Towards Unified Approaches to Nuclear Structure and Reactions for Nuclei

Guillaume Hupin

Collaborators

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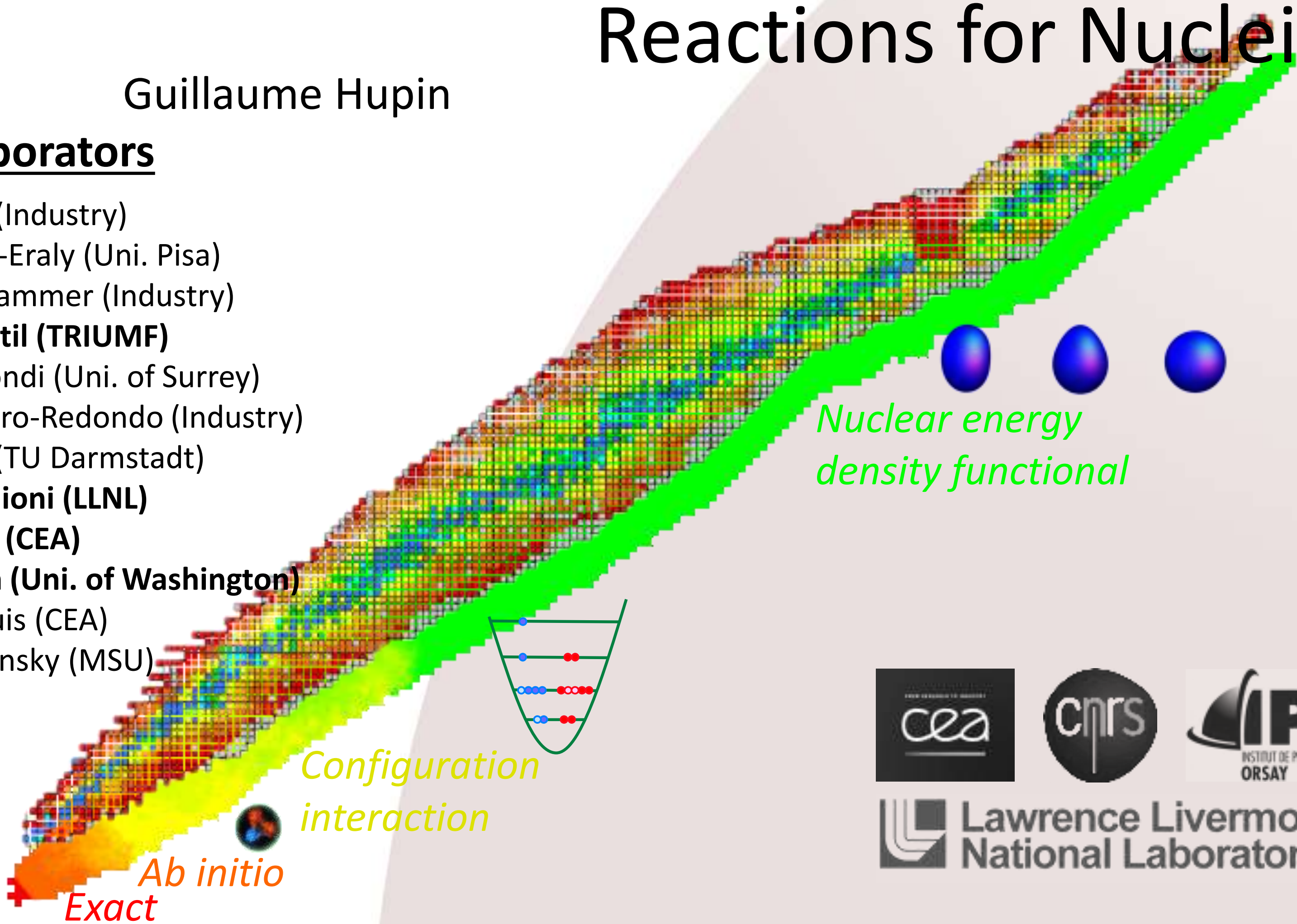

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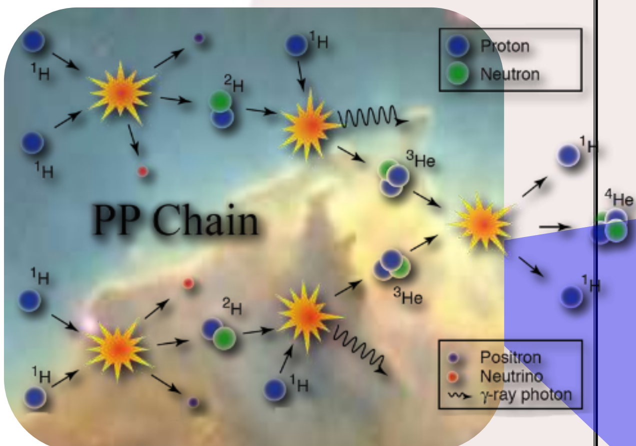
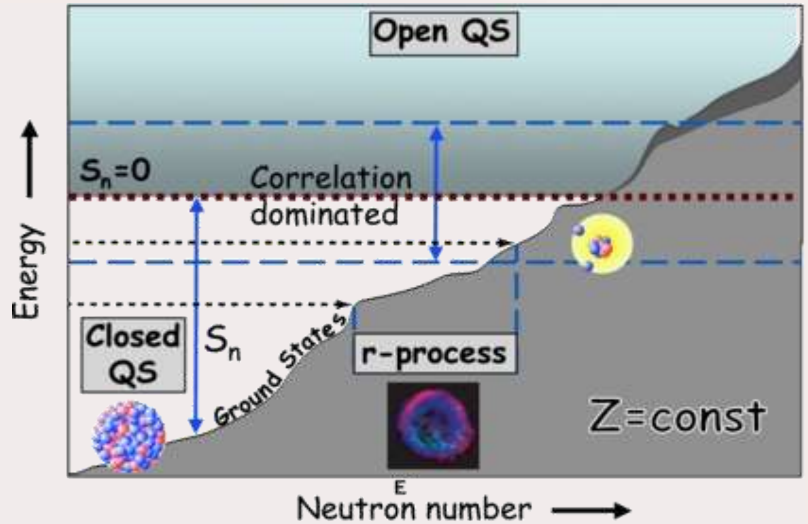
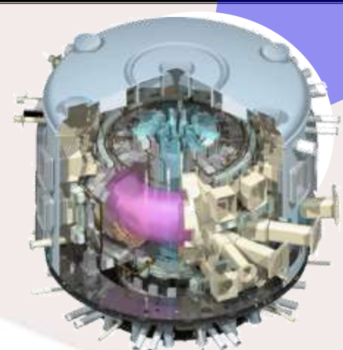
MOTIVATIONS: DESCRIPTION OF EXOTIC (NEUTRON RICH) AND RESONANT SCATTERING



Nuclear astrophysics



N. Michel, W. Nazarewicz, M. Płoszajczak et al. JPG36 (2008)

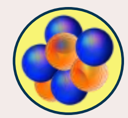


Fusion based energy generation

TRADITIONAL BOUND STATE TECHNIQUES

Methods developped in this presentation to solve the many body problem:

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

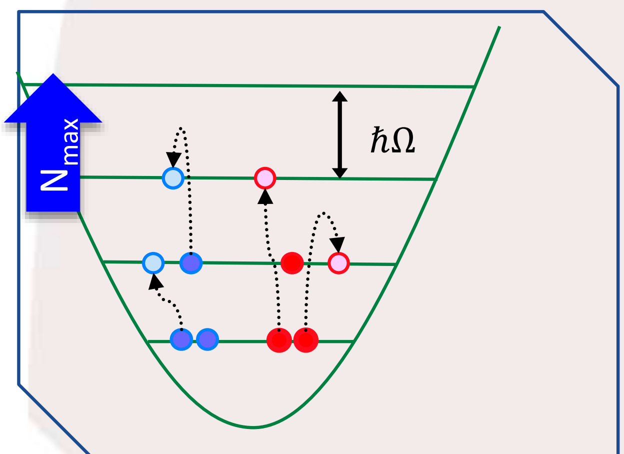


Mixing coefficients(unknown)

A-body harmonic oscillator states

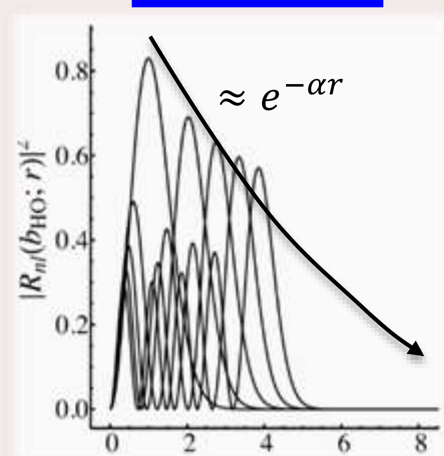
Second quantization

Can address **bound** and **low-lying resonances** (“short” range correlations).



No-Core Shell Model

HO basis

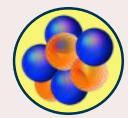


Unable to describe observables sensitive to the tail of the w.f. and **continuum states**.

EQUAL TREATMENT OF BOUND AND RESONANT STATES IN THE *AB INITIO* NO-CORE SHELL MODEL WITH CONTINUUM

Methods developped in this presentation to solve the many body problem:

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



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

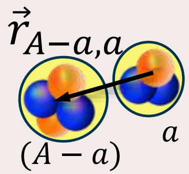
Mixing coefficients(unknown)

A-body harmonic oscillator states

Second quantization

Can address **bound** and **low-lying resonances** (“short” range correlations).

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



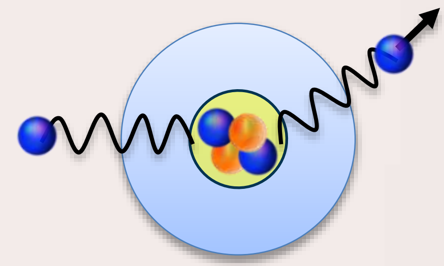
$\psi^{(A-a)}_{\alpha_1}\psi^{(a)}_{\alpha_2}\,\delta(\vec{r}-\vec{r}_{A-a,a})$

Relative wave function (unknown)

Antisymmetrizer

Channel basis

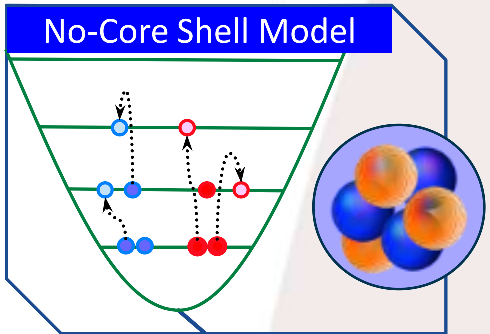
Cluster expansion technique

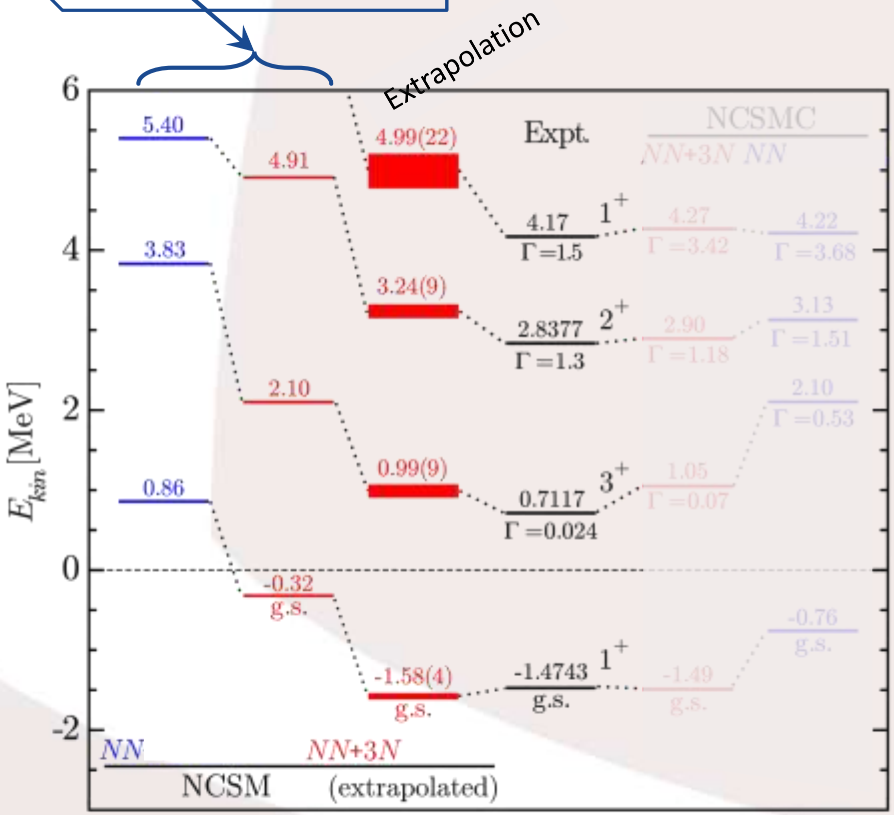


NCSM/RGM
Cluster formalism for elastic/inelastic

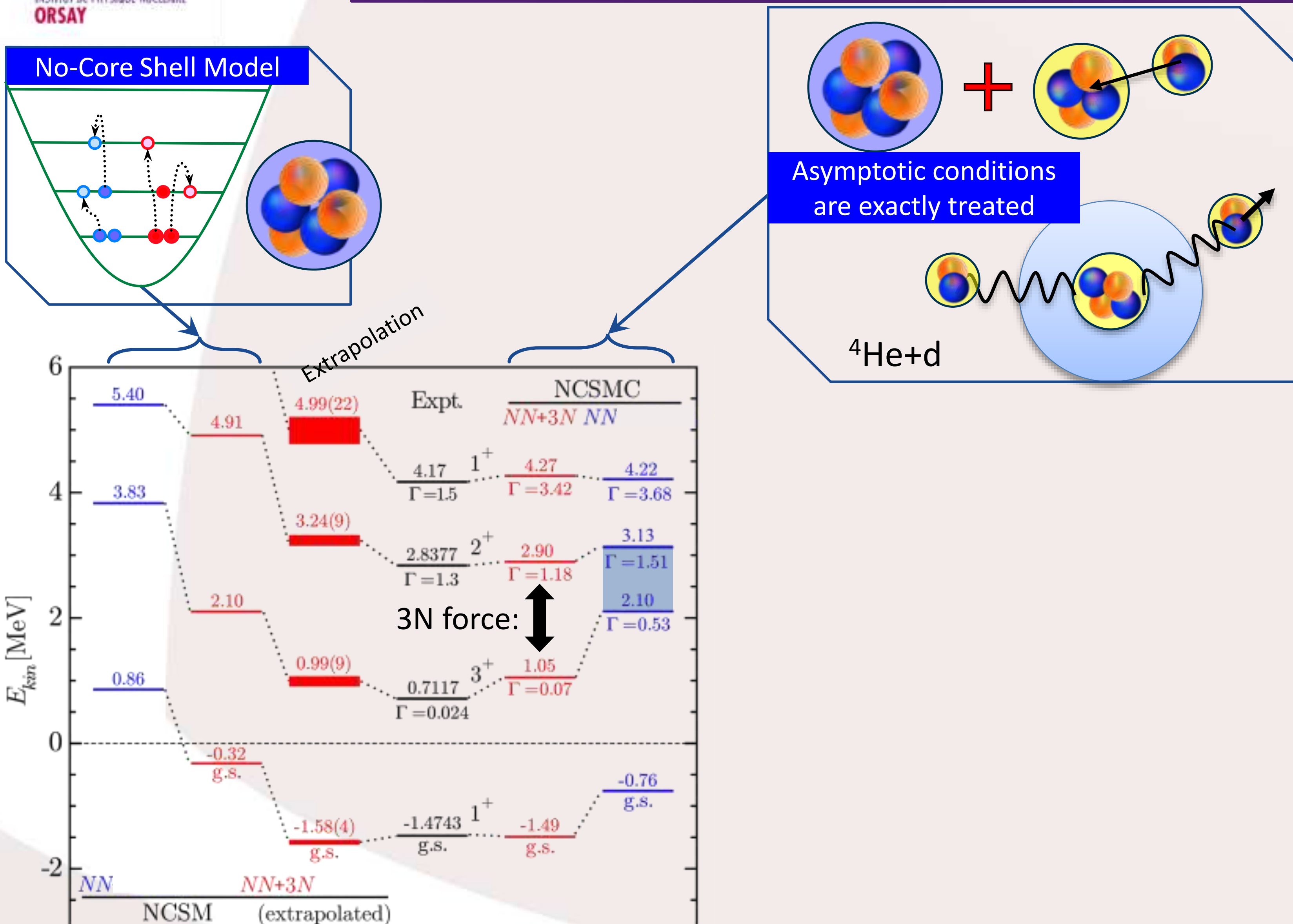
$$\Psi^{(A)}_{NCSMC} = \sum_{\lambda} c_{\lambda} |A\lambda J^{\pi}T\rangle + \sum_{v} \int d\vec{r} \, g_v(\vec{r}) \, \hat{A}_v \left| \Phi^{(A-a,a)}_{v\vec{r}} \right\rangle$$

UNDERSTANDING NUCLEAR STRUCTURE: ^{6}Li

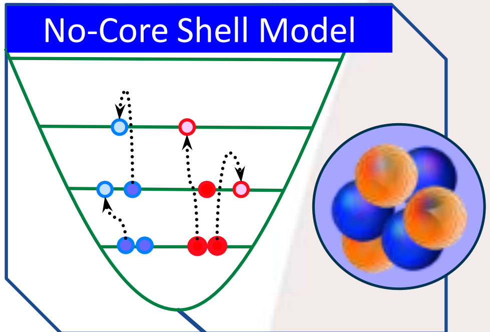


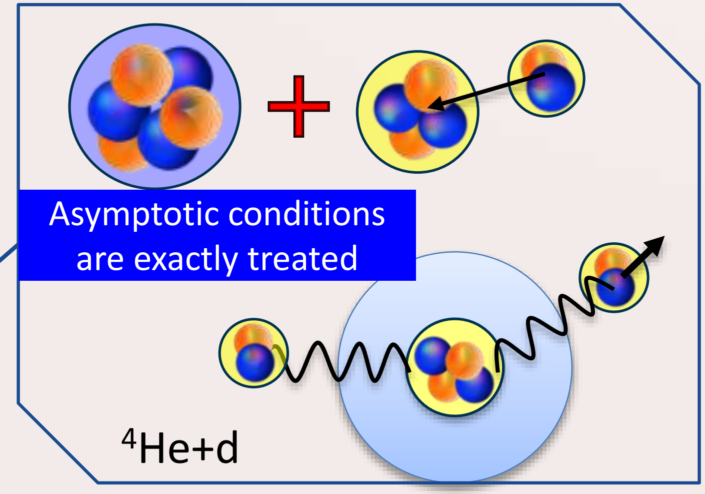


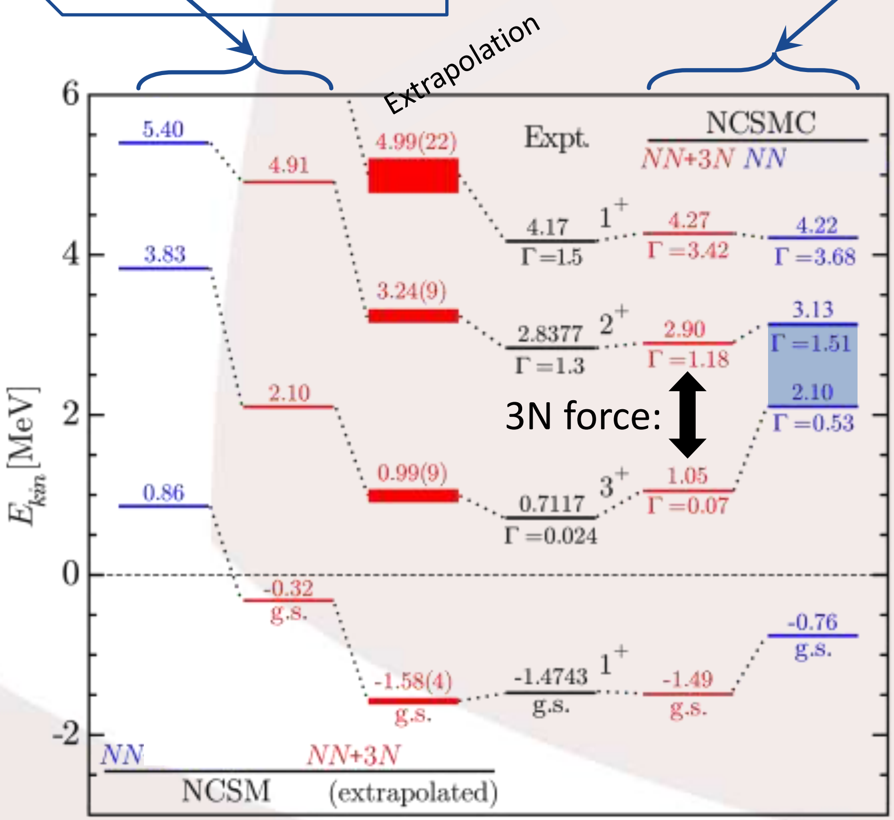
UNDERSTANDING NUCLEAR STRUCTURE: ^{6}Li



UNDERSTANDING NUCLEAR STRUCTURE: ^{6}Li



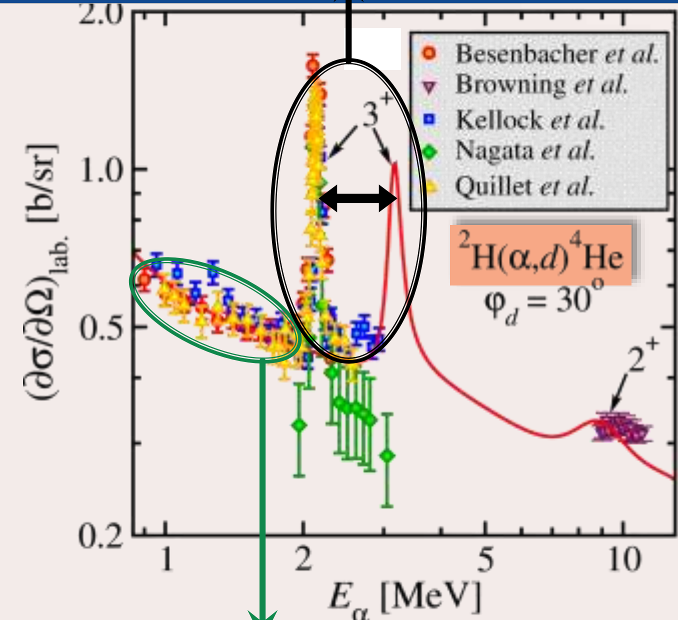




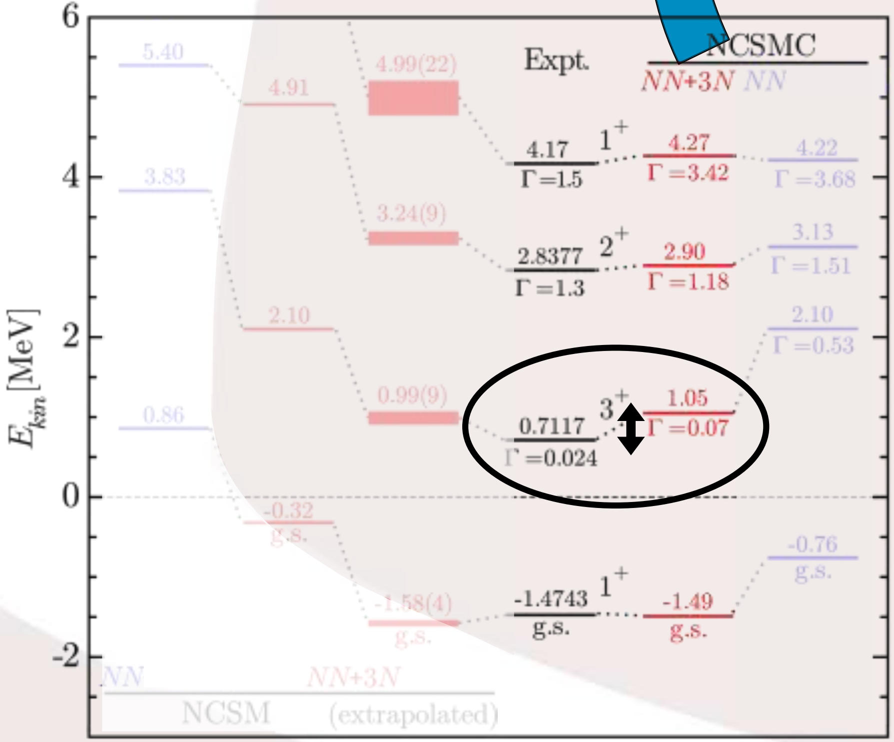
- Consistent ***ab initio*** calculation of this system.
- **Bound** and **resonant states** are **treated in the same way**.
- Effects of the chiral **3N force** are revealed.

CONCURRENTLY WITH NUCLEAR REACTION $^{2}H(\alpha,d)^{4}He$

Ability to probe the remaining inaccuracies of the **nuclear interaction**.



Correct treatment of continuum



High accuracy is achieved in the **low-energy** limit, important for:

1. Astrophysical S-factor.
2. Radiative capture at low energy.

G. Hupin, S. Quaglioni and P. Navrátil PRL**114** (2015)

p-^{10}C SCATTERING: STRUCTURE OF ^{11}N RESONANCES & TESTING χHAMILTONIAN

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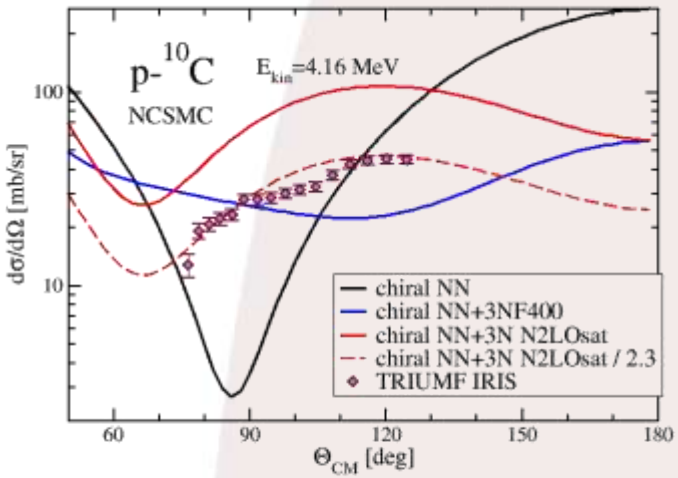
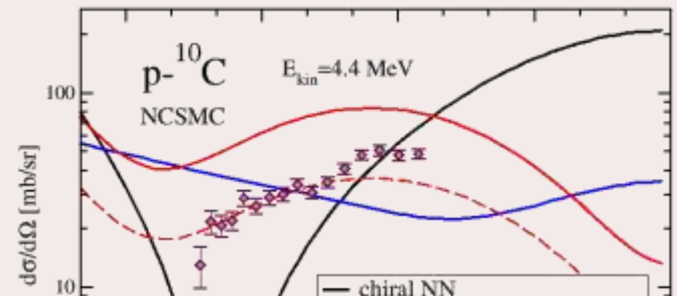
TRIUMF

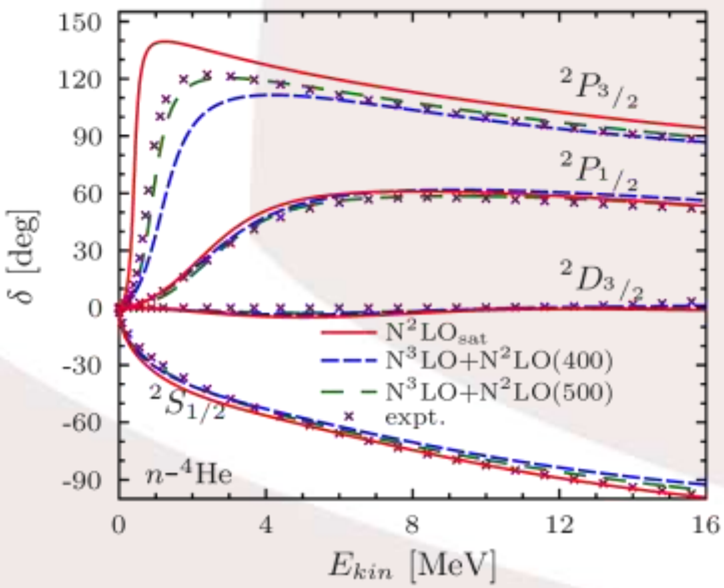
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

Possibility to discriminate between chiral nuclear forces ?





J^{π}	NN+3N400 E_r	NN+3N400 Γ	N^{2}LO$_{sat}$ E_r	N^{2}LO$_{sat}$ Γ	Data evaluation [12] E_r	Data evaluation [12] Γ
$1/2^+$	1.47	5.53	1.33	1.45	1.49(6)	0.83(3)
$1/2^-$	1.91	0.55	1.95	0.57	2.22(3)	0.6(1)
$5/2^+$	4.95	2.16	3.81	0.53	3.69(3)	0.54(4)
$3/2^-$	4.62	0.49	4.60	0.70	4.35(3)	0.34(4)
$3/2^+$	5.10	6.73	4.39	2.55	N/A	N/A
$5/2^-$	5.85	0.69	4.77	0.41		

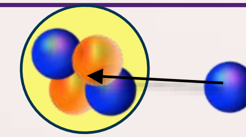


Some of the shortcomings of the nuclear interaction can already be **probed** in *p*-shell nuclei **through reactions**.
[NN *p*-waves are not perfectly reproduced by N^{2}LO$_{sat}$]

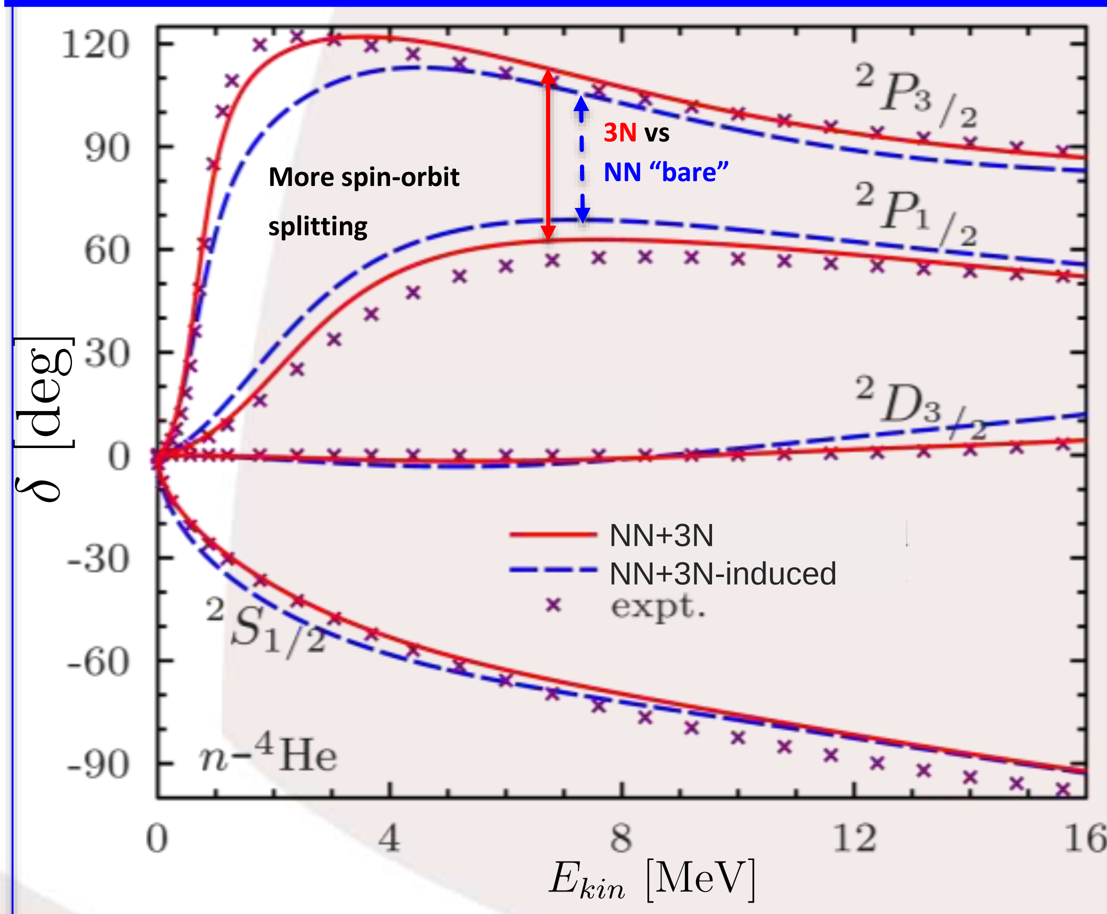
A. Kumar, R. Kanungo, A. Calci *et al.* PRL117 (2016).

n-^{4}He SCATTERING: NN VERSUS 3N INTERACTIONS

G. Hupin, J. Langhammer *et al.*, PRC88 (2013); P. Navrátil, S. Quaglioni, G. Hupin *et al.*, Phys. Scri.91 (2016) Celebrating the 1975 Nobel Prize



Three scenarii of nuclear Hamiltonians



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

Comparison between NN+3N-ind and NN+3N at N_{max}=13 with six ^{4}He states and 14 ^{5}He states.

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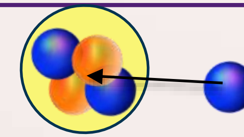
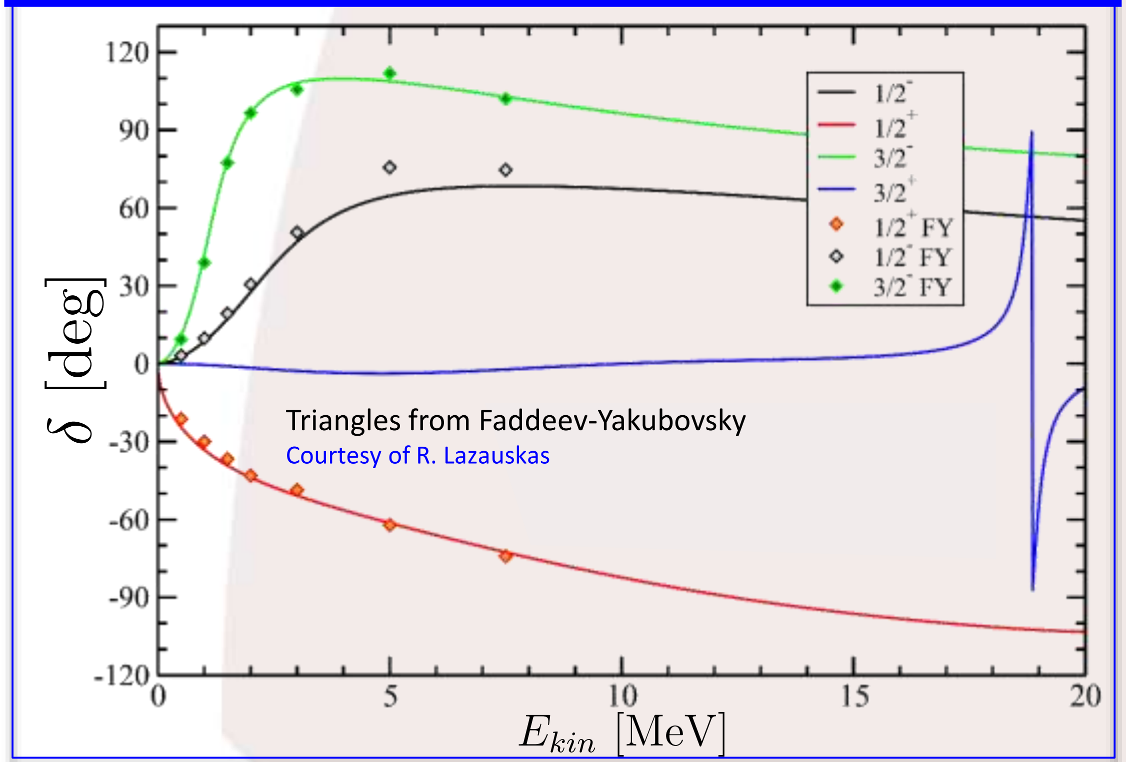
n-^{4}He SCATTERING: *AB INITIO* VS EXACT

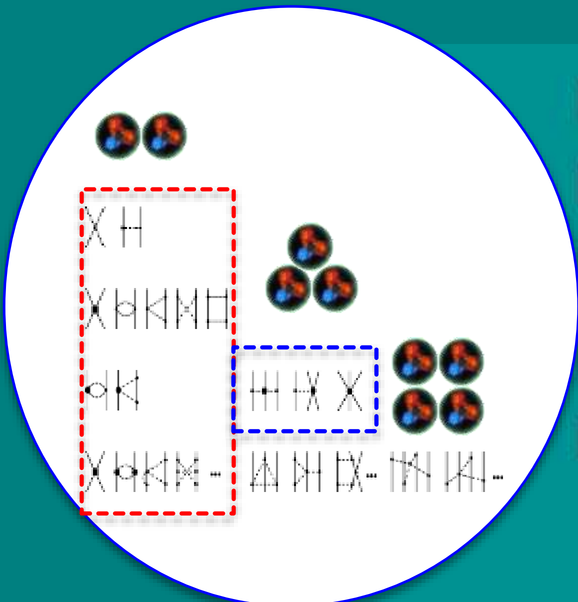


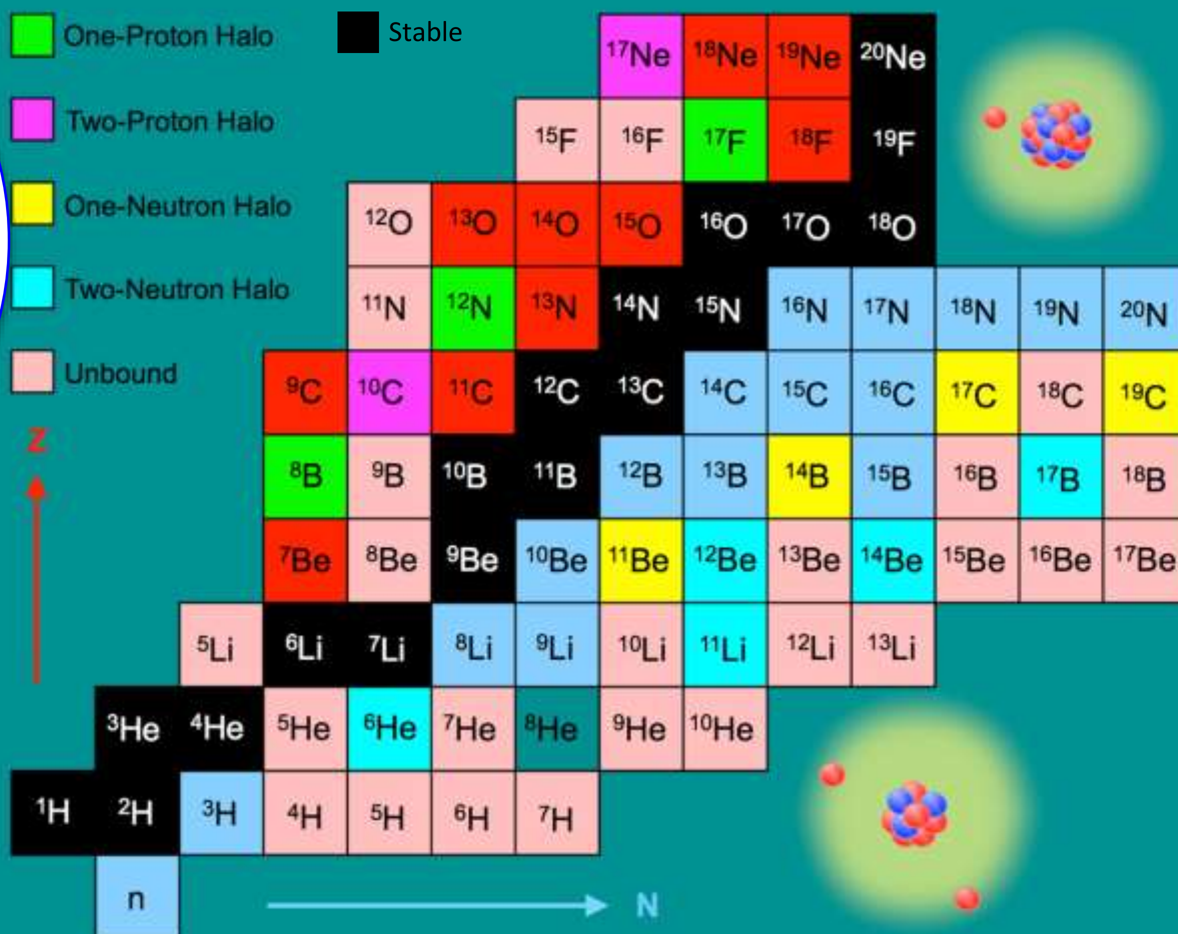
Scattering phase shifts NCSM/FY



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

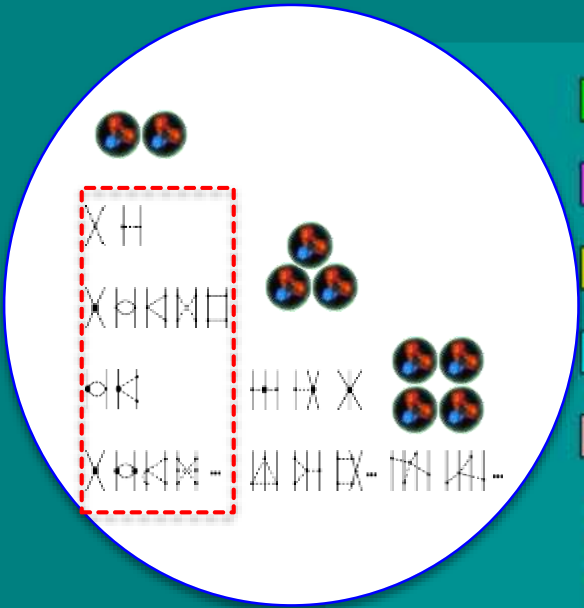
LIGHT SYSTEMS, FIRST TASTE OF EXOTIC PHENOMENA

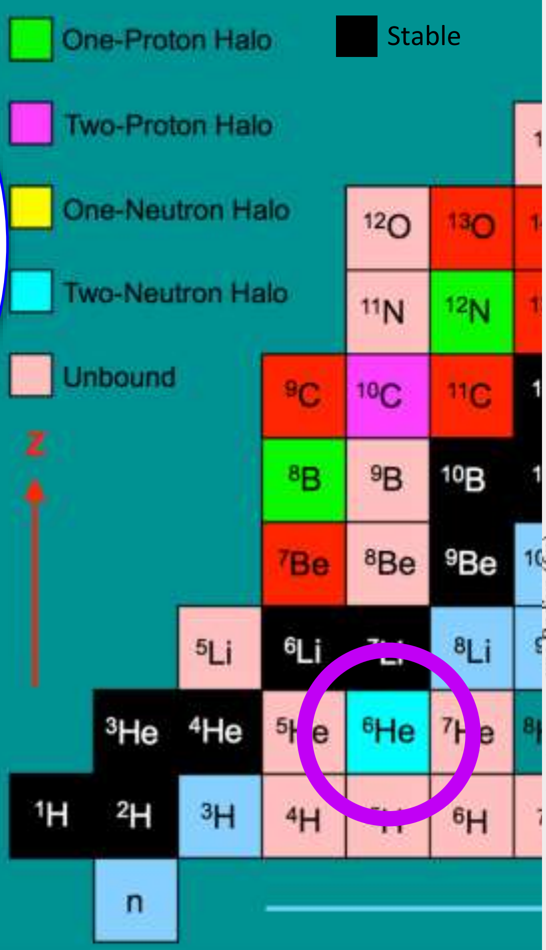


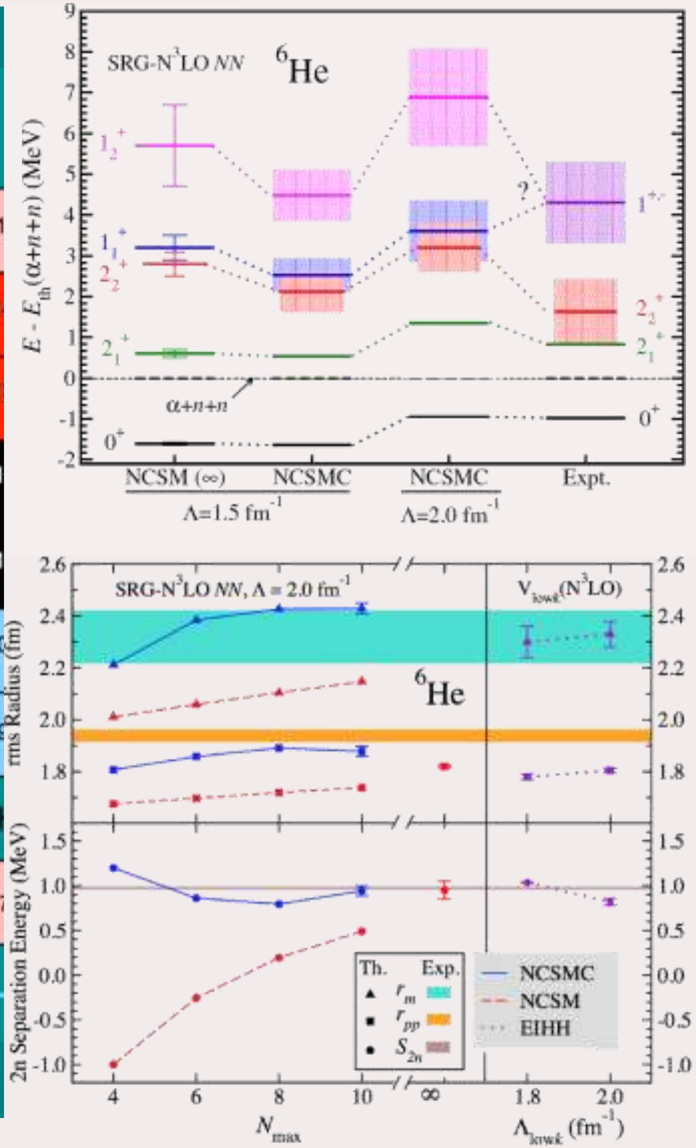


- Bound states
- Resonant states
- Scattering states
- Halo densities
- Clusterizations
- …

LIGHT SYSTEMS, FIRST TASTE OF EXOTIC PHENOMENA





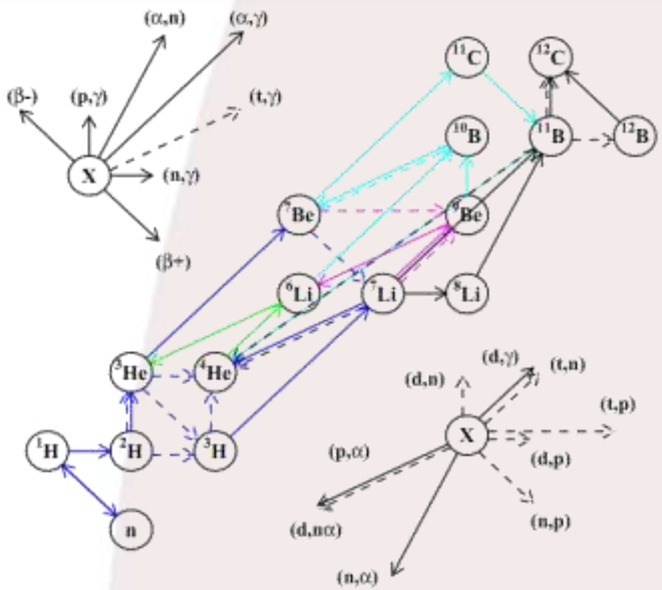


- Bound states
- Resonant states
- Scattering states
- Halo densities
- Clusterizations
- …

Carolina Romero-Redondo *et al.* PRL113 (2014); PRL117 (2016)

LOW-ENERGY TRANSFER REACTIONS (*d*,*N*)

Primordial Nucleosynthesis (blue)



LOW-ENERGY TRANSFER REACTIONS (*d*,*N*)

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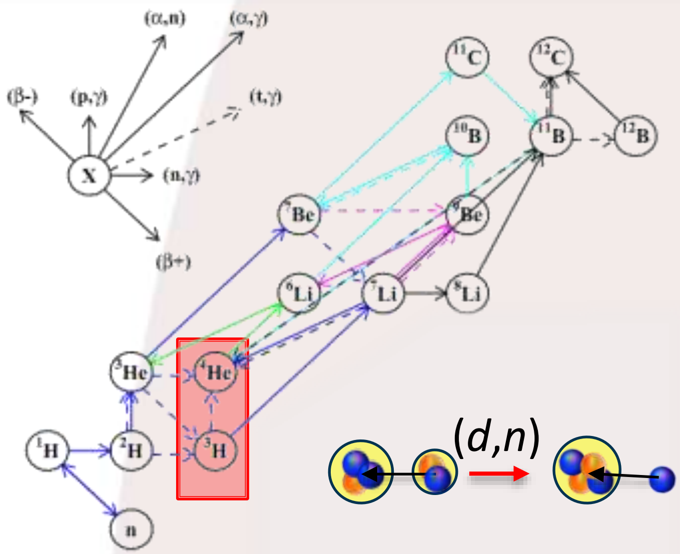
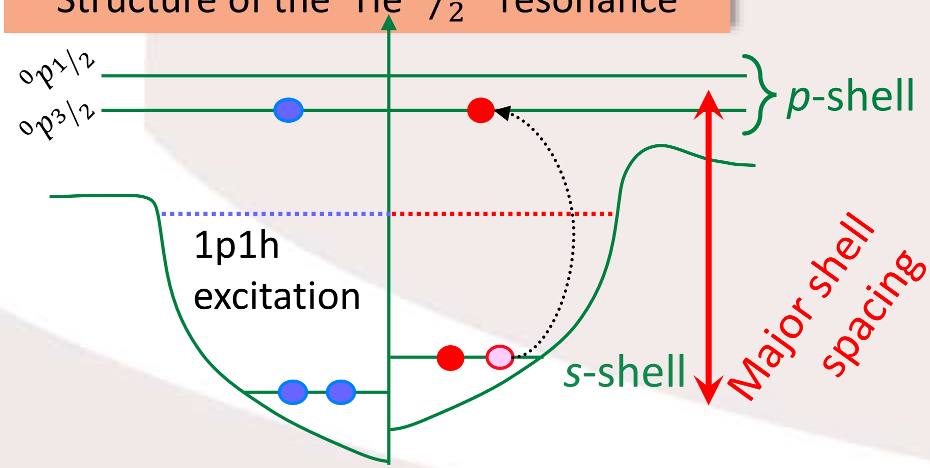
Primordial Nucleosynthesis (blue)

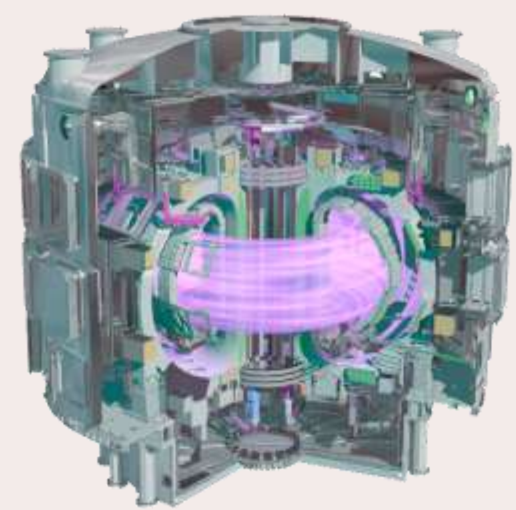


Structure of the ^{5}He $^{3}/_{2}^{+}$ resonance

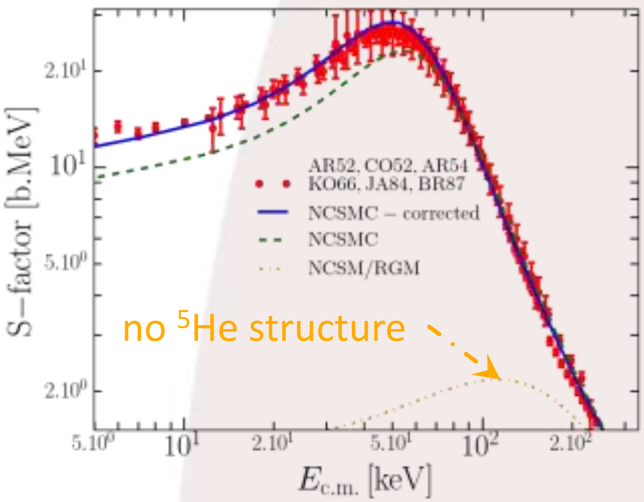


La science doit « nous rendre comme maîtres et possesseurs de la Nature »
R. Descartes *Discours de la méthode*.

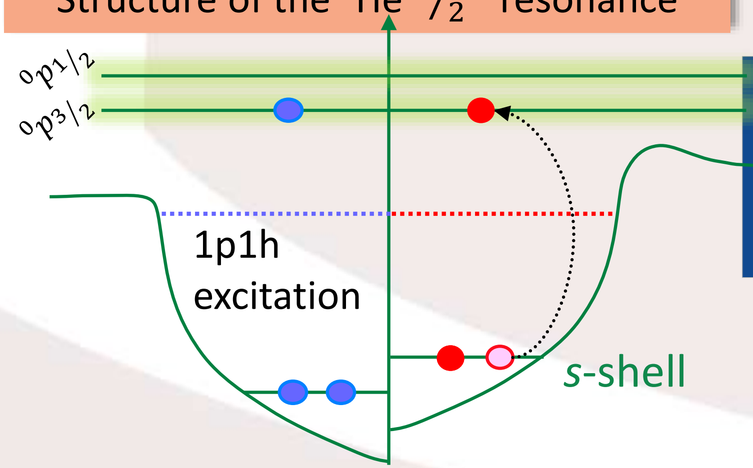
ITER design (Cadarache, France)



S-factor and angular distribution



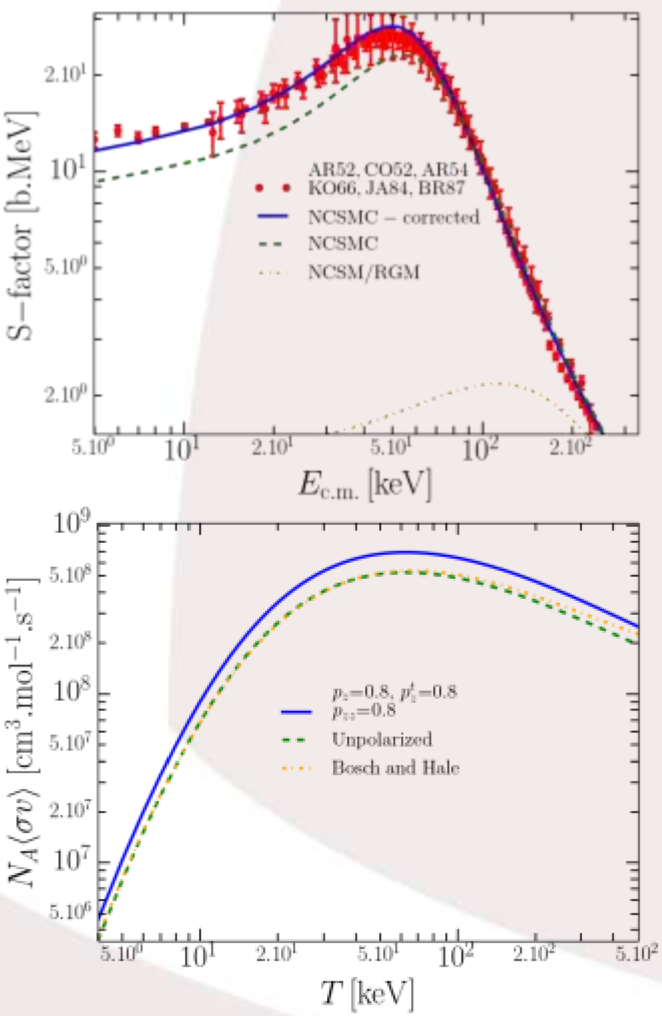
Structure of the ^{5}He $^3/_2{}^+$ resonance

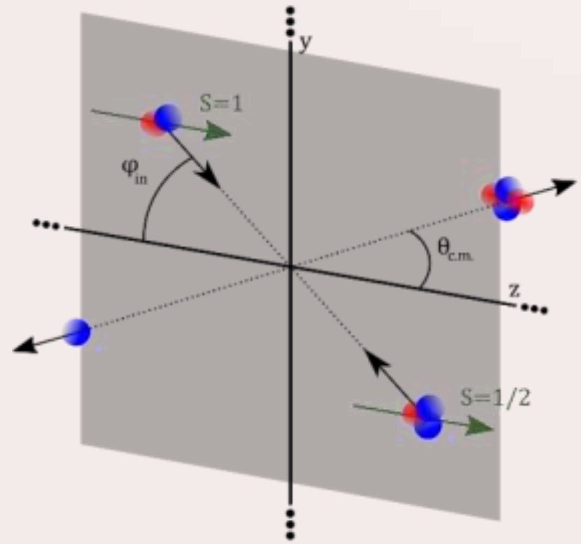


- **Importance** of **structure** of neighboring resonances is revealed in **transfer reactions**.

DT POLARIZED THERMONUCLEAR FUSION

S-factor and angular distribution





Reactant spins are prepared in a given configuration

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

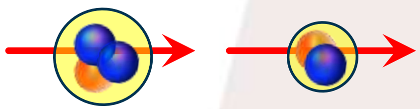
- **Importance** of **structure** of neighboring resonances is revealed in **transfer reactions.**
- **Predictions** for $^3\vec{\mathrm{H}}(\vec{d},n)^4\mathrm{He}$ reaction and its enhancement factor.

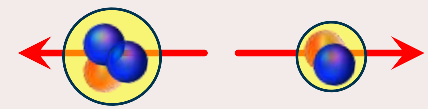
G. Hupin, S. Quaglioni and P. Navrátil to be submitted

POLARIZED THERMONUCLEAR FUSION:

Angular distribution in different polarization scenarios

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

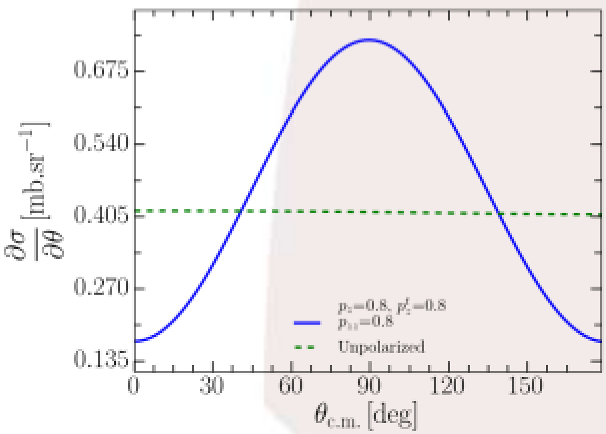


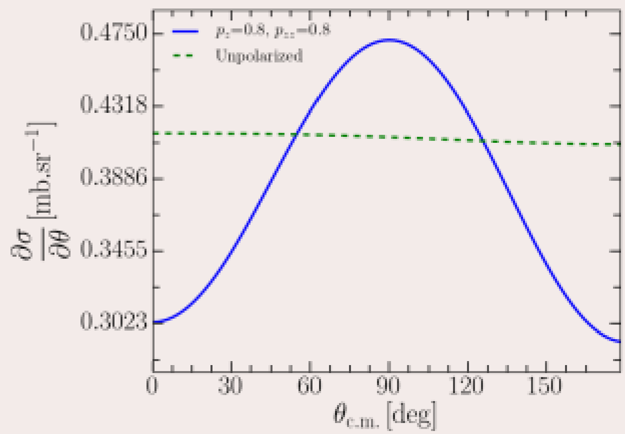


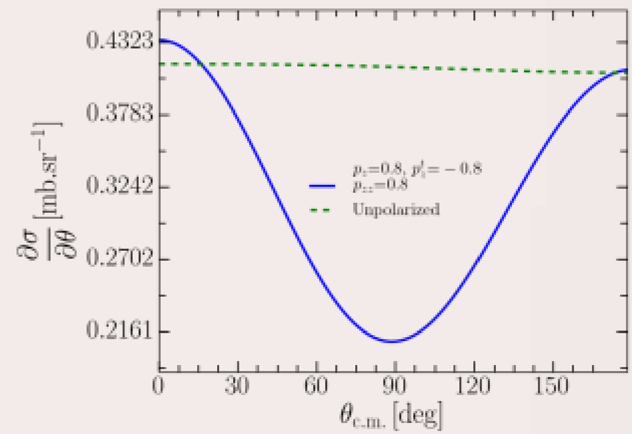
Total cross section increased

(on average) No changes

Total cross section decreased





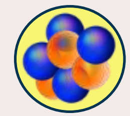


Spin tensor properties of the deuteron give the angular shape.
(Same as in $^3\overrightarrow{He}(\vec{d},p)^4He$)

MPMH METHOD: BRIEF INTRO

N. Pillet, J.-F. Berger, and E. Caurier, PRC78 (2008); C. Robin, N. Pillet, D. Peña Arteaga, and J.-F. Berger, PRC83 (2016)

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

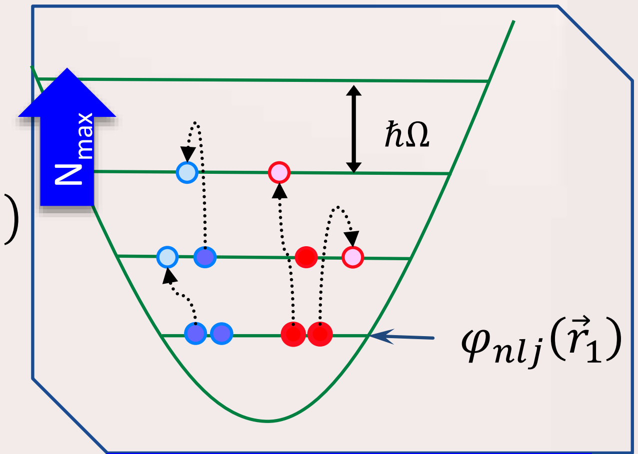


$$|A\lambda J^\pi T\rangle_{SD}\,\phi_{00}(\vec{R}^A_{c.m.})$$

Mixing coefficients(unknown)

A-body harmonic oscillator states

Second quantization



No-Core No-Shell Model

The MPMH is a double variational method

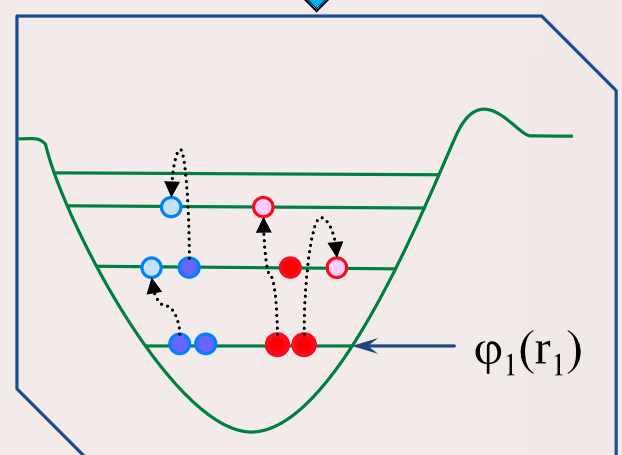
Variational amplitudes are the mixing coef. c_α and the single-particle orbitals $\varphi_i(\vec{r}_i)$, i.e.

$$\frac{\partial E}{\partial c_\alpha} = \frac{\partial E}{\partial \varphi_i} = 0$$

$$\Psi^{(A)}_{MPMH} = \sum_\alpha c_\alpha \mathcal{A}_\alpha \varphi_{\alpha,A}(\vec{r}_A)\varphi_{\alpha,A-1}(\vec{r}_{A-1}) \dots \varphi_{\alpha,1}(\vec{r}_1)$$

Mixing coefficients(unknown)

Single particle states(unknown)



MPMH « No-Core No-Shell »

MPMH METHOD: BRIEF INTRO

$$\Psi_{MPMH}^{(A)} = \sum_{\alpha} c_\alpha \mathcal{A}_\alpha \varphi_{\alpha,A}(\vec{r}_A)\varphi_{\alpha,A-1}(\vec{r}_{A-1}) \dots \varphi_{\alpha,1}(\vec{r}_1)$$

Mixing coefficients(unknown)

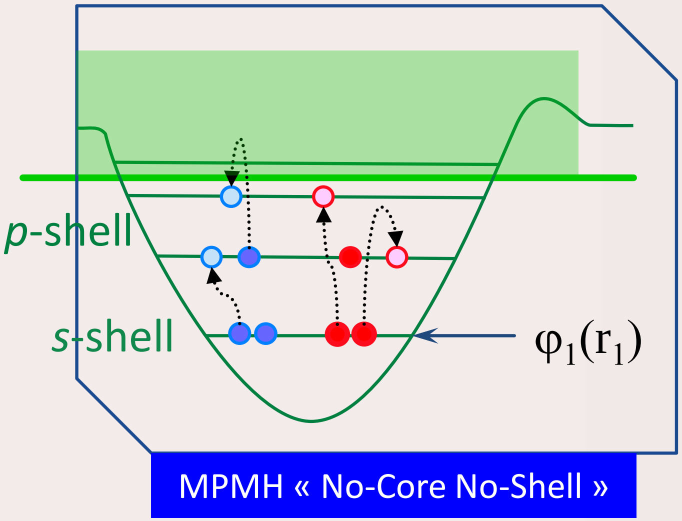
Single particle states(unknown)

For computational purpose we can truncate further

✓ Based on many-body energy:

Maximum s.p. energy

$$\Psi_{MPMH}^{(A)} = \sum_{\alpha}^{\alpha_{max}} c_\alpha \mathcal{A}_\alpha \varphi_{\alpha,A}(\vec{r}_A)\varphi_{\alpha,A-1}(\vec{r}_{A-1}) \dots \varphi_{\alpha,1}(\vec{r}_1)$$



MPMH METHOD: BRIEF INTRO

$$\Psi^{(A)}_{MPMH} = \sum_{\alpha} c_\alpha \mathcal{A}_\alpha \varphi_{\alpha,A}(\vec{r}_A)\varphi_{\alpha,A-1}(\vec{r}_{A-1}) \dots \varphi_{\alpha,1}(\vec{r}_1)$$

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- ✓ Based on many-body energy:

Maximum s.p. energy

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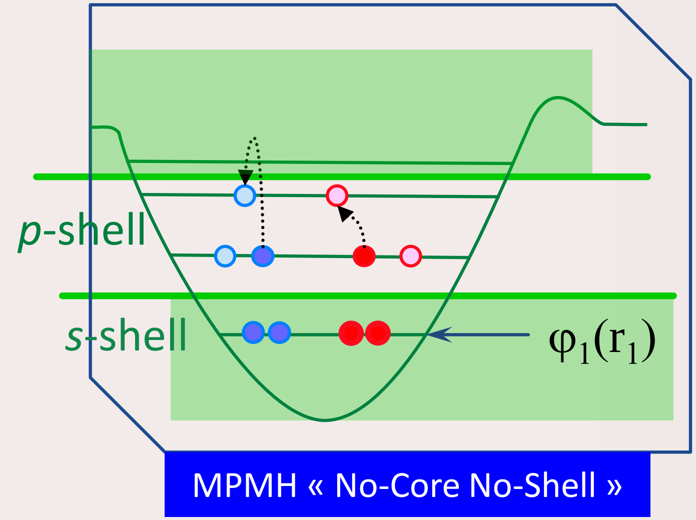


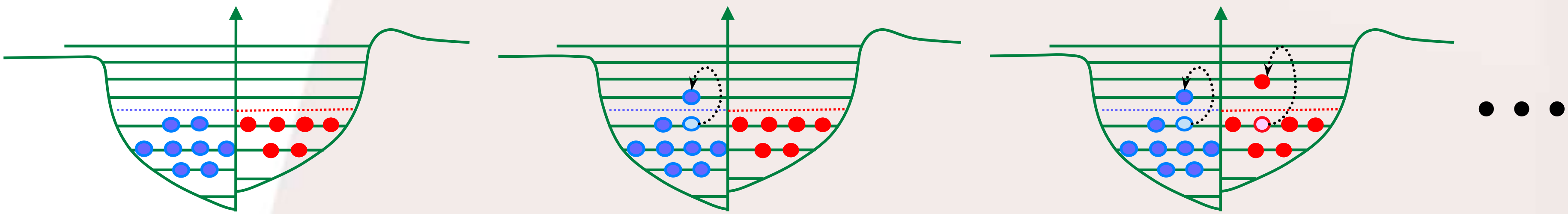
- ✓ Based on an active valence space and inactive core:

$$\Psi^{(A)}_{MPMH} = \sum_{\alpha=\alpha_{min}}^{\alpha_{max}} c_\alpha \, \Phi^{\varphi}_{\alpha,N}(\vec{r}_{A-a}, \dots, \vec{r}_A)\Phi^{\varphi}_{A-N}(\vec{r}_1, \dots, \vec{r}_{A-a})$$

Valence Core

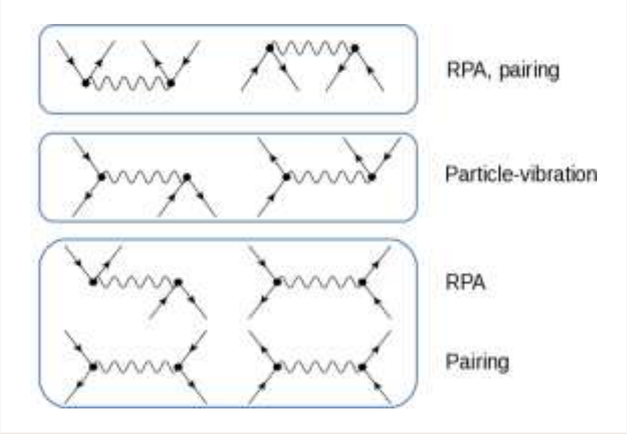
MPMH METHOD: BRIEF INTRO

✓ According to the type of many-body excitations



Reference state $|\phi\rangle$ $\qquad$ $|\phi_\alpha\rangle = |1p1h\rangle$ $\qquad$ $|\phi_\alpha\rangle = |2p2h\rangle$

- All nuclear correlations thought to be important in mean-field can be included.



- Some key features :
  - ✓ Systematically improvable, i.e. all the Hilbert space can be spanned.
  - ✓ All symmetries but translational invariance are conserved.

MPMH METHOD: ONE OR TWO PROPERTIES OF INTEREST

C. Robin, N. Pillet, D. Peña Arteaga, and J.-F. Berger PRC83 (2016)

Variation of mixing coefficients: **large-scale diagonalization.**

$$\delta_{c_\alpha^*}\big(E[\Psi] - \lambda(\langle\Psi|\Psi\rangle - 1)\big) = 0$$

$$\Leftrightarrow \sum_\beta \langle\Phi_\alpha|H|\Phi_\beta\rangle c_\beta = \lambda c_\alpha$$

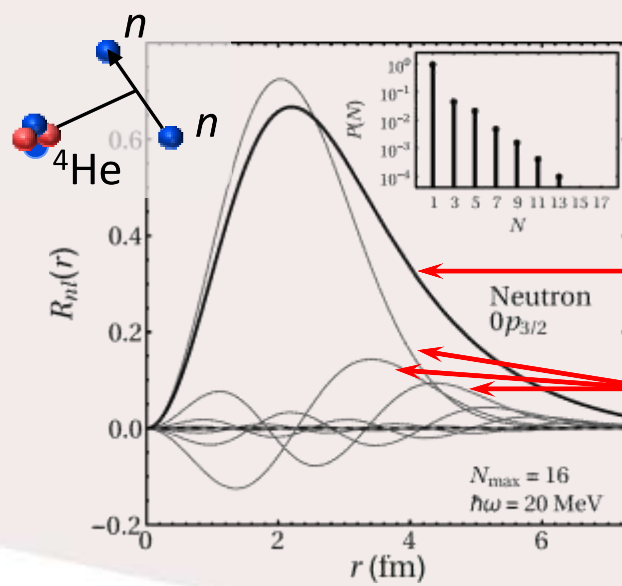
Variation of orbitals: generalized **one-body problem** embedded **in many-body space** spanned by Ψ.

$$\delta_{\varphi_i^*}\big(E[\Psi] - \lambda(\langle\Psi|\Psi\rangle - 1)\big) = 0$$

$$\Leftrightarrow \boxed{[h[\rho],\rho]} = G[\sigma]$$

Orbitals are optimum: $|\varphi\rangle = U|\varphi\rangle$

Mean-field adapted to a given type of many-body correlations (NCSMC, Shell-Model, 2p-2h…).



Opt. orbital

HO states

Ch. Constantinou, M. A. Caprio *et al.* arXiv:1605.04976

Illustration

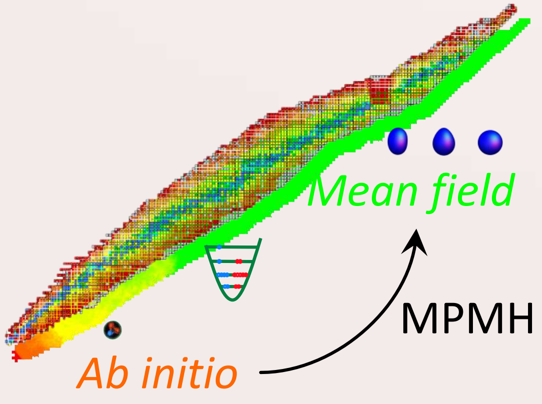
CONNECTING EDF TO BARE INTERACTION WITH MPMH

Ab initio ⟶ *Mean field*

use MPMH **for the first time**:

- To renormalize a bare nuclear interaction and **reveal** the corresponding **mean-field**.

→ MPMH can treat beyond mean-field correlations.



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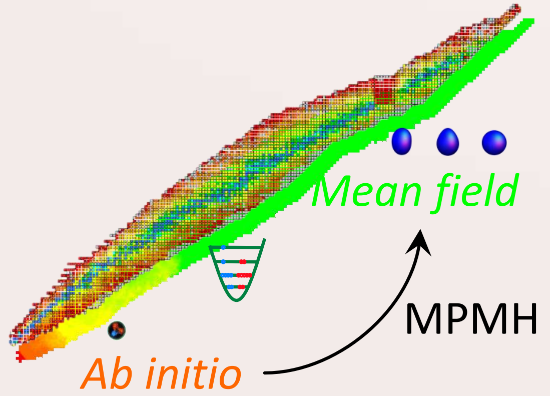
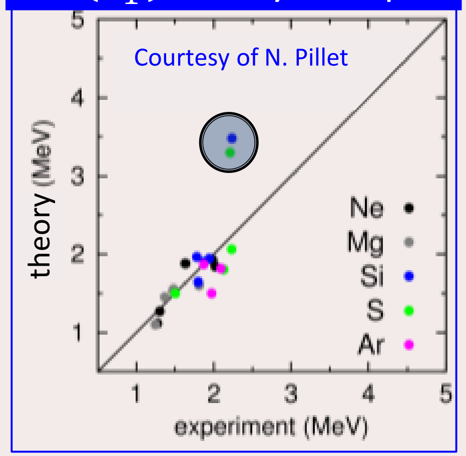


$E^*(2_1^+)$ theory vs expt.



$$v_{12}[\rho] = \sum_{j=1}^{2} \left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right) e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_j}$$

$$+\left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right) e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_3} \frac{\rho^\alpha(r_1)+\rho^\alpha(r_2)}{2(\mu_3\pi)^{3/2}}$$

$$+iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\vec{\nabla}_{12}(\vec{\sigma}_1+\vec{\sigma}_2)$$

$$+\ \text{tensor}$$

CONNECTING EDF TO BARE INTERACTION WITH MPMH

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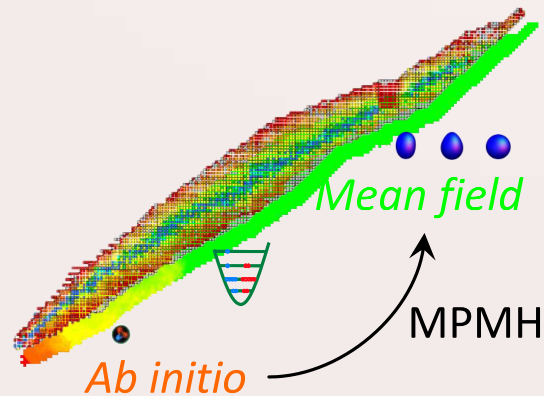

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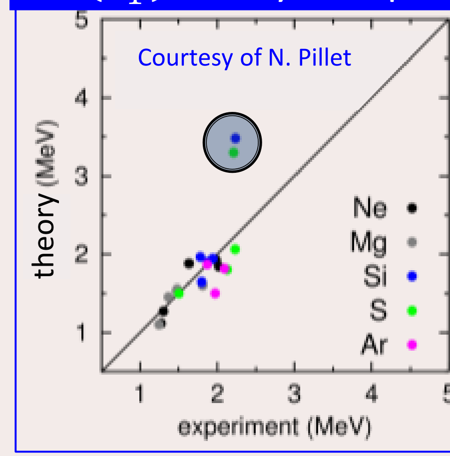
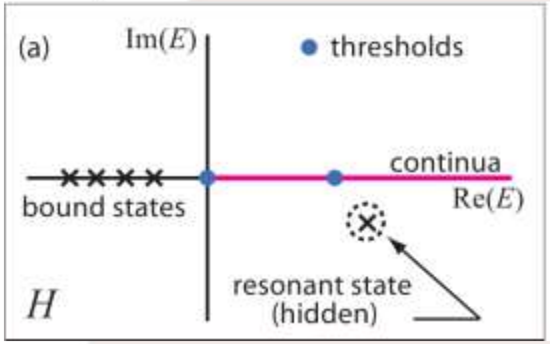
$E^*(2_1^+)$ theory vs expt.



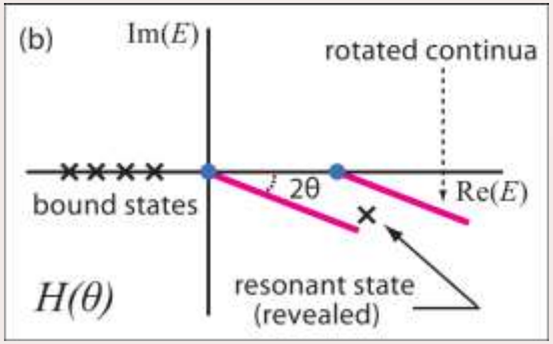
- Use **properties of the continuum** to infer an interaction fitted for exotic systems: a first step towards reactions.

Continuum properties of ^{11}N

	NN+3N400		N^{2}LO$_{sat}$		Data evaluation [12]	
J^π	E_r	Γ	E_r	Γ	E_r	Γ
$1/2^+$	1.47	5.53	1.33	1.45	1.49(6)	0.83(3)
$1/2^-$	1.91	0.55	1.95	0.57	2.22(3)	0.6(1)



Complex scaling



Kruppa *et al.* PRC89 (2014)

The complex scaling and the resonance states

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

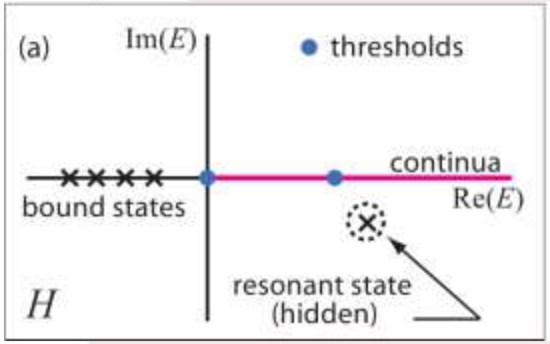
$$\hat{H}(\theta) = e^{-2i\theta}\hat{T} + \hat{V}\left(re^{i\theta}\right)$$
$$\hat{H}(r) = \hat{U}(\theta)\hat{H}(r)\hat{U}^{-1}(\theta)$$

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 Half-life

IN DEVELOPMENT: RESONANCES



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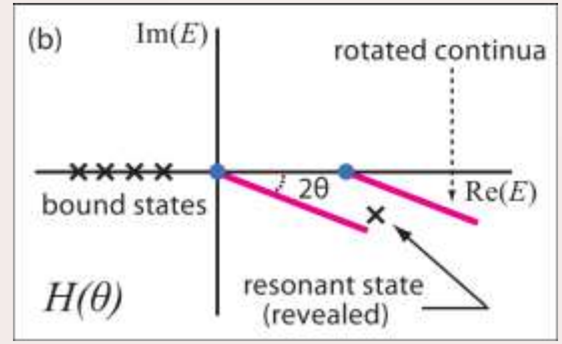

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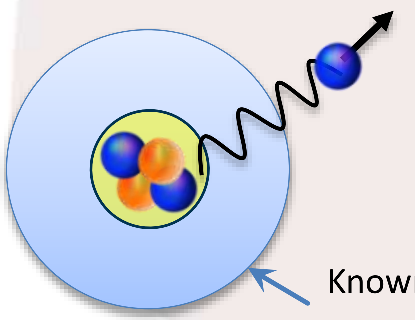
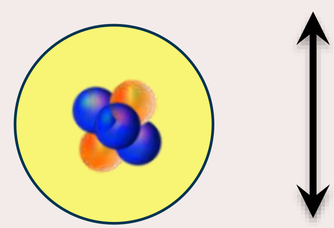


Known asymptotic

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

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



Spatially extended but falls off exponentially

Boundary limit problem

Bound state problem

IN DEVELOPMENT: APPLICATION TO NN SYSTEM

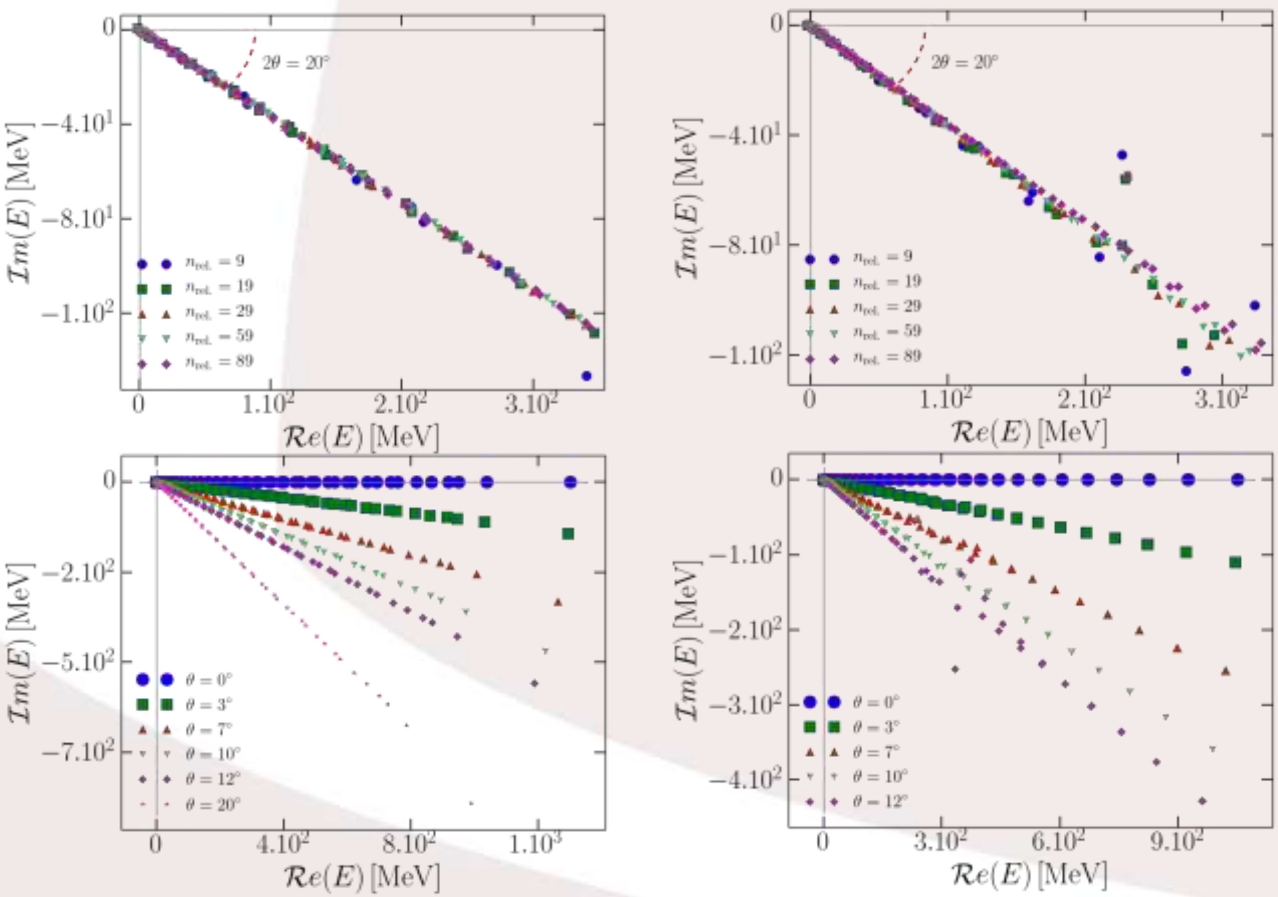
Collaboration with R. Lazauskas and J. Carbonell

Schematic case: the deuteron

- Use of an HO basis in Jacobi coordinates
- Diagonalization in the deuteron channel

Malfliet-Tjon

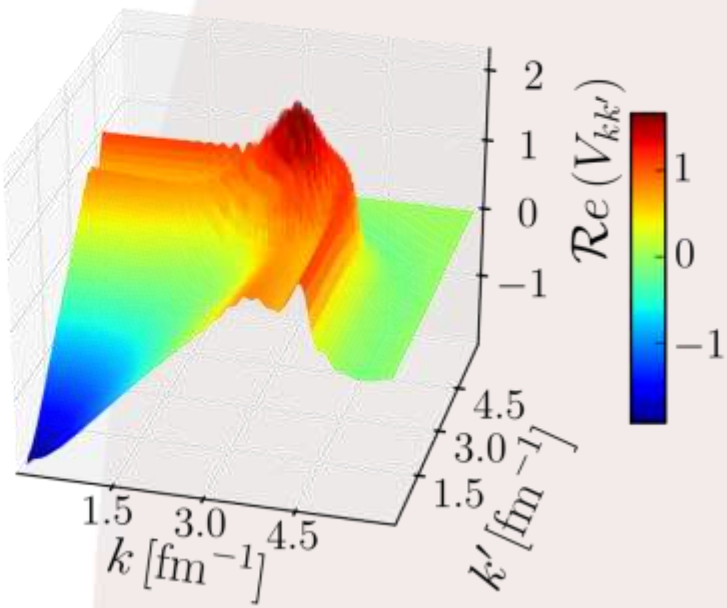
N^{3}LO

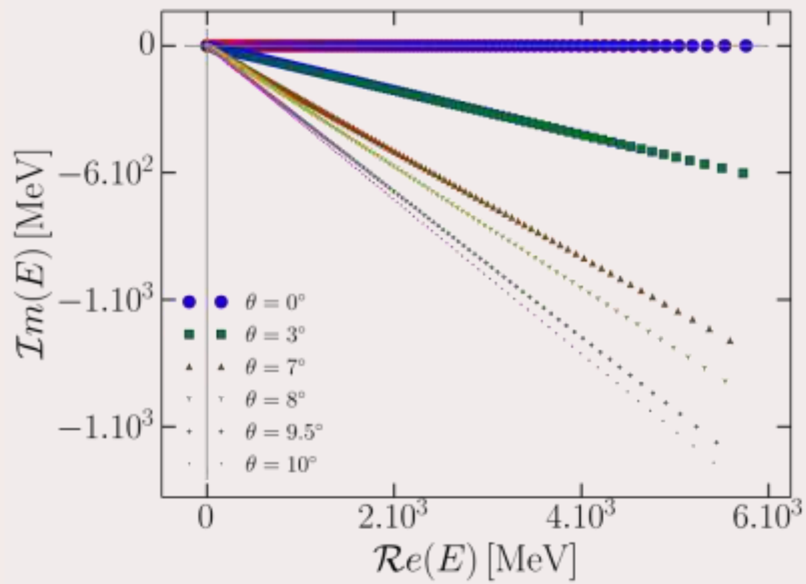


Generalization of the MPMH configuration mixing approach to symmetric non-hermitian complex matrices.

IN DEVELOPMENT: APPLICATION TO NN SYSTEM

$^1S_0$ N^{3}LO pn interaction at θ =10.0°

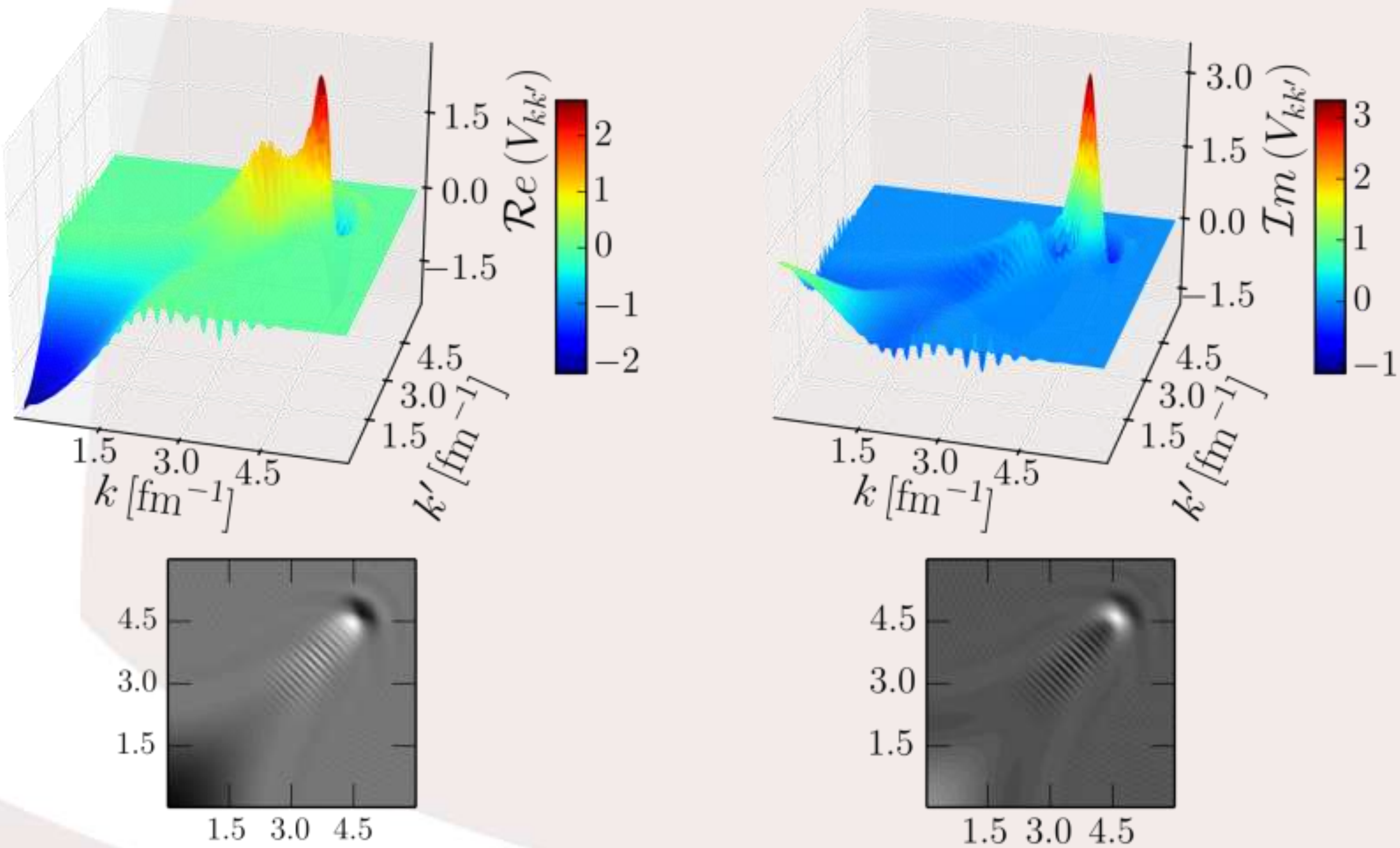




- SRG evolution requires spanning a large NN basis ($n_r \sim 150$). The typical scale of k is 10 fm^{-1} (V^{NN}).
- Complex scaling involves the integration of diverging polynomials (of order n) far from their zeroes.

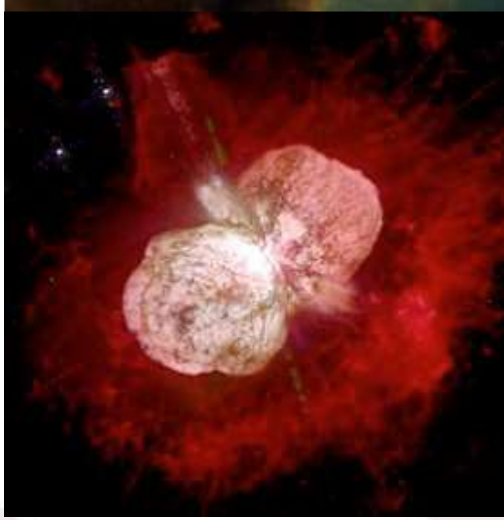
SOFT INTERACTION FOR CI METHODS WITH SRG

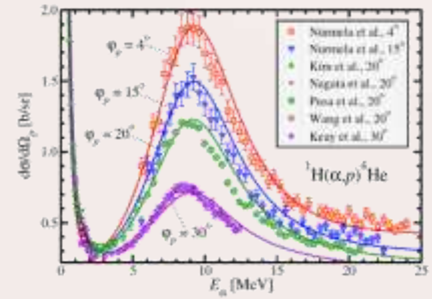
$^1S_0$ N^{3}LO pn interaction at $\theta = 10.0^\circ$ $\Lambda_{\text{SRG}} = 1.5\,\text{fm}^{-1}$



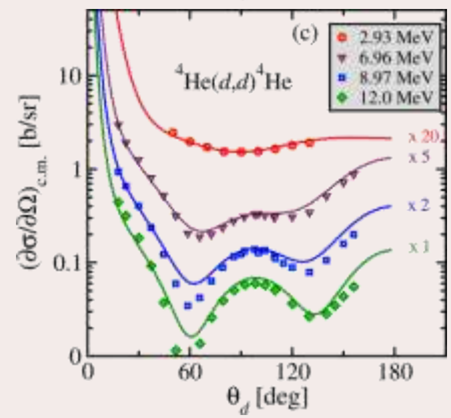
THANK YOU !



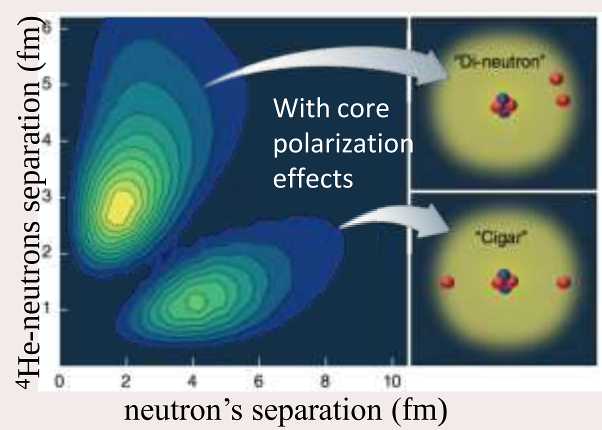


^{5}Li



^{6}Li



^{6}He