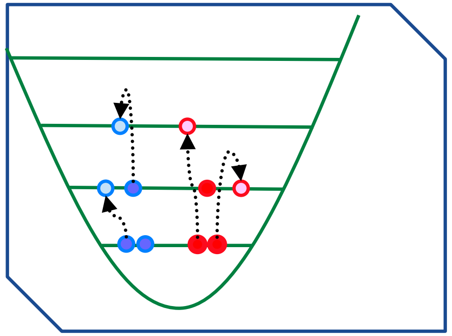
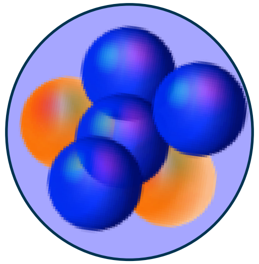
Guillaume Hupin, CNRS IJClab



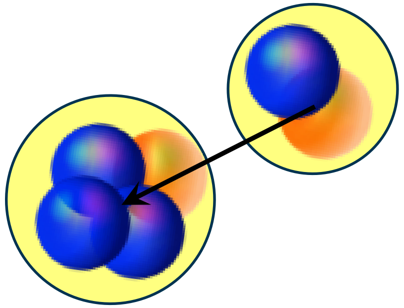


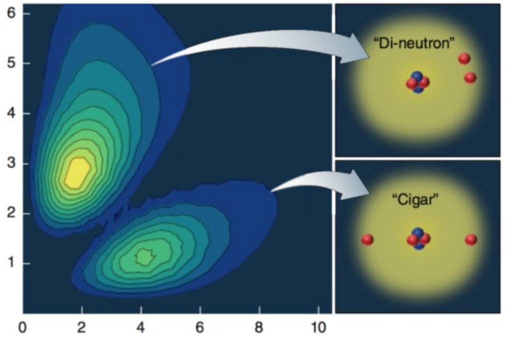
Collaborators

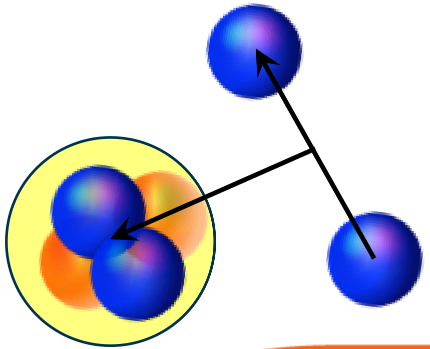
M. Aliotta (Edin)
K. Becker (Edin)
A. Dehghani (ULB)
P. Indelicato (LKB)
P. Navratil (TRIUMF)
S. Quaglioni (LLNL)
And a few others!
(PhD work of O. Yaghi, private sector)

Microscopic continuum physics: explicit channels and/or complex scaling?

NCSMC & NCSM Complex scaling







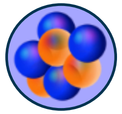
B.R. Barrett, P. Navrátil, J.P. Vary, J.P. Progr. Part. Nucl. Phys. 69 (2013)

One way to solve the many-body problem

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha}\, |A\alpha j_z{}^{\pi} t_z\rangle \quad \Longleftrightarrow \quad |A\lambda J^{\pi} T\rangle_{SD}\, \phi_{00}(\vec{R}^{A}_{c.m.})$$

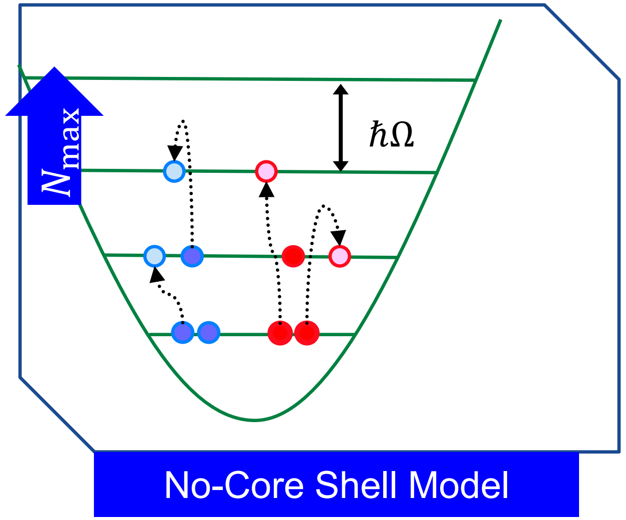
Mixing coefficients(unknown)

A-body harmonic oscillator states



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 derive s.p. to Jacobi coordinates transformation.
3. HO matrix elements can be transformed analytically between coordinate and momentum space
4. Localized HO basis → no explicit scattering asymptotics

S. Quaglioni, P. Navrátil PRL101 (2008).

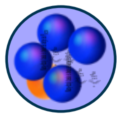
One way to solve the many-body problem when two scales appear

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

Mixing coefficients(unknown)

A-body harmonic oscillator states

$\Leftrightarrow$



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

Second quantization

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

Long-distance organization in the nuclear $|\Psi^A\rangle$

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

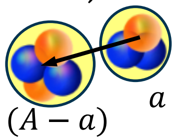
Relative wave function (unknown)

Antisymmetrizer

Channel basis

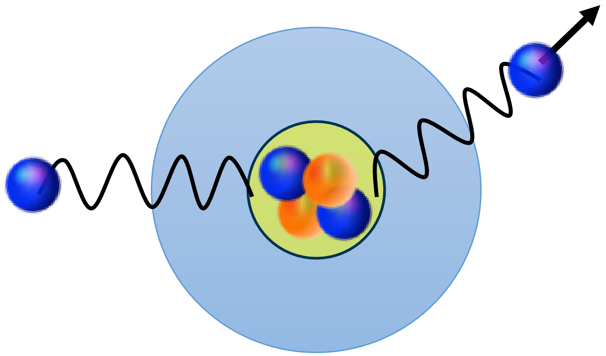
$\Leftrightarrow$

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



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

Cluster expansion technique



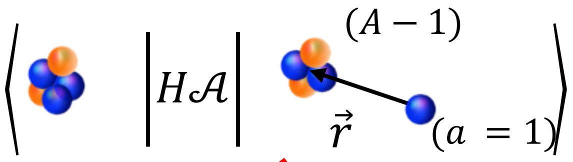
Many-body basis is twice as large as Ψ_{NCSM}

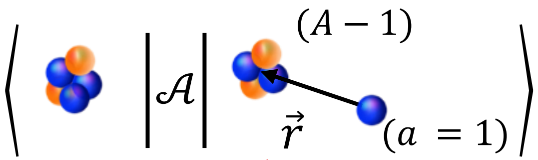
- $\psi^{(A-a)}_{\alpha_1} \in \mathcal{H}^{N_{\max}}$
- $\psi^{(a)}_{\alpha_2} \in \mathcal{H}^{N_{\max}}$

NCSM/RGM formalism for elastic/inelastic

NCSMC couples localized many-body states to explicit reaction channels

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

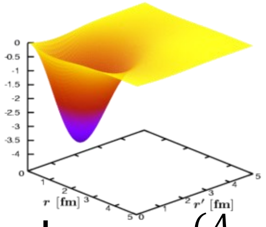


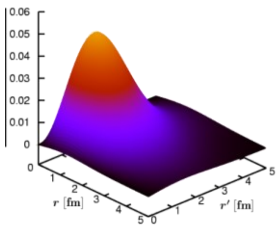


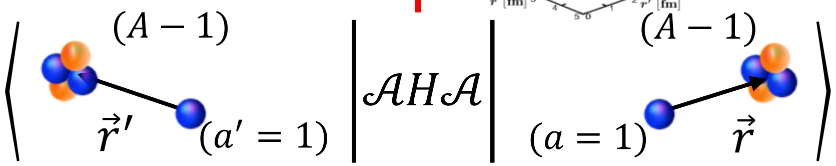
$E_\lambda \, \delta_{\lambda\lambda'}$

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

The coupling kernels play the role of microscopic reaction form factors.



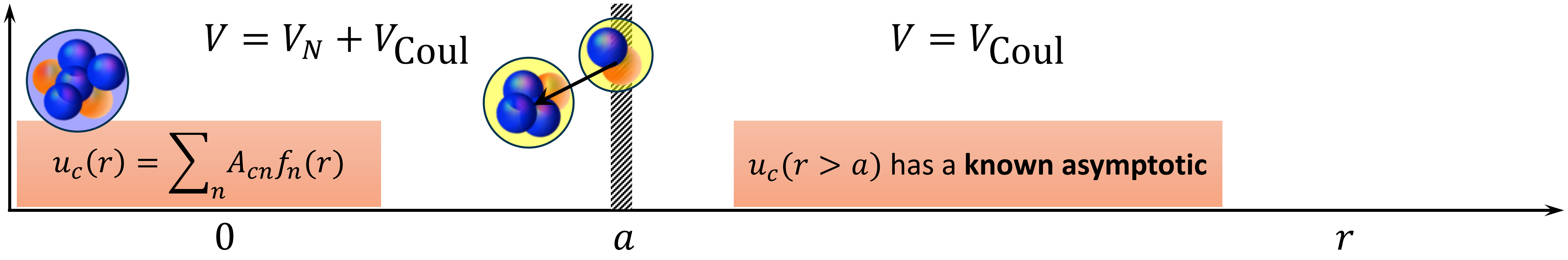




Scattering matrix (and observables) are obtained from matching to known asymptotic solutions using a scattering solver.

Internal region

External region



Decomposition on a Lagrange mesh.

NCSMC can be cast as Bloch-Schrödinger equation:

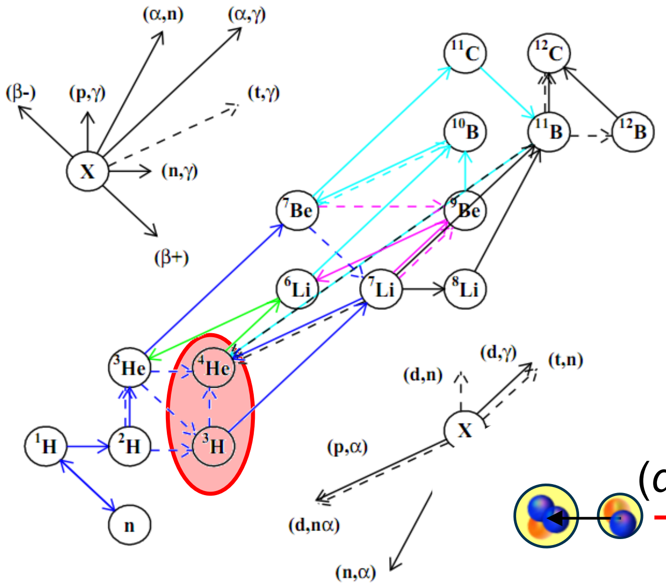
$$(C - EI)\vec{X} = Q(B)$$

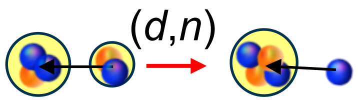
And solved using R-matrix, which in the eigen basis of $C - EI$ reads:

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

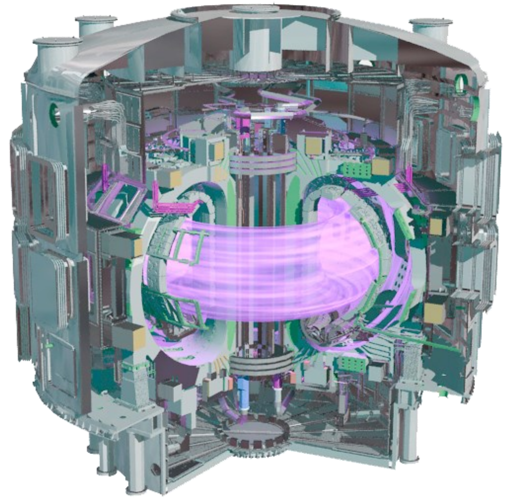
Explicit asymptotics are straightforward for binary channels, but become increasingly difficult for many-body breakup.

Primordial Nucleosynthesis (blue)

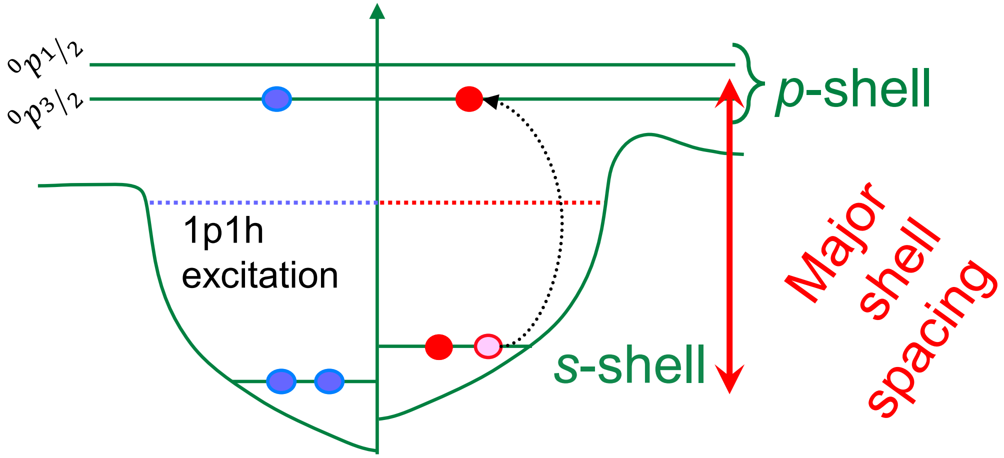




ITER design (Cadarache, France)

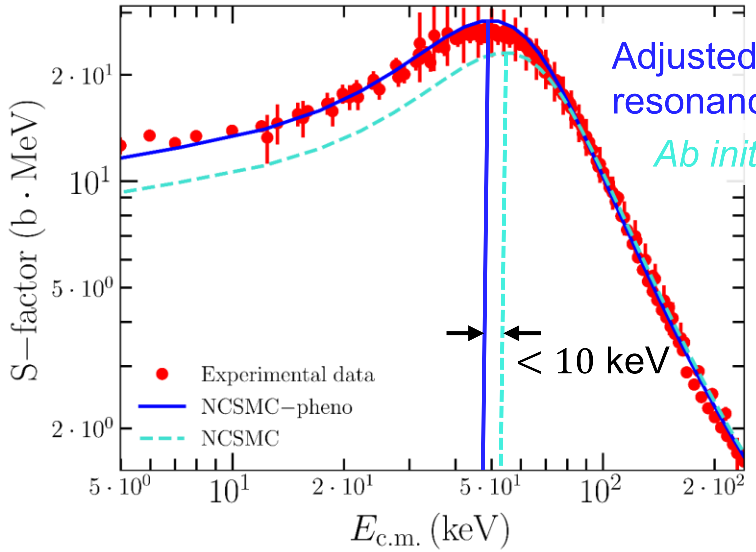


Structure of the ^{5}He $^3/_2{}^+$ resonance

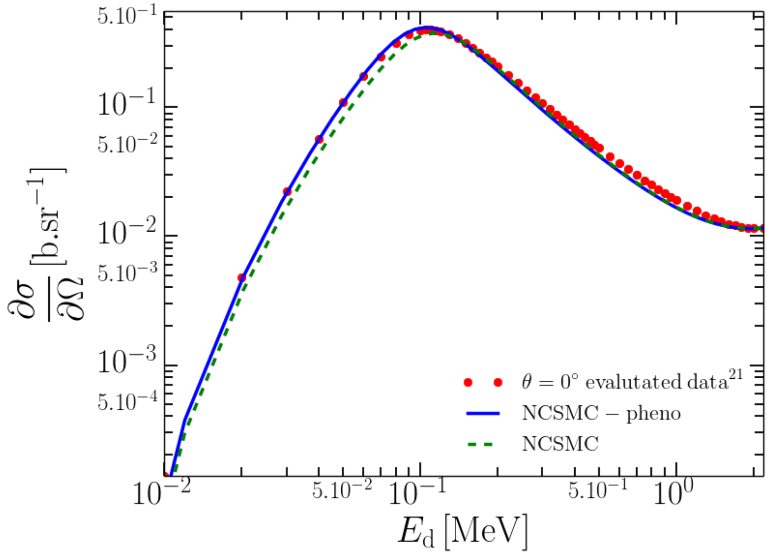


The low-energy fusion rate is controlled by a near-threshold resonance whose structure requires cross-shell configurations.

S-factor: computed and data



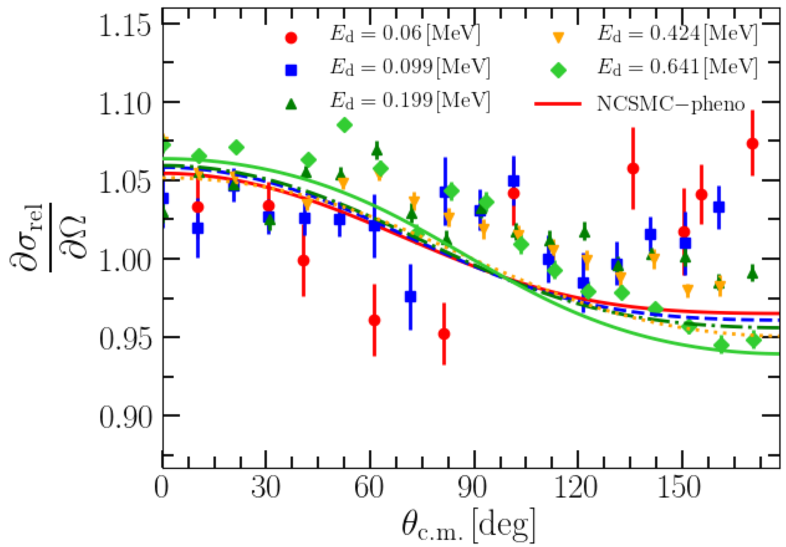
Angular distribution at $\theta = 0^\circ$

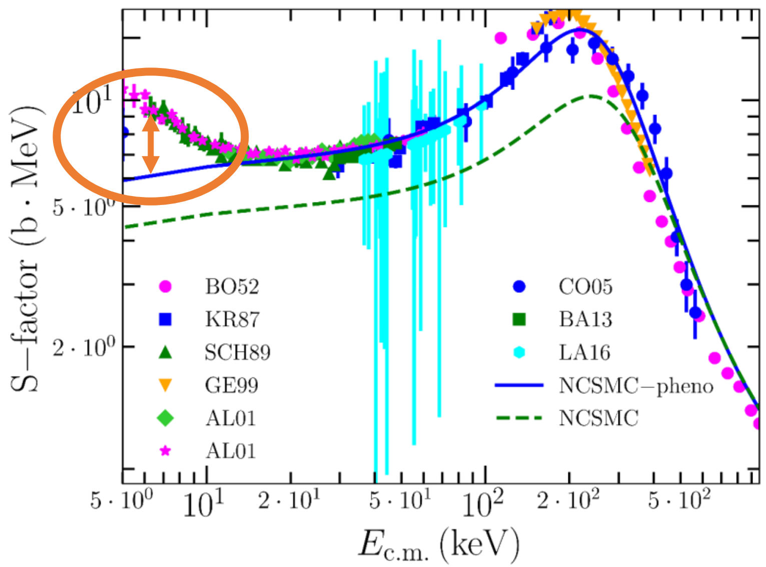


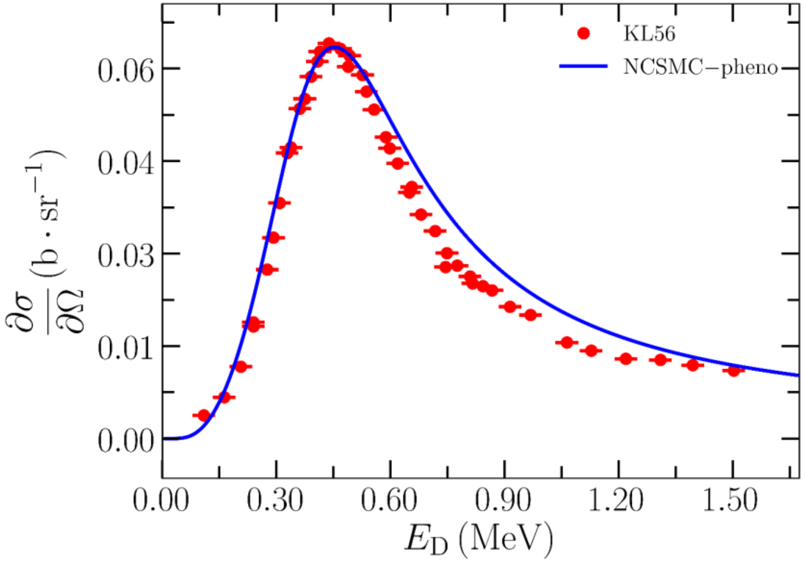
M. Drosg and N. Otuka, INDC(AUS)-0019 (2015).

- The S-factor is globally well reproduced;
- a shift of **only a few keV** in the 3/2+ pole strongly affects the low-energy S-factor: the accurate **reproduction** of the **resonance position**/width is **essential;**
- the angular distribution **agrees** with **evaluation**.

^{3}He(d,p)^{4}He fusion reaction: mirror reaction, globally similar to DT

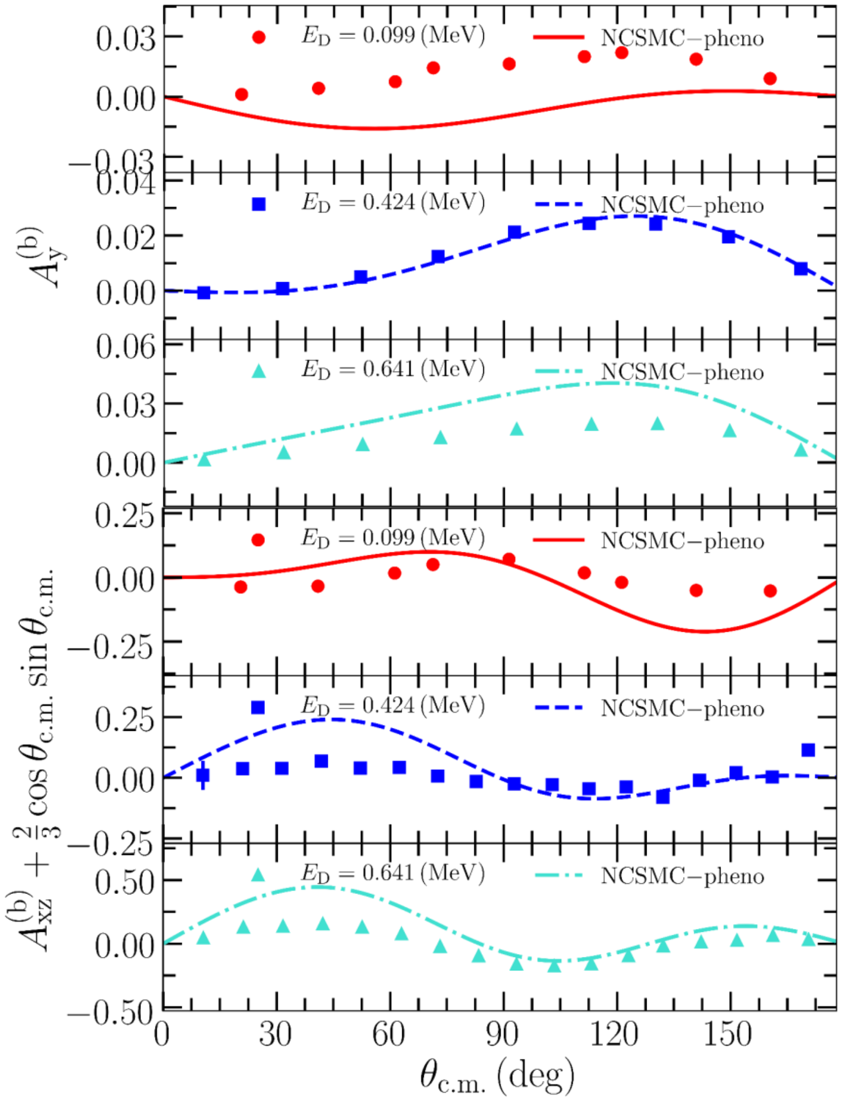


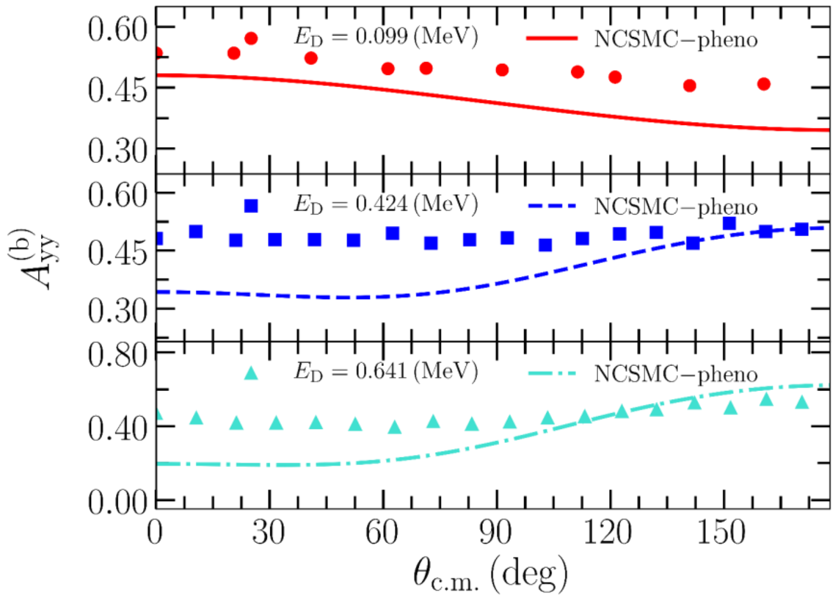




- The S-factor is globally well reproduced;
- However, there are **discrepancies** between data sets around the peak of the S-factor;
- Electron screening gives a significant contribution at the lowest energies.

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





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

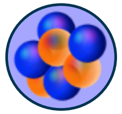
Analyzing tensors are globally reproduced in shape. **Getting a cross section right does not mean the wave function is perfect**.

One way to solve the many-body problem

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

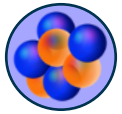
Mixing coefficients(unknown)

A-body harmonic oscillator states



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

Second quantization



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

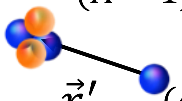
Second quantization

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

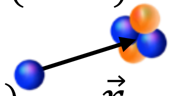
Advantage of HO CI methods:

1. Center of mass is factorized.

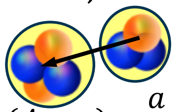
Span the same basis as



$$\left\langle \; {}^{(A-1)} \;\; \vec{r}\,' \;\; (a'=1) \; \middle| \mathcal{A}H\mathcal{A} \middle| \; (a=1) \;\; \vec{r} \;\; {}^{(A-1)} \right\rangle$$



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



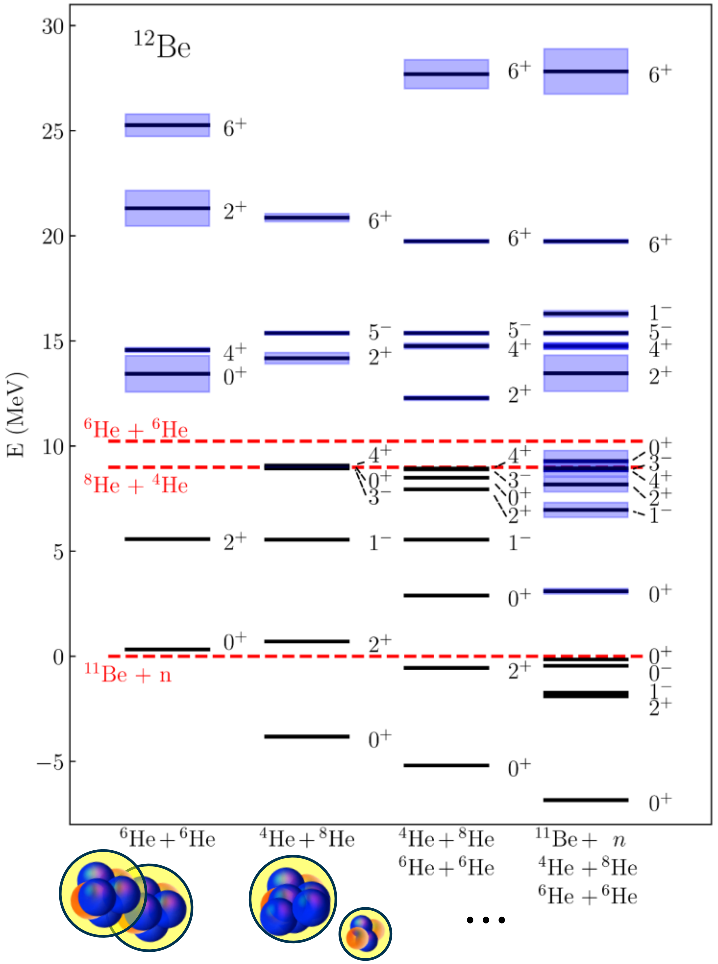
$(A-a)$ $\quad a$

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

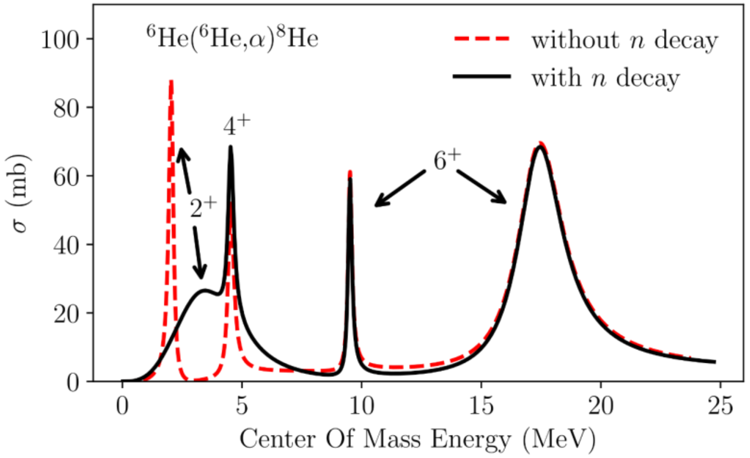
$$\phi^{A}_{n} = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_i(\vec{r}_1) & \dots & \phi_i(\vec{r}_A) \\ \vdots & \ddots & \vdots \\ \phi_l(\vec{r}_1) & \dots & \phi_l(\vec{r}_A) \end{vmatrix} = a^{\dagger}_{l}\dots a^{\dagger}_{i}|0\rangle$$

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

Evolution of ^{12}Be with cluster structure

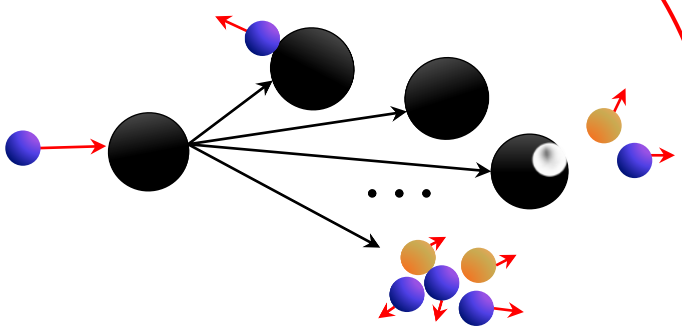


Evidence of channels selectivity



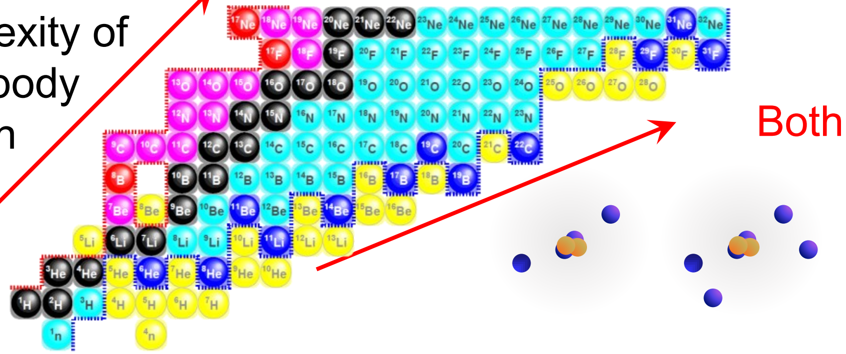
- Coupling to ^{11}Be+n channel reshapes ^{12}Be spectrum.
- Neutron decay strongly influences ^{6}He(^{6}He,α)^{8}He cross section.
- **Helium clustering survives** high above decay thresholds.

Where explicit-channel approaches become difficult



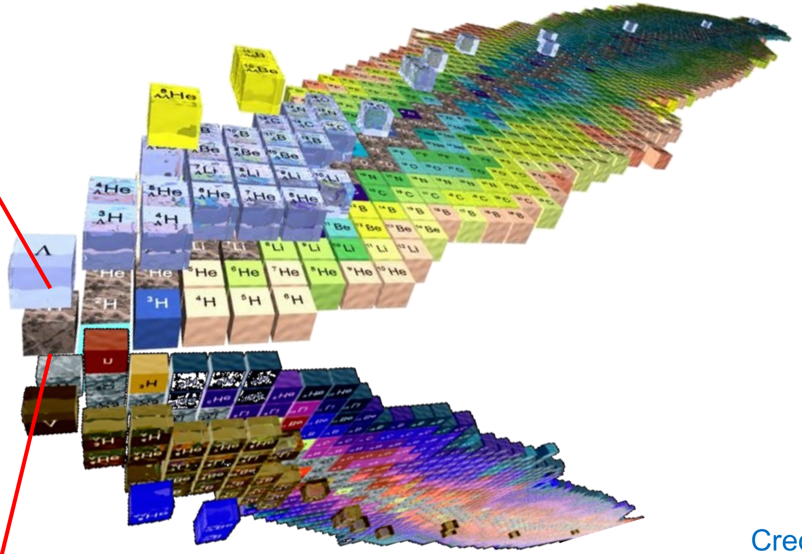
Complexity of scattering problem
clustering in the continuum

Complexity of many-body solution



Both

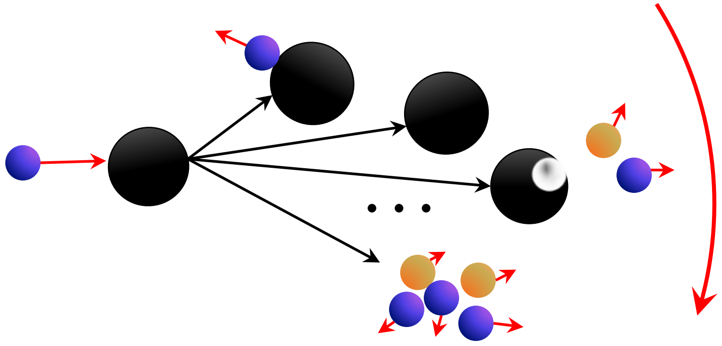
$\neq n, p$ particles interacting with strong force ($M_h \gg M_{n,p}$)
Exotic systems sensitive to clustering



$M_h \leq M_{n,p}$

☹ The challenge shifts from solving the many-body problem to organizing the continuum.

Credits H. Lenske



Complexity of scattering problem
clustering in the continuum

Complexity of many-body solution

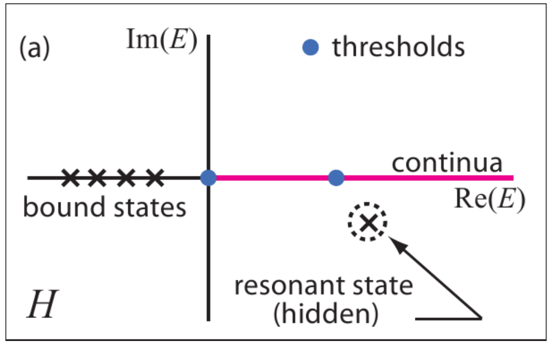
Both

$\neq n,p$ particles interacting with strong force ($M_h \gg M_{n,p}$)
Exotic systems sensitive to clustering

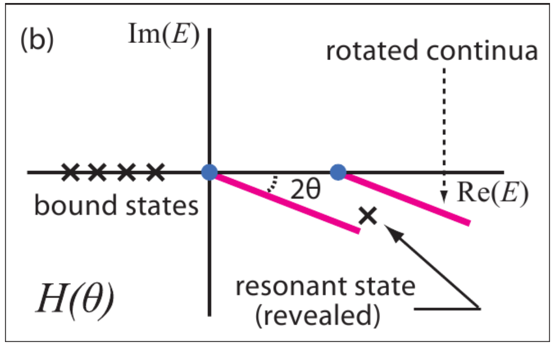
$M_h \leq M_{n,p}$

😐 Can resonance properties be obtained with a bound-state many-body solver?

Credits H. Lenske



Complex scaling



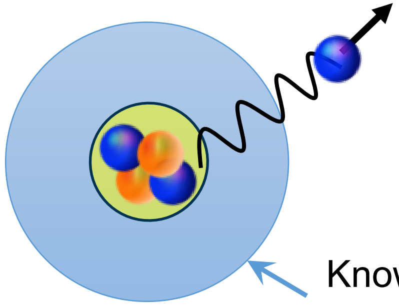
Kruppa *et al.* PRC**89** (2014)

"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.

The continuum rotates by 2θ, whereas an exposed resonance pole is stationary with respect to θ.

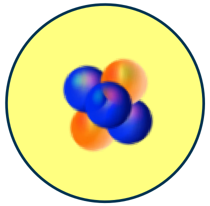
$$\hat{H}(r) = \hat{T} + \hat{V}(r)$$

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



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

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



Spatially extended but exponential fall off

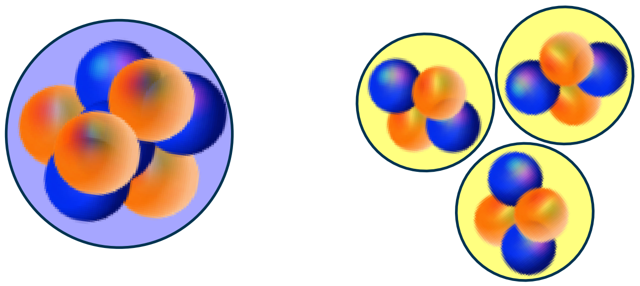
Boundary limit problem

Bound state problem

We want to develop a common framework applicable to both nuclear structure and reactions, to enhance our understanding of the strong force at low energy.

Structure

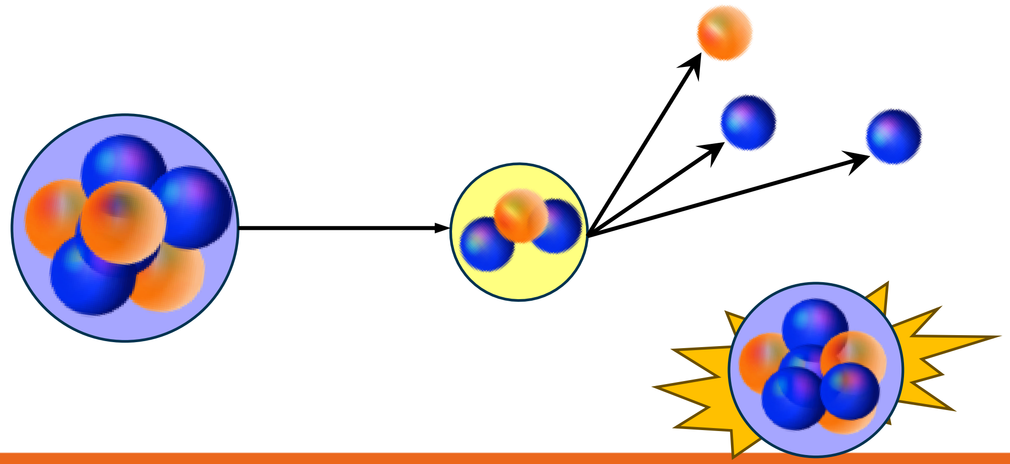
☺ Extraction of resonance properties (overlap function for indication of clustering) for fine tuning interactions and applications to astrophysics.



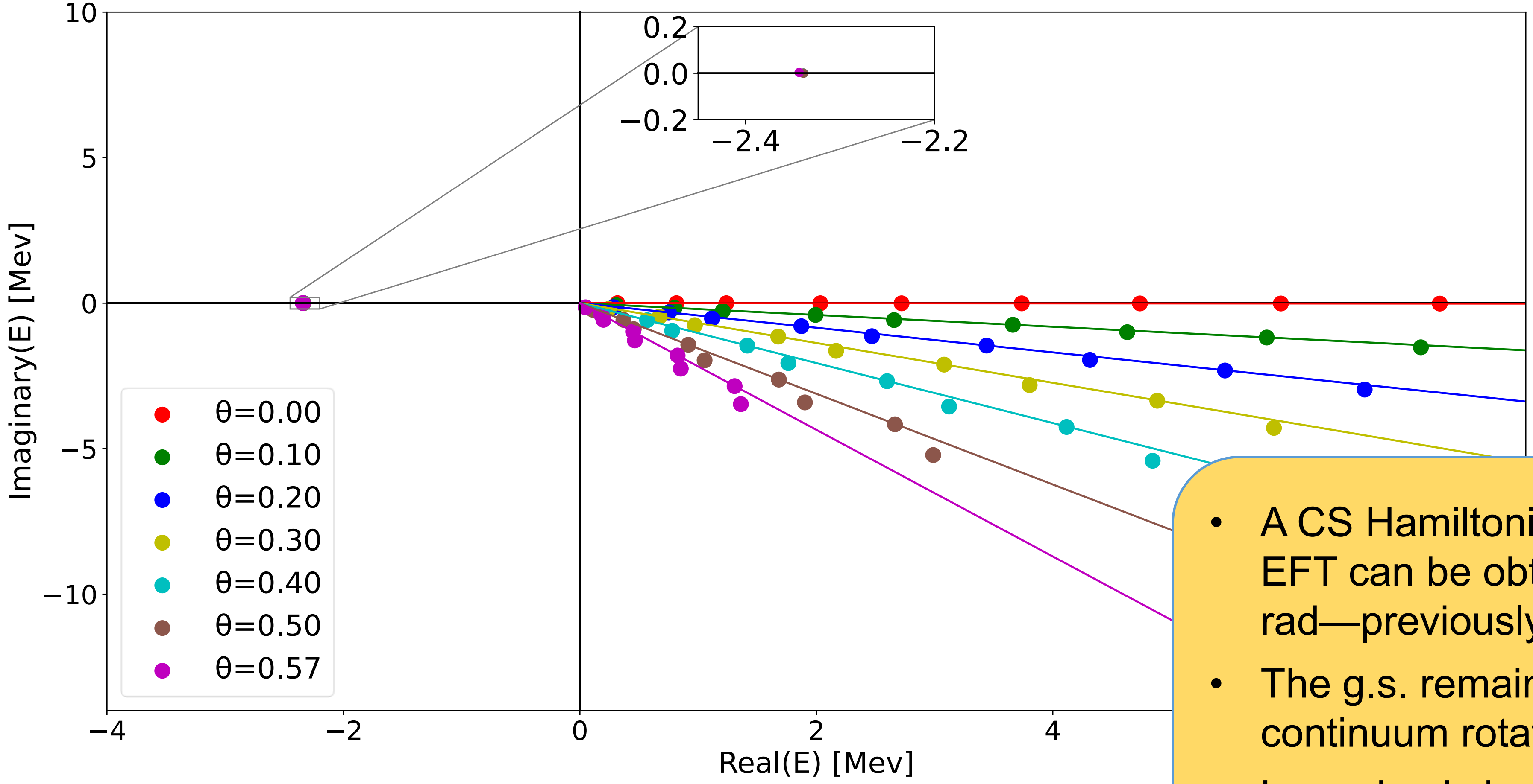
Reactions

☺ Enabling us to study nuclear breakup reactions including Final State Interaction (FSI)

☺ Calculation of complex charged (and multi-neutron) nuclear decay.

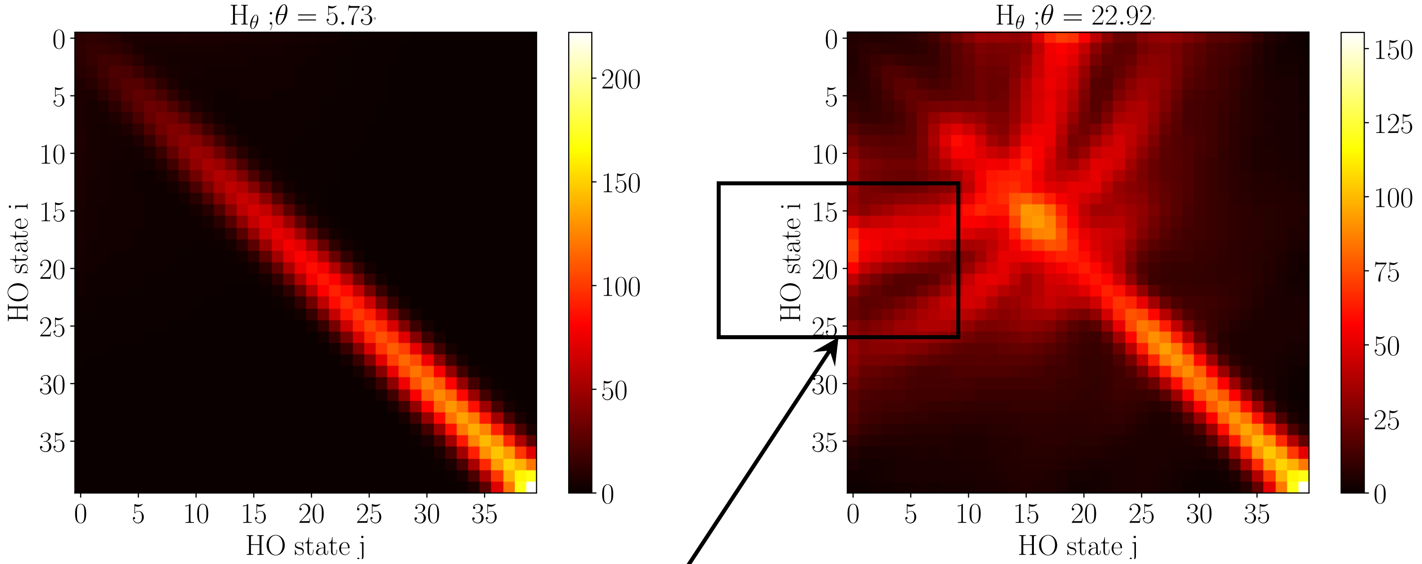


CS Hamiltonian eigenvalues using EM N3LO interaction



- A CS Hamiltonian derived from modern EFT can be obtained up to more than 0.57 rad—previously~ 0.3;
- The g.s. remains fixed and the discretized continuum rotates by 2θ;
- Large basis is required.

$A = 2$ Hamiltonian matrix elements with complex values*



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

Large off-diagonal coupling matrix elements

- The contour deformation from complex scaling induces a large off-diagonal couplings;
- This leads to very slow convergence in the HO basis.

* The absolute value of the elements are shown

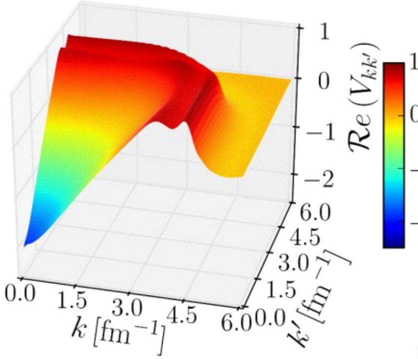
Complex-symmetric SRG restores low-/high-momentum decoupling

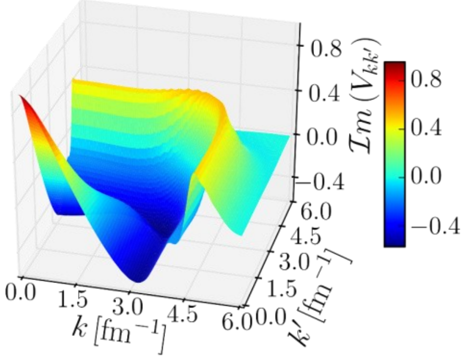
E. D. Jurgenson, P. Navrátil, R. J. Furnstahl PRL103 (2009); PRC83 (2011)

- In CI methods we need to decouple low- and high-momentum components to accelerate convergence. We use the Similarity-Renormalization-Group (SRG) method.
- SRG can be consistently extended to complex-symmetric Hamiltonian (including optical potential)

$$H_\lambda(\theta) = \underbrace{U_\lambda H(\theta) U_\lambda^T}_{\text{Similarity Transformation}}$$

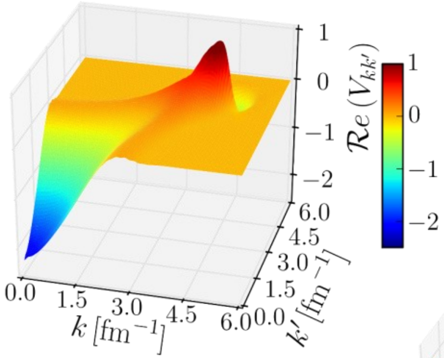
$$\begin{cases} \dfrac{dH_\lambda(\theta)}{d\lambda} = -\dfrac{4}{\lambda^5}[\eta(\lambda), H_\lambda(\theta)] \\ \eta(\lambda) = \dfrac{dU_\lambda}{d\lambda} U_\lambda^T \end{cases}$$

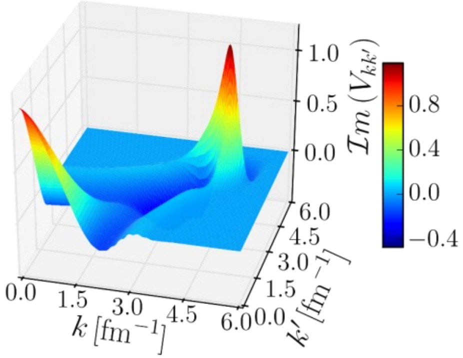




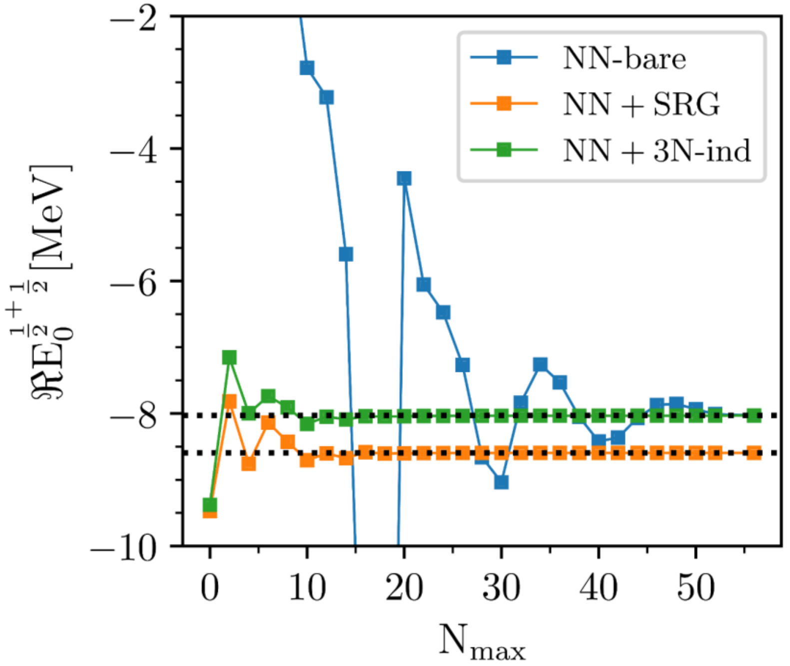
Evolution with flow parameter λ

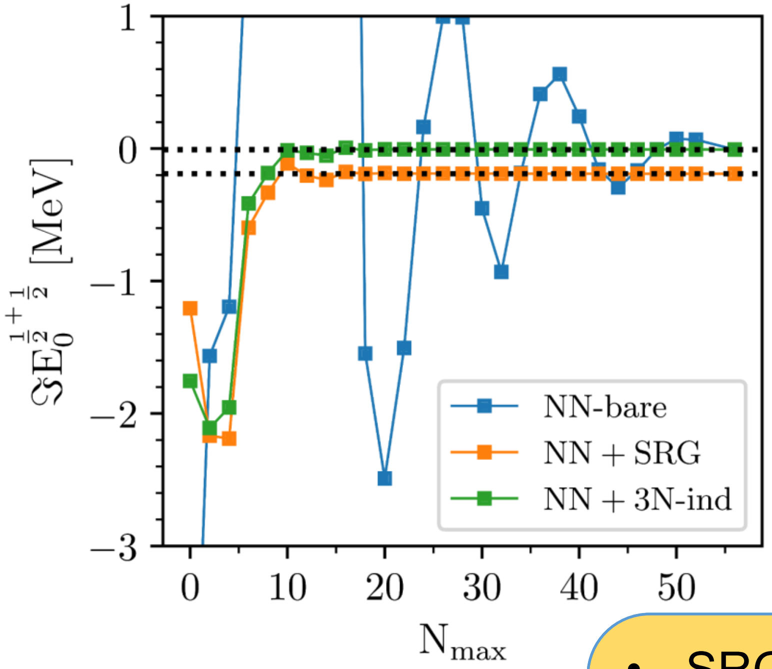
Consistent evolution of the imaginary part

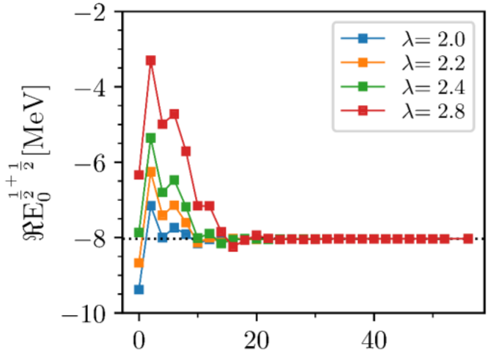


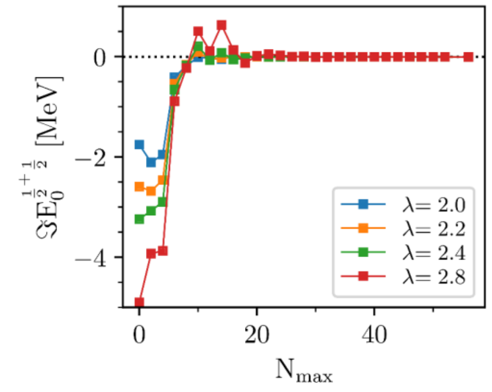


Triton g.s. convergence with CS-Hamiltonian ($\theta = 0.3$ rad)





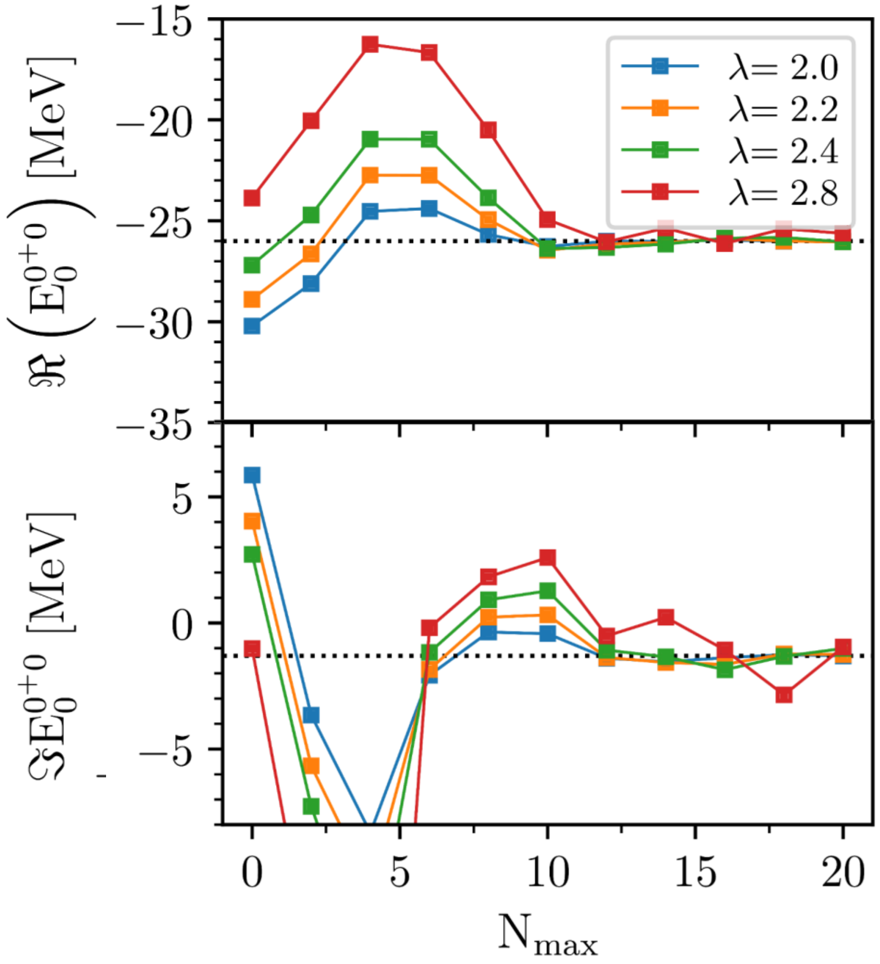


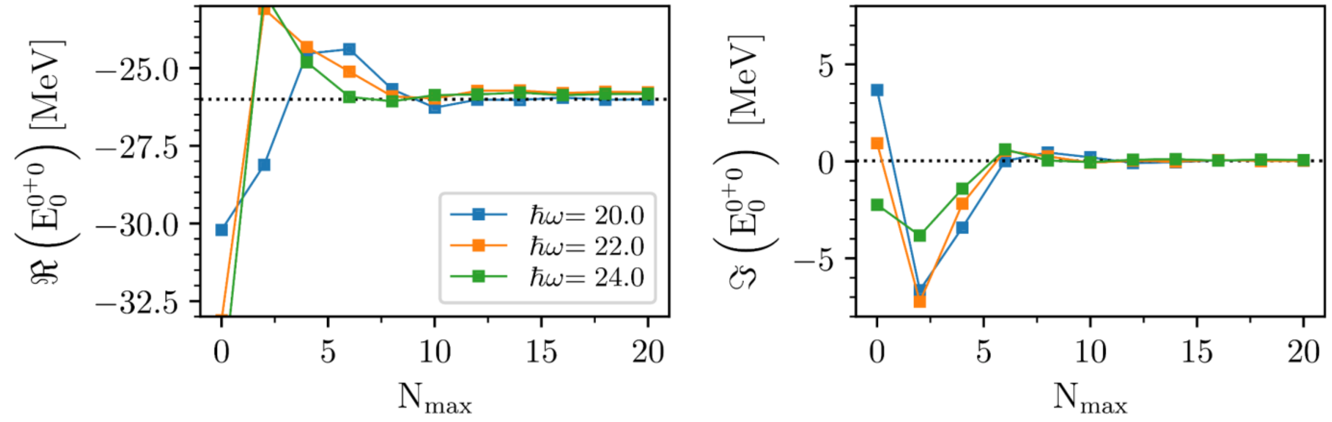


Maximum model space achievable $N_{\max}$~60 (30 nodes a box in excess of 15 fm)

- SRG leads to faster convergence;
- Induced 3N-interaction needs to be accounted for (as expected);
- the imaginary part of the bound-state energy converges back to zero.

α g.s. convergence with CS+SRG NN+3N Hamiltonian ($\theta = 0.3$ rad)



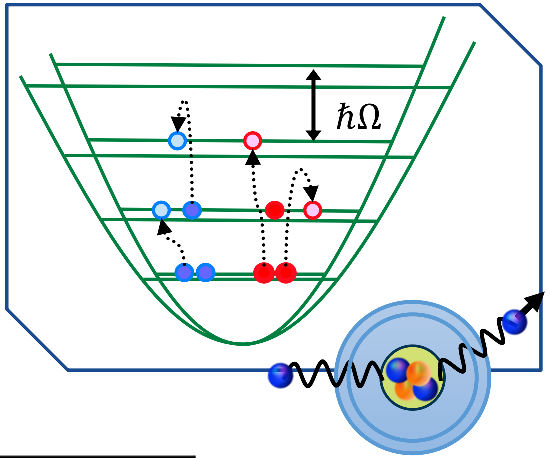


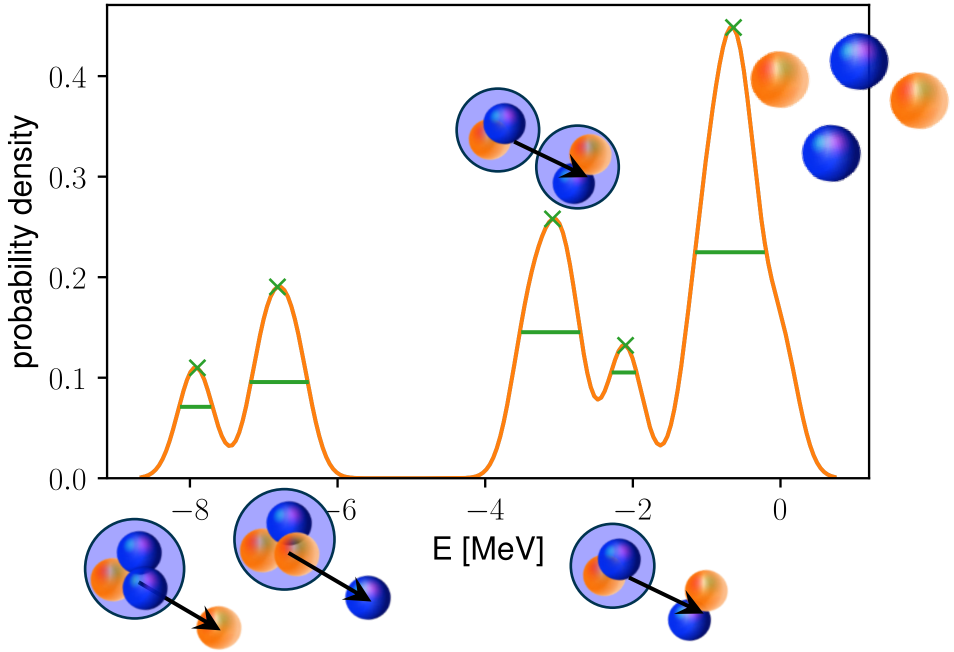
$A = 3$ evolution is made in the maximum model space achievable N_{max}~60

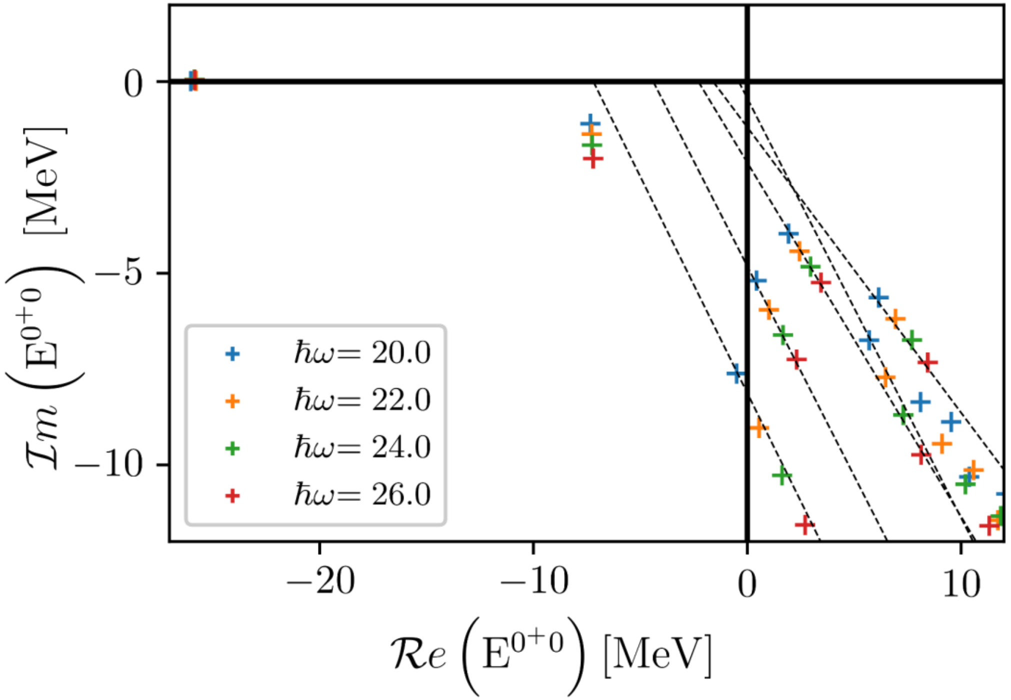
- Induced $A = 4$ appears small at the present accuracy;
- The flow parameter is limited to at best $1.8\ \mathrm{fm}^{-1}$ due to the $A = 3$ CI space needed for the evolution.

Each breakup threshold generates its own rotated continuum

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

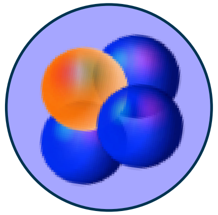


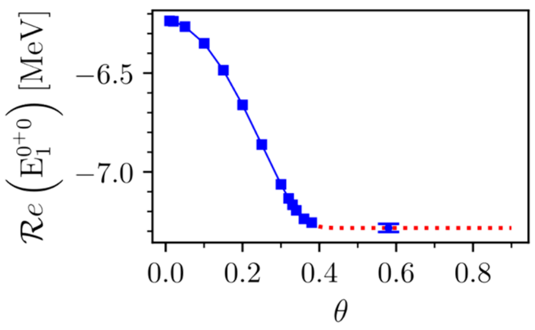


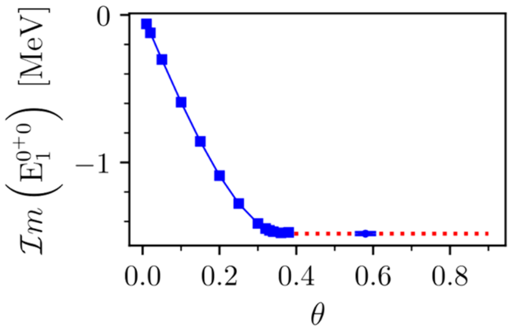


- Each breakup threshold generates its own rotated continuum ray. Therefore, identifying a resonance requires both the pole and the corresponding **theoretical fragment threshold;**
- Fragment thresholds and the A-body state converge at different rates with $N_{\max}$.

CS-NCSM agrees with the ^{4}H Faddeev benchmark within ~ 500 keV



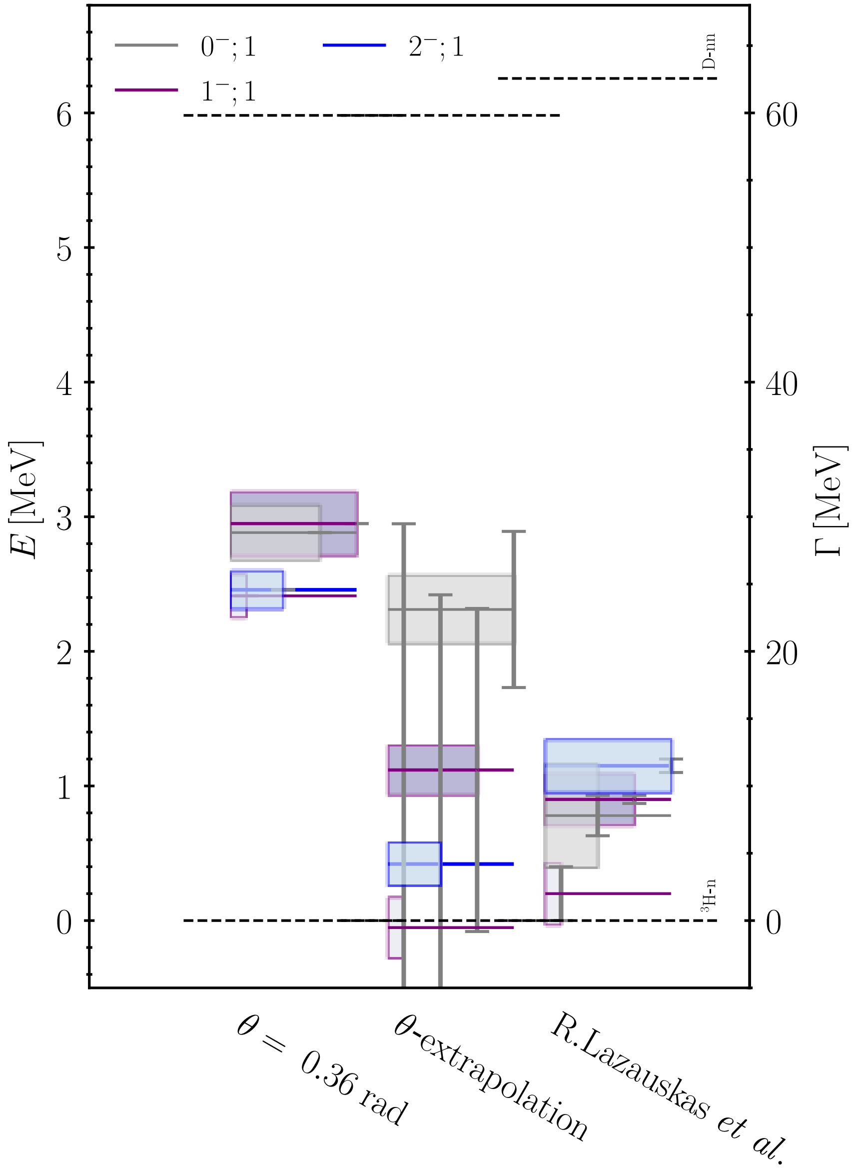


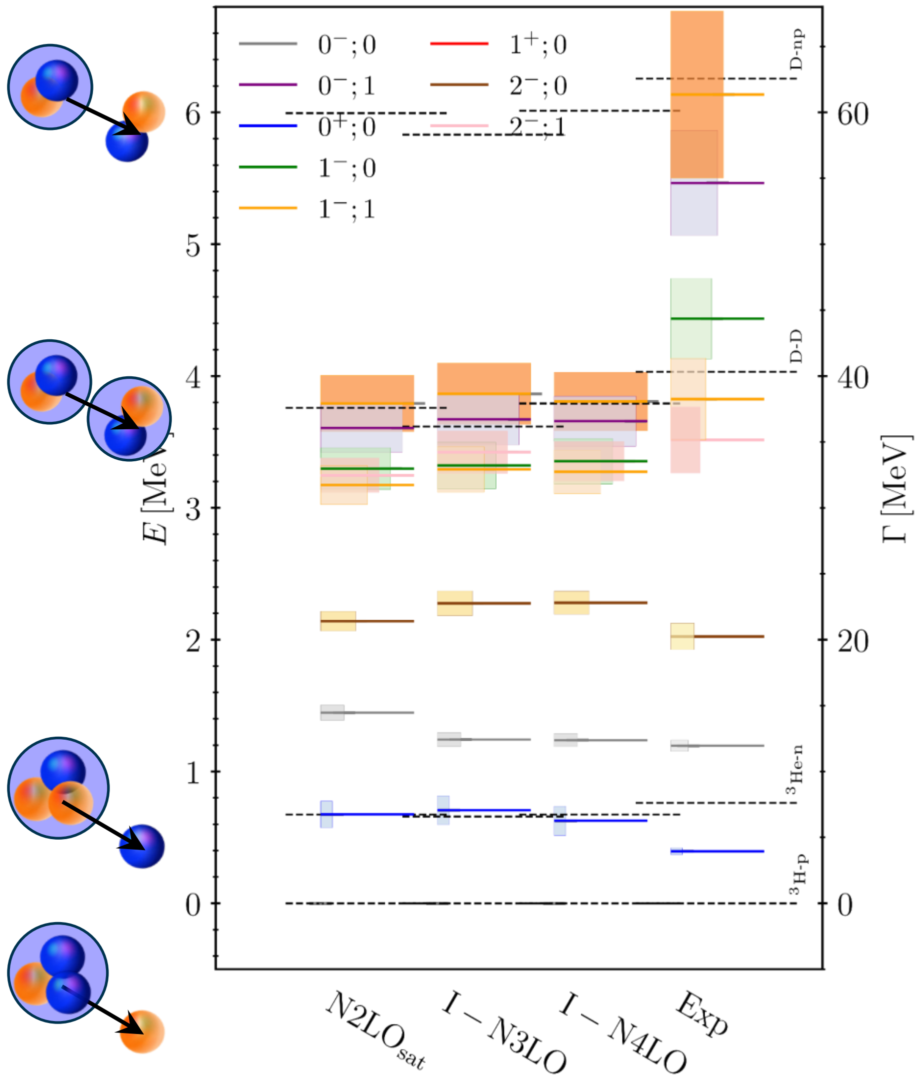


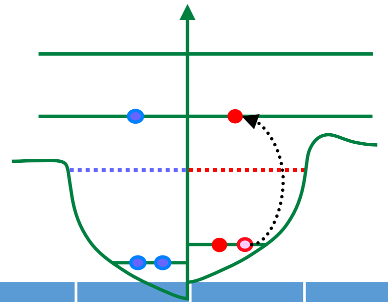
We compare with a calculation based on solving the Faddeev equations.

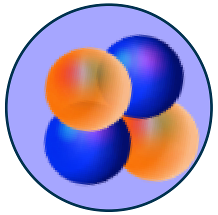
Deltuva & Lazauskas, 2019, PRC

- We perform a naïve extrapolation wrt to the CS rotation angle θ.
- We find an overall agreement of the calculation with the benchmark solution (within about 500 keV bias due to the extrapolation).





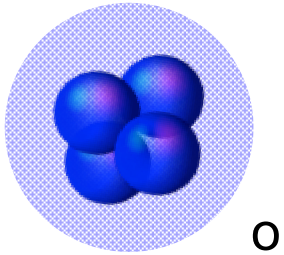




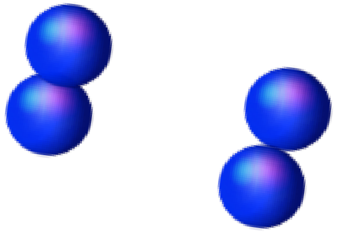
$J^\pi;T$	E_r [MeV]	$\epsilon_{N_{\max}}$	ϵ_θ	Γ_r	$\epsilon_{N_{\max}}$	ϵ_θ	R-matrix		FY, HH, AGS	
							E_r	Γ_r	E_r	Γ_r
$0^+;0$	0.40	−0.04	−0.43	2.00	−0.79	−0.80	0.391	0.50	0.12	0.25
$0^-;0$	1.31	+0.03	−0.52	1.20	−0.38	+0.02	1.199	0.84		
$2^-;0$	1.98	+0.02	−0.28	1.60	−0.45	+0.04	2.09	2.01		
$1^-;1$	2.93	−0.16	$\gtrsim -1$	3.36	−0.80	+0.52	3.829	6.20		

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 $A \sim 16$.

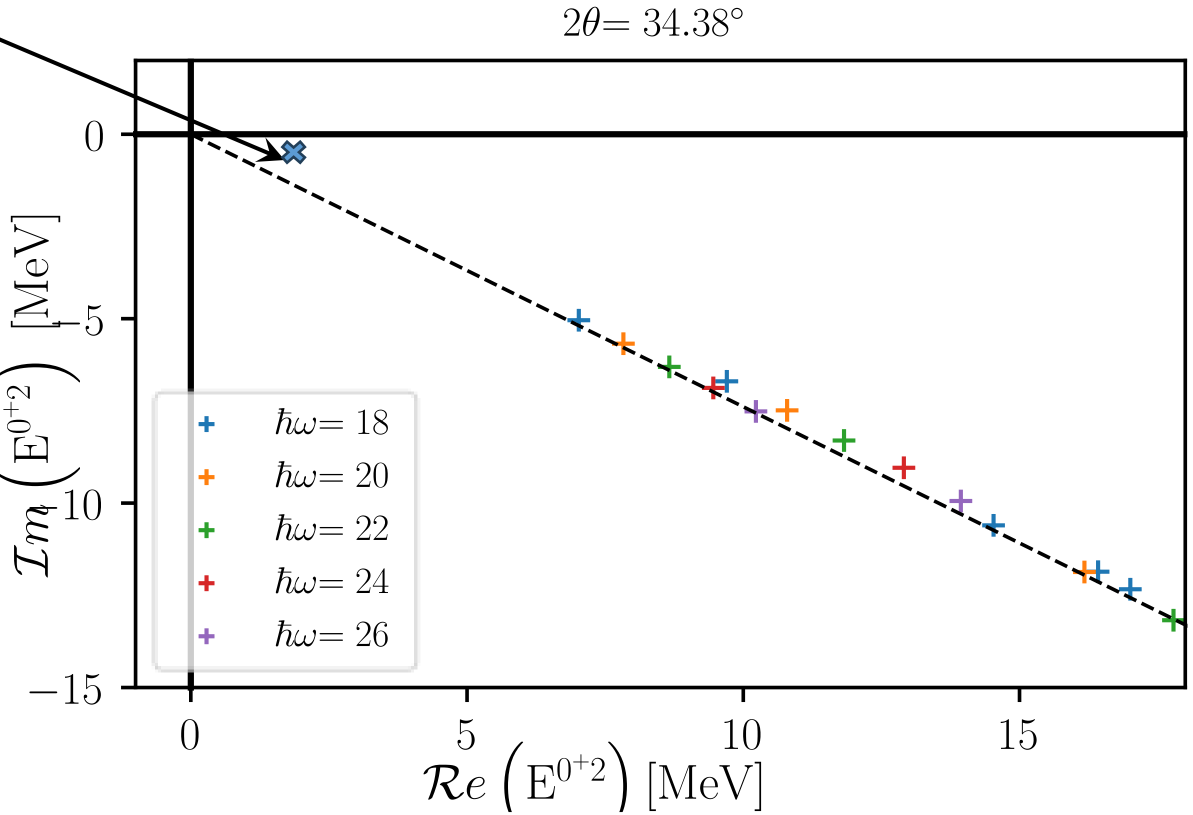
- The remaining discrepancies with experiment are larger than the 3N effects observed in the present calculations;
- Agreement with latest few-body benchmark.



or



Claimed by experiment



Within this Hamiltonian, accessible rotation angles, and the $J^{\pi}T = 1^+, 1^-, 0^+$ or 0^- sectors examined, we find no isolated CS pole compatible with the claimed resonance.

Using the maximum accessible rotation $2\theta_{\max} = 43.5°$, lower bound of :

$$\Gamma_r = 1.9\ E_r$$

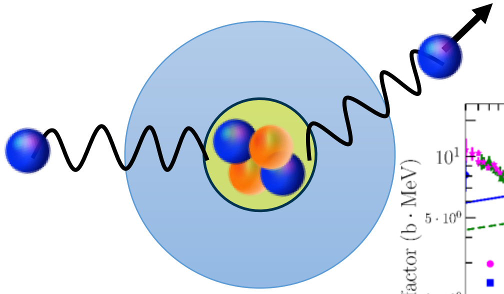
or :

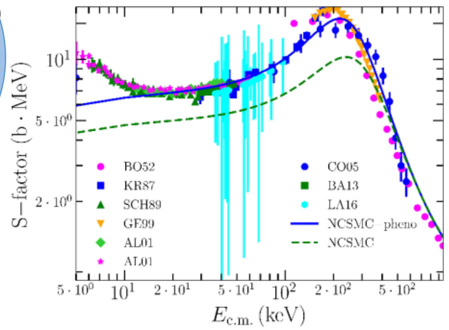
$$\Gamma_r = 4.5\ MeV$$

Conclusion

NCSMC

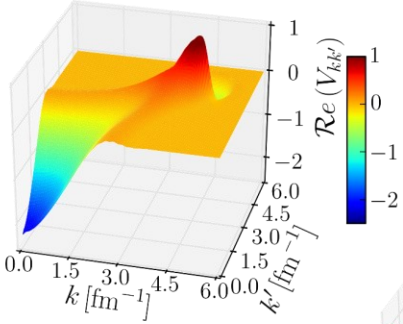
Correct asymptotics and direct reaction observables, but explicit-channel spaces become increasingly difficult for complex breakup.

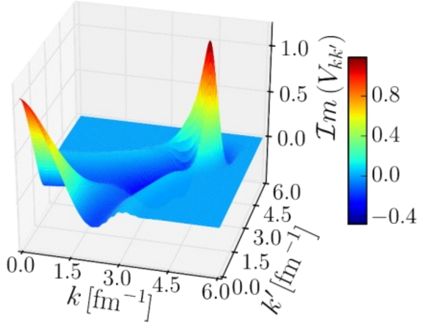




CS-NCSM

Resonance poles and wave functions can be accessed using bound-state many-body machinery, without selecting reaction channels.





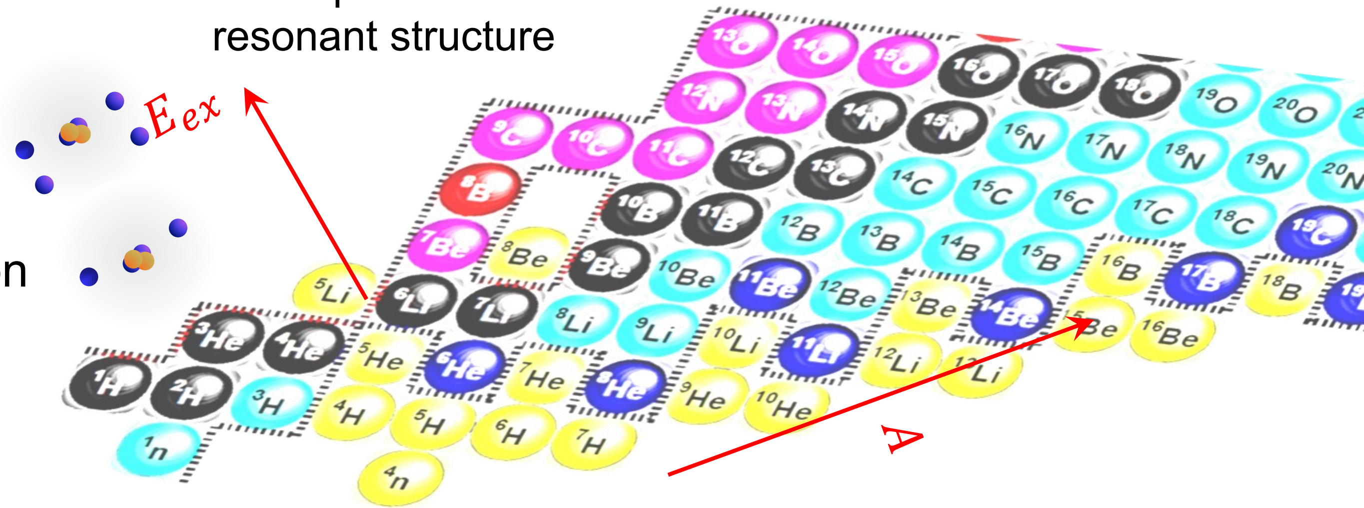
What we learned

Complex scaling of realistic interactions is feasible; SRG restores convergence; $A = 3 - 4$ benchmarks validate the approach, ~~while thresholds and broad resonances remain the principal numerical challenge~~.

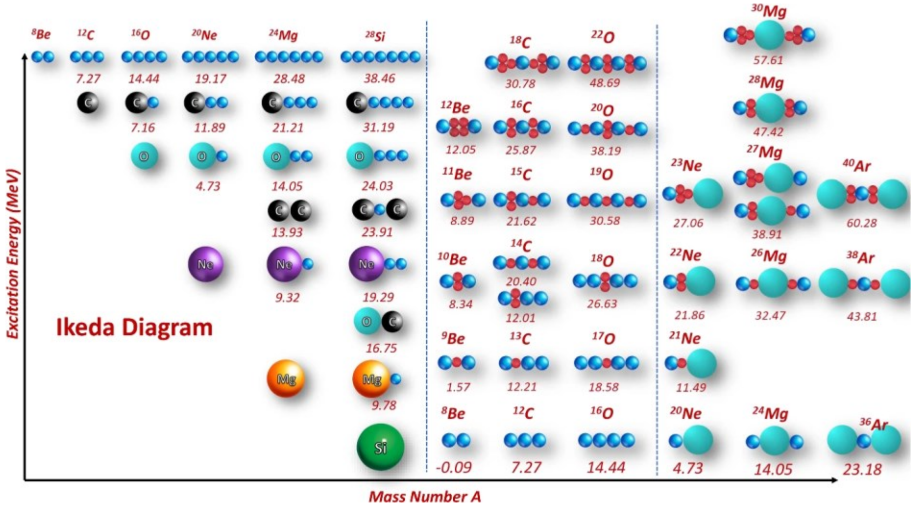
What I was planning to deliver for INT (still missing the manpower!)

Combine NCSMC with complex scaling to improve convergence and explore the extraction of optical potentials without explicit reaction channels.

Description of resonant structure

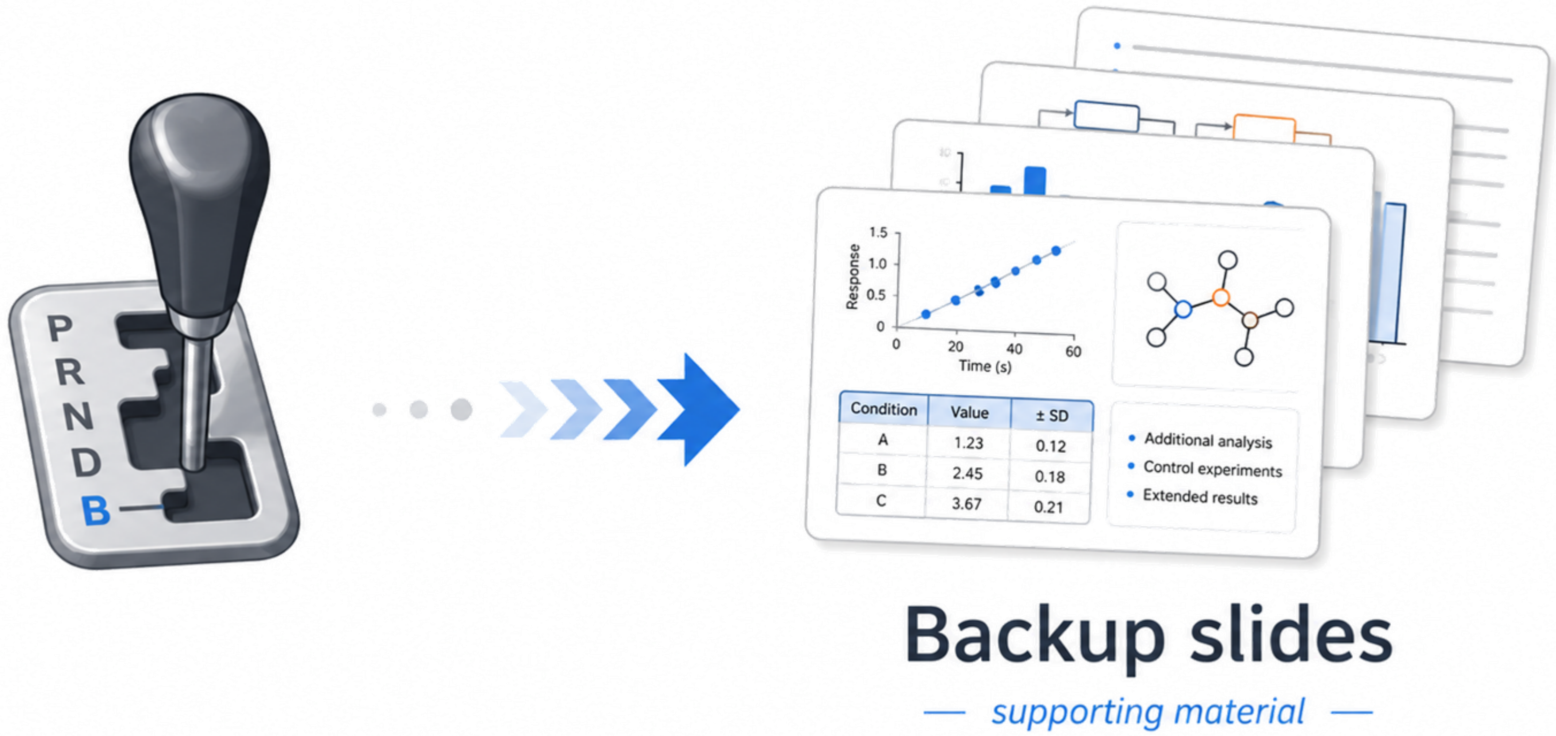


Clustering signatures from NCSM and other bound-state nuclear densities

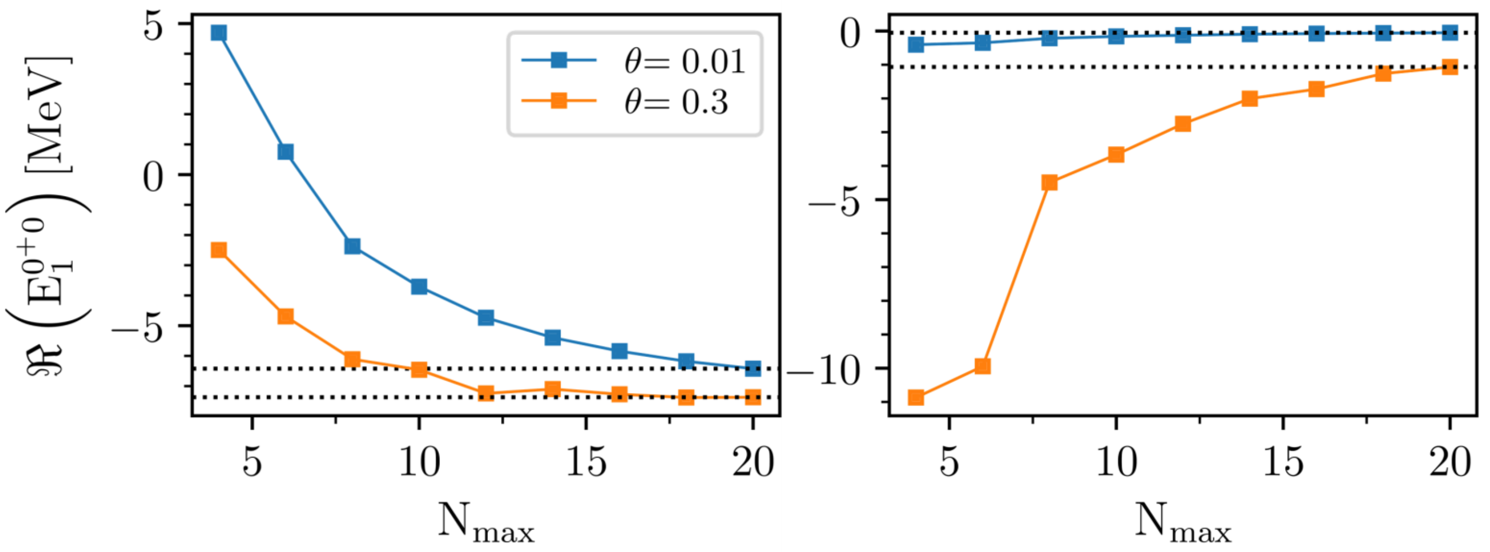


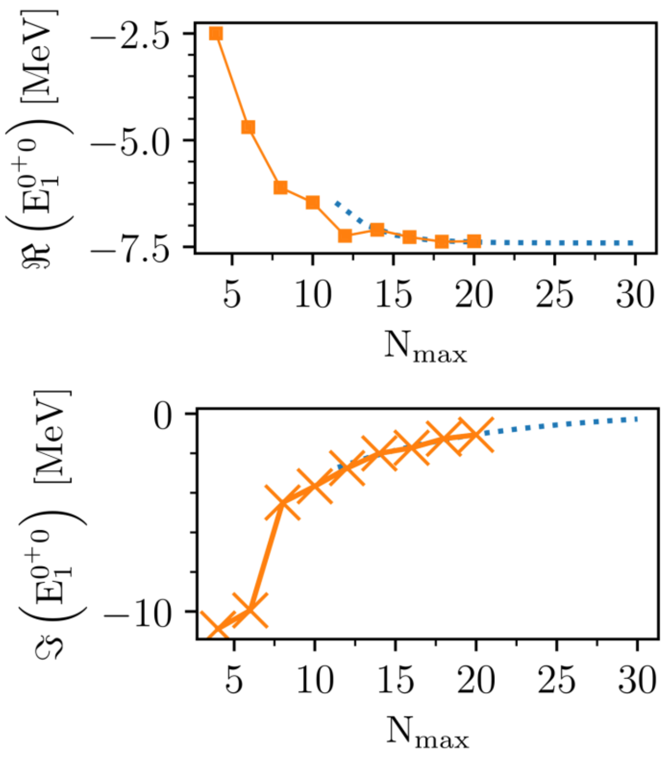
Future

- Implementation of Complex Scaling techniques to model breakup reactions Systematic study of low-lying resonance with CS-NCSM up to $A \sim 16$.
- Starting a project to develop PGCM using CS-SRG Hamiltonians to study cluster structure (most notably ^{12}C).


P
R
N
D
B
Response
1.5
1.0
0.5
0
0
20
40
60
Time (s)
Condition
Value
± SD
A
1.23
0.12
B
2.45
0.18
C
3.67
0.21
Additional analysis
Control experiments
Extended results
Backup slides
supporting material

$\alpha\, 0_1^+$ convergence with CS-Hamiltonian ($\theta = 0.3$ rad)

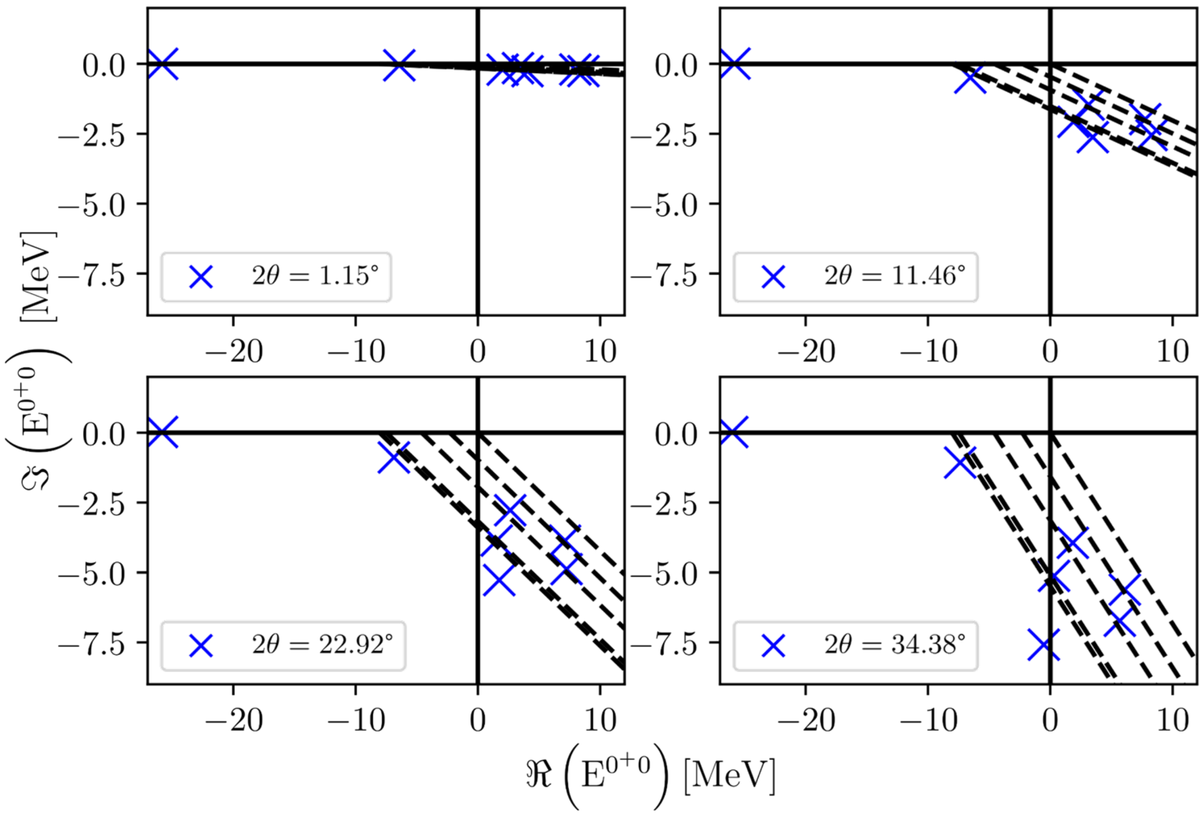


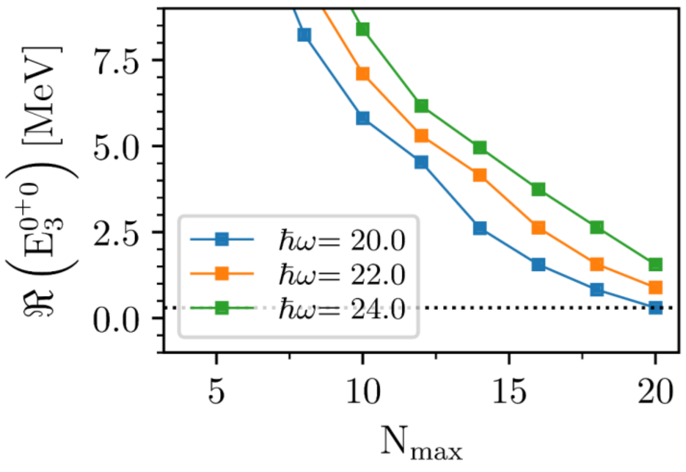


SRG permits a $\theta = 0.38$ rad rotation that gives a continuum rotation $2\theta = 43.5°$, allowing poles above this rotated cut to be exposed.

The pole can be isolated and numerically stabilized with a spectrum rotation of $34.4°$—but the calculated width is wrong.

α spectrum with CS-Hamiltonian ($\theta = 0.3$ rad)

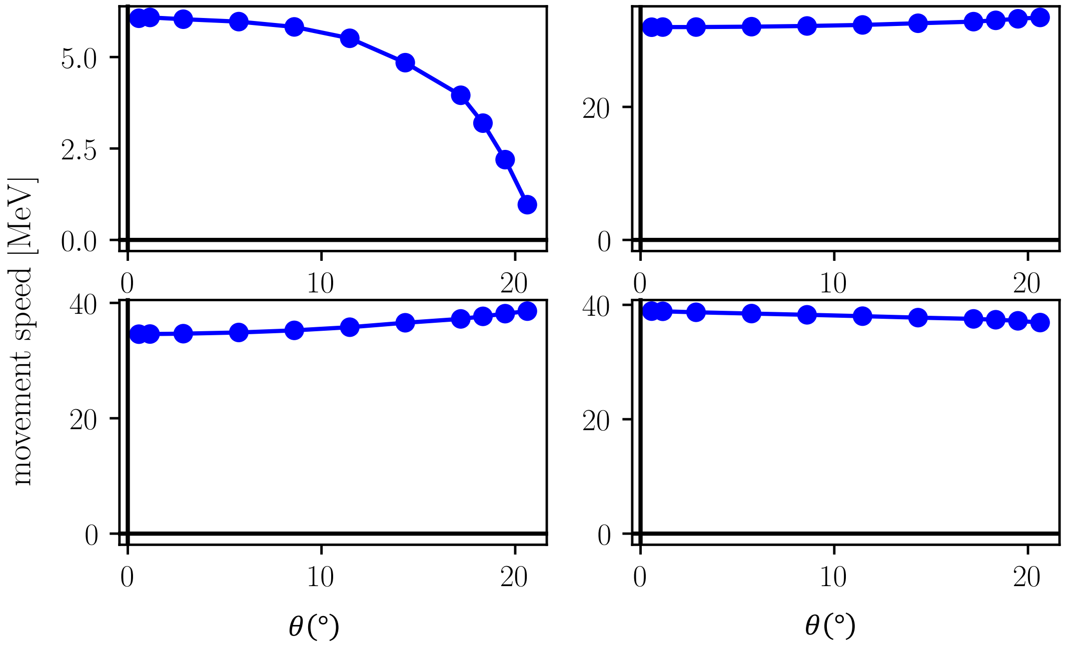


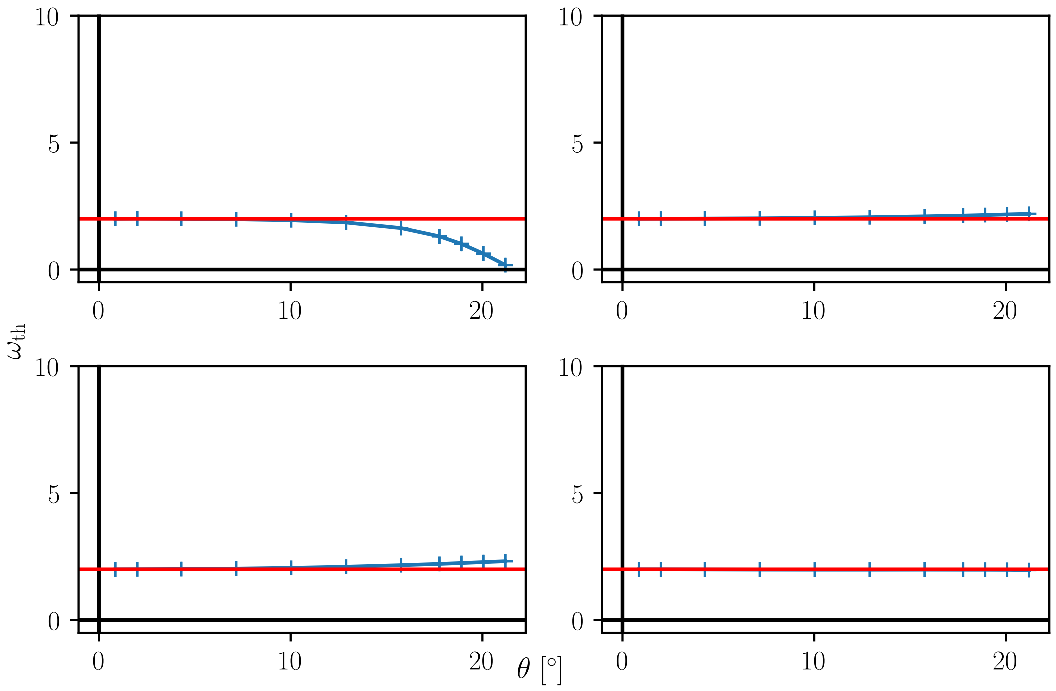


Further progress is needed with SRG to tackle non-Hermitian matrices

- Multiple rotated continua emerge from different thresholds and overlap with the finite-basis discretization;
- Convergence analysis with $h\Omega$ and Θ can help to identify resonances.

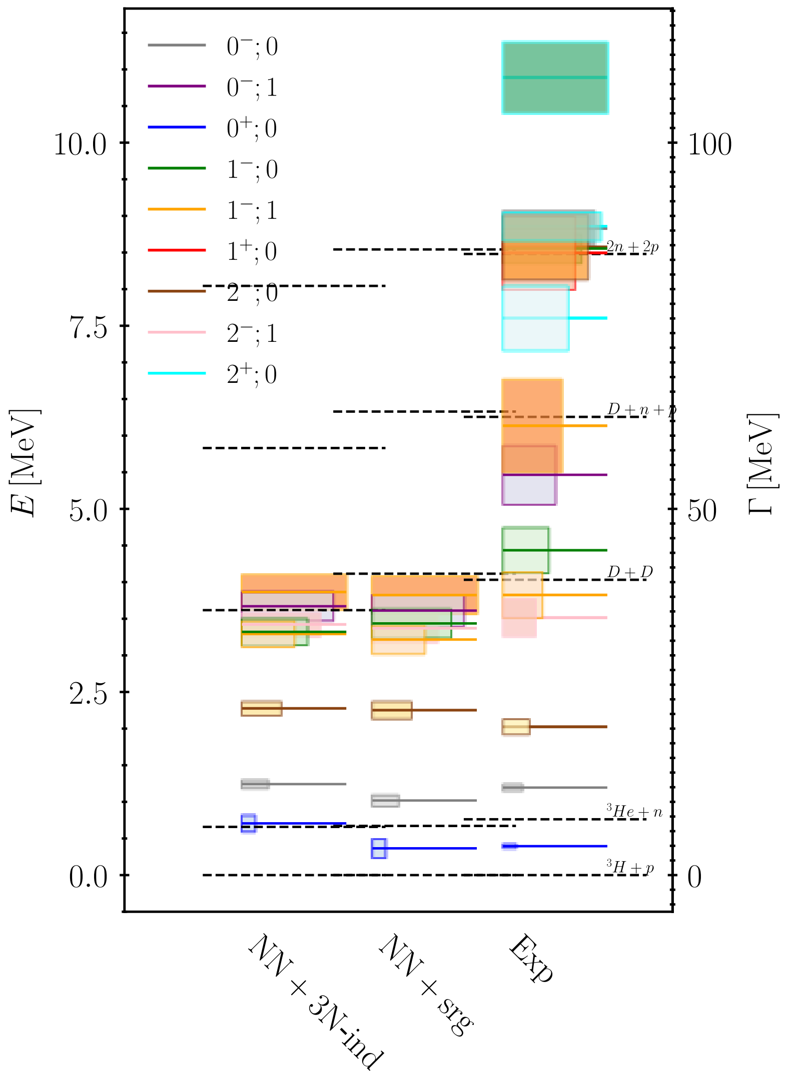
- Problem 1 : the threshold lives in a different mass partition;
- Problem 2 : converged values requires approximately **twice the N_{max}** : $A = 1 + 3 \rightarrow N_{\max} = 2X$ when $A = 4 \rightarrow N_{\max} = X$.

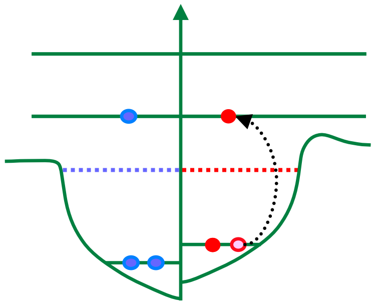


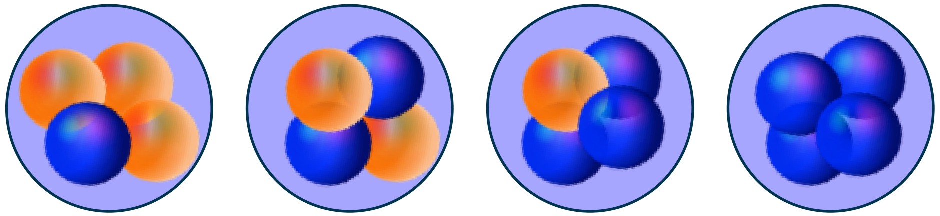


Current limitation: insufficient θ for some broad states → only lower bounds on Γ;
At larger rotation angles, instabilities develop in the SRG evolution, reducing its ability to restore smooth convergence with $N_{\max}$.

Wrap-up on the spectrum after analysis of the results



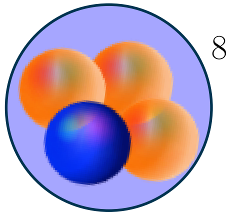




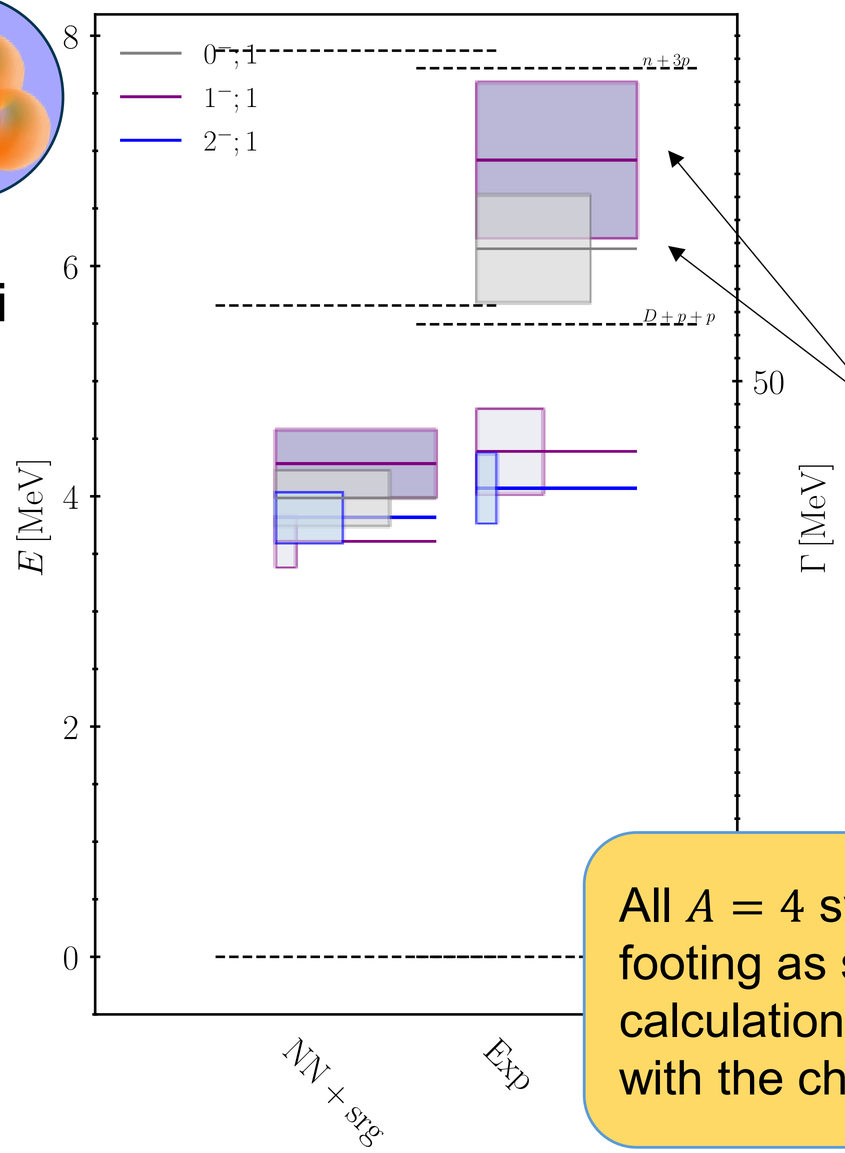
^{4}Li, ^{4}He, ^{4}H and 4n

The limited accessible rotation angle requires a convergence analysis, and only a lower bound on Γ can be extracted;
The resulting CS Hamiltonian can in principle be inserted into existing NCSM solvers up to the usual NCSM mass reach $A{\sim}16$.

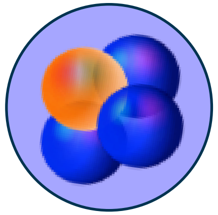
- The remaining discrepancies are larger than the 3N effects observed in the present calculations;
- Convergence analysis with $\hbar\Omega$ and Θ can help to identify resonances.



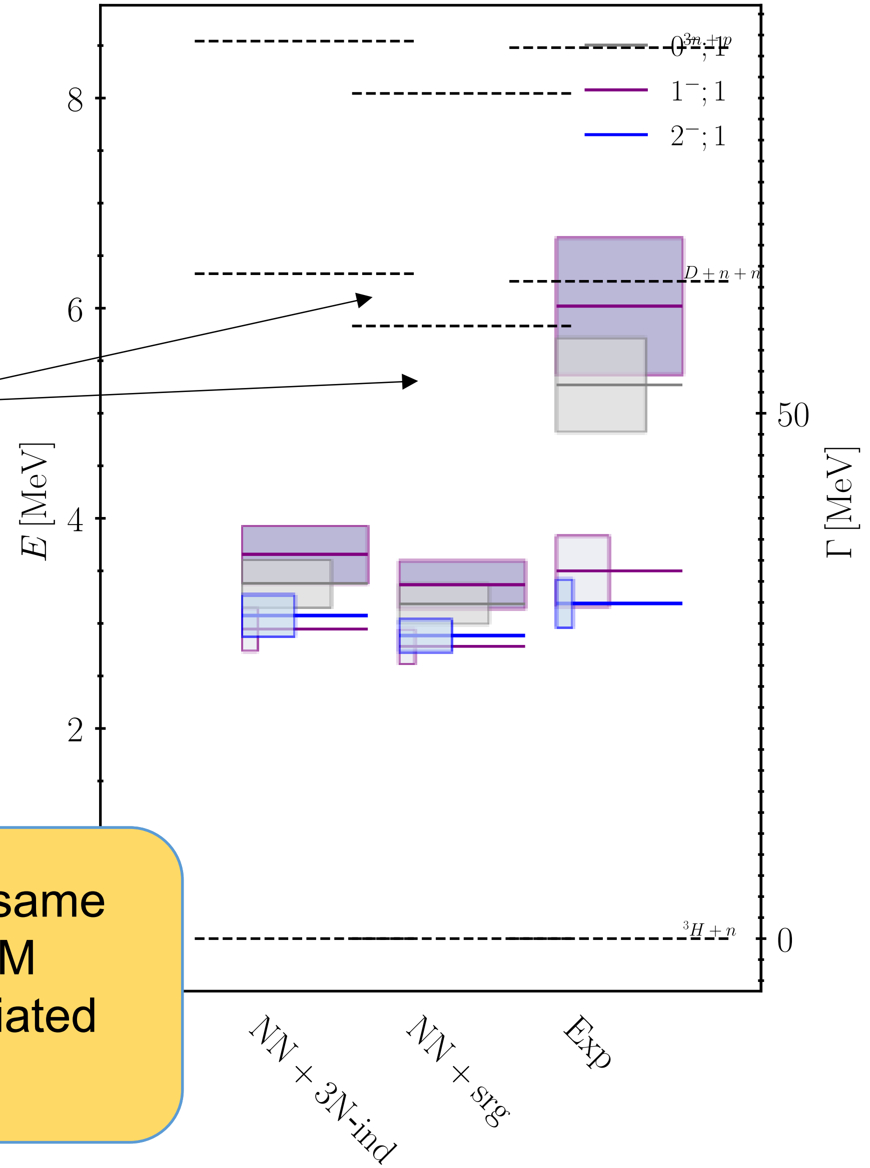
^{4}Li



Deviations from interpreted data (R-matrix analysis)



^{4}H



All $A = 4$ systems are treated on the same footing as standard bound-state NCSM calculations, with no ambiguity associated with the choice of reaction channels.