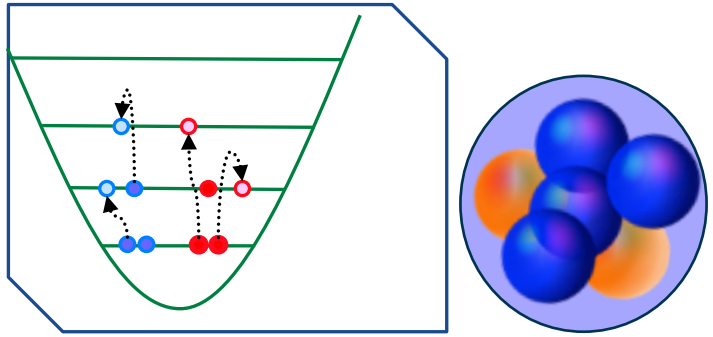
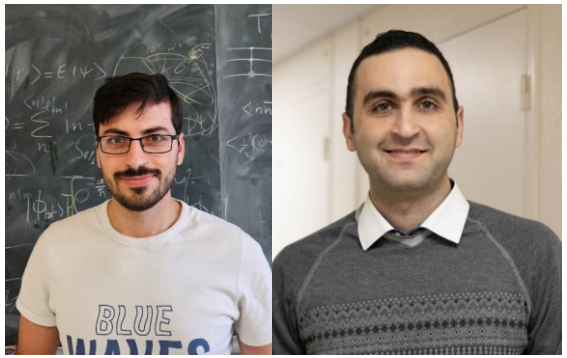
Guillaume Hupin, CNRS IJClab

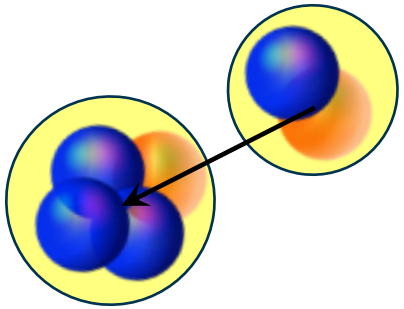


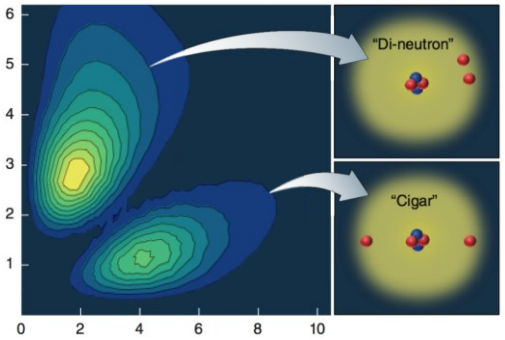
Collaborators

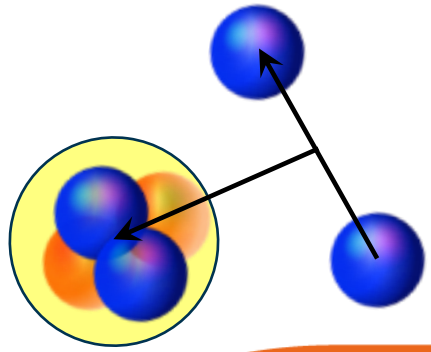
O. Yaghi (PhD, just defended)
A. Dehghani (PhD)

Reactions with clusters

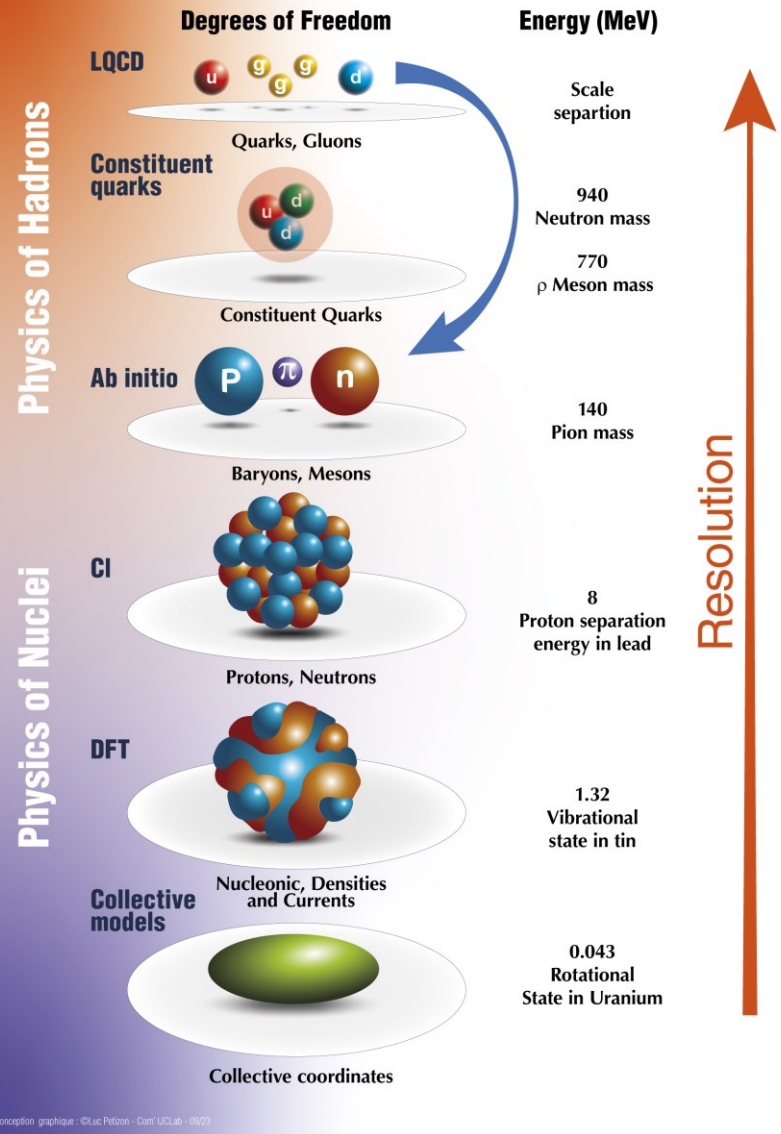








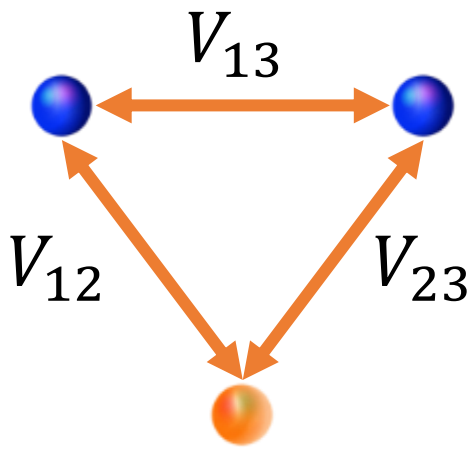
A story of multiple scale

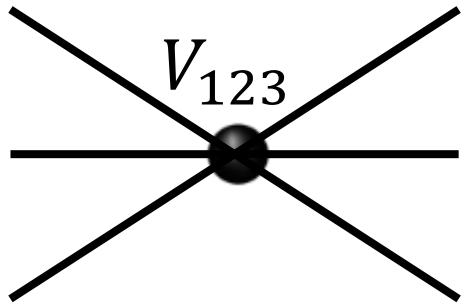


- Goal: Solving the Schrodinger equation (SE) for an A-body system:

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

- Nucleons are considered as point-like particles.
- The SE is solved by considering two and many-body interactions between nucleons



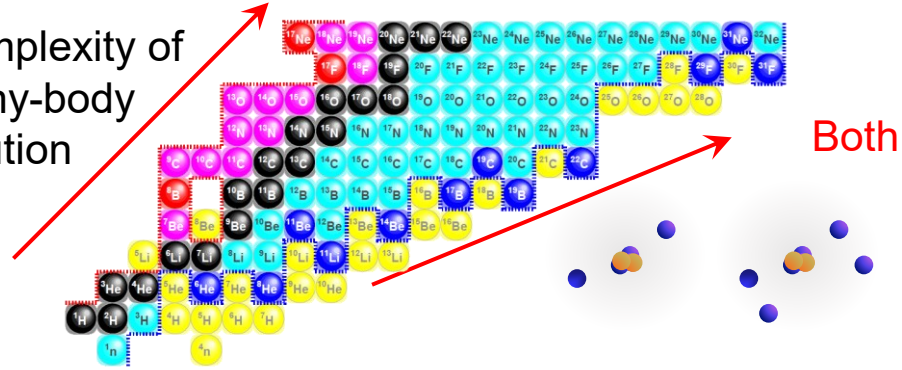


(i) Research directions

Complexity of scattering problem

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

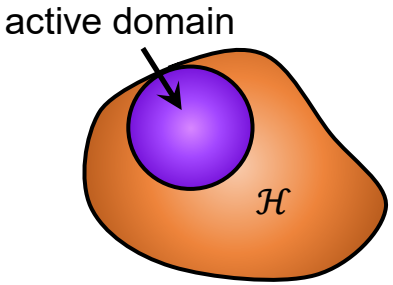
$M_h \leq M_{n,p}$



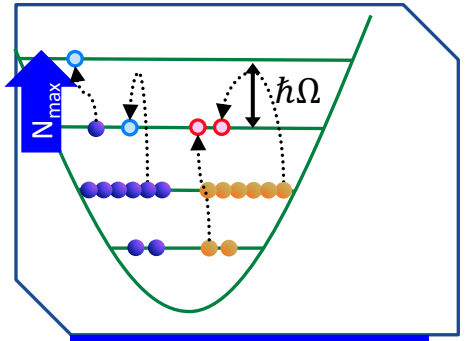
- 😐 Nuclear theory is **data driven**.
- ☹ The lack of accuracy of *ab initio* structure methods impedes the development of reactions modeling.

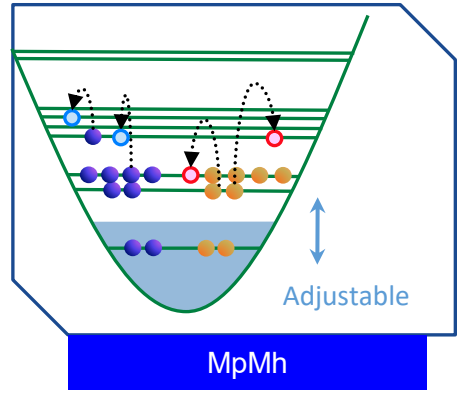
Credits H. Lenske

Configuration interaction methods suited for $A \gg 1$



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



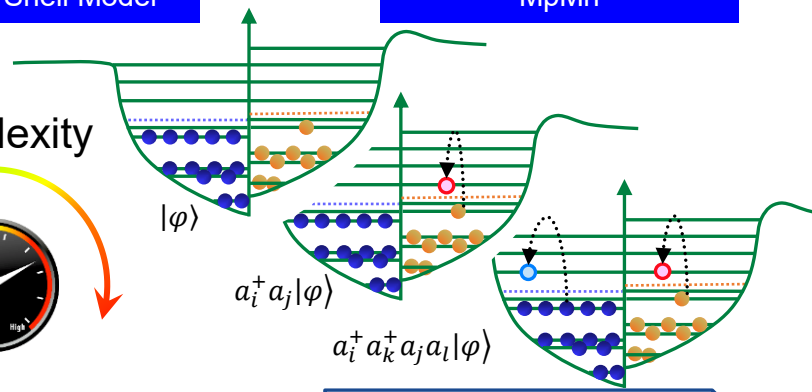


Superposition of Slater determinants:

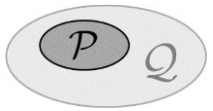
$$|\Psi^A\rangle = \sum_\alpha c_\alpha \Phi^\varphi_\alpha(\vec{r}_1, \ldots, \vec{r}_A) = A_0 \left|\Phi^0_{0p0h}\right\rangle + \sum_{\alpha'} A_{\alpha'} \left|\Phi^{\alpha'}_{1p1h}\right\rangle + \cdots$$

NCSM
IM-SH
MpMh

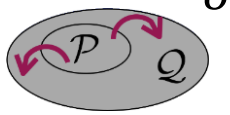
Complexity



Optimization of mixing coefficients, one-body Hilbert space:

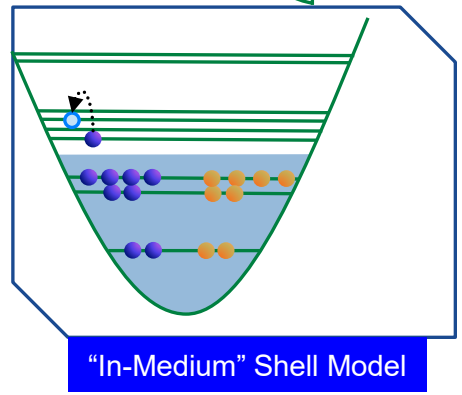


$$\delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \Longrightarrow \sum_\beta A_\beta \langle\Phi_\alpha|\hat{H}|\Phi_\beta\rangle = E A_\alpha$$

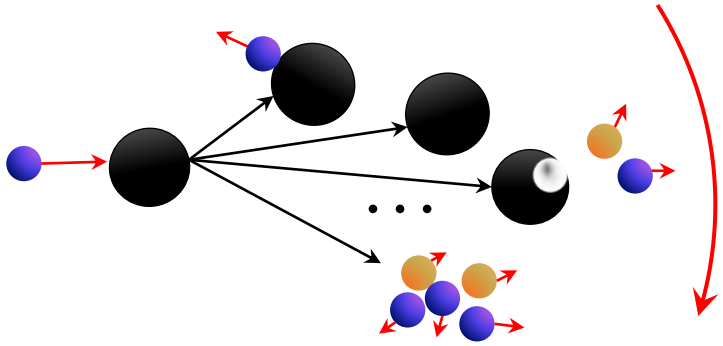


$$\delta\mathcal{E}[\Psi]_{/\{\varphi^*_\alpha\}} = \langle\Psi|[\hat{H}, \hat{T}]|\Psi\rangle = 0 \Leftrightarrow [\hat{h}(\rho), \hat{\rho}] = \hat{G}(\sigma)$$

Generalized Brillouin (GB) equation



(ii) Research directions



Complexity of scattering problem

Complexity of many-body solution

Both

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

$M_h \leq M_{n,p}$

😐 Nuclear theory is **data driven**.

☹ Few-body techniques scale **very bad** with the number of constituents in the continuum.

Credits H. Lenske

One way to solve the many-body problem

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

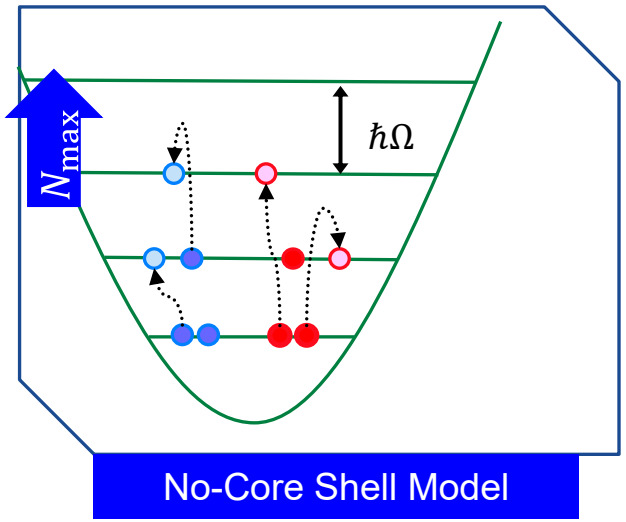
Mixing coefficients(unknown)

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.

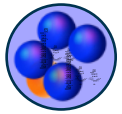
- One way to solve the many-body problem when two scales appear

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

Mixing coefficients(unknown)

A-body harmonic oscillator states

$\Leftrightarrow$



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

Second quantization

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

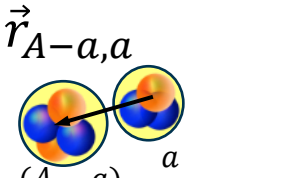
$$\Psi^{(A)}_{RGM} = \sum_v \int d\vec{r}\; g_v(\vec{r})\, \hat{A}_v \left|\Phi^{(A-a,a)}_{v\vec{r}}\right\rangle$$

Relative wave function (unknown)

Antisymmetrizer

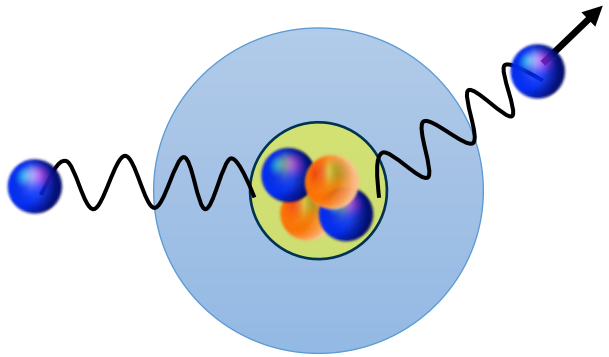
Channel basis

$\Leftrightarrow$



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

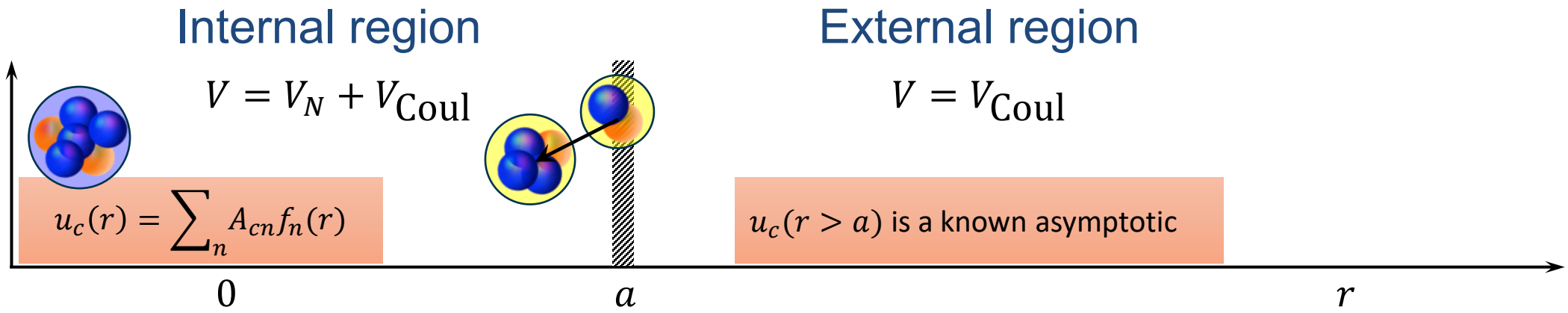
Cluster expansion technique



NCSM/RGM Cluster formalism for elastic/inelastic

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

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



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.

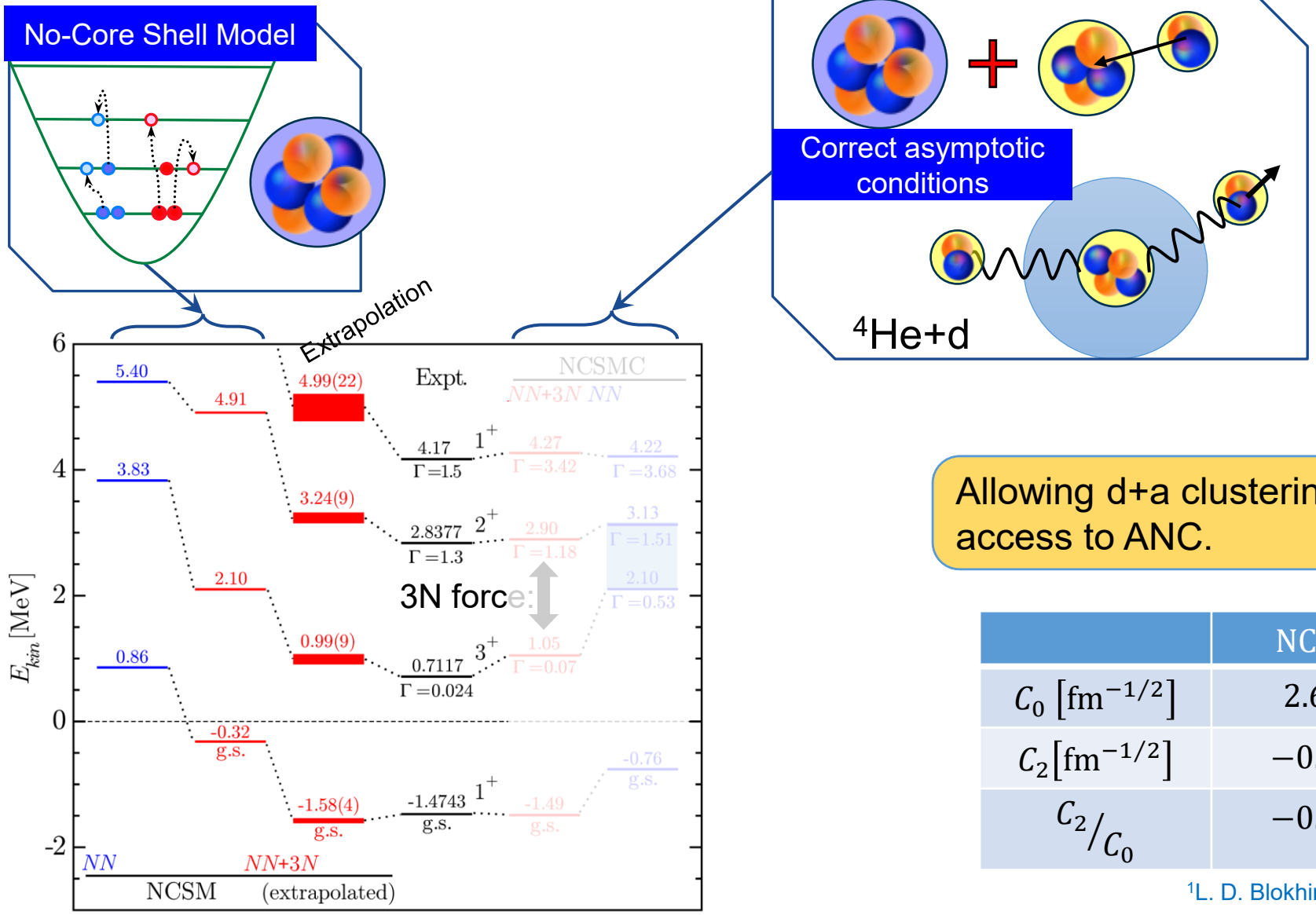
NCSM with continuum (NCSMC):

- For computing reactions and exotic nuclei.

Limitations:

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

Example: Structure of ^{6}Li continuum

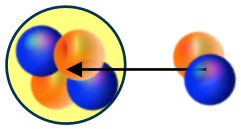


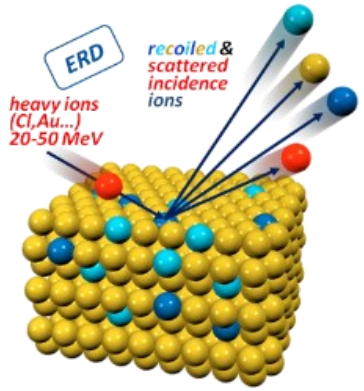
Allowing d+a clustering in the g.s. gives access to ANC.

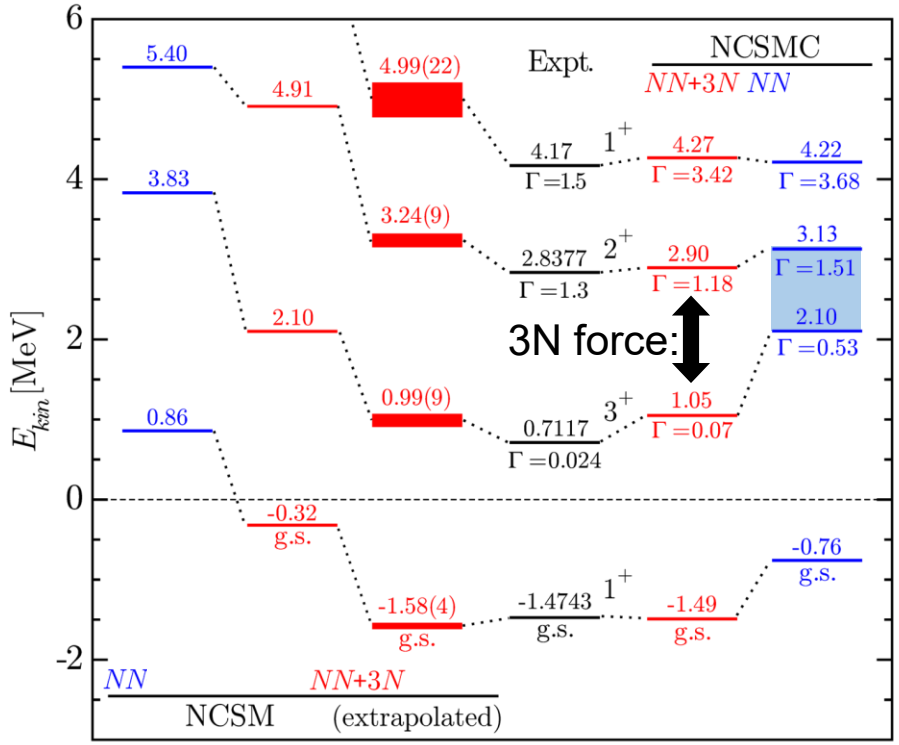
	NCSMC	Experiment[1]
C_0 $[\mathrm{fm}^{-1/2}]$	2.695	2.91 (9)
$C_2[\mathrm{fm}^{-1/2}]$	−0.074	−0,077 (18)
C_2/C_0	−0.027	0.025 (6)

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

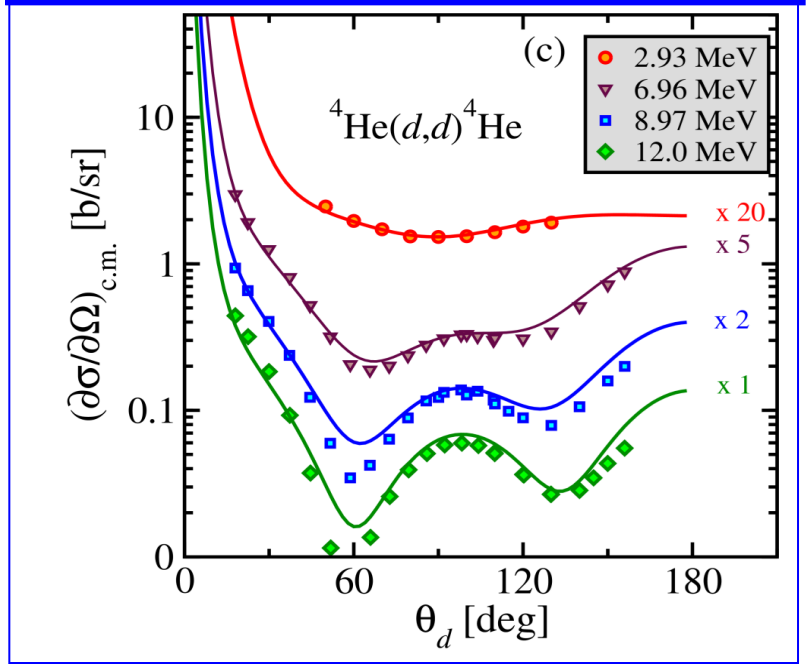
Example: Structure of ^{6}Li continuum



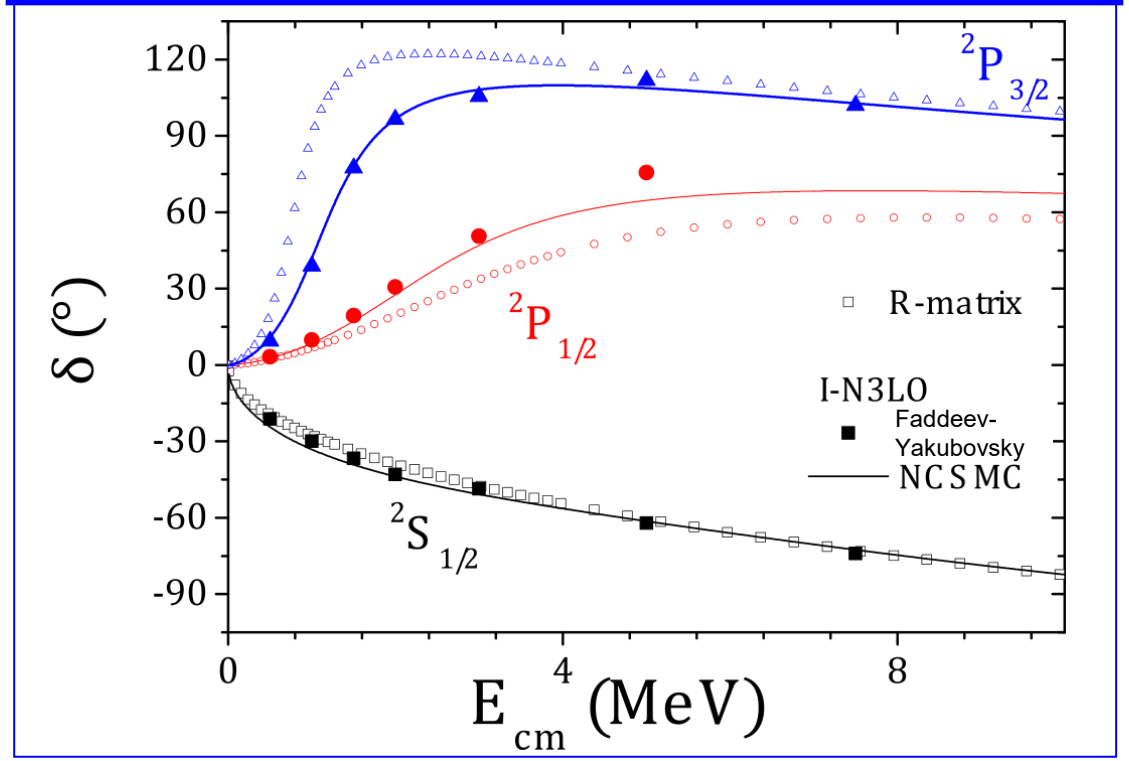




^{4}He(d,d) ^{4}He angular distribution

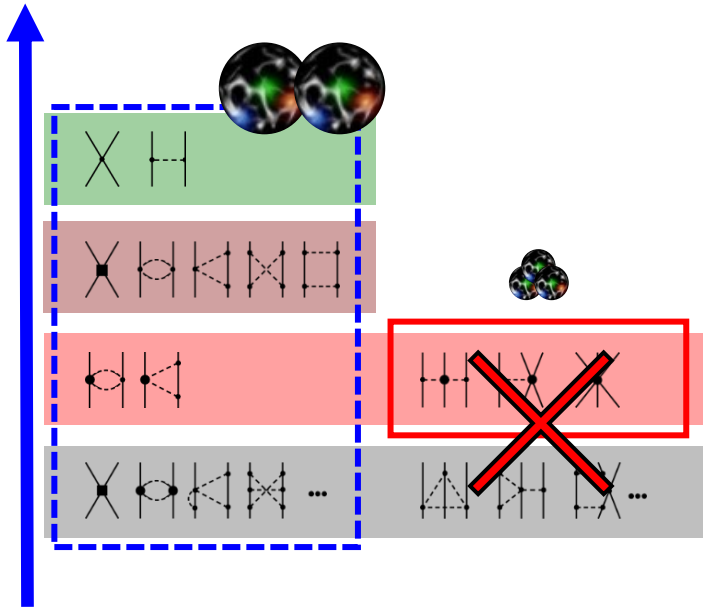


Benchmark: scattering phase shifts NCSMC/FY

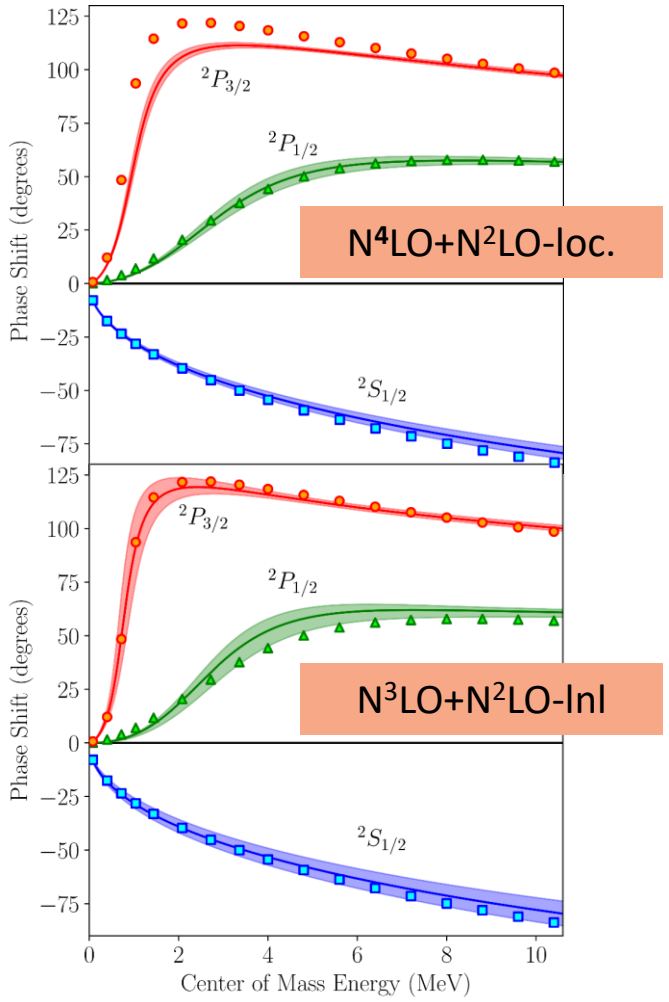


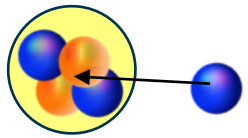
R. Lazauskas, PRC **97** (2018).*
*there is a more recent paper with 3N force.

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

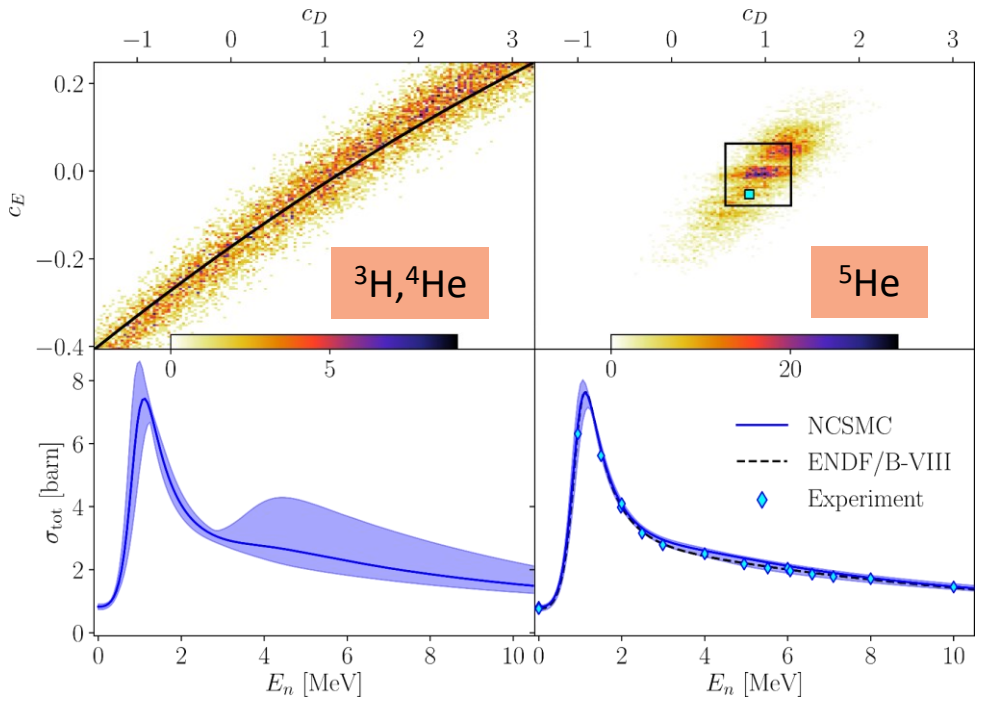


Sensitivity to c_D and c_E



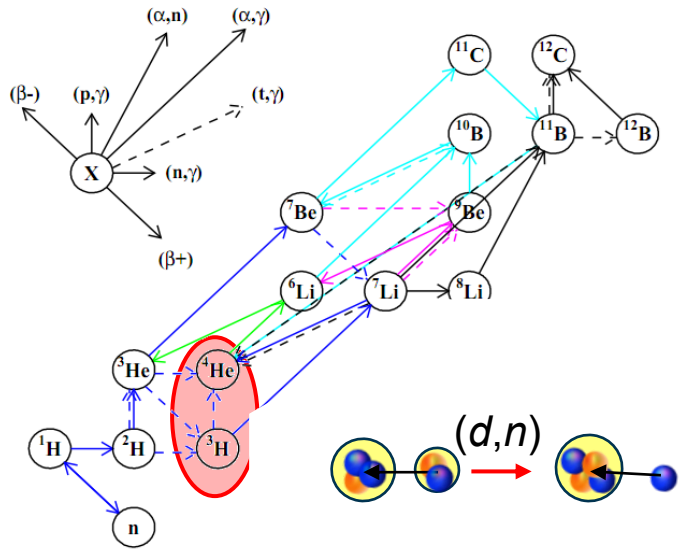


- NN-N4LO + 3N-N2LO **cannot reproduce** the p-wave splitting.
- Tighter posterior distribution if the properties of the ^{5}He are included in the fit of 3N LEC.

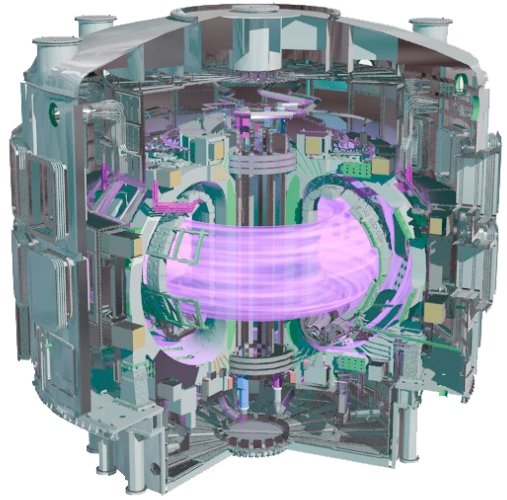


Low-energy Transfer reactions (*d*,*N*)

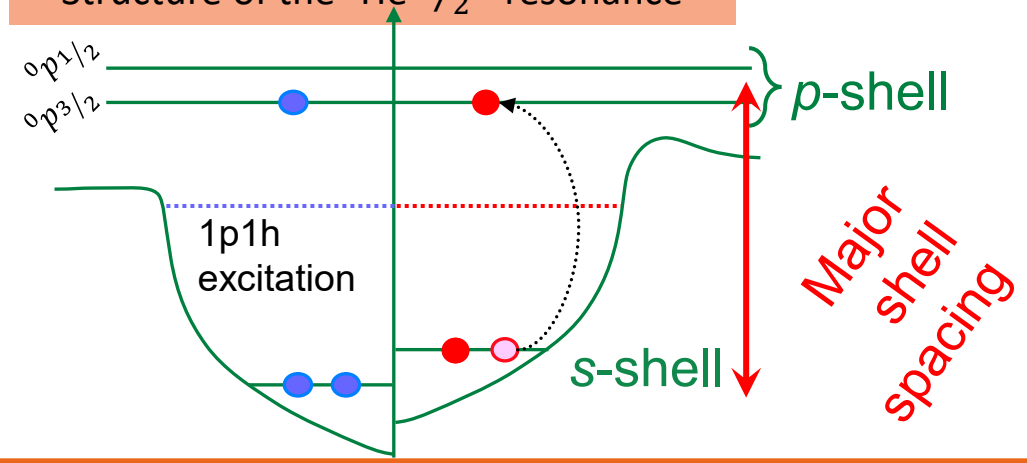
Primordial Nucleosynthesis **(blue)**



ITER design (Cadarache, France)

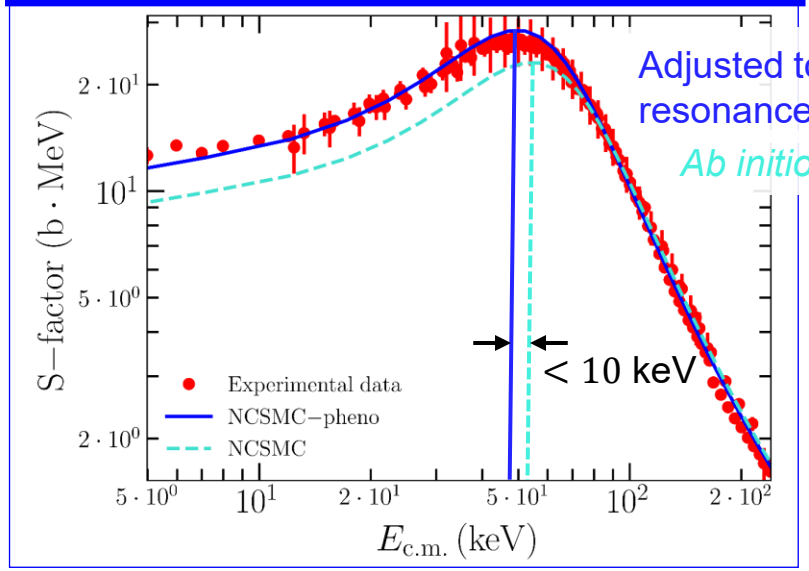


Structure of the ^{5}He $^{3}/_{2}^{+}$ resonance

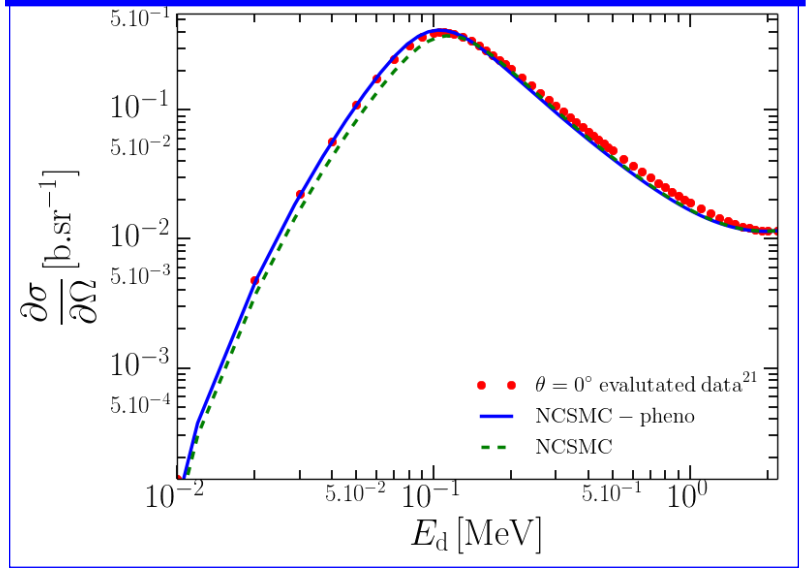


^{3}H(d,n)^{4}He fusion reaction: benchmark to data and evaluation

S-factor: computed and data



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

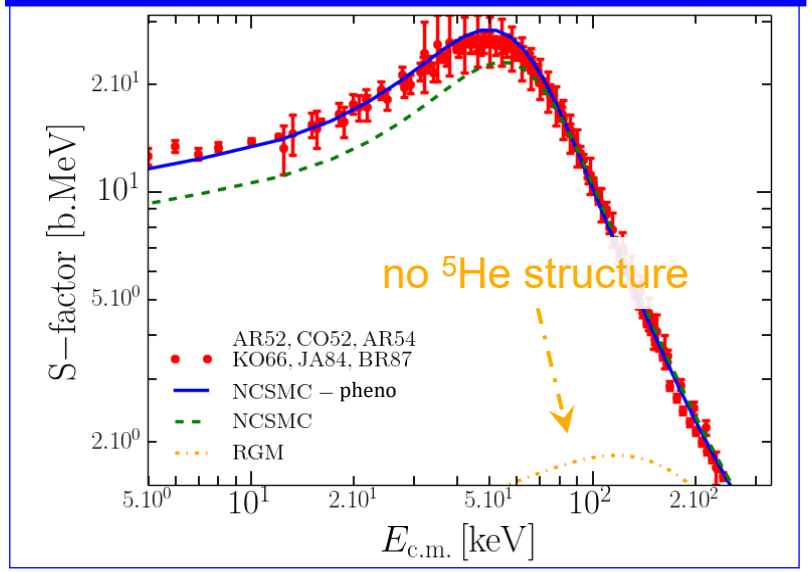


M. Drosg and N. Otuka, INDC(AUS)-0019 (2015).

- 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**.

^{3}H(d,n)^{4}He fusion reaction: impact of the resonance structure

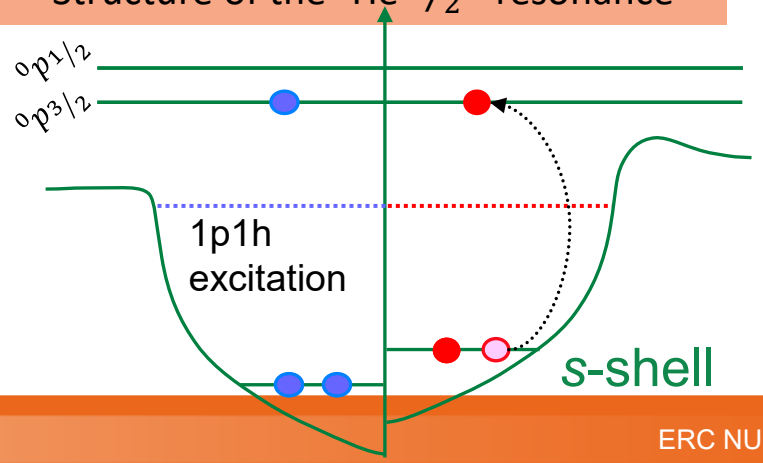
S-factor: NCSMC vs binary cluster



$^5\mathrm{He}(^4S_{3/2})$	$E_r\ (keV)$	$\Gamma_r\ (keV)$
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).

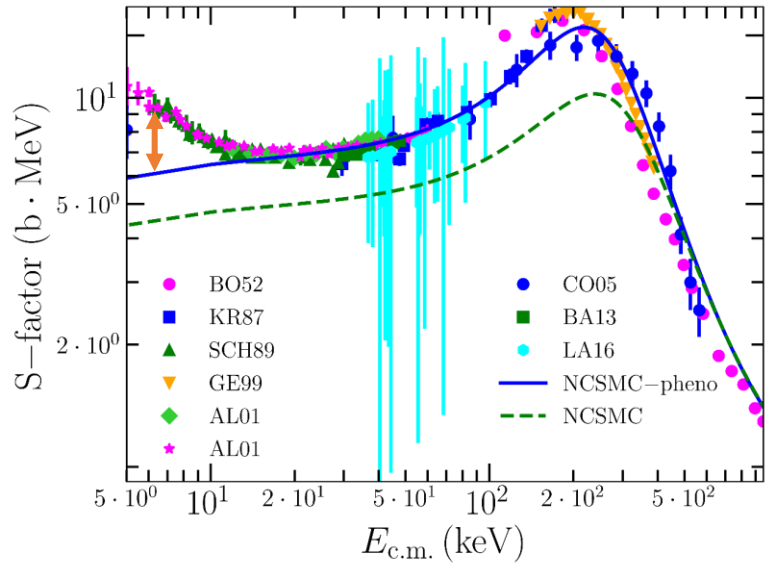
Structure of the ^{5}He $^3/_2^+$ resonance

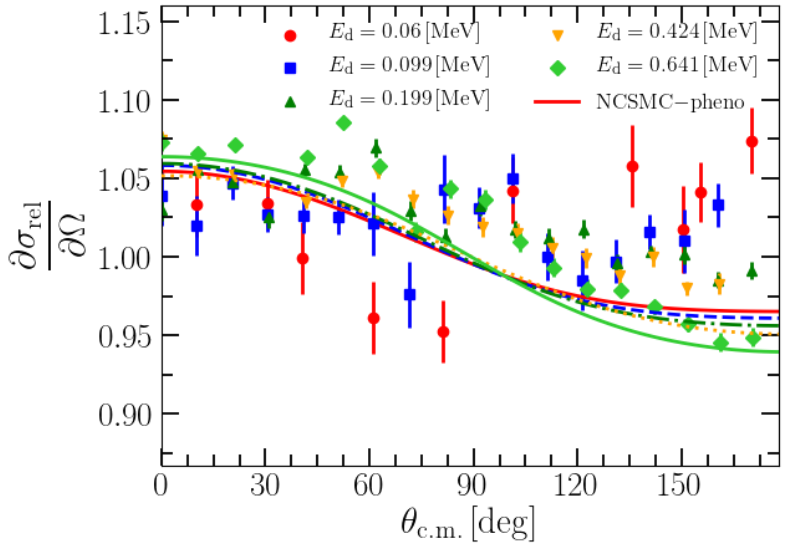


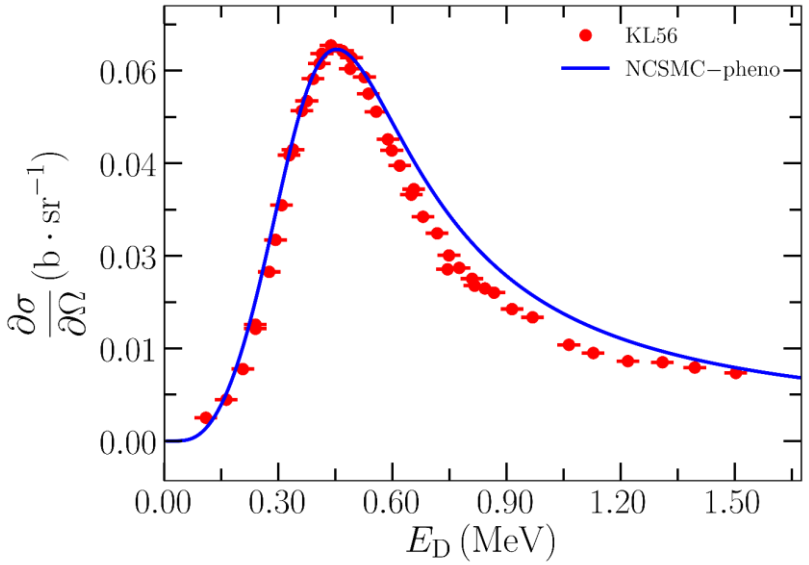
- Importance of structure of neighboring resonances is magnified in transfer reactions.

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

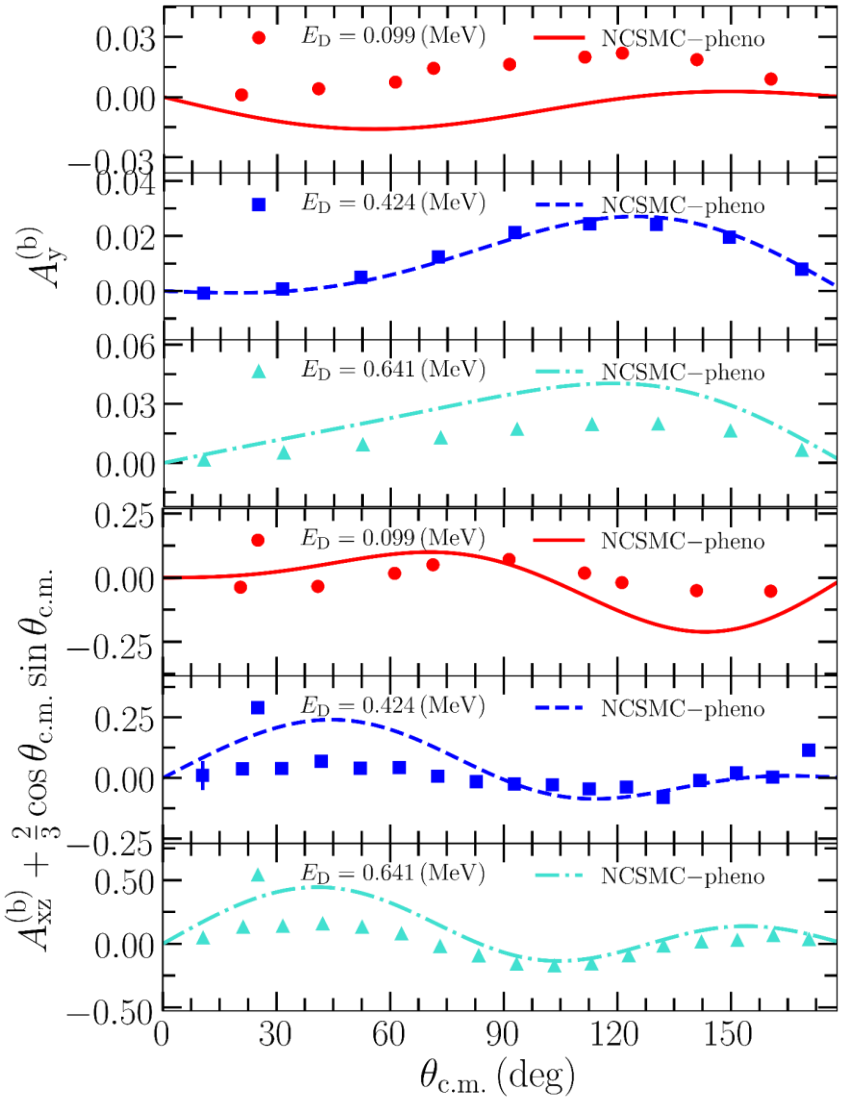
- The S-factor is globally well reproduced.
- However, there are **discrepancies** between data sets around the peak of the S-factor.
- Influence of p- and d-waves in agreement with data.

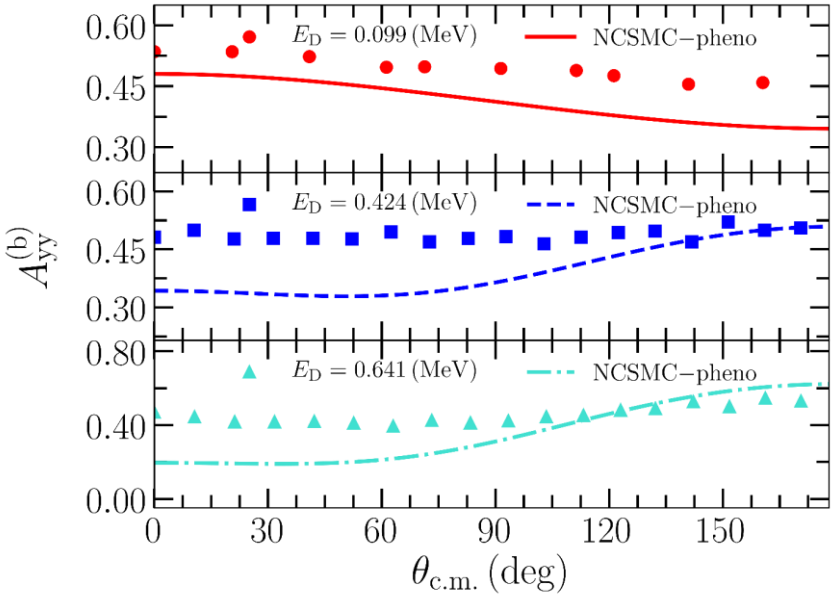






$^3\mathrm{He}(\vec{d},p)^4\mathrm{He}$: analyzing tensors





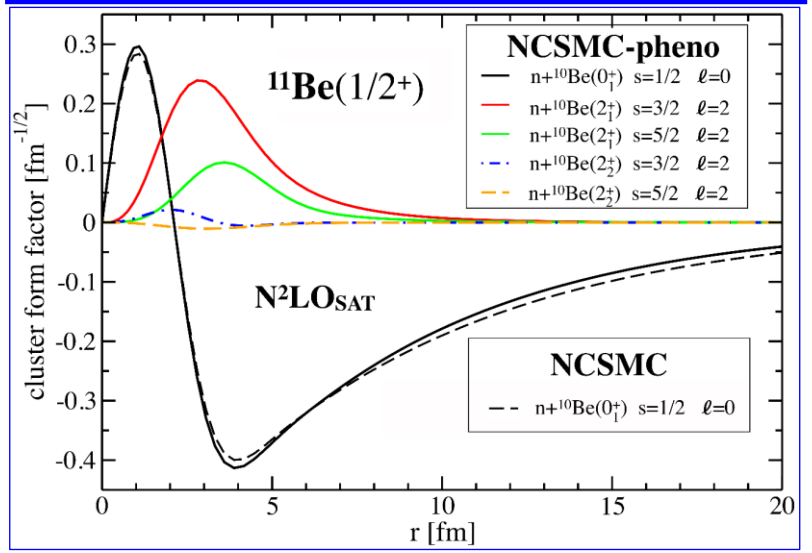
W.H. Geist, *et al.* PRC**60** (1999).

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

^{11}Be 1n Halo nuclei : EM probes

A. Calci, *et al.* PRL117 (2016)

Halo structure



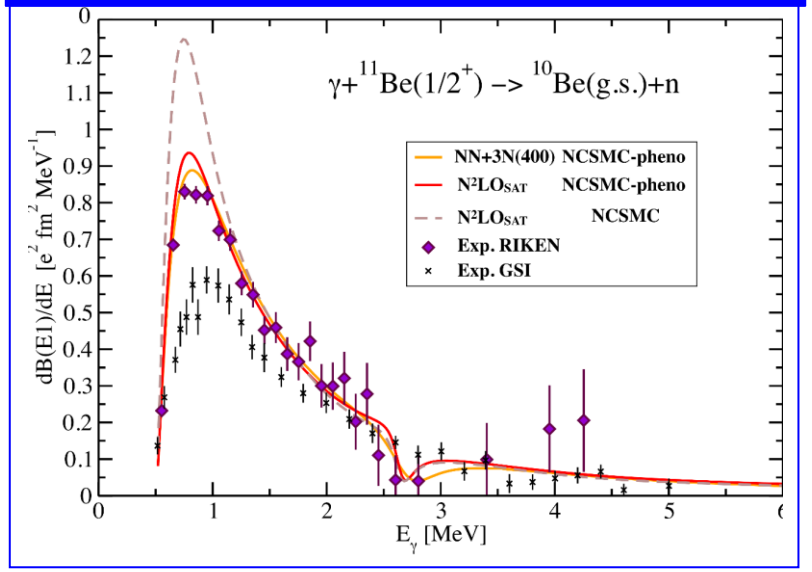
$N_{\max}$ =10 model space i.e. $r \approx 7$ fm HO spatial box

Parametric details of ^{11}Be ($^1/_2{}^+$), ANCs, ERE (a_ℓ, …) as output for free.

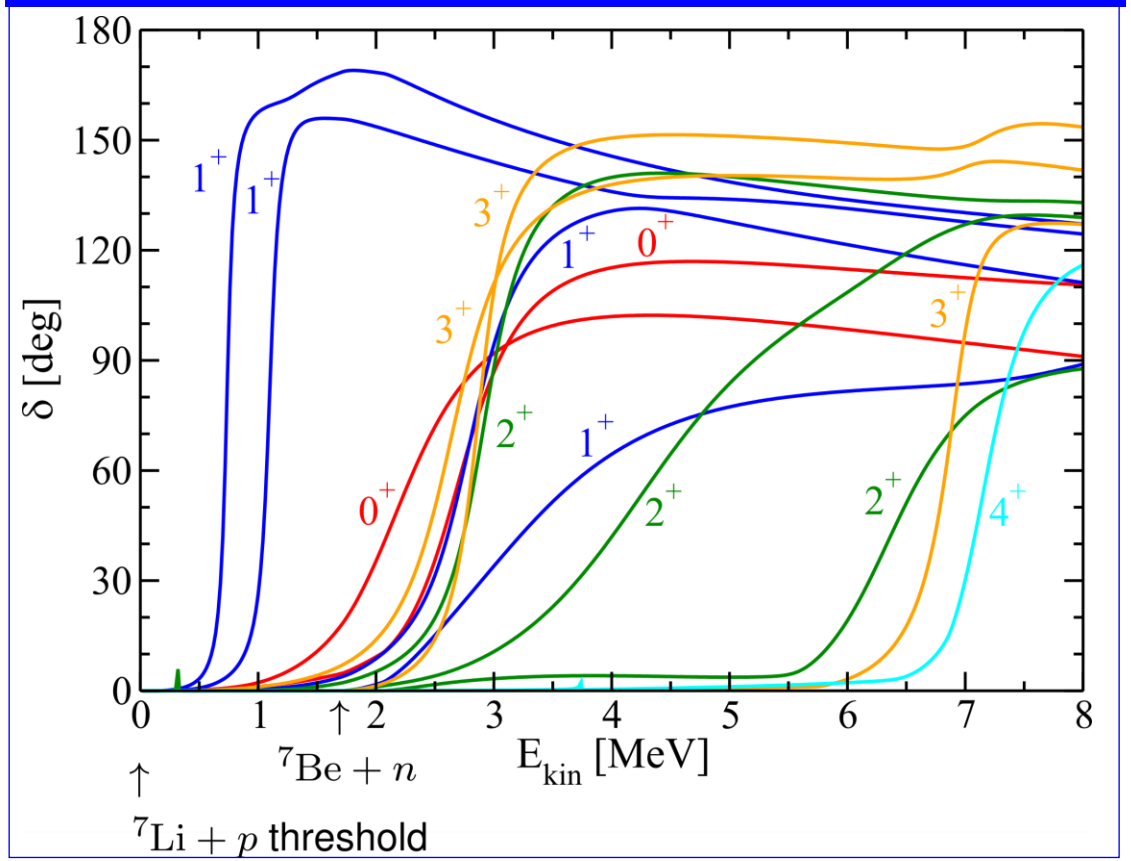
Bound to bound

	NCSM	NCSM-pheno	Expt.
$B\left(E1; \frac{1}{2}^+ \rightarrow \frac{1}{2}^-\right)$ $[e^2\ \mathrm{fm}^2]$	5.10^{-6}	0.118	0.102 (2)

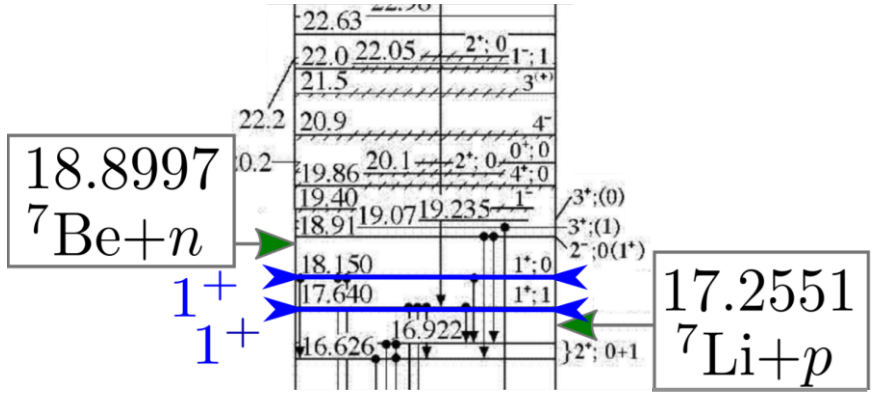
Bound to continuum



Positive parity eigen-phase shifts from NCSMC



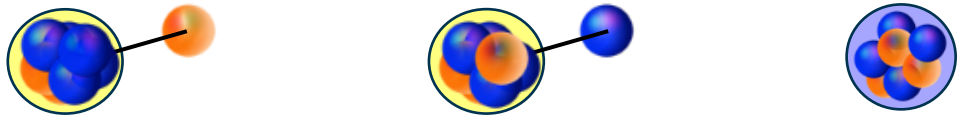
P. Gysbers *et al.* PRC **110** (2024)



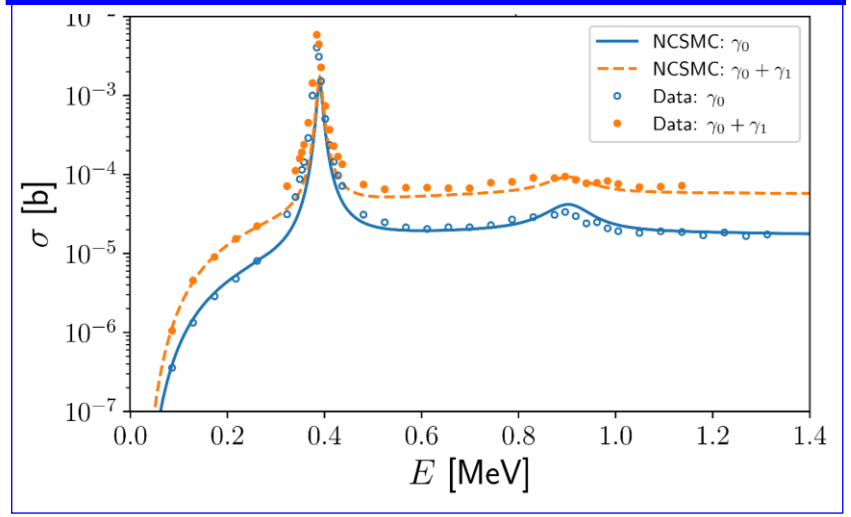
A number of resonances are unresolved in data/evaluation.

^{7}Li(p,γ)^{8}Be radiative capture, ^{7}Li(p,e^-e^+)^{8}Be pair production & X17 boson

- Motivated by ATOMKI experiments Firak, Krasznahorkay *et al.*, EPJ Web of Conf. 232, 04005 (2020)
- NCSMC with charge exchange channel included

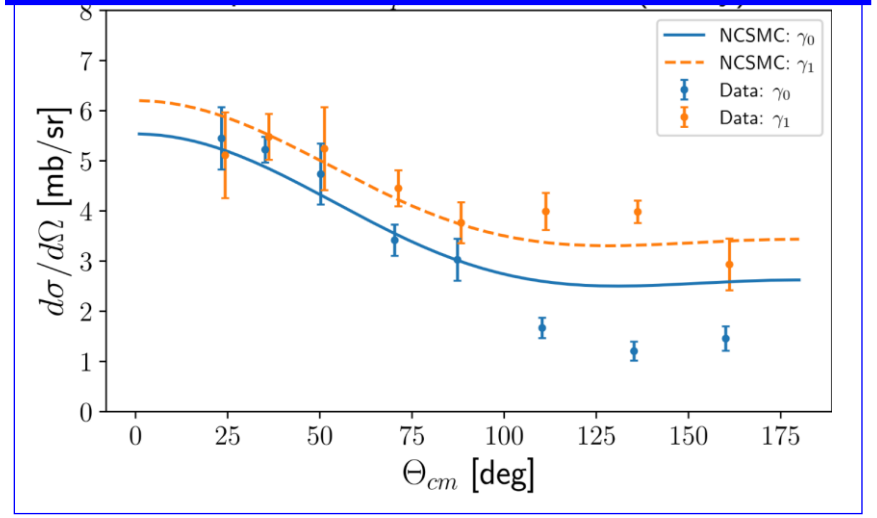


Cross-section $^7\mathrm{Li}_{3/2^-}(p,\gamma)^8\mathrm{Be}$



Zahnow *et al.* Z.Phys.A 351 229-236 (1995)

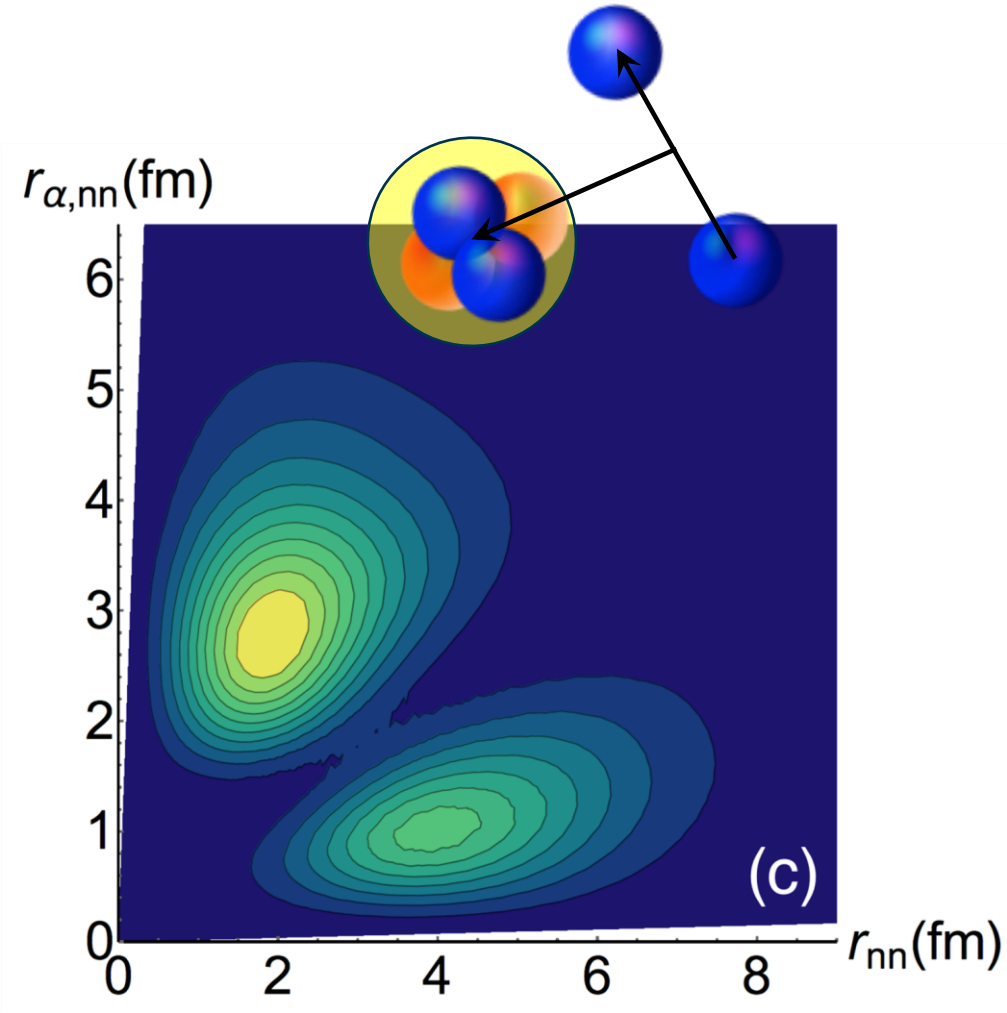
Capture $E_p = 1021.5$ keV (data Orsay)



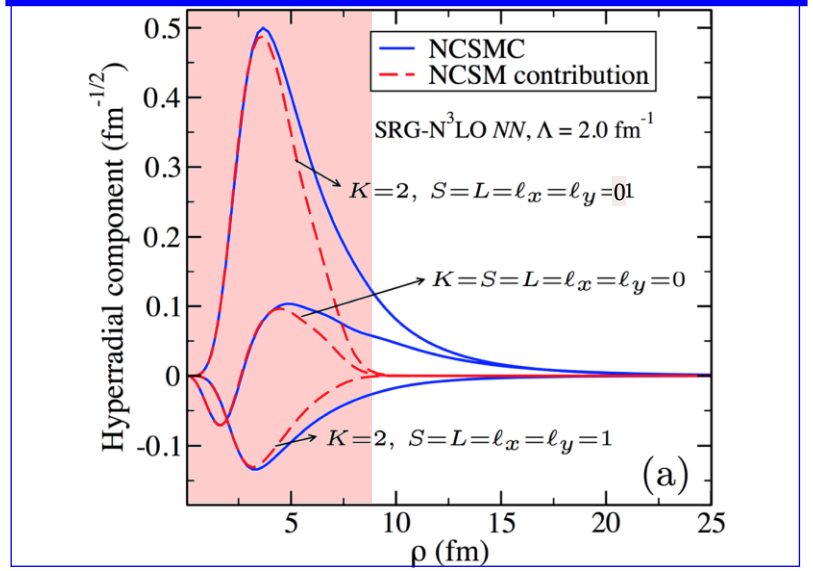
Isospin missing between the 1^+ is not well predicted.

^{6}He 2n Halo nuclei

C. Romero-Redondo, S. Quaglioni *et al.* PRL117 (2016); PRC97 (2018)



Halo structure



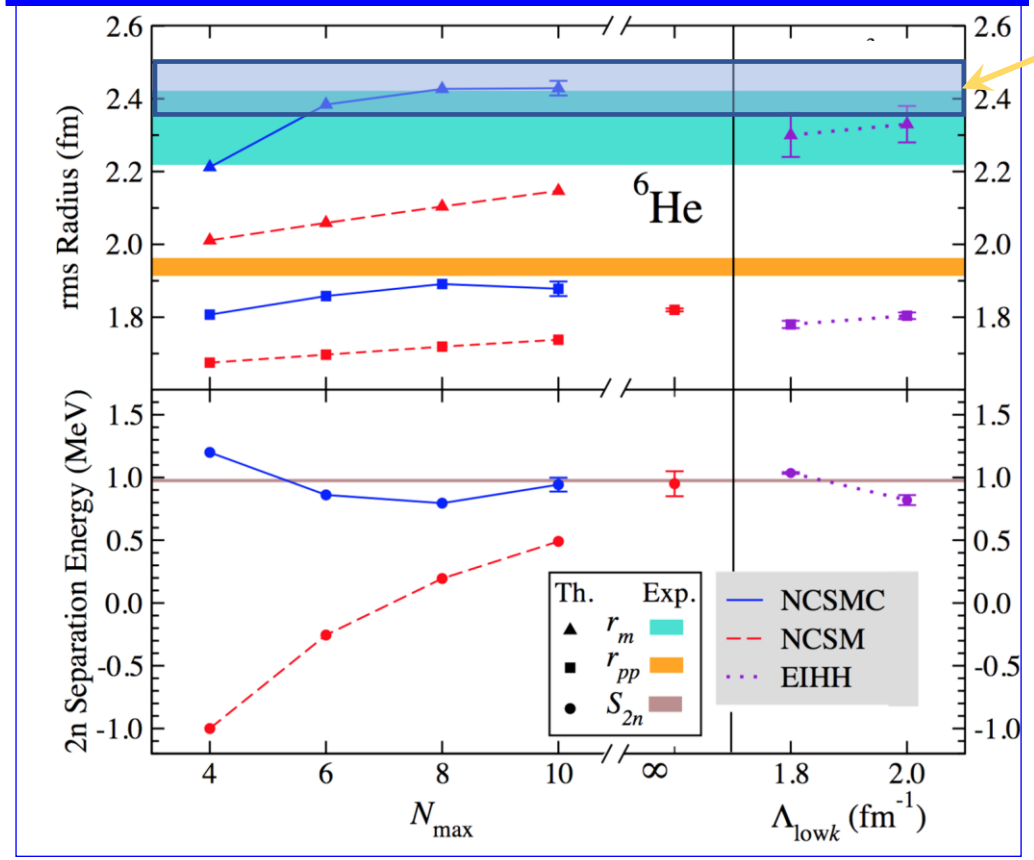
$N_{\max}$ =12 model space i.e. $r \approx 8$ fm HO spatial box

Long-distance components are mandatory to model ^{6}He.

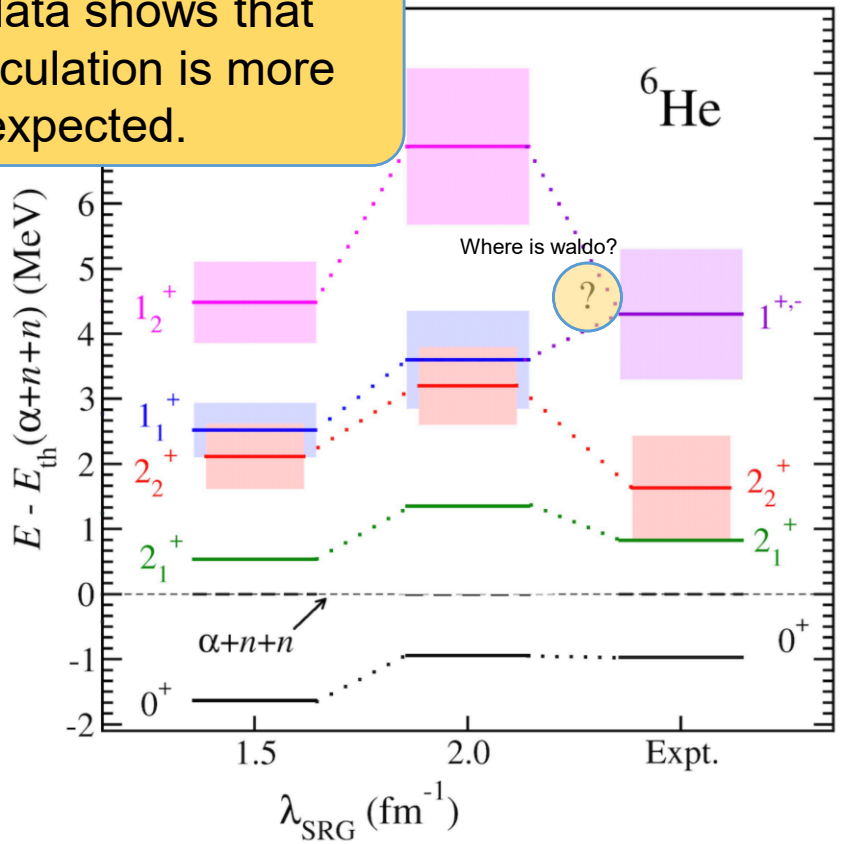
^{6}He 2n Halo nuclei

C. Romero-Redondo, S. Quaglioni *et al.* PRL117 (2016); PRC97 (2018)

^{6}He g.s. energy, proton and matter radii

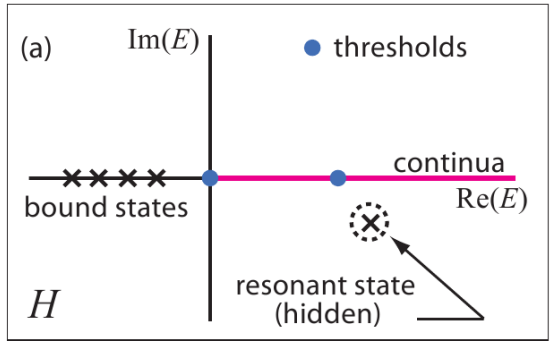


- Reanalysis of data shows that our *ab initio* calculation is more accurate than expected.

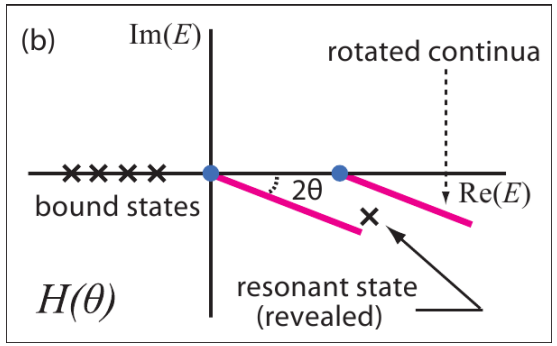


- Still significant room for improvements.
- Ab initio outputs from 2n-systems not yet used in reactions model.

Asymptotically vanishing equivalent problem



Complex scaling

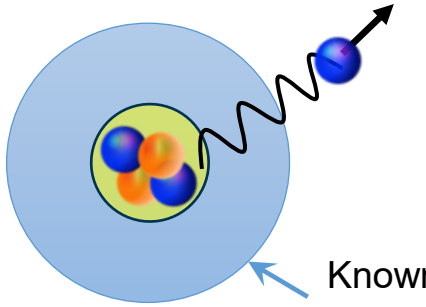


Kruppa *et al.* PRC**89** (2014)

"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.

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

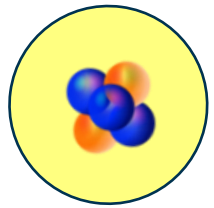
$$\hat{H}(\theta) = e^{-2i\theta}\hat{T} + \hat{V}\left(re^{i\theta}\right)$$
$$\hat{H}(r) = \hat{U}(\theta)\hat{H}(r)\hat{U}^{\intercal}(\theta)$$



Known asymptotic

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

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



Spatially extended but exponential fall off

Boundary limit problem

Bound state problem

Resonances are characterized by complex poles of the S-matrix.

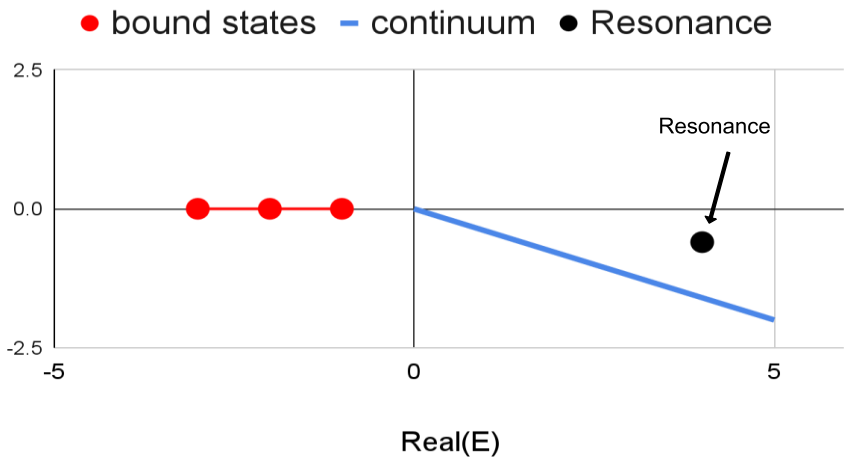
The scattering solutions linked to a resonance typically diverge.

However, complex scaling (CS) transforms these solutions into square-integrable forms, making them accessible via bound-state methods such as the NCSM.

$$\phi_{sc}(r \to \infty) = A(k)\mathrm{e}^{-\mathrm{i}kr} + B(k)\mathrm{e}^{+\mathrm{i}kr} \simeq \mathrm{e}^{-\mathrm{i}kr} + F(k)\mathrm{e}^{+\mathrm{i}kr}$$

At $E = \varepsilon_n - i\frac{\Gamma_n}{2}$

$$\phi_n^{\mathrm{res}}(r \to \infty) = B(k_n)\mathrm{e}^{+\mathrm{i}|k_n|\mathrm{e}^{-\mathrm{i}e\alpha}r} = B(k_n)\mathrm{e}^{\mathrm{i}a_n r}\mathrm{e}^{+b_n r} \to \infty$$



$\hat{S}$ definition of the CS operator:

$$\hat{U}f(r) = f\left(r\mathrm{e}^{\mathrm{i}\theta}\right)$$

$$\hat{U} = \mathrm{e}^{i\theta\frac{\partial}{\partial r}}$$

- $\hat{H}\phi_n = \varepsilon_n\phi_n$
- $\left(\hat{S}\hat{H}\hat{S}^{-1}\right)\left(\hat{S}\phi_n^{\mathrm{res}}\right) = (\varepsilon_n - (\mathrm{i}/2)\Gamma_n)\left(\hat{S}\phi_n^{\mathrm{res}}\right)$

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

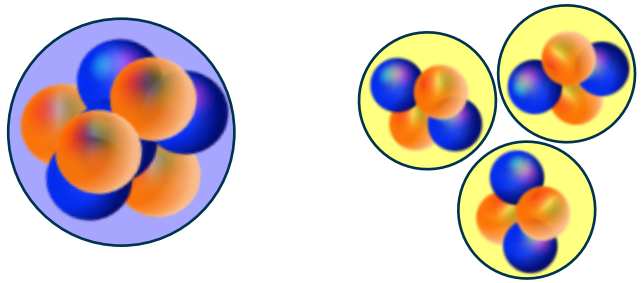
Structure

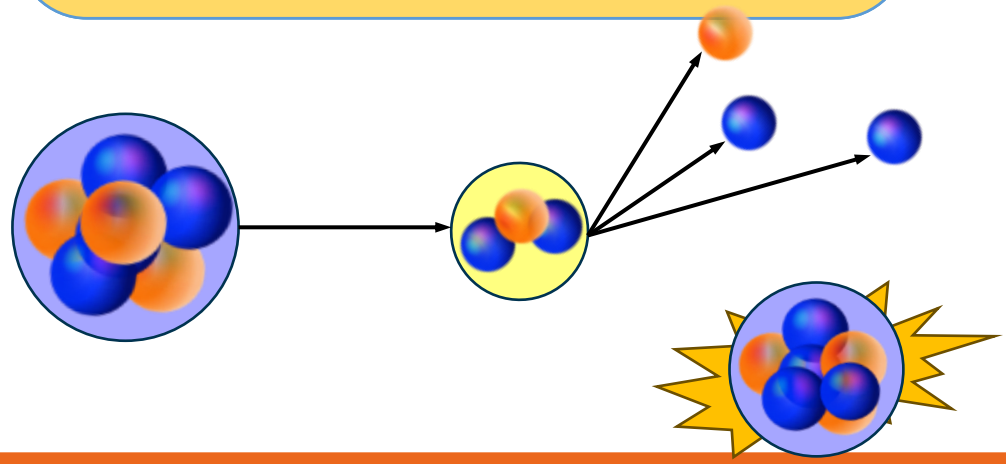
☺ Extraction of resonance properties for fine tuning interactions and applications to astrophysics.

Reactions

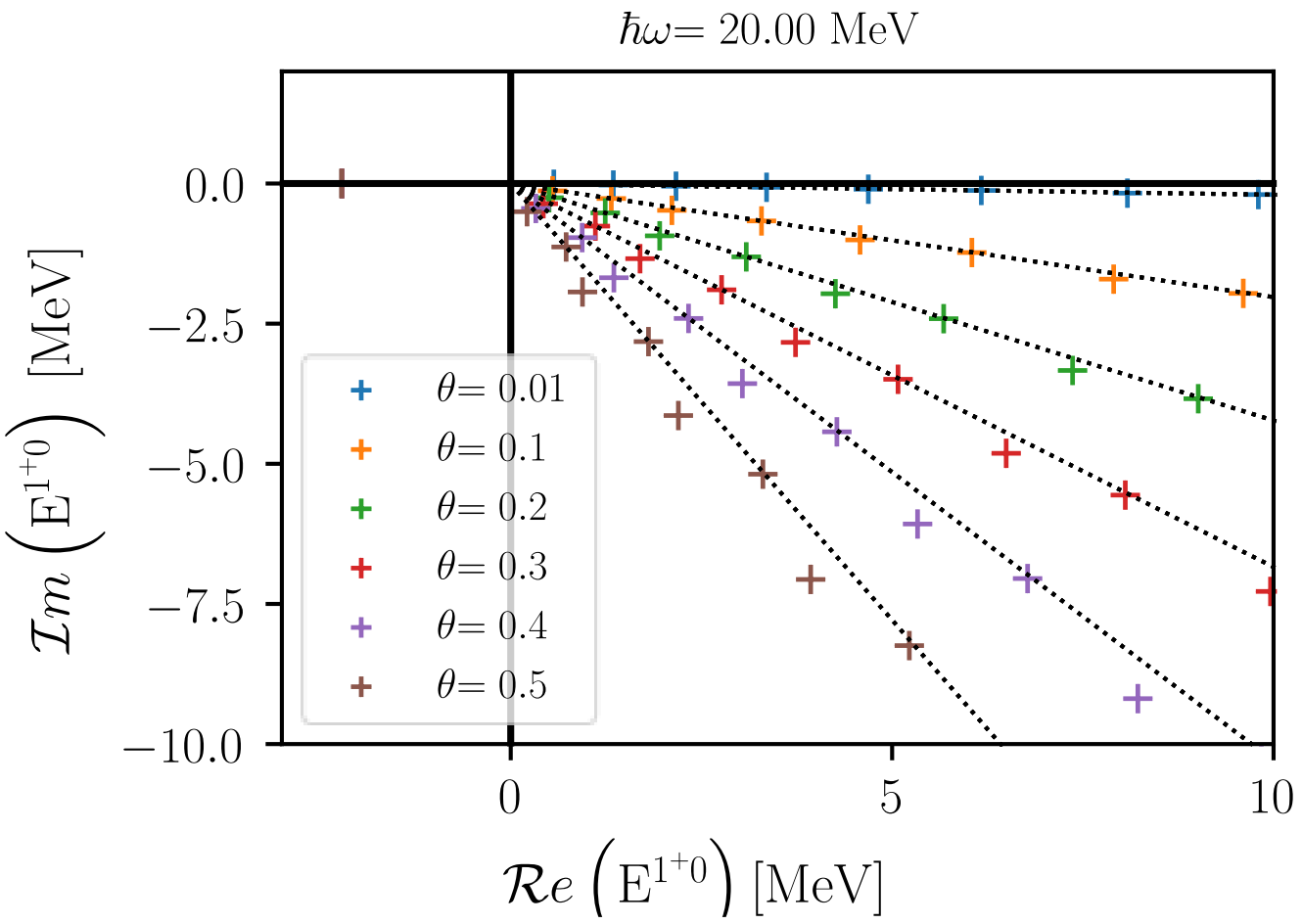
☺ Enabling us to study nuclear breakup reactions including Final State Interaction (FSI)

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



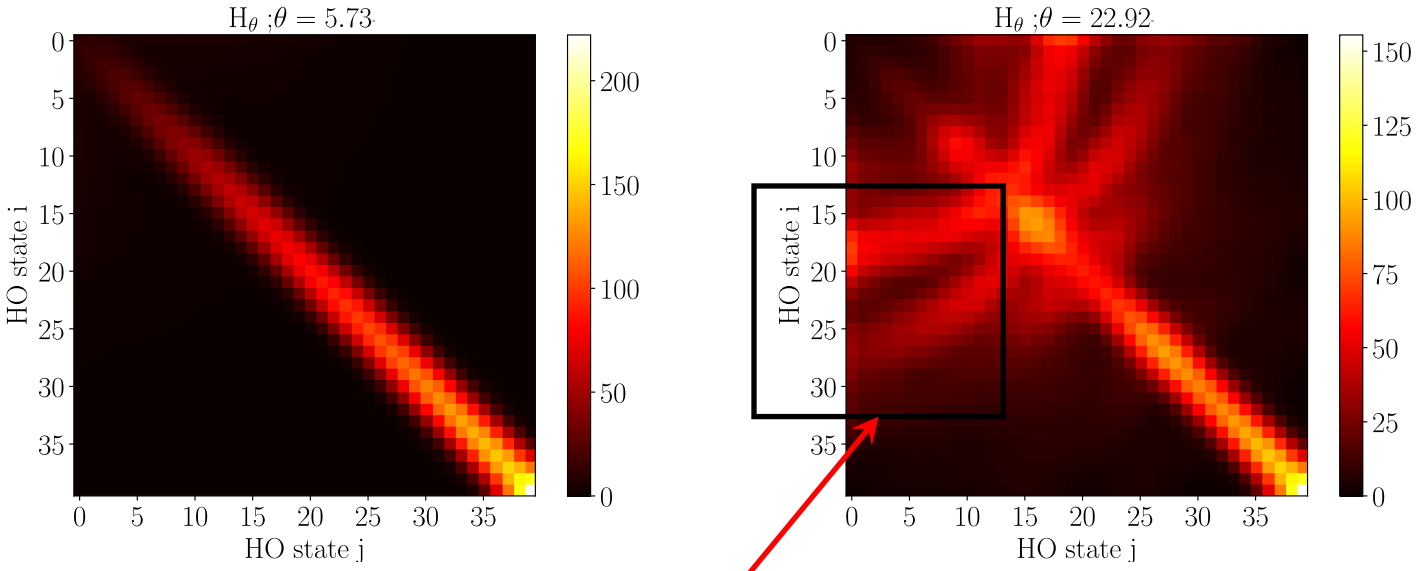


CS Hamiltonian eigenvalues using EM N3LO interaction



- 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 (known but not publicized).

A=2 Hamiltonian matrix elements with complex values*



Large off-diagonal coupling m.e.s

Maximum model space achievable $N_{\max}\sim 200$ (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.

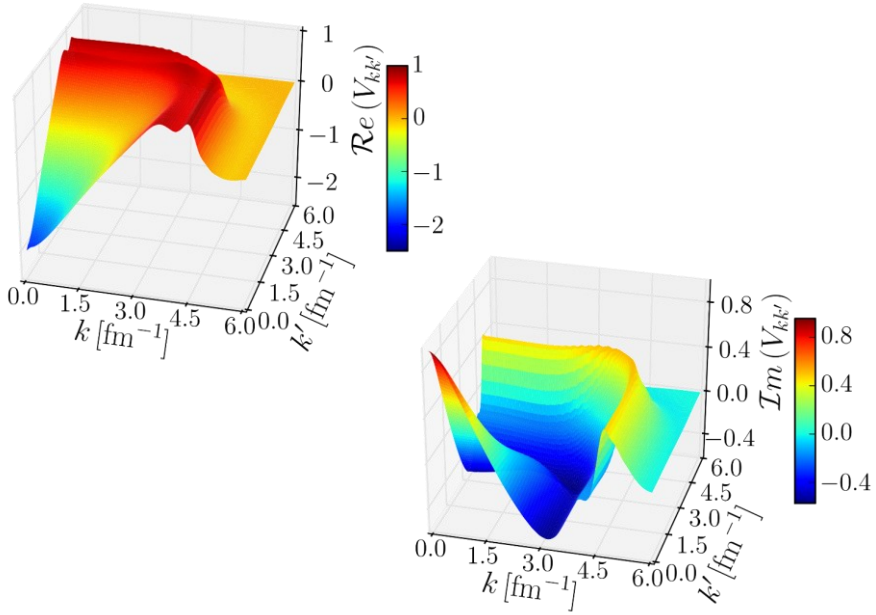
* The absolute value of the elements are shown

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

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

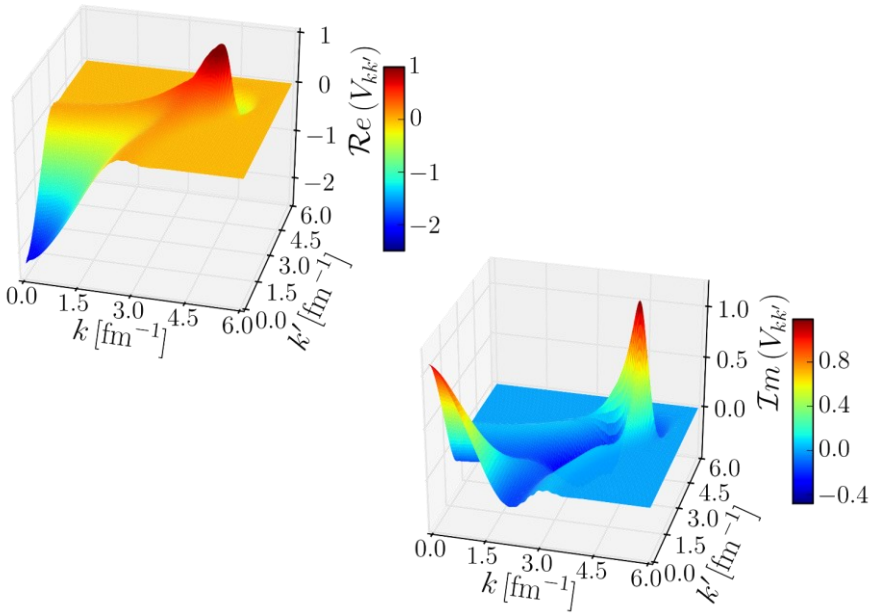
Similarity Transformation

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



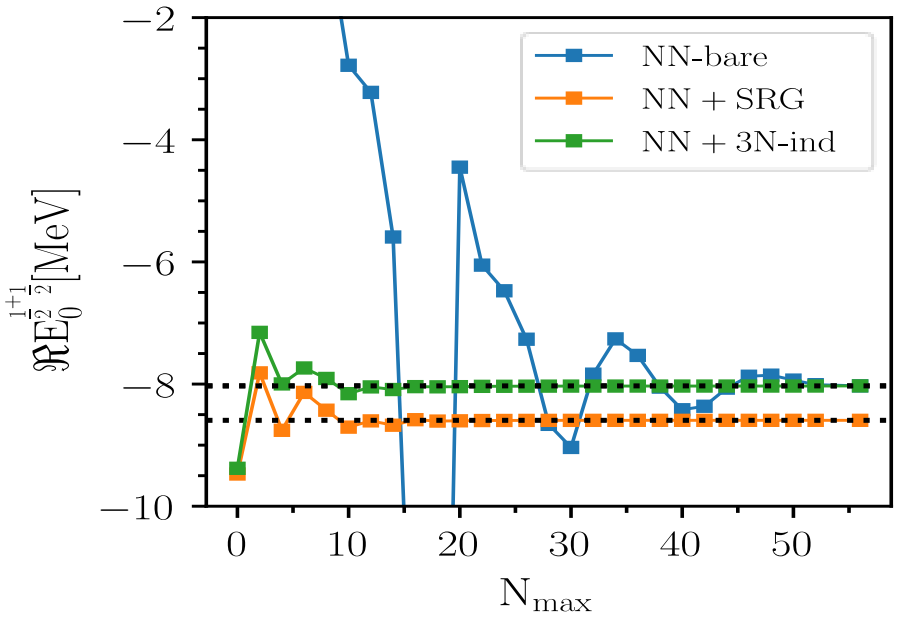
Evolution with flow parameter λ

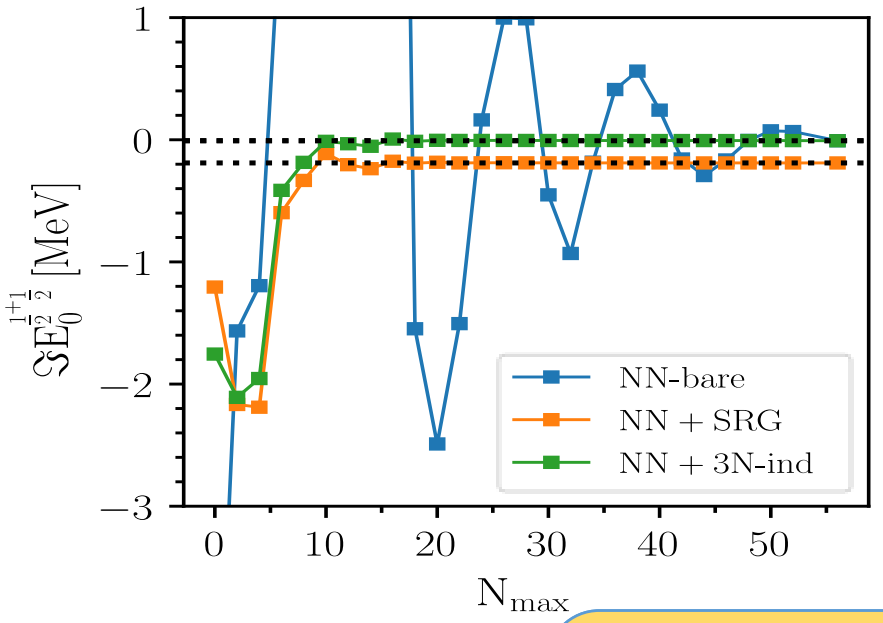
Consistent evolution of the imaginary part

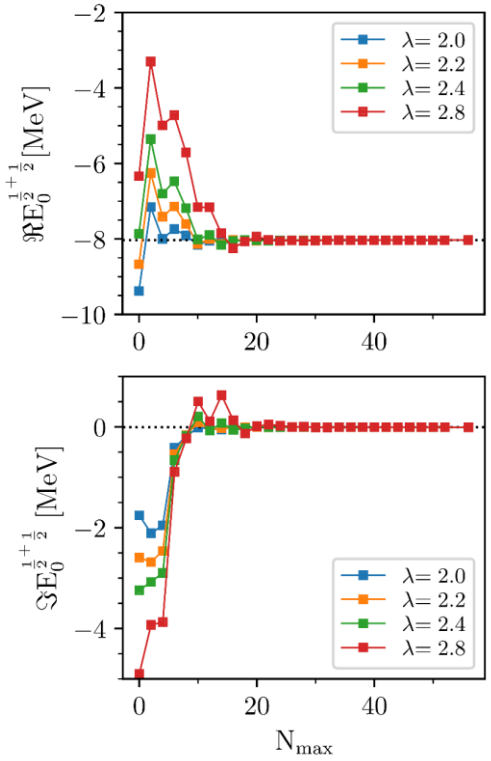


Quality of the rotated Hamiltonian evaluated in A=3

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



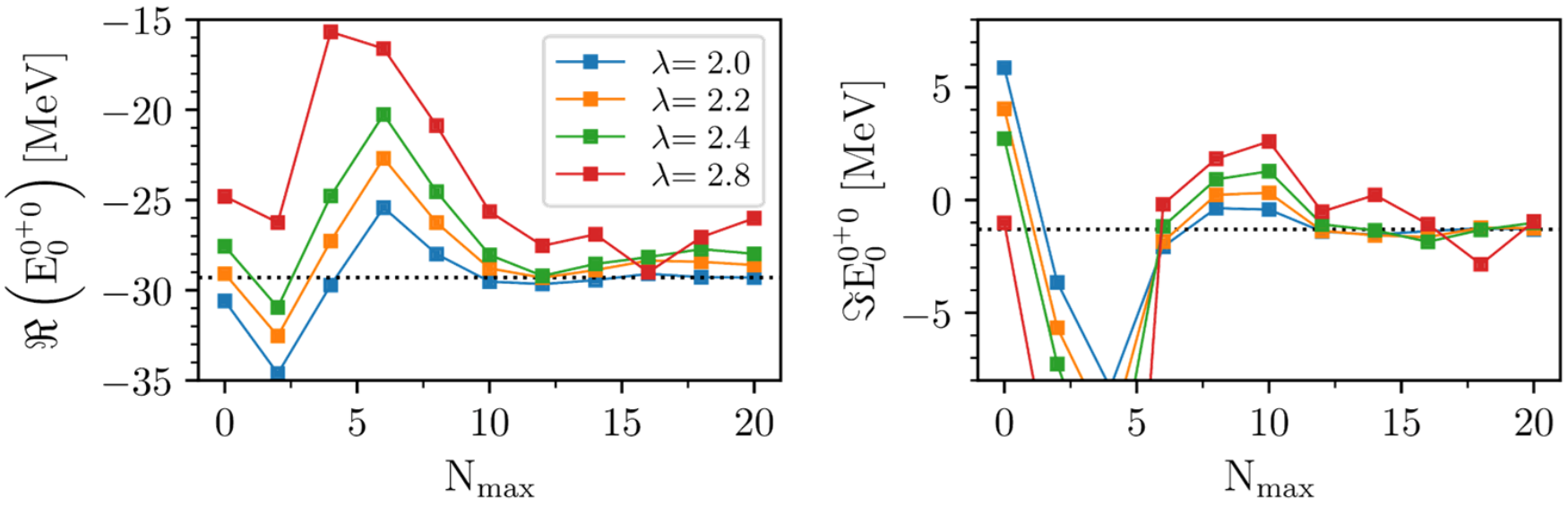




Maximum model space achievable N_{max}~60 (30 nodes a box in excess of 15 fm)

- SRG leads to faster convergence;
- Induced 3N-interaction needs to be accounted for (as expected from literature).

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

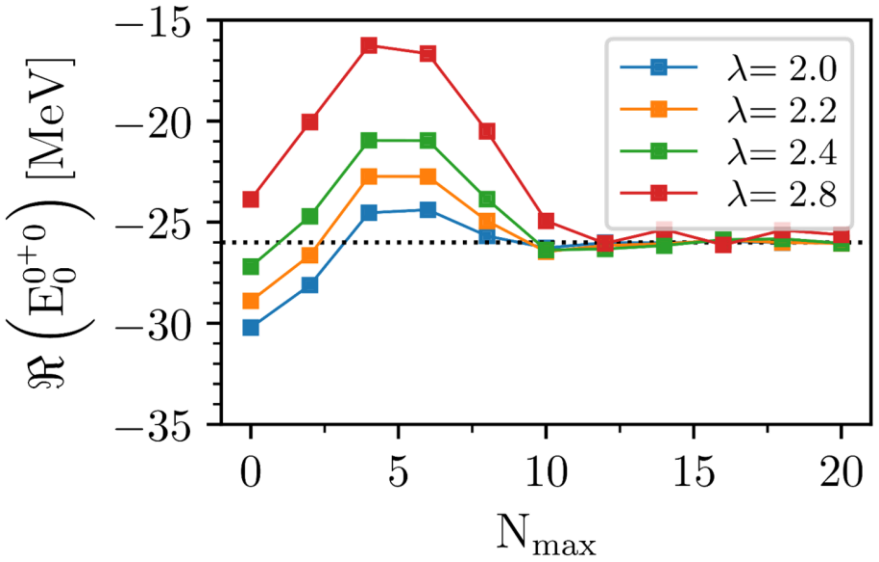


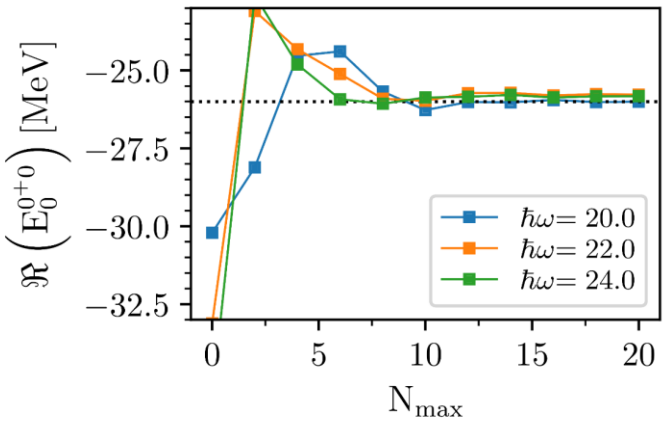
Maximum model space achievable $N_{\max}$~20 (10 nodes a box in excess of 8 fm)

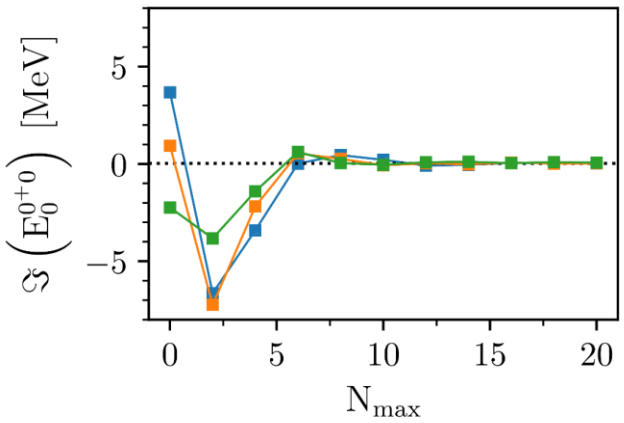
- Large λ makes the CS-Hamiltonian to converge monotonously;
- Smaller λ is better for convergence;
- Induced $A = 3$ interaction is important.

Quality of the rotated Hamiltonian evaluated in A=4

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





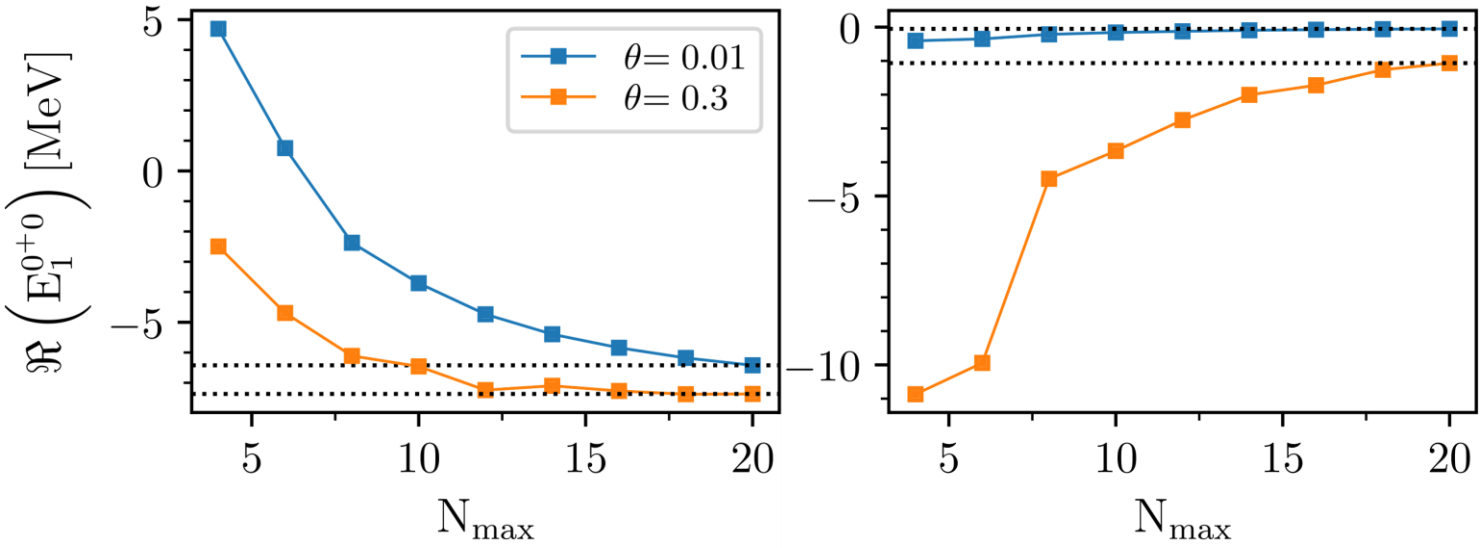


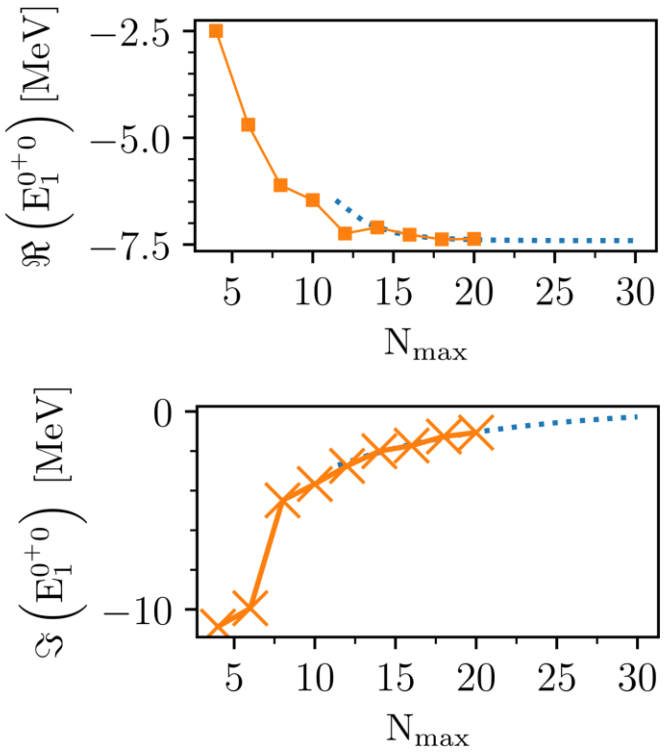
$A = 3$ evolution is made in the maximum model space achievable N_{max}~60

- Induced $A = 4$ interaction is not significant;
- The flow parameter is limited to at best $1.8\ \mathrm{fm}^{-1}$ due to the A=3 CI space needed for the evolution.

Quality of the rotated Hamiltonian evaluated in A=4

α 0_1^+ convergence with CS+SRG NN+3N Hamiltonian



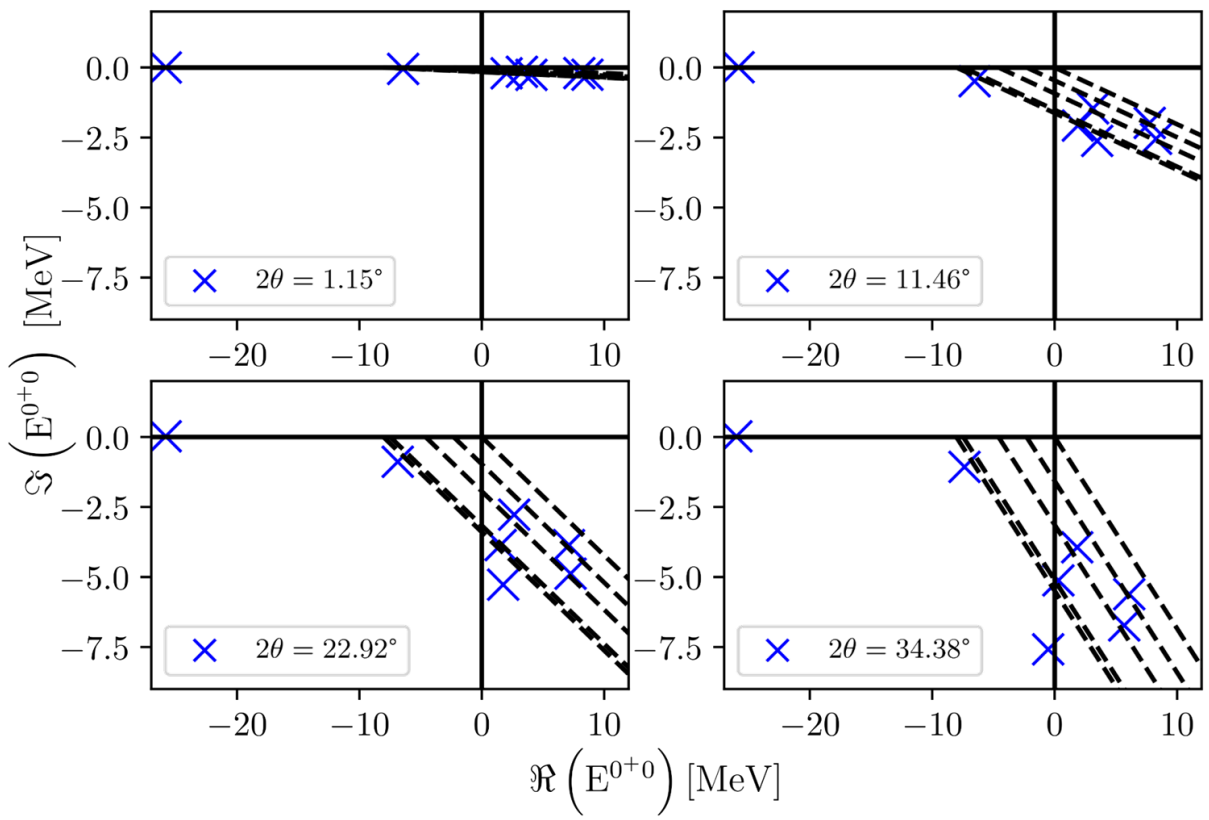


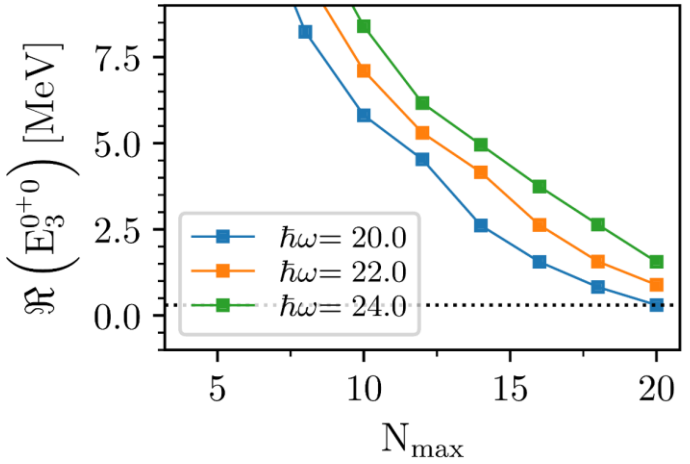
Advanced SRG research permits to reach a rotation of 0.38 rad, which corresponds to resonances of 43.5°

- The resonance is properly describes with a spectra rotation by 34.4°;
- This result totally fails to agree with experiment (± known).

Quality of the rotated continuum in A=4

α spectrum with CS+SRG NN+3N Hamiltonian





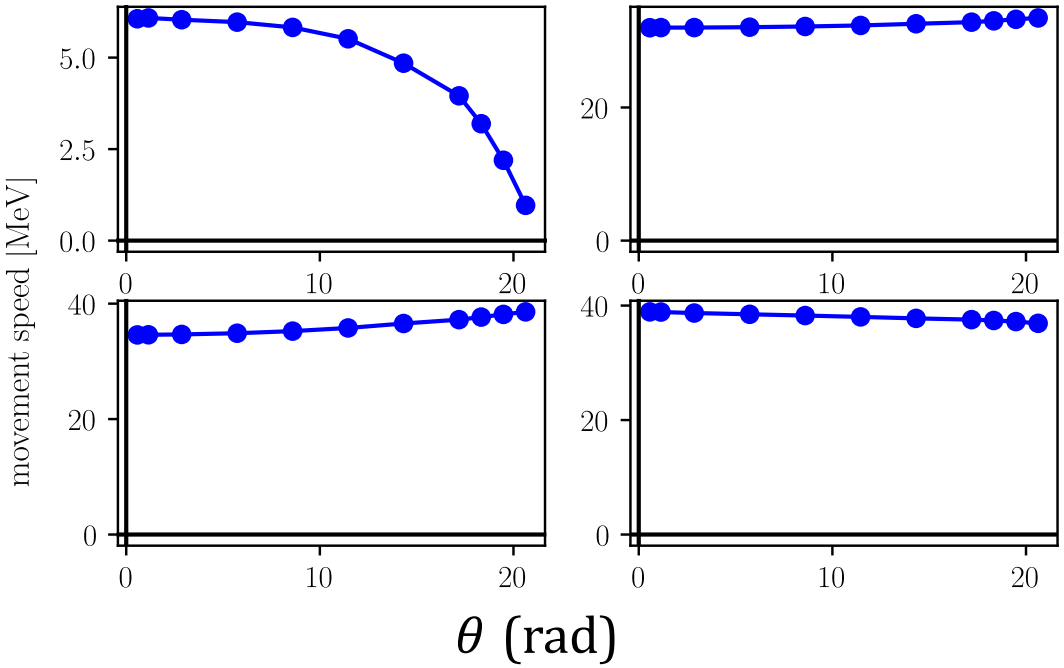
Further progress is needed with SRG to tackle non-Hermitician matrices

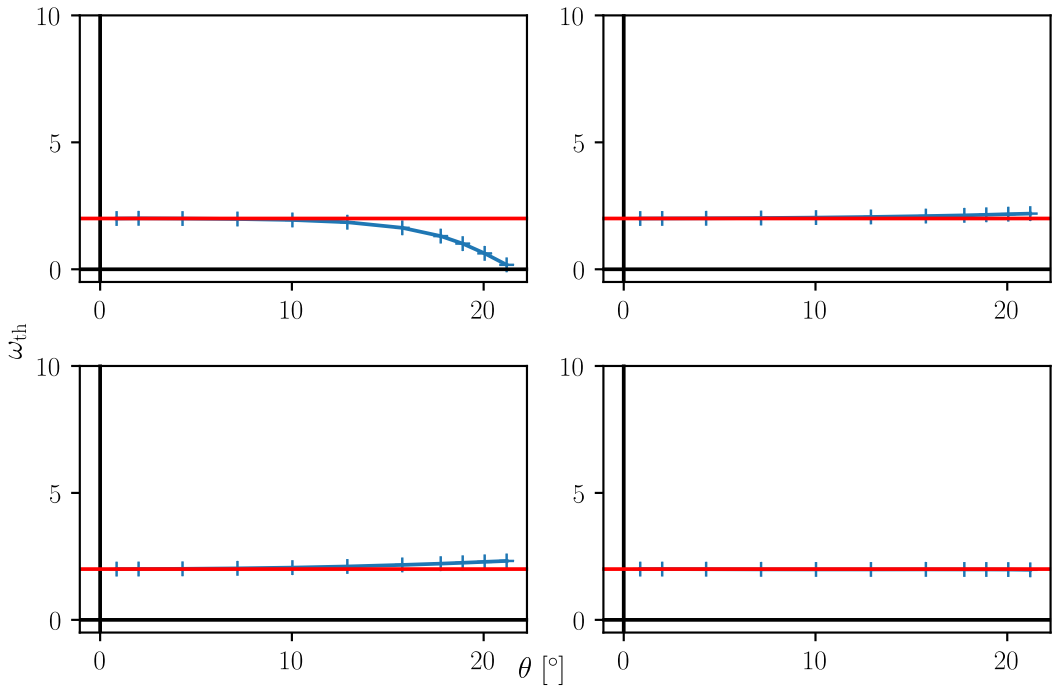
- The positive energy spectrum is challenging to disentangle;
- Convergence analysis with $\hbar\Omega$ and Θ can help to identify resonances.

How to extract the thresholds ?

Problem:

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

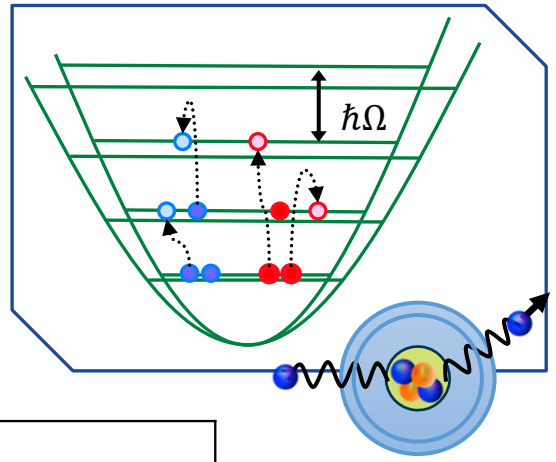


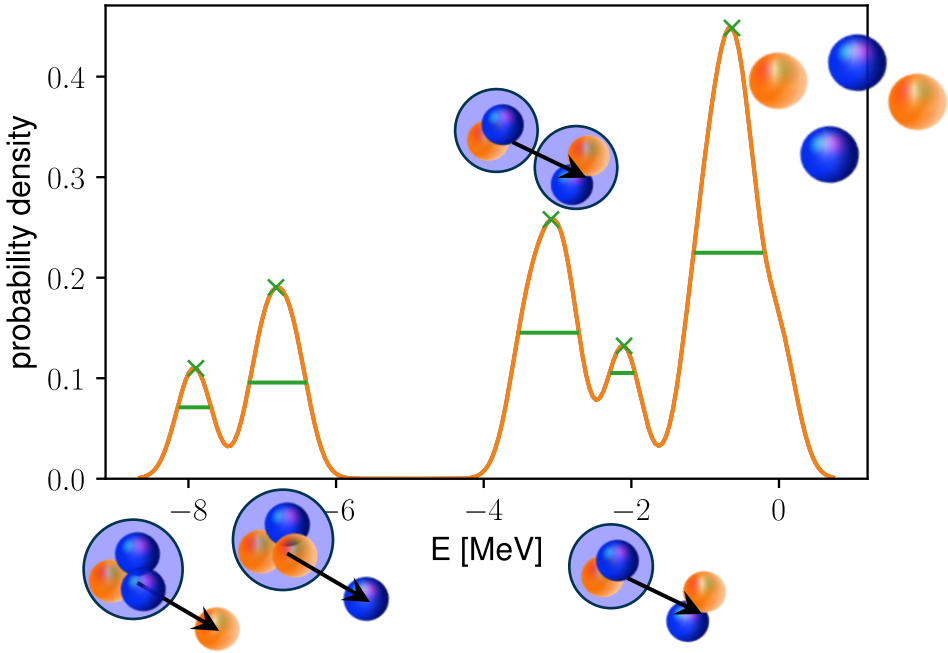


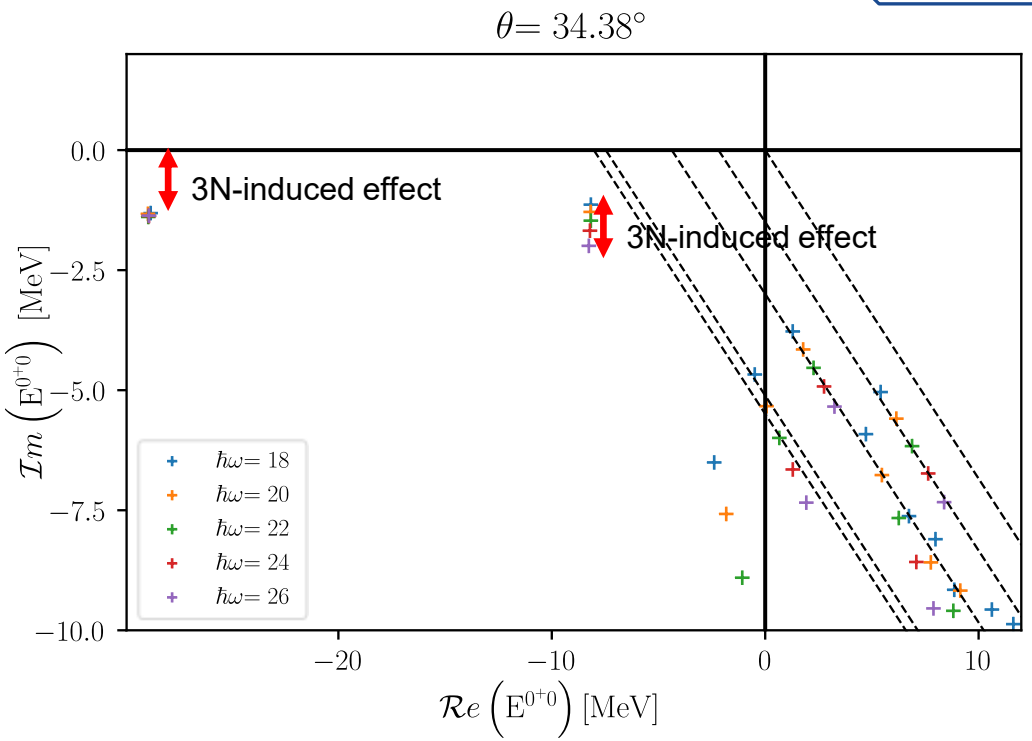
Preliminary, in the sense that insufficient rotation required convergence analysis (only lower bound of can be extracted);
Proof of principle that the CS-Hamiltonian is accurate and can be used in NCSM calculation up to $A{\sim}16$;

How to extract the thresholds ?

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

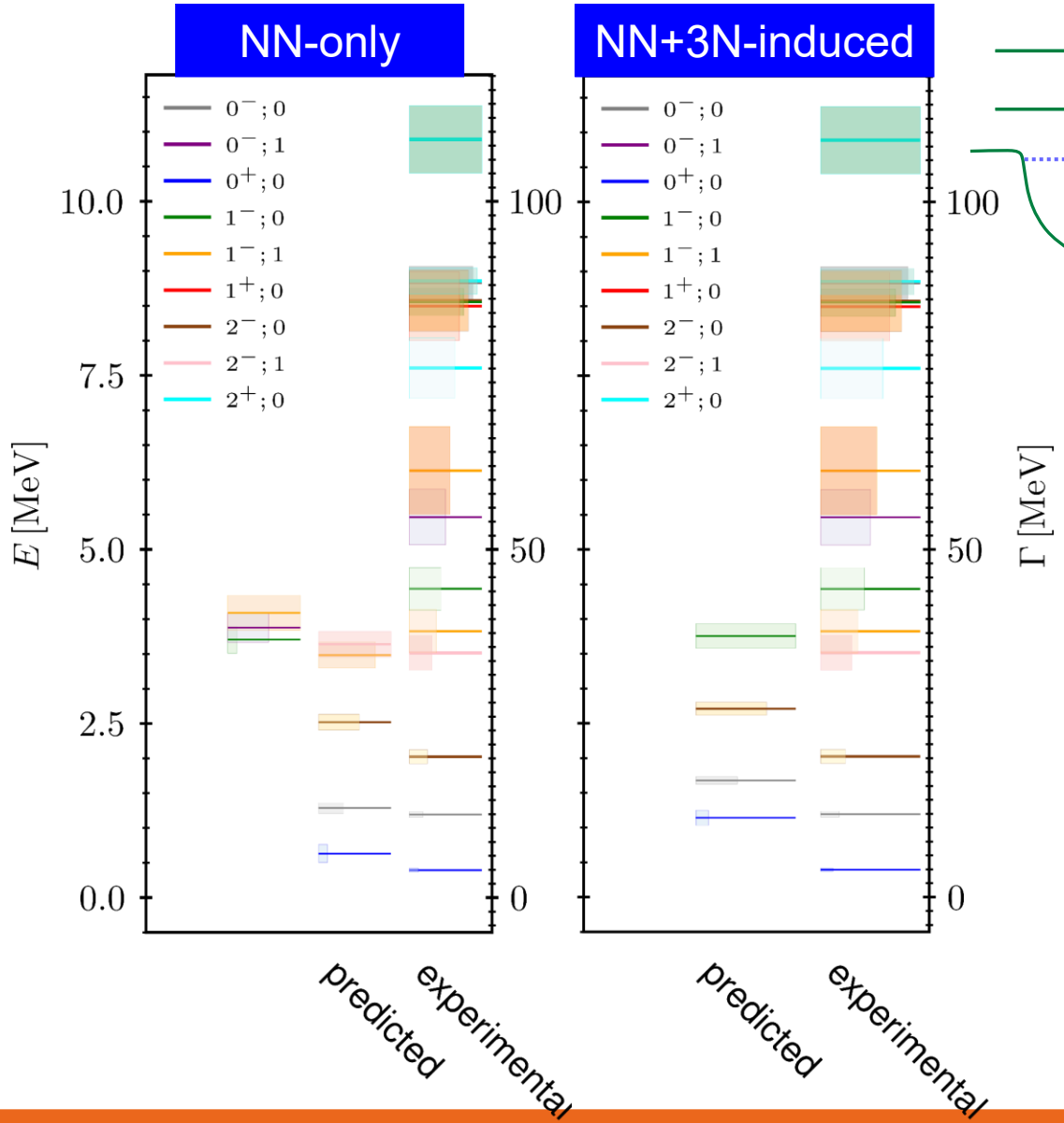


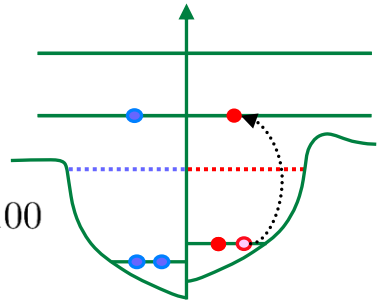


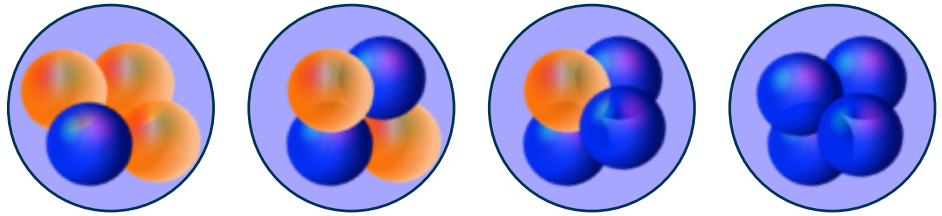


- The expected threshold are somewhat recovered w.r.t. experiments;
- Threshold energies does not converge at the same pace as the g.s.

Wrap-up on the spectrum after analysis of the results







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

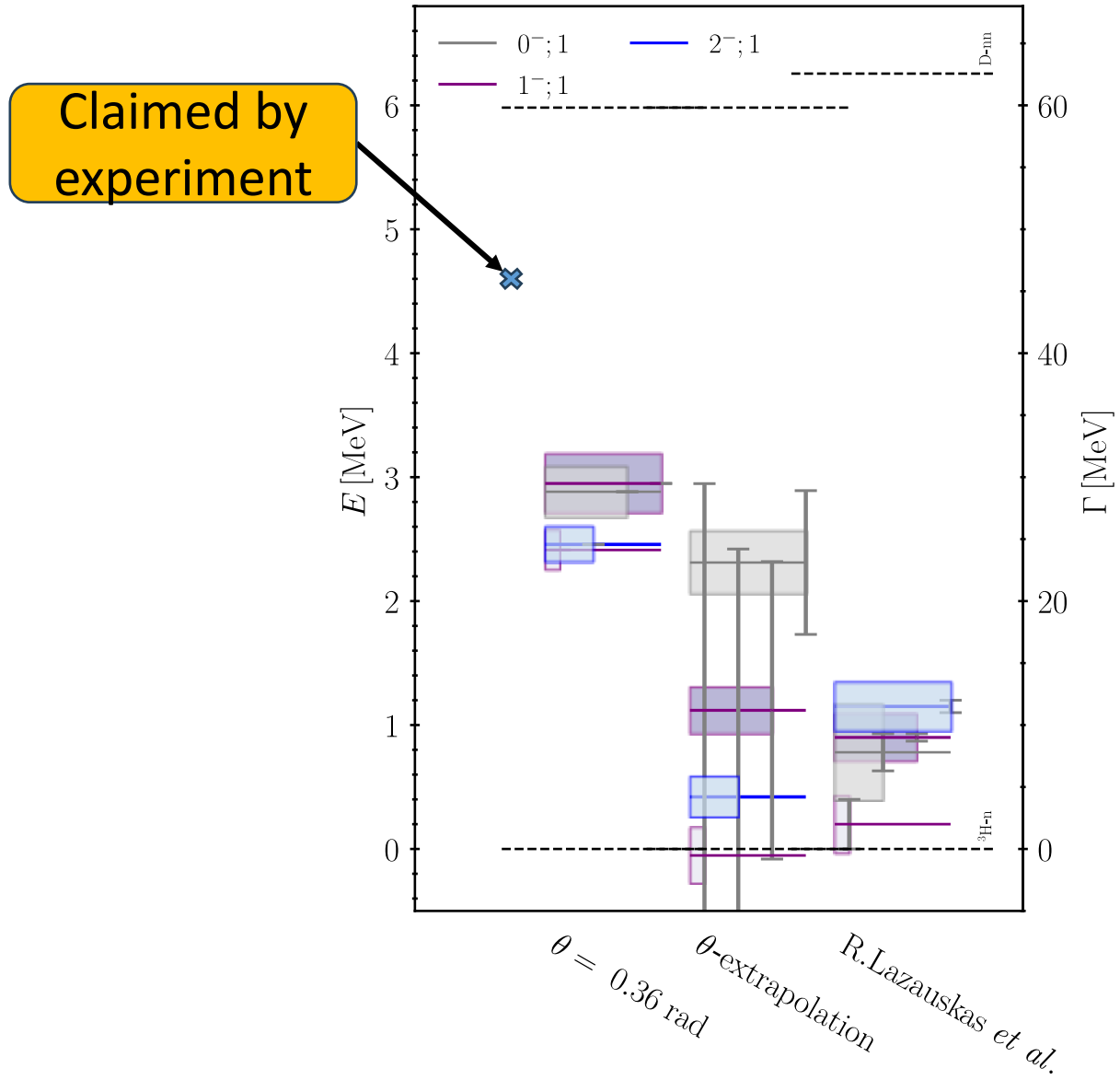
Preliminary, in the sense that insufficient rotation required convergence analysis (only lower bound of can be extracted);
Proof of principle that the CS-Hamiltonian is accurate and can be used in NCSM calculation up to $A{\sim}16$;

- Discrepancies with experiments too large to be corrected by 3N forces;
- Convergence analysis with $\hbar\Omega$ and Θ can help to identify resonances.

^{4}H system: a benchmark with Faddeev calculation

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).

Existence of the ^{4}n resonance

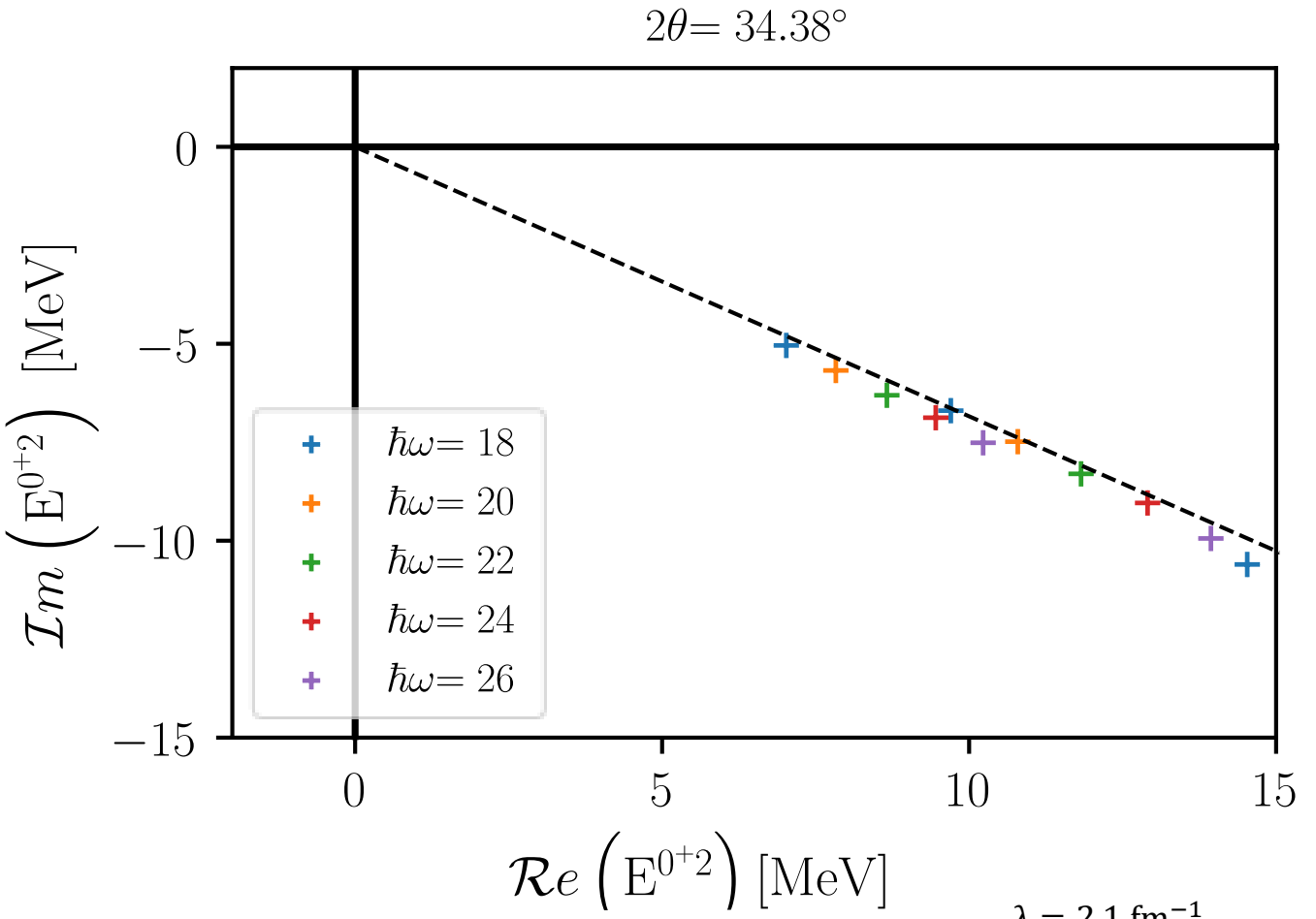
CS shows **no indication** of such a resonance in 1^+, 1^-, 0^+ or 0^-.

The results give a lower bound of:

$$\Gamma_r = 1.9\, E_r$$

or

$$\Gamma_r = 4.5\ \mathrm{MeV}$$



$\lambda = 2.1\ \mathrm{fm}^{-1}$,
$\theta = 0.3$ rad, $\mathrm{N_{max}}$~18,
$\hbar\omega = 20$ MeV, Nf = 12

No ^{4}n resonance exist in the vicinity of the real momentum energy axis.

(iii) Research directions

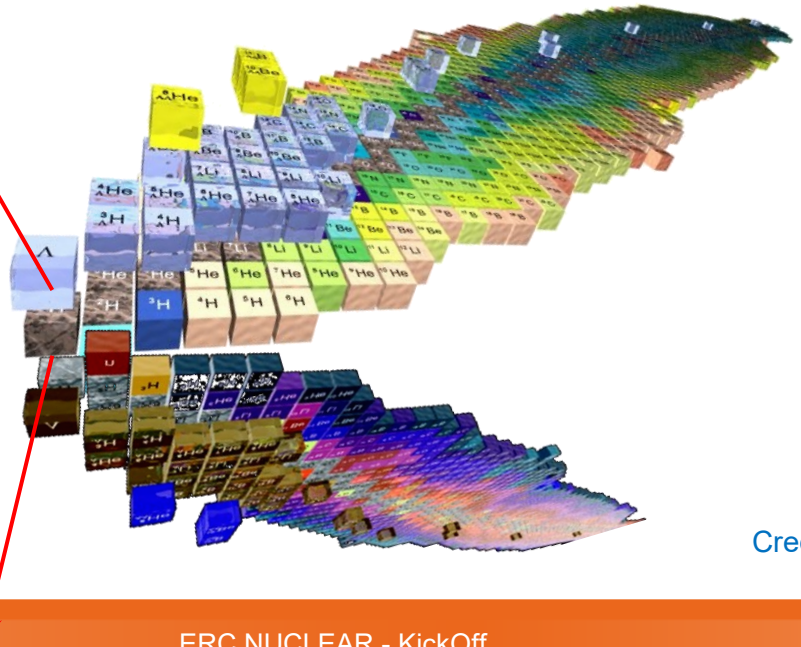
Complexity of scattering problem

Complexity of many-body solution

Both

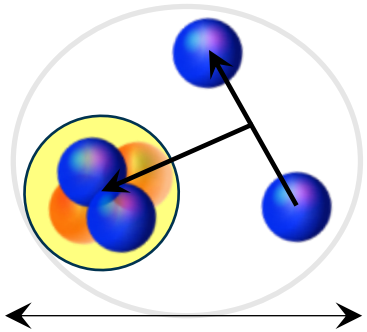
$\neq n, p$ particles interacting with strong force ($M_h \gg M_{n,p}$)

$M_h \leq M_{n,p}$



- 😐 Nuclear theory is **data driven**.
- ☹ Global optical models (NN or $N\bar{p}$ or $N\pi$ scattering) are not applicable to exotic systems.

Credits H. Lenske



r.m.s. radius ~2.4 fm

$\bar{\mathrm{N}} - \mathrm{A}$ capture

$Z = 2$ r.m.s. radius at annihilation ~50 fm

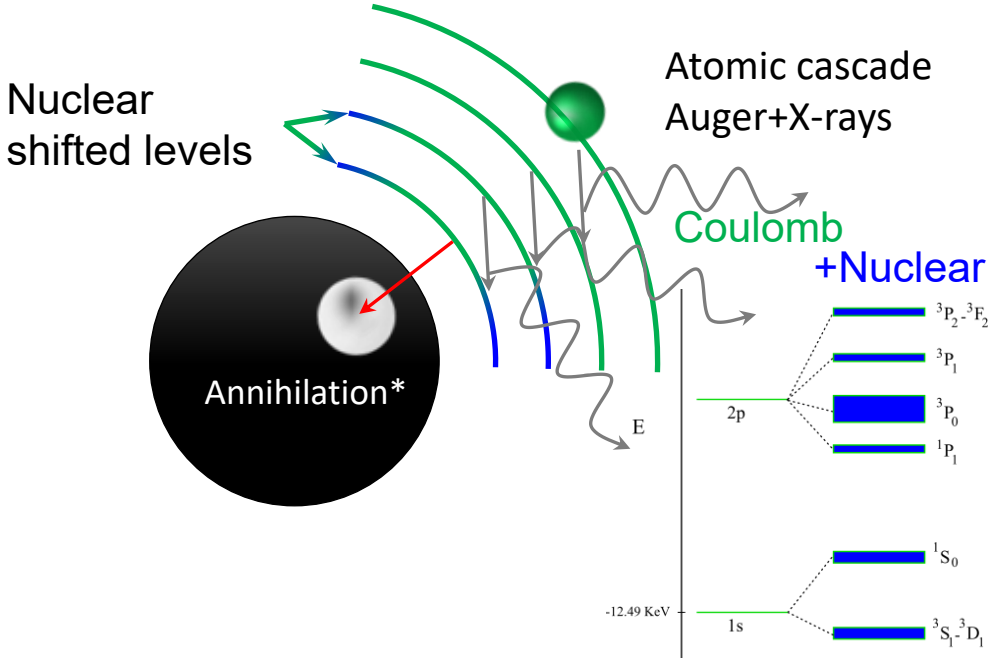
not scaled

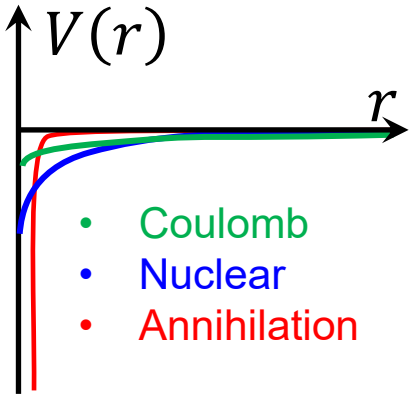
$Z \gg 2$

$r_n = \frac{57\ \mathrm{fm}}{Z} \frac{m}{2\mu} n^2$

$n \sim 4 - 9$

Ab initio for A < 10 then **Halo/pert**. EFT

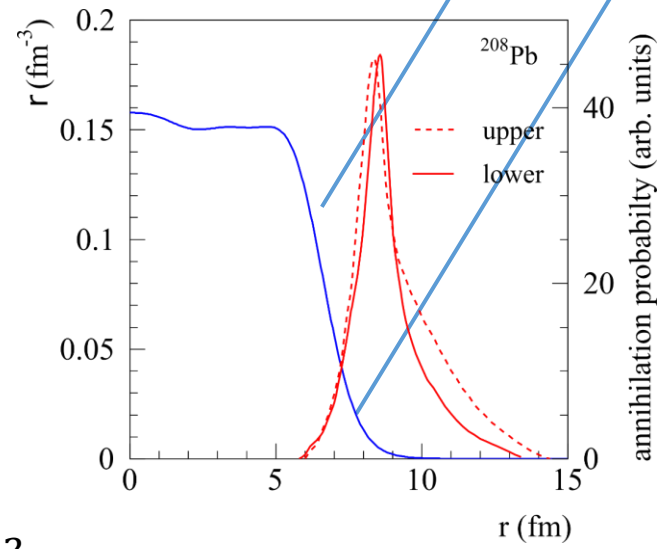




In flight capture

Cold capture

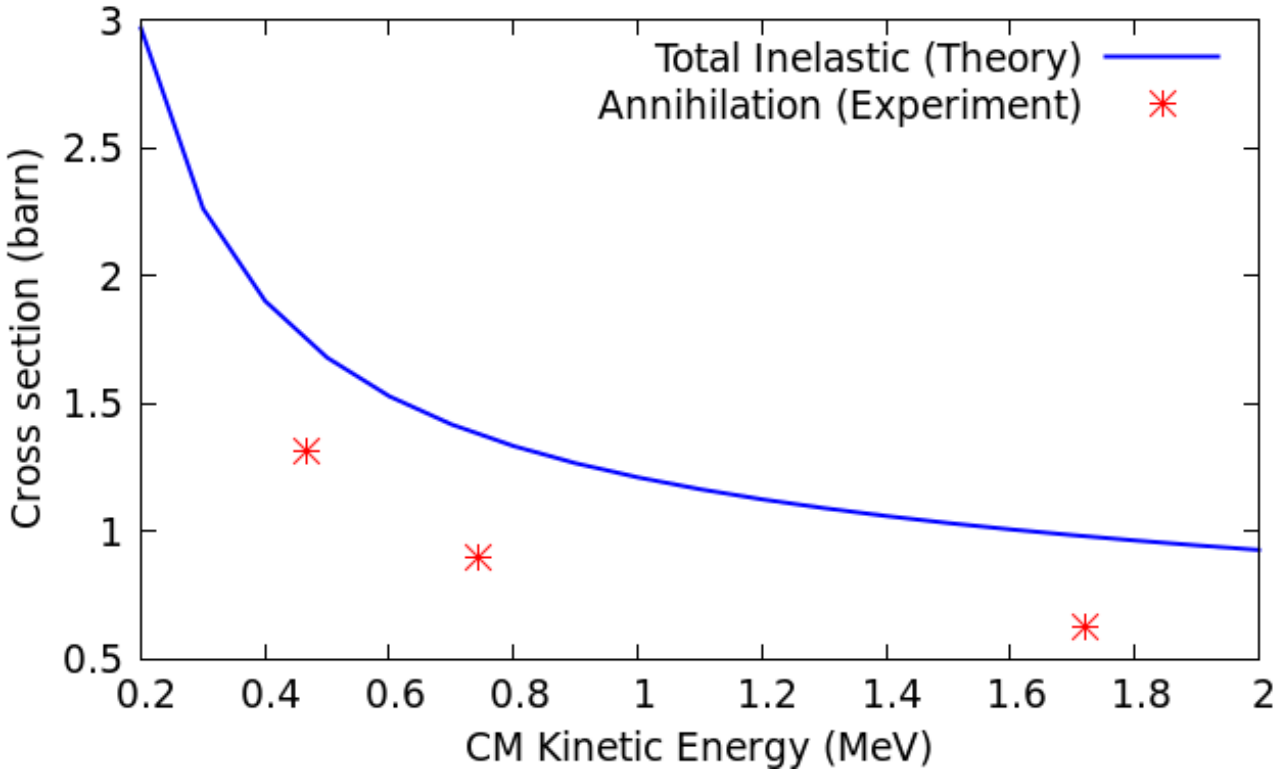
Trzcińska, *et al.* PRC**67** (2003)

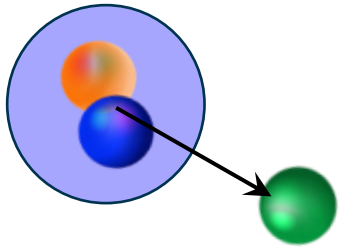


$$E = E_R - i\frac{\Gamma}{2}, \quad \Gamma = \Gamma_n + \Gamma_p$$

$$\frac{\Gamma_c}{2} = \int d\boldsymbol{R}\, \Im\left(W^c_{\bar{N}N}\right) \left|\Psi_{\mathrm{A}-\bar{\mathrm{p}}}(R)\right|^2$$

Level shifts and annihilation cross-section





Method	ϵ_{1S} (keV)	$\Gamma_{1S}/2$ (keV)
NCSM/RGM	2.43	1.27
Faddeev	1.92	0.89
Exp.	-1.05 ± 0.025	0.55 ± 0.0375

Annihilation cross-section of the $A = 3 + 1$ system N_{max}= 70 compared to data.

- Cross-section, differential cross-section, spin polarization, E.M. transitions to the continuum etc… all are calculated (or calculable).