

Description of Continuum States within No-Core Shell Model. Single-State HORSE Method



A. Mazur, I. Mazur

Pacific National University, Khabarovsk, Russia

A. Shirokov, L. Blokhintsev

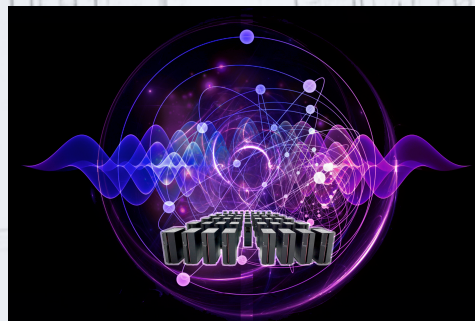
SINP Moscow State University, Moscow, Russia

Y. Kim, I. J. Shin

RISP, Institute for Basic Science, Daejeon, Korea

J. Vary *Iowa State University, USA*

*Count Muraviev-Amursky.
Khabarovsk.*



NTSE-2018

IBS Daejeon, Korea

29 Oct. – 2 Nov. 2018

RSF

Russian
Science
Foundation

Motivation

- *There are many ab initio approaches for describing bound states of light nuclei (for example, No Core Shell Model). In these approaches most states are in the continuum.*
- *Can we extract information about resonances and nonresonant scattering from shell model results?*

Motivation

- *There are many ab initio approaches for describing bound states of light nuclei (for example, NCSM).*
- *Can we extract information about resonances and nonresonant scattering from shell model results?*
- *We suggest an approach for describing scattering states based on shell model calculations of nuclei:
NCSM Single-State HORSE method.*
- *We suggest an interpretation of shell model results lying above decaying thresholds*

NCSM Single-State HORSE method:

No-Core Shell Model

+

Harmonic Oscillator Representation of Scattering Equation (Single-State version)

+

Low-energy phase shift parametrization

NCSM Single-State HORSE method:

No-Core Shell Model

+

Harmonic Oscillator Representation of Scattering Equation (Single-State version)

+

Low-energy phase shift parametrization

Application:

The resonance and non-resonance Na scattering within NCSM Single-State HORSE method with realistic NN-interactions JISP16 and Daejeon16

No-Core Shell Model

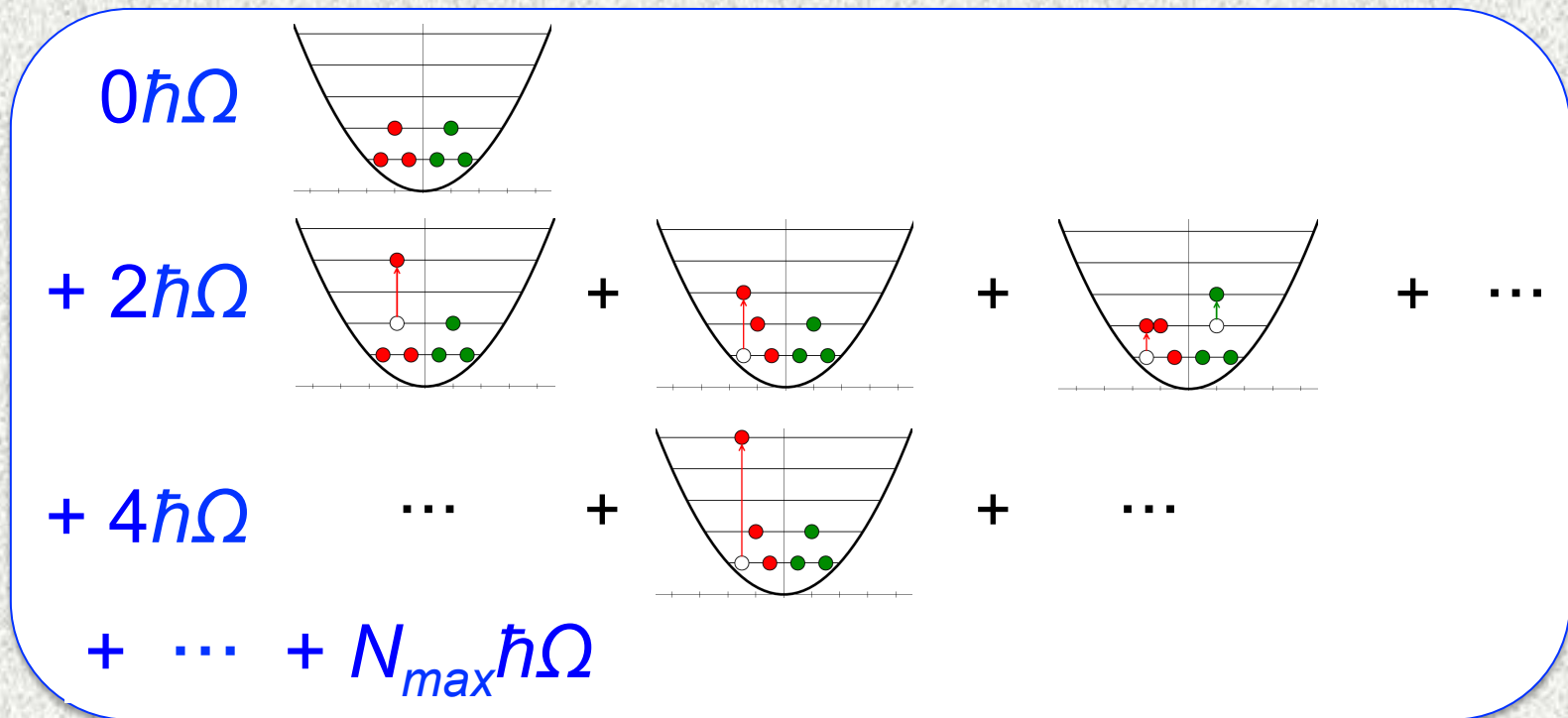
✓ *Modern version of Nuclear Shell Model*

B. R. Barrett, P. Navratil, J. P. Vary, **Progr. Part. Nucl. Phys.**, **69**, 131 (2013).

No-Core Shell Model

- ✓ *Modern version of Nuclear Shell Model*
- ✓ *All nucleons are spectroscopically active*

${}^6\text{Li}$:



N_{max} – *maximum number of excitation quanta*
 $\hbar\Omega$ – *parameter of oscillator function*

No-Core Shell Model

- ✓ *Modern version of Nuclear Shell Model*
- ✓ *All nucleons are spectroscopically active*
- ✓ *Basis: many-body oscillator functions*

Example: ^{14}F , model space $N_{max} = 8$
contains 1 990 061 078 basis functions

No-Core Shell Model

- ✓ *Modern version of Nuclear Shell Model*
- ✓ *All nucleons are spectroscopically active*
- ✓ *Basis: many-body oscillator functions*
- ✓ *Only NN (+ NNN) interaction as input*

Below we use realistic NN interactions:

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

a **Fortran code** generating the JISP16 matrix elements is available at
http://lib.dr.iastate.edu/energy_datasets/2/.

Daejeon16 A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris
and J. P. Vary, **Phys. Lett. B 761, 87 (2016).**

a **Fortran code** generating the Daejeon16 matrix elements is available at
http://lib.dr.iastate.edu/energy_datasets/1/

HORSE

Harmonic Oscillator Representation
of Scattering Equations

is the effective method to describe two-body scattering

$$H=T+V$$

$$H^l u_l(E, r) = E u_l(E, r)$$

$$u_l(E, r) = \sum_{N=N_0}^{\infty} a_{Nl}(E) R_{Nl}(r)$$

$$\sum_{N'=N_0}^{\infty} (H_{N,N'}^l - \delta_{N,N'}) a_{N'l}(E) = 0$$

$R_{Nl}(r)$ – Osc. functions

$$N = 2n + l$$

HORSE

N

$T+V$

0

0

T

Parameters $N, \hbar\Omega$

- ✓ Potential matrix elements $V_{NN'}$ decrease when N, N' grows while kinetic energy matrix elements T_{NN}, T_{NN+2} increase ($\sim N$).
So potential matrix V may be truncated.
- ✓ Tridiagonal kinetic matrix T is not truncated

**This is an
exactly solvable problem !**

HORSE

Phase shift:

$$\tan \delta_\ell(E) = -\frac{S_{N\ell}(E) - G_{NN}(E)T_{N,N+2}^\ell S_{N+2,\ell}(E)}{C_{N\ell}(E) - G_{NN}(E)T_{N,N+2}^\ell C_{N+2,\ell}(E)}$$

$$G_{NN'}(E) = -\sum_{\nu=0}^{N-1} \frac{\langle \nu | N\ell \rangle \langle N'\ell | \nu \rangle}{E_\nu - E}$$

**All information
about interaction**

$$\sum_{N'=N_0, N_0+2, \dots, N} H_{NN'}^\ell \langle N'\ell | \nu \rangle = E_\nu \langle N\ell | \nu \rangle$$

**Oscillator
free
solutions**

$$S_{N\ell}(E) = \sqrt{\frac{\pi n!}{\Gamma(n + \ell + \frac{3}{2})}} \left(\frac{2E}{\hbar\Omega}\right)^{\frac{\ell+1}{2}} \exp\left(-\frac{E}{\hbar\Omega}\right) L_n^{\ell+\frac{1}{2}}\left(\frac{2E}{\hbar\Omega}\right)$$
$$C_{N\ell}(E) = \sqrt{\frac{\pi n!}{\Gamma(n + \ell + \frac{3}{2})}} \frac{(-1)^n}{\Gamma(-\ell + \frac{1}{2})} \left(\frac{2E}{\hbar\Omega}\right)^{-\frac{\ell}{2}} \exp\left(-\frac{E}{\hbar\Omega}\right) \times$$
$$\times {}_1F_1\left(-n - \ell - \frac{1}{2}, -\ell + \frac{1}{2}; \frac{2E}{\hbar\Omega}\right)$$

HORSE: *charged particles*

J. M. Bang, A. I. Mazur, A. M. Shirokov, Yu. F. Smirnov, S. A. Zaytsev,
Ann. Phys. (N.Y.) 280, 299 (2000)

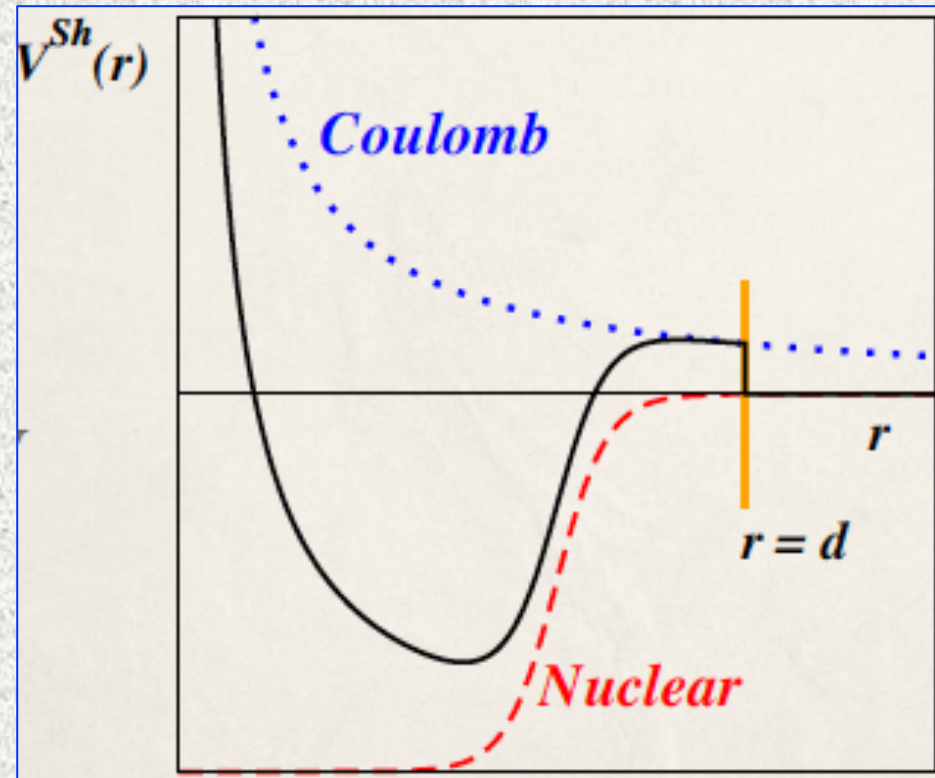
Auxiliary short range potential

$$V^{Sh} = \begin{cases} V^{Nucl} + V^{Coul}, & r \leq d \\ 0, & r > d \end{cases}$$

Optimal value of d is determined by classical turning point of basic state with oscillator quantum number $(N + 2)$

$$d = b_0 = 2r_0 \sqrt{N + 7/4}$$

$$r_0 = \sqrt{\frac{\hbar}{\mu\Omega}} \text{ is the oscillator radius}$$



HORSE: *charged particles*

Phase shift δ^{sh} can be calculated within HORSE

$$\tan \delta^{sh} = -\frac{S_{N,l} - G_{NN} T_{N,N+2}^l S_{N+2,l}}{C_{N,l} - G_{NN} T_{N,N+2}^l C_{N+2,l}}$$

Matching with Coulomb asymptotic at $r = b_0$

$$\tan \delta_l = -\frac{W_{b_0}(j_l, F_l) - W_{b_0}(n_l, F_l) \tan \delta_l^{Sh}}{W_{b_0}(j_l, G_l) - W_{b_0}(n_l, G_l) \tan \delta_l^{Sh}}$$

Quasi-Wronskians

$$W_{b_0}(j_l, F_l) = \left(\frac{dj_l(kr)}{dr} F_l(\eta, kr) - f_l(kr) \frac{dF_l(\eta, kr)}{dr} \right) \Big|_{r=b_0}$$

$$j_l(kr), \quad n_l(kr)$$

$$F_l(\eta, kr), \quad G_l(\eta, kr)$$

$$\eta = \frac{\mu Z_1 Z_2 e^2}{k}$$

Spherical Bessel and Neumann functions;

Coulomb wave functions;

Sommerfeld parameter.

Single-State HORSE

HORSE requires **ALL** shell model states:

$$\tan \delta_\ell(E) = - \frac{S_{N\ell}(E) - G_{NN}(E) T_{N,N+2}^\ell S_{N+2,\ell}(E)}{C_{N\ell}(E) - G_{NN}(E) T_{N,N+2}^\ell C_{N+2,\ell}(E)}$$

$$G_{NN'}(E) = - \sum_{\nu=0}^{N-1} \frac{\langle \nu | N\ell \rangle \langle N'\ell | \nu \rangle}{E_\nu - E}$$

So it is impossible for modern large-scale calculation in NCSM!

Single-State HORSE

A. M. Shirokov, A. I. Mazur, I. A. Mazur and J. P. Vary,
Phys. Rev. C 94, 064320 (2016); Phys. Part. Nucl. 48, 84 (2017).

But in the case $E = E_\nu$

$$\tan \delta_\ell(E_\nu) = -\frac{S_{N+2,\ell}(E_\nu)}{C_{N+2,\ell}(E_\nu)}$$

Now we get rid not only of the need to sum over a huge number of eigenstates but also from the shell model wave function component defining the desired channel.

Hence this equation can be used for scattering channels of any type.

By N , $\hbar\Omega$ variation, we get $\delta_\ell(E)$ in some energy interval!

Single-State HORSE: charged particles.

In the case $E = E_\nu$ phase shift

$$\tan \delta_l(E_\nu) = -\frac{W_{b_0}(n_l, F_l)S_{N+2,l}(E_\nu) + W_{b_0}(j_l, F_l)C_{N+2,l}(E_\nu)}{W_{b_0}(n_l, G_l)S_{N+2,l}(E_\nu) + W_{b_0}(j_l, G_l)C_{N+2,l}(E_\nu)}$$

also depends only on the energy E_ν .

Low-energy phase shift parametrization

An important feature of the Single-State HORSE method is the correct description a phase shift in the low-energy region.

Here we use the K -parametrization

Neutral particles ($\eta = 0$) $K_l^{(i)}(E) = k^{2l+1} \cot \delta_l(E_0^{(i)})$

Coulomb-modified effective radius function

$$K_l(k^2) = k^{2l+1} (c_{l\eta})^{-1} \left\{ \frac{2\pi\eta}{\exp(2\pi\eta) - 1} [\text{ctg } \delta_l(k) - i] + 2\eta H(\eta) \right\}$$

$$H(\eta) = \Psi(i\eta) + (2i\eta)^{-1} - \ln(i\eta)$$

Parametrization of the K -matrix by means of a Padé-approximant

$$K_l(k^2) = \frac{w_0 + w_1 k^2 + w_2 k^4}{1 + v_1 k^2}$$

Fitting procedure

The final values for w_0, w_1, w_2, v_1 are determined by minimizing the functional

$$\Xi = \sqrt{\frac{1}{d} \sum_{i=1}^d \left(E_0^{(i)} - \varepsilon^{(i)} \right)^2}$$

Here $E_0^{(i)}$ ($i = 1, 2, \dots, d$) are NCSM results with selected $N^{(i)}, \hbar\Omega^{(i)}$

and $\varepsilon_0^{(i)}$ are solutions of the transcendental equation

$$\frac{w_0 + w_1 k^2 + w_2 k^4}{1 + v_1 k^2} = k^{2l+1} (c_{l\eta})^{-1} \left\{ -\frac{2\pi\eta}{\exp(2\pi\eta) - 1} \times \right. \\ \left. \times \left[\frac{S_{N+2,l}(k) W_b(n_l, G_l) + C_{N+2,l}(k) W_b(j_l, G_l)}{S_{N+2,l}(k) W_b(n_l, F_l) + C_{N+2,l}(k) W_b(j_l, F_l)} + i \right] + 2\eta H(\eta) \right\}.$$

with fixed parameters w_0, w_1, w_2, v_1 for the same $N^{(i)}, \hbar\Omega^{(i)}$

Resonance energy and width

The renormalized
Coulomb-nuclear
scattering amplitude:

$$f_l = \frac{k^{2l}}{K_l(k^2) - 2\eta k^{2l+1} H(\eta) (c_{l\eta})^{-1}}$$

We obtain resonance energies E_r and widths Γ by a numerical location of the S -matrix poles which coincide with the poles of scattering amplitude, that is by solving the equation

$$K_l(k^2) - 2\eta k^{2l+1} H(\eta) (c_{l\eta})^{-1} = 0$$

$$E_r = \text{Re}(E_p), \quad \Gamma/2 = \text{Im}(E_p)$$

Neutral
particles

$$K_l(k^2) - i k^{2l+1} = 0$$

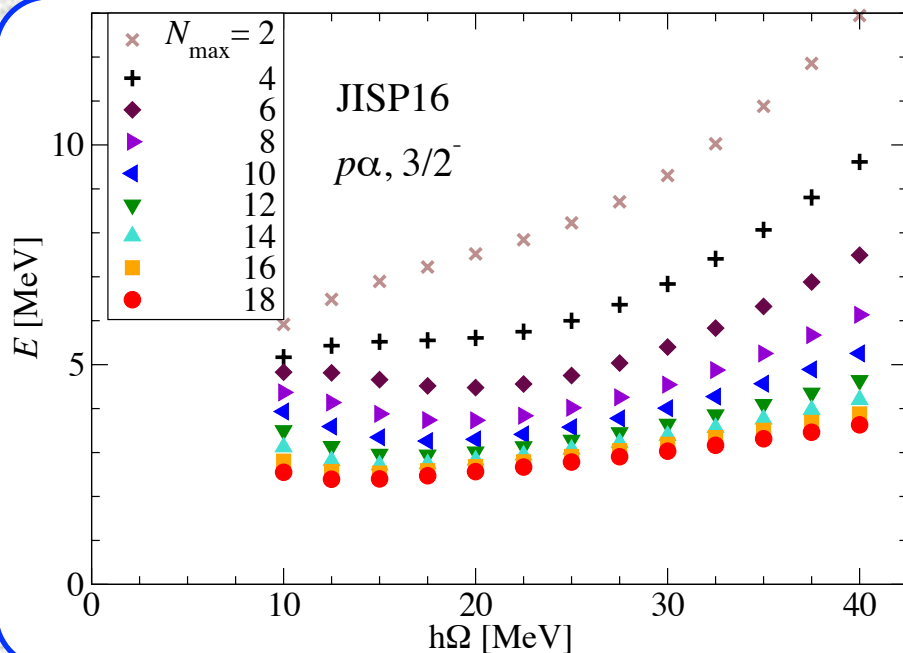
NCSM Single-State HORSE method:

how it works

${}^5\text{Li} (3/2^-)$

NCSM with JISP16

(Energies $E_\nu(\hbar\Omega)$ are measured from the proton- α threshold)



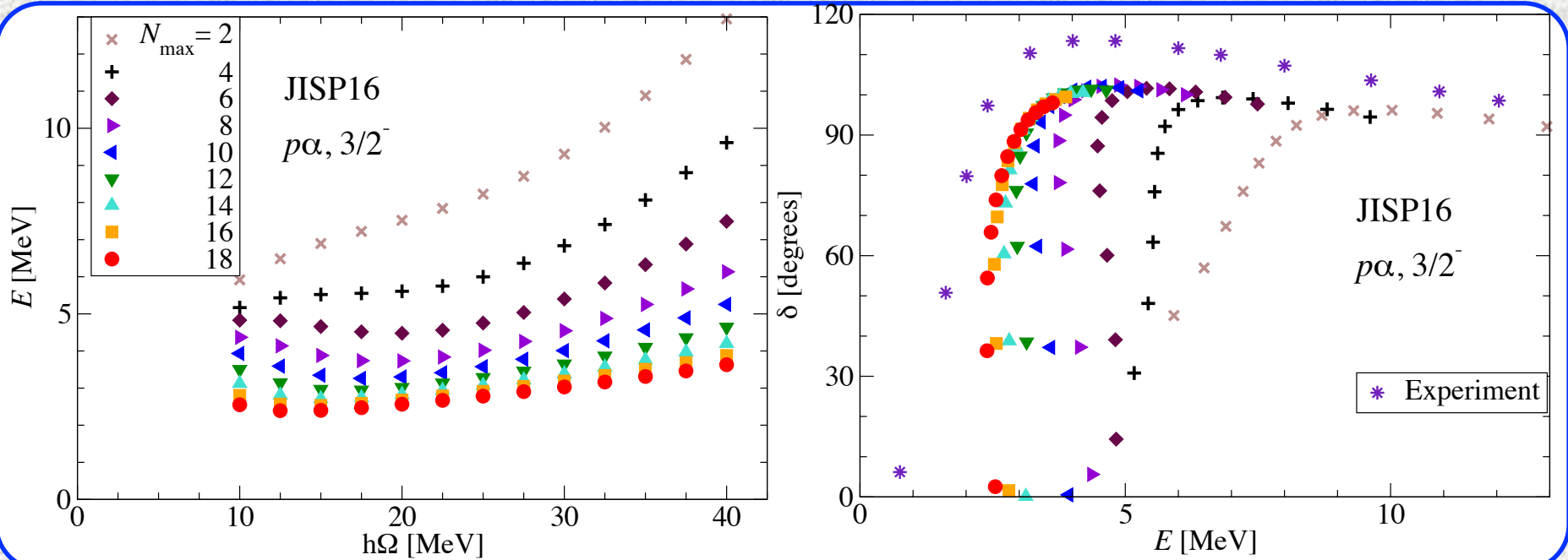
NCSM Single-State HORSE method

${}^5\text{Li} (3/2^-)$
NCSM with JISP16

Single-State HORSE
phase shifts

$$\tan \delta_l(E_\nu) = - \frac{W_{b_0}(n_l, F_l) S_{N+2,l}(E_\nu) + W_{b_0}(j_l, F_l) C_{N+2,l}(E_\nu)}{W_{b_0}(n_l, G_l) S_{N+2,l}(E_\nu) + W_{b_0}(j_l, G_l) C_{N+2,l}(E_\nu)}$$

$$N_{max} + N_0 = N$$

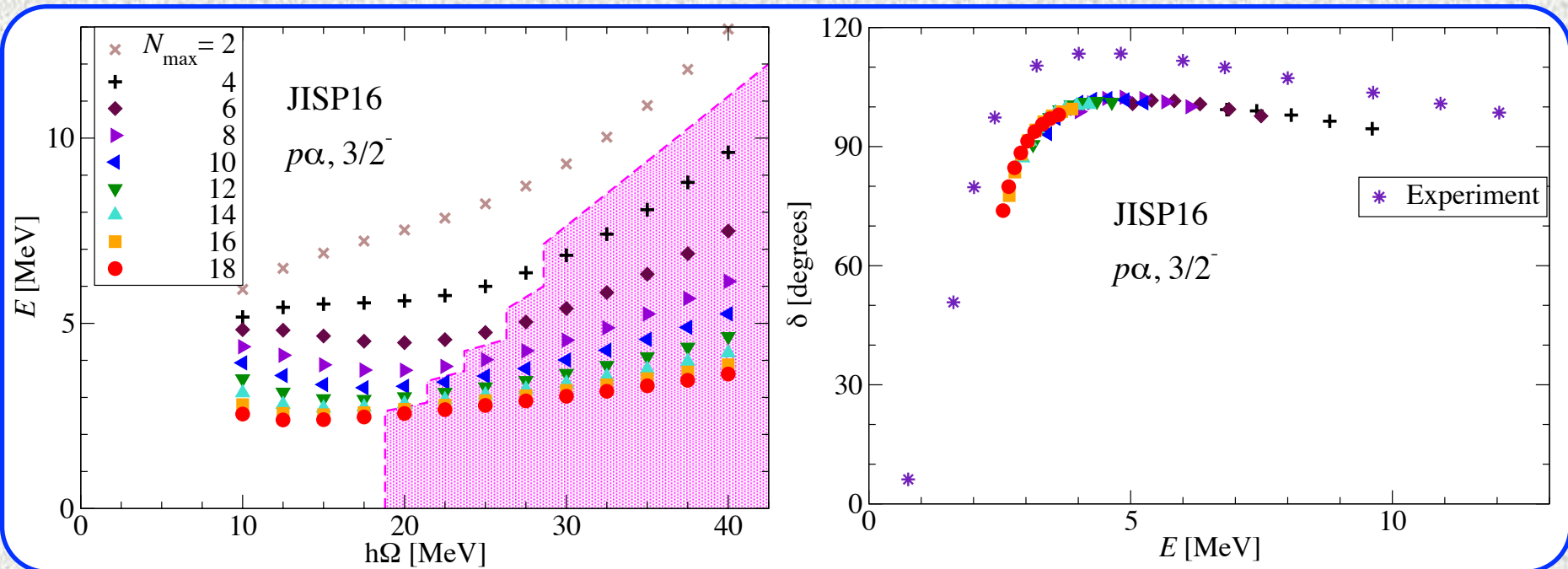


NCSM Single-State HORSE method

${}^5\text{Li} (3/2^-)$
NCSM (JISP16)

Single-State HORSE
phase shifts

+ the selection of the input data



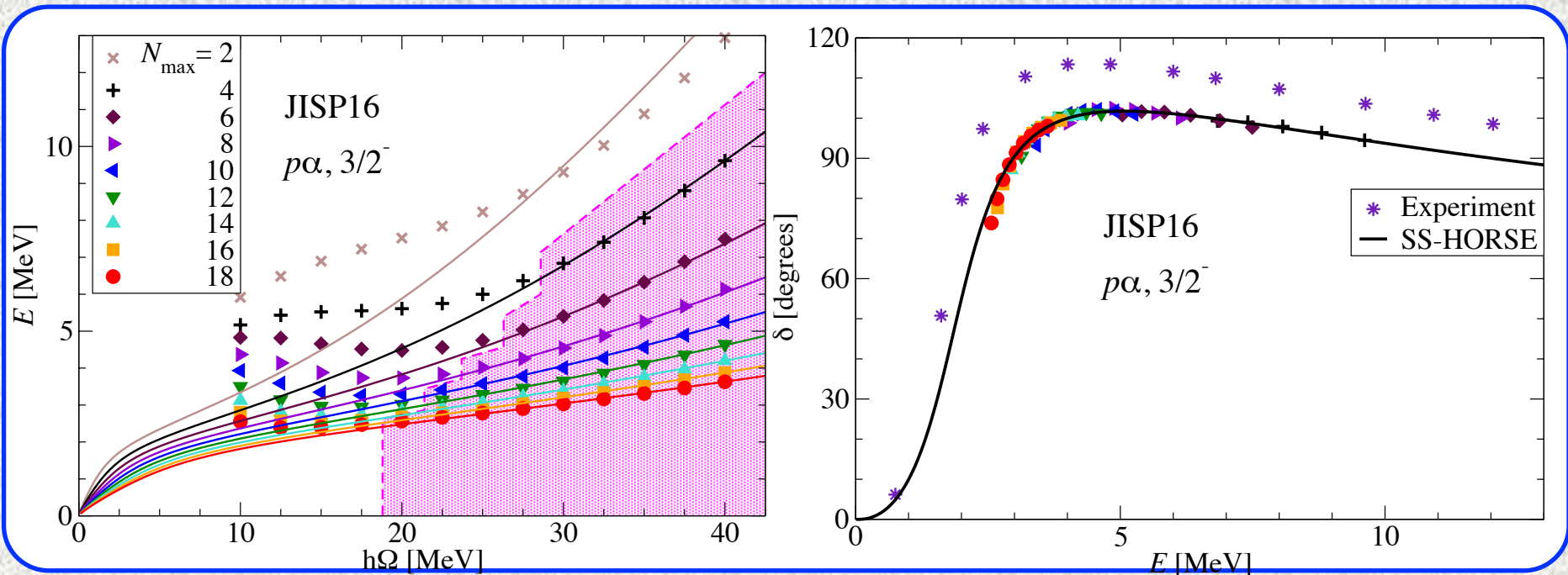
NCSM Single-State HORSE method

${}^5\text{Li} (3/2^-)$
NCSM (JISP16)

Single-State HORSE
phase shifts

+ the selection of the input data
+ phase shift parametrization

$$K_l(k^2) = \frac{w_0 + w_1 k^2 + w_2 k^4}{1 + v_1 k^2}$$



NCSM Single-State HORSE method

${}^5\text{Li} (3/2^-)$

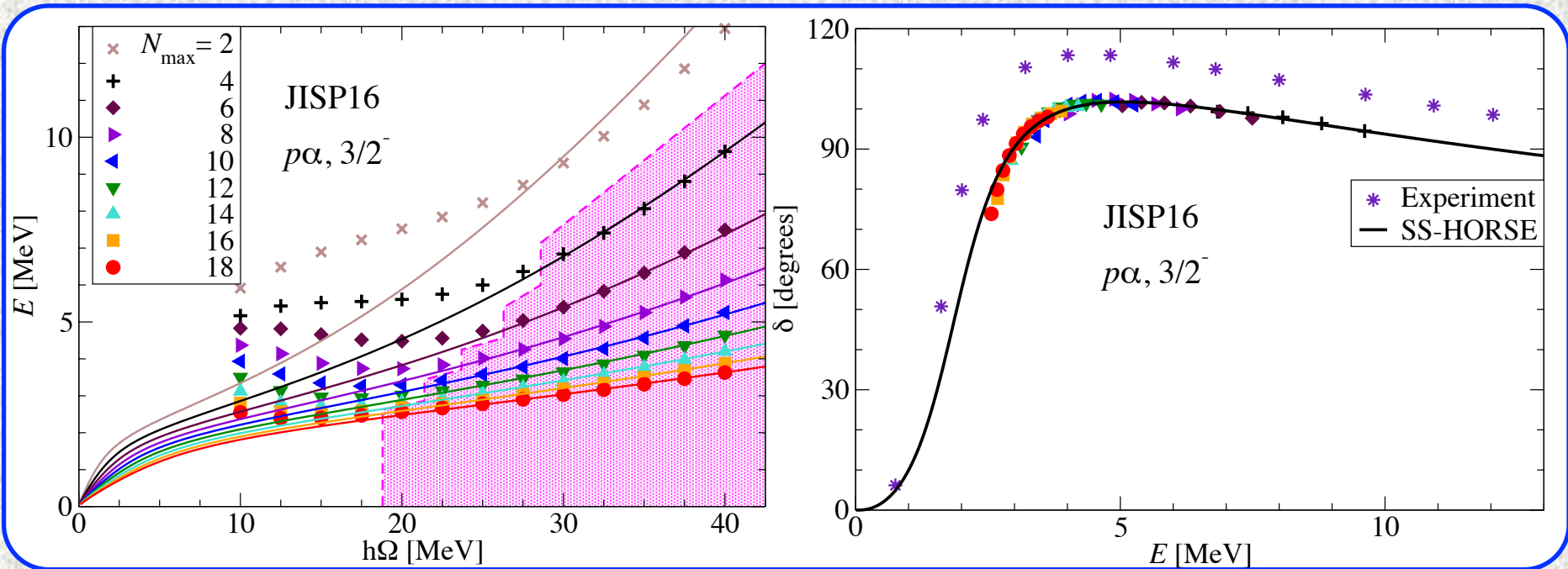
NCSM (JISP16)

Single-State HORSE

phase shifts

+ the selection of the input data

+ phase shift parametrization



S-matrix poles
 $E_p = E_r - i \Gamma/2$

$$K_l(k^2) - 2\eta k^{2l+1} H(\eta) (c_{l\eta})^{-1} = 0$$

Na-scattering. Results.

Within NCSM with interactions JISP16 and Daejeon16 we calculated:

- the lowest energy E_0 of the nuclei ${}^5\text{He}$ u ${}^5\text{Li}$ for states $3/2^-$, $1/2^-$, $1/2^+$ (in model spaces $N_{max} \leq 18$ with $10 \leq \hbar\Omega \leq 40$)*
- the lowest energy ground state of the nucleus ${}^4\text{He}$*

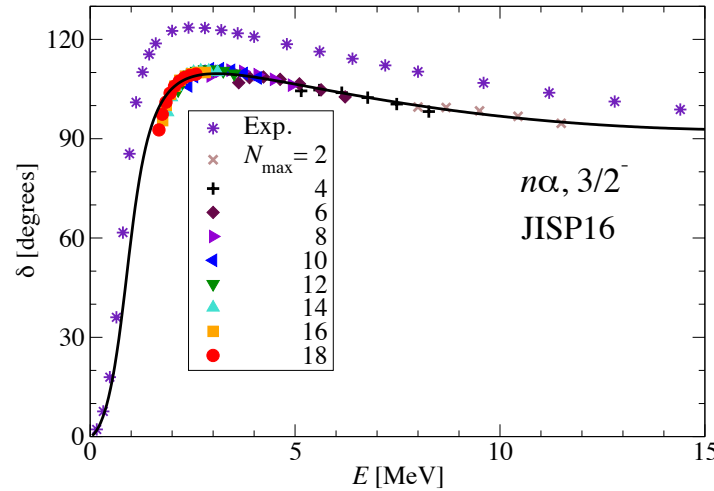
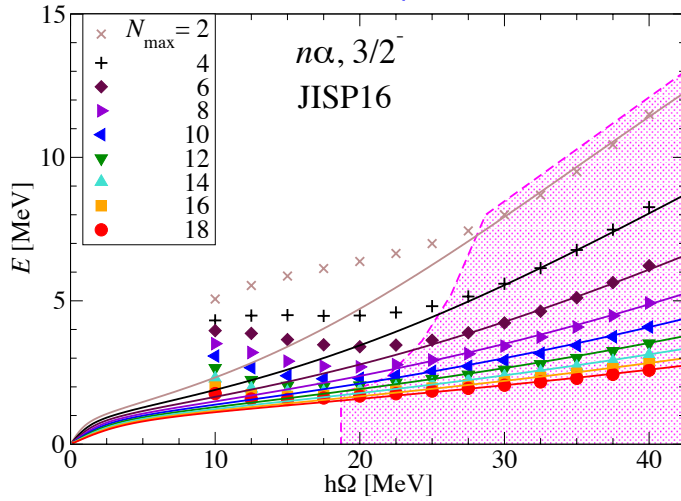
Single-State HORSE:

- Energies were measured from the threshold $N\alpha$*
- The total number of oscillator quanta of NCSM is identified with the number of quanta of relative $N\alpha$ motion in HORSE: $N_{max} + 1 = N$*

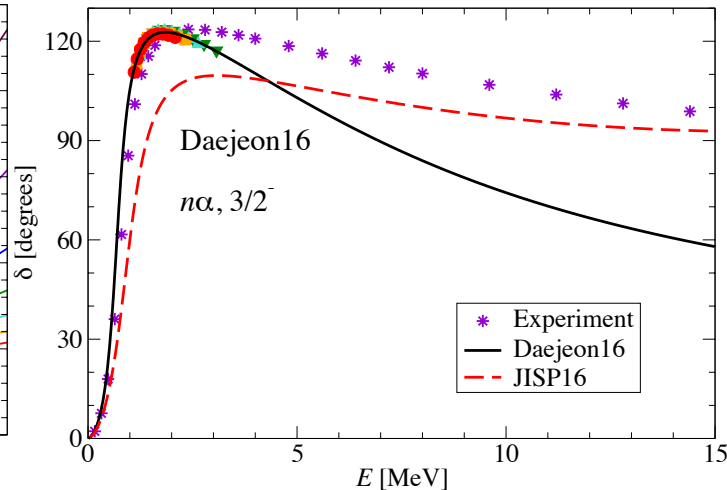
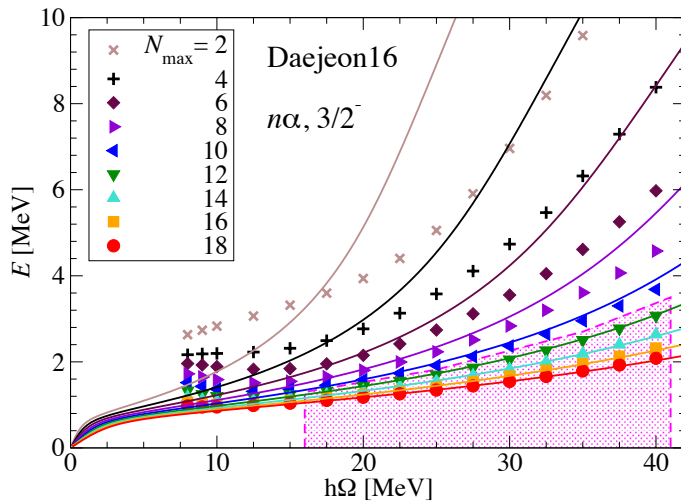
na scattering: resonant state 3/2-

JISP16 (Phys. Rev. C 94, 0624320, 2016)

	E_r MeV	Γ MeV
JISP	0.89	0.99
Dj16	0.68	0.52
Exp.	0.80	0.65



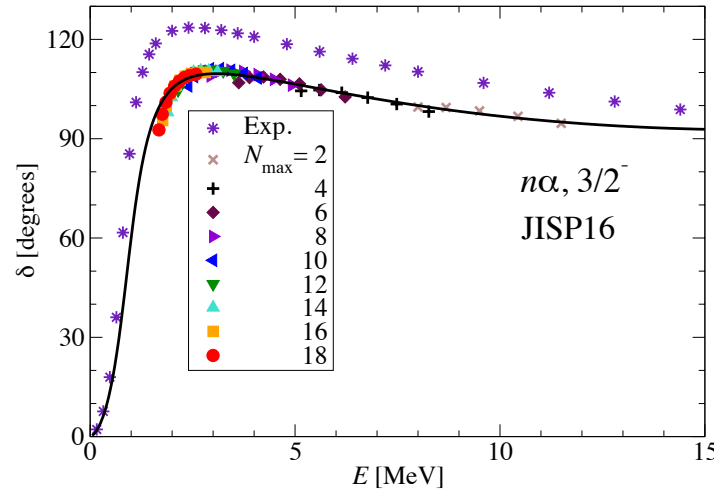
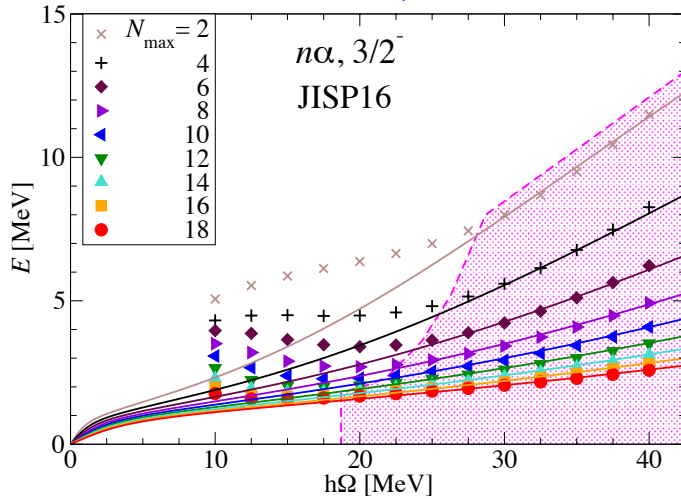
Daejeon16



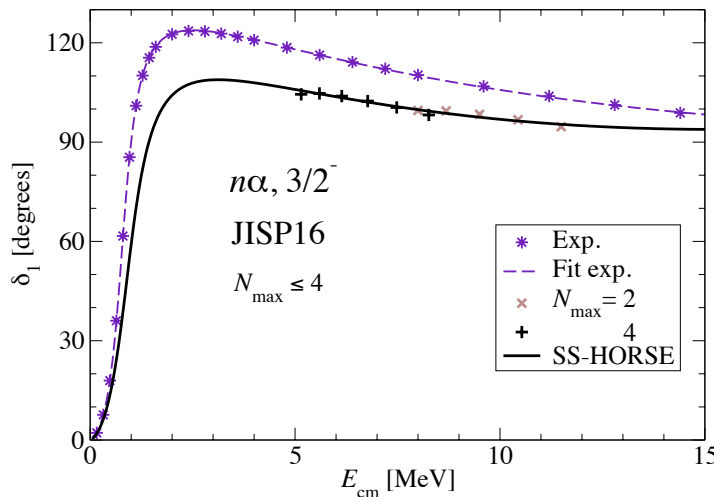
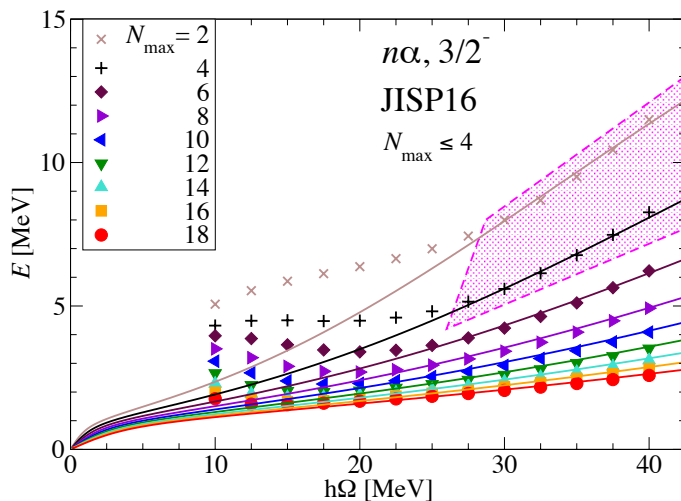
na scattering: resonant state 3/2-

JISP16 (Phys. Rev. C 94, 0624320, 2016)

	E_r MeV	Γ MeV
JISP	0.89	0.99
JISP (2-4)	0.89	1.01
Exp.	0.80	0.65

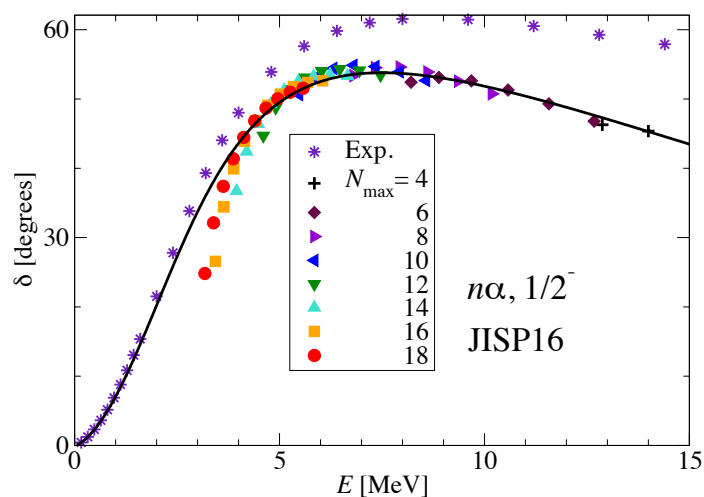
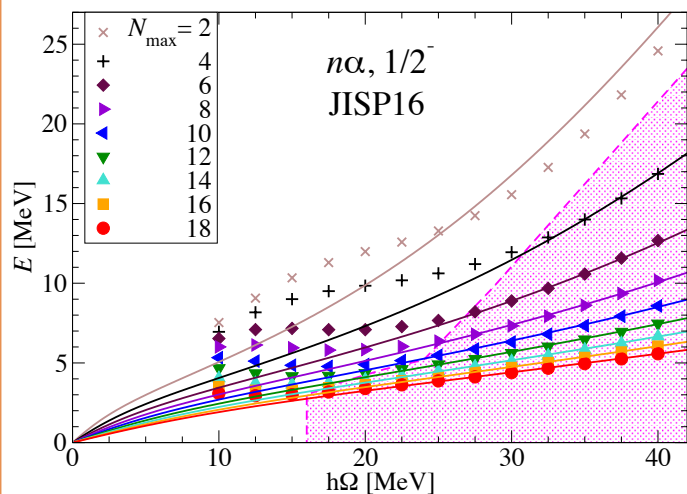


JISP16 ($N_{\max} = 2, 4$ only)

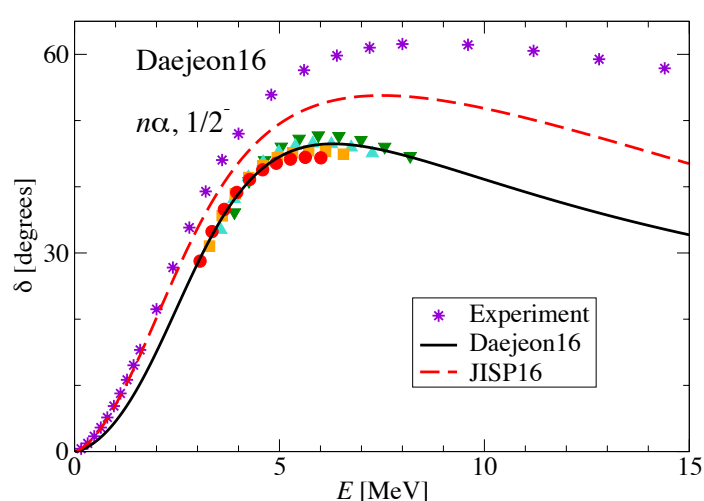
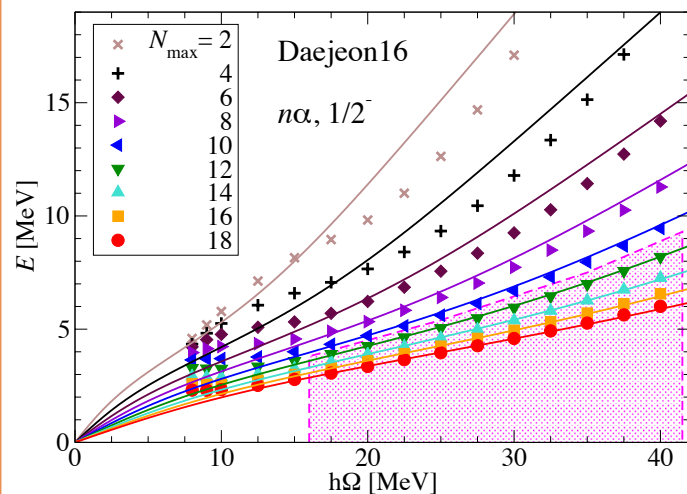


na scattering: resonant state 1/2-

JISP16 (Phys. Rev. C 94, 0624320, 2016)



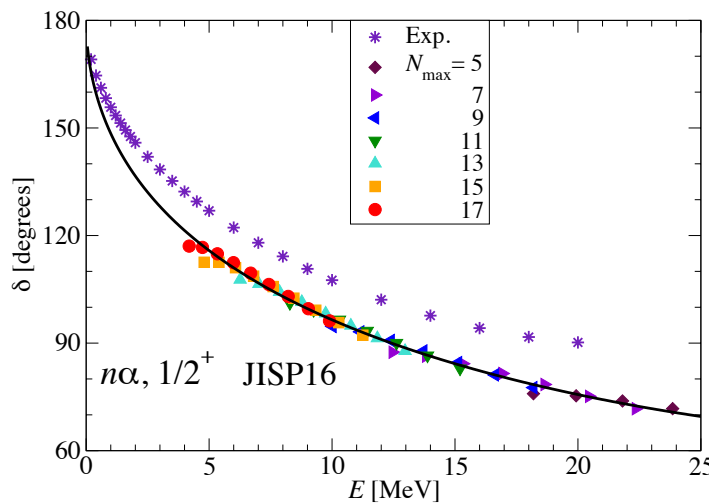
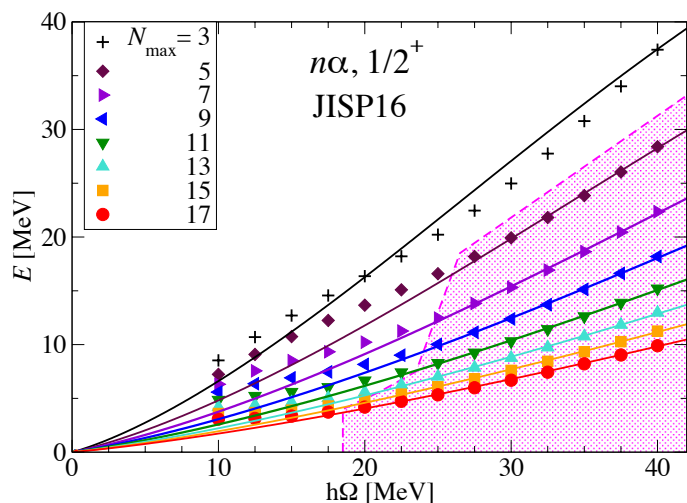
Daejeon16



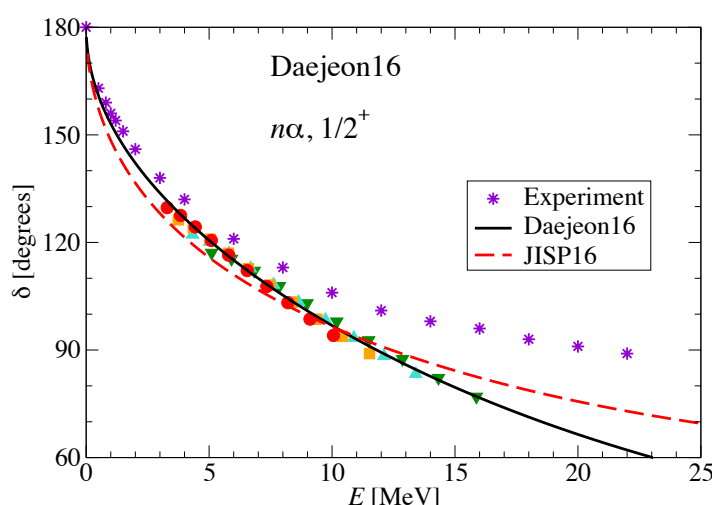
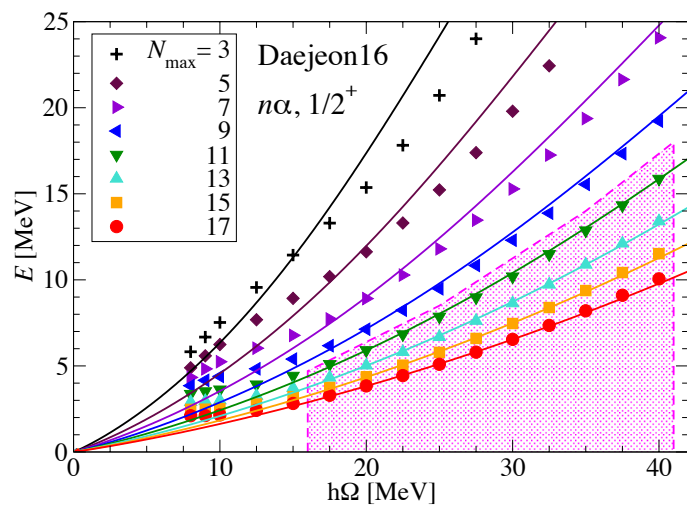
	E_r MeV	Γ MeV
JISP	1.86	5.46
Dj16	2.22	5.13
Exp.	2.07	5.57

Non-resonant na scattering: $1/2^+$

JISP16 (Phys. Rev. C 94, 0624320, 2016)

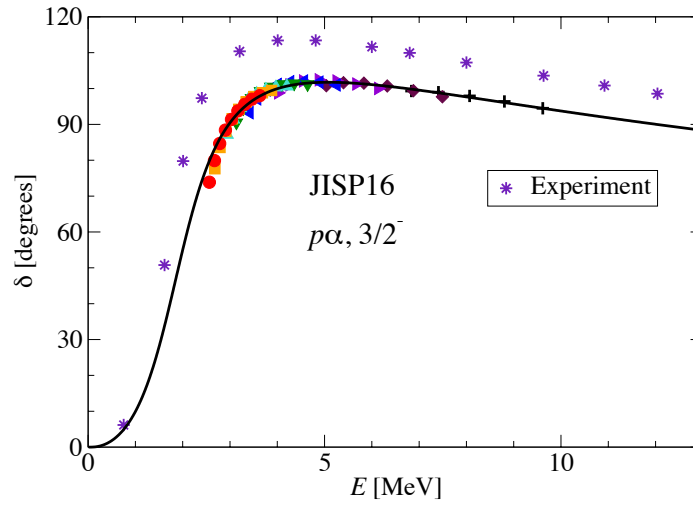
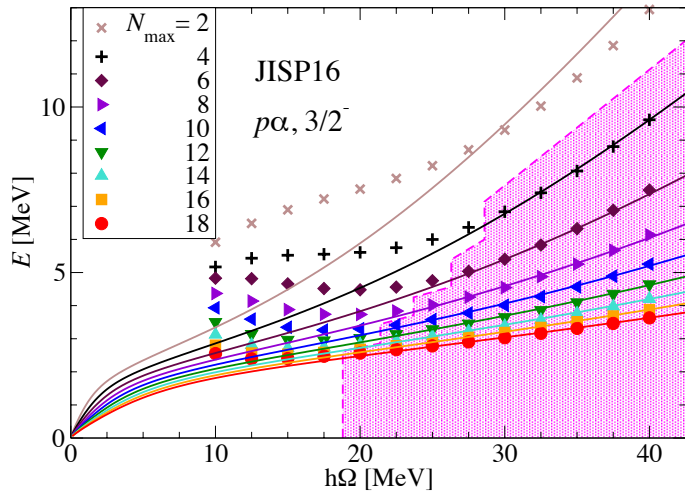


Daejeon16

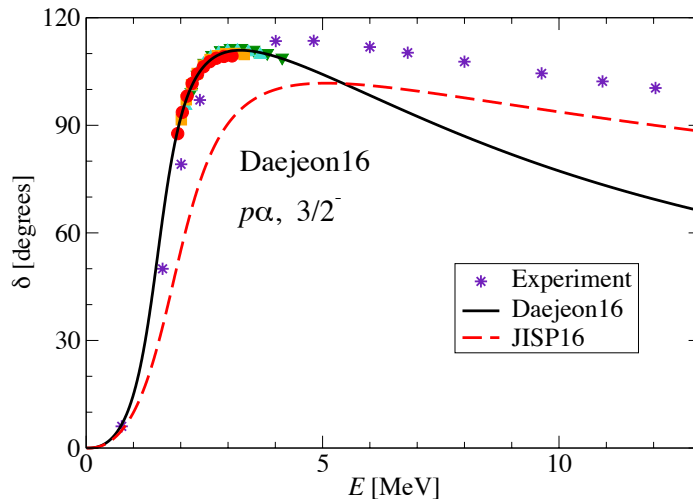
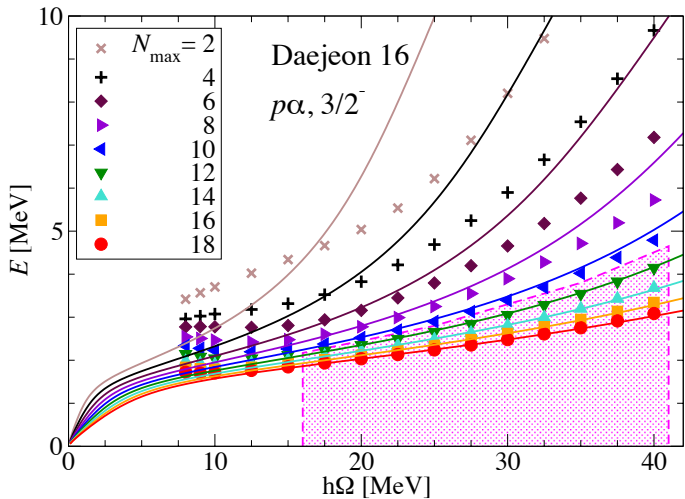


pa scattering: resonant state $3/2^-$

JISP16



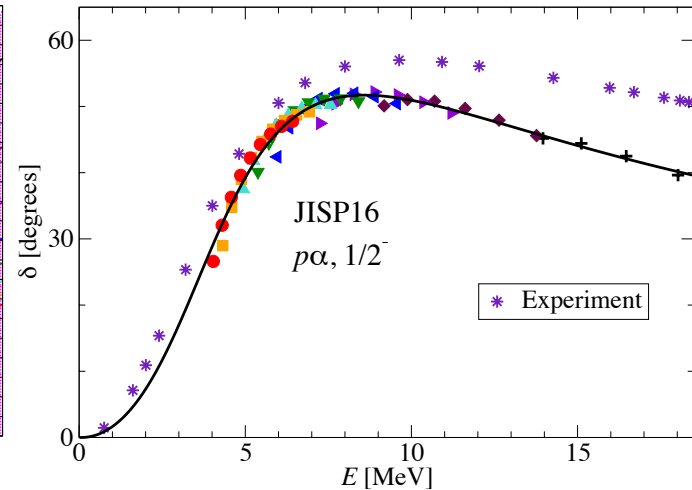
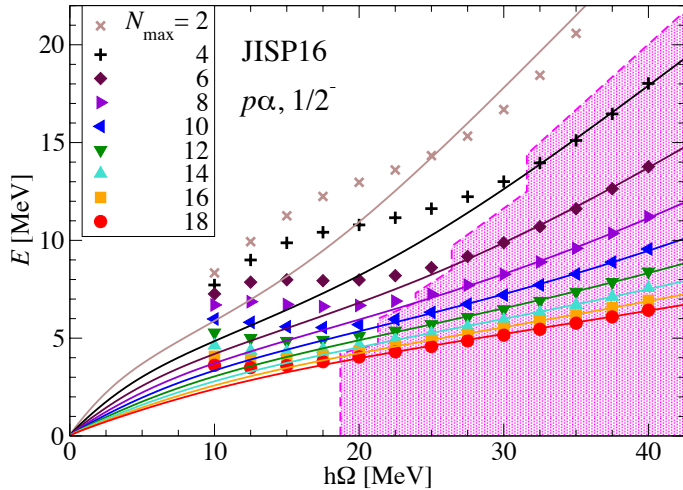
Daejeon16



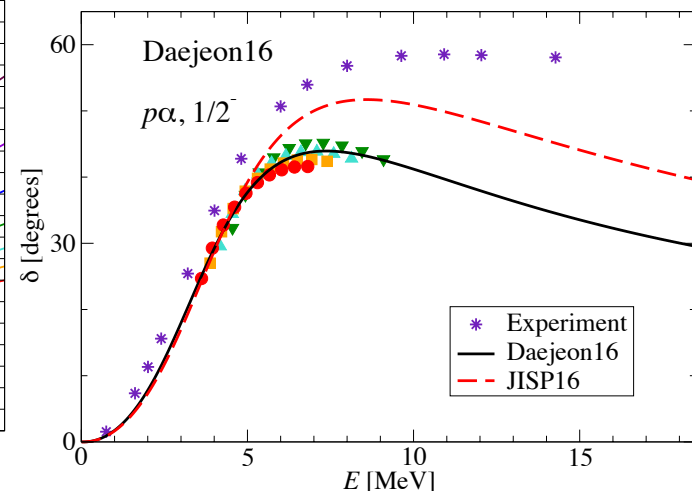
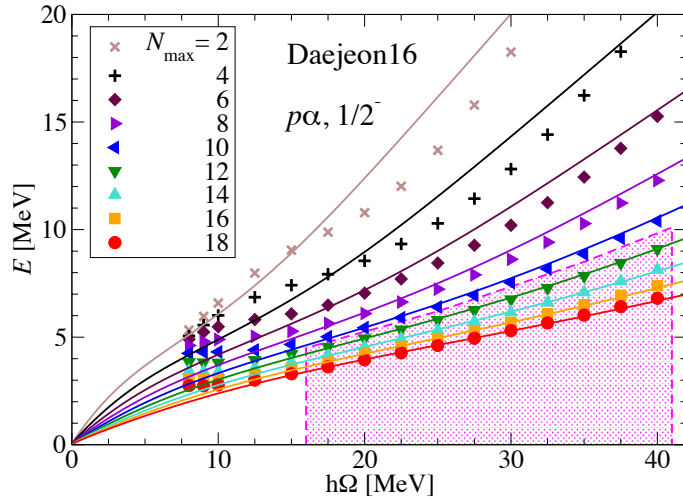
	E_r MeV	Γ MeV
JISP	1.81	1.78
Dj16	1.52	1.05
Exp.	1.69	1.23

pa scattering: resonant state $1/2^-$

JISP16



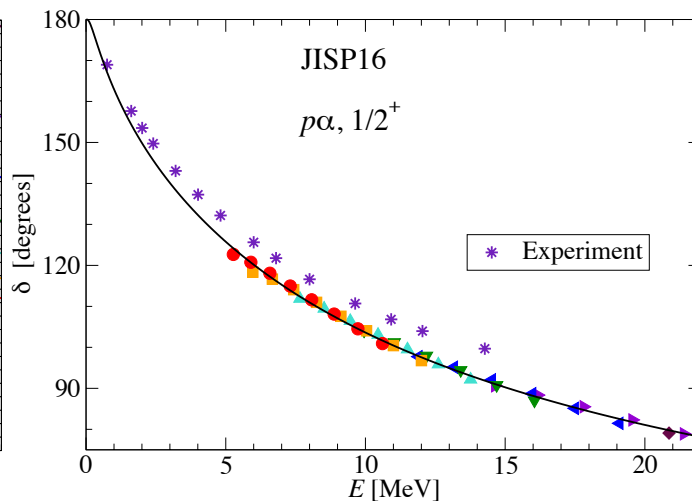
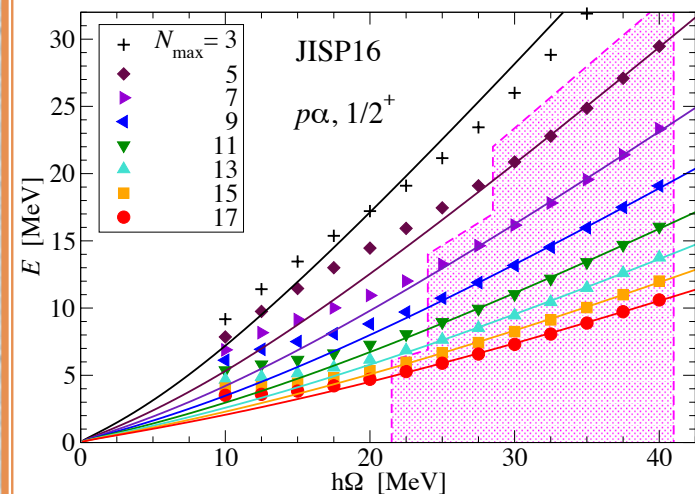
Daejeon16



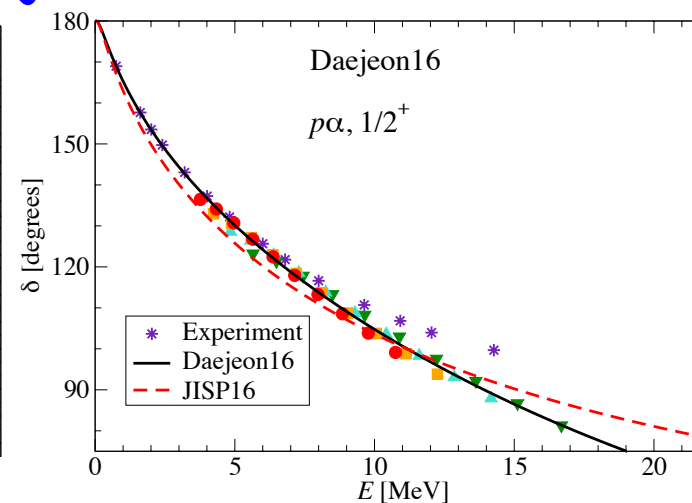
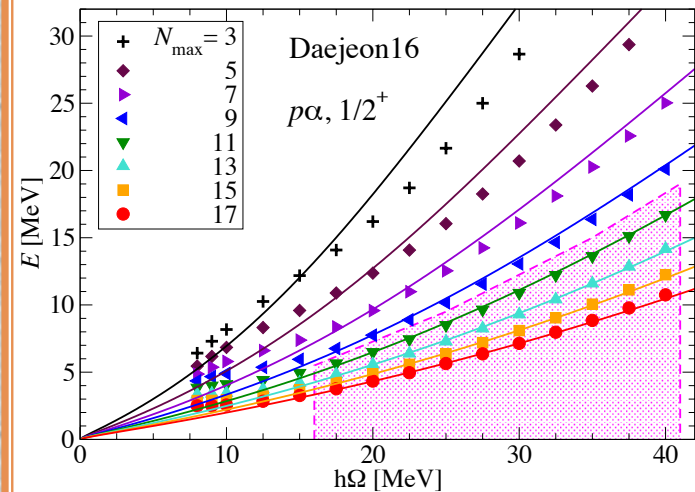
	E_r MeV	Γ MeV
JISP	3.54	6.05
Dj16	3.18	5.63
Exp.	3.18	6.60

Non-resonant pa scattering: $1/2^+$

JISP16



Daejeon16



Energies and widths

	E_r MeV	Γ MeV	Ξ keV		E_r MeV	Γ MeV	Ξ keV	Δ MeV
	${}^5\text{Li}, 3/2^-$				${}^5\text{Li}, 1/2^-$			
<i>Experim.</i>	1.69	1.23			3.18	6.60		1.49
JISP16	1.81	1.78	44		3.54	6.05	66	1.73
Daejeon16	1.52	1.05	24		3.18	5.63	50	1.66
	${}^5\text{He}, 3/2^-$				${}^5\text{He}, 1/2^-$			
<i>Experim.</i>	0.80	0.65			2.07	5.57		1.27
JISP16	0.89	0.99	37		1.86	5.46	53	0.97
Daejeon16	0.68	0.52	22		2.22	5.13	48	1.54

$$\Delta = E_r^{(1/2^-)} - E_r^{(3/2^-)}$$

Conclusions

- ✓ Method *NCSM Single-State HORSE* for description scattering states, based on shell model calculations of nuclei, is suggested
- ✓ This method has been applied to Na resonant and non-resonant scattering

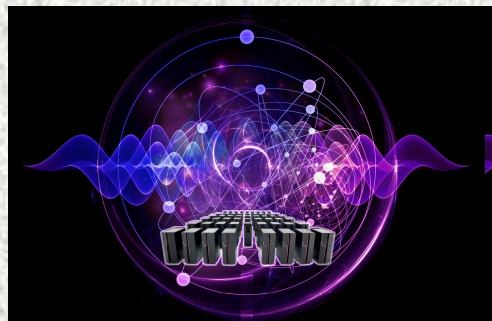
Phys. Rev. C 98, 044624 (2018)

RSF

Russian
Science
Foundation

*This work was supported by the
Russian Science Foundation
(project No 16-12-10048)*

THANKS YOU
for YOUR ATTENTION



NTSE-2018

IBS Daejeon, Korea

29 Oct. – 2 Nov. 2018