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# Study of Low-energy Phase Shifts using NCSM with Three NN Interactions

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KAERI 한국원자력연구원 Korea Atomic Energy Research Institute

# Outline

- About KNDC/KAERI
- Motivation
- Ab initio approaches
- Harmonic Oscillator Representation of Scattering Equations (HORSE) formalism
- Single-State (SS) HORSE
- Application to (n,α) scattering
- Summary and Further works

# Korea Atomic Energy Research Institute



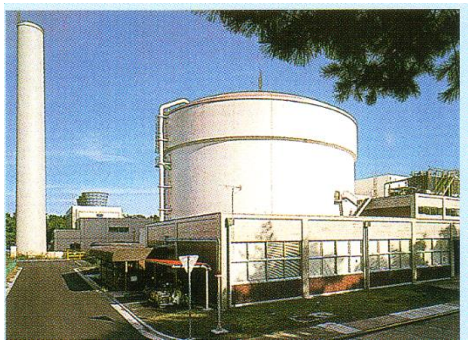
- ✓ Nuclear basic research
- ✓ Nuclear safety research
- ✓ Nuclear reactor research
- ✓ Nuclear fuel and fuel cycle research
- ✓ Radiation and radioisotope application
- ✓ Nuclear Fusion Technology
- ✓ Proton Accelerator Development
- ✓ Nuclear Manpower Training
- ✓ Nuclear policy research

# Nuclear Data

- Nuclear data are physical parameters that describe the internal structure of nuclei, their decay and interactions.
  - Nuclear Structure Data
    - Mass, half-life, and decay modes of nucleus
  - Nuclear Reaction Data
    - Reaction cross sections and energy-angle distributions
  - Atomic and molecular data
    - Level structures, transition probabilities
- Nuclear data, as brides between nuclear/atomic physics and their applications, play a basis in the research and development of nuclear energy and radiation applications.

# Nuclear Data Needs

➢ Nuclear data are needed in a variety of applications.



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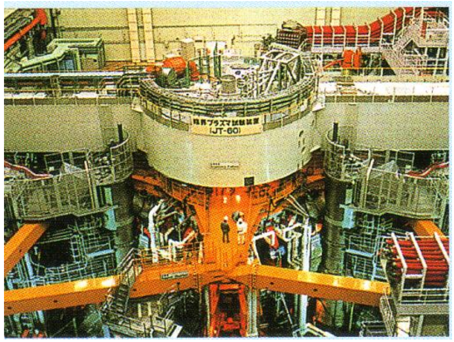

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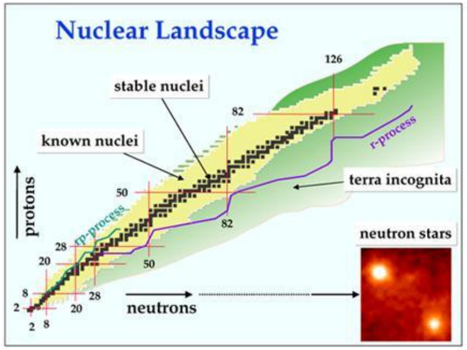
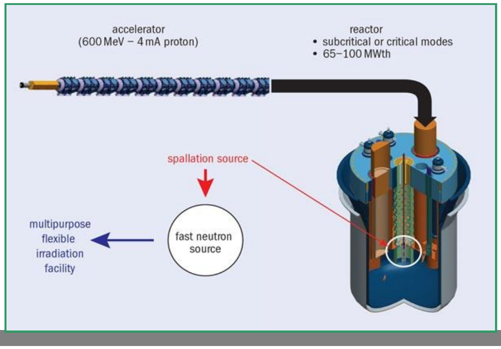



| Nuclear energy development | Basic science |
|---|---|
| Accelerator applications | Space engineering |

*ADS*

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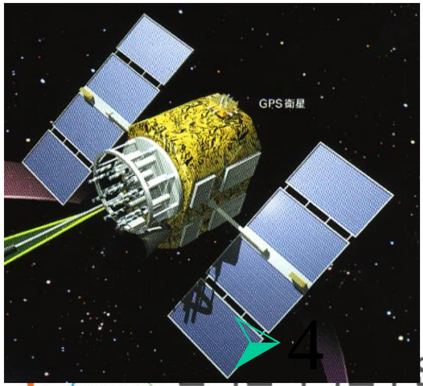


# Korea Nuclear Data Center @ KAERI

- KNDC/KAERI is performing the various activities of the nuclear data complication/evaluation, processing, validation, and measurement.
  - Measurement of nuclear reaction cross sections
  - Evaluation of nuclear reaction/decay data
  - Development of evaluation technique for nuclear reaction
  - Process/validation/dissemination of the evaluated data files for applications
- The mission (aim) of KNDC is to provide nuclear data on time for nuclear physics, nuclear power and related fields such as nuclear energy developments, ADS, medical and basic science.
- Within this regard, improving and updating the nuclear structure and decay data become important.
- In order to obtain more precise nuclear data, we require advanced nuclear theory and approaches based on microscopic description (first principles on nucleon level).

# Motivation

- ✓ A more consistent treatment of reactions within ab initio framework is a challenge of nuclear theory.
- ✓ Describe nuclei from first principles as systems of nucleons that interact by fundamental interactions.
- ✓ Why it has not been solved yet?
  - ➢ High-quality nucleon-nucleon (NN) potentials constructed for many years
    - Difficult to use in many-body calculations
  - ➢ NN interaction not enough for $A > 2$
    - Three-nucleon interaction not well known
  - ➢ Need sophisticated approaches and big computing power.

# Motivation

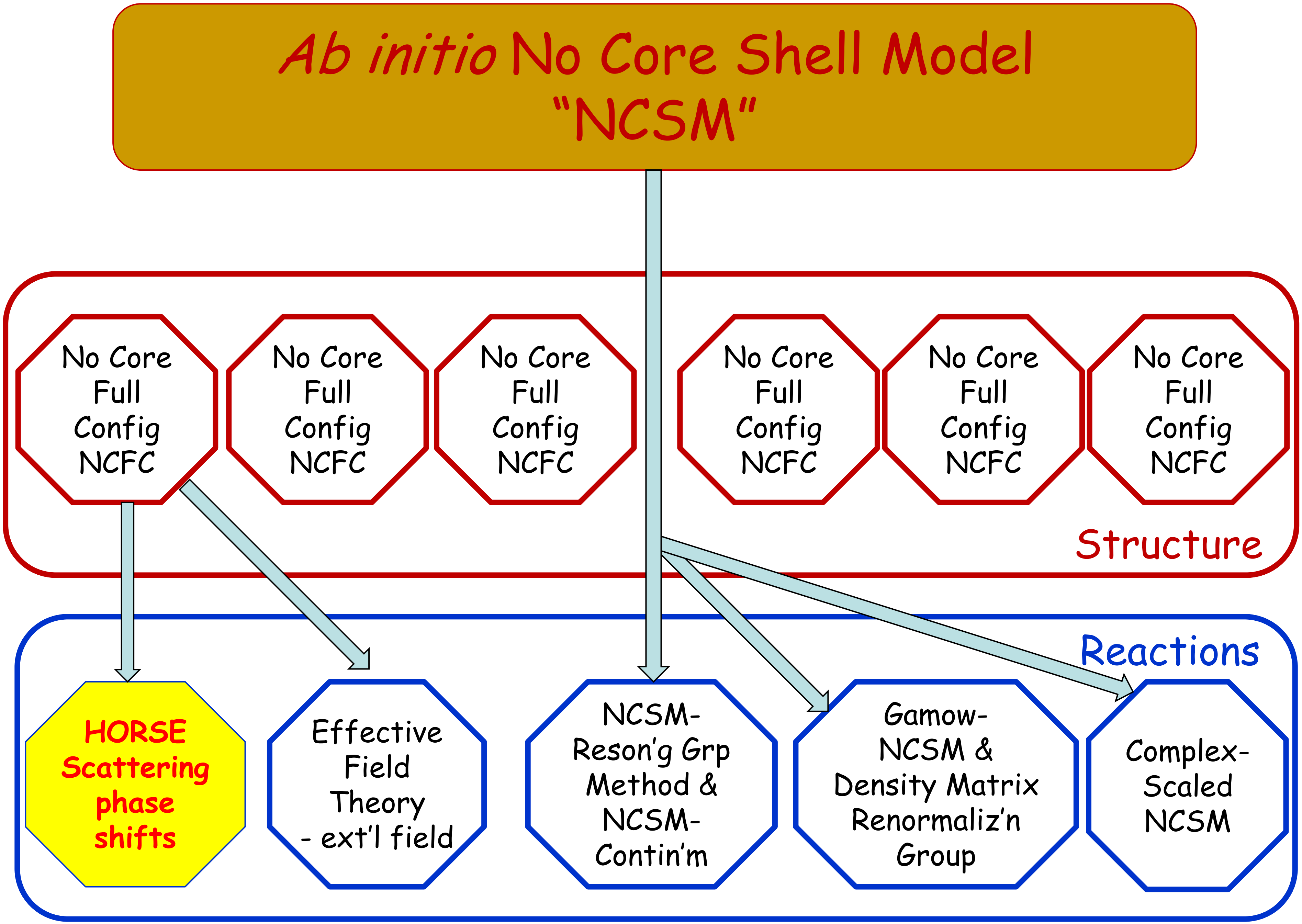
- ✓ The microscopic description of nuclear reactions, continuum spectra and widths of nuclear resonant states have been significantly developed.
- ✓ Ab initio no-core shell model (NCSM) is a powerful tool to solve the nuclear structure problem for light nuclei.
  - ➢ This is technique for the solution of the A-nucleon bound-state problem.
  - ➢ This is not appropriate to deal with the continuum states; not clear how to interpret states in continuum at low-energies and how to calculate scattering phase shifts or resonance widths.
- ✓ We propose a simple method (SS HORSE) based on *J*-matrix formalism.

# Ab initio approaches

- To understand the properties of nuclei from the first principles
- To achieve a predictive theory for the light nuclear systems
- Ab initio calculations for unbound states and scattering processes is very difficult.
- A = 3, 4 nucleon systems
  - Faddeev method
  - Faddeev–Yakubovsky (FY) method
  - Hyperspherical Harmonics (HH) method
  - Alt, Grassberger and Sandhas (AGS) method
- A > 4 nucleon systems
  - Green's Function Monte Carlo (GFMC)
    - First ab initio calculation for neutron-4He scattering
    - Scattering boundary conditions at large radius ($R \geq 7$ fm)
  - Coupled-Cluster Method (CCM)
    - Applicable mostly to closed shell nuclei (A = 4, 16, 40, 48, 56, …)
    - Resonant and scattering single-particle states within a Gamow basis
  - Ab Initio No-Core Shell Model (NCSM)

# Ab initio No Core Shell Model

- ✓ Ab initio
  - To describe nuclei from first principles using fundamental interactions without uncontrolled approximations.
- ✓ No core
  - All nucleons are active and no inert core
- ✓ Shell model
  - Use harmonic oscillator basis
- ✓ Needs huge computing resources.




From the talk by J.P. Vary

# Ab initio NCSM calculations (by Ik Jae Shin)

- ✓ MFDn : Many Fermion Dynamics for nuclear physics (J. Vary et al.)
  - Scalable and load-balanced CI code for nuclear structure
  - M-scheme
  - Hybrid OpenMP/MPI
- ✓ Tachyon II @ KISTI
  - 3,200 nodes
  - 2 quad-core Intel Xeon x5570 2.93-GHz processors per node
  - 24 GB memory per node
- ✓ NN interactions
  - JISP16
  - $NNLO_{opt}$
  - Deajeon16

# NN Interactions

- JISP16 : J-matrix Inverse Scattering Potential (ref. A.M.Shirokov's talk)
  - Constructed to reproduce np scattering data (Phase shifts)
  - Use Phase-Equivalent Transformations (PET)
  - Non-local phenomenological NN interaction
  - Appropriate description for light nuclei
  - Good convergence behavior for binding energies
- $\text{NNLO}_{\text{opt}}$ : Optimized chiral interaction at next-to-next-to-leading order (A. Ekstrom, et al. Phys. Rev. Lett. 110 (2013) 192502)
  - Optimized NN interaction at NNLO using POUNDerS
  - 3 pion-nucleon couplings and 11 partial wave contract parameters
- Daejeon16 (ref. A.M.Shirokov's talk and Phys. Letts. B 761, 87 (2016))
  - Based on SRG'd chiral N3LO, uses PETs to fit properties of light nuclei
  - Useful for normal p-shell nuclei
  - Gives reliable results even though for exotic nuclei

# HORSE
## (Harmonic Oscillator Representation of Scattering Equations)

- ✓ Based on the J-matrix formalism in scattering theory
  - ✓ J-matrix formalism with oscillator basis: HORSE

- ✓ Aim
  - ➢ To calculate low-energy phase shifts
  - ➢ To extract resonant energies and widths

- ✓ Advantage
  - ➢ Calculate directly from the NCSM results without additional complexities
    - NCGSM: introducing additional Berggren basis states
    - NCSM/RGM: additional RGM calculations

# HORSE

- Schrodinger equation

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

- Expanded wave function  in oscillator functions

$$u_l(E,r) = \sum_{n=0}^{\infty} a_{nl}(E)\, R_{nl}(r)$$

$$R_{nl}(r) = (-1)^n \sqrt{\frac{2n!}{r_0 \Gamma(n+l+3/2)}} \left(\frac{r}{r_0}\right)^l \exp\left(-\frac{r^2}{2r_0^2}\right) L_n^{l+1/2}\left(\frac{r^2}{r_0^2}\right)$$

  - $L_n^{\alpha}(x)$ : the associated Laguerre polynomial
  - $r_0 = \sqrt{\hbar/m\Omega}$: the oscillator radius
  - $a_{nl}(E)$:  a solution of an infinite set of algebraic equations

$$\sum_{n'=0}^{\infty} (H^l_{nn'} - \delta_{nn'} E)\ a_{n'l}(E) = 0$$

# HORSE

## ✓ Structure of the infinite Hamiltonian

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

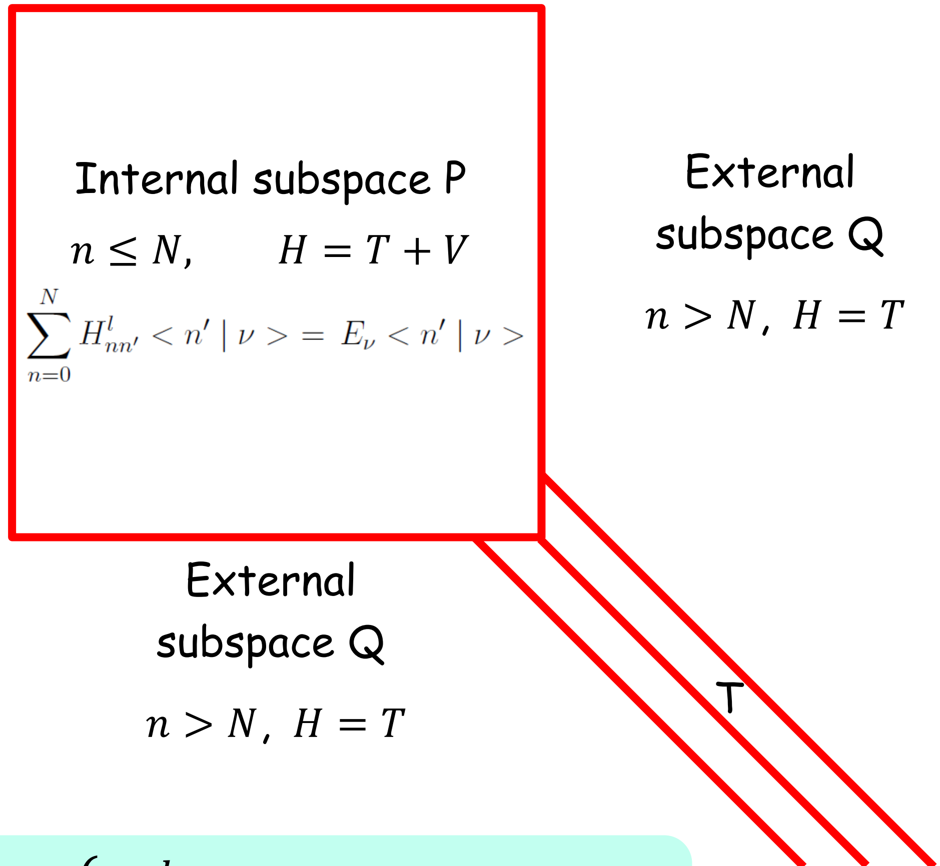
➢ Kinetic energy matrix

- $T^l_{nn} = \frac{\hbar\omega}{2}(2n + l + \frac{3}{2})$
- $T^l_{n,n\pm1} = -\frac{\hbar\omega}{2}\sqrt{(n+1)(n+l+\frac{3}{2})}$

$$T^l_{nn'} \sim n, increase\ with\ n, n' \to \infty$$

➢ Potential energy matrix

$$V^l_{nn'}: decrease\ with\ n, n' \to \infty$$




Truncated potential matrix →

$$\tilde{V}^l_{nn'} = \begin{cases} V^l_{nn'}, & if\ n\ and\ n' \le N \\ 0, & if\ n\ or\ n' > N \end{cases}$$

# HORSE

✓ Phase shift

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN}(E)\, T^{l}_{N,N+2}\, S_{N+2,l}}{C_{Nl}(E) - G_{NN}(E)\, T^{l}_{N,N+2}\, C_{N+2,l}}$$

$$G_{NN}(E) = -\sum_{\nu=0}^{N} \frac{< N \mid \nu >^2}{E_\nu - E}$$

➢ Regular and irregular oscillator solutions

$$S_{nl}(E) = \sqrt{\frac{2r_0 n!}{\Gamma(n+l+3/2)}}\; q^{l+1} \exp\left(-\frac{q^2}{2}\right) L_n^{l+1/2}(q^2)\ ,$$

$$C_{nl}(E) = \sqrt{\frac{2r_0 n!}{\Gamma(n+l+3/2)}}\; \frac{\Gamma(l+1/2)}{\pi\, q^l} \exp\left(-\frac{q^2}{2}\right) \Phi(-n-l-1/2, -l+1/2; q^2)\ .$$

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# Problems with direct HORSE application

- P-space: associated with many-body SM basis

$$< N \mid \nu > \Longrightarrow < N[\alpha]J\Gamma \mid \nu >$$

$$G_{NN}(E) = -\sum_{\nu=0}^{N} \frac{< N \mid \nu >^2}{E_\nu - E} \quad \longrightarrow \quad G_{NN}(E) = -\sum_{\nu=0}^{N} \frac{< N[\alpha]J\Gamma \mid \nu >^2}{E_\nu - E}$$

- The P-space dimensionality $d$ increases drastically.
- A lot of $E_\nu$ eigenstates needed while NCSM usually calculate few lowest states only.
- Need $\langle \mathcal{N}[\alpha]J\Gamma|\nu\rangle$ for the relative N-nucleus coordinate $r_{nA}$ but NCSM provides $\langle \mathcal{N}[\alpha]J\Gamma|\nu\rangle$ for the coordinate $r_n$ .
- Therefore, the HORSE formalism can't directly apply in nucleon-nucleus scattering problem.

→ Single-State (SS) HORSE

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# Single State (SS) HORSE

- ✓ Suppose: a shell model eigenstate defines all the properties of a nearby resonant state.

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN}(E)\,T^{l}_{N,N+2}\,S_{N+2,l}}{C_{Nl}(E) - G_{NN}(E)\,T^{l}_{N,N+2}\,C_{N+2,l}} \qquad G_{NN}(E) = -\sum_{\nu=0}^{N} \frac{< N[\alpha]J\Gamma \mid \nu >^2}{E_\nu - E}$$

$$E = E_\nu \;; \qquad G_{NN}(E_\nu) \Longrightarrow \infty$$

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

- ✓ We calculate a set of $E_\nu$ eigenstates with different *$\hbar\Omega$ and $N_{max}$* within NCSM.
- ✓ We obtain a set of δ(E) values at low energies.

# Application to (n,α) scattering

- ✓ Calculate the (n,α) scattering phase shifts using the results of the NCSM calculations of $^5$He with the JISP16, $NNLO_{opt}$ and Daejeon16 NN interactions.
- ✓ The model space of NCSM is conventionally truncated using $N_{max}$, the maximal excitation oscillator quanta.
- ✓ The model space of NCSM should be associated with the P space of the SS HORSE method.
  - ➢ This is defined using total oscillator quanta in the many-body system, $\mathcal{N}$, in the SS HORSE formulas.
  - ➢ In the case of $^5$He
    - $\mathcal{N} = N_{max} + 1$ for the $\frac{1}{2}^-$, $\frac{3}{2}^-$ and $\frac{1}{2}^+$ state

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# Application to (n,α) scattering

- ✓ Pick up for further scattering calculations the lowest NCSM eigenenergies $E^{NCSM}$ in $^5$He nuclei with $J^\pi = \frac{1}{2}^-, \frac{3}{2}^-$ and $\frac{1}{2}^+$ states.
  - $E^{NCSM} < 0$ (Since they are defined regarding to the 5-nucleon decay threshold.)
  - But the SS HORSE method requires positive eigenenergies $E_0$ defined in respect to the N + α threshold.
  - Define $E_0 = E^{NCSM} - E^{\alpha}$
  - $E^{\alpha}$ : the $^4$He ground state energy obtained in NCSM
    - Same $\hbar\Omega$
    - Same $N_{max}$ in the case of $\frac{3}{2}^-$ and $\frac{1}{2}^-$ states of $^5$He
    - Excitation quanta $N_{max}$ - 1 in the case of $\frac{1}{2}^+$ state of $^5$He

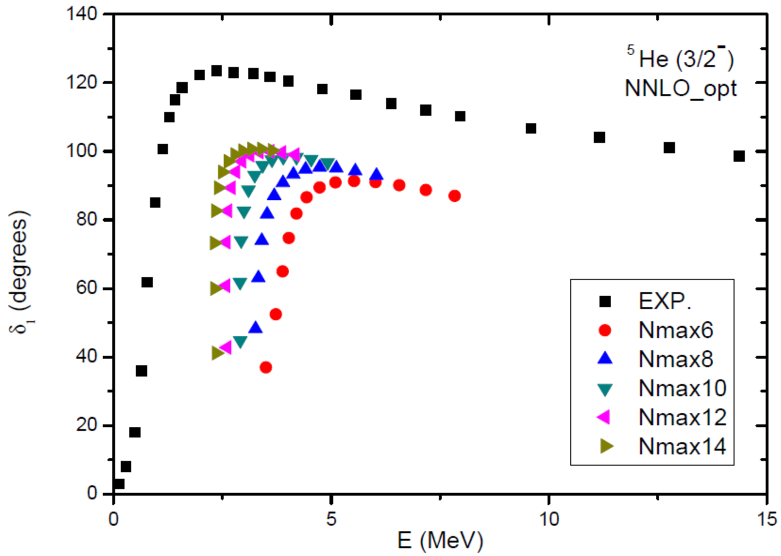
$$E_\nu(\hbar\Omega, N_{\max}) = E_\nu^{A=5}(\hbar\Omega, N_{\max}) - E_\nu^{A=4}(\hbar\Omega, N_{\max})$$

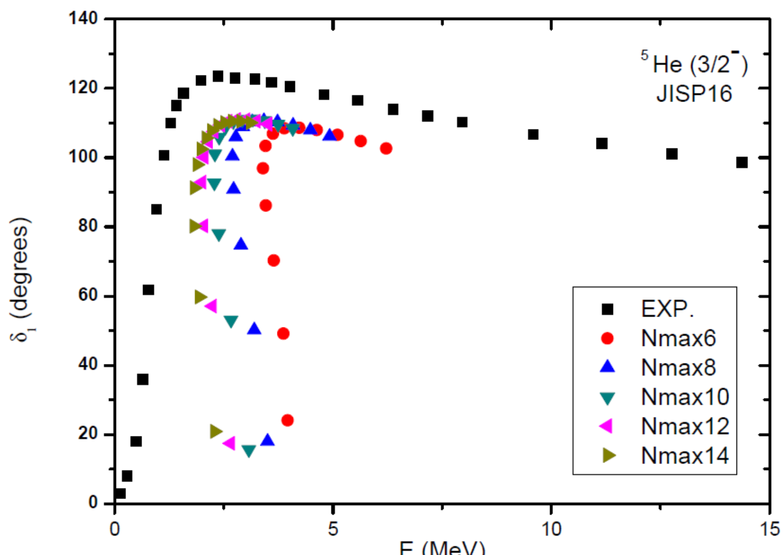
$$E_\nu(\hbar\Omega, N_{\max}) = E_\nu^{A=5}(\hbar\Omega, N_{\max}) - E_\nu^{A=4}(\hbar\Omega, N_{\max} - 1)$$

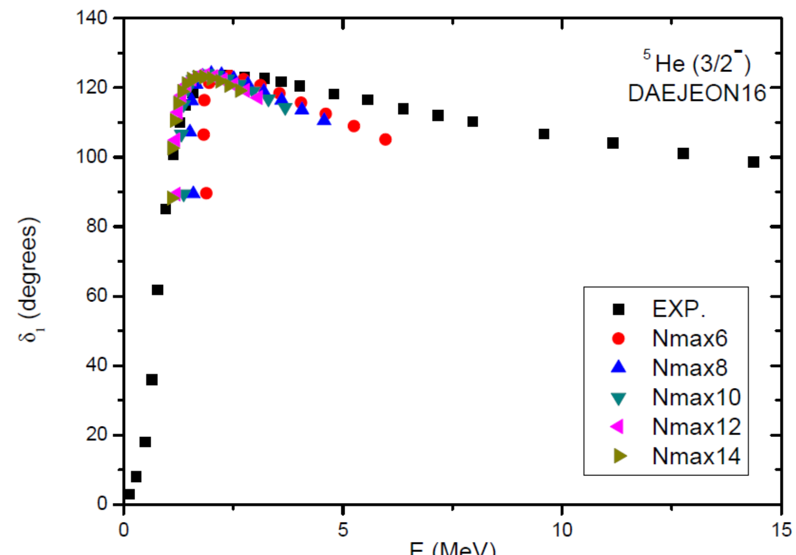
# Results: (n,α) scattering in the $\frac{3}{2}^-$ state

- ✓ $^5$He calculation
  - $N_{max}$ = 6, 8, 10, 12, 14
  - $\hbar\Omega$ : 10 to 40 MeV (2.5 MeV step)
  - Three different NN interactions
    - JISP16
    - $NNLO_{opt}$
    - Daejeon16

Exp. Data: J. E. Bond et. Al, Nucl. Phys. A **287**, 317 (1977).



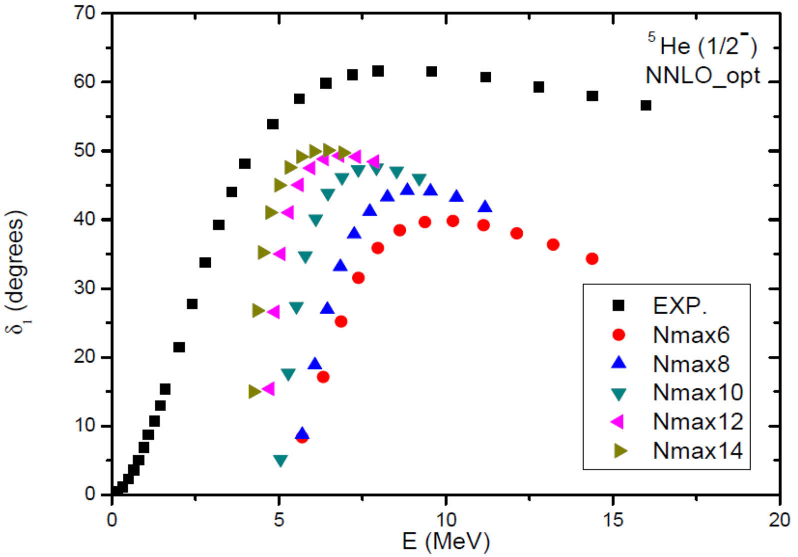



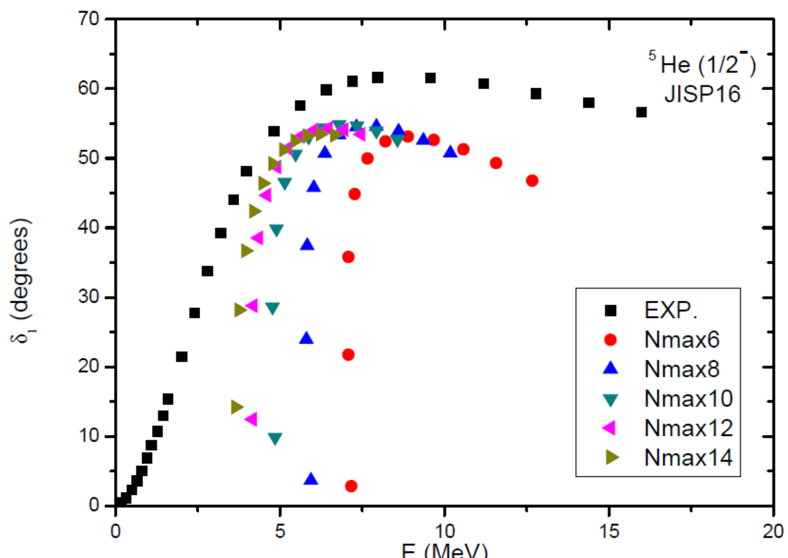



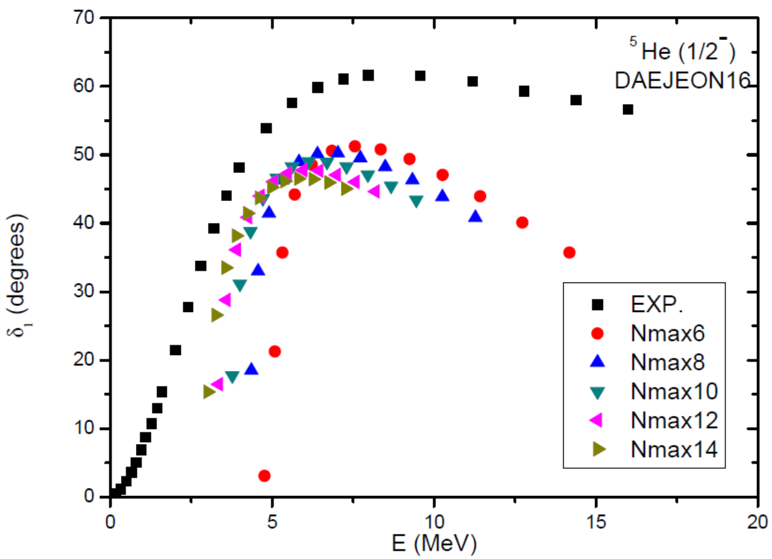
# Results: (n,α) scattering in the $\frac{1}{2}^{-}$ state

- ✓ $^{5}$He calculation
  - $N_{max}$ = 6, 8, 10, 12, 14
  - $\hbar\Omega$ : 10 to 40 MeV (2.5 MeV step)
  - Three different NN interactions
    - JISP16
    - $NNLO_{opt}$
    - Daejeon16

Exp. Data: J. E. Bond et. Al, Nucl. Phys. A **287**, 317 (1977).



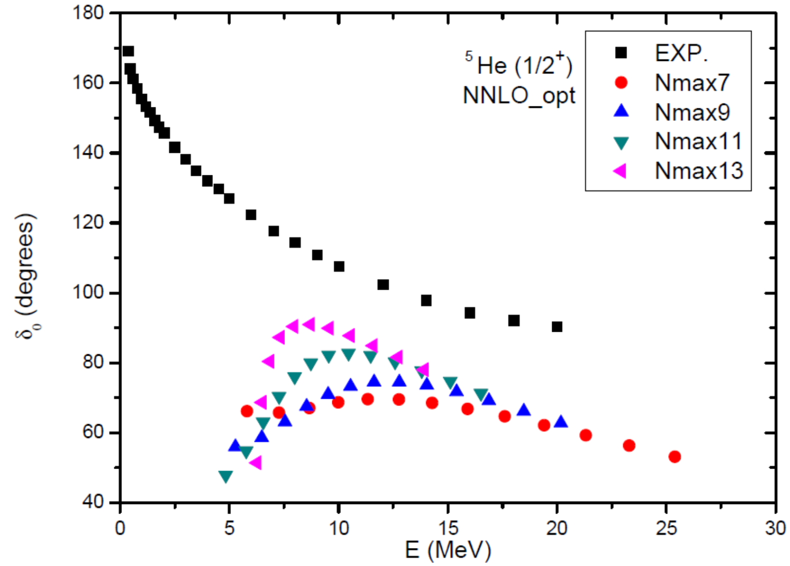



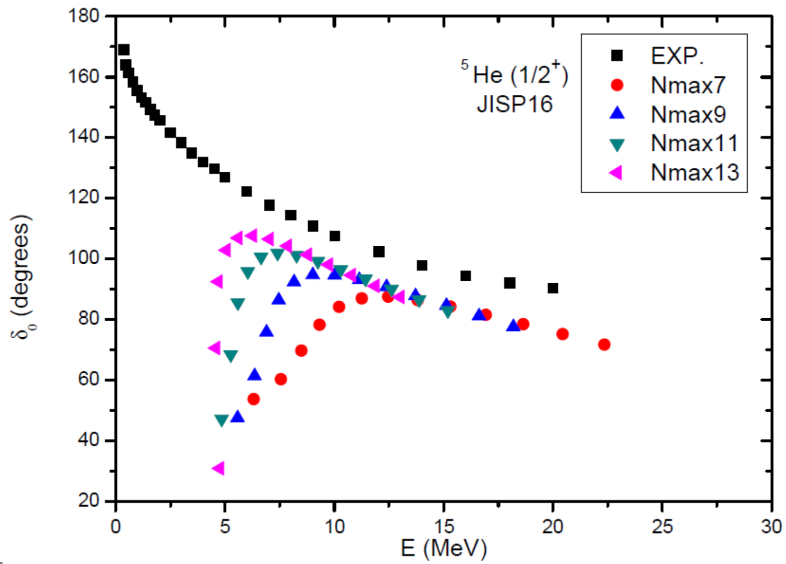



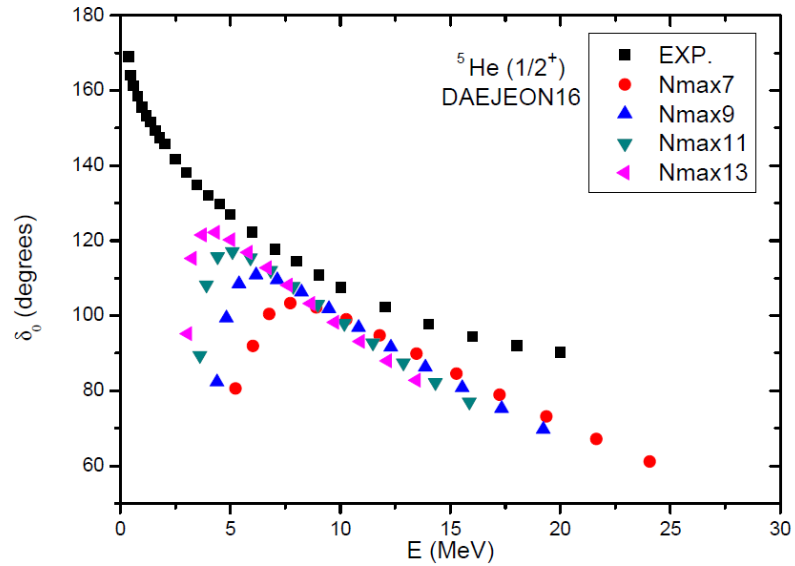
# Results: (n,α) scattering in the $\frac{1}{2}^+$ state

- ✓ $^5$He calculation
  - $N_{max}$ = 6, 8, 10, 12, 14
  - $\hbar\Omega$ : 10 to 40 MeV (2.5 MeV step)
  - Three different NN interactions
    - JISP16
    - $NNLO_{opt}$
    - Daejeon16

Exp. Data: J. E. Bond et. Al, Nucl. Phys. A **287**, 317 (1977).



# Summary and Further works

- ✓ Neutron-induced nuclear reaction data play a key role in the nuclear physics and related fields. Within this regard, improving and updating the nuclear structure and decay data become important.
- ✓ We propose a SS HORSE method to calculate phase shifts and to treat light-ion reactions at low-energy.
  - Based on the J-matrix inverse scattering approach
  - Calculate the low-energy phase shifts directly from the NCSM results without additional complexities
- ✓ We calculate the (n,α) scattering phase shifts using the results of the NCSM calculations of $^5$He nuclei with three different NN interactions.
- ✓ Further works
  - Parametrize the low-energy phase shift
  - Extract resonant energy and width
  - Calculate and evaluate cross section of neutron-induced light nuclei reactions

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THANK YOU!