12)	0.28(4)	0.430(3)		
		Γ	0.57(4)	0.13(2)	0.182(5)		
$1/2^+$	0^+	E_r					
		Γ					
$1/2^-$	0^+	E_r	2.7(8)	2.7(4)	3.0(1)	3.5	1.0(1)
		Γ	5.0(6)	4.3(3)	2	10	0.75(8)
$5/2^-$	0^+	E_r	4.4(4)	3.63(16)			
		Γ	1.56(4)	1.36(3)			
	2^+	E_r	3.85(15)	3.23(25)			
		Γ	2.5(2)	2.28(8)			
Predictions		E_r	4.1(7)	3.4(4)	3.36(9)		
		Γ	2.0(7)	1.8(5)	1.99(17)		
$3/2^-_2$	0^+	E_r	5.8(5)	5.0(3)			
		Γ	4.11(23)	2.84(24)			
	2^+	E_r	5.3(4)	4.4(4)			
		Γ	3.9(6)	3.9(3)			
Predictions		E_r	5.6(7)	4.7(7)			
		Γ	4.0(7)	3.4(8)			

We describe all experimentally known ^{7}He resonances and suggest an interpretation of an observed wide resonance of unknown spin-parity

I. A. Mazur, I. J. Shin, Y. Kim, A. I. Mazur, A. M. Shirokov, P. Maris and J. P. Vary, PRC 106, 064320 (2022)

Summary

- A few important and interesting results from ab initio NCSM with Daejeon 16 are briefly presented.
- The guidance of James, needless to say, was essential in developing Daejeon 16 and its applications to ab initio nuclear structure studies!