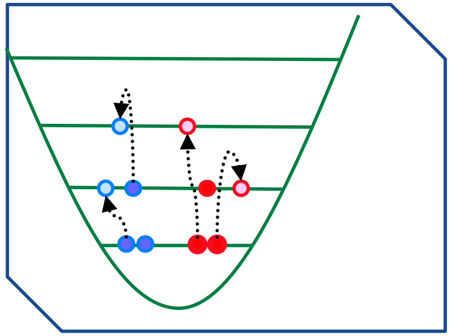
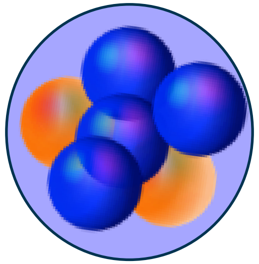
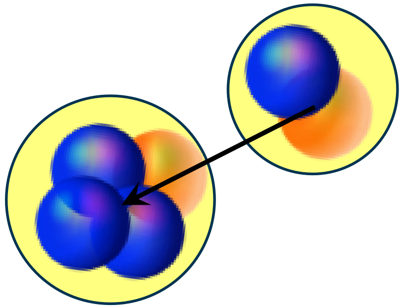
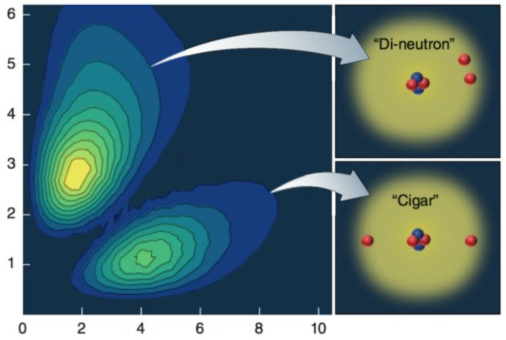
Guillaume Hupin, CNRS IJClab

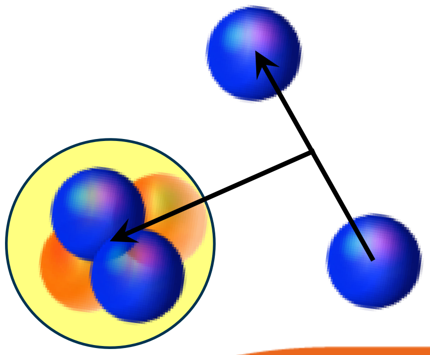
Ab initio predictions for thermonuclear fusion



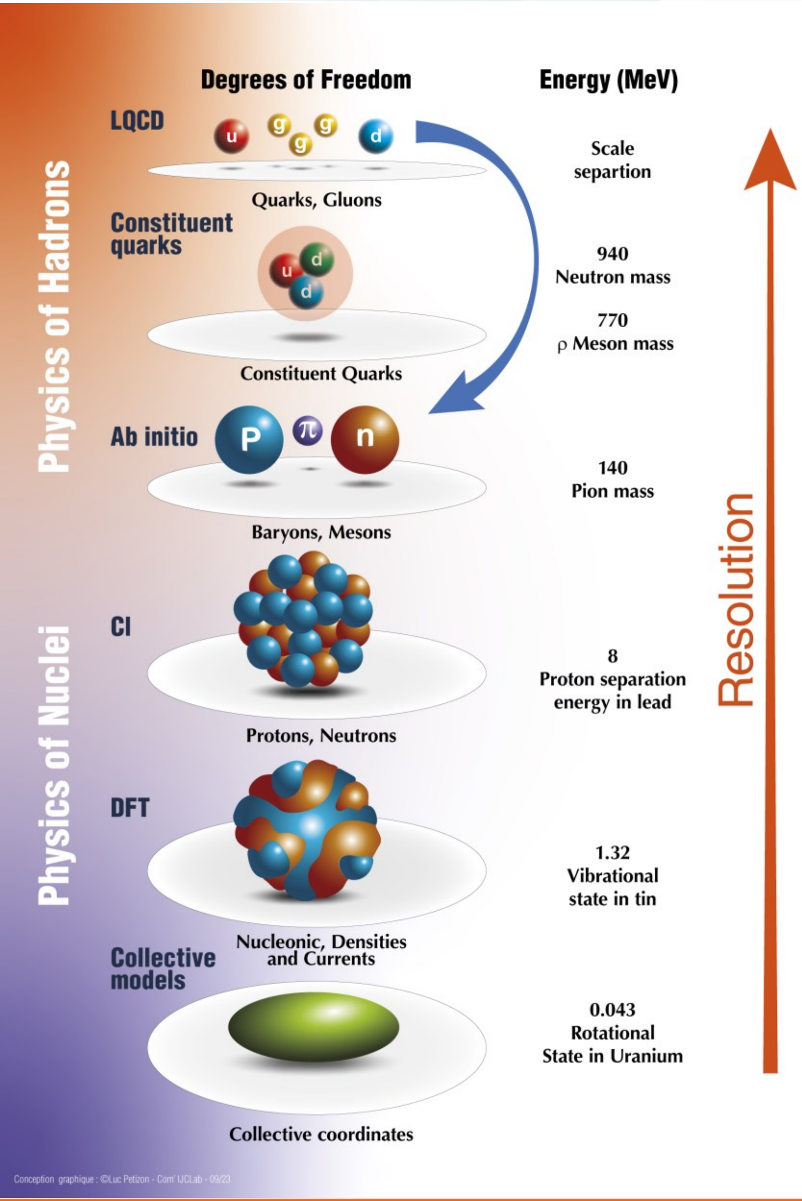








A story of multiple scale

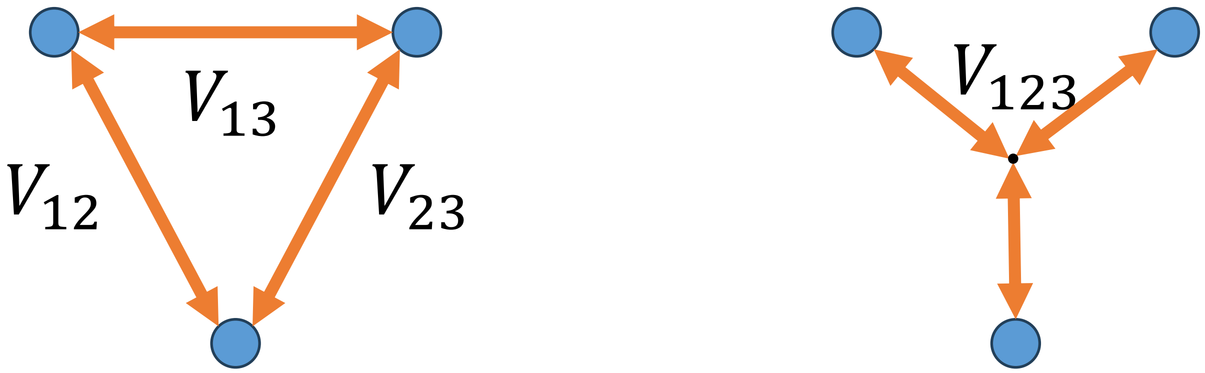


- Goal: Solving the Schrodinger equation (SE) for an A-body system:

$$H|\psi^{J^\pi T}> = E|\psi^{J^\pi T}>$$

- Nucleons are considered as point-like particles.

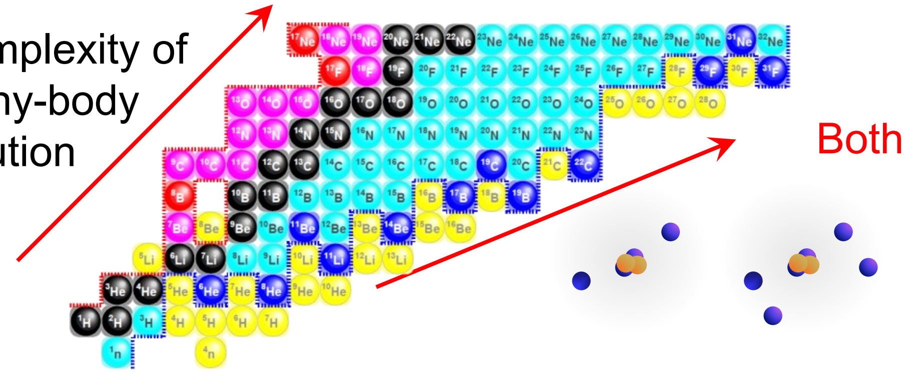
- The SE is solved by considering two and many-body interactions between nucleons



Complexity of scattering problem

$\neq n,p$ particles interacting with strong force ($M_h \gg M_{n,p}$)

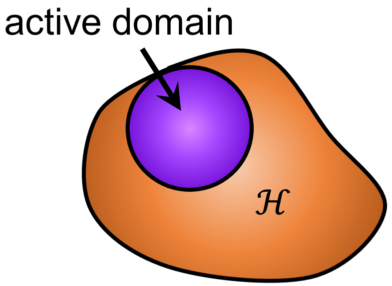
Complexity of many-body solution



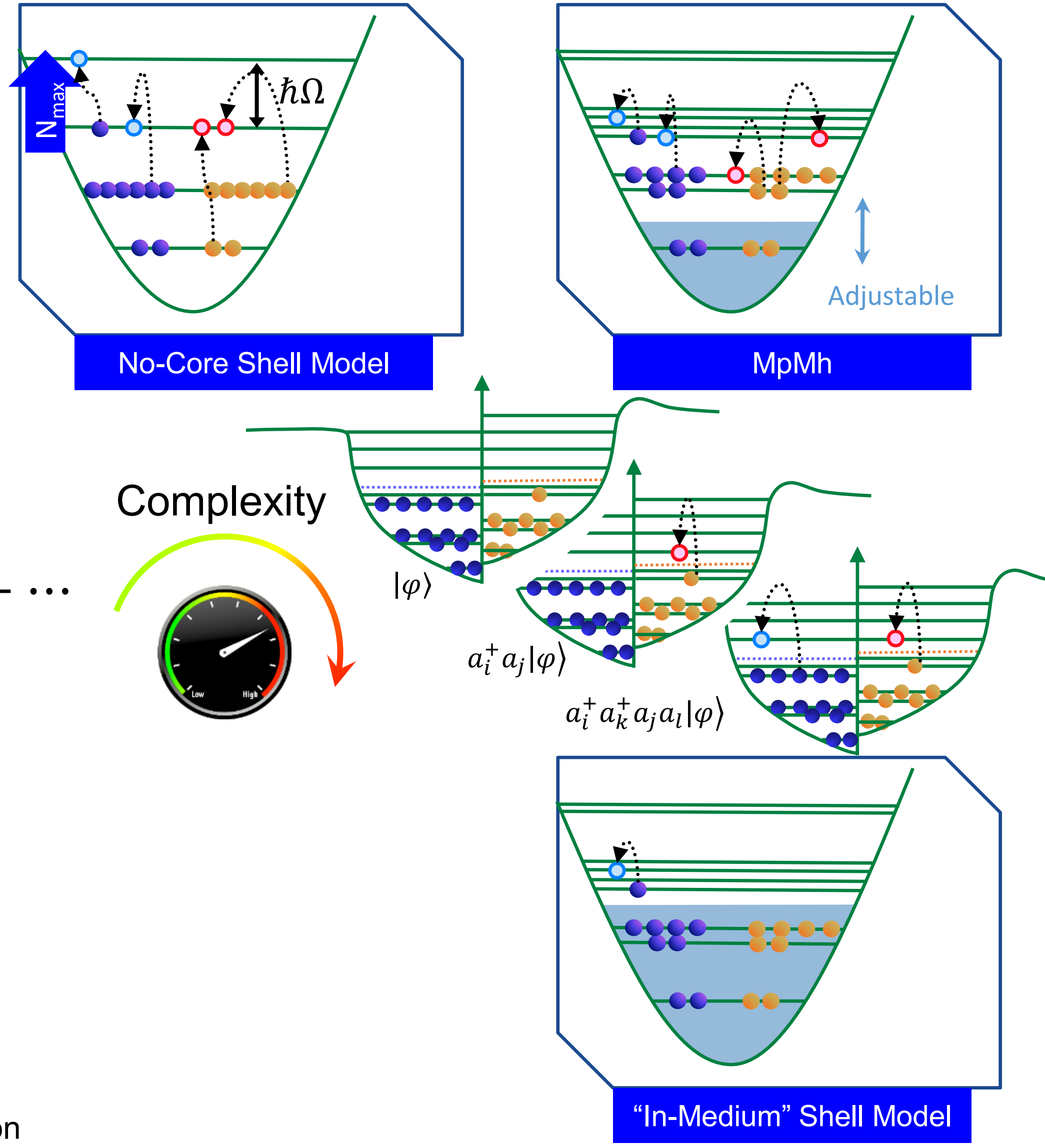
$M_h \leq M_{n,p}$

- 😐 Nuclear theory is **data driven**.
- ☹ The lack of accuracy of *ab initio* structure methods impedes the development of reactions modeling.

Credits H. Lenske



- Variational;
- Orthonormal basis;
- Controllable parameters ($N_{\max}$, $E1_{\max}$etc…);
- UV/IR convergence.

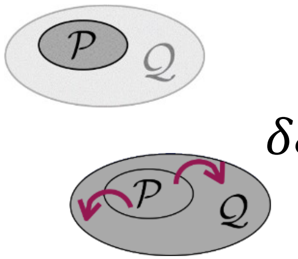


Superposition of Slater determinants:

$$|\Psi^A\rangle = \sum_\alpha c_\alpha \Phi_\alpha^\varphi(\vec{r}_1, \dots, \vec{r}_A) = A_0 \left|\Phi^0_{0p0h}\right\rangle + \sum_{\alpha'} A_{\alpha'} \left|\Phi^{\alpha'}_{1p1h}\right\rangle + \cdots$$

NCSM
IM-SH
MpMh

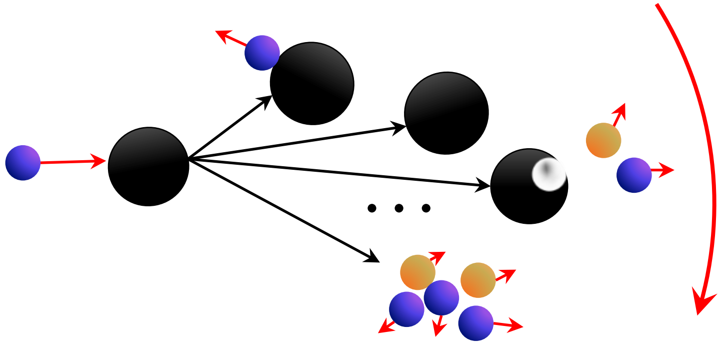
Optimization of mixing coefficients, one-body Hilbert space:



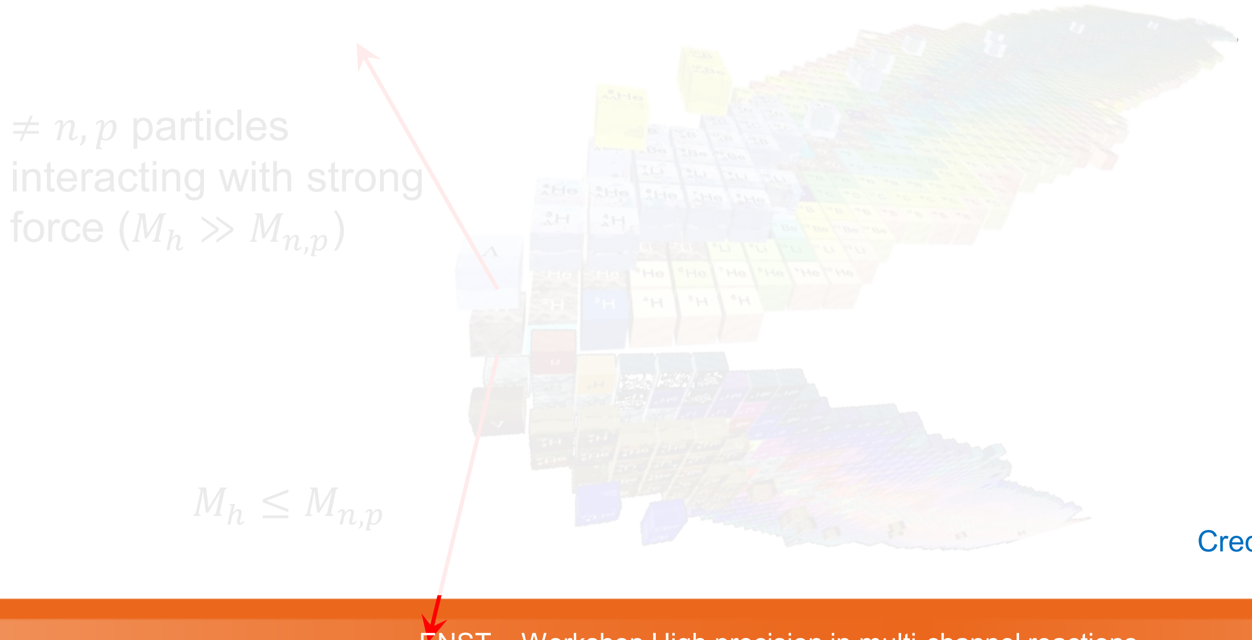
$$\delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \Longrightarrow \sum_\beta A_\beta \langle \Phi_\alpha | \hat{H} | \Phi_\beta \rangle = E A_\alpha$$

$$\delta\mathcal{E}[\Psi]_{/\{\varphi^*_\alpha\}} = \left\langle \Psi \left| \left[\hat{H}, \hat{T}\right] \right| \Psi \right\rangle = 0 \Longleftrightarrow \left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma)$$

Generalized Brillouin (GB) equation



Complexity of scattering problem



- 😐 Nuclear theory is **data driven**.
- ☹ Few-body techniques scale **very bad** with the number of constituents in the continuum.

Credits H. Lenske

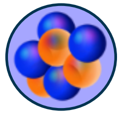
B.R. Barrett, P. Navrátil, J.P. Vary, J.P. Progr. Part. Nucl. Phys. 69 (2013)

One way to solve the many-body problem

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \; |A\alpha j_z{}^{\pi} t_z\rangle$$

Mixing coefficients(unknown)

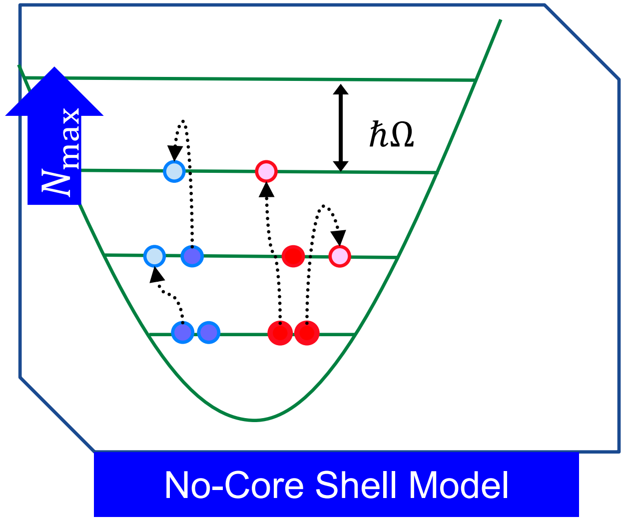
A-body harmonic oscillator states



$|A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$

Second quantization

Can address bound and low-lying resonances (short range correlations)



Advantage of HO CI methods:

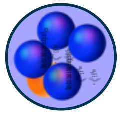
1. Center of mass is factorized.
2. Mathematically possible to derived s.p. to Jacobi coordinates transformation.
3. Fourier transform is trivial: NCSM, RGM with HO CI is equivalent in momentum or position space.

- One way to solve the many-body problem when two scales appear

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \; |A\alpha j_z{}^{\pi} t_z\rangle$$

Mixing coefficients(unknown)

A-body harmonic oscillator states

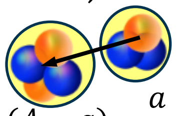


$|A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$

Second quantization

Can address bound and low-lying resonances (short range correlations)

$\vec{r}_{A-a,a}$



$$\Psi^{(A)}_{RGM} = \sum_{v} \int d\vec{r}\; g_v(\vec{r})\, \hat{A}_v \left| \Phi^{(A-a,a)}_{v\vec{r}} \right\rangle$$

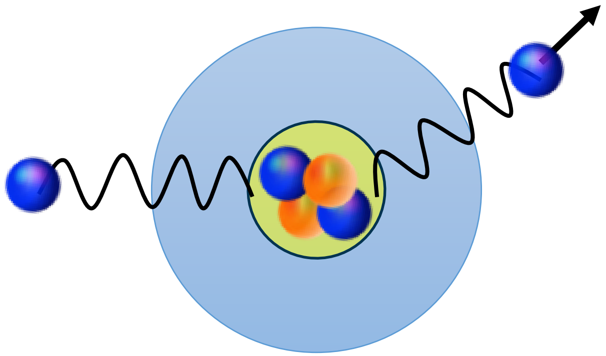
Relative wave function (unknown)

Antisymmetrizer

Channel basis

$\psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2}\, \delta(\vec{r} - \vec{r}_{A-a,a})$

Cluster expansion technique

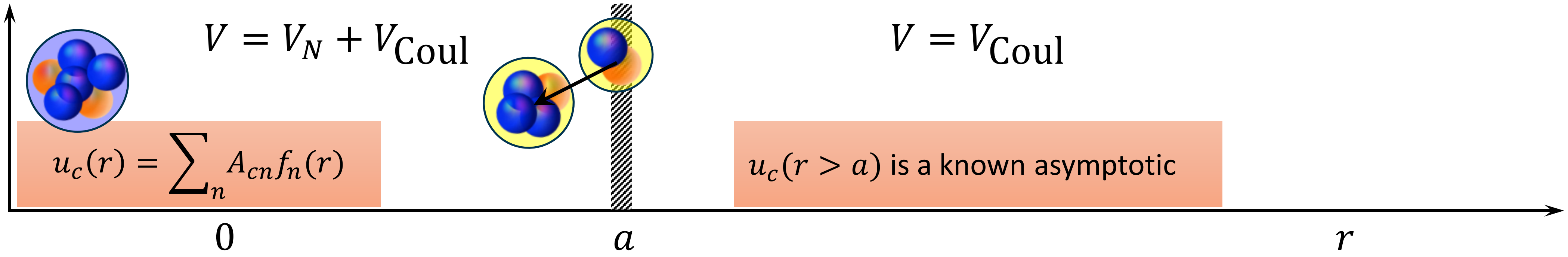


NCSM/RGM
Cluster formalism for elastic/inelastic

Many-body basis is twice as large as Ψ_{NCSM}

- $\psi^{(A-a)}_{\alpha_1} \in \mathcal{H}^{N_{\max}}$
- $\psi^{(a)}_{\alpha_2} \in \mathcal{H}^{N_{\max}}$

Internal region / External region



Decomposition on a Lagrange mesh.

NCSMC can be cast as Bloch-Schrödinger equation:

$$(C - EI)\vec{X} = Q(B)$$

And solved using R-matrix, which in the eigen basis of $C - EI$ reads:

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

Simple for binary reacting system, more involved for neutral ternary system and extremely challenging for charged breakup.

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \, |A\alpha j_z{}^{\pi} t_z\rangle$$

Mixing coefficients (unknown)

A-body harmonic oscillator states

$$\Psi^{(A)}_{RGM} = \sum_{v} \int d\vec{r}\, g_v(\vec{r})\, \hat{A}_v \left|\Phi^{(A-a,a)}_{v\vec{r}}\right\rangle$$

Relative wave function (unknown)

Antisymmetrizer

Channel basis

Configuration Interaction (CI):

- Eigen-value problem → Matrix diagonalization: $\hat{H}\phi_n = \varepsilon_n \phi_n$

No Core Shell Model (NCSM):

- HO wavefunctions;
- Single particle basis;
- Jacobi basis.

NCSM with continuum (NCSMC):

- For computing reactions and exotic nuclei.

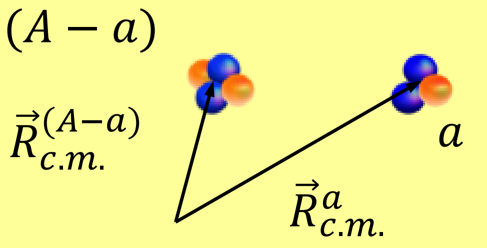
Limitations:

- Resonance properties cannot be accessed directly.
- Reaction channels must be introduced manually.

- Translational invariance is preserved (exactly!) also with SD cluster basis

$$ {}_{\mathrm{SD}}\left\langle \Phi_{f}^{J^{\pi}T} \middle| \hat{\mathcal{O}}\left(\vec{\xi}_1 \ldots \vec{\xi}_{A-1}\right) \middle| \Phi_{i}^{J^{\pi}T} \right\rangle_{\mathrm{SD}} = \sum_{i'f'} \mathcal{U}_{if,i'f'} \; {}_{\mathrm{SD}}\left\langle \Phi_{f'}^{J^{\pi}T} \middle| \hat{\mathcal{O}}\left(\vec{\xi}_1 \ldots \vec{\xi}_{A-1}\right) \middle| \Phi_{i'}^{J^{\pi}T} \right\rangle $$

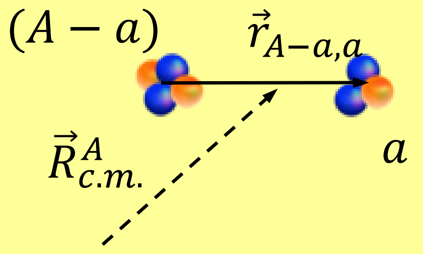
What we calculate in the "SD" channel basis



$$ \left|\psi_{\alpha_1}^{(A-a)}\right\rangle_{\mathrm{SD}} \left|\psi_{\alpha_2}^{a}\right\rangle \varphi_{nl}(\vec{R}_{c.m.}^{a}) $$

Matrix inversion →

Observables calculated in the translationally invariant basis



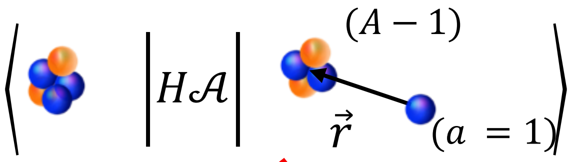
$$ \left|\psi_{\alpha_1}^{(A-a)}\right\rangle \left|\psi_{\alpha_2}^{a}\right\rangle \varphi_{nl}(\vec{r}_{A-a,a}) $$

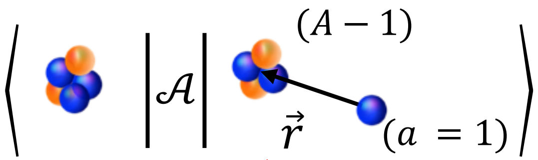
- Advantage: can use powerful second quantization techniques

$$ {}_{\mathrm{SD}}\left\langle \Phi_{\nu' r'}^{J^{\pi}T} \middle| \hat{\mathcal{O}}(\vec{\xi}_1 \ldots \vec{\xi}_{A-1}) \middle| \Phi_{\nu\, r}^{J^{\pi}T} \right\rangle_{\mathrm{SD}} \propto {}_{\mathrm{SD}}\left\langle \Phi_{\nu' r'}^{J^{\pi}T} \middle| a^{\dagger} a \middle| \Phi_{\nu\, r}^{J^{\pi}T} \right\rangle_{\mathrm{SD}}, \; {}_{\mathrm{SD}}\left\langle \Phi_{\nu' r'}^{J^{\pi}T} \middle| a^{\dagger} a^{\dagger} a a \middle| \Phi_{\nu\, r}^{J^{\pi}T} \right\rangle_{\mathrm{SD}}, \text{etc} $$

S. Baroni, P. Navrátil and S. Quaglioni PRL110 (2013); PRC93 (2013)

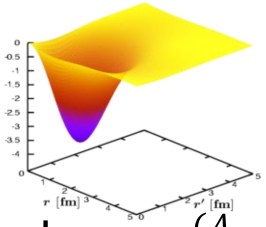
$E_\lambda \, \delta_{\lambda\lambda'}$

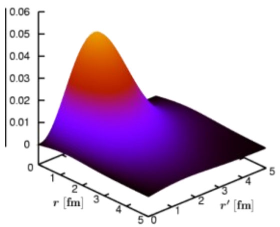


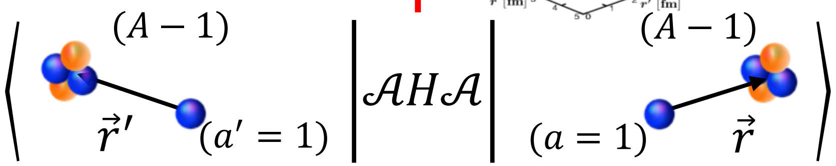


$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix}$$

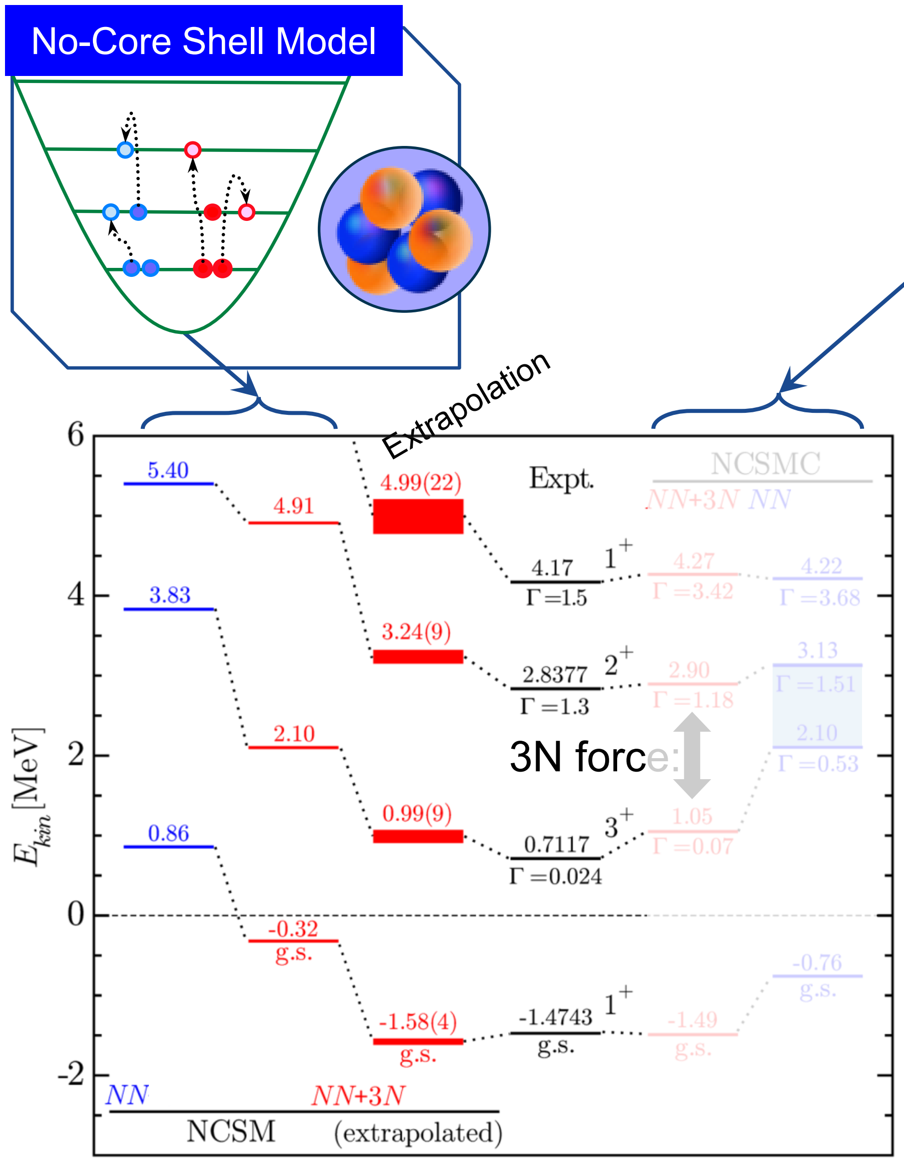
These are basically the "form factors" is used in reaction theory.

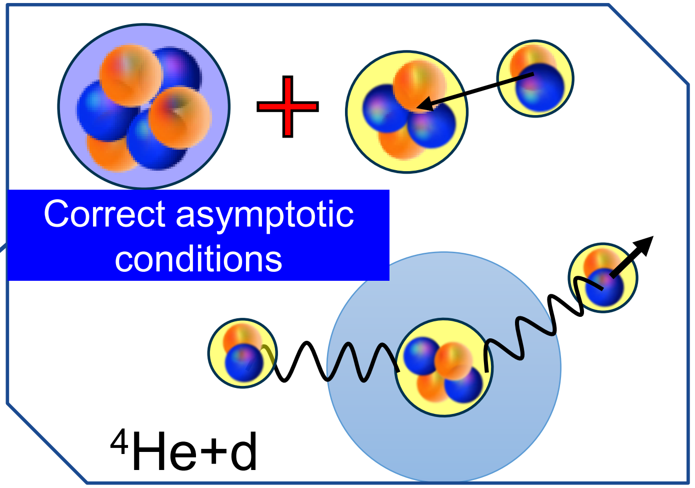






Scattering matrix (and observables) are obtained from matching to known asymptotic solutions using whatever scattering solver.



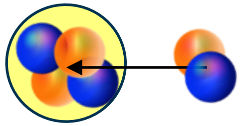


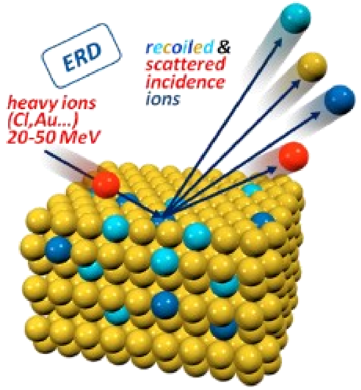
Allowing d+a clustering in the g.s. gives access to ANC.

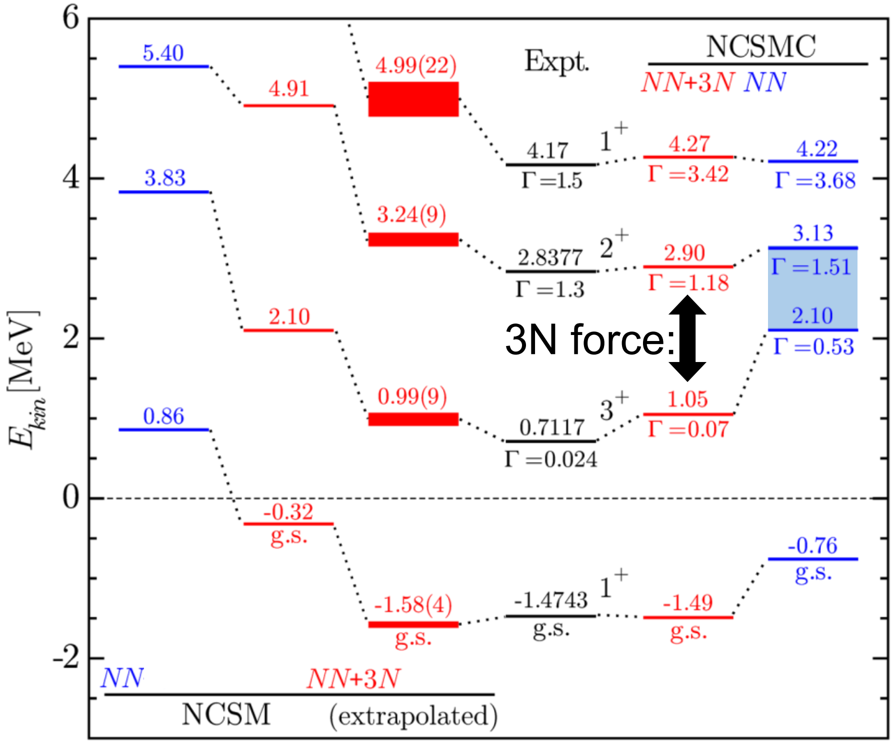
	NCSMC	Experiment[1]
C_0 $[\mathrm{fm}^{-1/2}]$	2.695	2.91 (9)
C_2 $[\mathrm{fm}^{-1/2}]$	−0.074	−0,077 (18)
C_2/C_0	−0.027	0.025 (6)

[1]L. D. Blokhintsev *et al.* PRC**48** (1993).

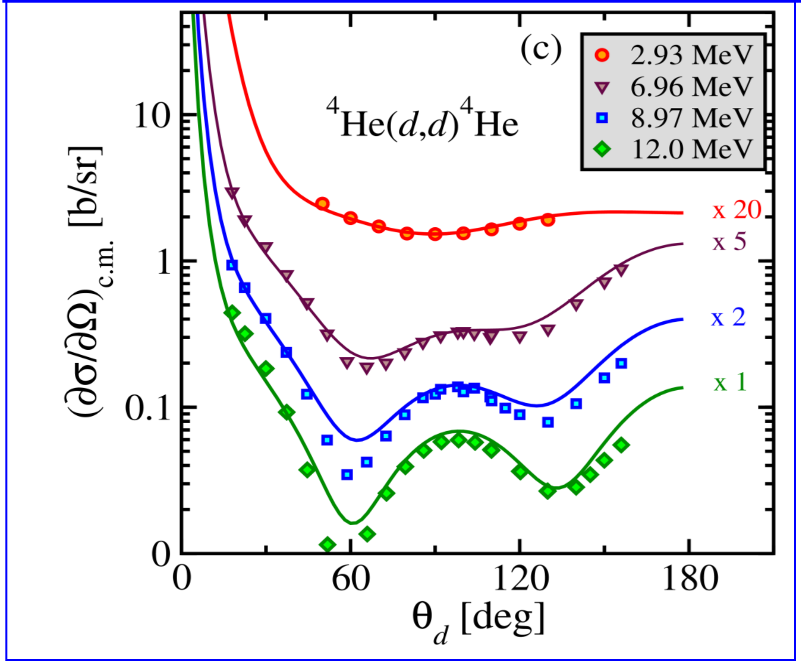
Example: Structure of ^{6}Li continuum





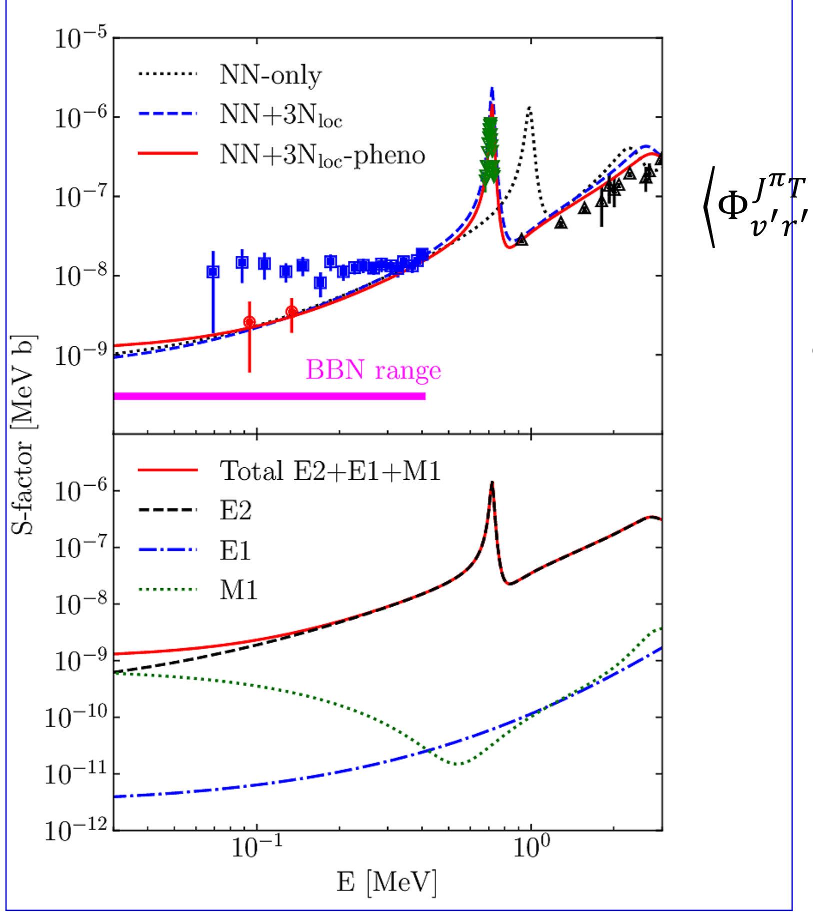


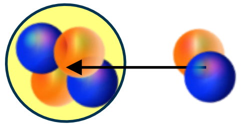
^{4}He(d,d) ^{4}He angular distribution

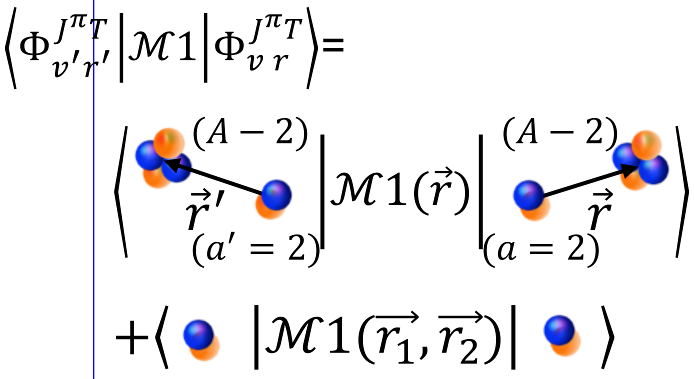


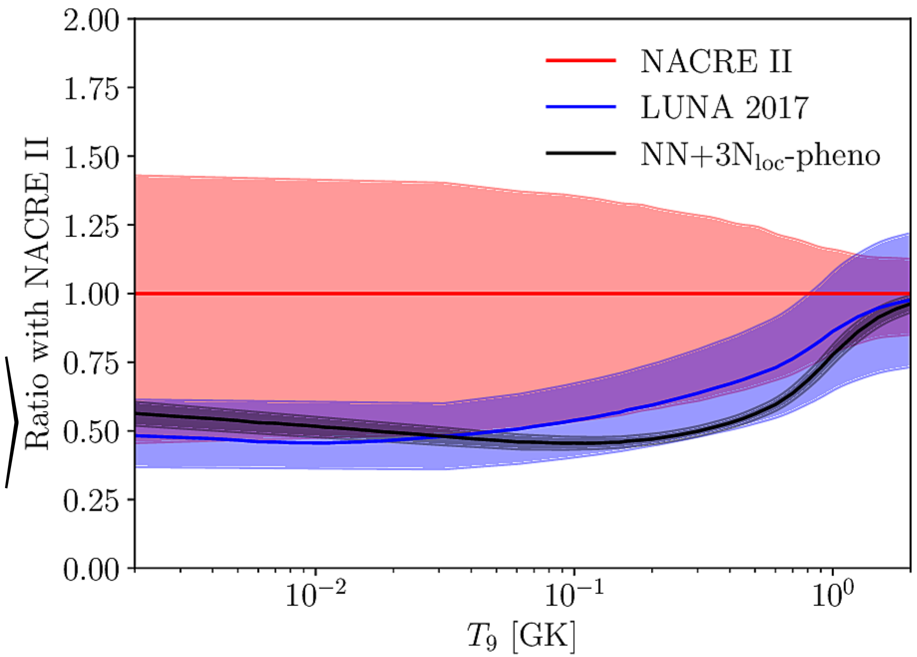
C. Hebborn, G. Hupin *at al.* PRL129 (2022)

S-factor of radiative capture and EM contributions

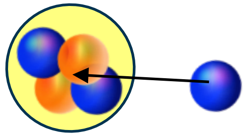




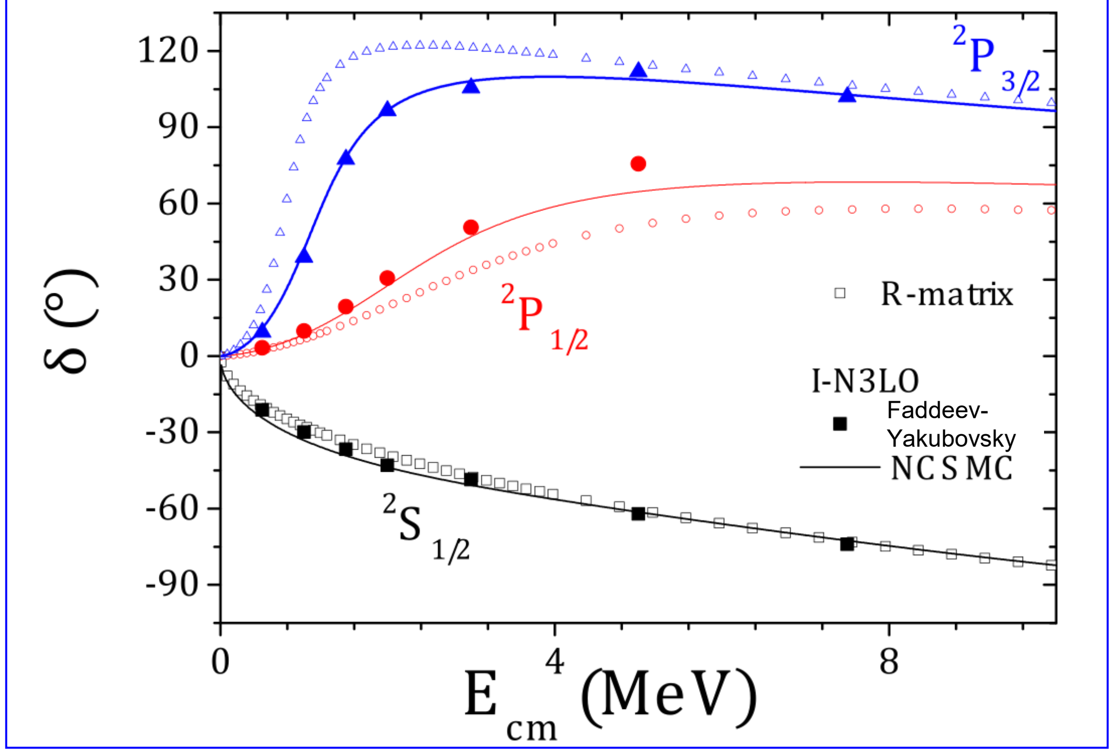




- *Ab initio* calculations show the importance of the $\mathcal{M}1$ **transition** (neglected in cluster models).
- **Reduction** of the capture rate **uncertainty** by factor of 7 compared to data evaluation.



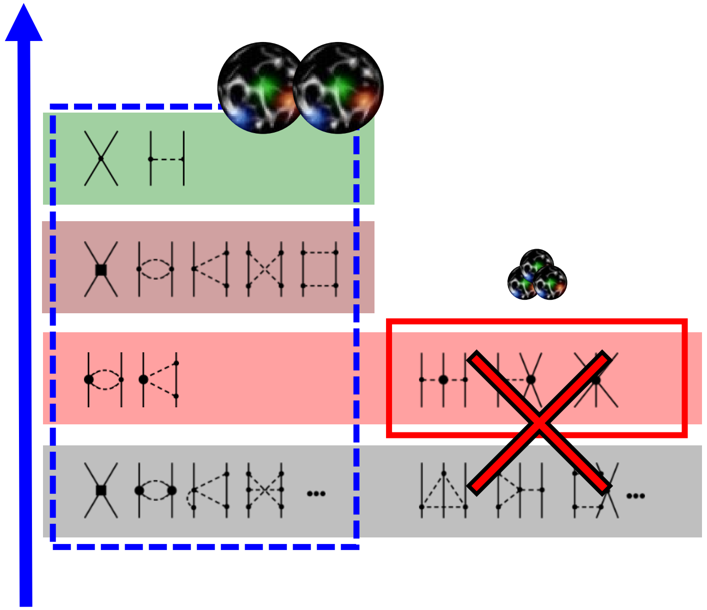
Benchmark: scattering phase shifts NCSMC/FY

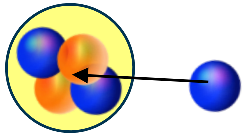


R. Lazauskas, PRC **97** (2018).*

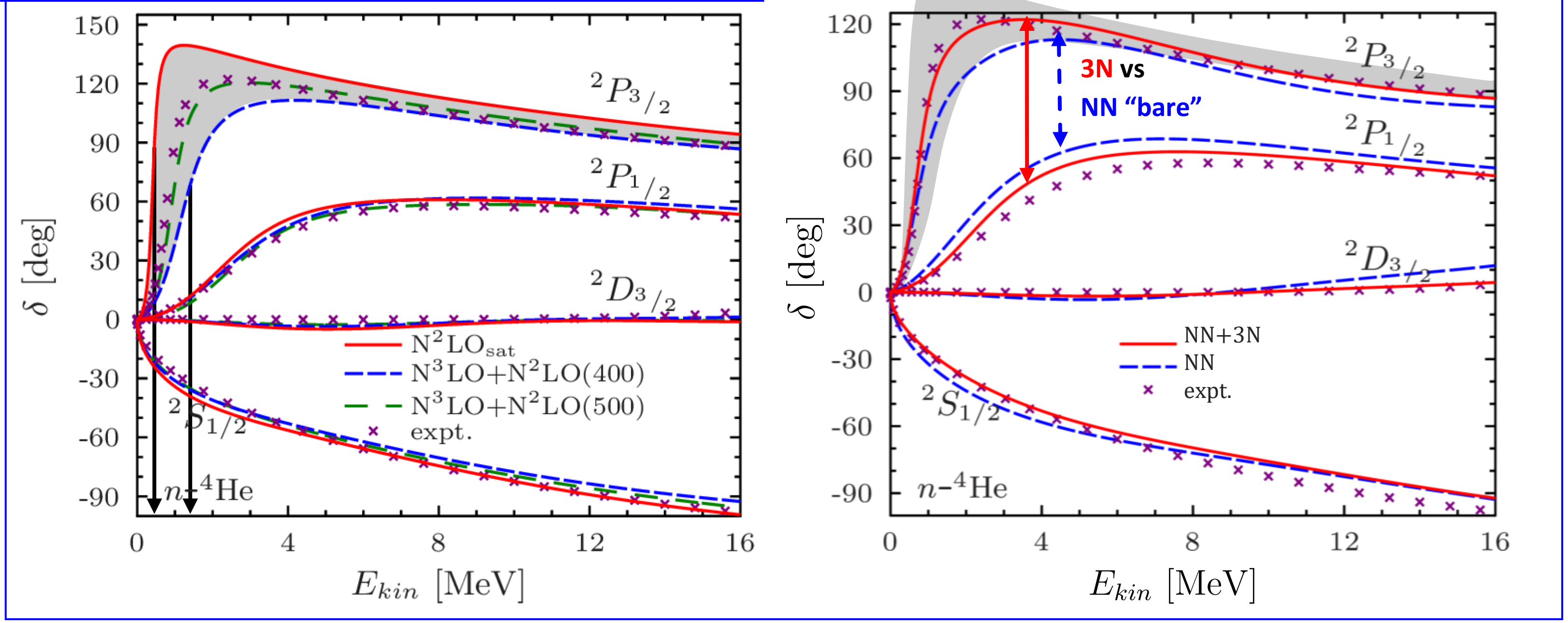
*there is a more recent paper with 3N force.

- **Good** agreement between the two methods.





n-^{4}He scattering phase shifts



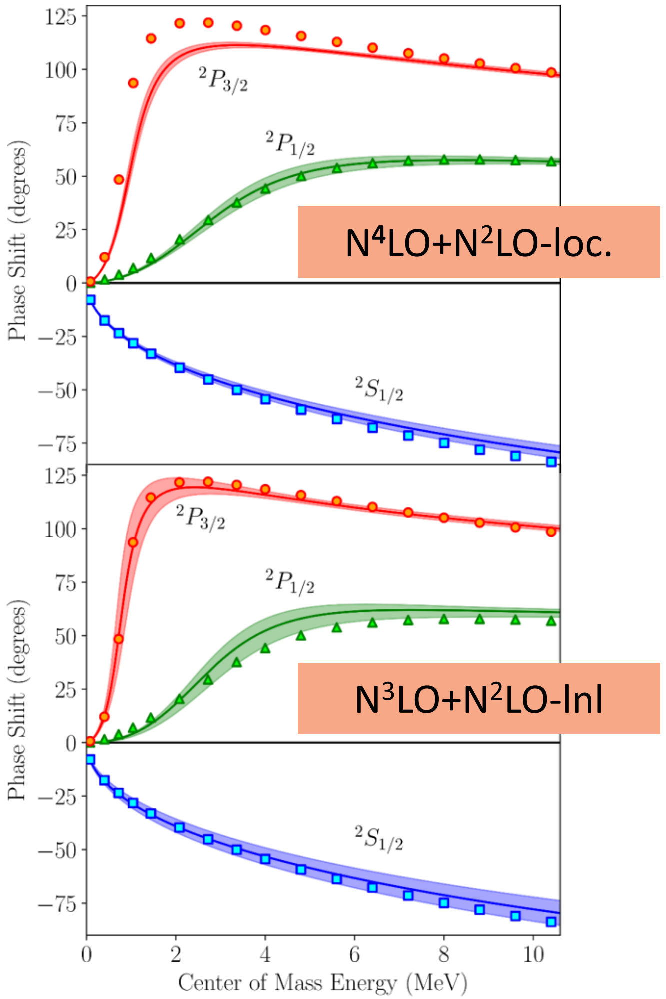
R-matrix results from G. Hale

Some of the shortcomings of the nuclear interaction can already be **probed** in p-shell nuclei **through reactions**.

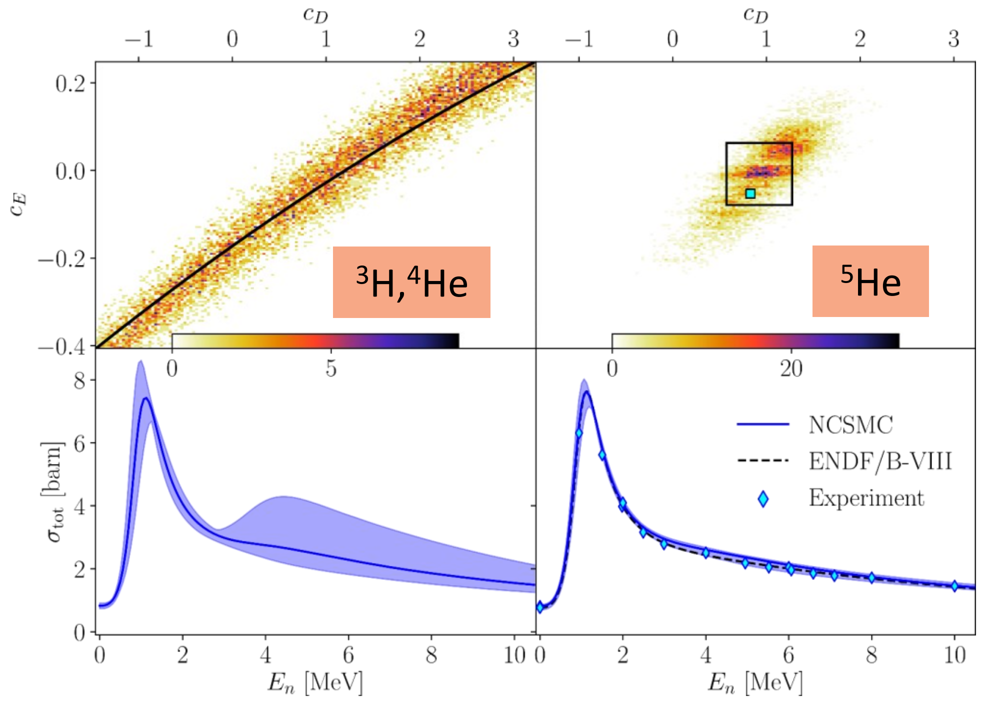
[known since the work of K. Nollett]

- The 3N interactions **influence** mostly the **p-waves**.
- Conservative estimate of EFT accuracy illustrated by the spread of 3N force predictions.

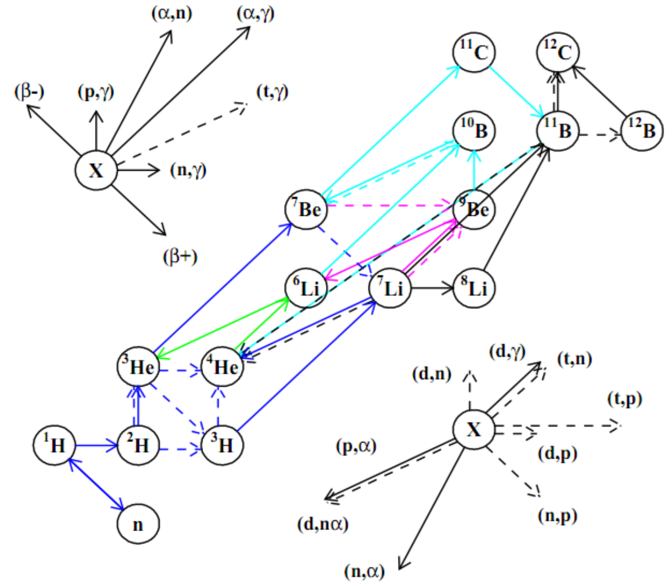
Sensitivity to c_D and c_E

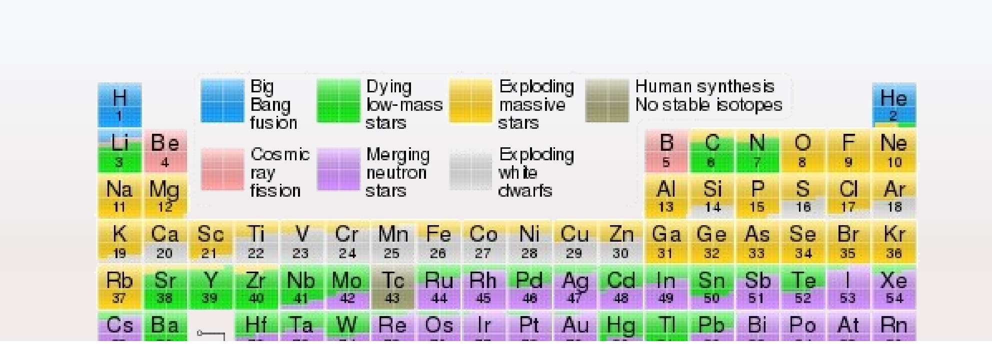


- NN-N4LO + 3N-N2LO **cannot reproduce** the p-wave splitting.
- Tighter posterior distribution if the properties of the ^{5}He are included in the fit of 3N LEC.

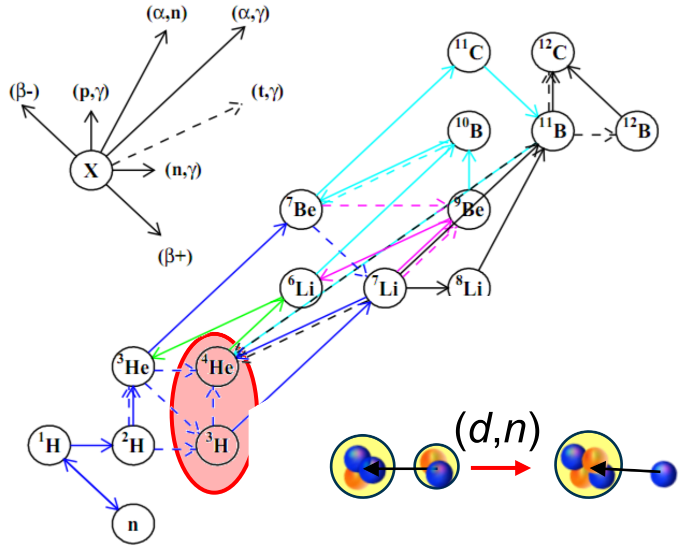


Primordial Nucleosynthesis **(blue)**

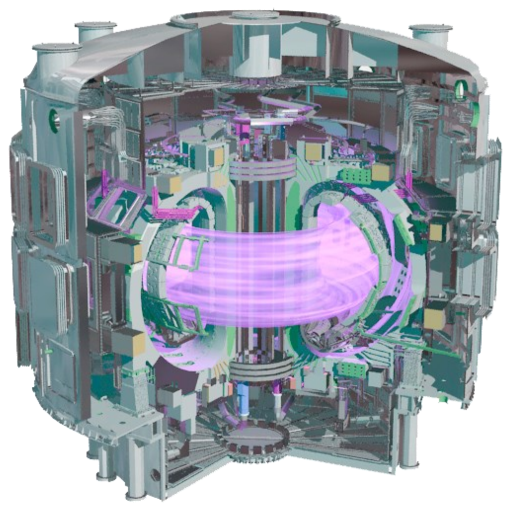




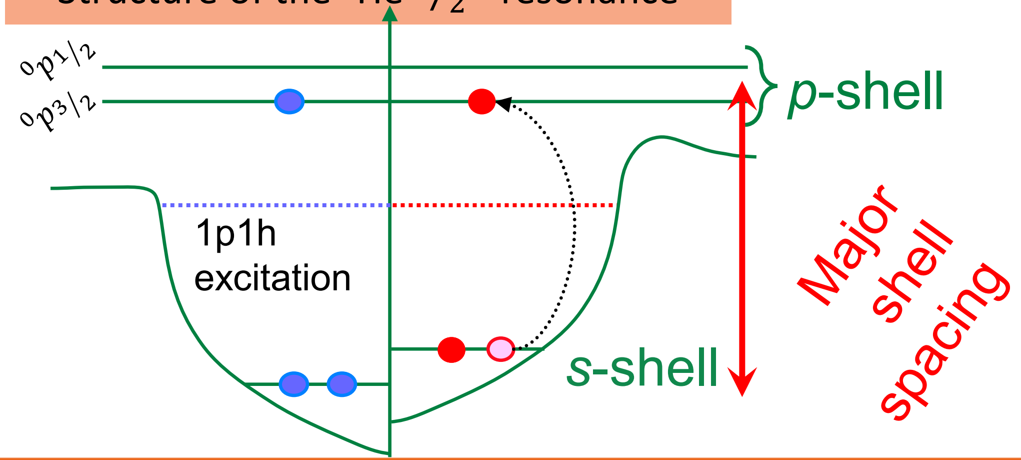
Primordial Nucleosynthesis **(blue)**



ITER design (Cadarache, France)

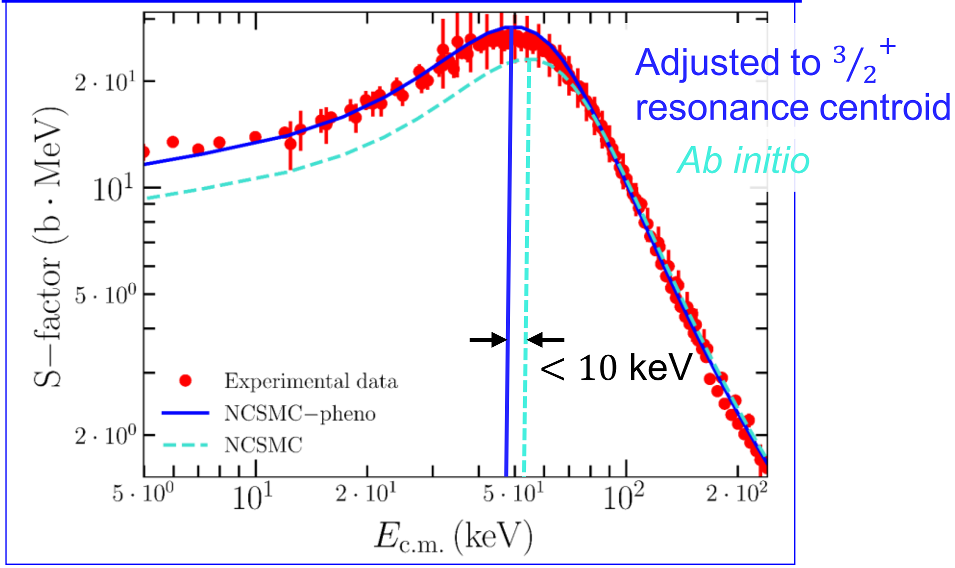


Structure of the ^{5}He $^3/_2{}^+$ resonance

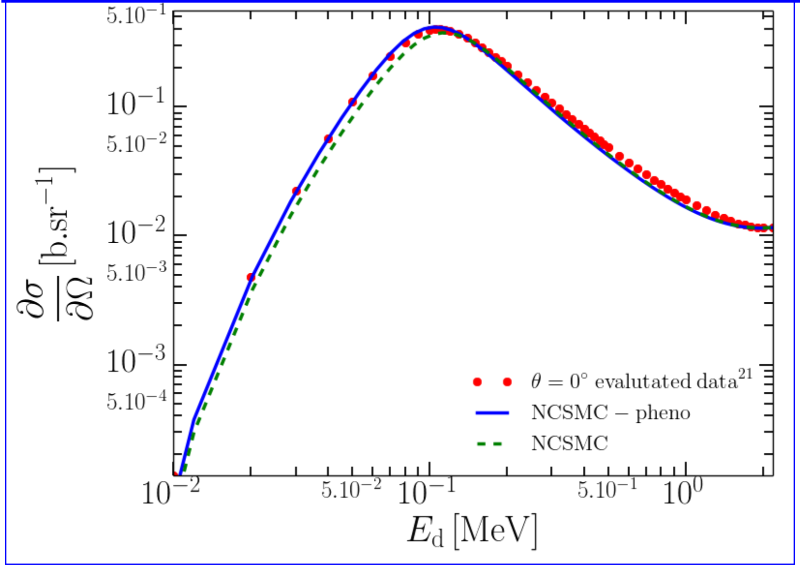


$^3H(d,n)^4He$ fusion reaction: benchmark to data and evaluation

S-factor: computed and data



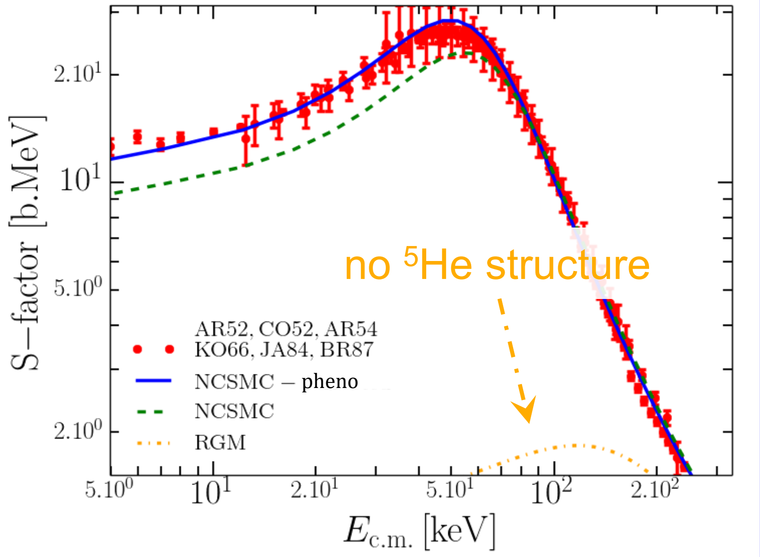
Angular distribution at $\theta = 0^\circ$



M. Drosg and N. Otuka, INDC(AUS)-0019 (2015).

- The S-factor is globally well reproduced.
- The accurate **reproduction** (of the order of keV) of the **resonance position**/width is **essential**.
- Shape of the angular distribution **agrees** with recent **evaluation**.

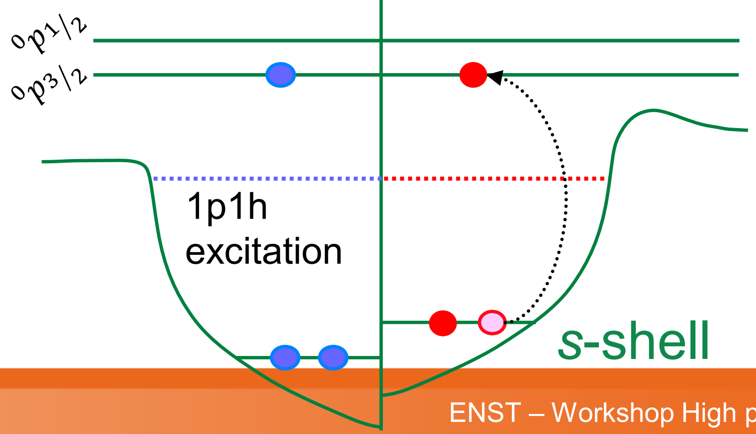
S-factor: NCSMC vs binary cluster



$^{5}\text{He}(^{4}S_{3/2})$	E_r (keV)	Γ_r (keV)
Cluster basis (D g.s. only)	105	1100
Cluster basis	120	570
NCSMC (D g.s. only)	65	160
NCSMC	55	110
NCSMC-pheno	50	98
R-matrix	48	74

G.M. Hale, *et al.* PRL **59** (1987).

Structure of the ^{5}He $^{3}/_{2}^{+}$ resonance

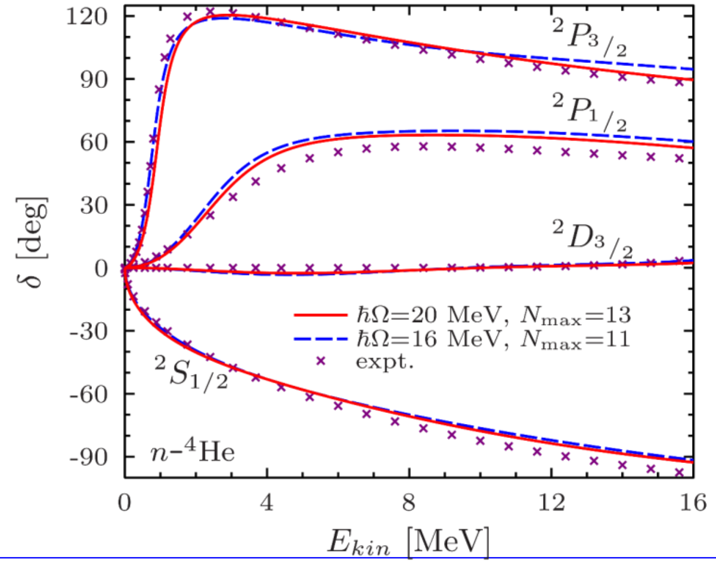


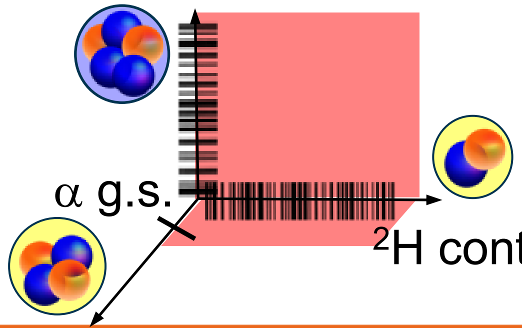
- Importance of structure of neighboring resonances is magnified in transfer reactions.

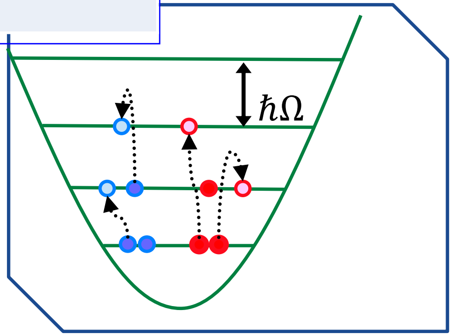
Convergence of $^3/_2{}^+$ resonance

N_{max}	$\hbar\omega$=20 MeV Λ_{SRG}=2.0 fm^{-1}	$\hbar\omega$=16 MeV Λ_{SRG}=1.7 fm^{-1}
7	78.70%	42.29%
9	45.04%	18.85%
11	25.68%	8.41%
13	13.78%	-

n-^{4}He phase shifts

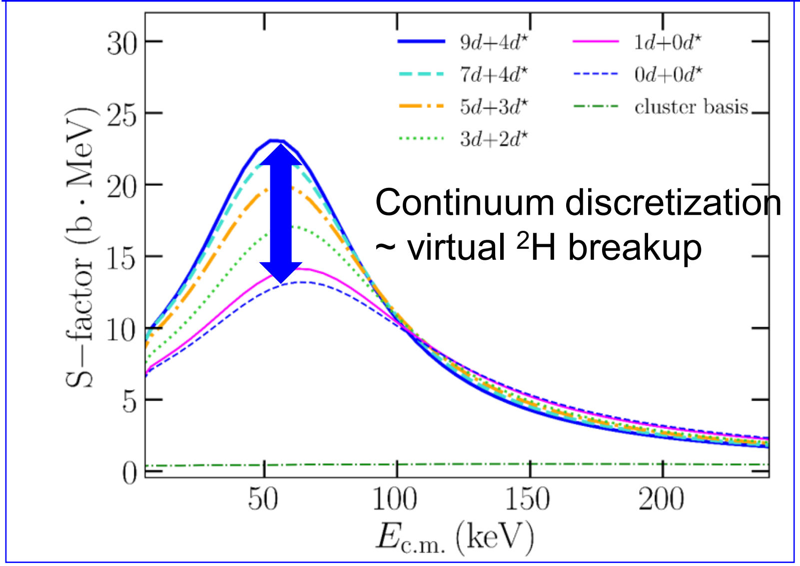




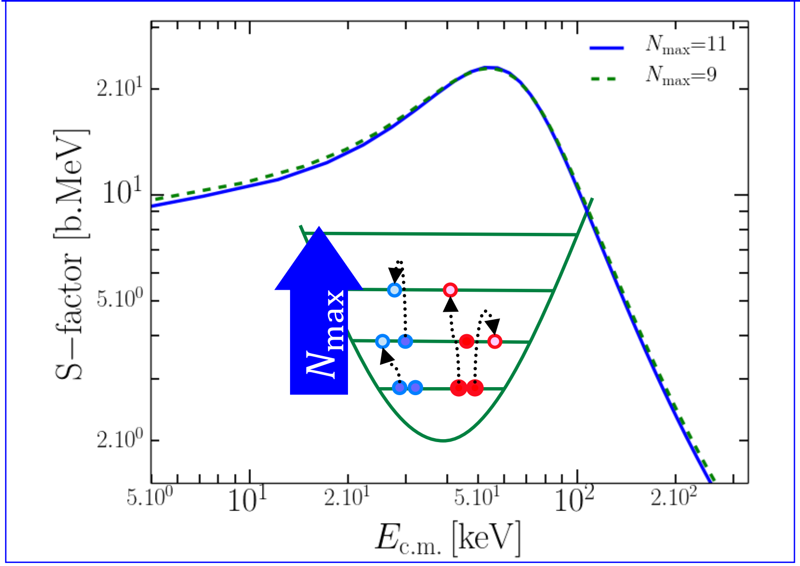


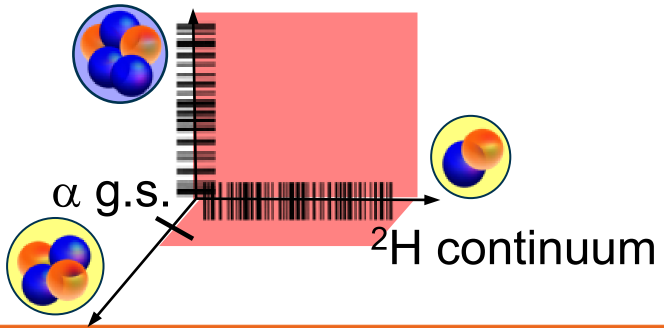
- $^3/_2{}^+$ resonance converges the fastest with $\hbar\omega = 16$ MeV, understood from **major shell splitting**.
- n-^{4}He elastic scattering independent of HO frequency and SRG flow.

Convergence wrt ^2H continuum



Convergence with N_{max}

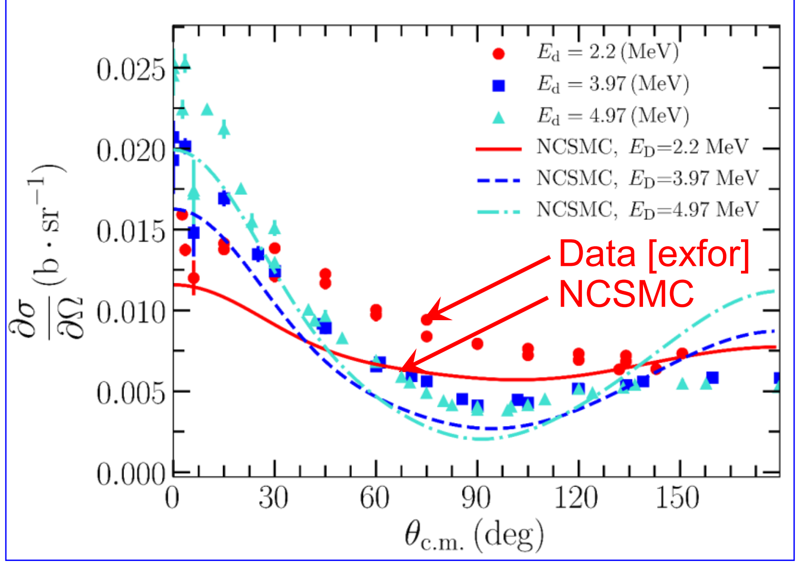


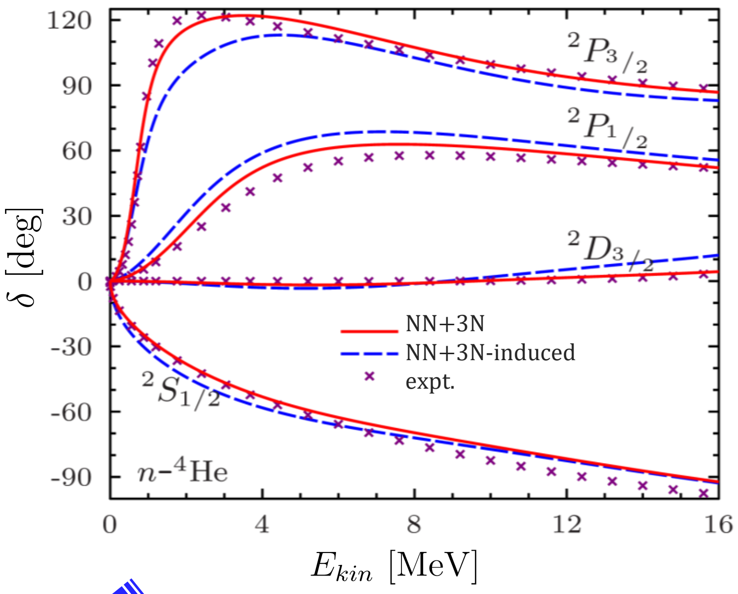


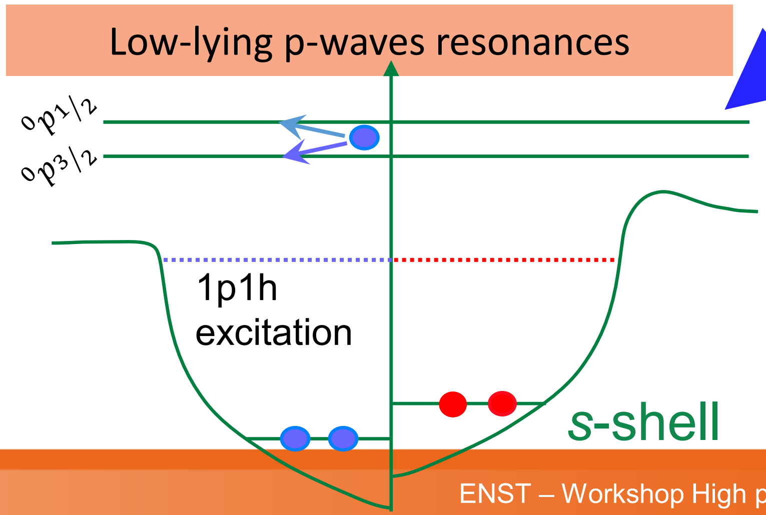
correlated

- Discretization of ^2H is **essential** for the reproduction of the S-factor.
- Stable behavior with respect to the number of ^2H pseudo states.
- Converged with N_{max}.

Differential cross section $E > E_{3/2^+}$

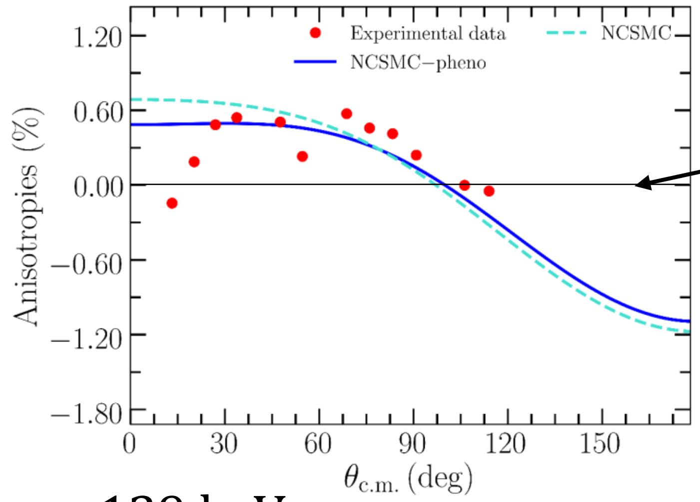






- Away from the **DT** fusion peak, the **remaining discrepancies** of low-lying **background phase-shifts** can be seen.
- No effects of the adjustment of the $^3/_2{}^+$ resonance position (i.e. **NCSMC≡NCSMC-pheno**).

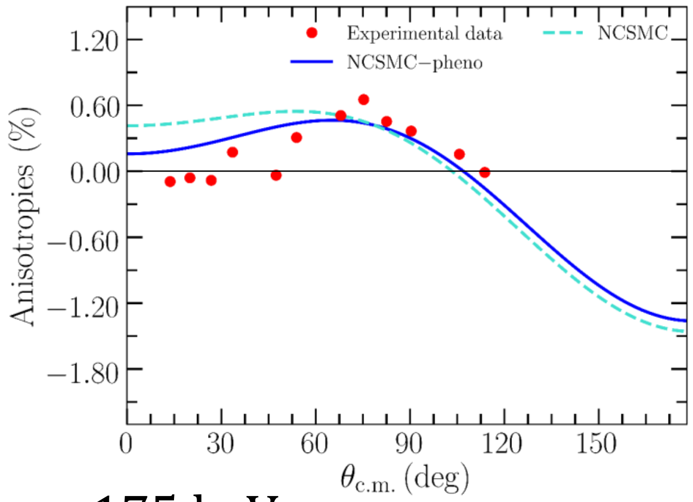
Deviations from pure s-wave



$E_D = 139$ keV

Isotropic case

Deviations from pure s-wave

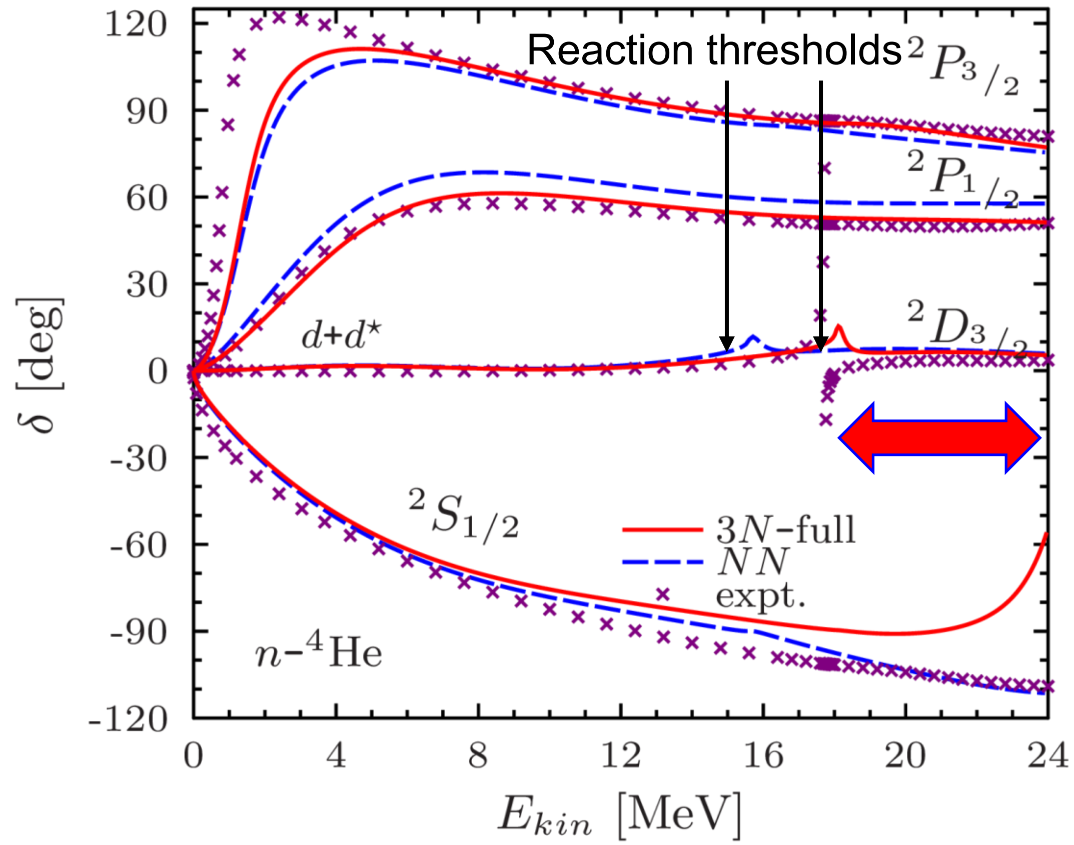


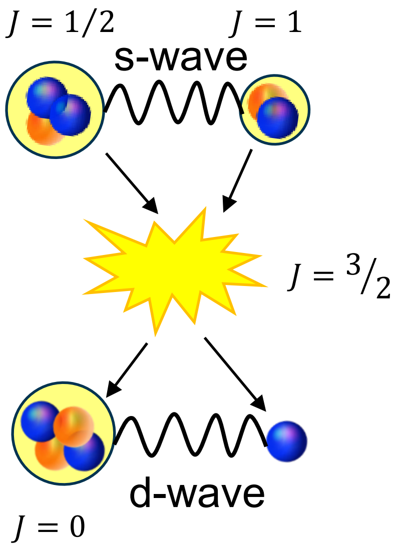
$E_D = 175$ keV

P. Bém *et al.*, Few-Body Syst. **22** (1997).

- Influence of p- and d-waves in the slope and bump of $\partial\sigma_{\text{rel}}/\partial\Omega$, respectively.
- Overall good reproduction of data: **collision matrix** is expected to be **accurate**.

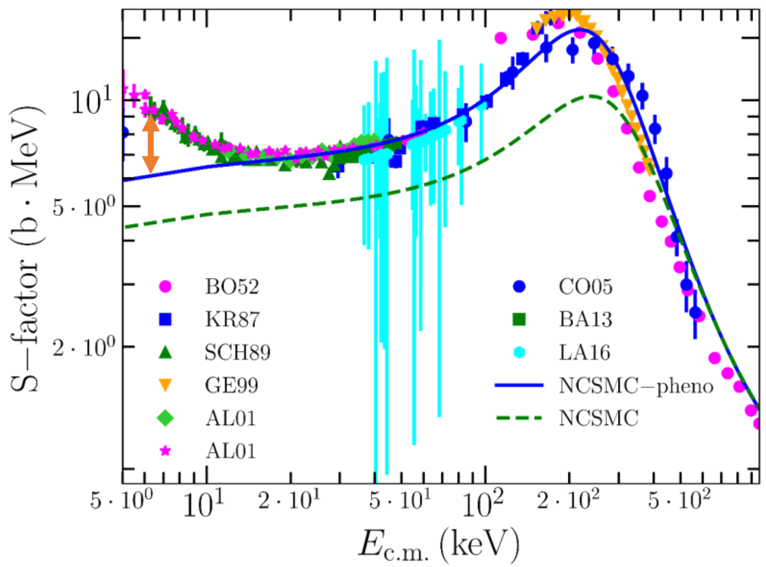
^{3}H(d,n)^{4}He fusion reaction: impact of 3N force

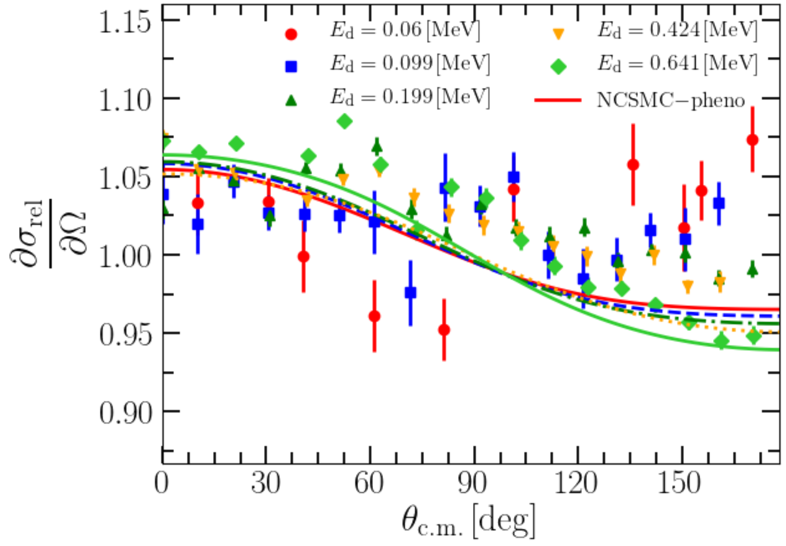


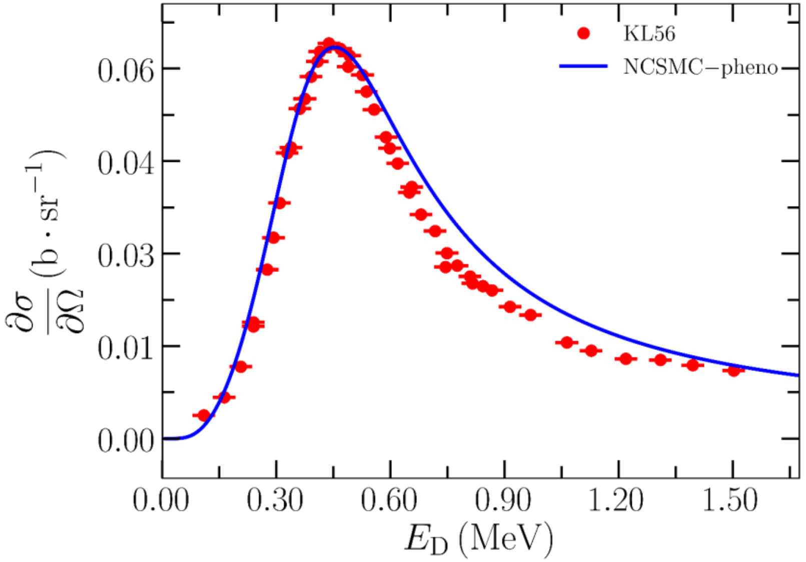


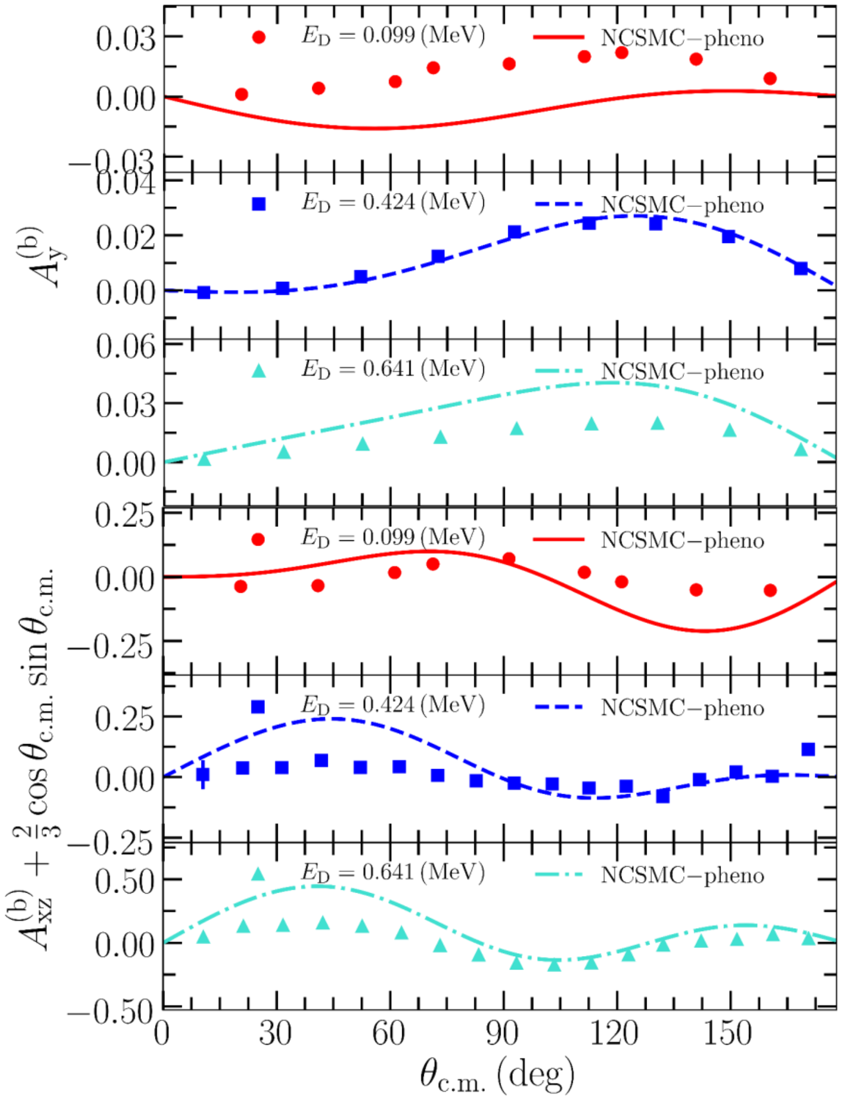
- 3N force impacts:
  - The thresholds (i.e. nuclear masses).
  - The positions and splitting between the $^3/_2{}^+$ and $^1/_2{}^+$ resonances.
- Tensor like force is essential to model the ^{3}H(d,n)^{4}He transfer reaction.

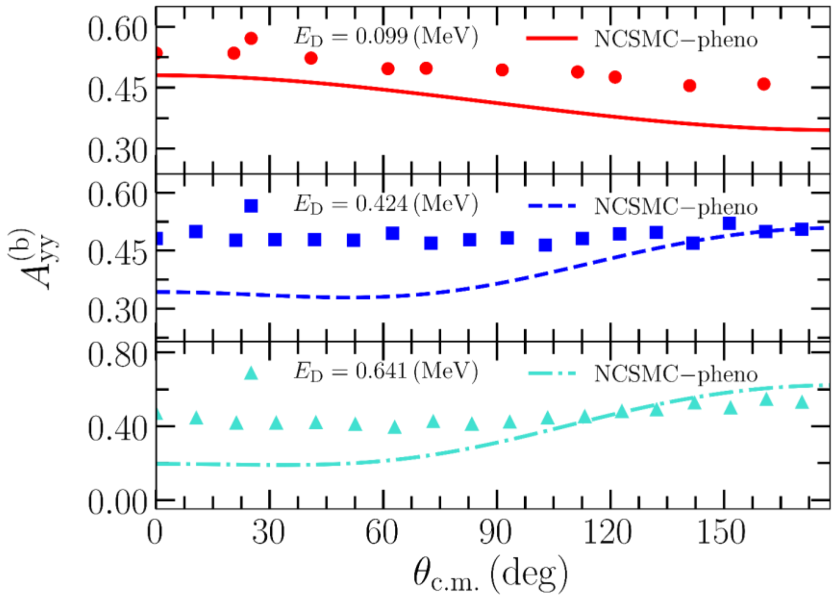
- The S-factor is globally well reproduced.
- However, there are **discrepancies** between data sets around the peak of the S-factor.
- Influence of p- and d-waves in agreement with data.







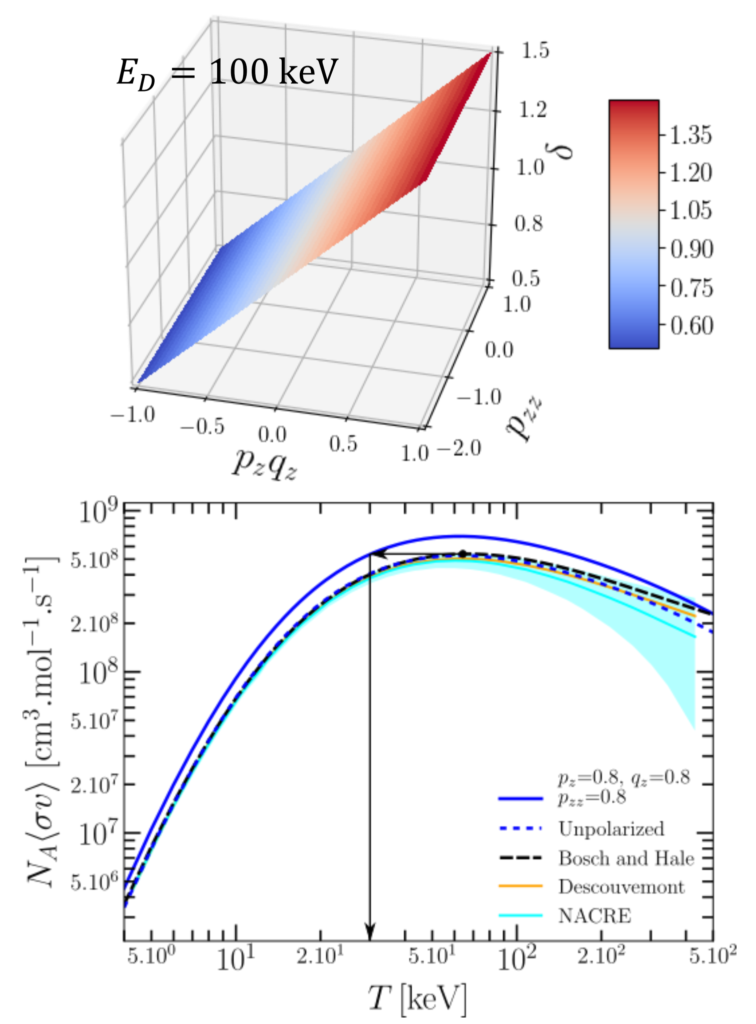


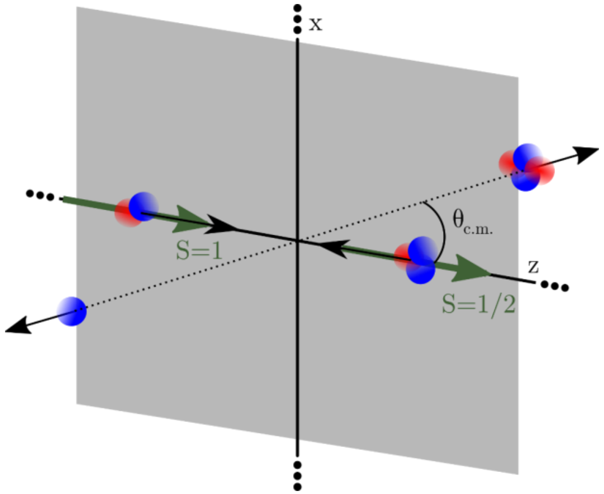


W.H. Geist, *et al.* PRC**60** (1999).

Deviations from a pure s-wave of the analyzing tensors are globally reproduced in shape but their amplitude is not.

Enhancement factor and reaction rate



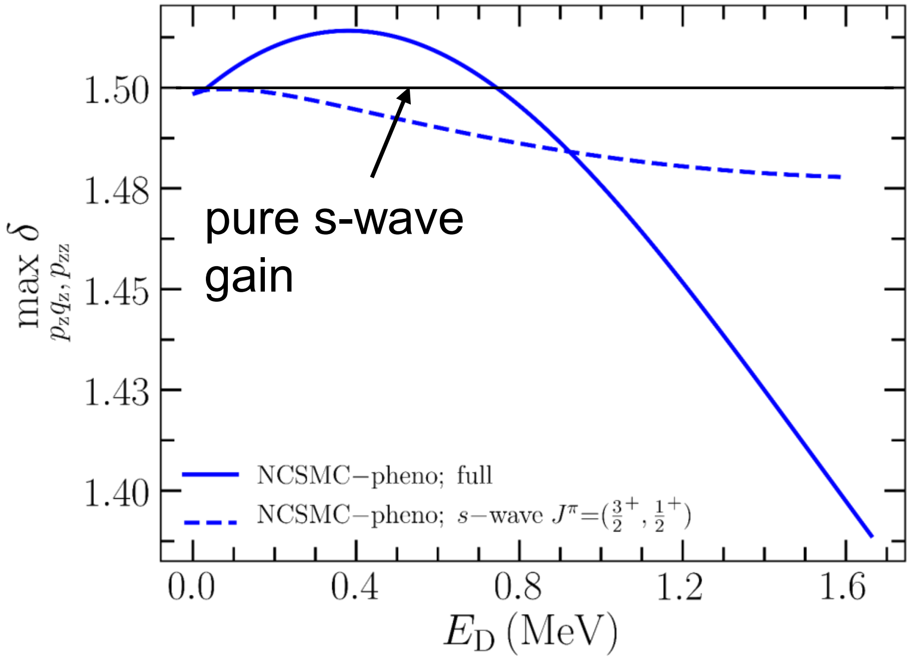


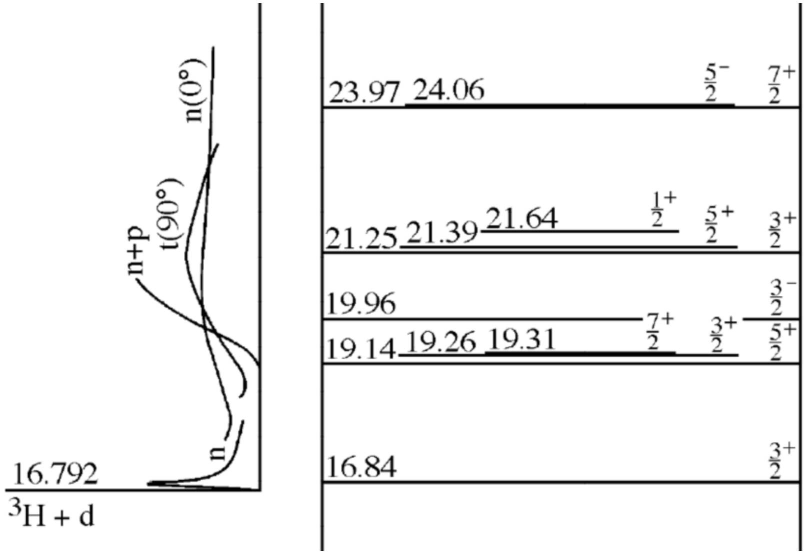
Reactant spins are prepared in a configuration

$$\frac{\partial \sigma^{\text{polar}}}{\partial \Omega}(\theta) = \frac{\partial \sigma}{\partial \Omega}(\theta)\left(1 + \frac{1}{2} p_{zz} A_{zz}(\theta) + \frac{3}{2} p_z q_z C_{z,z}(\theta)\right)$$

- **Predictions** for polarized $^3\vec{\mathrm{H}}(\vec{d},n)^4\mathrm{He}$ enhancement factor and reaction rate.
- **Confirmation** of maximum enhancement ($\delta = 1.5$) scenario.
- *Ab initio* calculation shows that $\delta = 1.38$ can be achieved in lab.

Maximum enhancement as $f(E)$



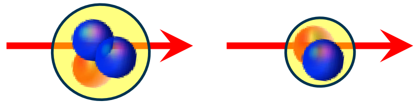


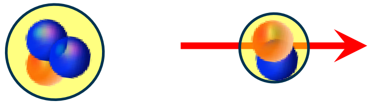
- $\delta = 1.5$ only valid at $E \sim 0$.
- δ can be greater than 1.5 due to d-wave.
- Pure s-wave picture gives the right order of magnitude but not the shape of the **energy dependence**.

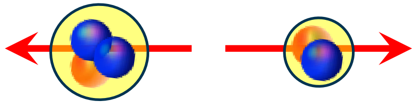
Anisotropies from polarized reaction

Angular distribution in different polarization scenarios

$J = 1/2$ $J_z = -1/2$ $J = 1$ $J_z = 1$



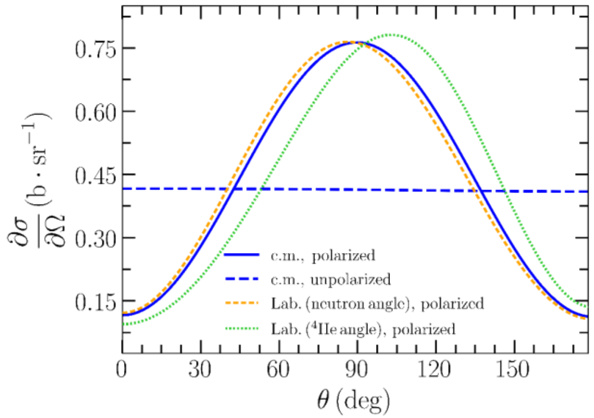


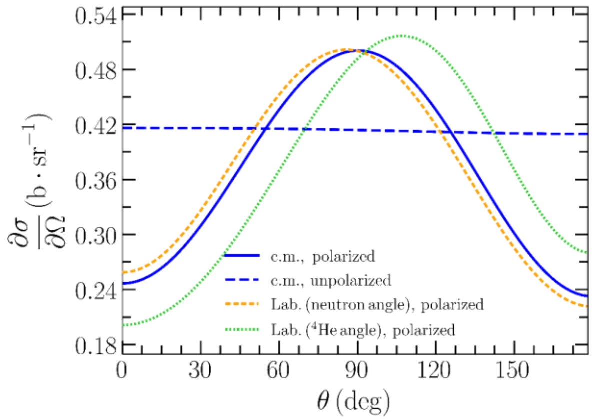


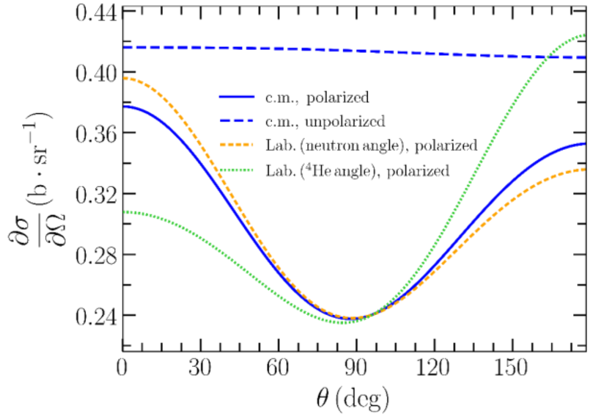
Total cross section increased

On average no effects

Total cross section decreased







Spin tensor properties of the deuteron give the angular shape.
(same as in $^3\overrightarrow{\mathrm{He}}(\vec{d},p)^4\mathrm{He}$)

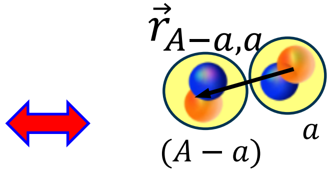
DD fusion: a more complicated situation

$$\Psi_{RGM}^{(A)} = \sum_{v} \int d\vec{r}\, g_v(\vec{r})\, \hat{A}_v \left| \Phi_{v\vec{r}}^{(A-a,a)} \right\rangle$$

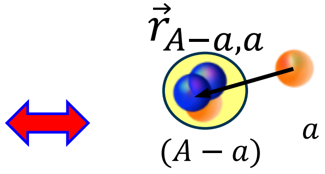
Relative wave function (unknown)

Antisymmetrizer

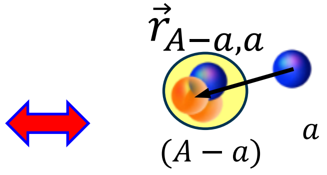
Channel basis



$$\psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

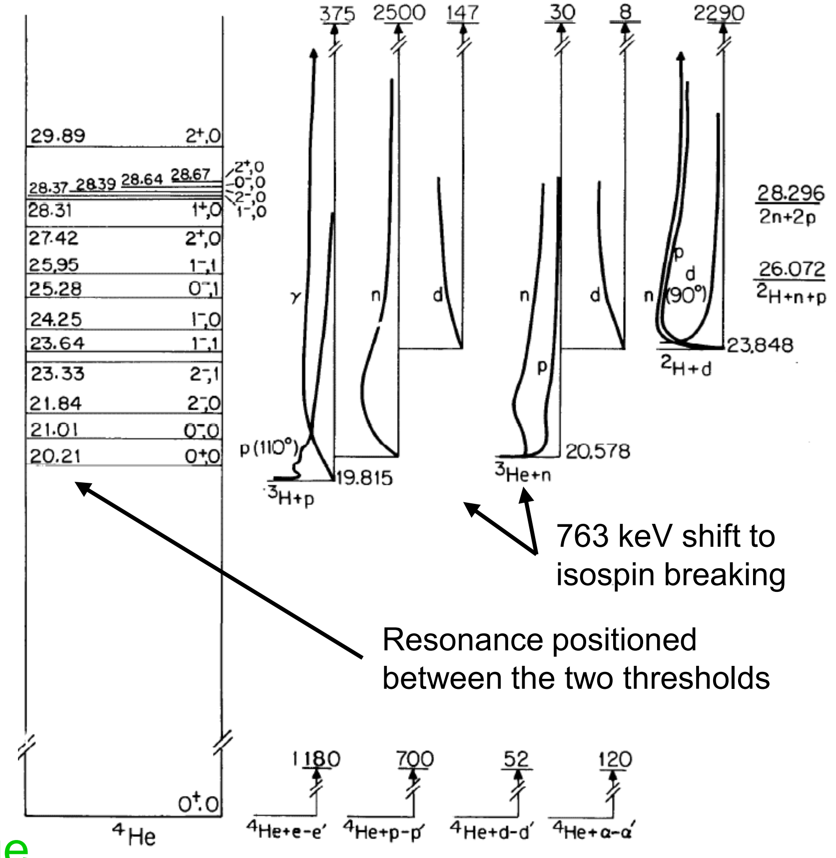


$$\psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$



$$\psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

Lightly bound& identical particle

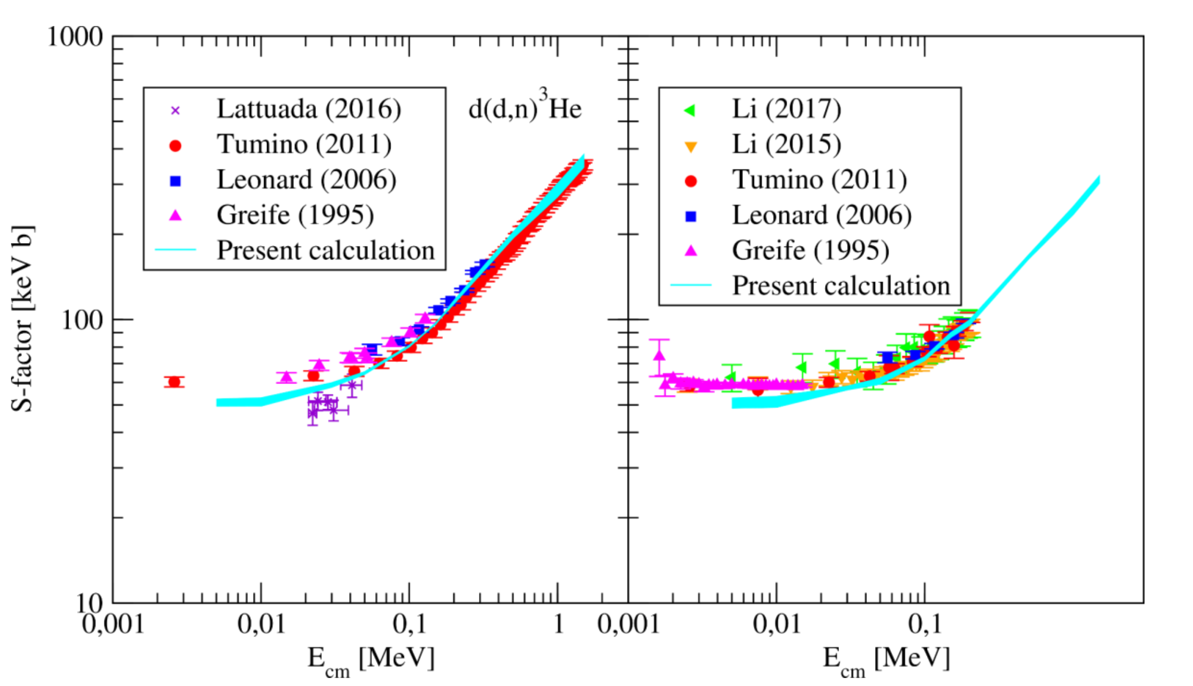


763 keV shift to isospin breaking

Resonance positioned between the two thresholds

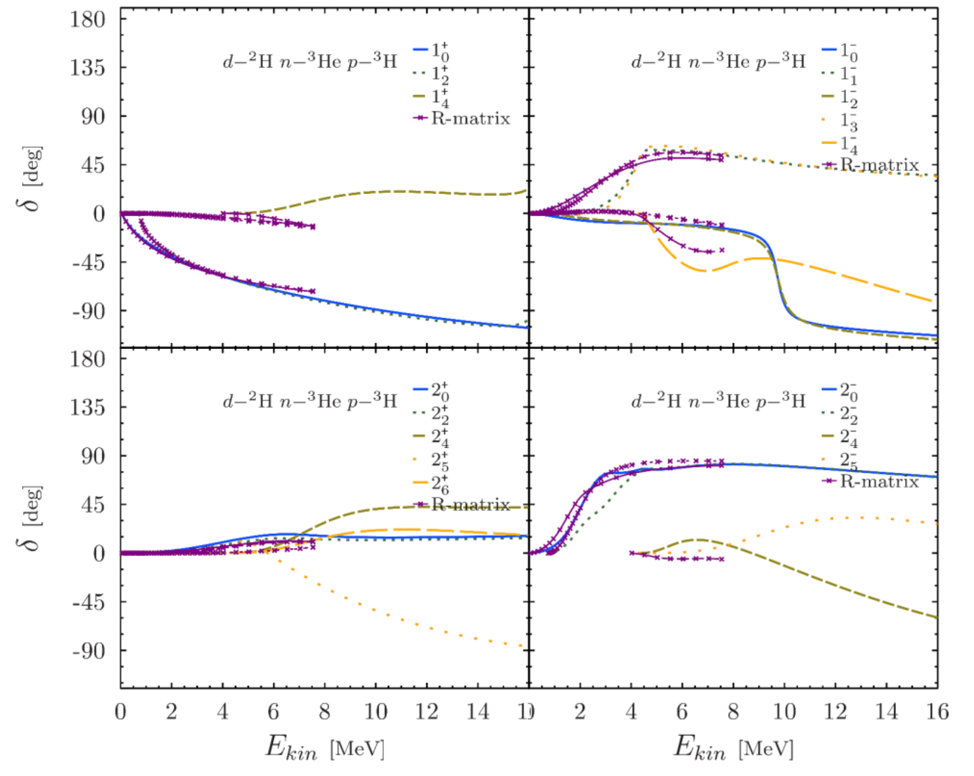
Charged exchange channel.. “fine tuning of nuclear interaction”

HH and Kohn variational principle for DD fusion



M. Viviani, L. Girlanda *et al.* PRL**130** 122501 (2023).

NCSMC phase shifts NN+3N-LNL



Excellent agreement with data for the low-energy fusion.

Reasonable agreement with R-matrix analysis of data over large energy range.

K. Kravvaris, S. Quaglioni *et al.* PLB856, 138930 (2024)

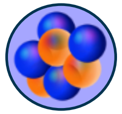
One way to solve the many-body problem

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \; |A\alpha j_z{}^{\pi} t_z\rangle$$

Mixing coefficients (unknown) → c_α

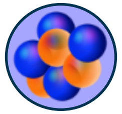
A-body harmonic oscillator states → $|A\alpha j_z{}^{\pi} t_z\rangle$

⇔



$|A\lambda J^{\pi}T\rangle_{SD}\,\phi_{00}(\vec{R}^{A}_{c.m.})$

Second quantization



$|A\lambda J^{\pi}T\rangle_{SD}\,\phi_{nl}(\vec{R}^{A}_{c.m.})$

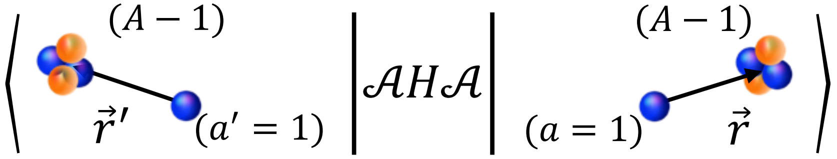
Second quantization

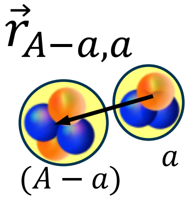
"Trivial" to create a **basis of boosted NCSM** wave functions

Advantage of HO CI methods:

1. Center of mass is factorized.

Span the same basis as

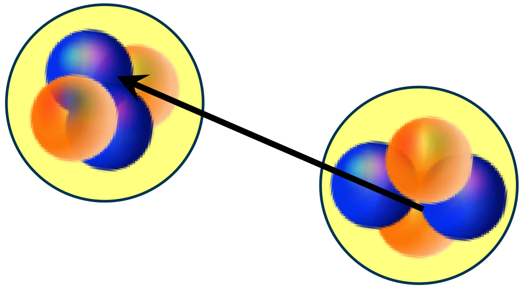




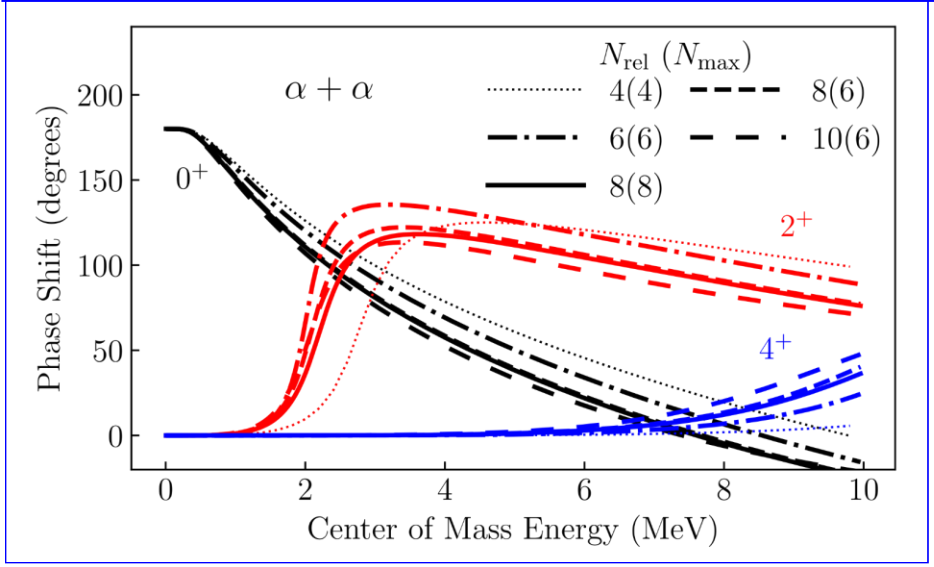
$\psi^{(A-a)}_{\alpha_1}\psi^{(a)}_{\alpha_2}\,\delta(\vec{r}-\vec{r}_{A-a,a})$

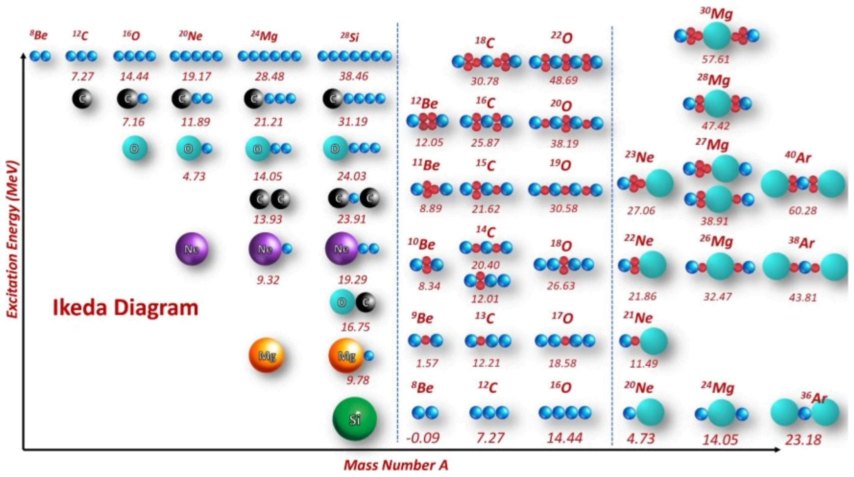
⇔

$$\phi^{A}_{n} = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_i(\vec{r}_1) & \dots & \phi_i(\vec{r}_A) \\ \vdots & \ddots & \vdots \\ \phi_l(\vec{r}_1) & \dots & \phi_l(\vec{r}_A) \end{vmatrix} = a^{\dagger}_{l} \dots a^{\dagger}_{i}|0\rangle$$



α+α scattering phase-shift

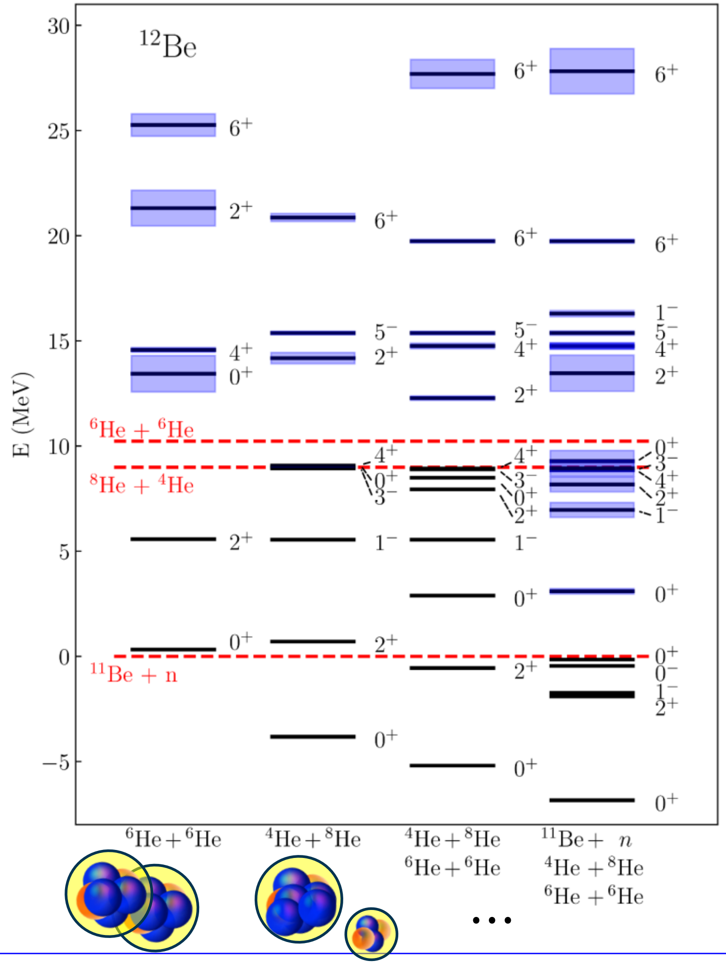




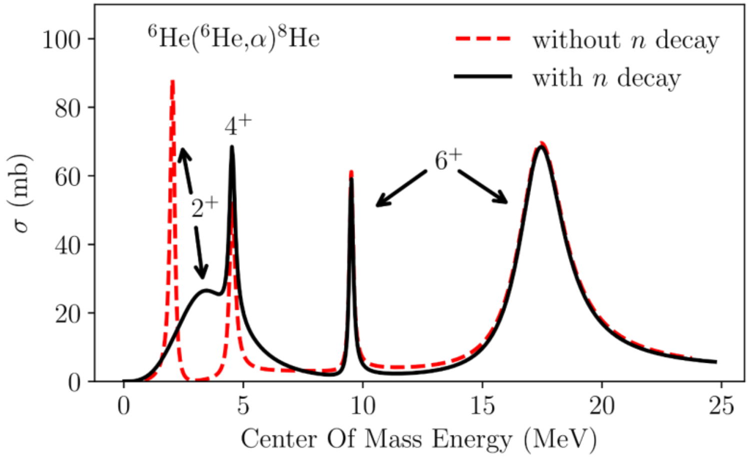
I. Lombardo *et al.* Riv. Nuovo Cim. **46** (2023)

- *Ab initio* NCSM/RGM calculation of α–α scattering using chiral NN+3N;
- **3N regulator** choice strongly **affected** resonance positions;
- **NN+3NlnI** give best agreement with experimental data.

Evolution of ^{12}Be with cluster structure



Evidence of channels selectivity



- Coupling to ^{11}Be+n channel reshapes ^{12}Be spectrum.
- Neutron decay strongly influences ^{6}He(^{6}He,α)^{8}He cross section.
- **Helium clustering survives** high above decay thresholds.