Ab initio calculations of reactions and exotic nuclei

Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart (INT 17-1a)

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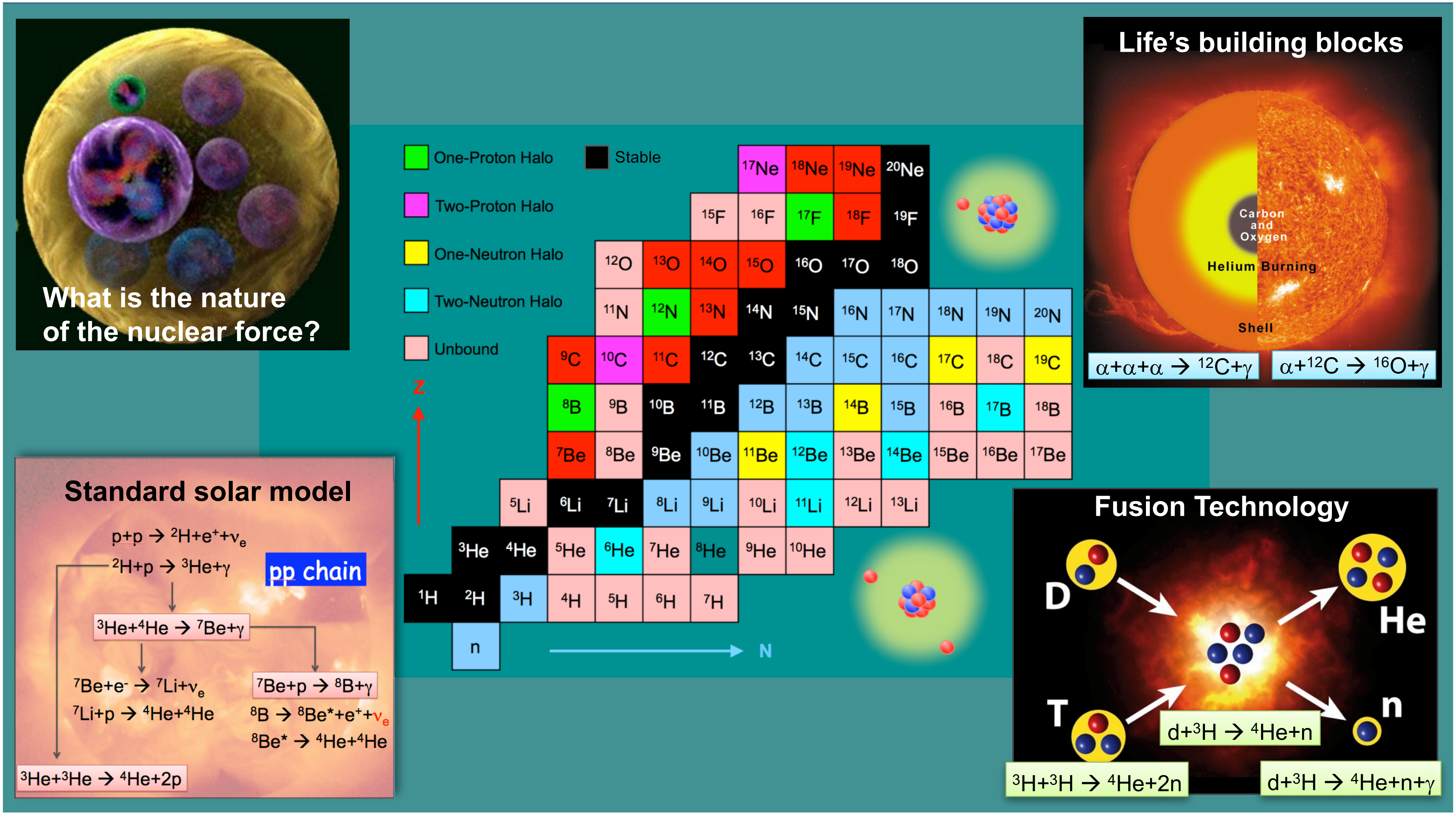
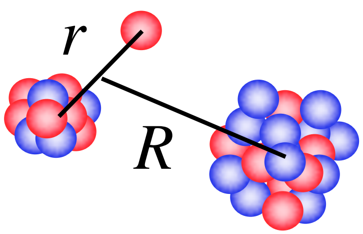
A predictive theory of light-nuclei reactions is essential for both basic and applied science



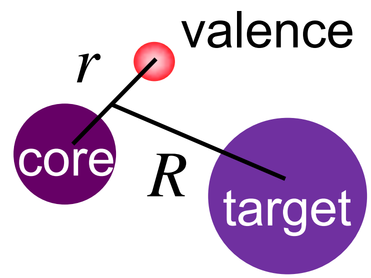
Our problem: quantum mechanical scattering. The 'idealist' and the 'pragmatic' approach

Ab Initio Theory



- A nucleon degrees of freedom
- 'Realistic' nucleon-nucleon (NN) and three-nucleon (3N) forces
- Pauli principle treated exactly
- Extremely difficult multichannel scattering problem
  - Exactly solvable for A = 3,4
  - What to do for heavier light nuclei?

Few-Body Model



- Few (3 or 4) relevant 'cluster' d.o.f.
- Structure of clusters is neglected
- Effective (optical) potential between core, valence and target
- Pauli principle approximated
- Easier to solve, more widely applicable

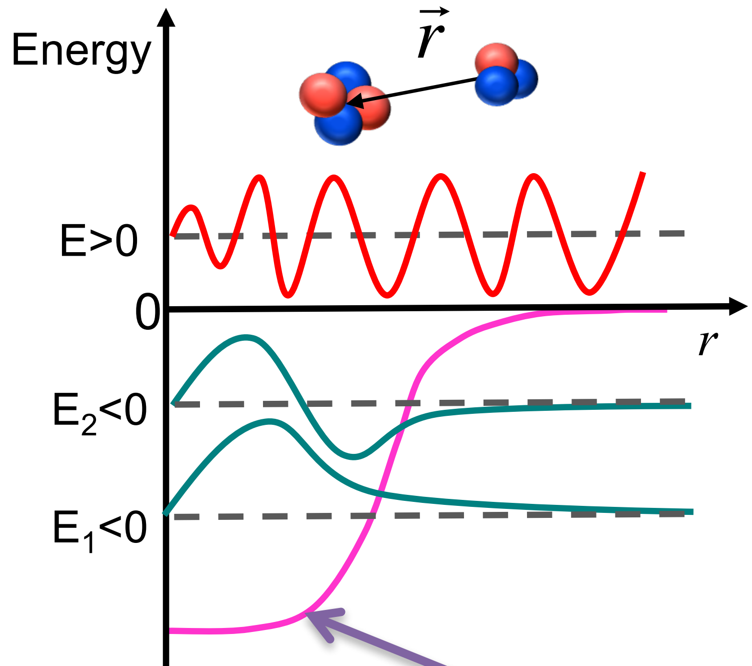
At low-energies, when only a few reaction channels are open, 'adiabatic' two-step solution

1) Reconstruct the interaction potential between a projectile and a target starting from:

   – *Ab initio* square-integrable wave functions of the clusters

   – 'Realistic' nucleon-nucleon (NN) and three-nucleon (3N) interactions

2) Solve for projectile-target relative motion



Overall interaction potential between projectile and target

This is the main concept behind the no-core shell model with continuum approach … albeit with a small tweak

Ab initio no-core shell model with continuum (NCSMC)

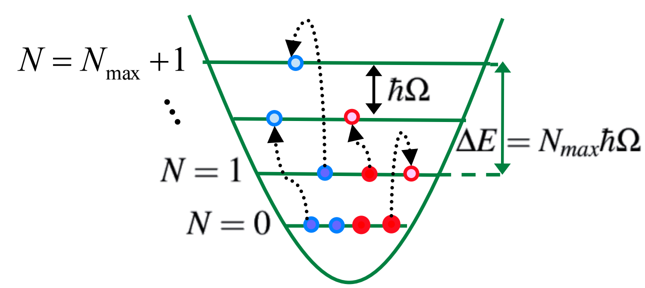
- Seeks many-body solutions in the form of a generalized cluster expansion

NCSM eigenstates — **NCSM/RGM continuous states**

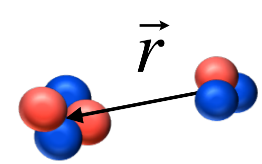
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\, u_{\nu}(\vec{r}\,) \hat{A}_{\nu} \left| {}_{(A-a)} \xrightarrow{\vec{r}} {}_{(a)} , \nu \right\rangle$$

Unknowns

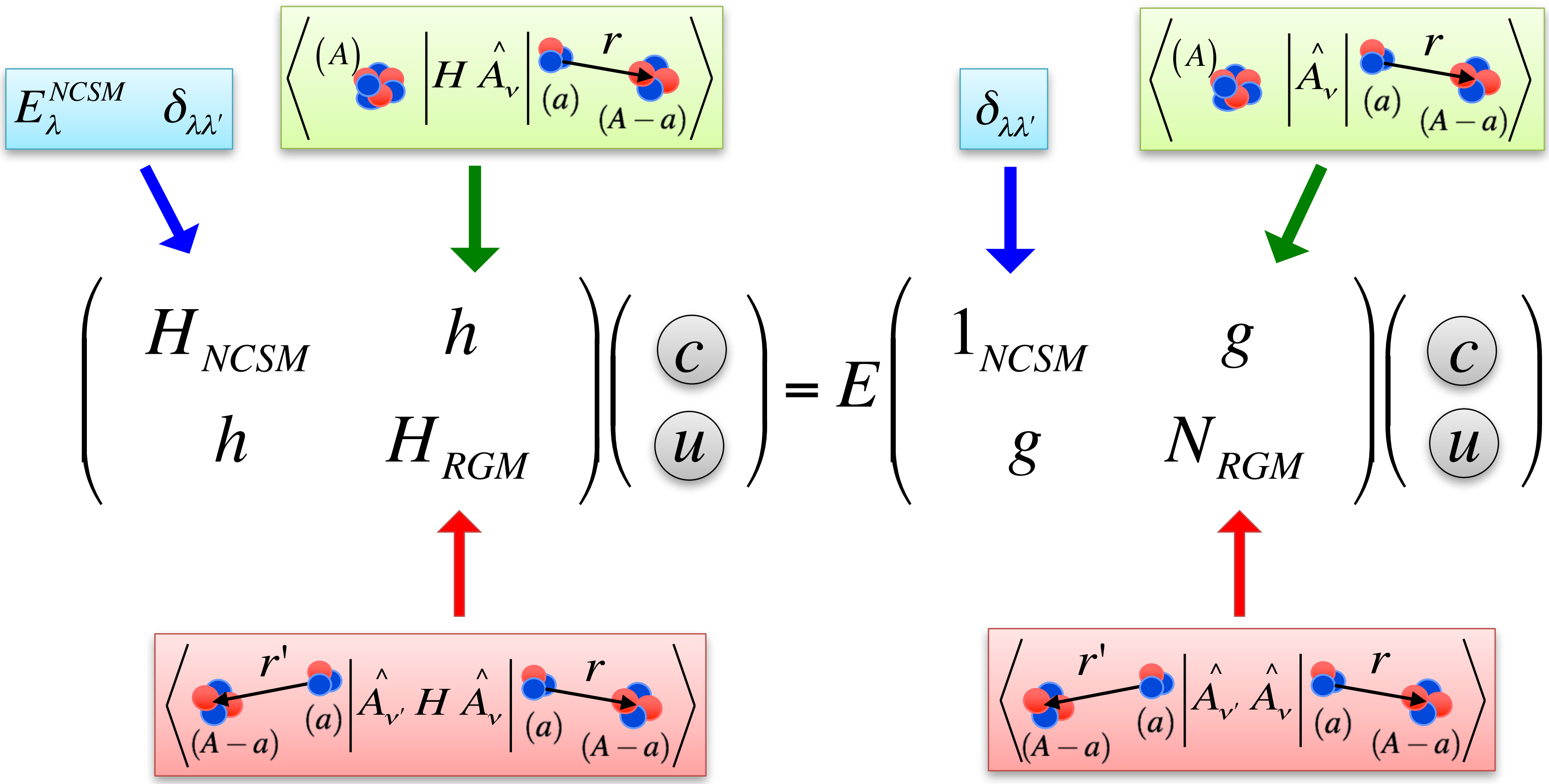
- *Ab initio* no-core shell model (NCSM):
  - Clusters' structure, short range



- Resonating-group method (RGM):
  - Dynamics between clusters, long range



Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations



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

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

Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

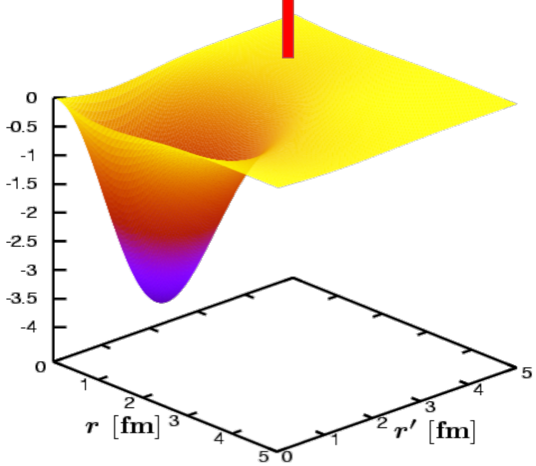
$$E_\lambda^{NCSM}\,\delta_{\lambda\lambda'}$$

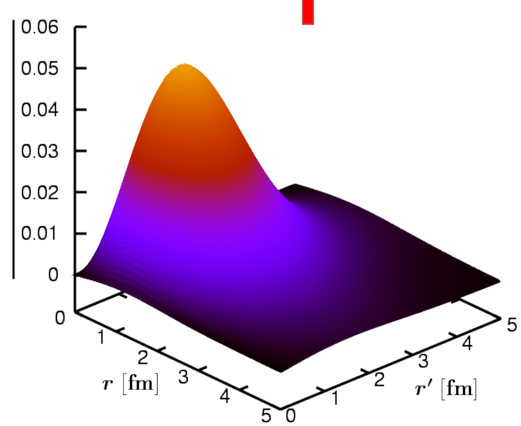
$$\left\langle (A) \middle| H\,\hat{A}_\nu \middle| (a) \xrightarrow{r} (A-a) \right\rangle$$

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

$$\left\langle (A) \middle| \hat{A}_\nu \middle| (a) \xrightarrow{r} (A-a) \right\rangle$$

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





A few words about the RGM portion of the basis

- NCSMC generalized cluster expansion:

NCSM eigenstates — **NCSM/RGM continuous states**

$$\Psi^{(A)} = \sum_\lambda c_\lambda \left| {}^{(A)} \text{(nucleus)}, \lambda \right\rangle + \sum_\nu \int d\vec{r}\, u_\nu(\vec{r})\, \hat{A}_\nu \left| \text{(nucleus)}_{(A-a)} \xrightarrow{\vec{r}} \text{(nucleus)}_{(a)}, \nu \right\rangle$$

Unknowns: c_λ, $u_\nu(\vec{r})$

Jacobi channel basis

$$\left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left[\left(\left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}$$

- These are **translational invariant** basis states, describing only the internal motion
- Note: Here the target and projectile are **both translational invariant** states

Since we are using NCSM eigenstates, it is convenient to introduce HO channel states

- Jacobi channel states in the harmonic oscillator (HO) space:

$$\left|\Phi_{\nu n}^{J^\pi T}\right\rangle = \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} R_{n\ell}(r_{A-a,a})$$

- Notes:
  - Formally, the coordinate space channel sates given by:

$$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle = \sum_n R_{n\ell}(r) \left|\Phi_{\nu n}^{J^\pi T}\right\rangle$$

    – I used the closure properties of HO radial wave functions

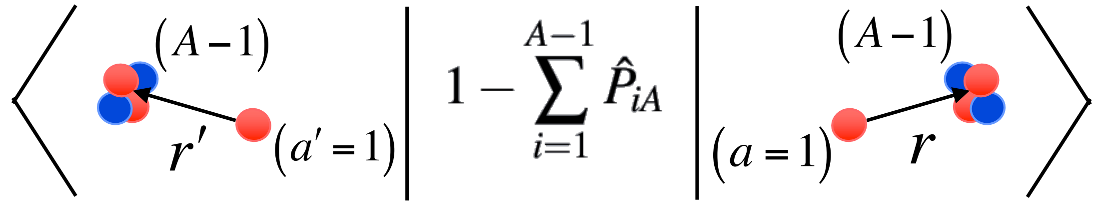
$$\delta(r - r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

  - Again: target and projectile are both translational invariant eigenstates
    – Works for the projectiles up to ^{4}He
    – Not practical if we want to describe reactions with p-shell targets!

In practice, expansion is truncated and only works for short-range components of NCSM/RGM kernels

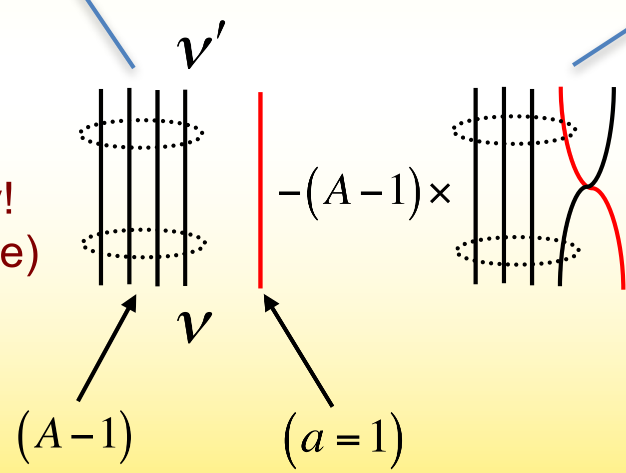
An example: the RGM norm kernel for nucleon-nucleus channel states

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



$$N^{\mathrm{RGM}}_{\nu'\nu}(r',r) = \delta_{\nu'\nu} \frac{\delta(r'-r)}{r'r} - (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

Direct term:
Treated exactly!
(in the full space)



Exchange term:
Obtained in the model space!
(**Short-range** many-body correction due to the exchange of particles)

$$\delta(r - r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

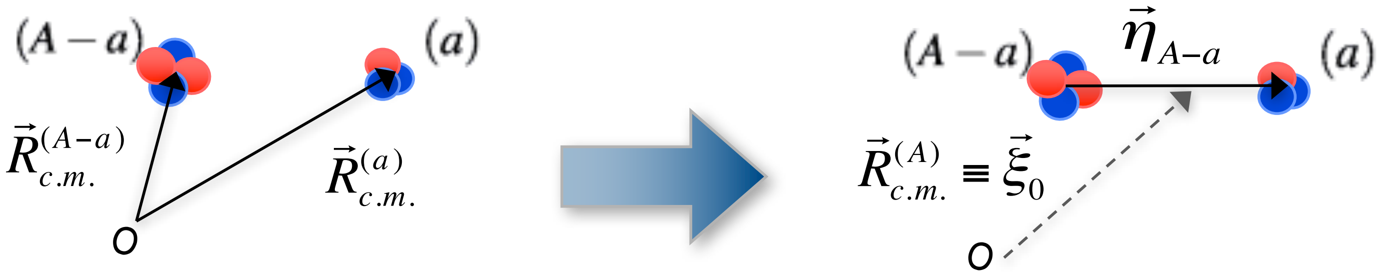
Define Slater-Determinant (SD) channel states in which the target is described by a SD eigenstates

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle_{SD} \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell\left(\hat{R}^{(a)}_{c.m.}\right)\right]^{(J^\pi T)} R_{n\ell}\left(R^{(a)}_{c.m.}\right)$$

$$\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)$$

Vector proportional to the c.m. coordinate of the A-a nucleons

Vector proportional to the c.m. coordinate of the a nucleons



$$\left(\varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)\varphi_{n\ell}\left(\vec{R}^{(a)}_{c.m.}\right)\right)^{\ell} = \sum_{n_r\ell_r,NL} \left\langle 00,n\ell,\ell \middle| n_r\ell_r,NL,\ell\right\rangle_{d=\frac{a}{A-a}} \left(\varphi_{n_r\ell_r}\left(\vec{\eta}_{A-a}\right)\varphi_{NL}\left(\vec{\xi}_0\right)\right)^{\ell}$$

c.m. motion

In this 'SD' channel basis, translation-invariant matrix elements are mixed with c.m. motion …

- More in detail:

c.m. motion

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n_r\ell_r,NL,J_r} \hat{\ell}\hat{J}_r(-1)^{s+\ell_r+L+J}\begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix}\langle 00,n\ell,\ell|n_r\ell_r,NL,\ell\rangle_{d=\frac{a}{A-a}}\left[\left|\Phi^{J_r^{\pi_r}T}_{\nu_r n_r}\right\rangle\varphi_{NL}(\vec{\xi}_0)\right]^{(J^\pi T)}$$

- The spurious motion of the c.m. is mixed with the intrinsic motion

$$_{SD}\left\langle\Phi^{J^\pi T}_{\nu' n'}\left|\hat{O}_{t.i.}\right|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n'_r\ell'_r,n_r\ell_r,J_r}\left\langle\Phi^{J_r^{\pi_r}T}_{\nu'_r n'_r}\left|\hat{O}_{t.i.}\right|\Phi^{J_r^{\pi_r}T}_{\nu_r n_r}\right\rangle$$

$$\times\sum_{NL}\hat{\ell}\hat{\ell}'\hat{J}_r^2(-1)^{s+\ell-s'-\ell'}\begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix}\begin{Bmatrix} s' & \ell'_r & J_r \\ L & J & \ell' \end{Bmatrix}$$

$$\times\langle 00,n\ell,\ell|n_r\ell_r,NL,\ell\rangle_{d=\frac{a}{A-a}}\langle 00,n'\ell',\ell'|n'_r\ell'_r,NL,\ell'\rangle_{d'=\frac{a'}{A-a'}}$$

Interested in this

Compute these

… but they can be extracted exactly from the 'SD' matrix elements by applying the inverse of the mixing matrix

- More in detail:

c.m. motion

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n_r \ell_r, NL, J_r} \hat{\ell}\hat{J}_r (-1)^{s+\ell_r+L+J} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a}{A-a}} \left[\left|\Phi^{J_r^{\pi_r} T}_{\nu_r n_r}\right\rangle \varphi_{NL}(\vec{\xi}_0) \right]^{(J^\pi T)}$$

- The spurious motion of the c.m. is mixed with the intrinsic motion

Matrix inversion

$$_{SD}\left\langle \Phi^{J^\pi T}_{f_{SD}} \middle| \hat{O}_{t.i.} \middle| \Phi^{J^\pi T}_{i_{SD}} \right\rangle_{SD} = \sum_{i_R f_R} M^{J^\pi T}_{i_{SD} f_{SD}, i_R f_R} \left\langle \Phi^{J^\pi T}_{f_R} \middle| \hat{O}_{t.i.} \middle| \Phi^{J^\pi T}_{i_R} \right\rangle$$

Calculate these

Interested in these

Working within the 'SD' channel basis we can access reactions involving p-shell targets

- Can use second quantization representation
  - Matrix elements of translational operators can be expressed in terms matrix elements of density operators on the target eigenstates
  - E.g., the matrix elements appearing in the RGM norm kernel for nucleon-nucleus channel states:

$$
{}_{SD}\left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| P_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle_{SD} = \frac{1}{A-1} \sum_{jj'K\tau} \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{K}\hat{\tau} (-1)^{I_1'+j'+J} (-1)^{T_1+\frac{1}{2}+T}
$$

$$
\times \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I_1' & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix} \begin{Bmatrix} I_1 & K & I_1' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T_1' \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix}
$$

$$
\times {}_{SD}\left\langle A-1\ \alpha_1' I_1'^{\pi_1'} T_1' \right\| \left(a^+_{n\ell j\frac{1}{2}} \tilde{a}_{n'\ell' j'\frac{1}{2}} \right)^{(K\tau)} \left\| A-1\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle_{SD}
$$

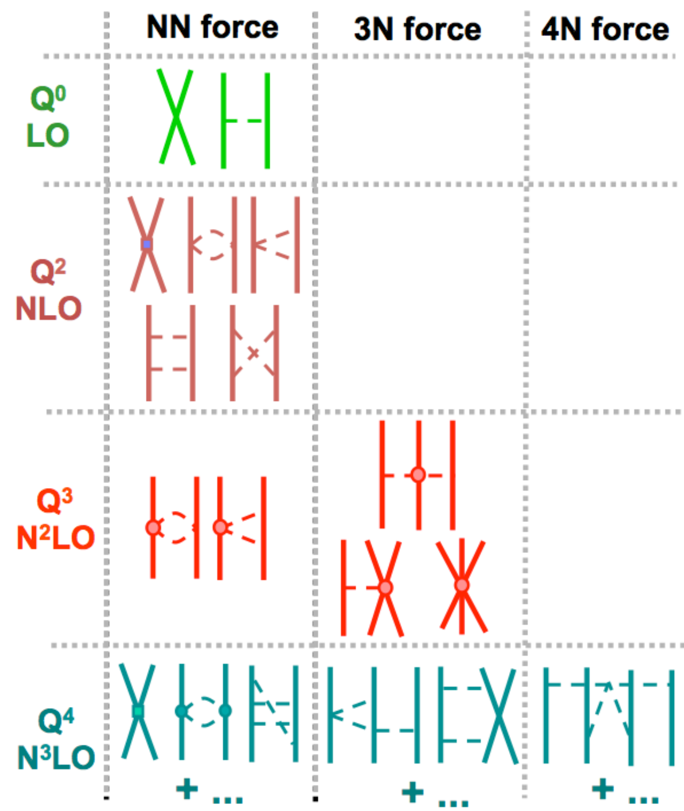
One-body density matrix elements

In the following I will review some results

Adopted interactions:

- NN: potential at N^3LO, 500 MeV cutoff (by Entem & Machleidt)
- NN+3N(500): NN plus 3N force at N^2LO, 500 MeV cutoff (local form by Navrátil)
- NN+3N(400): NN plus 3N force at N^2LO, 400 MeV cutoff (local form by Navrátil)
- N^2LOsat : NN+3N at N^2LO, fitted simultaneously (by Ekström et al.)

Chiral Effective Field Theory

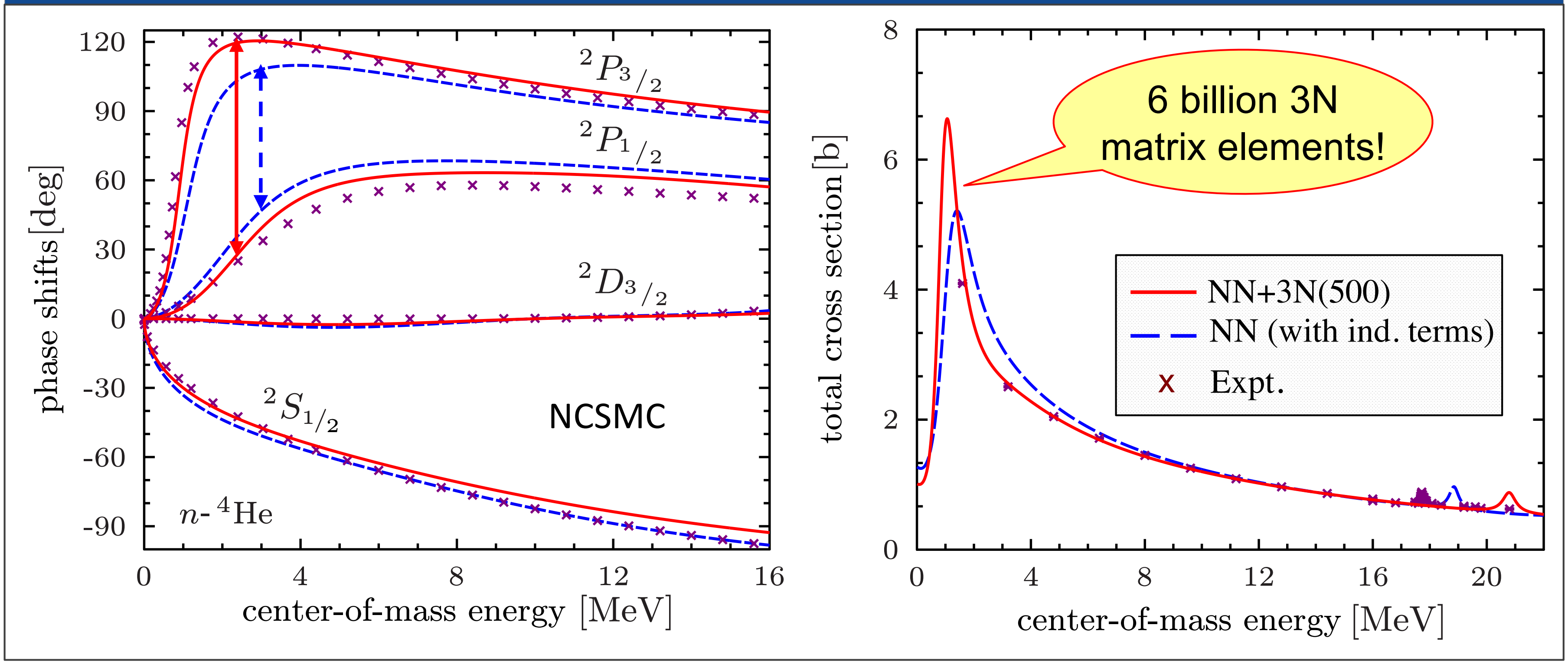


Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

Neutron-^{4}He scattering: a magnifying glass for 3N forces

- 3N force enhances $1/2^-$ ←→ $3/2^-$ splitting; essential at low energies!

Elastic scattering of neutrons on ^{4}He

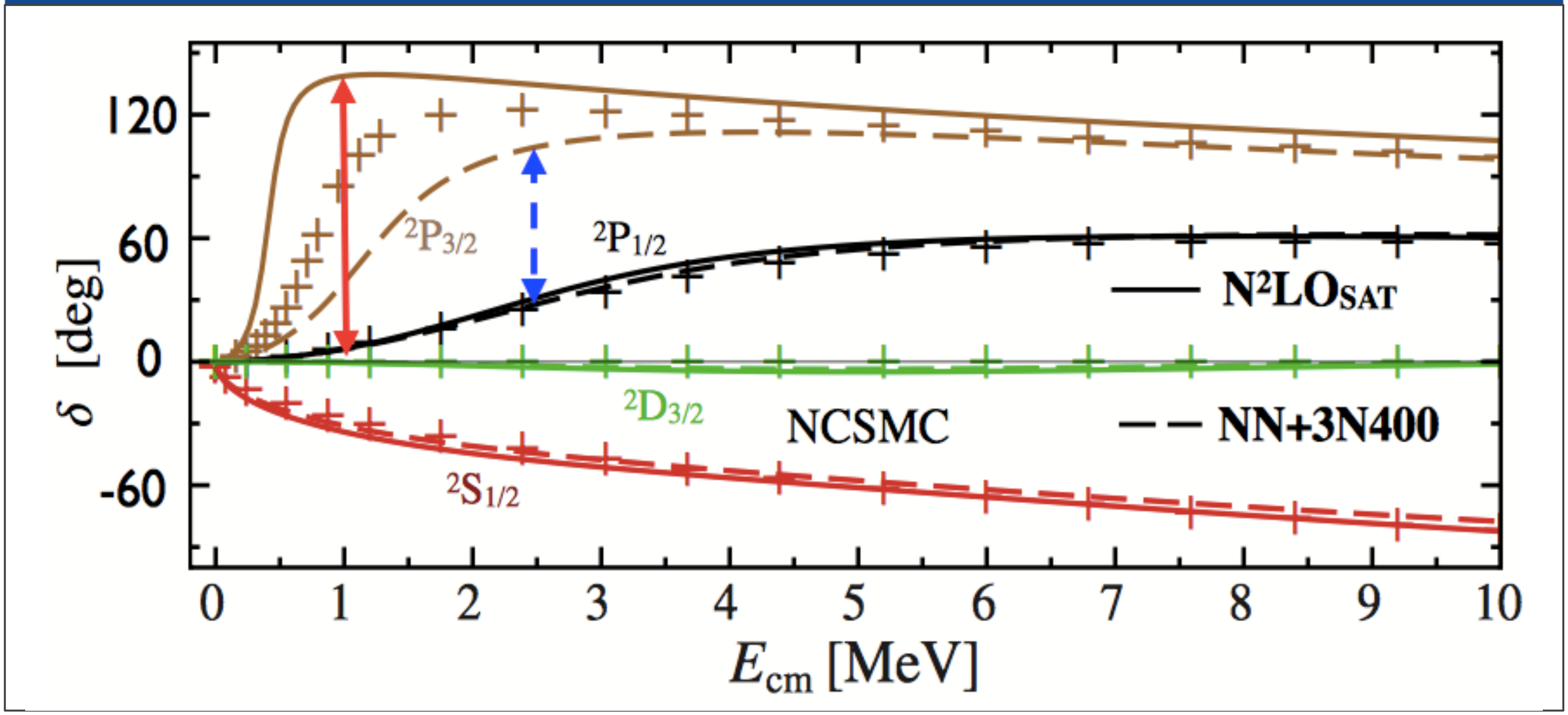


G. Hupin, S. Quaglioni, and P. Navratil, JPC Conf. Proc. (2015)

Neutron-^{4}He scattering: a magnifying glass for 3N forces

- $1/2^{-} \leftarrow\rightarrow 3/2^{-}$ splitting sensitive to 3N force, strength of spin-orbit

Elastic scattering of neutrons on ^{4}He

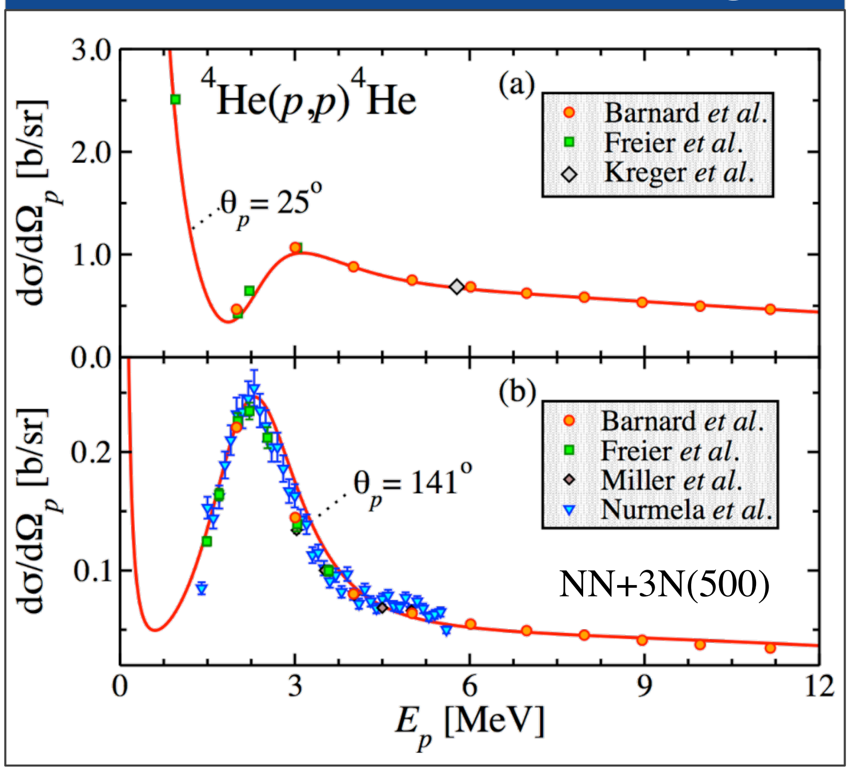


G. Hupin, S. Quaglioni, and P. Navratil, JPC Conf. Proc. (2015)

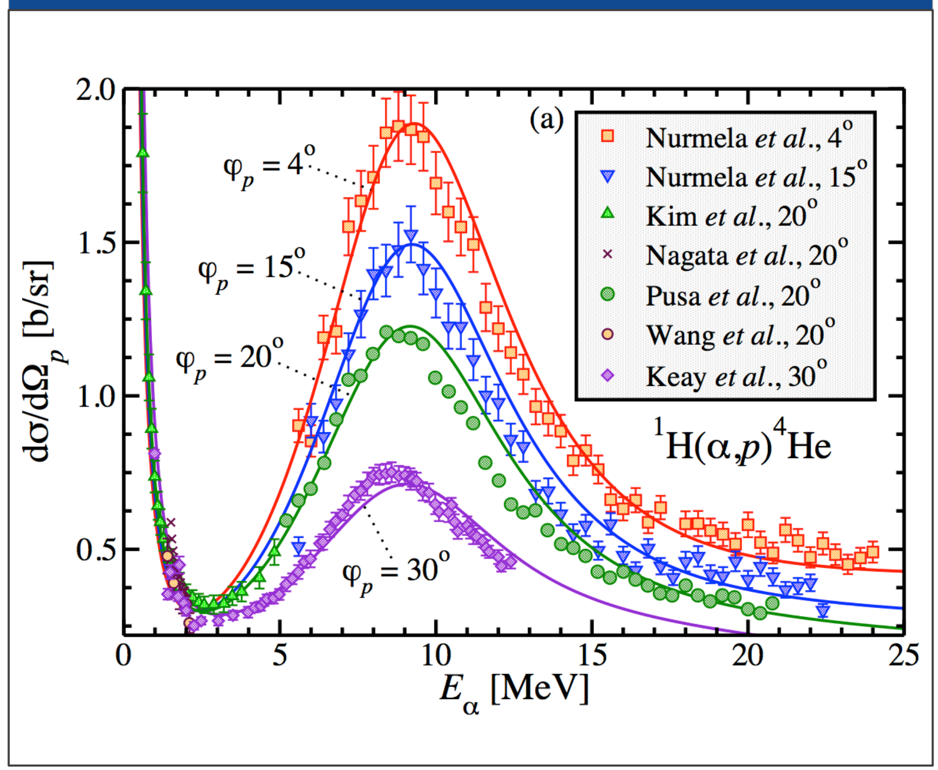
We can reproduce the elastic scattering and recoil of protons off ^{4}He based on chiral NN+3N(500) interactions

- Used to characterize ^{1}H and ^{4}He impurities in materials' surfaces

Proton elastic scattering



Proton elastic recoil

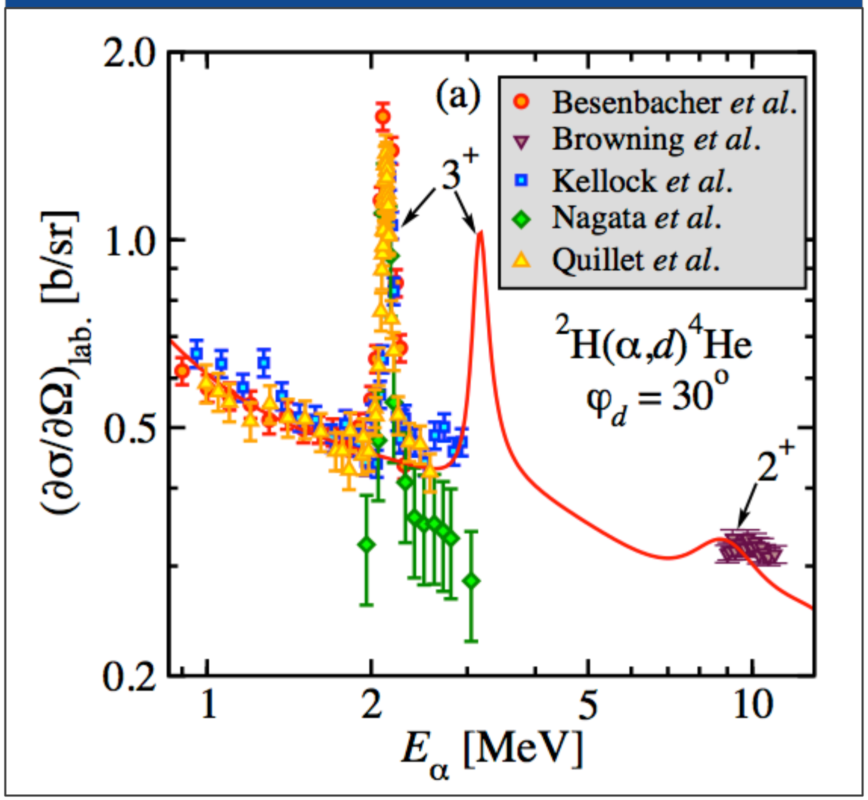


G. Hupin, S. Quaglioni, and P. Navratil, Phys. Rev. C **90**, 061601(R) (2014)

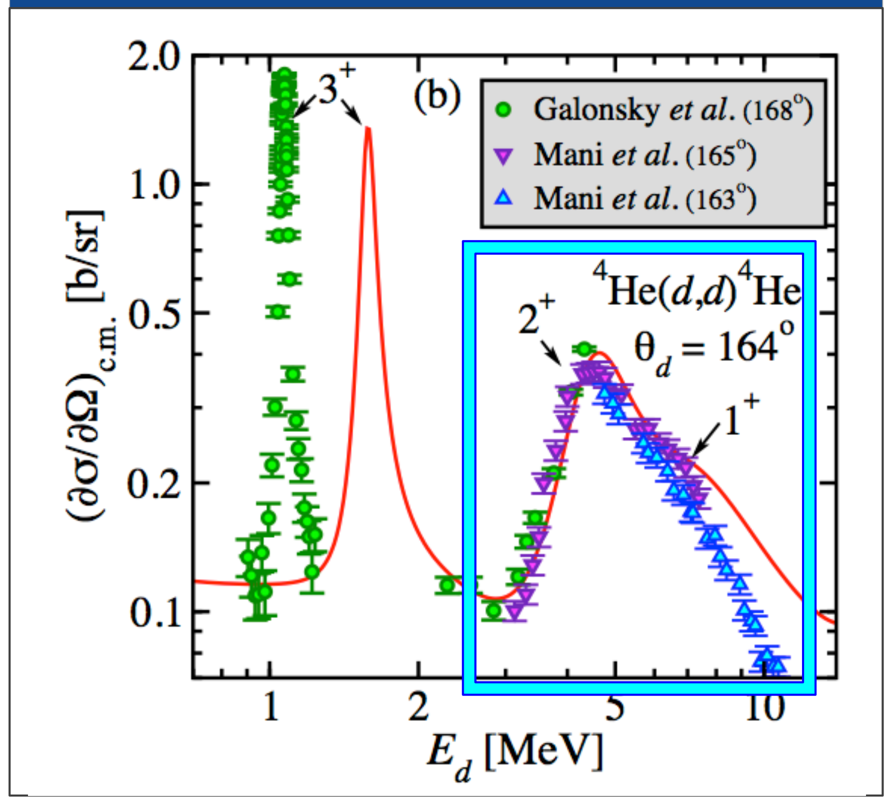
Elastic scattering and recoil of deuterons off ^{4}He

- Narrow 3^+ resonance not well described by NN+3N(500) force

^{2}H(α,d)^{4}He elastic recoil



^{4}He(d,d)^{4}He elastic scattering

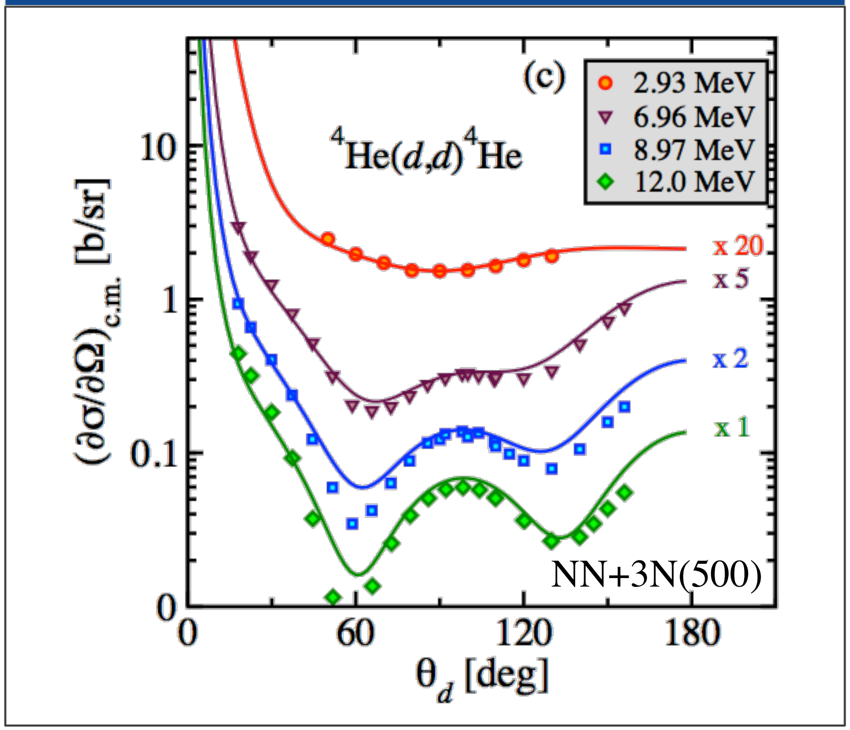


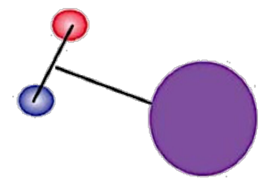
G. Hupin, S. Quaglioni, and P. Navratil, Phys. Rev. Lett. **114**, 212502 (2015)

Opportunity to root three-body reaction model in ab initio many-body framework (F. Nunes)

Ab initio many-body → Three-Body Model

Elastic d-^{4}He Scattering





- 3 relevant 'cluster' d.o.f.
- Structure of target is neglected
- Effective (optical) potential between nucleons and target
- Pauli principle approximated
- Expect need for effective 3-body force to recover ab initio results

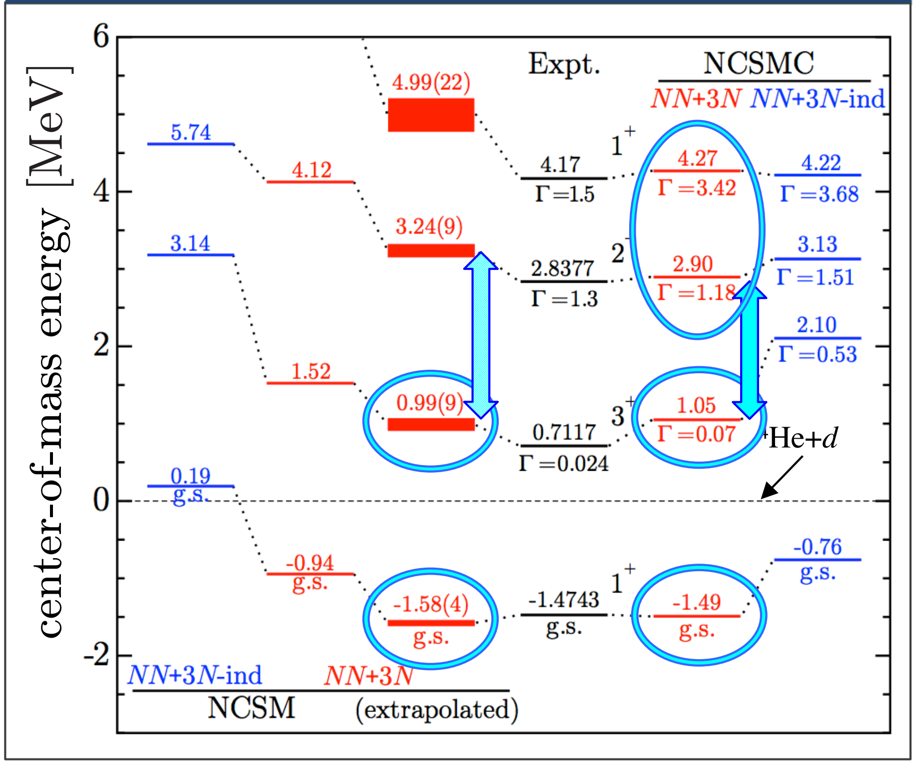
What is more important in shaping energy spectra: the proximity to a breakup threshold or 3N-force effects?

- The ^{6}Li ground state lies only 1.47 MeV (compared to its absolute binding energy of nearly 32 MeV) below the ^{4}He+d separation energy

- To find answer, we compared energies obtained with and without the coupling of d+^{4}He continuum states

It would be interesting to compare with symmetry-adapted NCSM

^{6}Li vs. (^{4}He+d)+^{6}Li calculation



G. Hupin, S. Quaglioni, and P. Navratil, Phys. Rev. Lett. **114**, 212502 (2015)

^{6}Li asymptotic *D*- to *S*-state ratio in d+^{4}He configuration

- In the NCSMC, bound state wave functions have (correct) Whittaker asymptotic – as opposed to traditional NCSM!

$$u_c(r) = C_c W(k_c r)$$

- Asymptotic D- to S-state ratio (C^2/C^0) of ^{6}Li g.s. in d+^{4}He configuration
  - Not well determined, even as to its sign
  - Our results do not support a near-zero value

G. Hupin, S. Quaglioni, and P. Navratil, Phys. Rev. Lett. **114**, 212502 (2015)

^{6}Li(g.s.)	NCSMC	Experiment	
E [MeV]	-32.01	-31.994	
C_0 [fm$^{-1/2}$]	2.695	2.91(9)	2.93(15)
C_2 [fm$^{-1/2}$]	-0.074	-0.077(18)	
C_2/C_0	-0.027	-0.025(6)(10)	0.0003(9)

George & Knutson, PRC **59**, 598 (1999): Determination from ^{6}Li-^{4}He elastic scattering

K.D. Veal et al., PRL **81**, 1187 (1998): Determination from ($^{6}\vec{\text{Li}}$,d) reactions on medium-heavy targets.

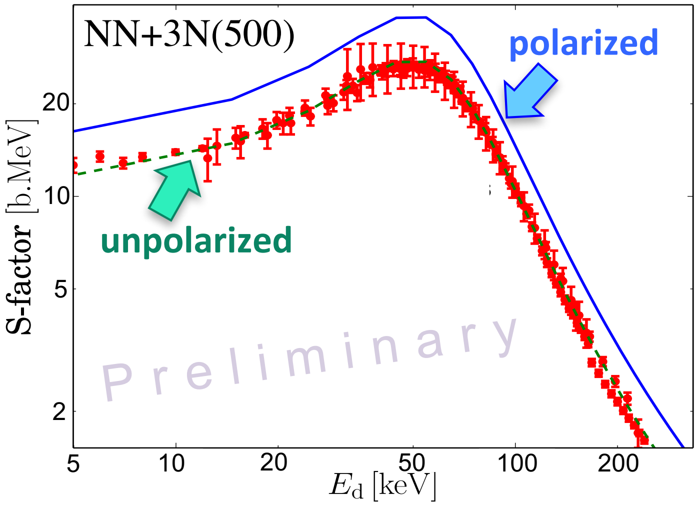
With the same NN+3N forces, we can also make predictions for more complex transfer reactions

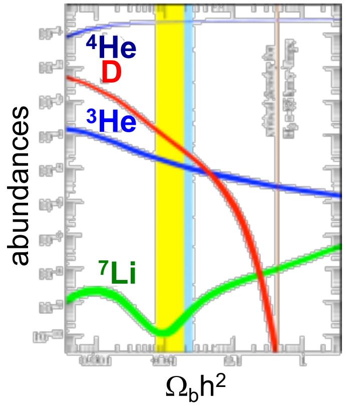
- Deuterium-Tritium fusion
  - Big Bang nucleosysthesis of light nuclei
  - Fusion research and plasma physics

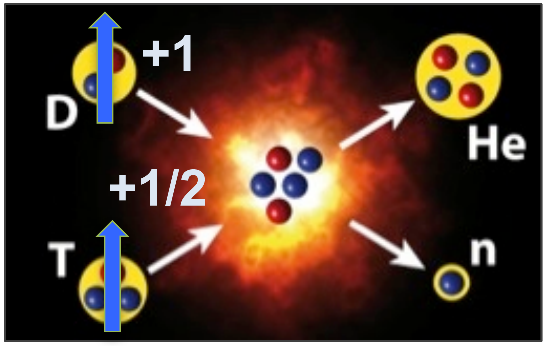
G. Hupin

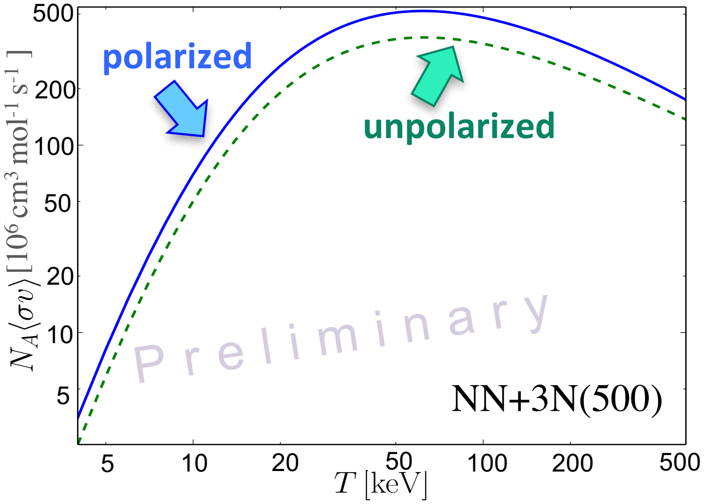
- What is the effect of spin polarization on the reaction rate?

$$N_A\langle\sigma v\rangle = \sqrt{\frac{8}{\pi\mu}}\frac{N_A}{(k_BT)^{3/2}}\int_0^\infty dE\ S(E)\ \exp\left(-\frac{2\pi Z_1Z_2e^2}{\hbar\sqrt{2mE}}-\frac{E}{k_BT}\right)$$



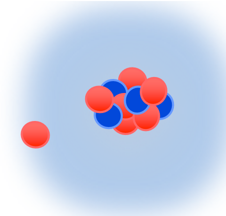






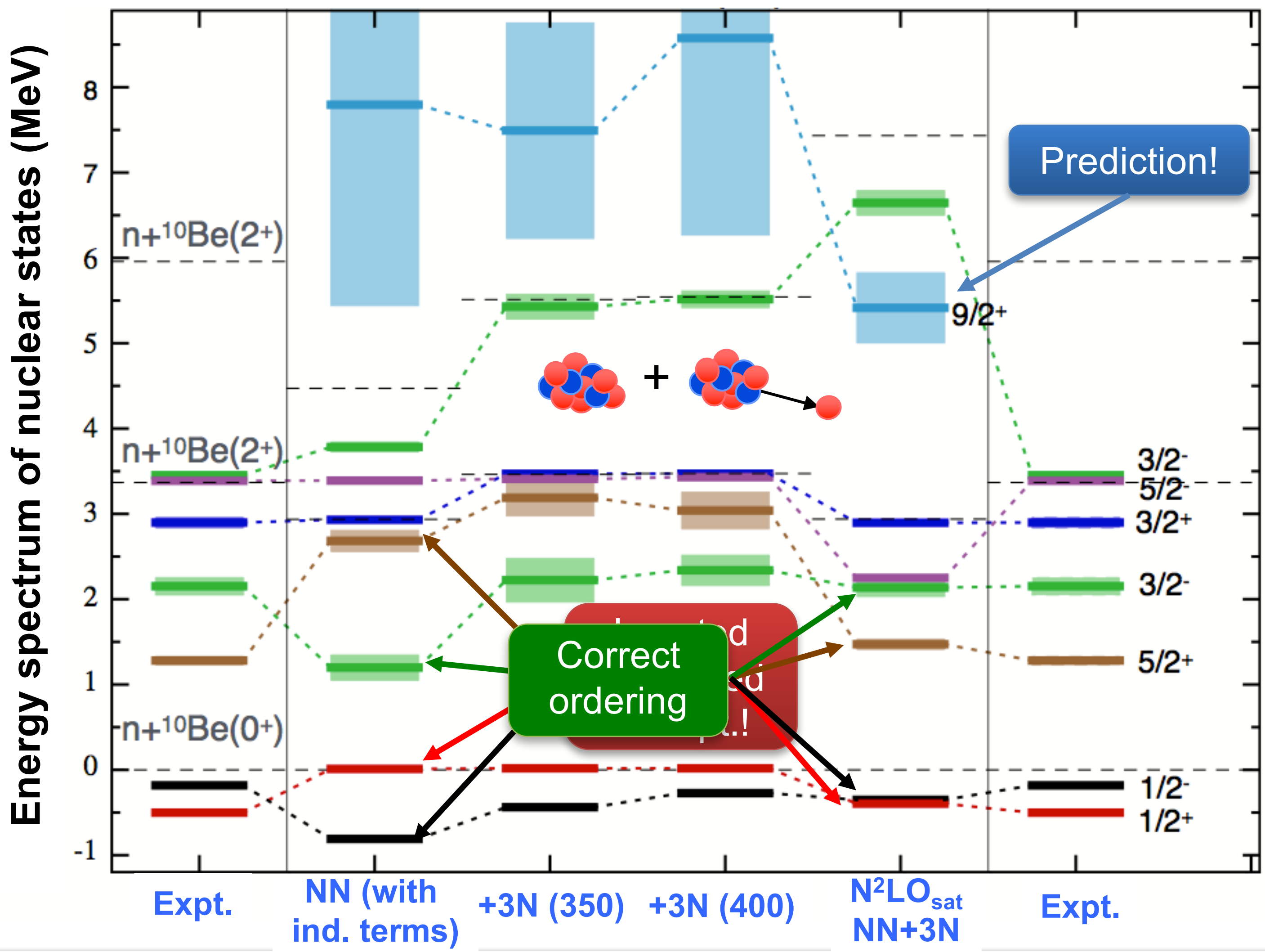
G. Hupin, S. Quaglioni, and P. Navrátil, in progress

Can ab initio theory explain the phenomenon of parity inversion in ^{11}Be?

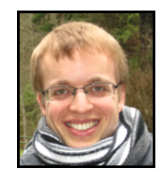


^{11}Be

A. Calci, P. Navratil, R. Roth, **J. Dohet-Eraly**, S.Q., and G. Hupin, Phys. Rev. Lett. 117, 242501 (2016)

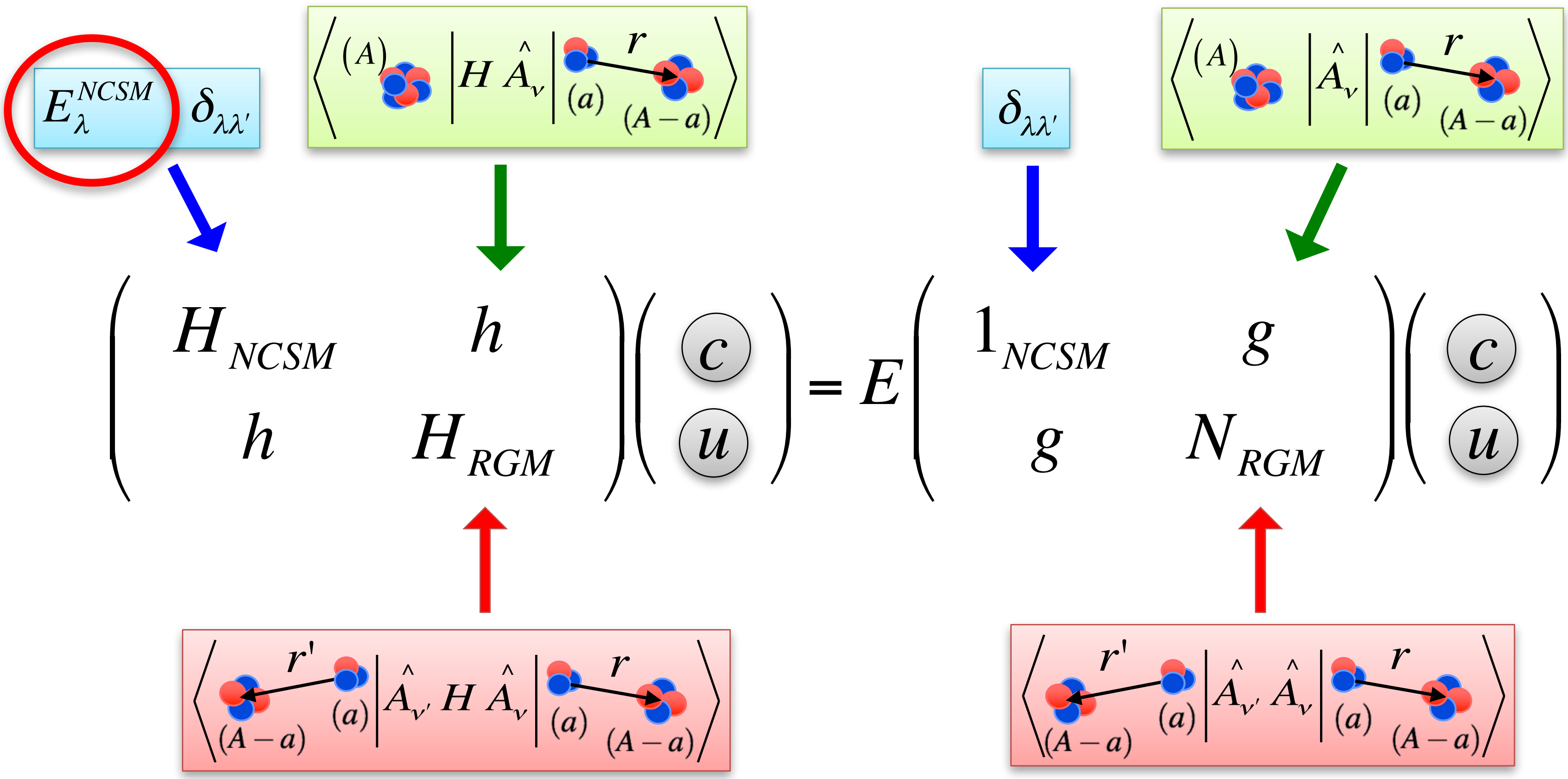


A. Calci



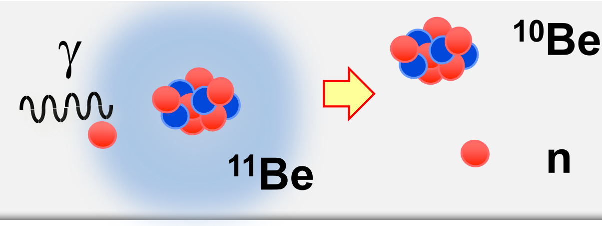
J. Dohet-Eraly

Phenomenologically adjusted NCSMC

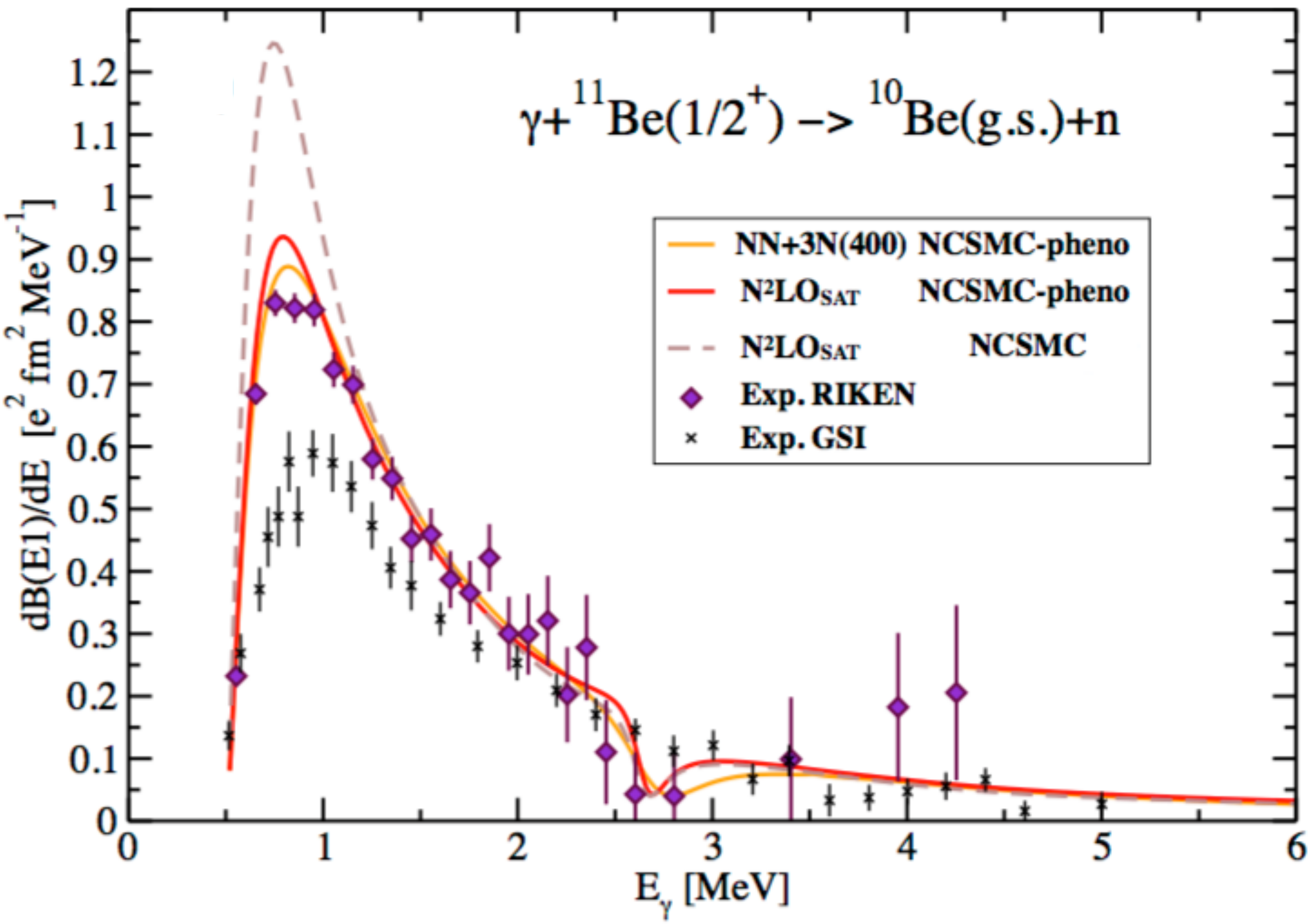


NCSM energy eigenvalues treated as adjustable parameters; clusters' excitation energies set to experimental value

Can ab initio theory explain the photodisintegration of ^{11}Be?



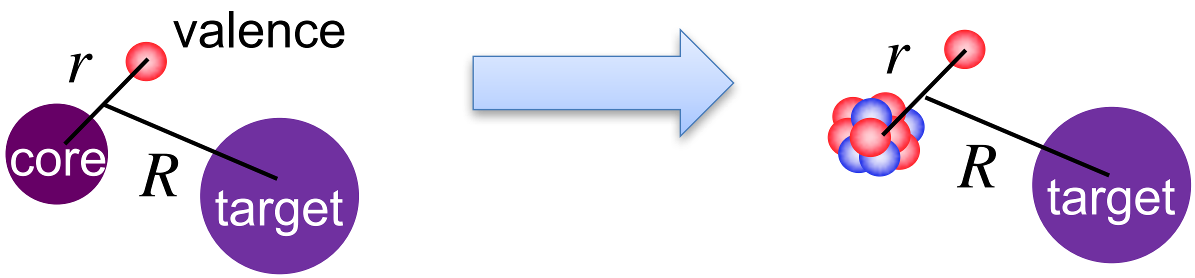
A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S.Q., and G. Hupin, Phys. Rev. Lett. 117, 242501 (2016)



Opportunity to arrive at a more realistic description of the projectile in few-body models

Few-Body Model

Semi-microscopic model



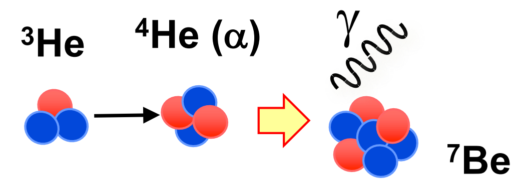
Few-Body Model

- Few (3 or 4) relevant 'cluster' d.o.f.
- Structure of clusters is neglected
- Effective (optical) potential between core, valence and target
- Pauli principle approximated
- Easier to solve, more widely applicable

Semi-microscopic model

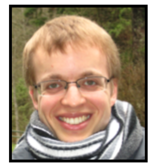
- Structure of target is still neglected
- Connection to ab initio many-body theory for the projectile
- Ab initio wave functions (S-matrix) of projectile (**see talk of A. Bonaccorso**)
- Effective valence-core interaction fitted to ab initio phase shifts (**see talk of P. Capel**)

Now gradually building up capability to describe solar pp-chain reactions



The ^{3}He(α,γ)^{7}Be fusion rate is essential to evaluate the fraction of pp-chain terminations resulting in ^{7}Be versus ^{8}B solar neutrinos

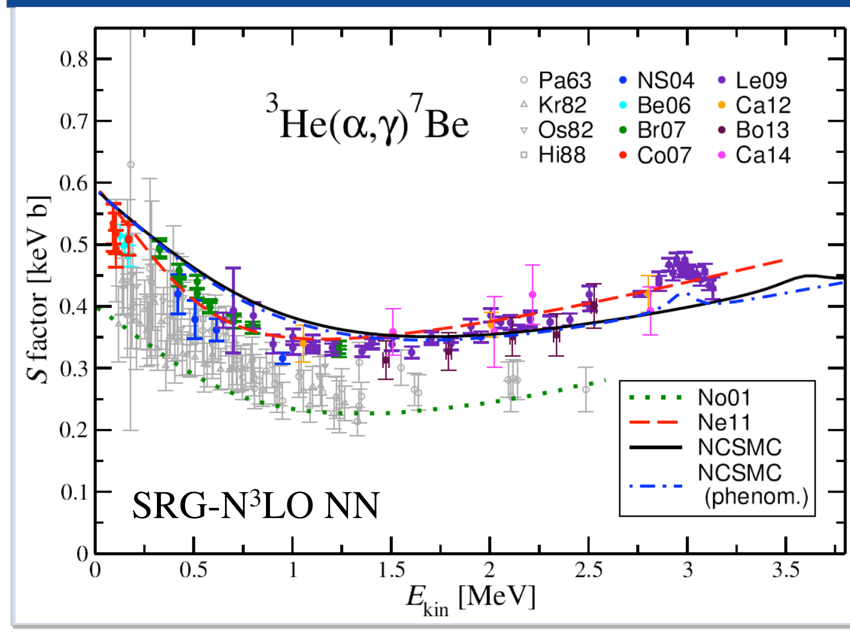
- Quantitative comparison still requires inclusion of 3N forces

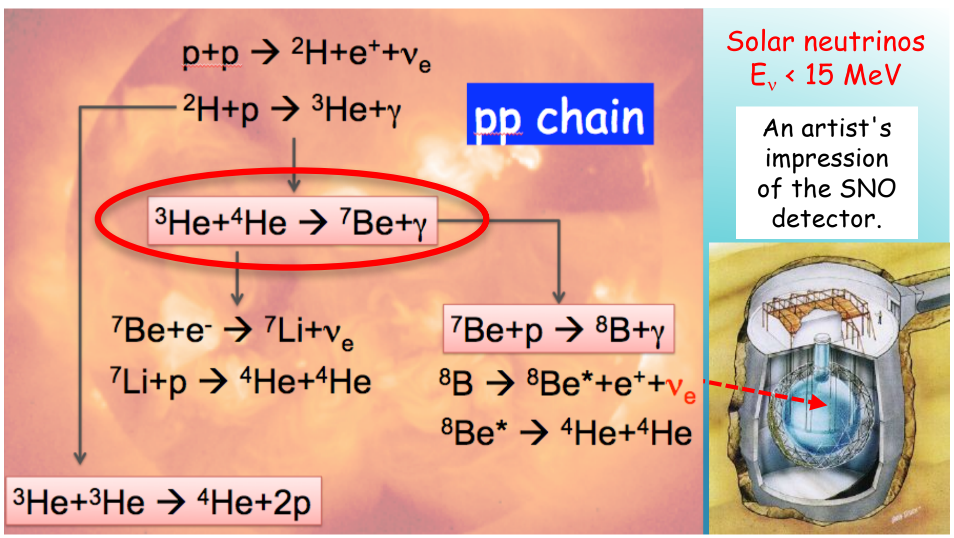


J. Dohet-Eraly

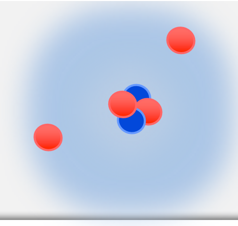
J. Dohet-Eraly, P. Navrátil, S.Q., W. Horiuchi, and F. Raimondi, Physics Letters B **757,** 430 (2016)

^{3}He(α,γ)^{7}Be Astrophysical S-factor





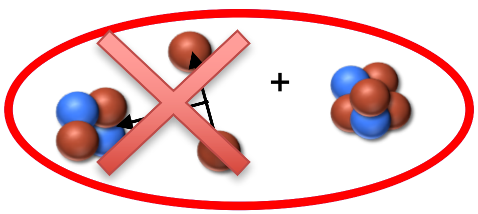
Ab initio calculations simultaneously address many-body correlations and 3-cluster dynamics

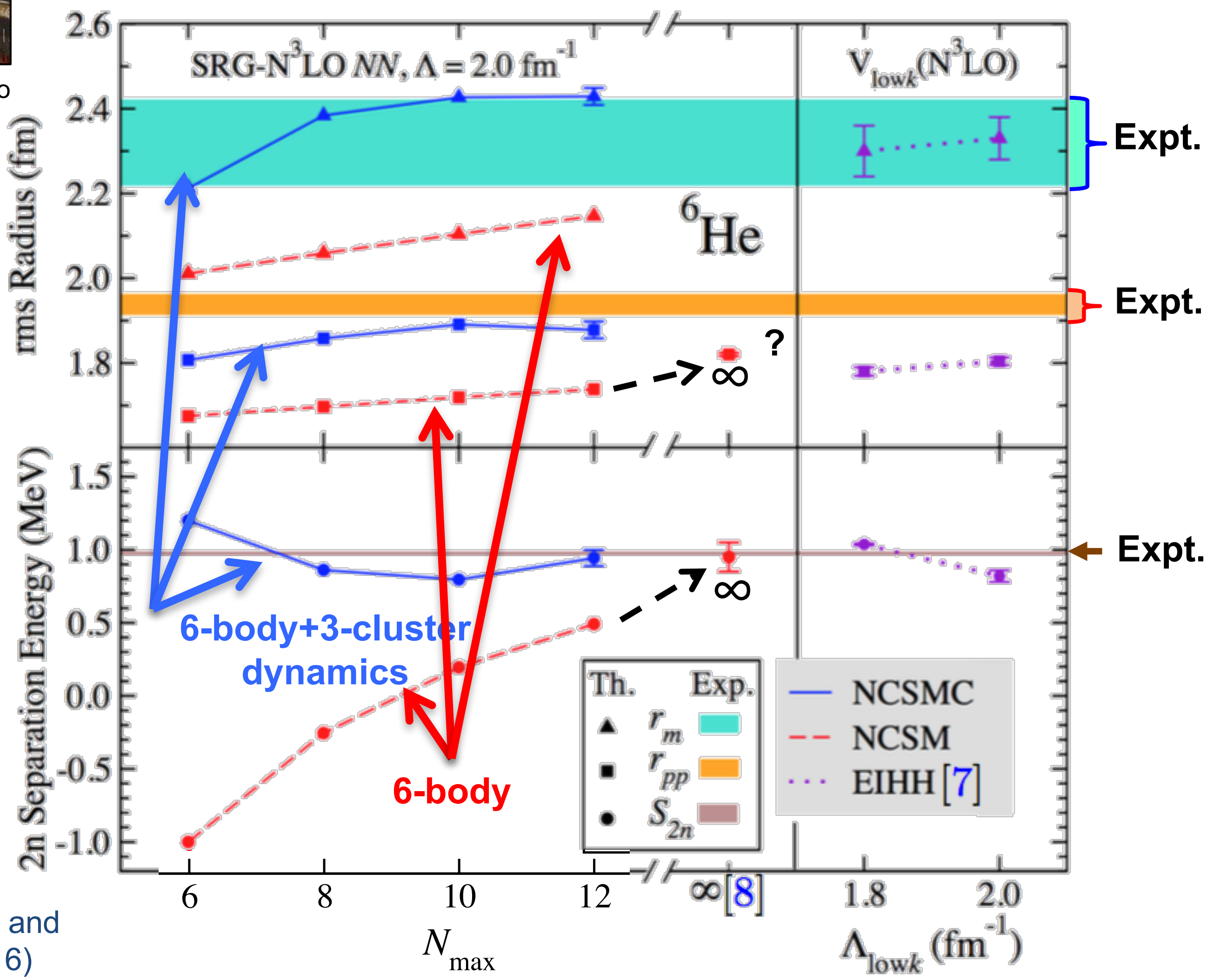


Borromean halos (dripline nuclei)

C. Romero

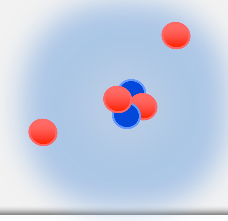
- ^{6}He (= ^{4}He+n+n), ^{11}Li (= ^{9}Li+n+n), ^{14}Be (= ^{12}Be+n+n), …
- Constituents do not bind in pairs!
- 3-cluster NCSMC





C. Romero-Redondo, S. Quaglioni, P.Navratil, and G. Hupin, Phys. Rev. Lett. 117, 222501 (2016)

Ab initio calculations simultaneously address many-body correlations and 3-cluster dynamics



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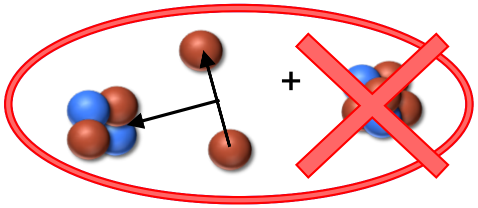

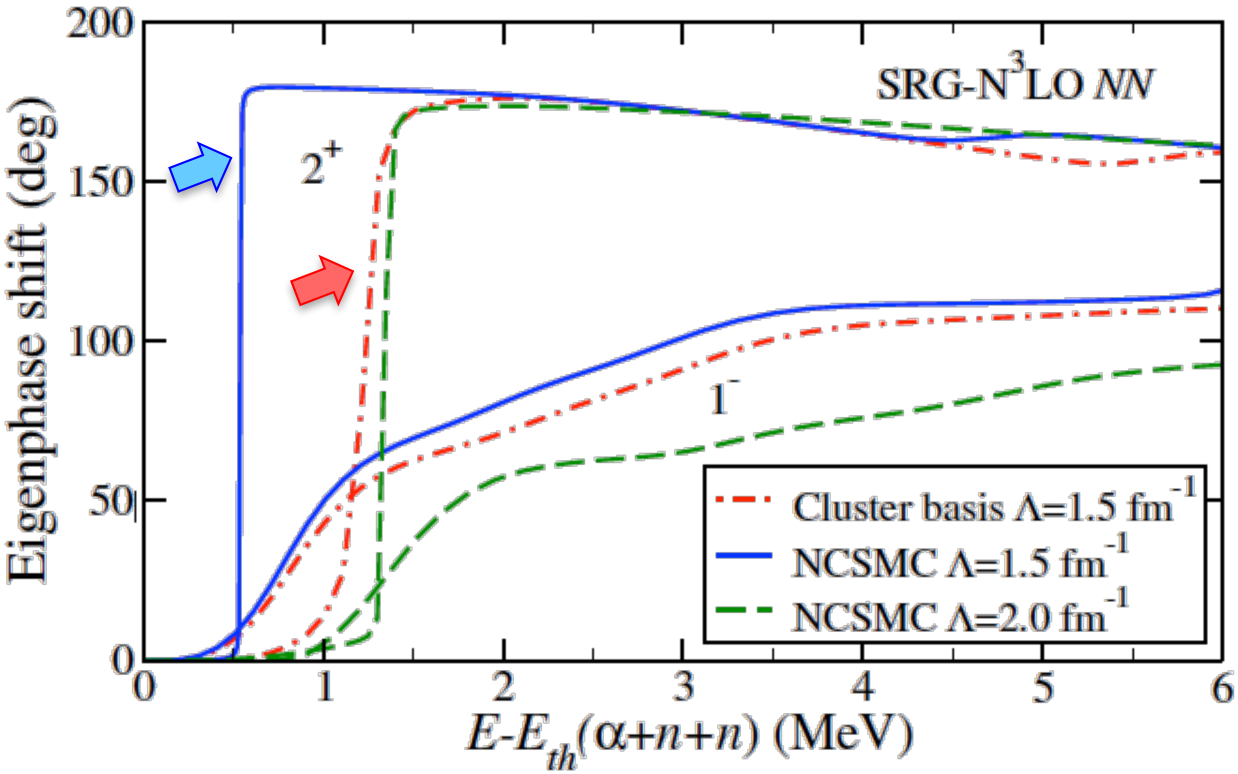

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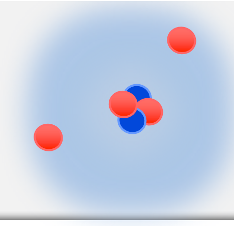
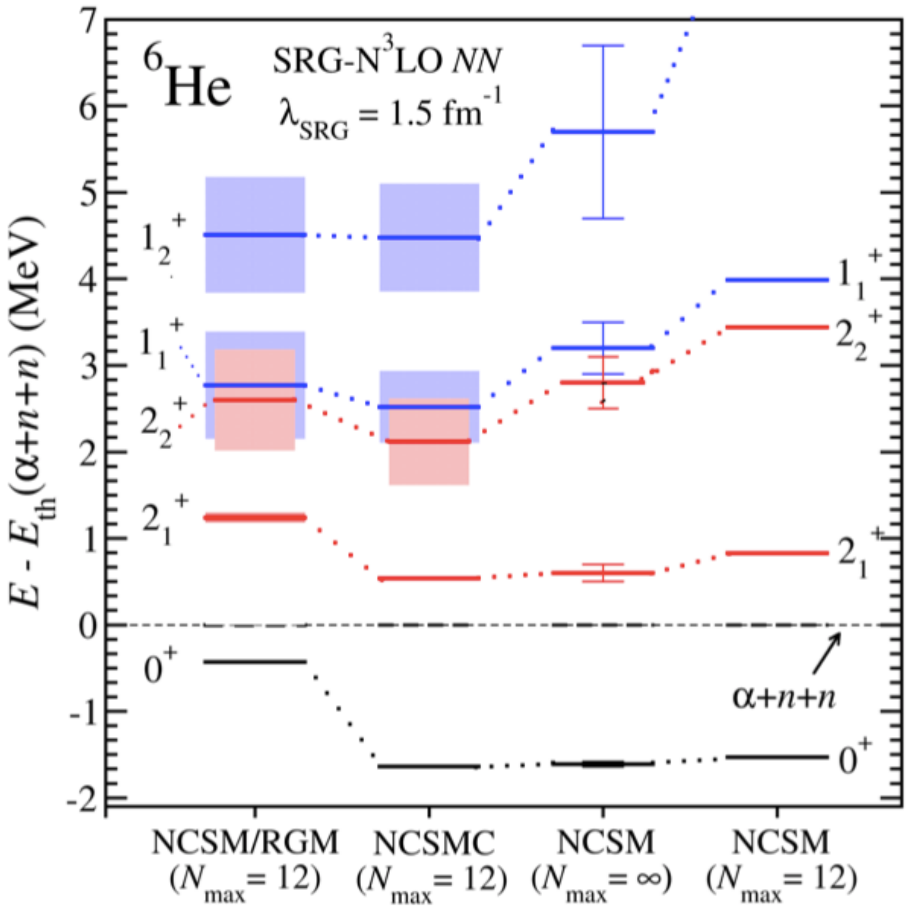
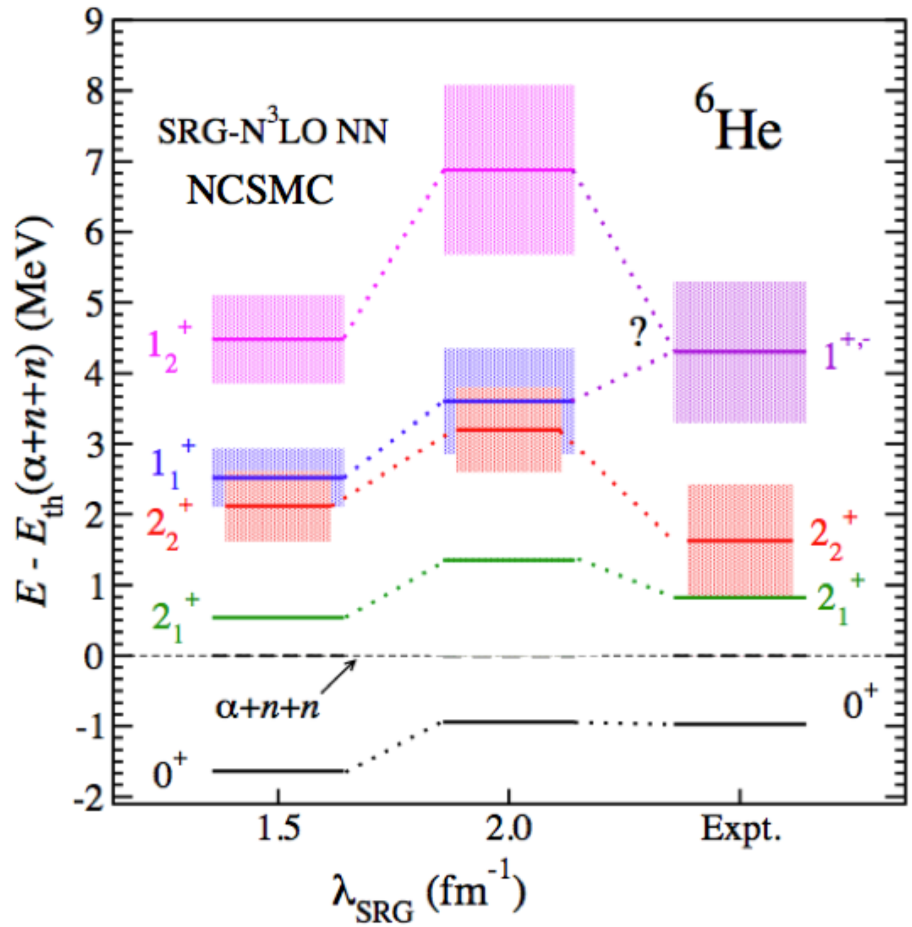


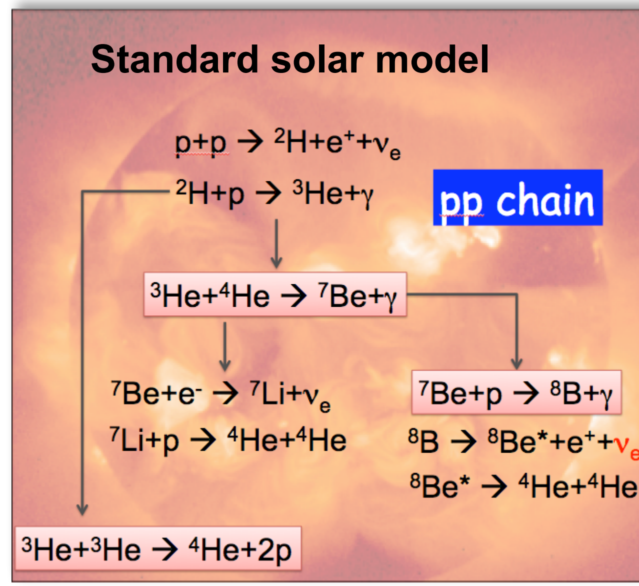


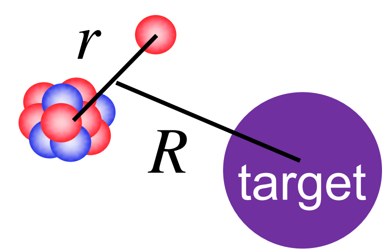


Quantitative comparison still requires inclusion of 3N forces

Conclusions and Prospects

- Working within the ab initio no-core shell model with continuum we have made great strides in the description of reactions and exotic nuclei
- We are on the verge of predicting Solar fusion cross sections and reaction rates for fusion technology from chiral NN+3N forces
- These developments are also allowing to further expose and will help overcome deficiencies in chiral NN+3N forces
- New opportunities to forge a connection between ab initio many-body theory and few-body reaction models are emerging





Collaborators

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- P. Navratil (TRIUMF)
- C. Romero-Redondo (LLNL)
- R. Roth (TU Darmstadt)

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