

Ab initio theory for reactions and exotic nuclei

Guillaume Hupin, CNRS IPNO

Recent advances and challenges in the description of nuclear reactions at the limit of stability, March 6th 2018

Collaborators

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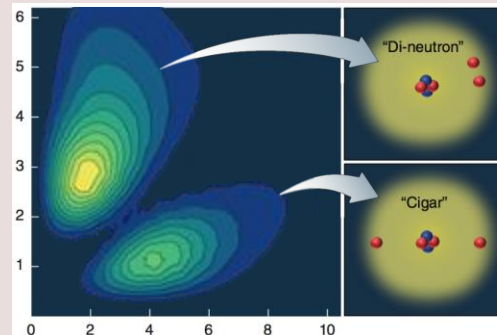
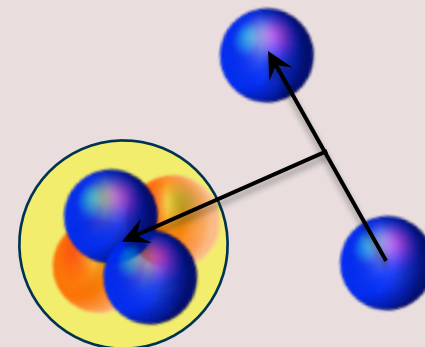
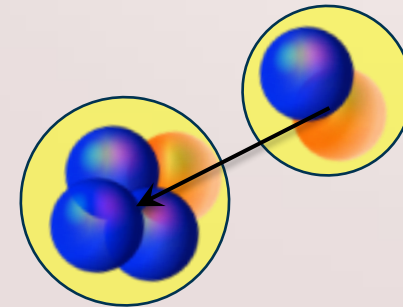
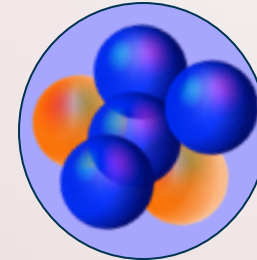
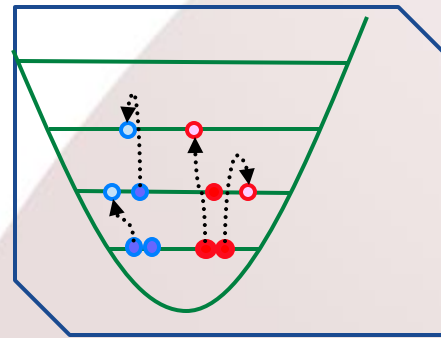
F. Raimondi (Uni. of Surrey)

C. Romero-Redondo (Industry)

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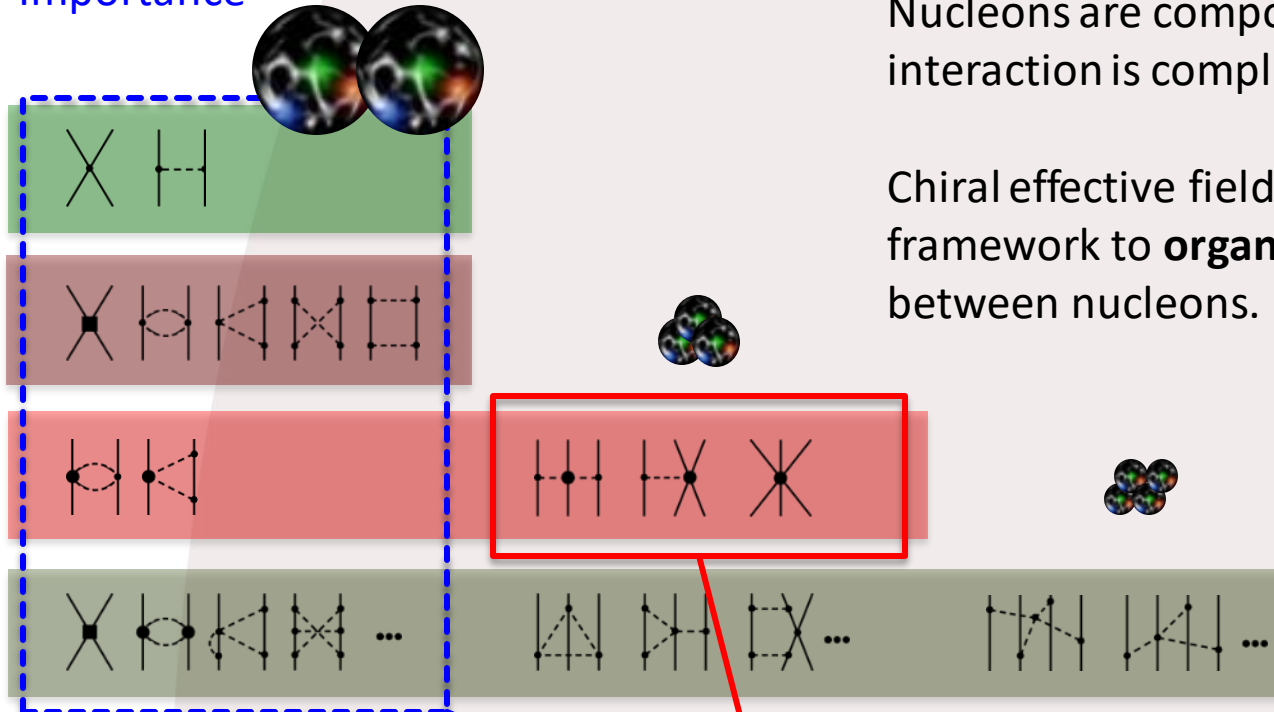
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CHIRAL EFFECTIVE FIELD THEORY, A MODERN DERIVATION OF NUCLEAR EFFECTIVE INTERACTION

Importance



Nucleons are composite objects. The nuclear interaction is complex by nature.

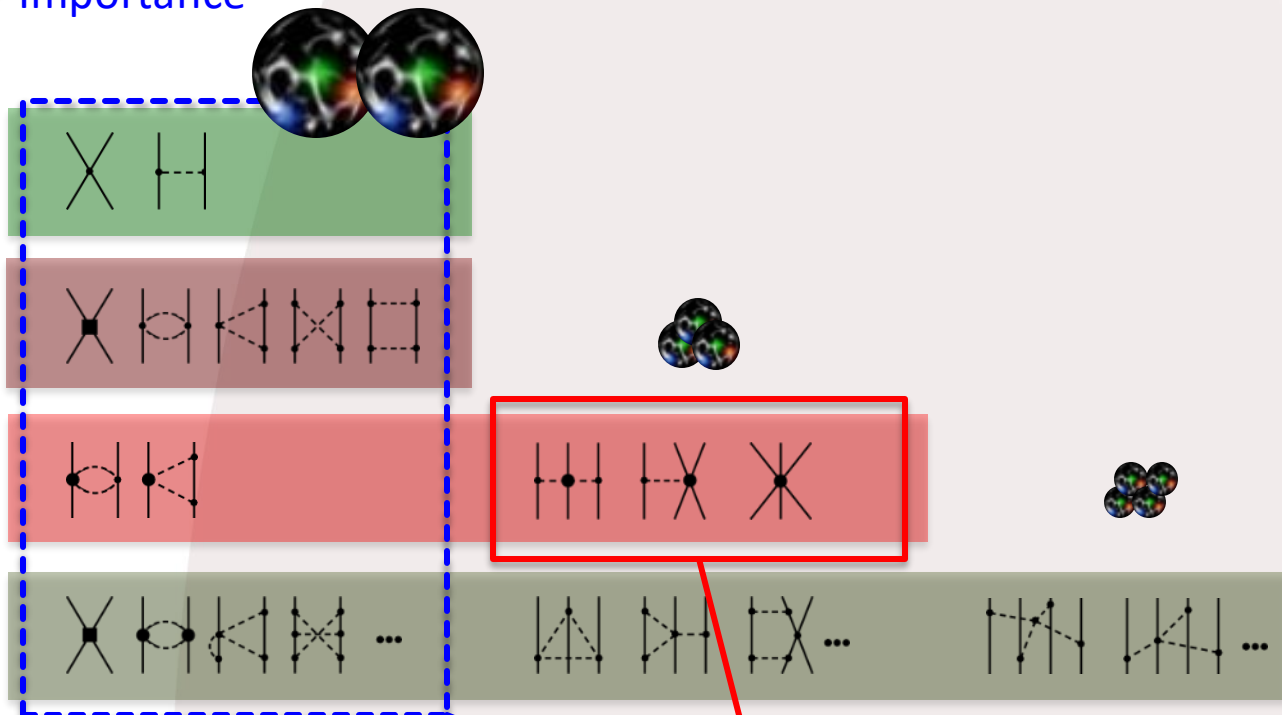
Chiral effective field theory offer a **consistent** framework to **organize** the interaction between nucleons.

- Yet uncompleted...

Constrained to provide an accurate description of the $A=2$ and $A=3$ systems.

Predictions for nuclear structure and dynamic ($A>3$).

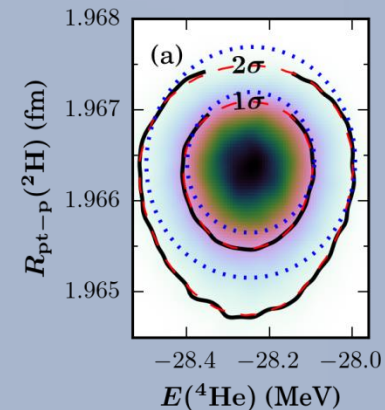
Importance



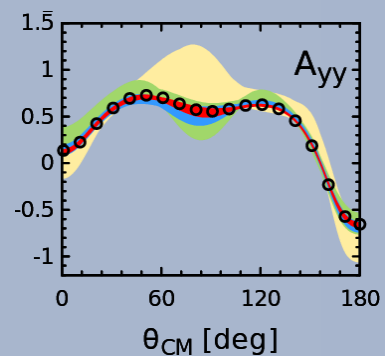
• Yet uncompleted...

Constrained to provide an accurate description of the $A=2$, $A=3$ and $A=4$ or $A>3$ systems?

Predictions for nuclear structure and dynamic ($A>3$).



B. D. Carlsson *et al.*
PRX6 (2016)



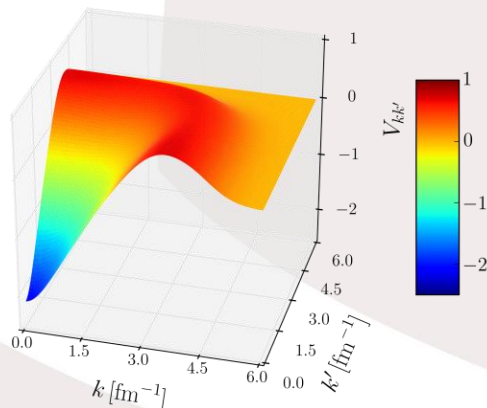
E. Epelbaum, *et al.*
PRL115 (2015)

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

$$H_\lambda = \underbrace{U_\lambda H U_\lambda^\dagger}_{\substack{\text{Unitary} \\ \text{transformation}}} \quad \left\{ \begin{array}{l} \frac{dH_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), H_\lambda] \\ \eta(\lambda) = \frac{dU_\lambda}{d\lambda} U_\lambda^\dagger \end{array} \right.$$

Flow parameter

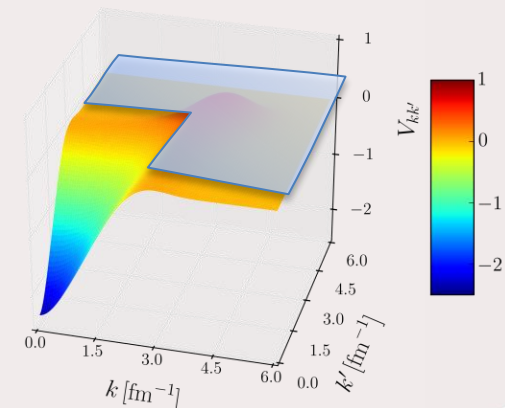
Bare potential



Evolution with flow parameter λ

- Preserves the physics
- Decouples high and low momentum
- Induces many-body forces

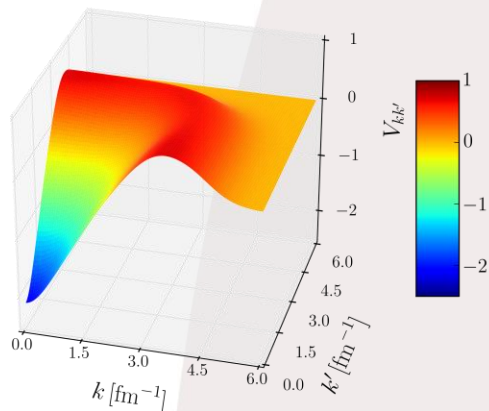
Evolved potential



EFFECTIVE INTERACTION ADAPTED TO MANY-BODY MODEL SPACE (I.E. PREDIAGONALIZED)

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

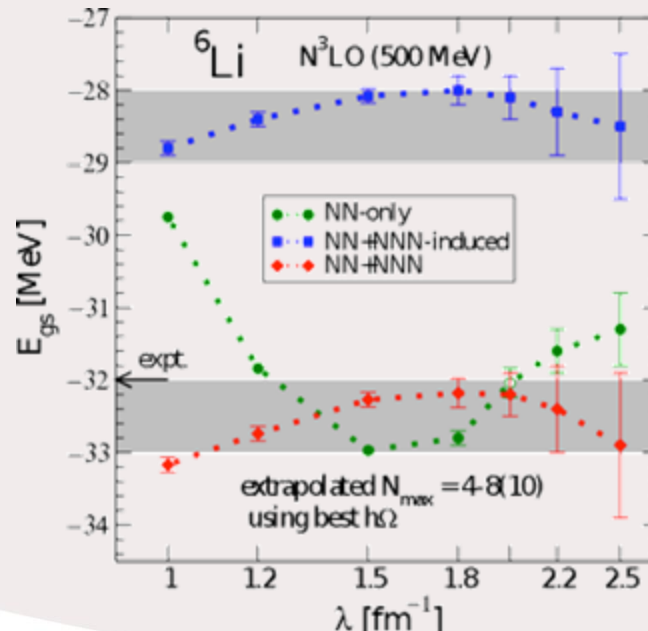
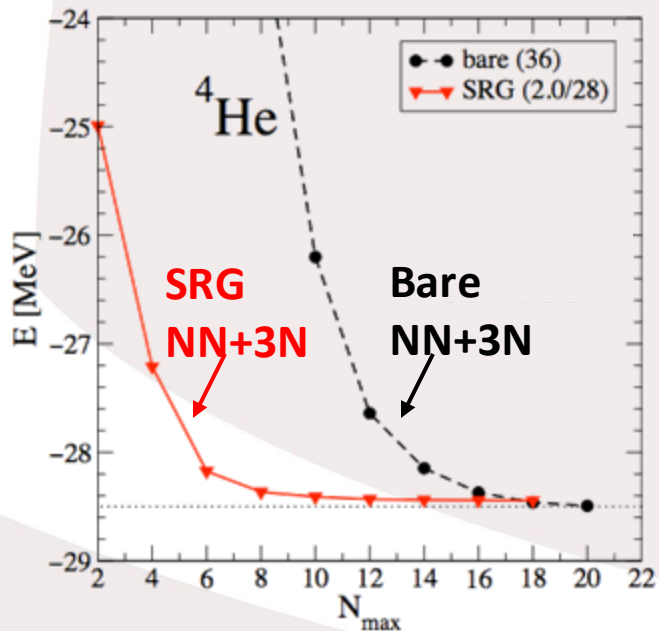
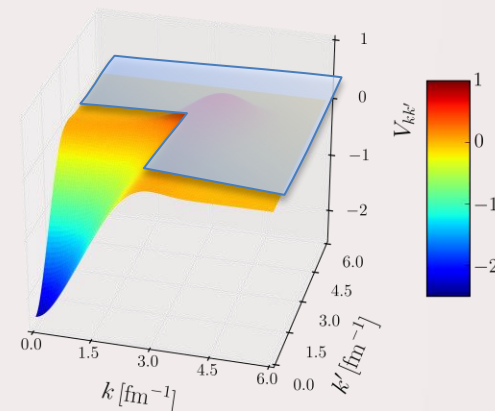
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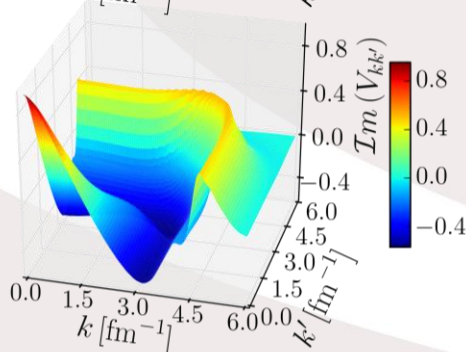
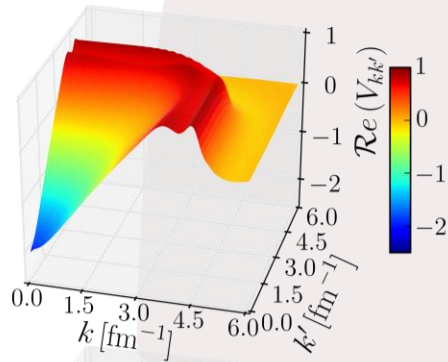


Effective techniques applied to the non-Hermitian world.
 Maybe a technical way to study shape and non-localities in optical potential? "R. Lazauskas"

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

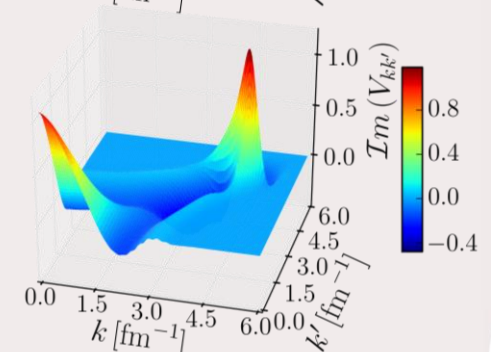
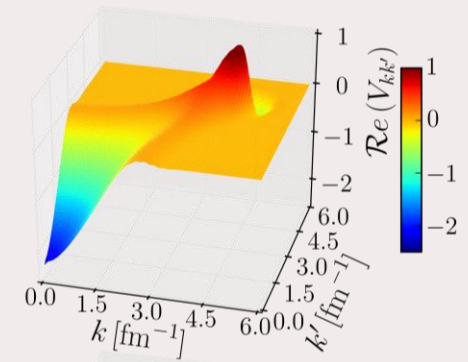
Similarity Transformation

$$\left\{ \begin{aligned} \frac{dH_\lambda(\theta)}{d\lambda} &= -\frac{4}{\lambda^5} [\eta(\lambda), H_\lambda(\theta)] \\ \eta(\lambda) &= \frac{dU_\lambda}{d\lambda} U_\lambda^T \end{aligned} \right.$$

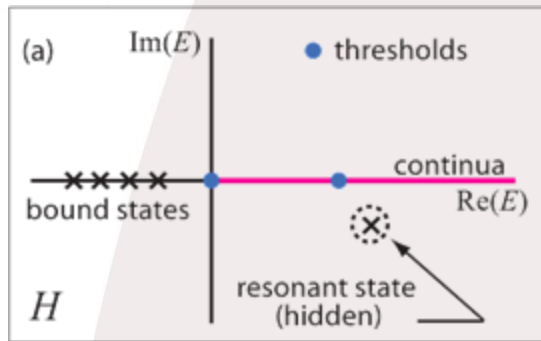


Evolution with flow parameter λ

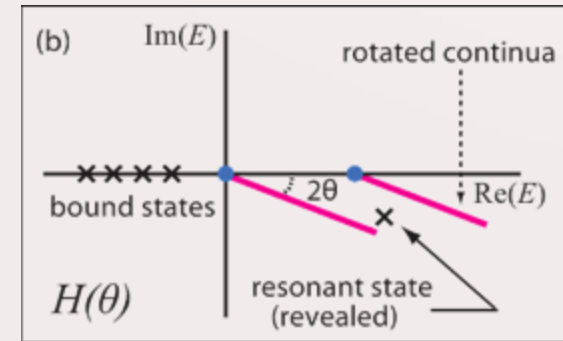
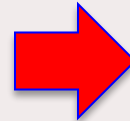
Consistent evolution of the imaginary part



NON-HERMITIAN POTENTIAL TYPICALLY USED IN THE CONTEXT OF COMPLEX SCALING TECHNIQUE



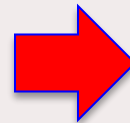
Complex scaling



Kruppa *et al.* PRC89 (2014)

The complex scaling and the resonance states

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



$$\hat{H}(\theta) = e^{-2i\theta}\hat{T} + \hat{V}(re^{i\theta})$$

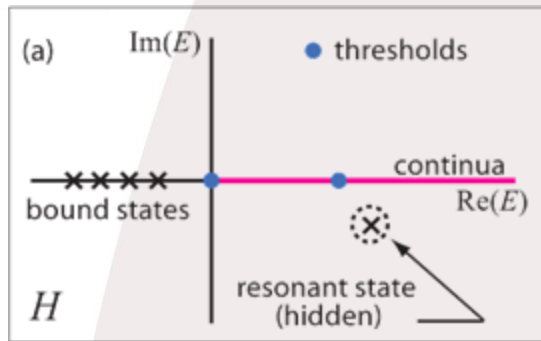
$$\hat{H}(r) = \hat{U}(\theta)\hat{H}(\theta)\hat{U}^{-1}(\theta)$$

Aguilar-Balslev-Combes theorem: the resonant states of the original Hamiltonian are invariant and the non-resonant scattering states are rotated and distributed on a 2θ ray that cuts the complex energy plane with a corresponding threshold being the rotation point.

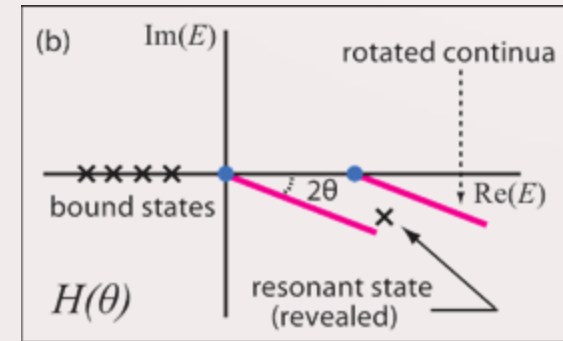
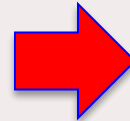
$$\hat{H}(r, \theta)\psi(r, \theta) = (E + i\Gamma)\psi(r, \theta)$$

Energy \uparrow \uparrow Half-life

NON-HERMITIAN POTENTIAL TYPICALLY USED IN THE CONTEXT OF COMPLEX SCALING TECHNIQUE



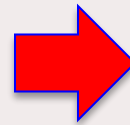
Complex scaling



Kruppa et al. PRC89 (2014)

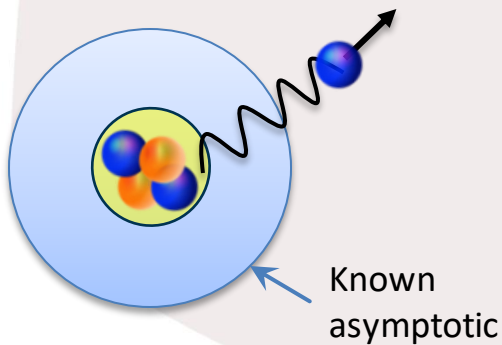
The complex scaling and the resonance states

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

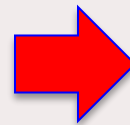


$$\hat{H}(\theta) = e^{-2i\theta}\hat{T} + \hat{V}(re^{i\theta})$$

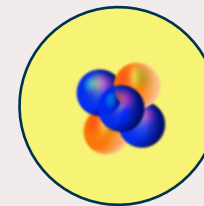
$$\hat{H}(r) = \hat{U}(\theta)\hat{H}(\theta)\hat{U}^{-1}(\theta)$$



$$U(\theta)H(r)U(\theta)^{-1}$$



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



Spatially extended
but falls off
exponentially

Boundary limit problem

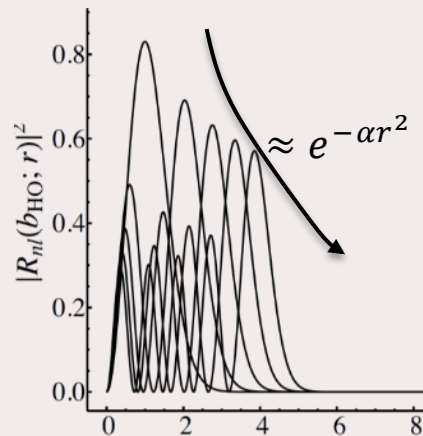
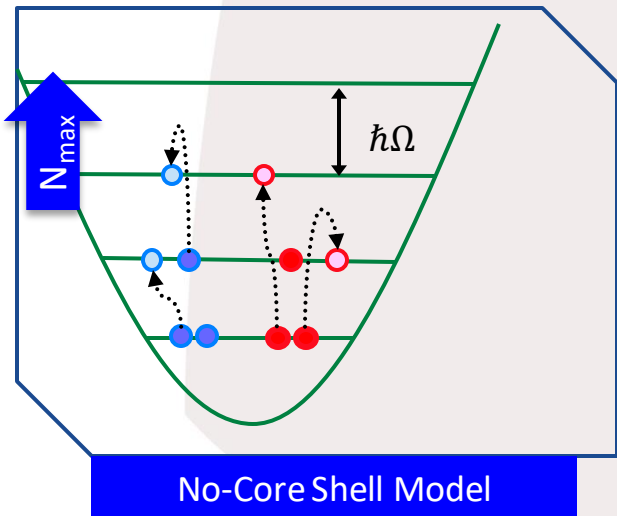
Bound state problem

- Methods develop in this presentation to solve the many body problem

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

Mixing coefficients (unknown) A-body harmonic oscillator states Second quantization

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




$$\Psi_{NCSMC}^{(A)} = \sum_{\lambda} c_{\lambda} |A\lambda J^\pi T\rangle$$

- Methods develop in this presentation to solve the many body problem

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

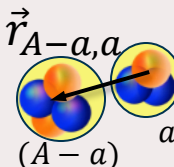
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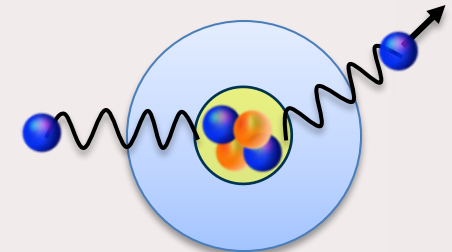


Can address bound and low-lying resonances (short range correlations)

$$\Psi_{RGM}^{(A)} = \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v |\Phi_{v\vec{r}}^{(A-a,a)}\rangle \longleftrightarrow \psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$

Relative wave function (unknown) Antisymmetrizer Channel basis Cluster expansion technique



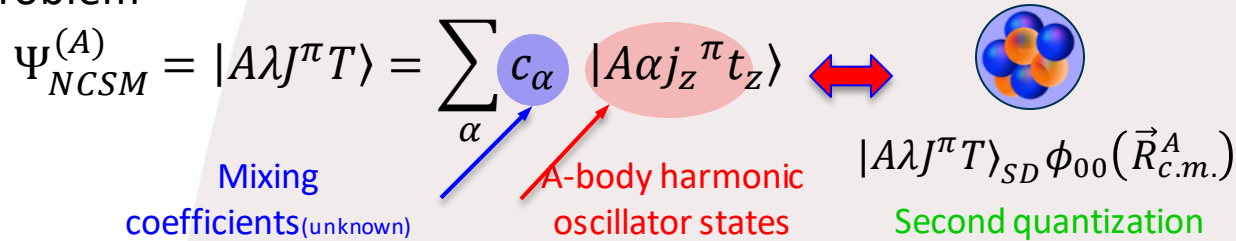


NCSM/RGM
Cluster formalism for elastic/inelastic

- Methods develop in this presentation to solve the many body problem

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

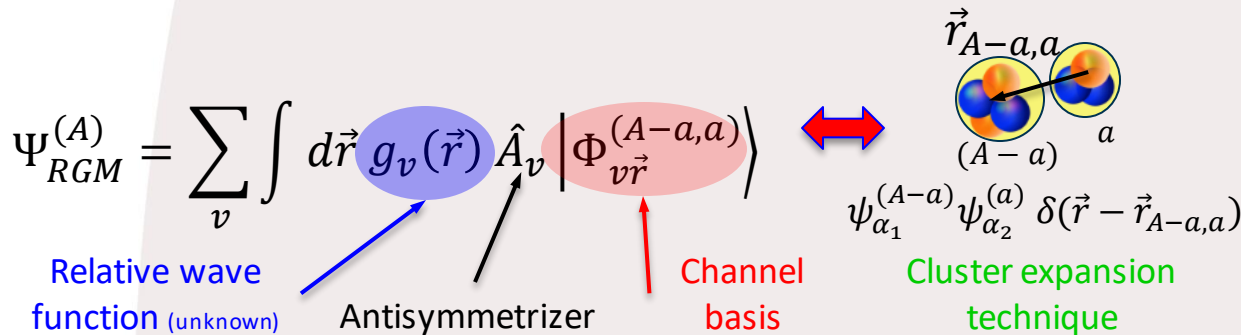
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Can address bound and low-lying resonances (short range correlations)

$$\Psi_{RGM}^{(A)} = \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v |\Phi_{v\vec{r}}^{(A-a,a)}\rangle \longleftrightarrow \psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$

Relative wave function (unknown) Antisymmetrizer Channel basis Cluster expansion technique



Design to account for scattering states (best for long range correlations)

- The many body quantum problem is best described by the superposition of both type of wave functions


$$\Psi_{NCSMC}^{(A)} = \sum_{\lambda} c_{\lambda} |A\lambda J^\pi T\rangle + \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v |\Phi_{v\vec{r}}^{(A-a,a)}\rangle$$

NCSMC

- Methods develop in this presentation to solve the many body problem

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

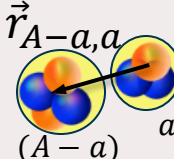
Mixing coefficients (unknown) A-body harmonic oscillator states Second quantization



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

$$\Psi_{RGM}^{(A)} = \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v |\Phi_{v\vec{r}}^{(A-a,a)}\rangle \leftrightarrow \psi_{\alpha_1}^{(A-a)} \psi_{\alpha_2}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$

Relative wave function (unknown) Antisymmetrizer Channel basis Cluster expansion technique

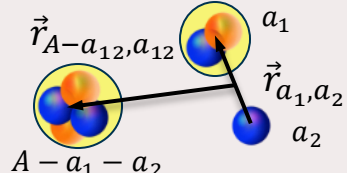


Design to account for scattering states (best for long range correlations)

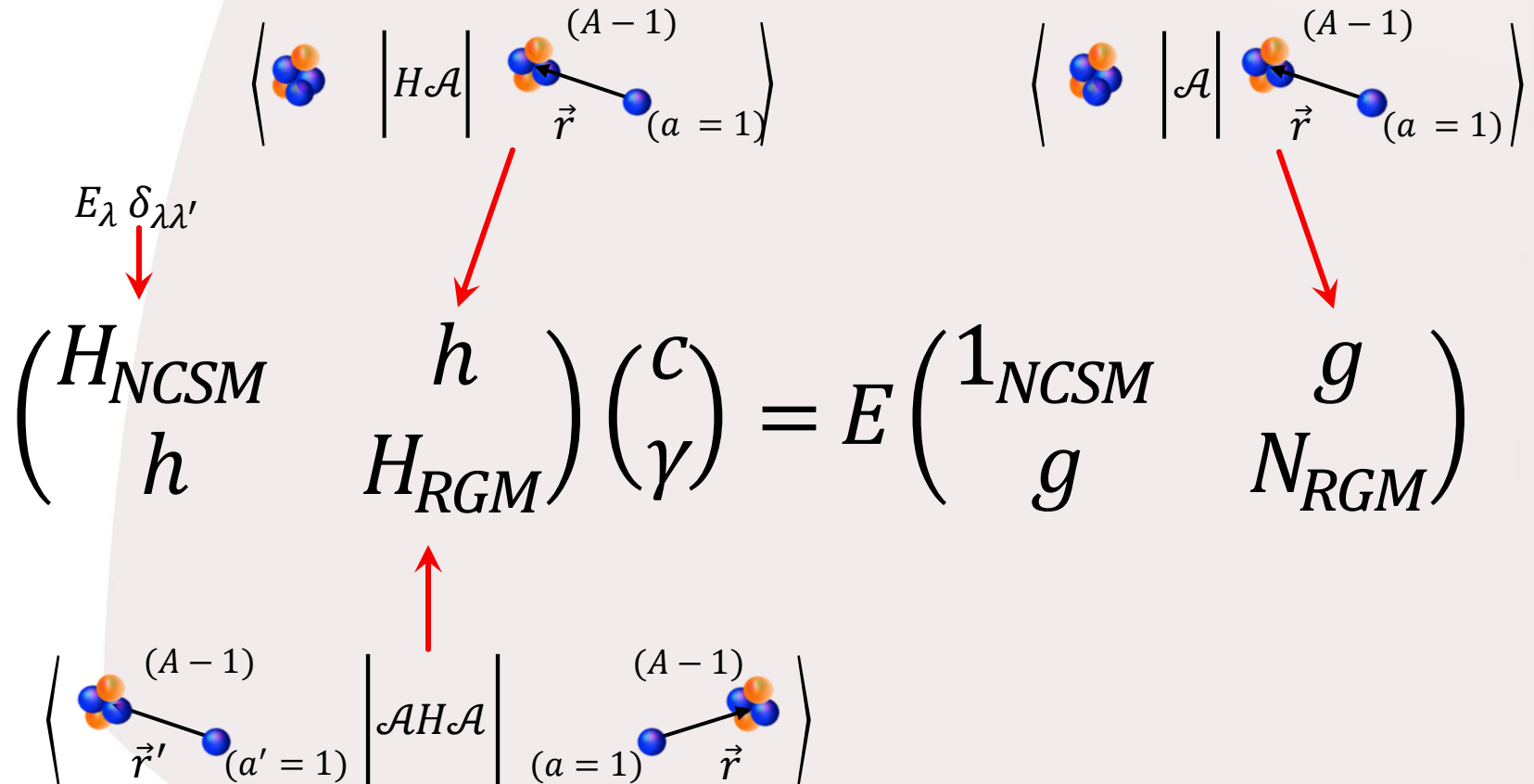
- Adding three-cluster degrees of freedom:

$$+ \sum_v \iint d\vec{x} d\vec{y} x^2 y^2 G_v(\vec{x}, \vec{y}) \hat{A}_v |\Phi_{v\vec{x}\vec{y}}^{(A-a_1-a_2, a_1, a_2)}\rangle \leftrightarrow \psi_{\alpha_1}^{(A-a_1-a_2)} \psi_{\alpha_2}^{(a_1)} \psi_{\alpha_3}^{(a_2)} \delta(\vec{r} - \vec{r}_{a_1, a_2}) \times \delta(\vec{r} - \vec{r}_{A-a_1-a_2, a_1, a_2})$$

Cluster expansion technique

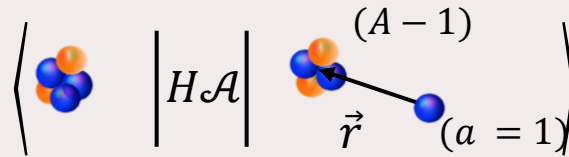


...



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

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic R-matrix on Lagrange mesh.



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

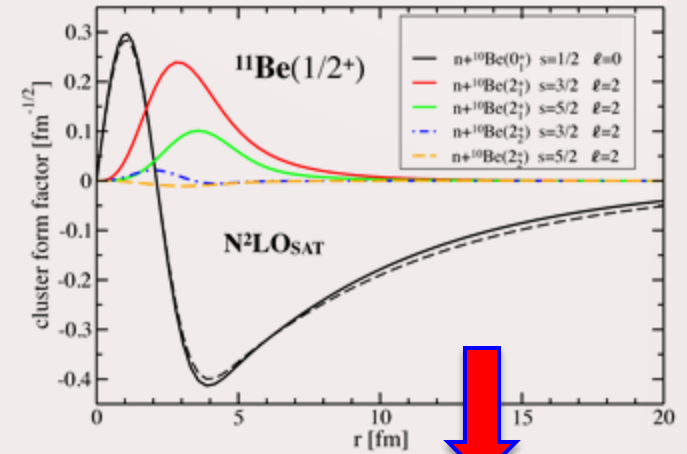
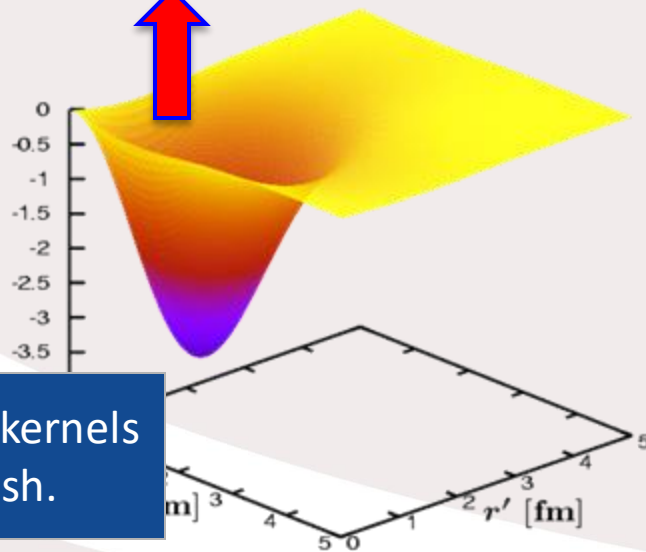
$$\begin{pmatrix} H_{NCSM} \\ h \end{pmatrix}$$

$$\begin{pmatrix} h \\ H_{RGM} \end{pmatrix}$$

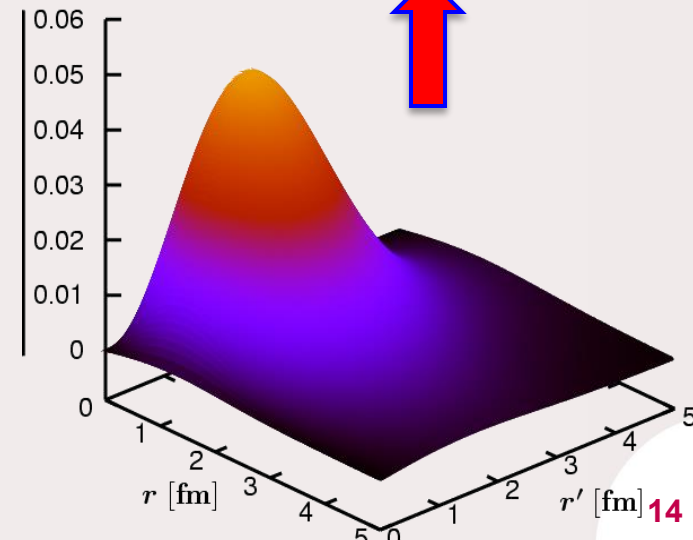
$$\begin{pmatrix} c \\ \gamma \end{pmatrix}$$

$$= E \begin{pmatrix} 1_{NCSM} \\ g \end{pmatrix}$$

$$\begin{pmatrix} g \\ N_{RGM} \end{pmatrix}$$

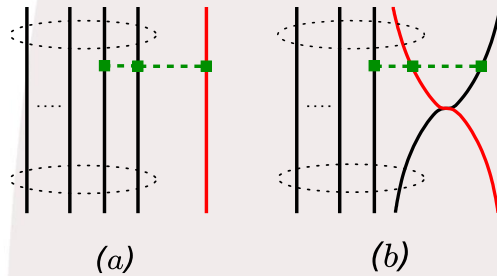


Long-range part of the kernels is computed on the mesh.



$$\langle \Phi_{v' r'}^{J^{\pi T}} | \hat{A}_{v'} V^{NNN} \hat{A}_v | \Phi_{v r}^{J^{\pi T}} \rangle = \left\langle \begin{array}{c} (A-1) \\ \text{diagram} \\ (a' = 1) \end{array} \middle| V^{NNN} (1 - \sum_{i=1}^{A-1} \hat{P}_{iA}) \middle| \begin{array}{c} (A-1) \\ \text{diagram} \\ (a = 1) \end{array} \right\rangle$$

$$\mathcal{V}_{v'v}^{NNN}(r, r') = \sum R_{n'l'}(r') R_{nl}(r) \left[\frac{(A-1)(A-2)}{2} \langle \Phi_{v'n'}^{J^{\pi T}} | V_{A-2A-1A} (1 - 2P_{A-1A}) | \Phi_{vn}^{J^{\pi T}} \rangle \right.$$



Direct potential:

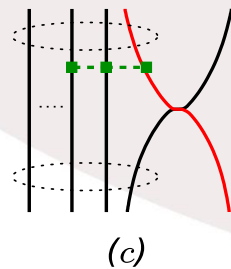
$$\propto_{SD} \langle A - a\alpha'_1 I_1^{\pi'1} T'_1 | a^\dagger a^\dagger a a | A - a\alpha_1 I_1^{\pi 1} T_1 \rangle_{SD} \sim 1\text{Go}$$

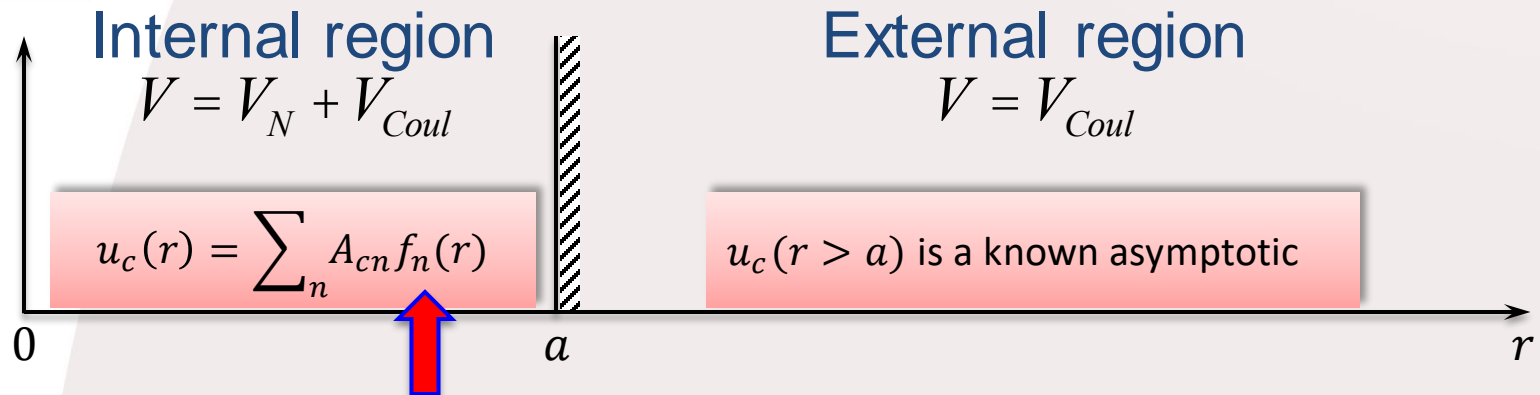
$\sim 7.10^3$ two-body states

$$- \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi_{v'n'}^{J^{\pi T}} | P_{A-1A} V_{A-3A-2A-1} | \Phi_{vn}^{J^{\pi T}} \rangle \cdot$$

Exchange potential:

$$\propto_{SD} \langle A - a\alpha'_1 I_1^{\pi'1} T'_1 | a^\dagger a^\dagger a^\dagger a a a | A - a\alpha_1 I_1^{\pi 1} T_1 \rangle_{SD}$$





Decomposition on a Lagrange mesh.

NCSMC can be cast as Bloch-Schrödinger equation:

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

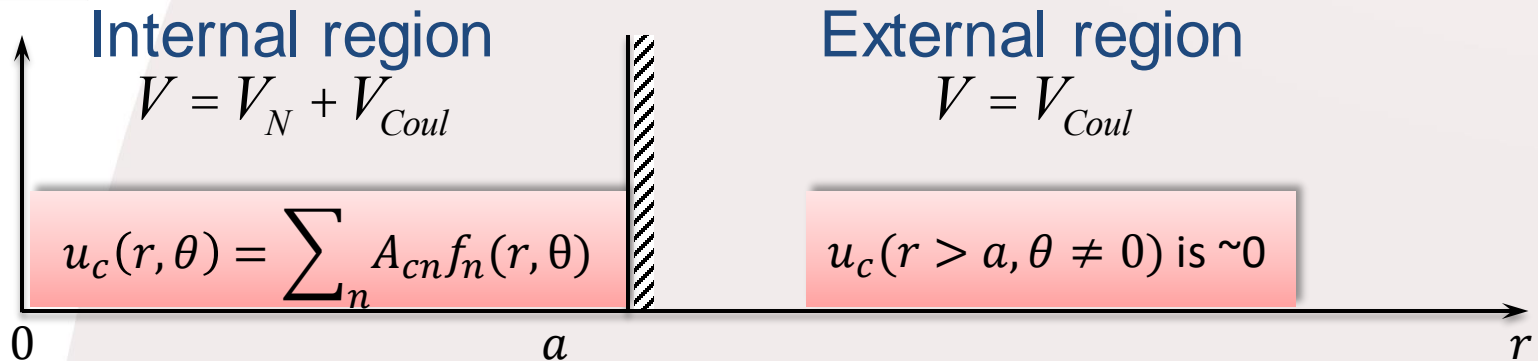
And solved using R-matrix, which in the eigen basis of $C - EI$ reads:

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

Simple for binary reacting system,
more involved for neutral ternary

system and extremely challenging for
charged breakup !

ALTERNATIVE: COMPLEX SCALING



Complex scaling brings us back to Hilbert space; NCSMC will be solved with (two-body) Schrödinger equation

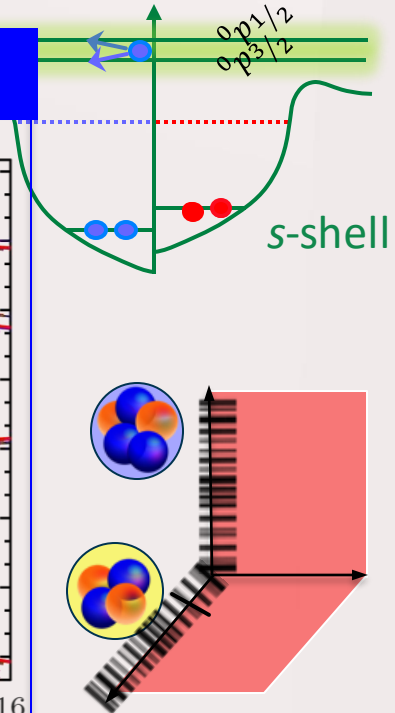
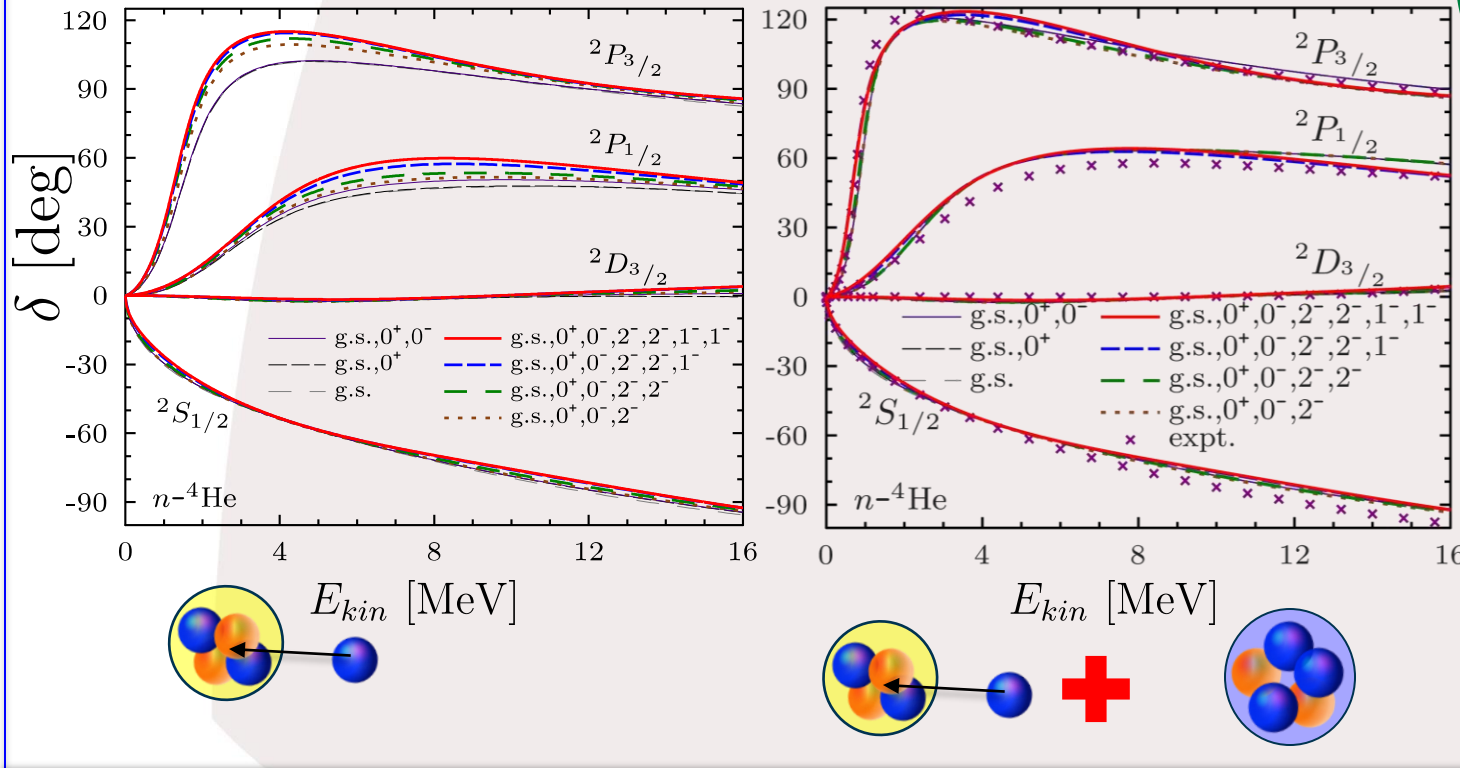
$$(H(\theta) - EI)\psi(\Theta) = 0$$

i.e. no inhomogeneous term. Scattering observables need to be derived using integral relations like Green's theorem

$$A(\mathbf{k}) = \frac{m}{\hbar} \left[\left\langle F^{\text{in}}(\mathbf{k}e^{i\theta}) \middle| V(\theta) \middle| \psi(\mathbf{k}, \theta) \right\rangle - \left\langle \psi(\mathbf{k}, \theta) \middle| V(\theta) \middle| F^{\text{in}}(\mathbf{k}e^{i\theta}) \right\rangle \right]$$

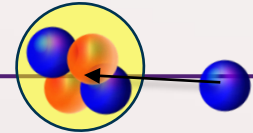
- Long-range coulomb problem is avoided.
- "Simple" to solve.
- Useful for charged breakup.

Convergence with respect to the # of ^4He low-lying states

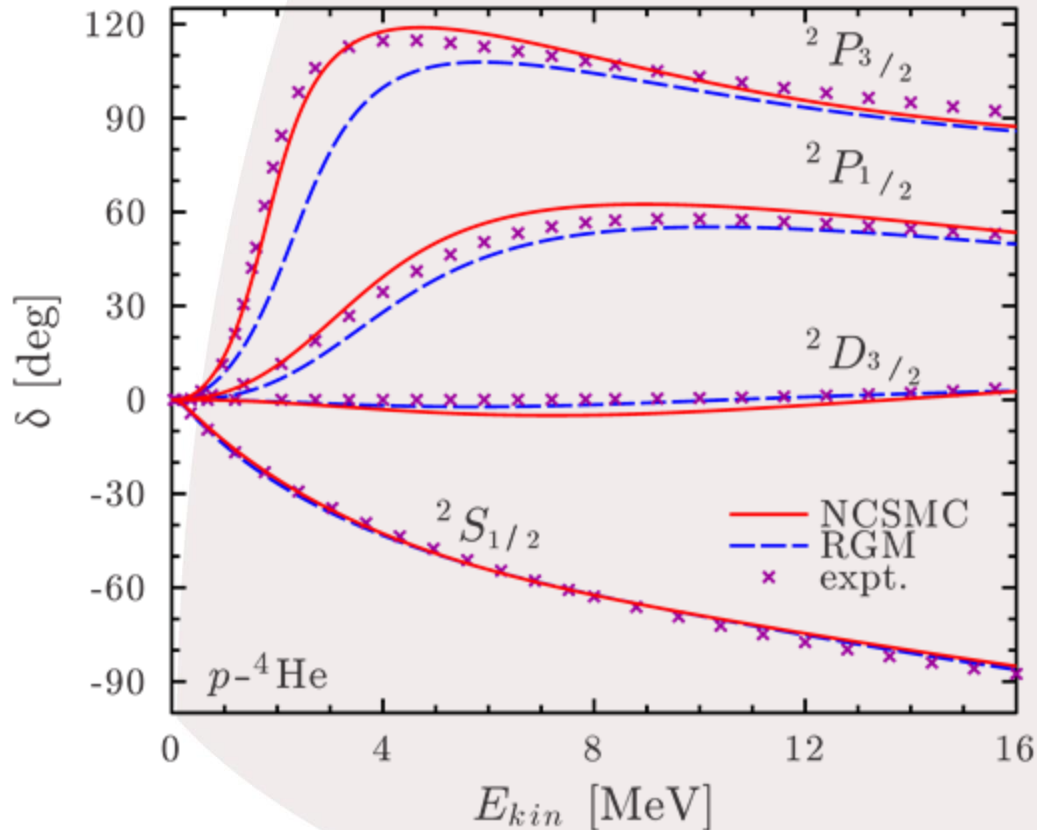


$n-^4\text{He}$ scattering phase-shifts for NN+3N potential with $\lambda=2.0 \text{ fm}^{-1}$.

- The convergence pattern much better with NCSMC
- The experimental phase-shifts are well reproduced.

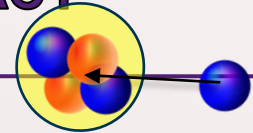


Two scenarii of nuclear Hamiltonians

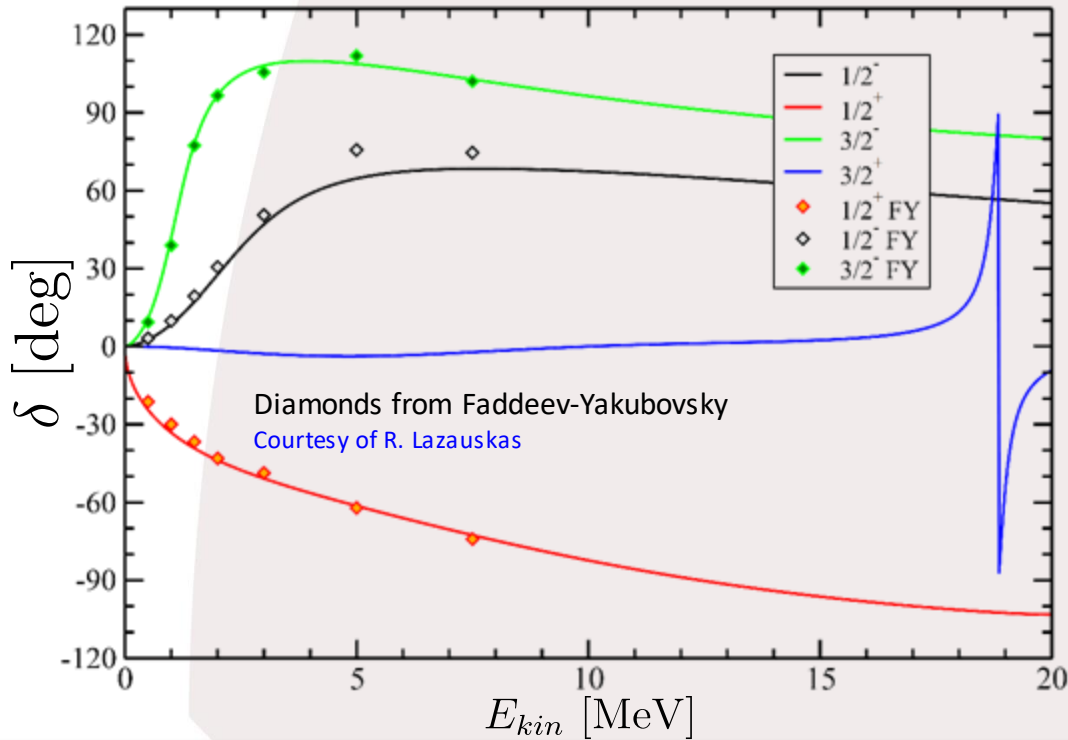


- NCSMC outperforms the binary cluster model for all resonant waves.
- Good agreement of NCSMC with experiment.

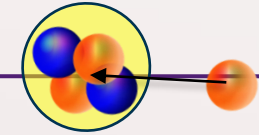
Comparison between NCSM/RGM (i.e. a binary cluster approximation) and NCSMC



Benchmark: scattering phase shifts NCSMC/FY

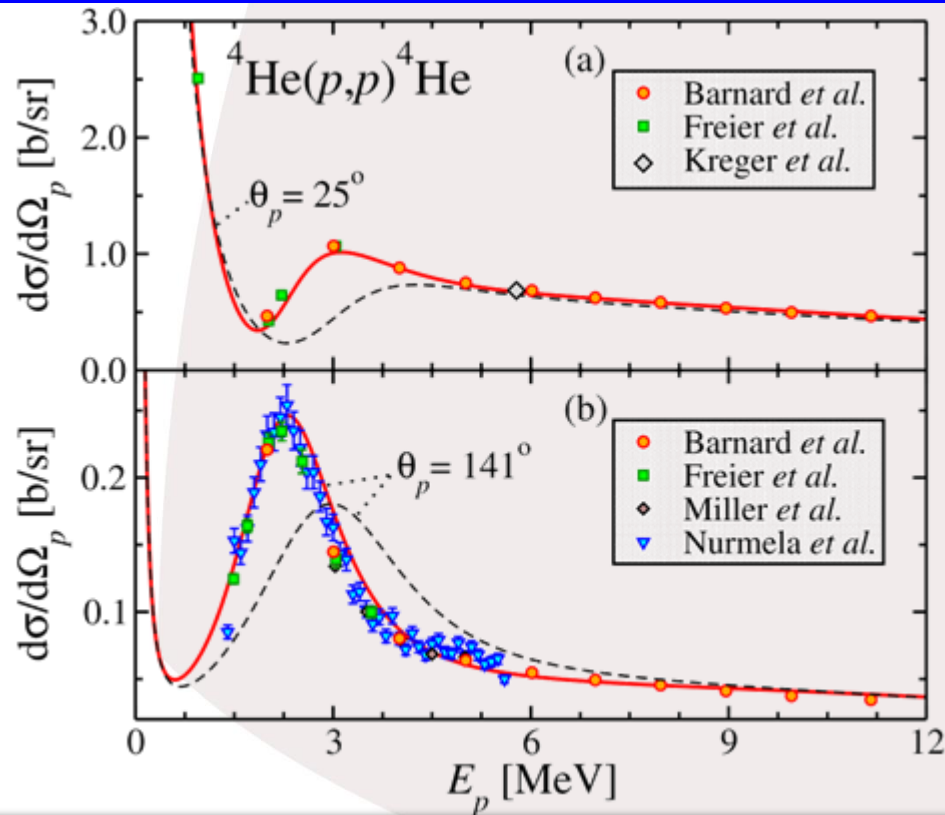


- Good agreement between the two methods.



p - ^4He scattering

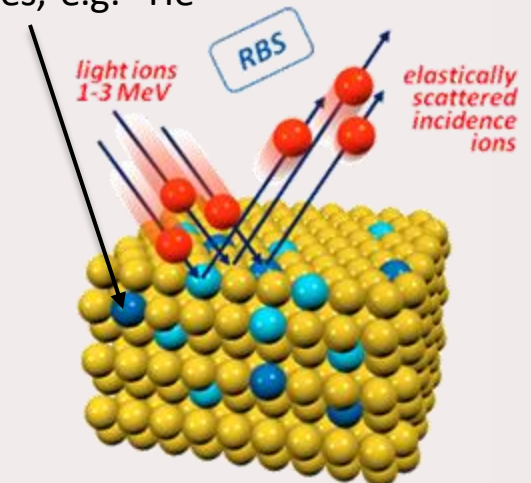
p - ^4He differential cross-section compared to experiment



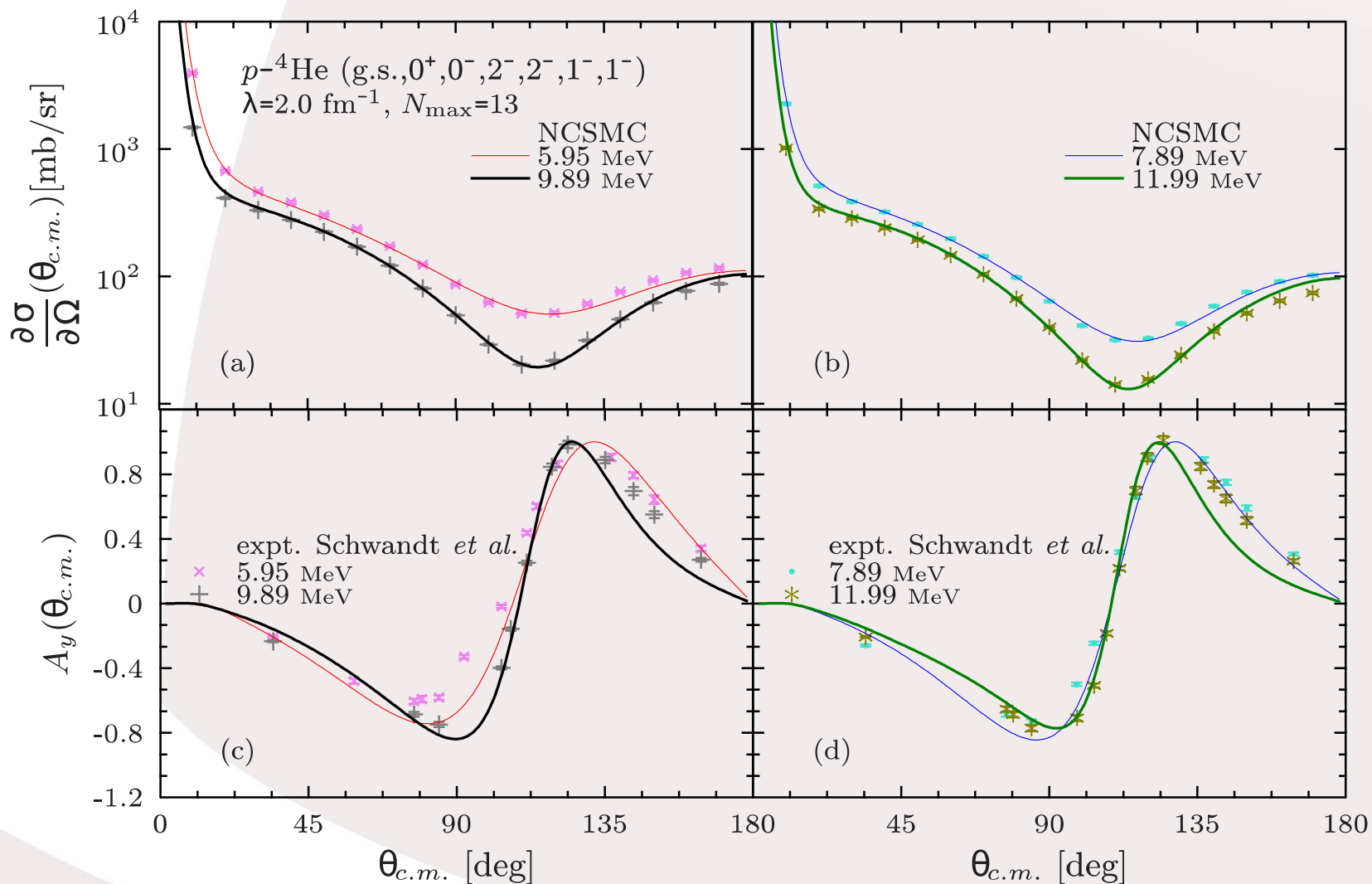
p - ^4He differential cross-section for NN+3N.

For the non-destructive physical, electrical and chemical characterization of materials, nuclear physics is routinely used for energies above the Rutherford scattering.

Impurities, e.g. ^4He



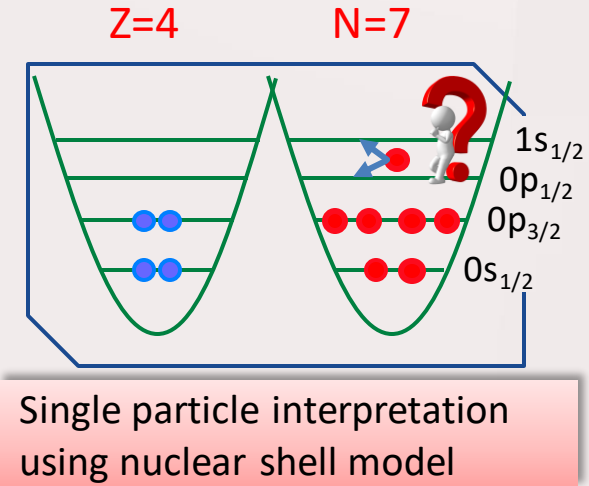
p - ^4He SCATTERING FOLLOWS THE TREND OBSERVED IN p - ^3He CONCERNING THE REDUCED A_y PROBLEM



ν -RICH HALO NUCLEUS ^{11}Be

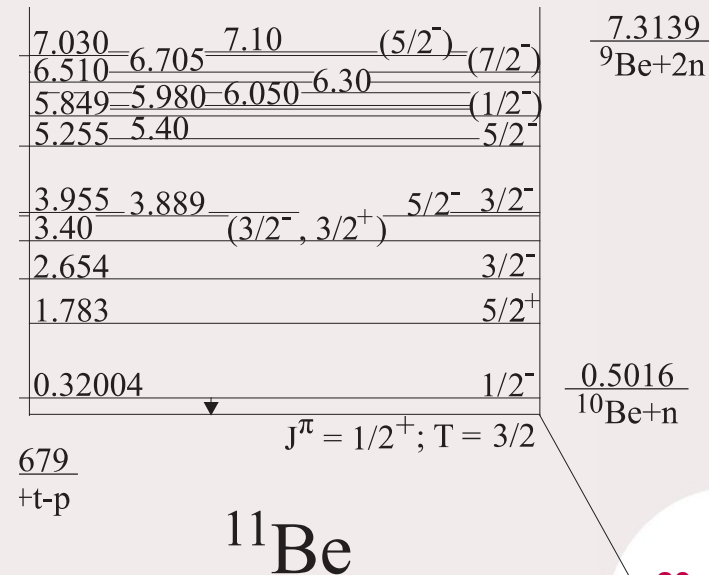


- In a shell model picture, the g.s. expected to be $J^\pi = 1/2^-$.
- In reality, ^{11}Be g.s. is $J^\pi = 1/2^+$ -- **parity inversion**.
- Very weakly bound: $E_{\text{th}} = -0.5$ MeV **Halo state** -- dominated by n - ^{10}Be in a S -wave.
- The $1/2^-$ state also bound -- **only by 180 keV**.

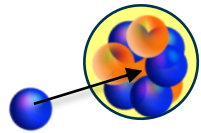


Can we describe ^{11}Be in *ab initio* calculations?

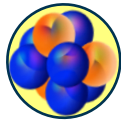
- Continuum must be included.
- Does the 3N interaction play a role in the parity inversion?



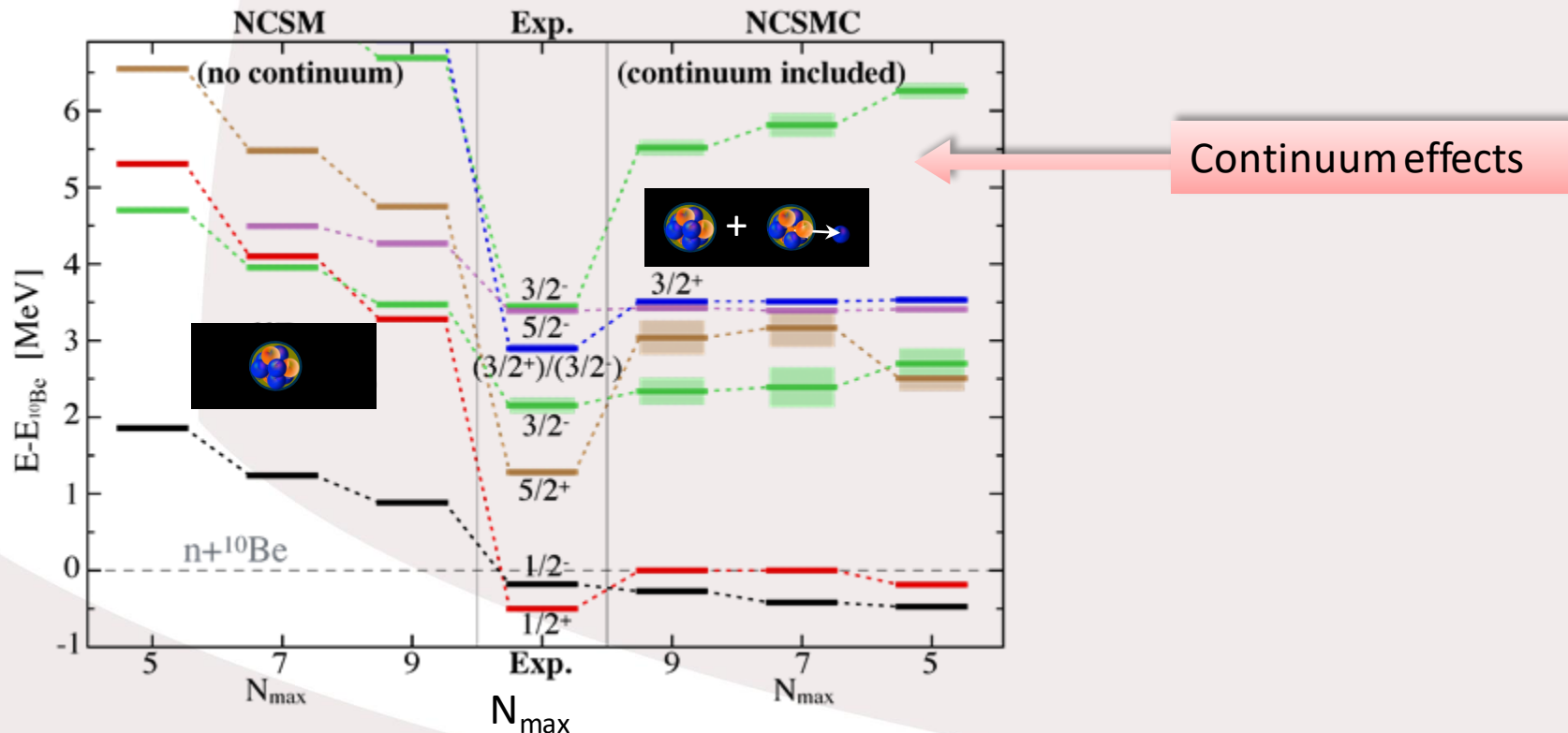
NCSMC calculations including chiral 3N ($N^3\text{LO NN}+N^2\text{LO 3NF400}$)

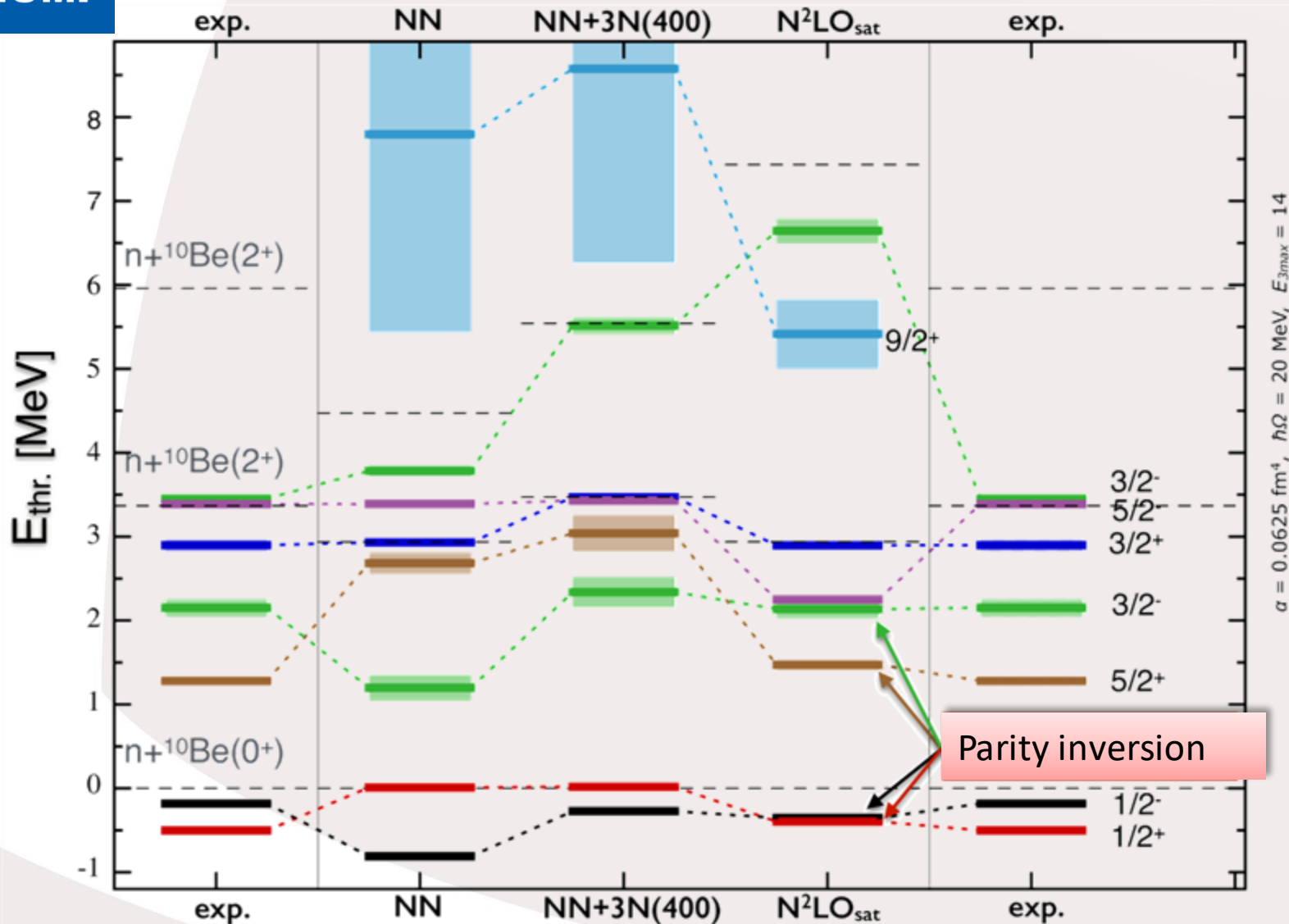


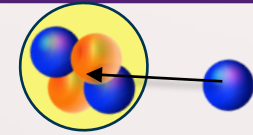
^{10}Be : 0^+ , 2^+ , 2^+ NCSM eigenstates



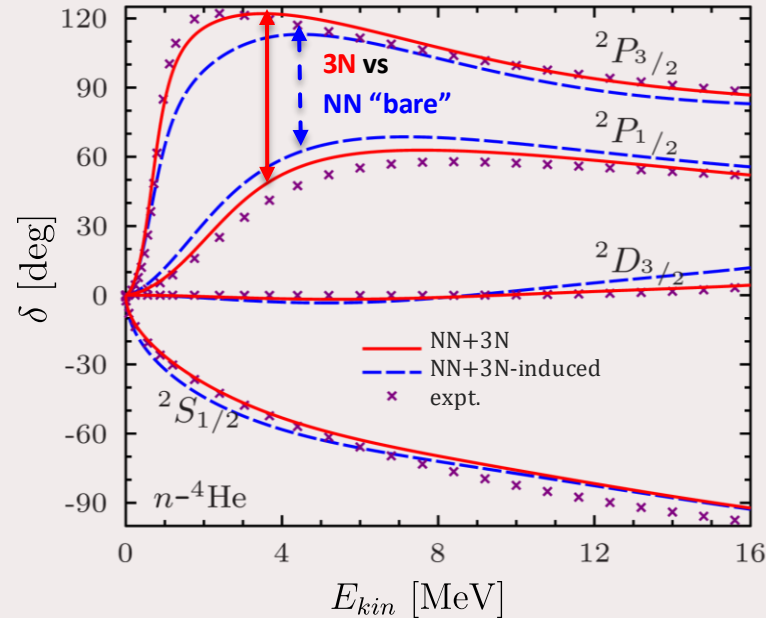
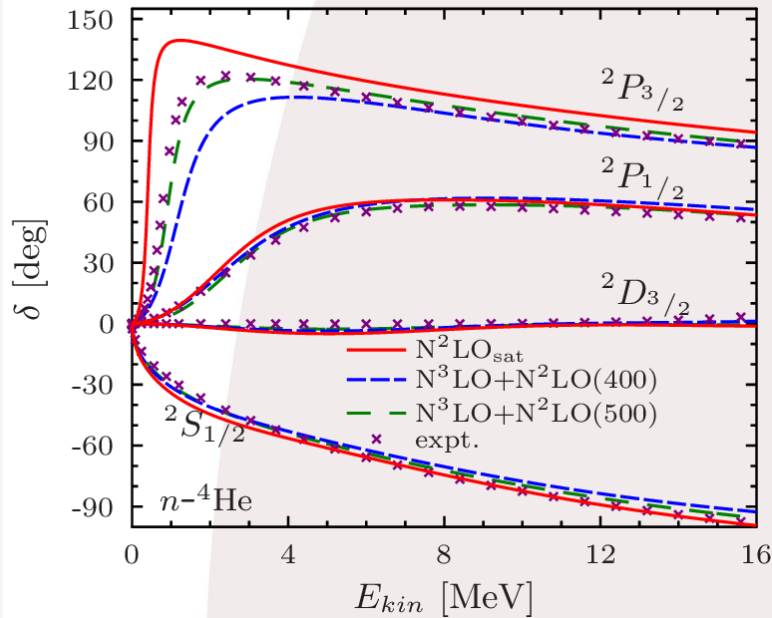
^{11}Be : ≥ 6 ($\pi=-1$) and ≥ 3 ($\pi=1$) NCSM eigenstates







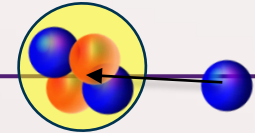
n - ^4He scattering phase shifts



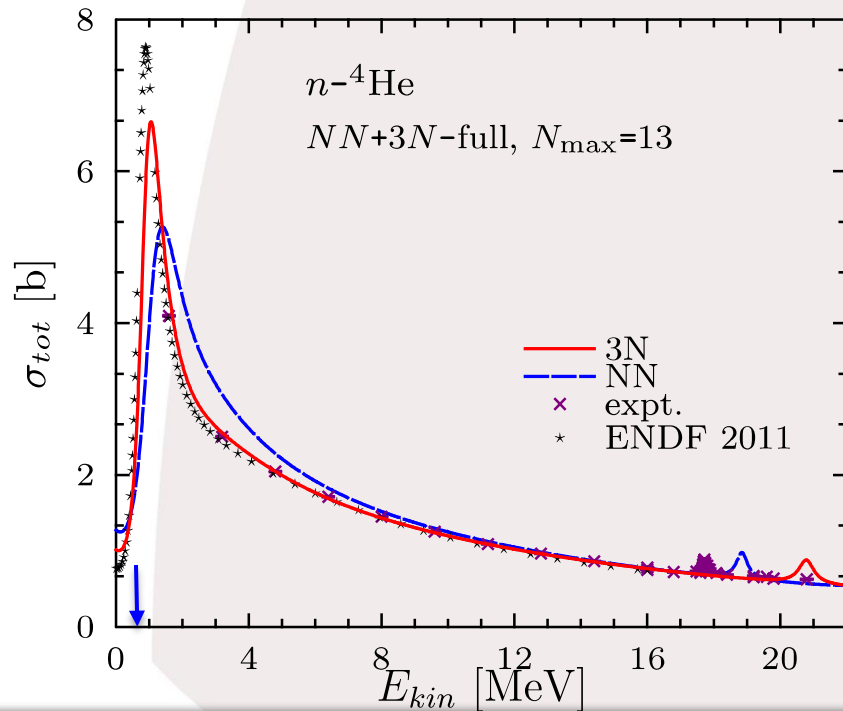
Some of the shortcomings of the nuclear interaction can already be **probed** in p -shell nuclei **through reactions**.

[NN p -waves are not perfectly reproduced by $N^2\text{LO}_{\text{sat}}$]

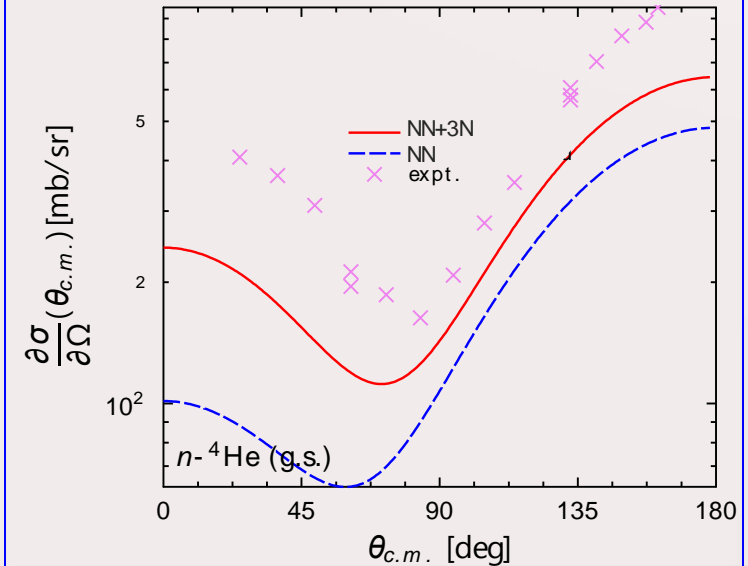
- The 3N interactions **influence** mostly the P waves.
- The **largest splitting** between P waves is obtained with **NN+3N**.



Comparison of the elastic cross-section between NN and NN+3N with ^4He (g.s.)

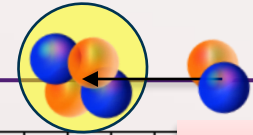


n - ^4He elastic cross-section for NN+3N-induced, NN+3N potentials compared to expt. and ENDF evaluation.

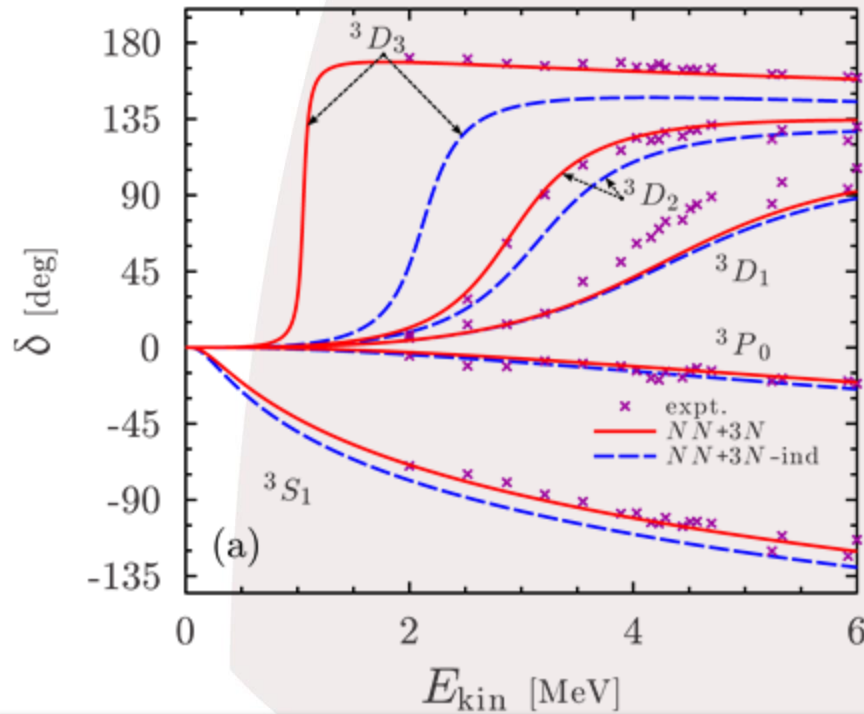


Differential cross-section at $E_{\text{neutron}}=0.84$ MeV between NN+3N-ind and NN+3N.

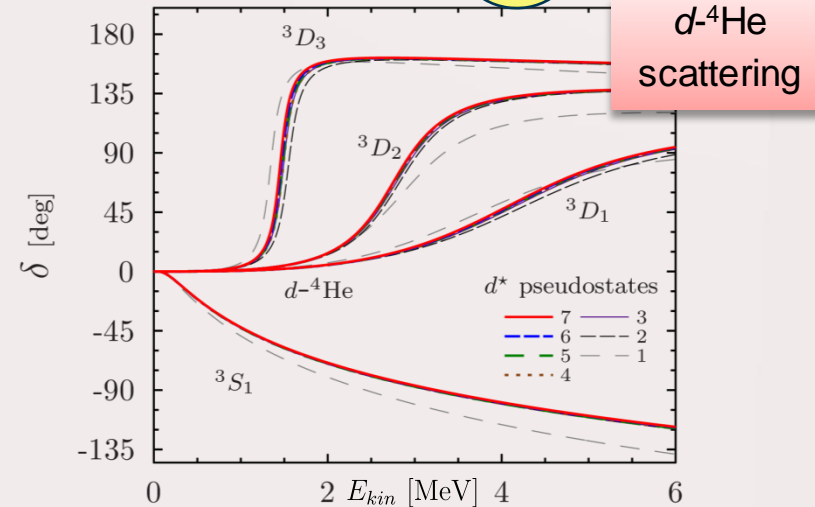
- We obtained a better agreement with data when using NN+3N.
- The 3N force is constitutive to the reproduction of the $3/2^+$ resonance.



Comparison of the d - α phase-shifts with different interactions ($N_{\text{max}}=11$)

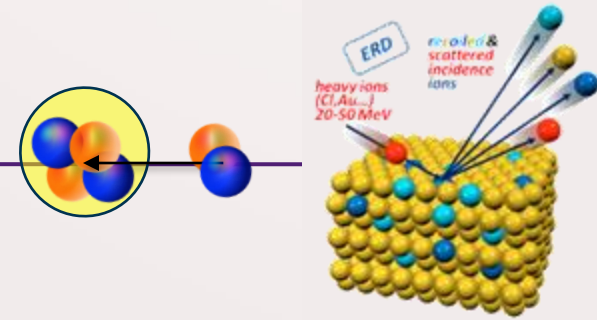


d - ^4He (g.s.) scattering phase-shifts for NN-only, NN+3N-induced, NN+3N-full potential with $\lambda=2.0 \text{ fm}^{-1}$.

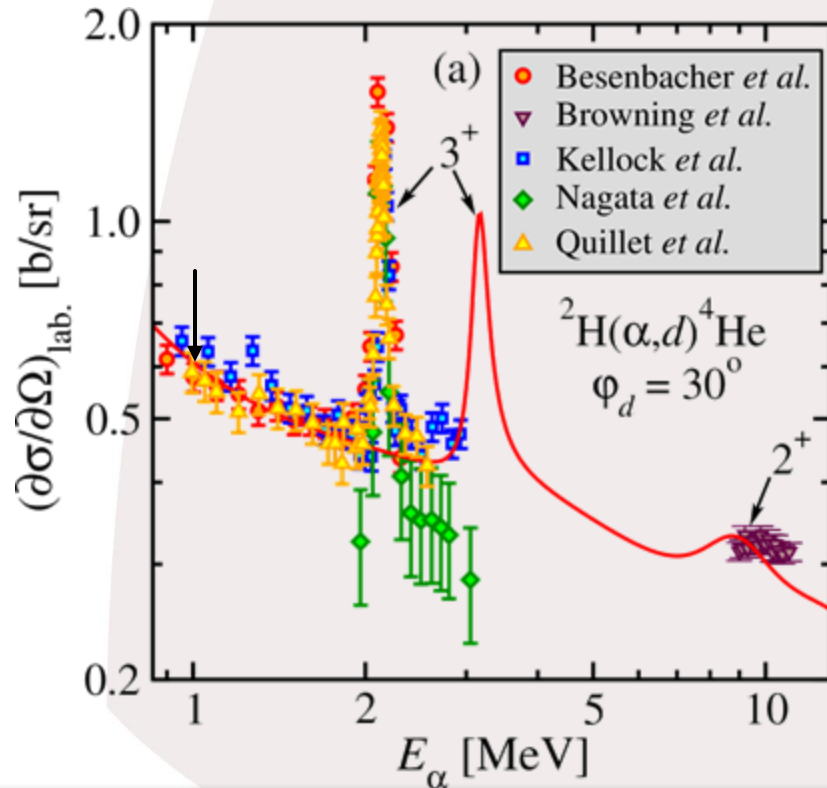


- Best results in a decent model space ($N_{\text{max}}=11$).
- The 3D_3 resonance is reproduced but the 3D_2 and 3D_1 resonance positions are underestimated.
- The 3N force corrects the D -wave resonance positions by increasing the spin-orbit splitting.
- There is room for improvements.

$^4\text{He}(d,^4\text{He})d$ CROSS-SECTION

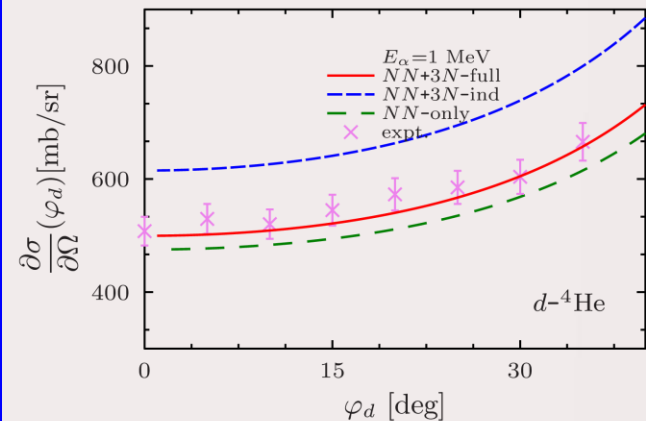


$^4\text{He}(d,^4\text{He})d$ differential cross section at $\varphi=30^\circ$



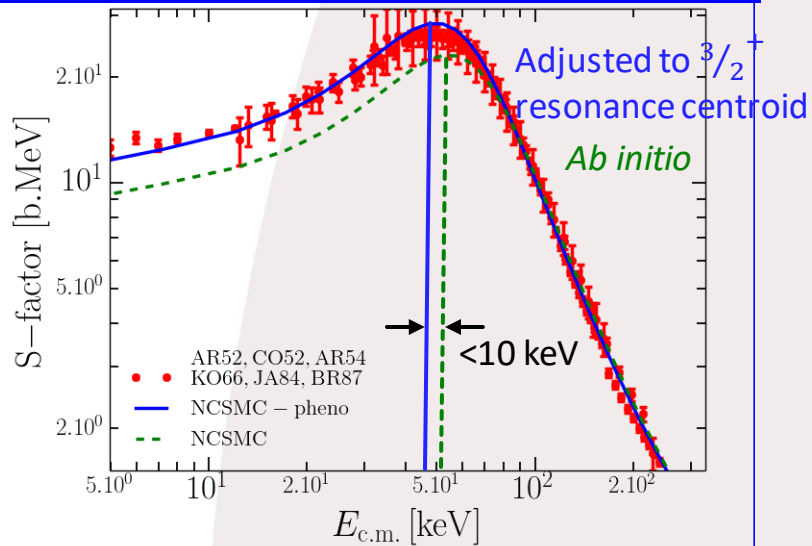
Comparison to experiment of the $d\text{-}^4\text{He}$ elastic recoil differential cross section of NCSMC with NN+3N potential at $\lambda=2.0\text{ fm}^{-1}$.

Comparison between potentials

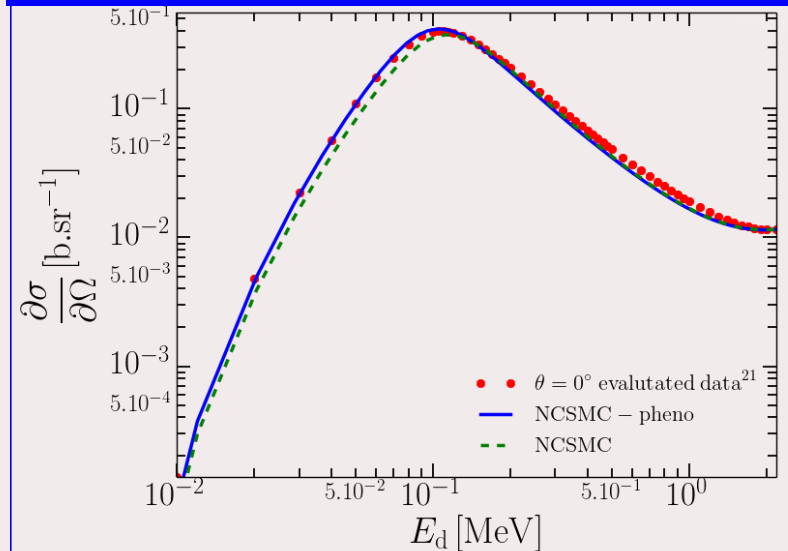


The 3^+ resonance is missed. As its width is very narrow, it has little impact and the bulk of the cross-section.

S-factor: computed and data



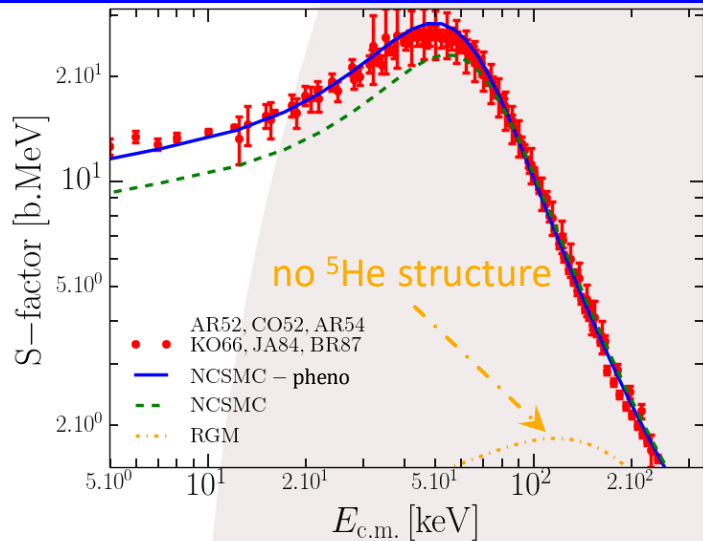
Angular distribution at $\theta = 0^\circ$



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

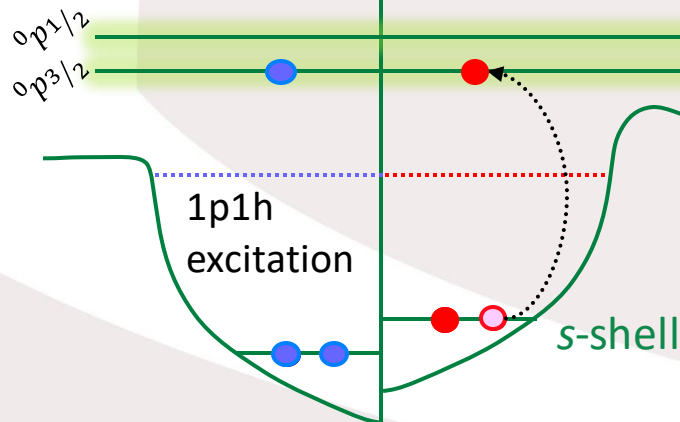
- The S-factor is globally well reproduced.
- The accurate reproduction (of the order of keV) of the **resonance position/width is essential**.
- Shape of a the angular distribution agrees with recent **evaluation**.

S-factor: NCSMC vs binary cluster



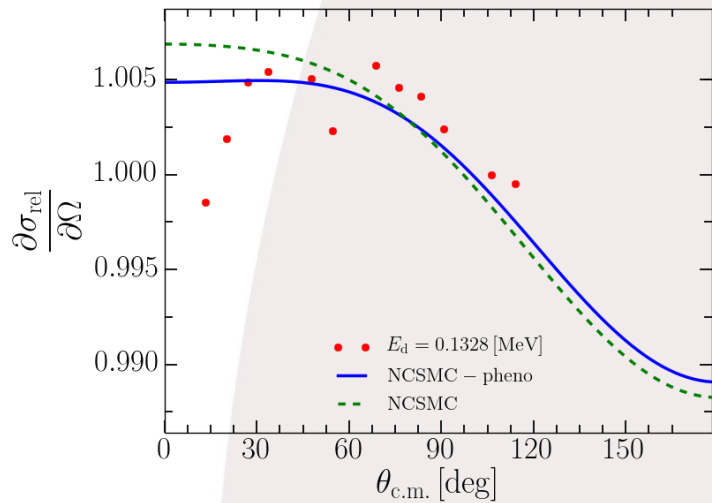
${}^5\text{He}({}^4S_{3/2})$	E_r (keV)	Γ_r (keV)
Cluster basis (D g.s. only)	105	1100
Cluster basis	120	570
NCSMC (D g.s. only)	65	160
NCSMC	55	110
NCSMC-pheno	50	98
R-matrix	48	25

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

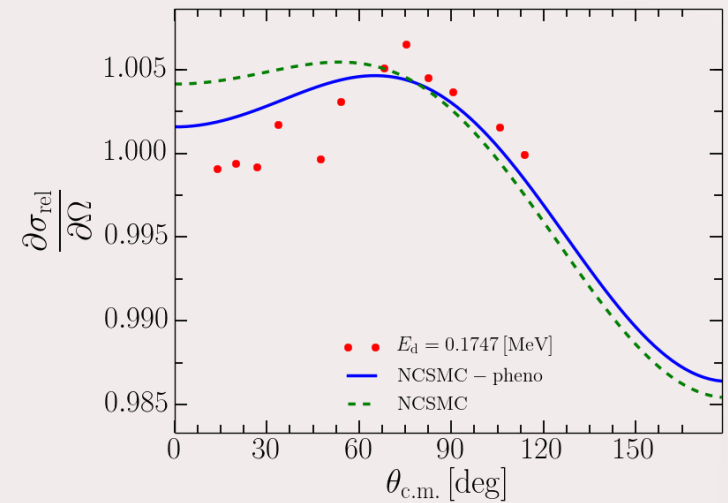


- Importance of structure of neighboring resonances is magnified in transfer reactions.

Angular distribution relative to integral



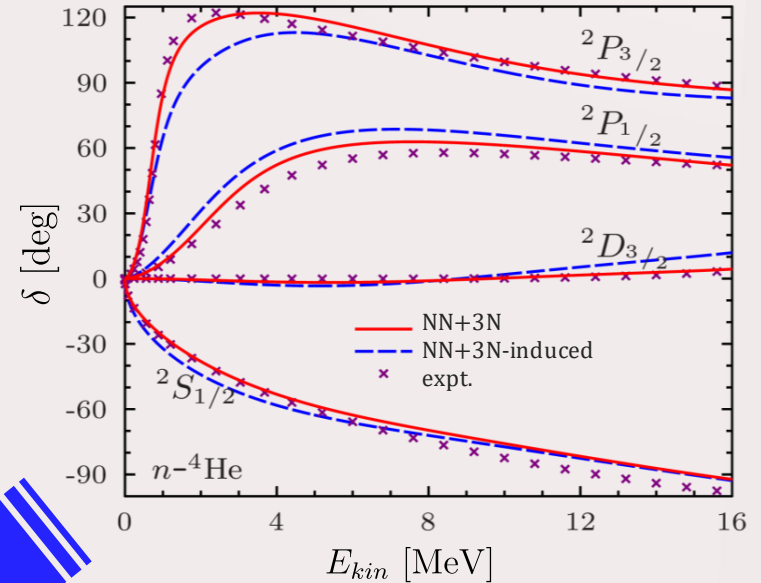
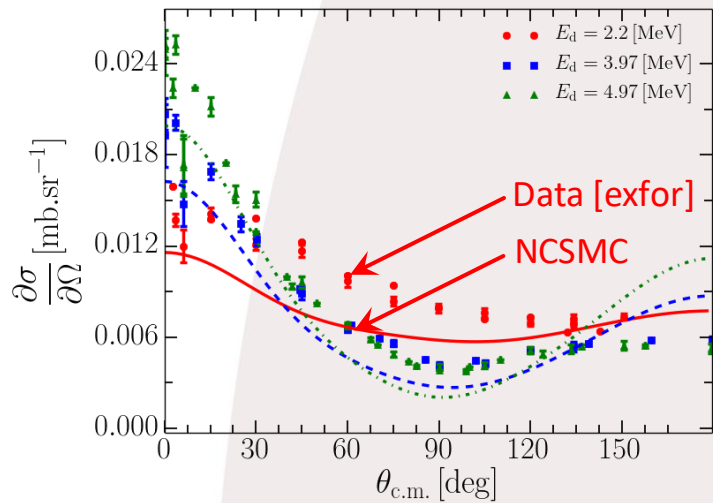
Angular distribution relative to integral



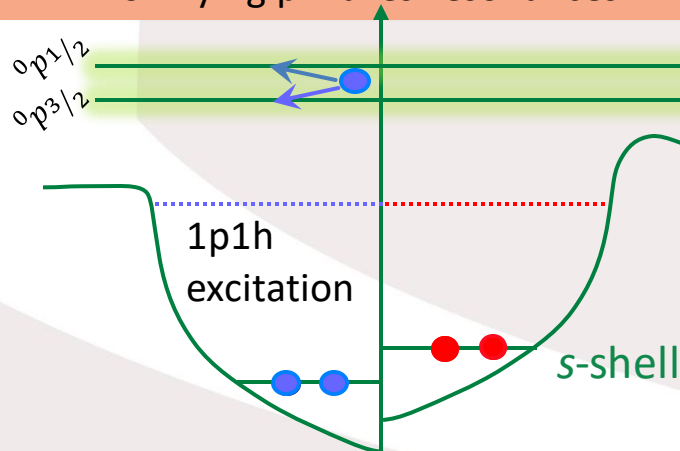
P. Bém *et al.*, *Few-Body Syst***22**, 77 (1997).

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

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

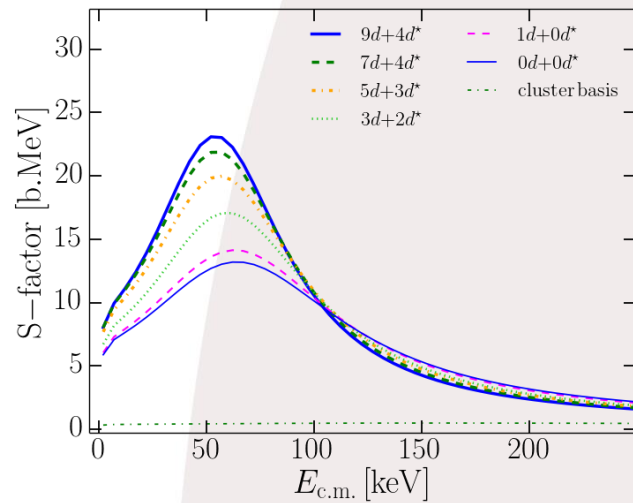


Low-lying p-waves resonances

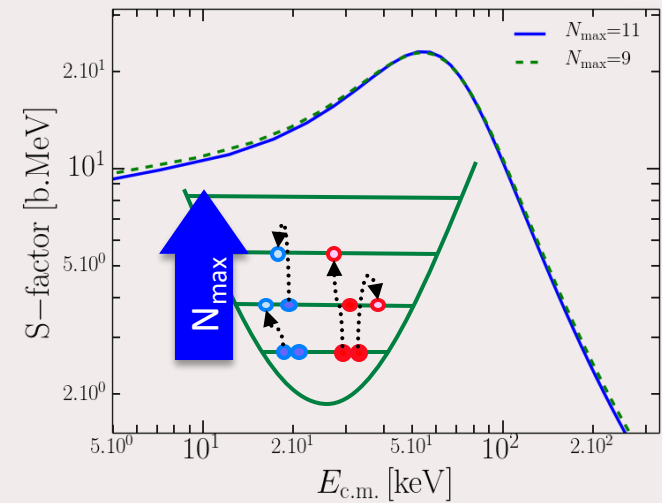


- Away from the DT fusion peak, the effects of low-lying background phase-shifts can be seen.
- No effects of the adjustment of the $3/2^+$ resonance position (i.e. NCSMC \equiv NCSMC-pheno).

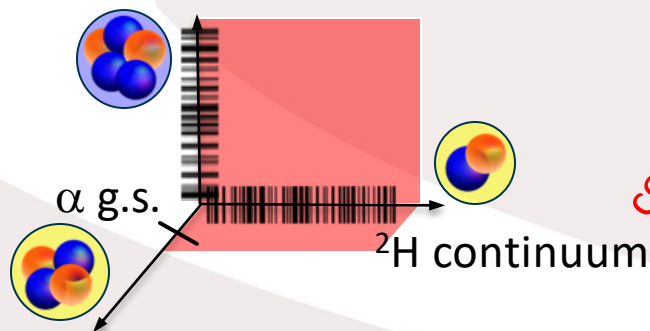
Convergence wrt ${}^2\text{H}$ continuum



Convergence with N_{max}



${}^5\text{He}$ resonances



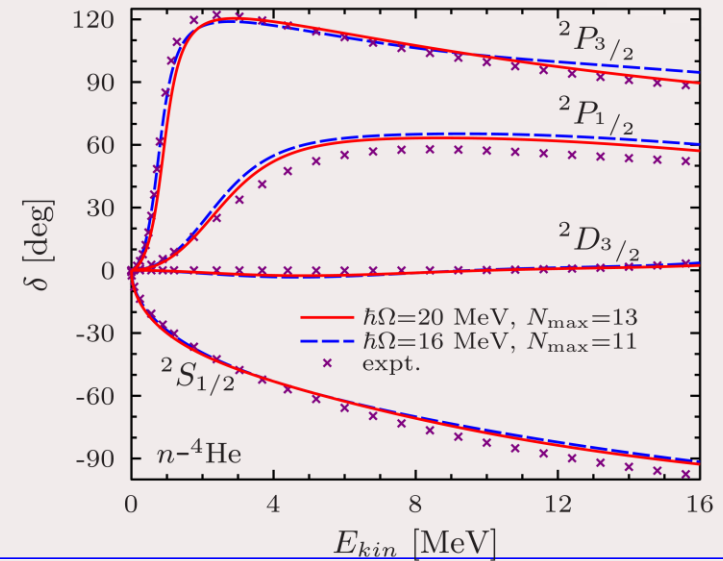
correlated

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

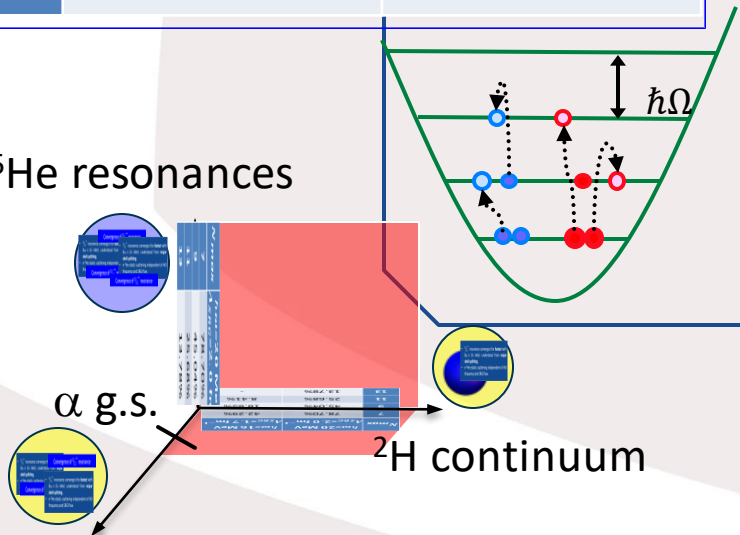
Convergence of ${}^{3/2}^+$ resonance

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

$n-{}^4\text{He}$ phase shifts

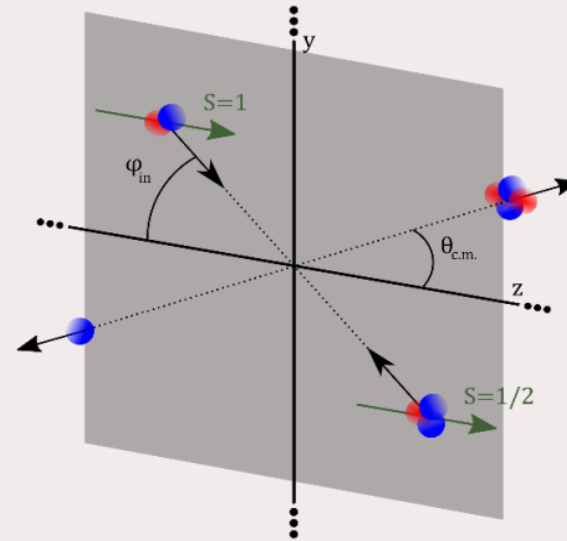
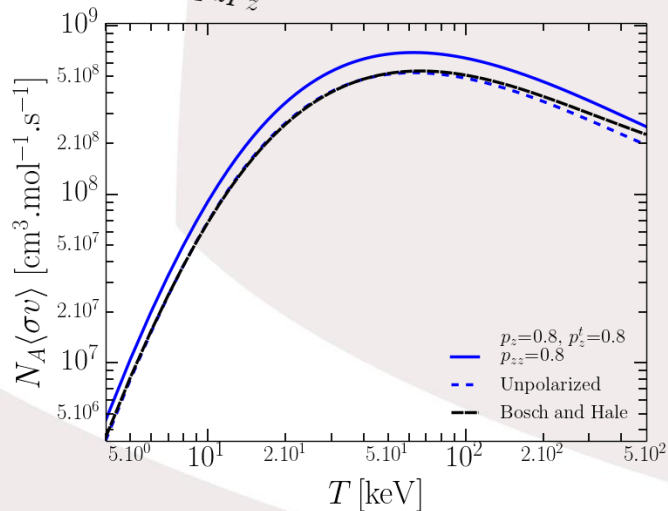
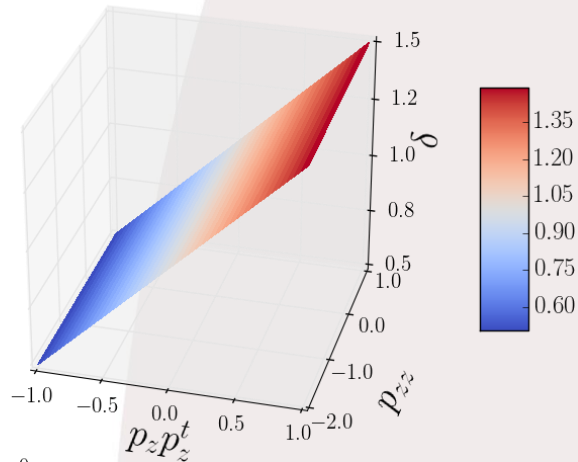


${}^5\text{He}$ resonances



- ${}^{3/2}^+$ resonance converges the **fastest** with $\hbar\omega = 16$ MeV, understood from **major shell splitting**.
- $n-{}^4\text{He}$ elastic scattering independent of HO frequency and SRG flow.

Enhancement factor and reaction rate



Reactant spins are prepared in a configuration

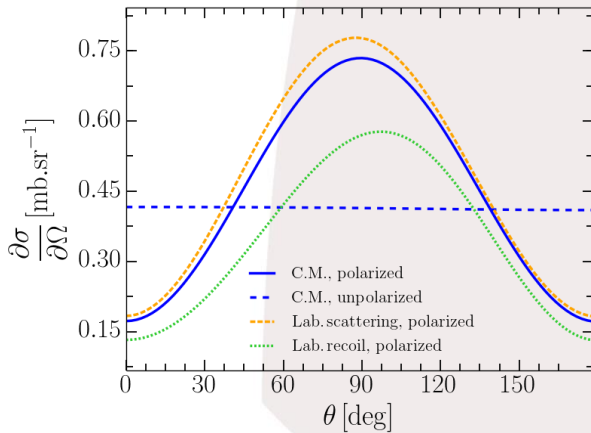
$$\sigma^{\text{polar}}(\theta) = \sigma(\theta) \left(1 + \frac{1}{3} p_{zz} A_{zz} + \frac{3}{2} p_z p_z^t C_{z,z^t} \right)$$

- **Predictions** for polarized ${}^3\text{H}(\vec{d}, n){}^4\text{He}$ 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.

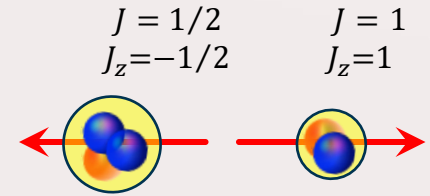
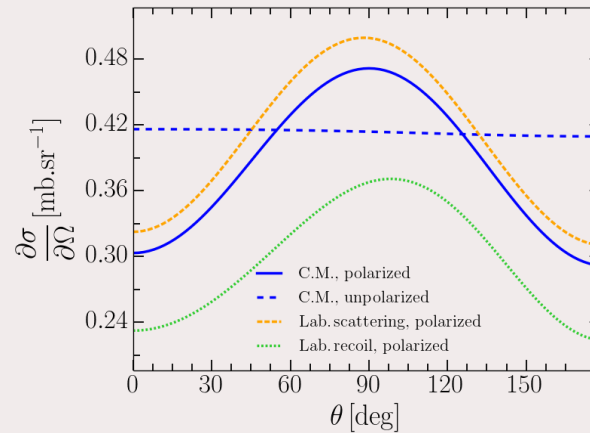
Angular distribution in different polarization scenarios



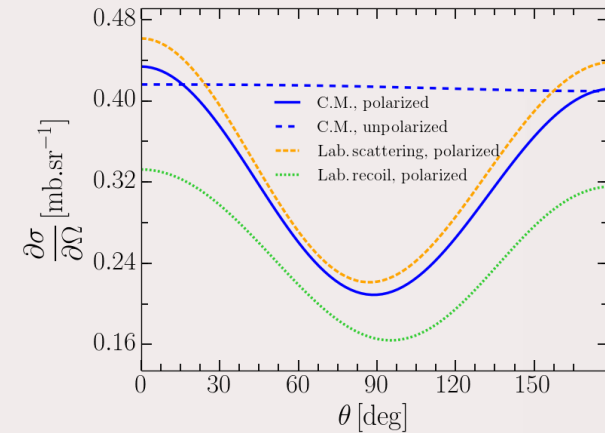
Total cross section increased



on average no effects



Total cross section decreased



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

Summary:

- Binary cluster states and (elastic, transfer..) reactions with NN and 3N.
- Three-cluster bound state and continuum with NN (and 3N).
- Reasonable control over model uncertainties.
- Challenging for heavier systems.
- Reaction observables/complete information on the continuum to probe nuclear forces.

Personal questions:

- How to use *ab initio* reactions to test approximations in reaction modeling ?
- Effective method to study optical potential ?