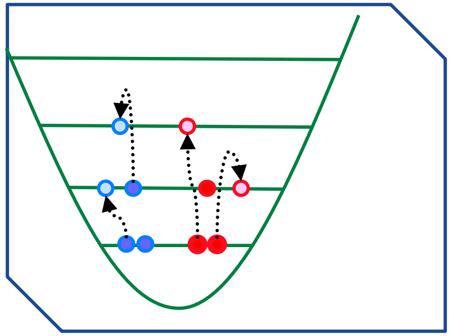
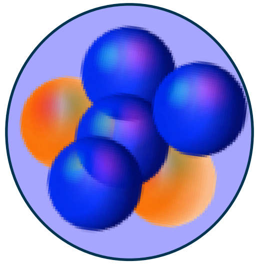
Guillaume Hupin, CNRS IJClab

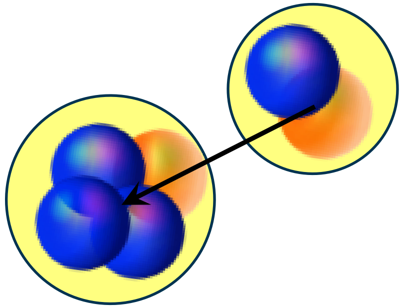


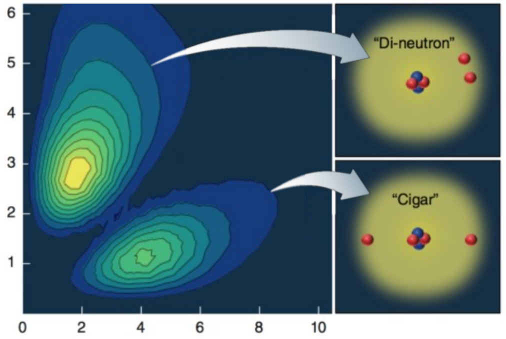


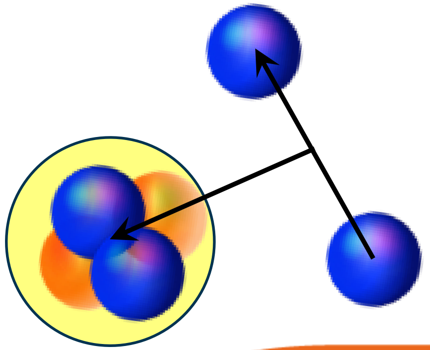
Collaborators

S. Quaglioni (LLNL)
K. Kravvaris (LLNL)
P. Navratil (TRIUMF)
M. Aliotta (UoE)
and many other distinguished colleagues!

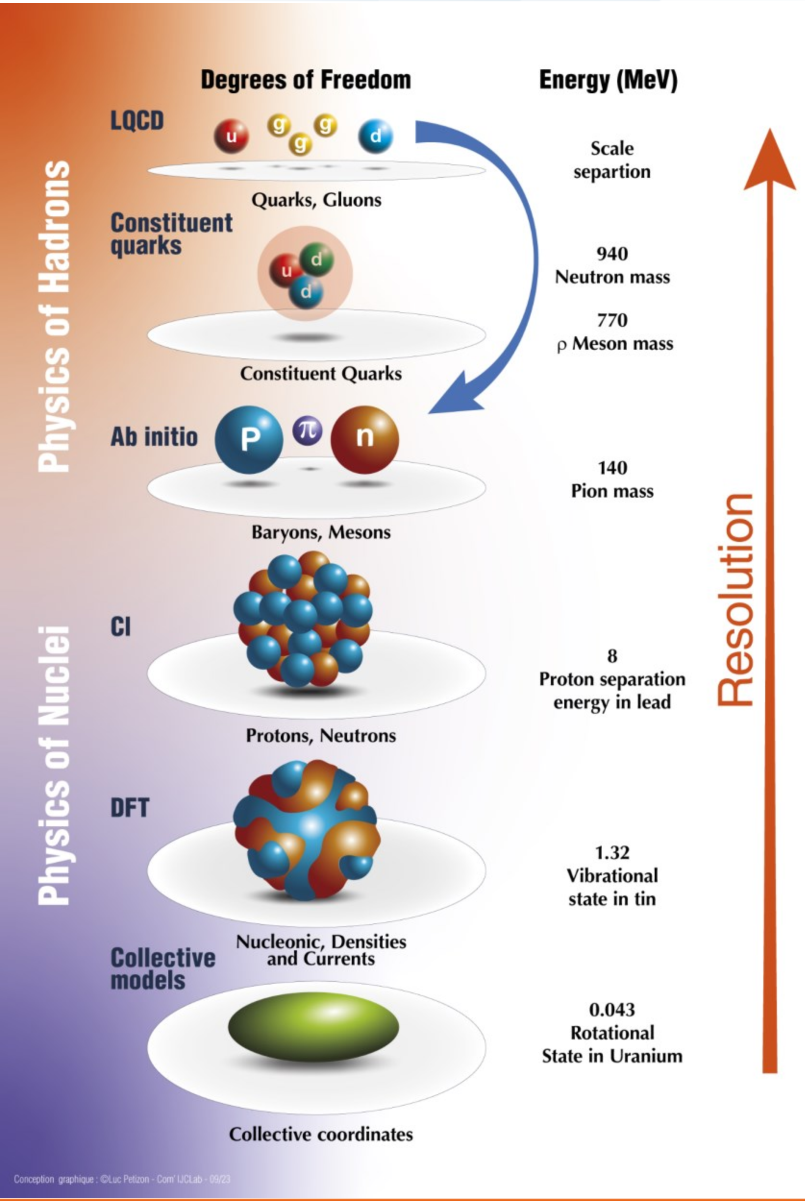
Ab initio framework for nuclear fusion reactions







A story of multiple scale

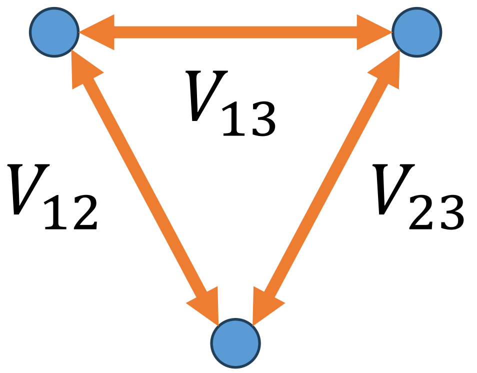


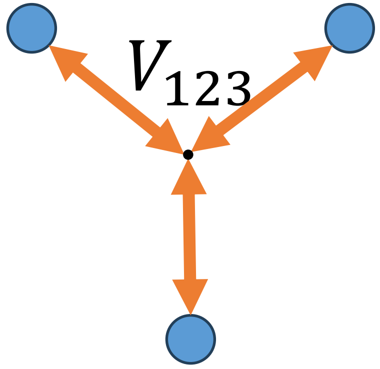
- Goal: Solving the Schrodinger equation (SE) for an A-body system:

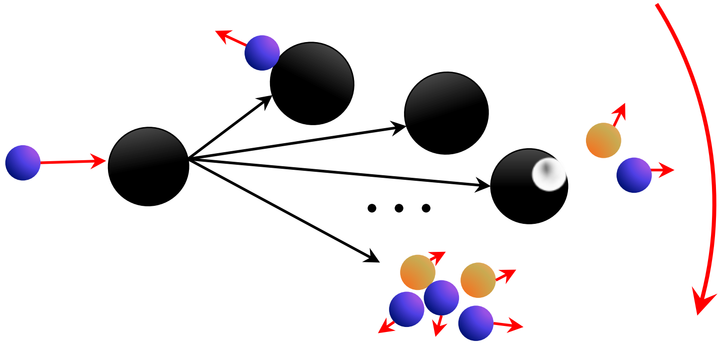
$$H|\psi^{J^{\pi}T}>=E|\psi^{J^{\pi}T}>$$

- Nucleons are considered as point-like particles.

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







Complexity of scattering problem

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

Credits H. Lenske

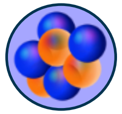
B.R. Barrett, P. Navrátil, J.P. Vary, J.P. Progr. Part. Nucl. Phys. 69 (2013)

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)

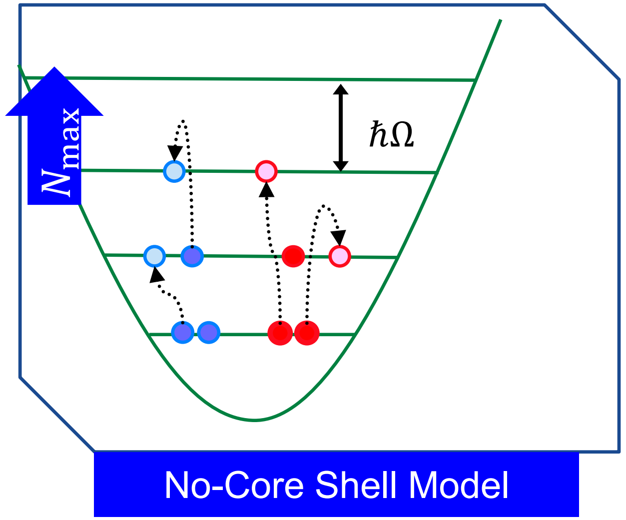
A-body harmonic oscillator states



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

Second quantization

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



Advantage of HO CI methods:

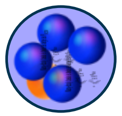
1. Center of mass is factorized.
2. Mathematically possible to derived s.p. to Jacobi coordinates transformation.
3. Fourier transform is trivial: NCSM, RGM with HO CI is equivalent in momentum or position space.

- 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

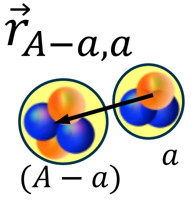
Can address bound and low-lying resonances (short range correlations)

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

Relative wave function (unknown)

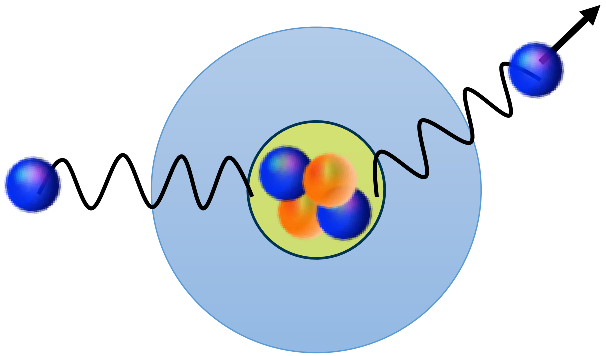
Antisymmetrizer

Channel basis



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

Cluster expansion technique

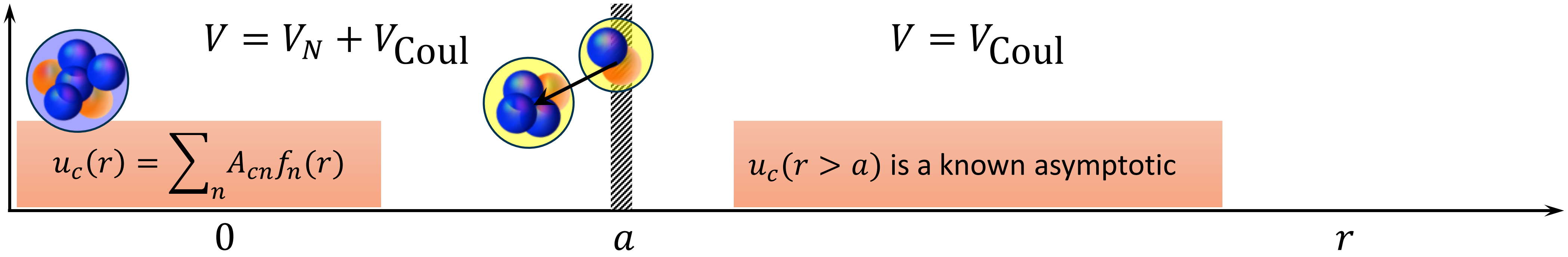


NCSM/RGM Cluster formalism for elastic/inelastic

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):

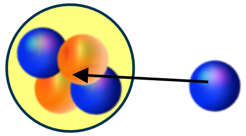
- HO wavefunctions;
- Single particle basis;
- Jacobi basis.

NCSM with continuum (NCSMC):

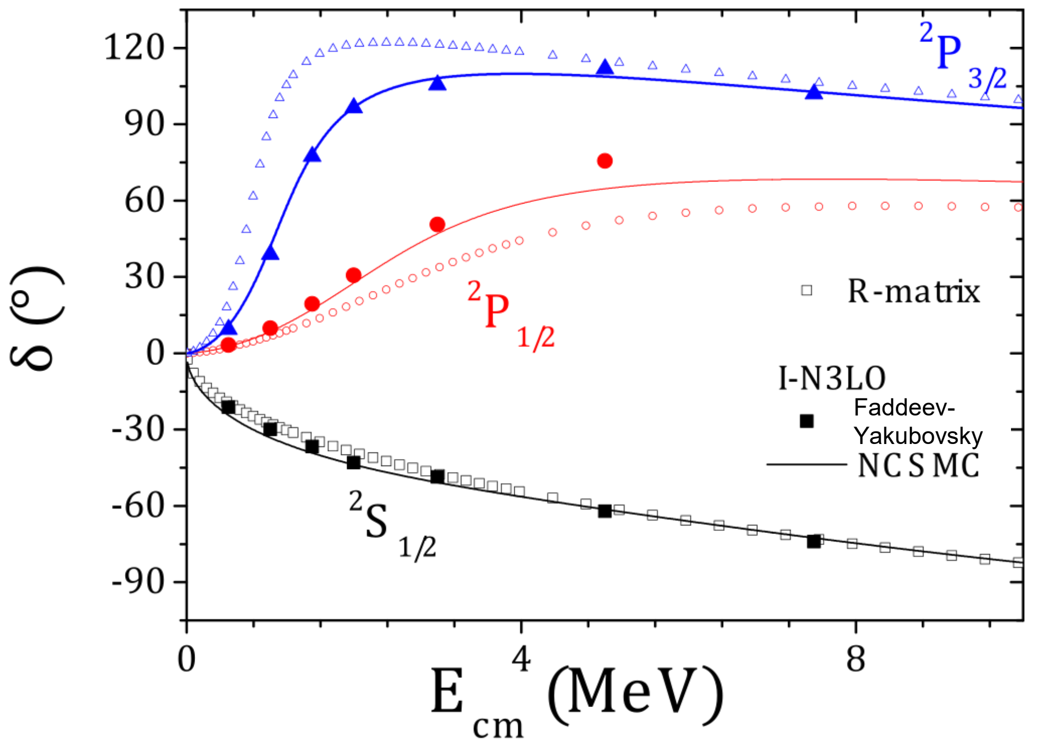
- For computing reactions and exotic nuclei.

Limitations:

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



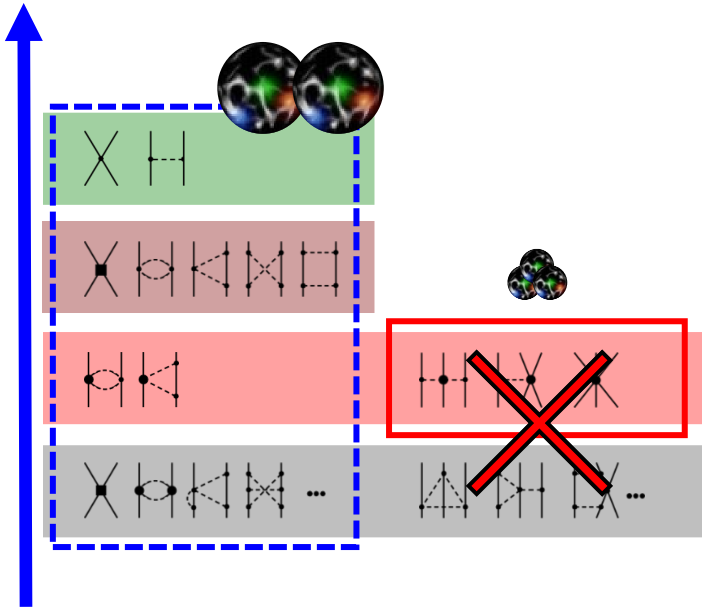
Benchmark: scattering phase shifts NCSMC/FY

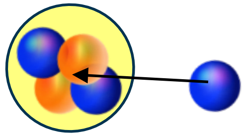


R. Lazauskas, PRC **97** (2018).*

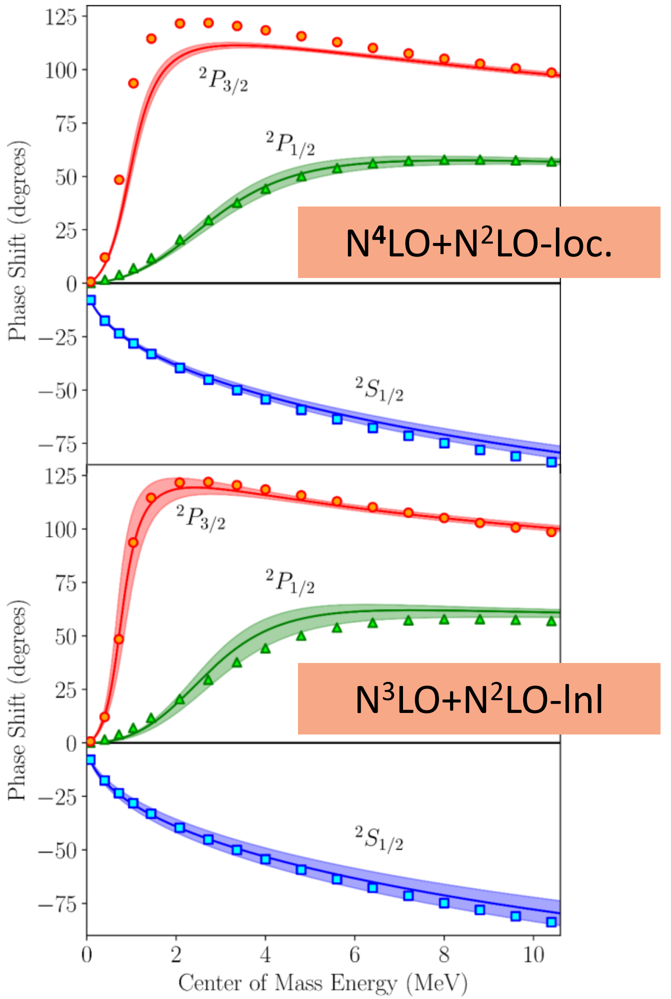
*there is a more recent paper with 3N force.

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

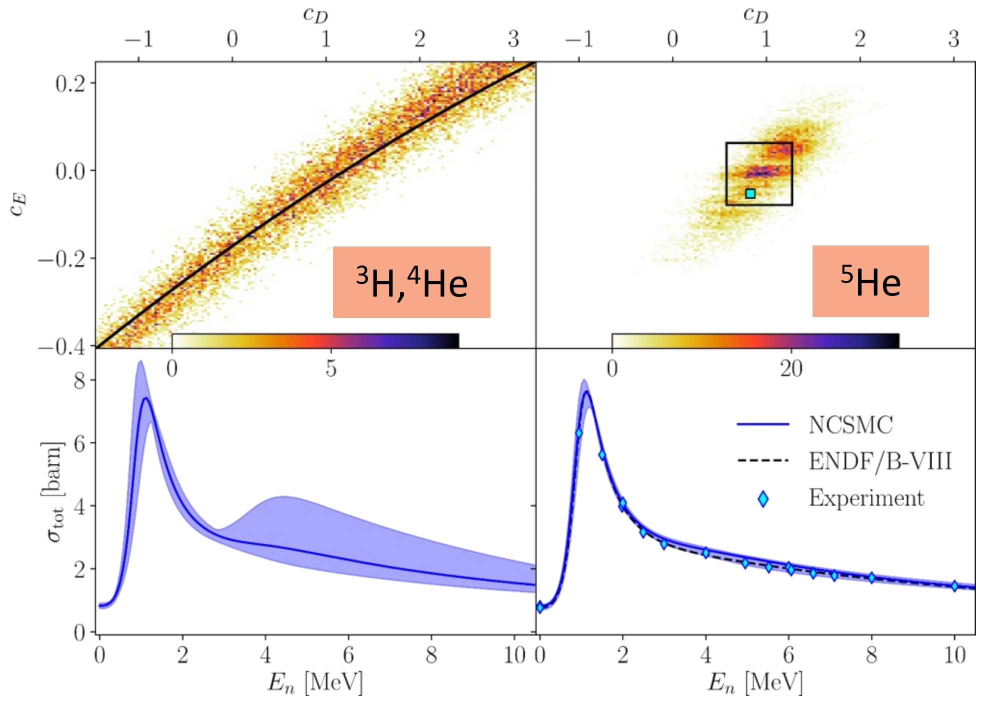




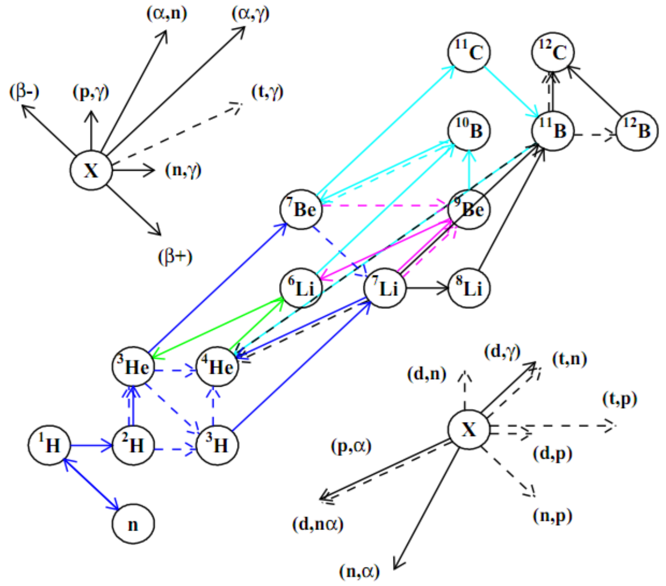
Sensitivity to c_D and c_E

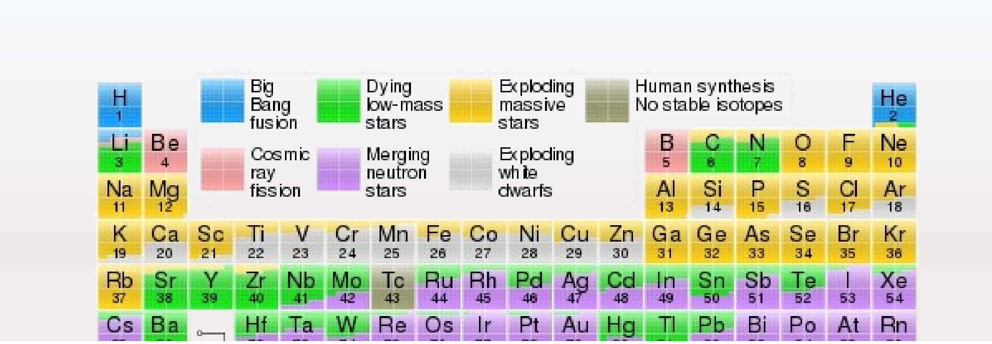


- NN-N4LO + 3N-N2LO **cannot reproduce** the p-wave splitting.
- Tighter posterior distribution if the properties of the ^{5}He are included in the fit of 3N LEC.

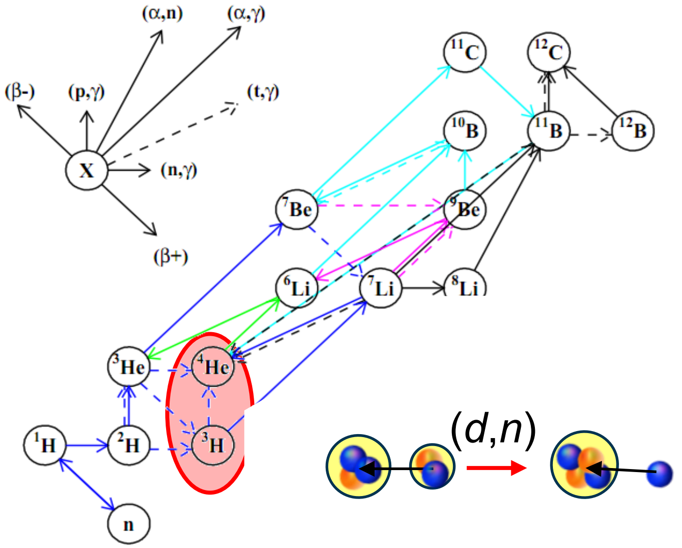


Primordial Nucleosynthesis **(blue)**

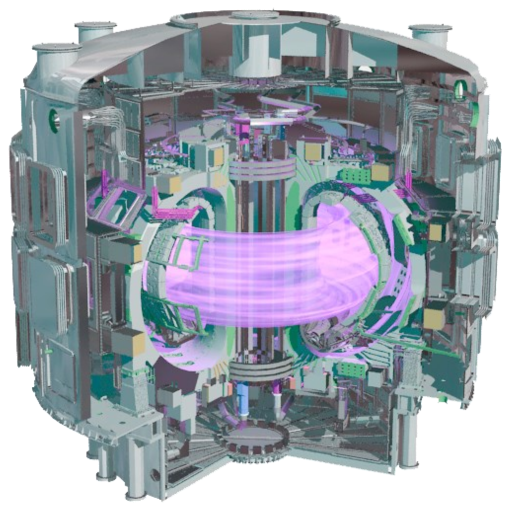




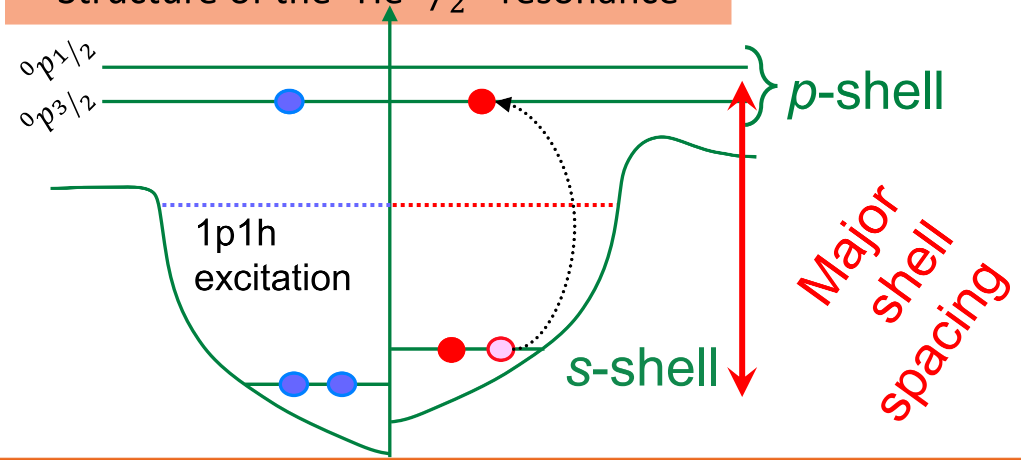
Primordial Nucleosynthesis **(blue)**



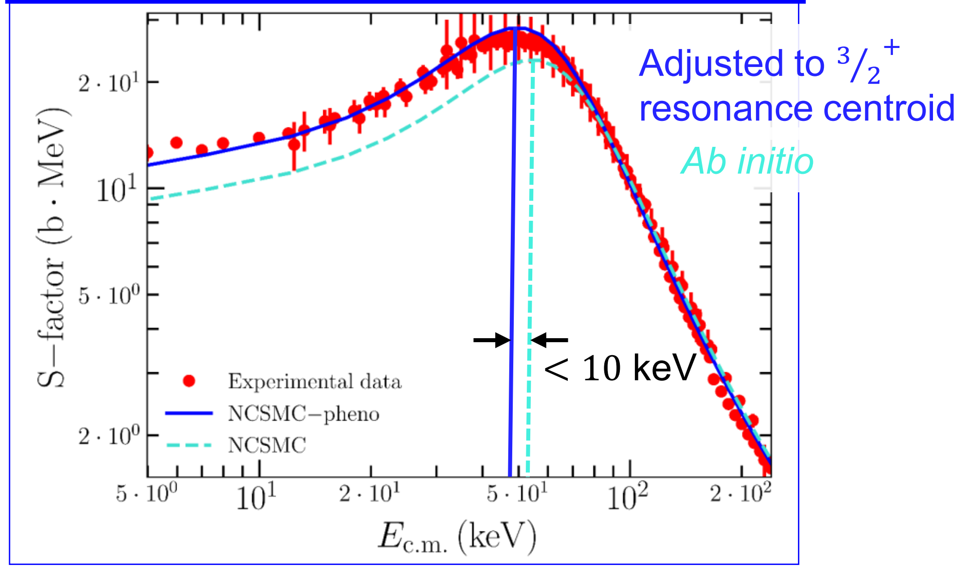
ITER design (Cadarache, France)



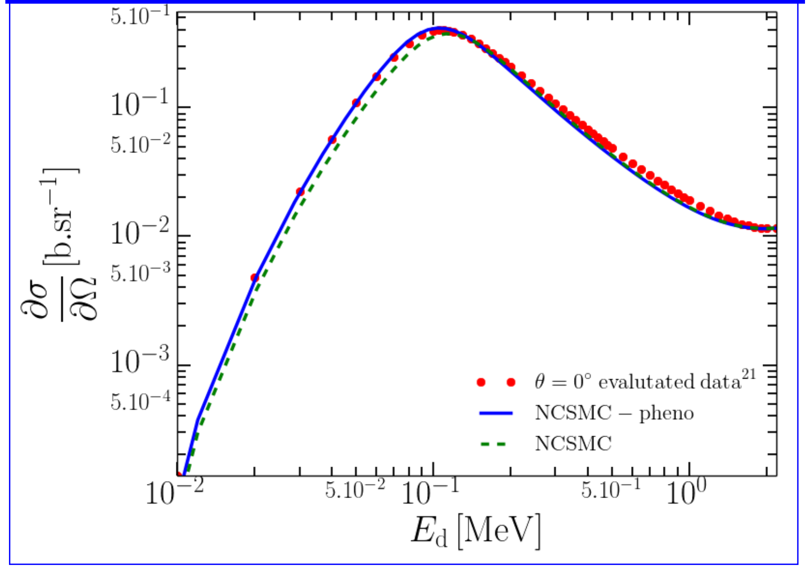
Structure of the ^{5}He $^3/_2{}^+$ resonance



S-factor: computed and data



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

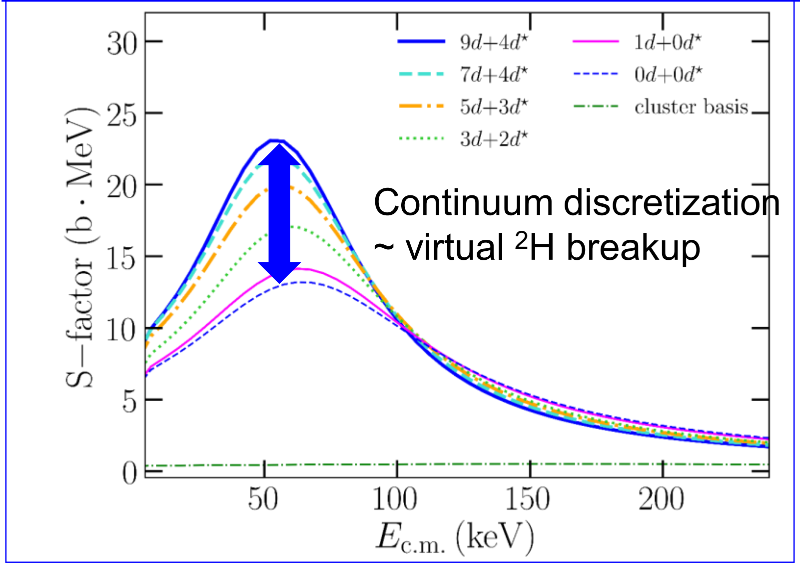


M. Drosg and N. Otuka, INDC(AUS)-0019 (2015).

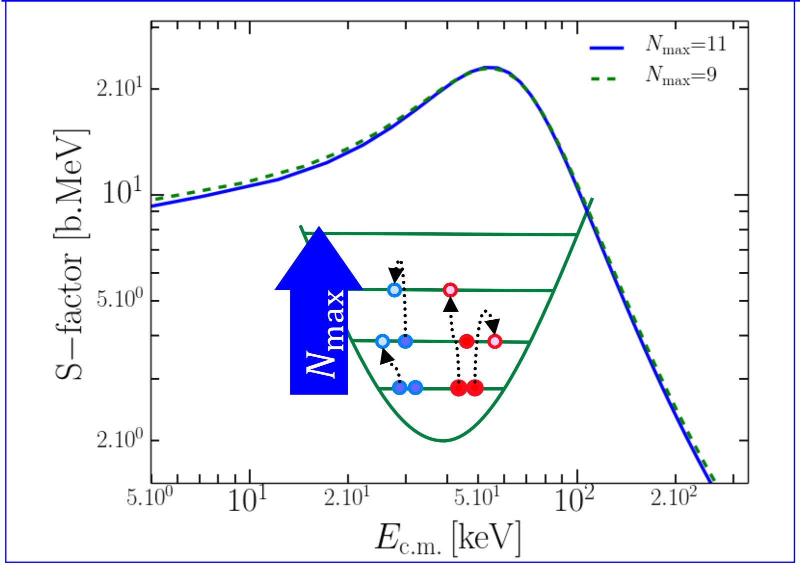
- The S-factor is globally well reproduced.
- The accurate **reproduction** (of the order of keV) of the **resonance position**/width is **essential**.
- Shape of the angular distribution **agrees** with recent **evaluation**.

^{3}H(d,n)^{4}He fusion reaction: Model convergence

Convergence wrt ^{2}H continuum



Convergence with $N_{\max}$

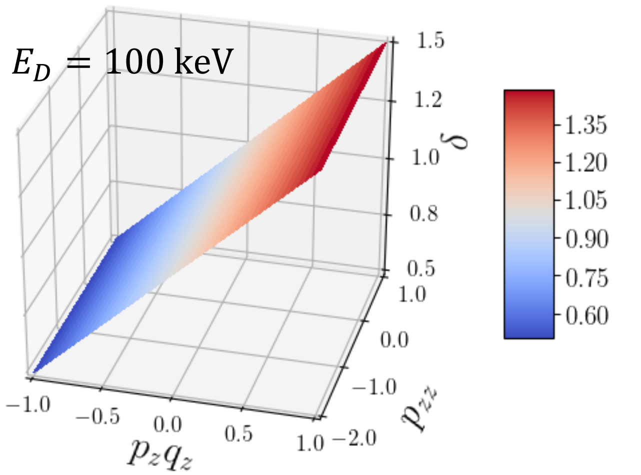


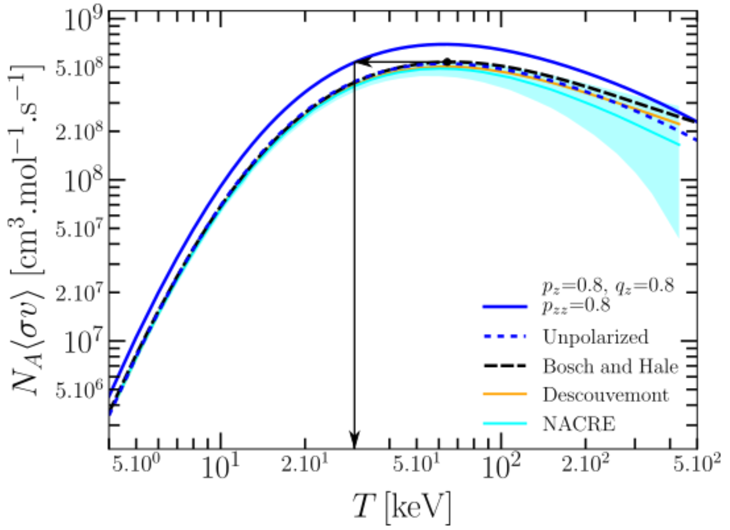
^{5}He($^4S_{3/2}$)	E_r (keV)	Γ_r (keV)
Cluster basis (D g.s. only)	105	1100
Cluster basis	120	570
NCSMC (D g.s. only)	65	160
NCSMC	55	110
NCSMC-pheno	50	98
R-matrix G.M. Hale, *et al.* PRL **59** (1987).	48	74

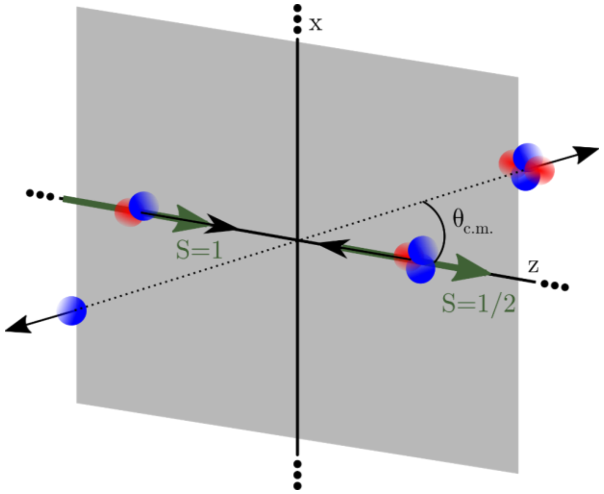
correlated

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

Enhancement factor and reaction rate





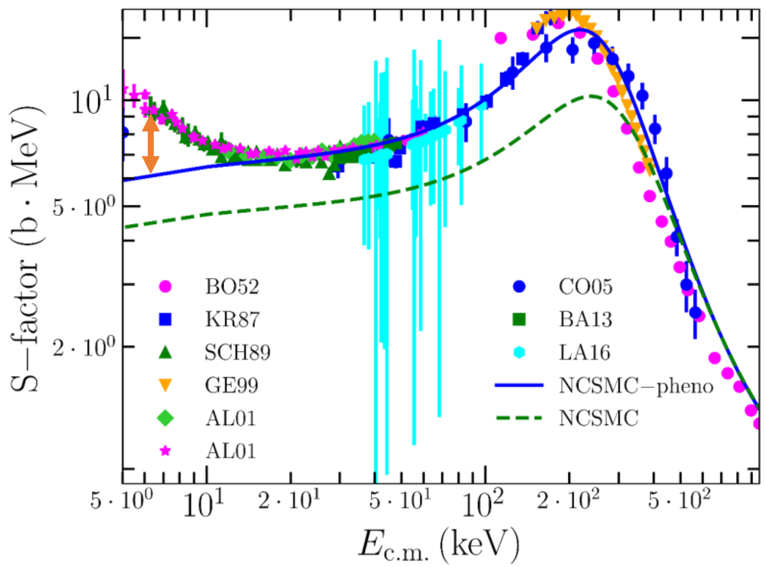


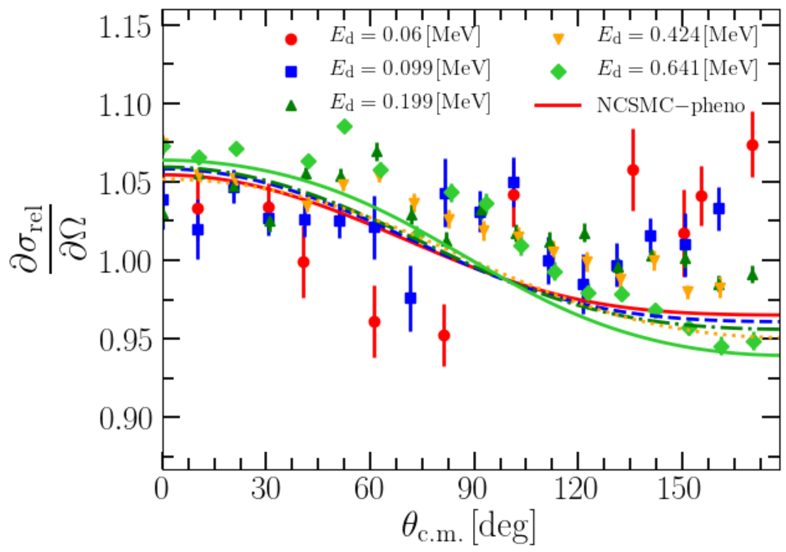
Reactant spins are prepared in a configuration

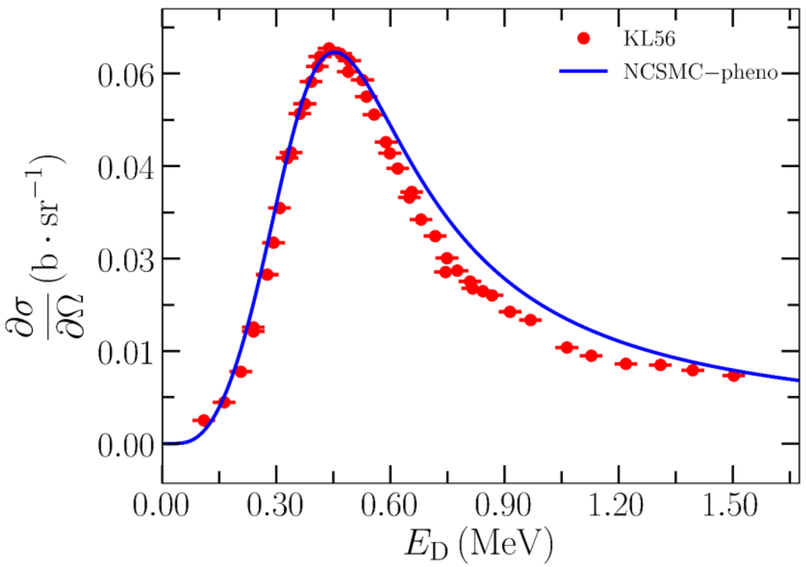
$$\frac{\partial \sigma^{\text{polar}}}{\partial \Omega}(\theta) = \frac{\partial \sigma}{\partial \Omega}(\theta)\left(1 + \frac{1}{2} p_{zz} A_{zz}(\theta) + \frac{3}{2} p_z q_z C_{z,z}(\theta)\right)$$

- **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.

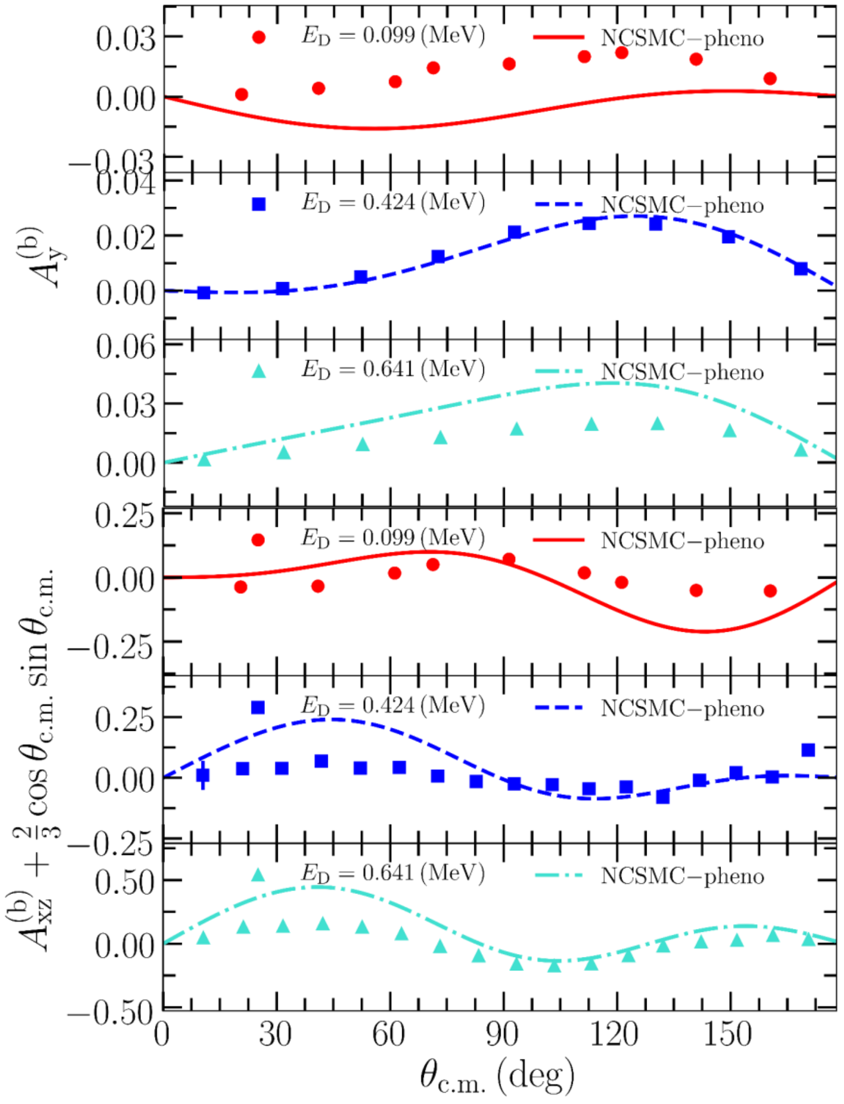
- The S-factor is globally well reproduced.
- However, there are **discrepancies** between data sets around the peak of the S-factor.
- Influence of p- and d-waves in agreement with data.

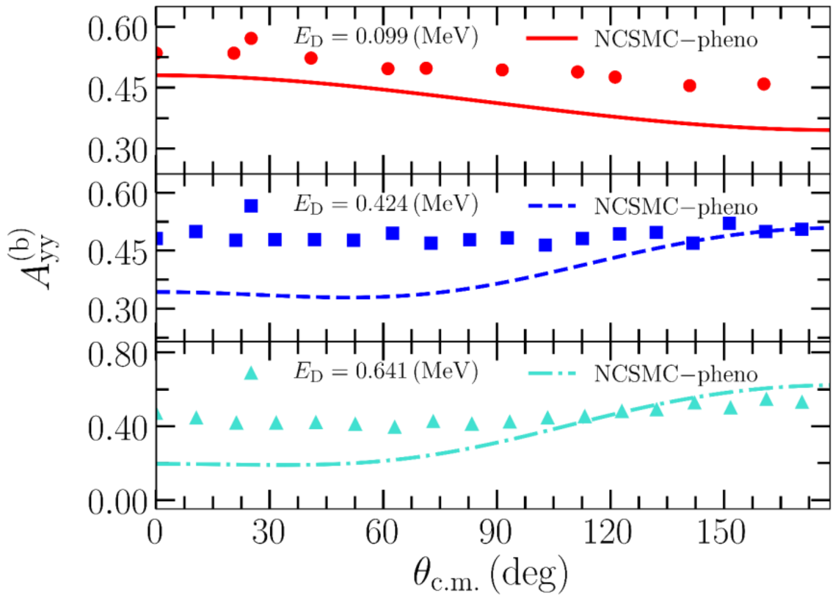






$^3He(\vec{d},p)^4He$: analyzing tensors

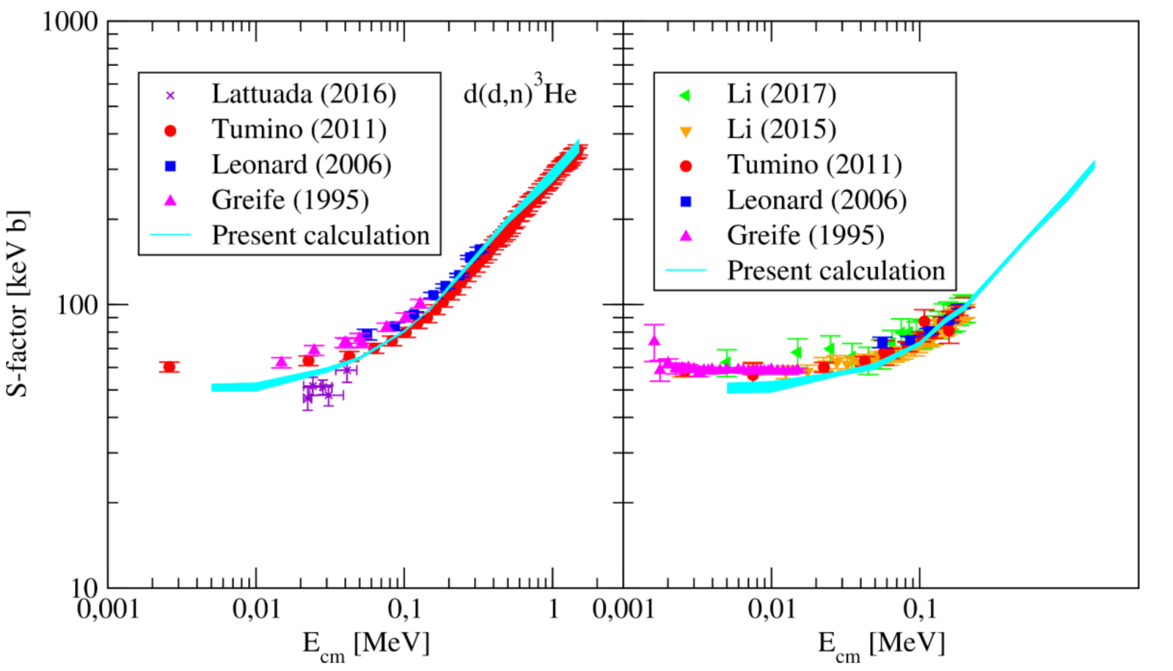




W.H. Geist, *et al.* PRC**60** (1999).

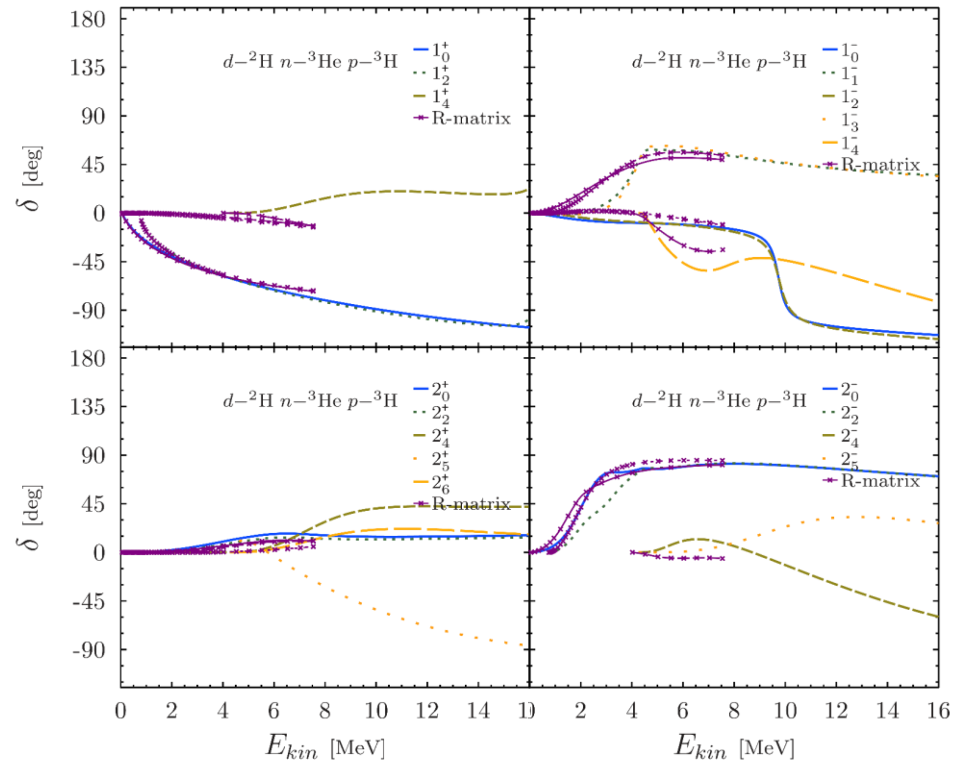
Deviations from a pure s-wave of the analyzing tensors are globally reproduced in shape but their amplitude is not.

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.

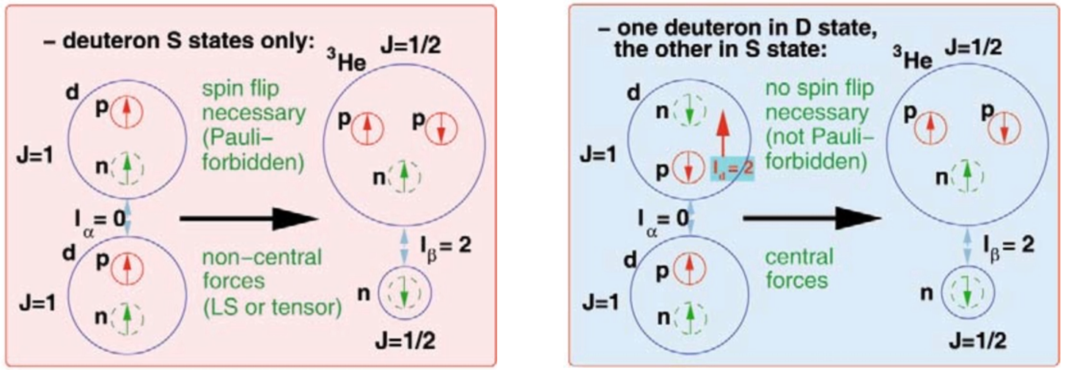
Reasonable agreement with R-matrix analysis of data over large energy range.

DD fusion: quintet suppression for fusion

Advanced design for an aneutronic reactor..

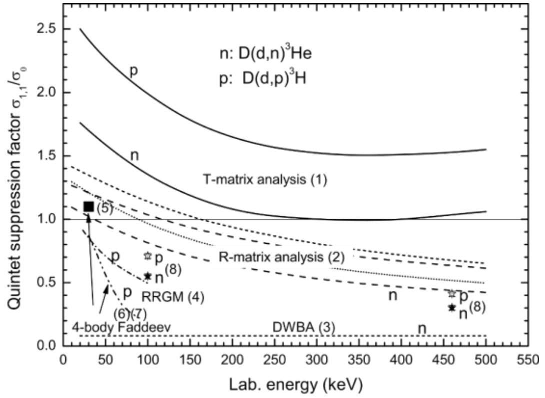
$$\sigma_{tot} = \frac{1}{9}\left(2\sigma_{1,1} + 4\sigma_{1,0} + \sigma_{0,0} + \sigma_{1,-1}\right)$$

quintet triplet singlets

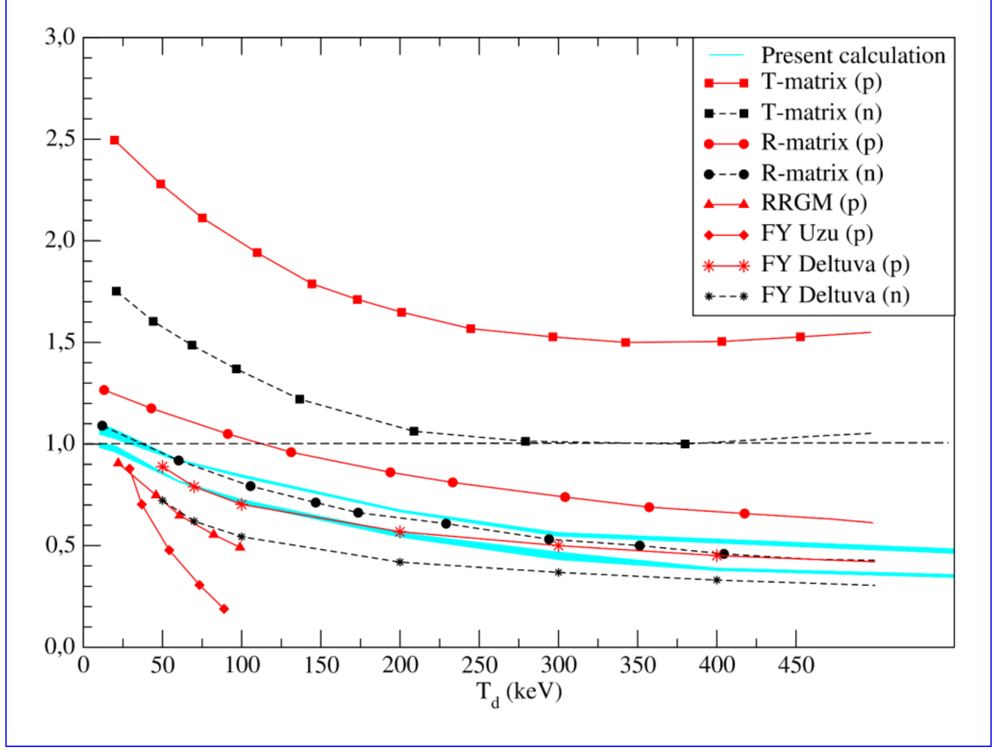


H.P. gen. Schieck EPJA**44** (2010).

- No experimental data
- No clear cut evidence from calculations:
  1. Low-energy
  2. Coulomb.
  3. Lack of complete nuclear interaction.



Quintet suppression factor



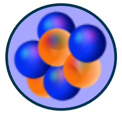
M. Viviani, L. Girlanda *et al.* PRL**130** 122501 (2023).

One way to solve the many-body problem

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

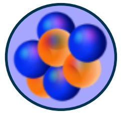
Mixing coefficients(unknown)

A-body harmonic oscillator states



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

Second quantization



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

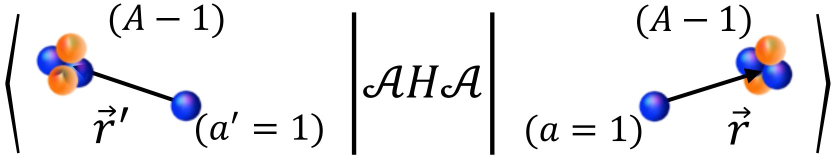
Second quantization

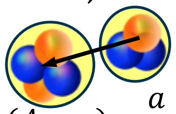
"Trivial" to create a **basis of boosted NCSM** wave functions

Advantage of HO CI methods:

1. Center of mass is factorized.

Span the same basis as

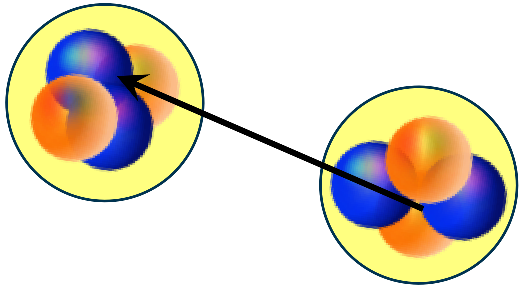




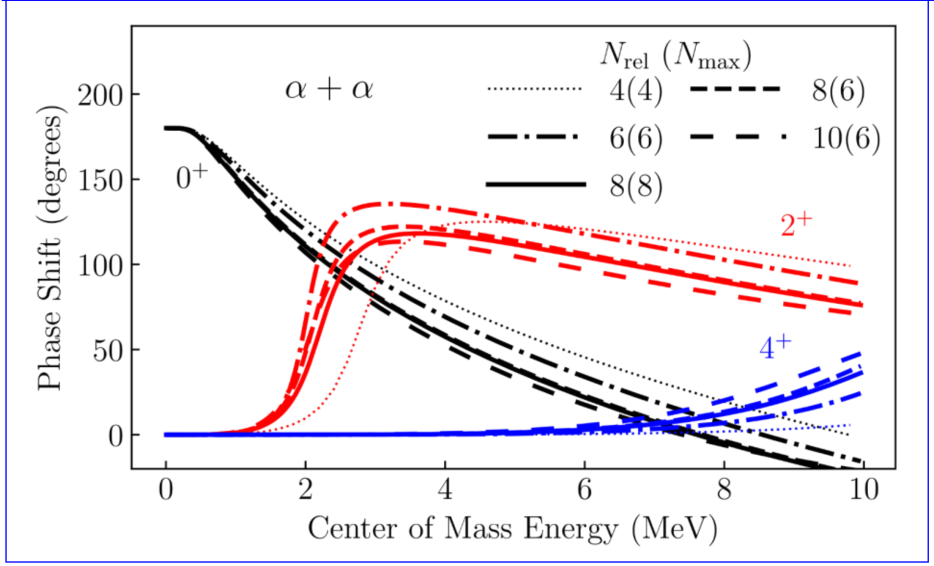
$\psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2} \, \delta(\vec{r} - \vec{r}_{A-a,a})$

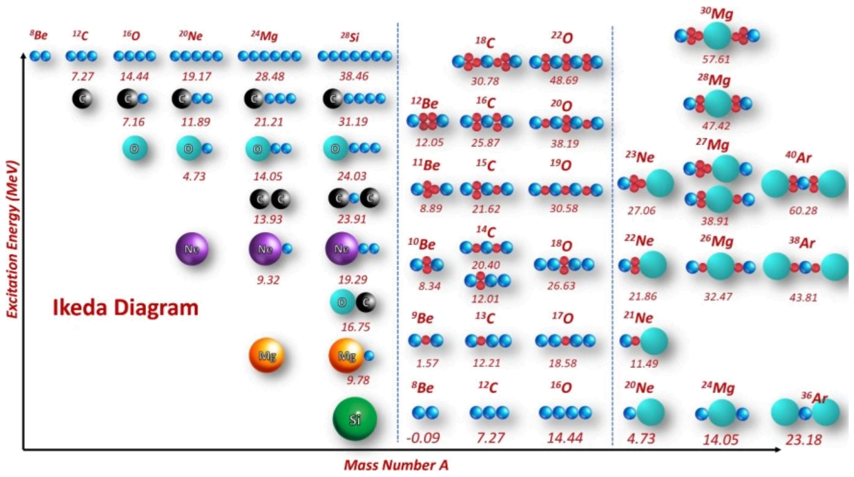
$$\phi^{A}_{n} = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\vec{r}_1) & \dots & \phi_i(\vec{r}_A) \\ \vdots & \ddots & \vdots \\ \phi_l(\vec{r}_1) & \dots & \phi_l(\vec{r}_A) \end{vmatrix} = a^{\dagger}_{l} \dots a^{\dagger}_{i} |0\rangle$$

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



α+α scattering phase-shift

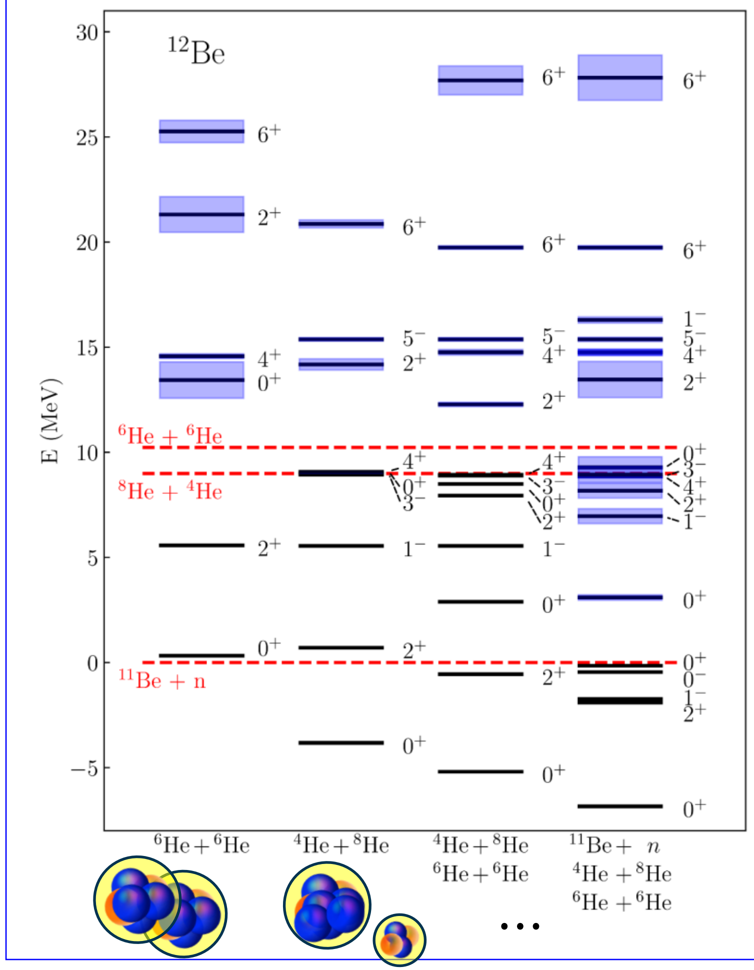




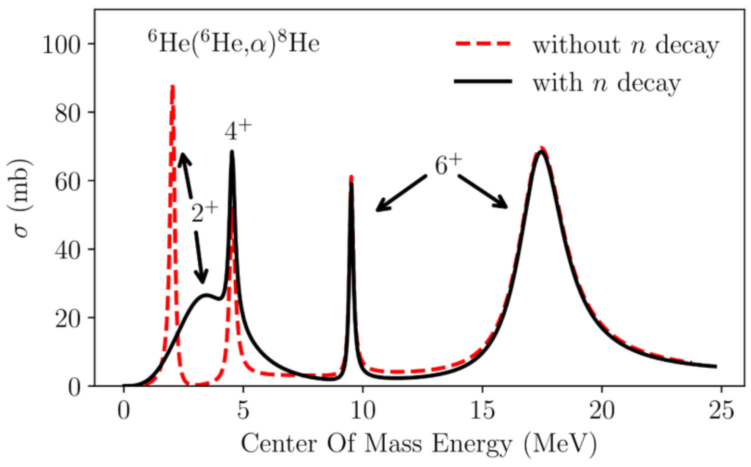
I. Lombardo *et al.* Riv. Nuovo Cim. **46** (2023)

- *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.

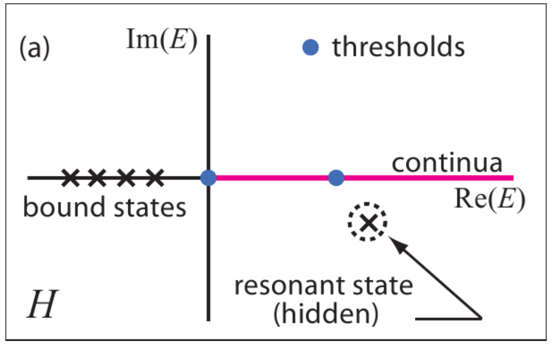
Evolution of ^{12}Be with cluster structure



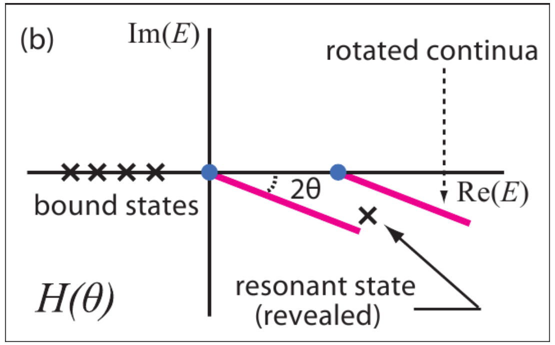
Evidence of channels selectivity



- 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.



Complex scaling

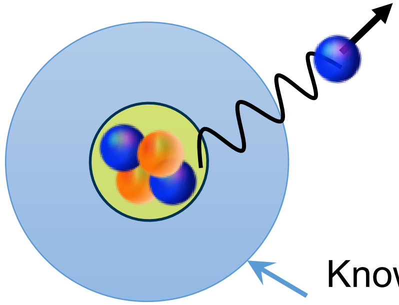


Kruppa *et al.* PRC**89** (2014)

"A" definition of a resonance is that it corresponds to a pole in the S-matrix at the complex energy associated with the resonance location.

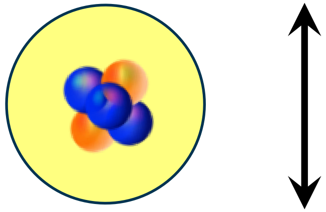
$$\hat{H}(r) = \hat{T} + \hat{V}(r)$$

$$\hat{H}(\theta) = e^{-2i\theta}\hat{T} + \hat{V}\left(re^{i\theta}\right)$$
$$\hat{H}(r) = \hat{U}(\theta)\hat{H}(r)\hat{U}^{\intercal}(\theta)$$



$$U(\theta)H(r)U(\theta)^{\intercal}$$

$$\psi(r,\theta) \underset{\infty}{\sim} e^{-\boldsymbol{kr}\sin\theta}$$

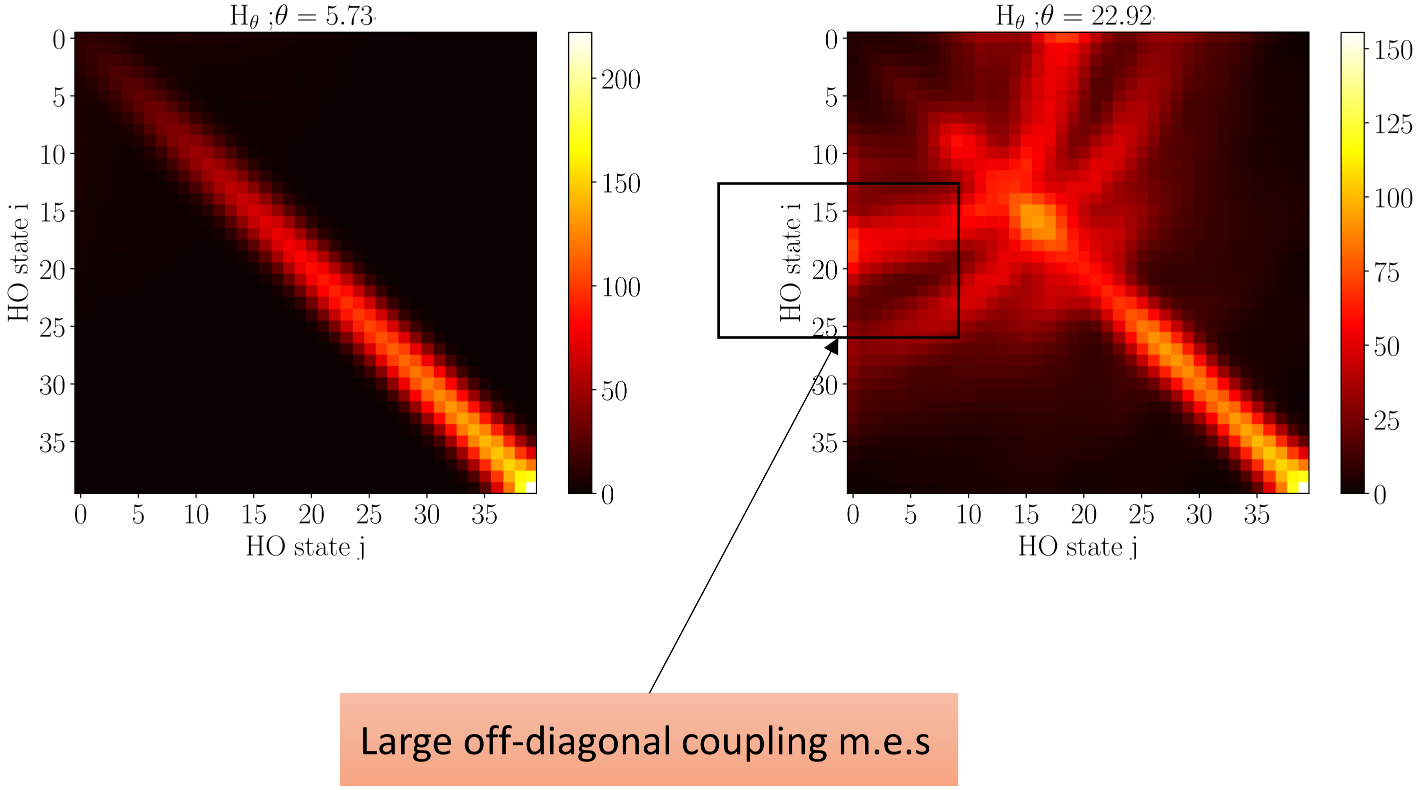


Spatially extended but exponential fall off

Boundary limit problem

Bound state problem

A=2 Hamiltonian matrix elements with complex values*



Maximum model space achievable $N_{\max}$~200 (100 nodes a box in excess of 20 fm)

- The contour deformation from complex scaling induces a large off-diagonal couplings;
- The latter is a no-go theorem for many-body practitioner as it implies slow UV convergence.

* The absolute value of the elements are shown

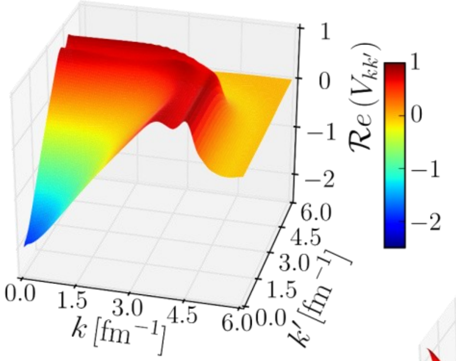
E. D. Jurgenson, P. Navrátil, R. J. Furnstahl PRL103 (2009); PRC83 (2011)

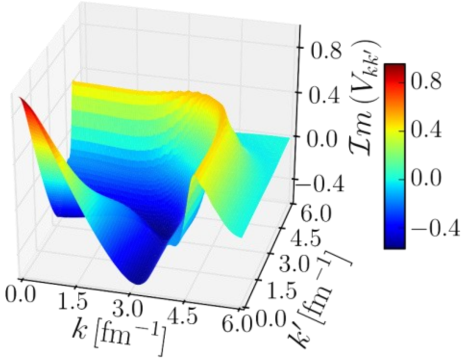
In configuration interaction methods we need to soften interaction to address the hard core. We use the Similarity-Renormalization-Group (SRG) method

$$H_\lambda(\theta) = U_\lambda H(\theta) U_\lambda^T$$

Similarity Transformation

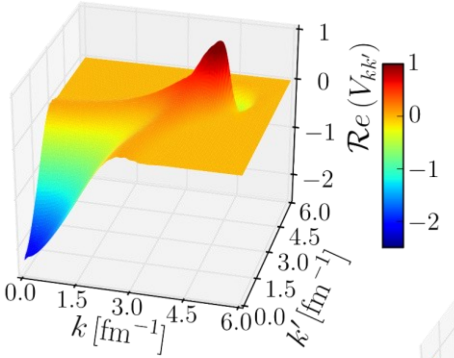
$$\begin{cases} \dfrac{dH_\lambda(\theta)}{d\lambda} = -\dfrac{4}{\lambda^5}[\eta(\lambda), H_\lambda(\theta)] \\ \eta(\lambda) = \dfrac{dU_\lambda}{d\lambda} U_\lambda^T \end{cases}$$

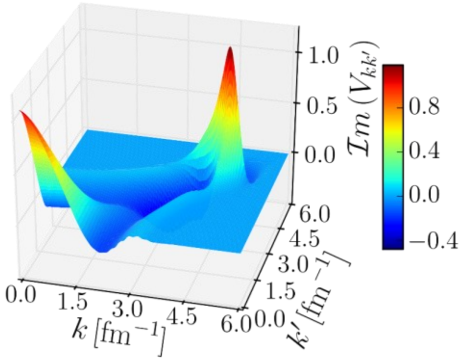




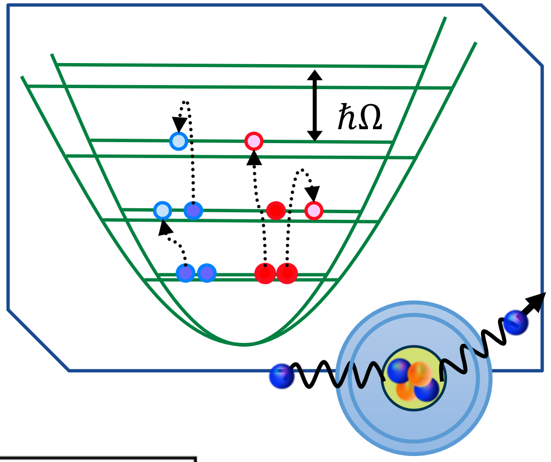
Evolution with flow parameter λ

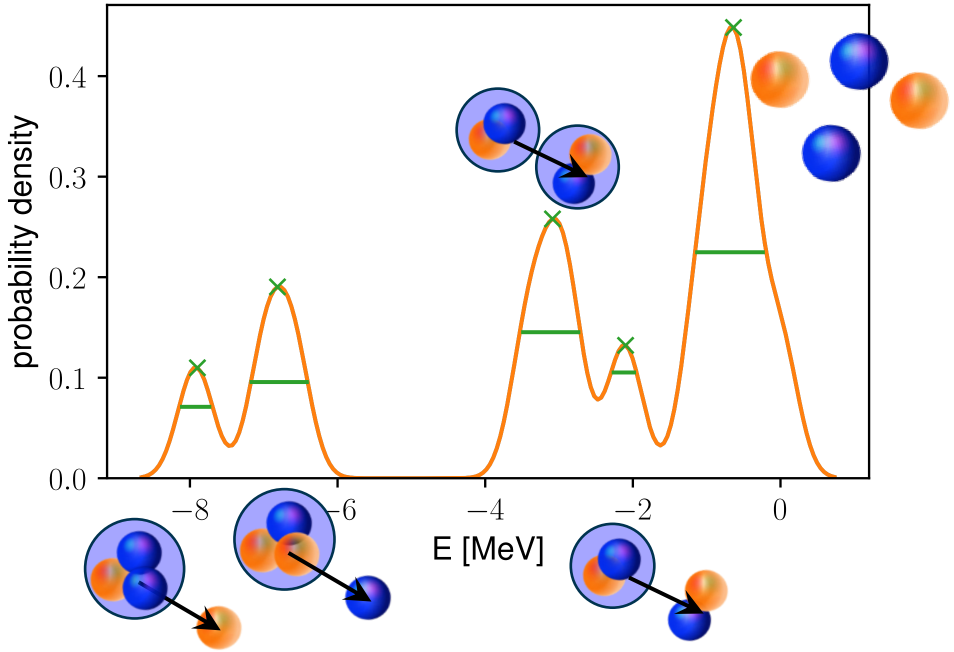
Consistent evolution of the imaginary part

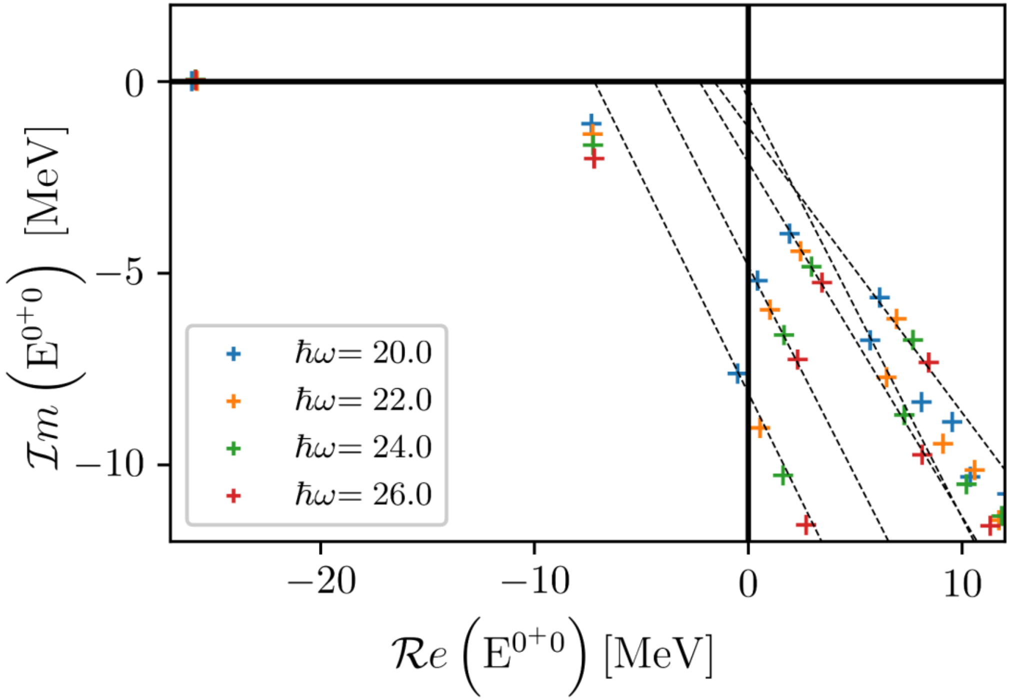




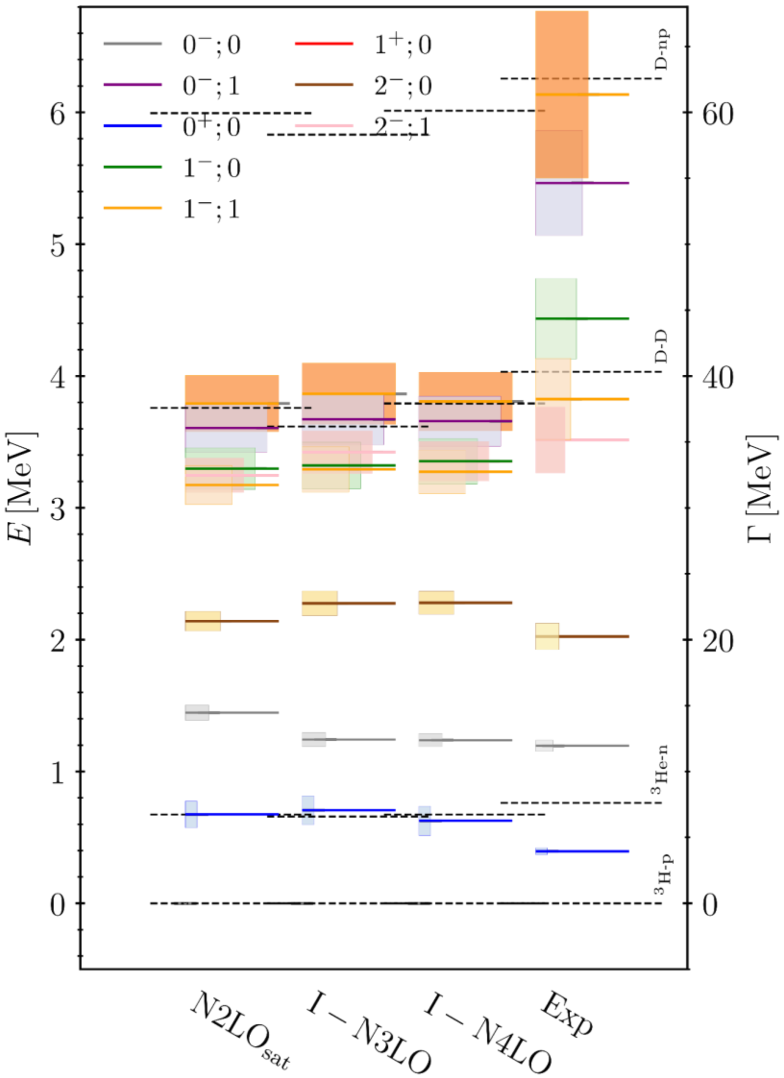
This analysis is made without the induced 3bdy force because of the numerical cost.

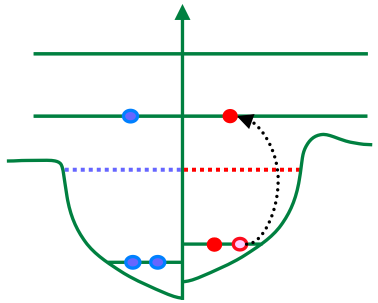


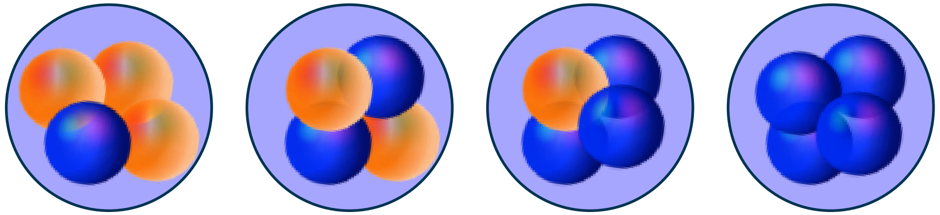




- The expected threshold are somewhat recovered w.r.t. experiments;
- Threshold energies do not converge at the same pace as the g.s.





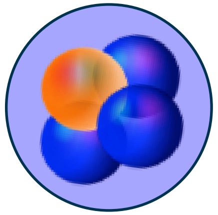


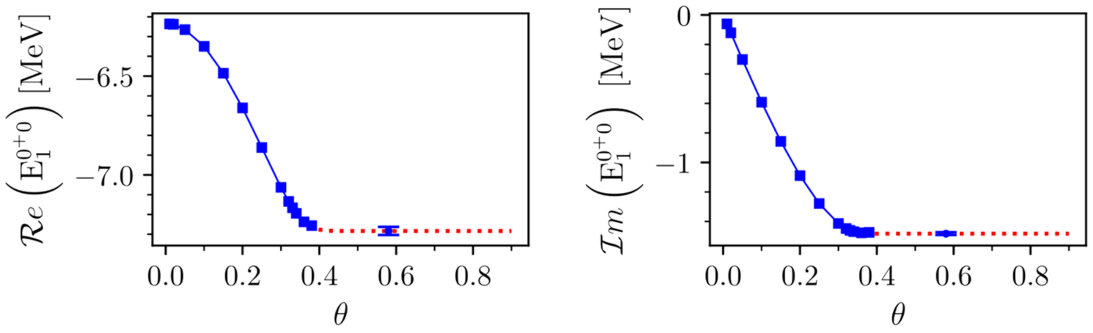
^{4}Li, ^{4}He, ^{4}H and 4n

$J^\pi;T$	E_r [MeV]	$\epsilon_{N_{max}}$	ϵ_θ	Γ_r	$\epsilon_{N_{max}}$	ϵ_θ	R-matrix		Δ
							E_r	Γ_r	
$0^+;0$	0.40	−0.04	−0.43	2.00	−0.79	−0.80	0.391	0.50	0.75
$0^-;0$	1.31	+0.03	−0.52	1.20	−0.38	+0.02	1.199	0.84	0.85
$2^-;0$	1.98	+0.02	−0.28	1.60	−0.45	+0.04	2.09	2.01	2.25
$1^-;1$	2.93	−0.16	$\gtrsim -1$	3.36	−0.80	+0.52	3.829	6.20	3.66
$1^-;0$	3.21	−0.11	$\gtrsim -1$	3.94					
$2^-;1$	3.02	−0.31	$\gtrsim -1$	3.00					
$0^-;1$	3.37	−0.15	$\gtrsim -1$	4.20					
$1^-;1$	3.45	−0.48	$\gtrsim -1$	4.89					

Careful extrapolation techniques need to be designed;
Proof of principle that the CS-Hamiltonian is accurate and can be used in NCSM calculation up to $A \sim 16$;

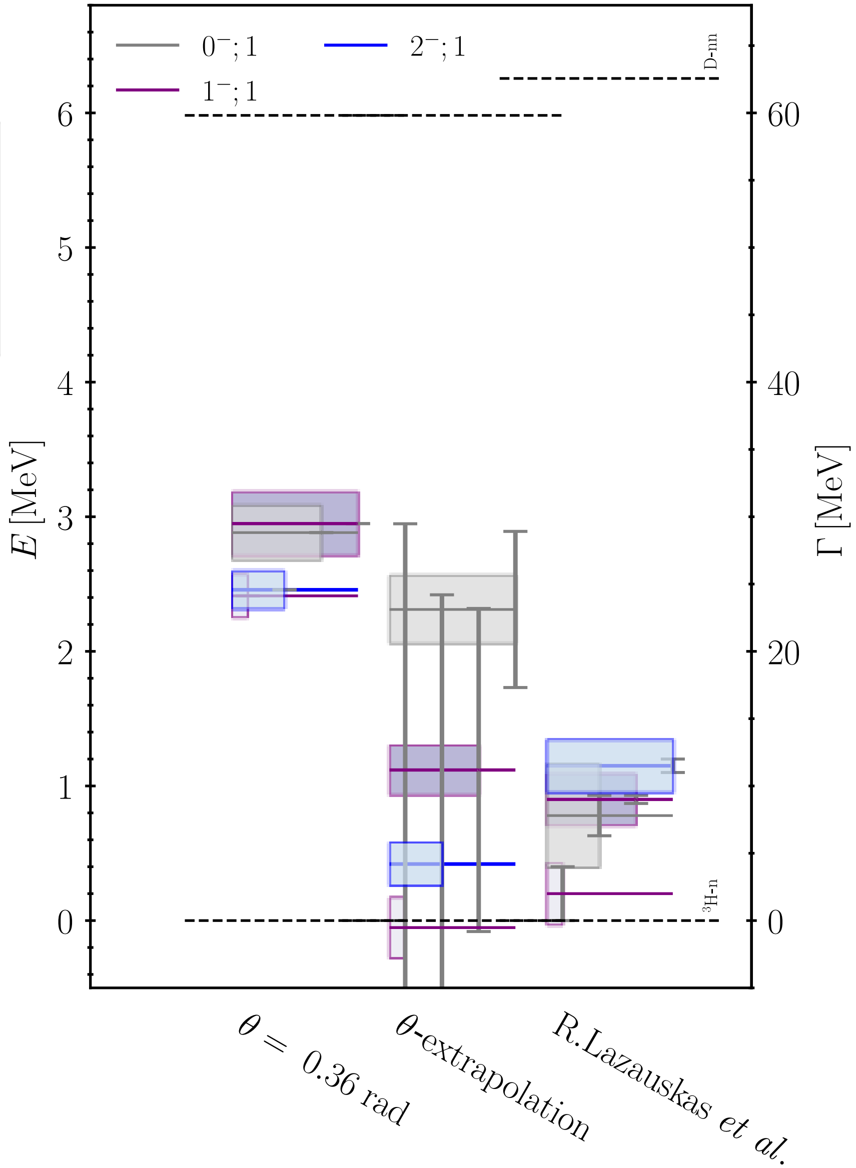
- Discrepancies with experiments too large to be corrected by 3N forces;





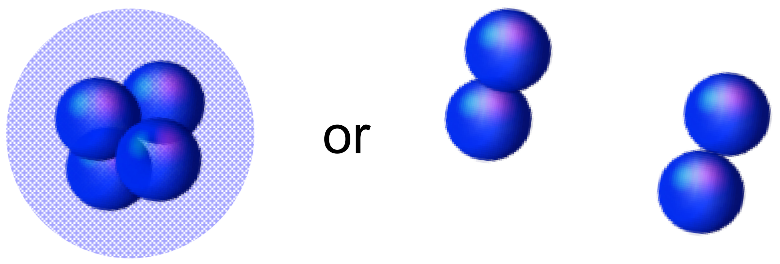
We compare with a calculation based on solving the Faddeev equations.

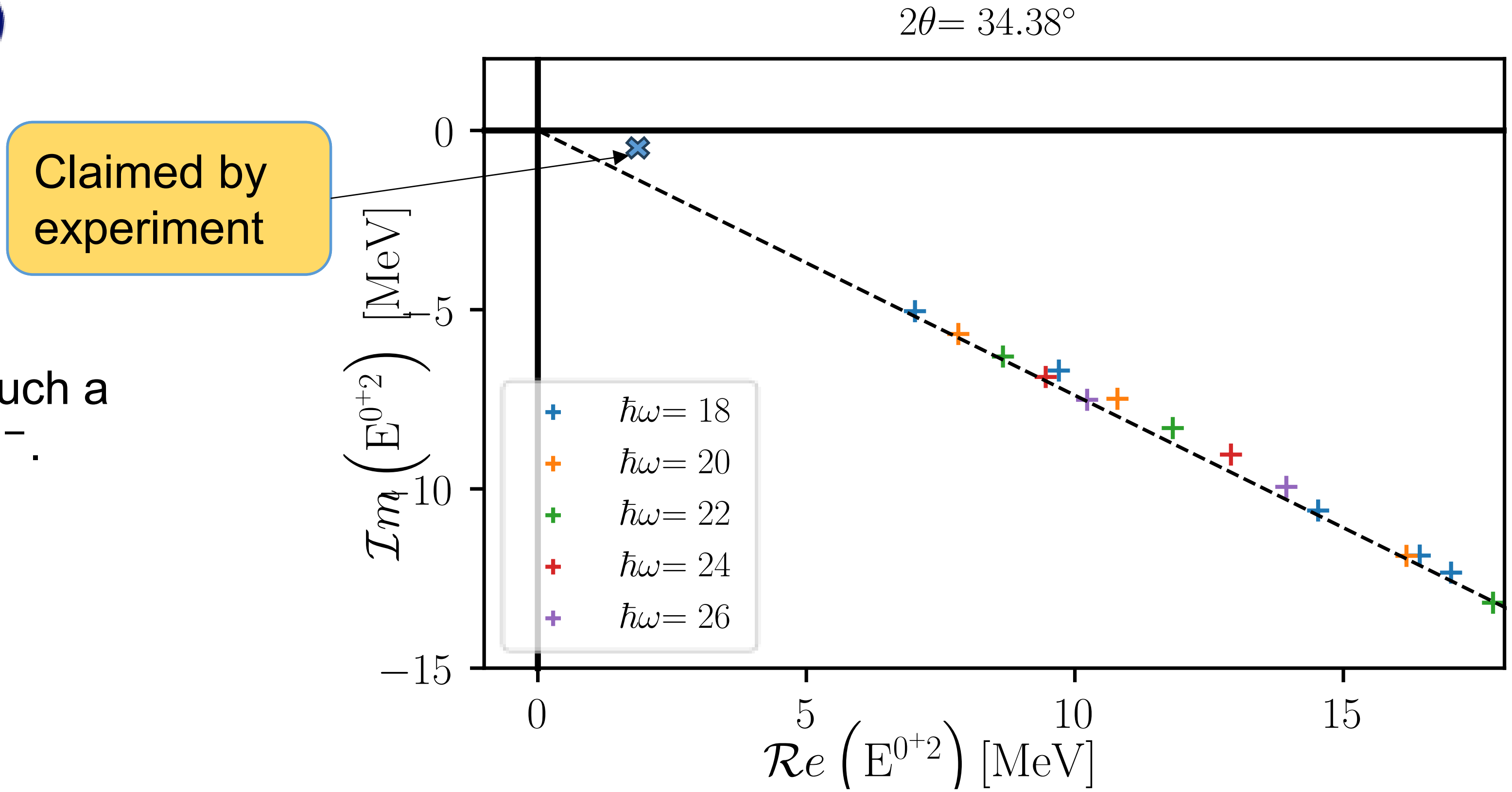
Deltuva & Lazauskas, 2019, PRC



We perform a naïve extrapolation wrt to the CS rotation angle θ.

We find an overall agreement of the calculating with the exact solution (up to 500 keV bias due to the extrapolation).





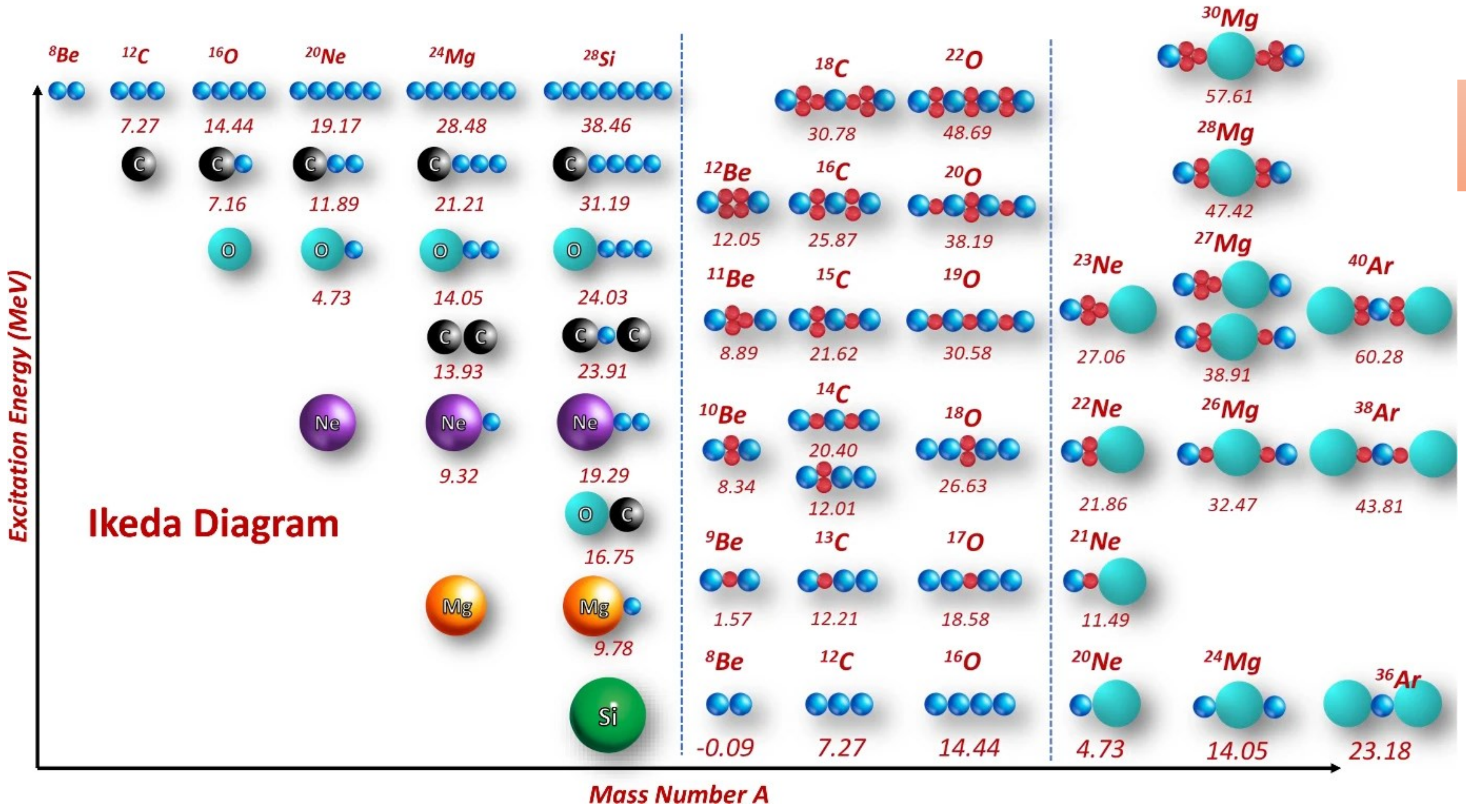
CS shows no indication of such a resonance in 1^+, 1^-, 0^+ or 0^-.

Lower bound of :

$$\Gamma_r = 1.9\, E_r$$

or :

$$\Gamma_r = 4.5\, MeV$$


Ikeda Diagram
Excitation Energy (MeV)
Mass Number A
⁸Be
¹²C
¹⁶O
²⁰Ne
²⁴Mg
²⁸Si
7.27
14.44
19.17
28.48
38.46
7.16
11.89
21.21
31.19
4.73
14.05
24.03
13.93
23.91
9.32
19.29
16.75
9.78
¹⁸C
30.78
²²O
48.69
¹²Be
12.05
¹⁶C
25.87
²⁰O
38.19
¹¹Be
8.89
¹⁵C
21.62
¹⁹O
30.58
¹⁰Be
8.34
¹⁴C
20.40
12.01
¹⁸O
26.63
⁹Be
1.57
¹³C
12.21
¹⁷O
18.58
⁸Be
-0.09
¹²C
7.27
¹⁶O
14.44
³⁰Mg
57.61
²⁸Mg
47.42
²⁷Mg
38.91
²³Ne
27.06
⁴⁰Ar
60.28
²²Ne
21.86
²⁶Mg
32.47
³⁸Ar
43.81
²¹Ne
11.49
²⁰Ne
4.73
²⁴Mg
14.05
³⁶Ar
23.18

Thank you！