Capture reactions, αN scattering, and bremsstrahlung within the NCSMC

Jérémy Dohet-Eraly (TRIUMF)

Collaborators:
Petr Navratil (TRIUMF)
Sofia Quaglioni (LLNL Livermore)
Guillaume Hupin (LLNL Livermore)
Wataru Horiuchi (Hokkaido University)

Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, BC, Canada, February 18th, 2015.

Outline

- What?
- Why?
- How?

Outline

- What? Electromagnetic transitions and elastic scattering
- Why?
- How?

Outline

- What? Electromagnetic transitions and elastic scattering
- Why? It's quite interesting!
- How?

TRIUMF

Outline

- What? Electromagnetic transitions and elastic scattering
- Why? It's quite interesting!
- How? With the No-Core Shell Model with Continuum/Clustering (NCSMC) approach

Radiative captures

Motivation: the nuclear reaction in stars

- Radiative captures play an important role in the synthesis of elements in the stars
- Rates of these reactions are essential for describing quantitatively the evolution of the stars
- Radiative capture processes take place at low energies, out of reach of the experiments
- $\Rightarrow$ NUCLEAR MODELS ARE NEEDED

Motivation: *pp*-chains

- Among the nuclear reactions which take place in the stars, the *pp*-chains play a central role. Indeed, they are the first reactions which synthesize nuclear elements since they do not require any catalyst.

$$p + p \rightarrow {}^2\mathrm{H} + e^+ + \nu_e$$

$$^2\mathrm{H} + p \rightarrow {}^3\mathrm{He} + \gamma$$

$$^3\mathrm{He} + {}^3\mathrm{He} \rightarrow \alpha + p + p$$

$$^3\mathrm{He} + \alpha \rightarrow {}^7\mathrm{Be} + \gamma$$

$$^7\mathrm{Be} + e^- \rightarrow {}^7\mathrm{Li} + \nu_e$$

$$^7\mathrm{Li} + p \rightarrow \alpha + \alpha$$

$$^7\mathrm{Be} + p \rightarrow {}^8\mathrm{B} + \gamma$$

$$^8\mathrm{B} \rightarrow \alpha + \alpha + e^+ + \nu_e$$

Branch I	Branch II	Branch III
$\approx 69\%$	$\approx 30.9\%$	$\approx 0.1\%$

- The relative rates of the $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ and $^3\mathrm{He}(^3\mathrm{He},2p)^4\mathrm{He}$ reactions determines which percentage of the *pp*-chain terminations produces neutrinos.

Outline

- What? Radiative captures: $^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$ and $^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$
- Why? Nuclear astrophysical interest.
- How?

Starting point: microscopic approach

- A pointlike nucleons interacting via inter-nucleon potentials
- Pauli-antisymmetrization between nucleons taken into account
- all physical quantities are derived from the internal many-body Schrödinger equation

$$H\Psi = \left(\sum_{i=1}^{A} \frac{p_i^2}{2m_N} + \sum_{i>j=1}^{A} v_{ij} + \sum_{i>j>k=1}^{A} v_{ijk} - T_{\rm c.m.} \right) \Psi = E_T \Psi,$$

where

- v_{ij} and v_{ijk} are two- and three-nucleon interactions (chiral N^3LO NN interaction*+chiral N^2LO NNN interaction† softened via the similarity-renormalization-group‡)

*D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)

† P. Navrátil, Few-Body Syst. 41, 117 (2007)

‡ S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C 75, 061001 (2007)

Describing a radiative capture

$$\underbrace{\alpha + {}^3\mathrm{He}}_{\textit{scattering state}} \rightarrow \underbrace{{}^7\mathrm{Be}}_{\textit{bound state}} + \underbrace{\gamma}_{\textit{photon emission}}$$

Method

- Solving the Scrödinger equation to find the $^7\mathrm{Be}$ bound state(s)
- Solving the Scrödinger equation at the positive initial energy (scattering state$\Rightarrow$ non-square-integrable wave function)
- Evaluating the matrix element of the photon emission operator between the initial and final wave functions

Studying the bound states

Key principle: the VARIATIONAL approach

- Expanding the wave function in a chosen set of N basis functions

$$\Psi = \sum_{n}^{N} \underbrace{c_n}_{unknown} \Psi_n$$

- Evaluating the norm and Hamiltonian matrices

$$\langle \Psi_i | \Psi_j \rangle \text{ and } \langle \Psi_i | H | \Psi_j \rangle \text{ for } i, j = 1, \ldots, N$$

- Solving the generalized eigenvalue problem to determine c_n

$$\begin{pmatrix} \langle \Psi_1 | H | \Psi_1 \rangle & \cdots & \langle \Psi_1 | H | \Psi_N \rangle \\ \vdots & & \vdots \\ \langle \Psi_N | H | \Psi_1 \rangle & \cdots & \langle \Psi_N | H | \Psi_N \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = E \begin{pmatrix} \langle \Psi_1 | \Psi_1 \rangle & \cdots & \langle \Psi_1 | \Psi_N \rangle \\ \vdots & & \vdots \\ \langle \Psi_N | \Psi_1 \rangle & \cdots & \langle \Psi_N | \Psi_N \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}$$

- If the basis is orthonormal $\Rightarrow$ standard eigenvalue problem

No-Core Shell Model

- No-Core Shell Model (NCSM) functions are Slater determinants of harmonic-oscillator functions (frequency:Ω)

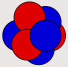
$$\psi_i = \mathcal{A}\varphi_{n_1 l_1 j_1 m_1}(\boldsymbol{r}_1)\varphi_{n_2 l_2 j_2 m_2}(\boldsymbol{r}_2)\ldots\varphi_{n_N l_N j_N m_N}(\boldsymbol{r}_N)$$

Properties

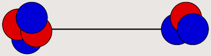
- With a complete $N_{max}\hbar\Omega$, the translational invariance is guaranteed (even if single-nucleon coordinates are used).
- Second-quantization techniques (very efficient) can be used
- Gaussian asymptotic behavior

Gaussian extension

- For $N_{max} \to \infty$, the NCSM states are able to describe any square-integrable function
- However, describing short- and long-range correlation needs huge values of N_{max} (unreachable)
- NCSM basis functions (one center) unadapted to describe cluster states (two centers, at least)



not convenient for describing



Solution: adding cluster basis functions

TRIUMF

NCSM/Resonating Group Method

- In the No-Core Shell Model/Resonating Group Method, the basis states have the following cluster structure

$$|\psi_i\rangle = \; = \left[\left(|A_1 \alpha_1 I_1^{\pi_1} T_1\rangle |A_2 \alpha_2 I_2^{\pi_2} T_2\rangle\right)^{IT} Y_\ell(\Omega_{12})\right]^{JM} \frac{\gamma_\nu(r_{12})}{r_{12}}$$

= Cluster states where the clusters are approximate eigenstates (ground state and excited states) of the A_1- or A_2- nucleon Schrödinger equation within the No−Core Shell Model

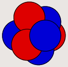
- For $N_{max} \to \infty$, if all excited states of the clusters are considered, any square-integrable function can be described.
- BUT including many excited cluster states is too time consuming
- $\Rightarrow$ Combining both approaches

NCSM with Continuum (Clustering) (NCSMC)

- In the NCSMC, the A-nucleon wave function is expanded as

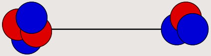
$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda \underbrace{|A\lambda J^\pi T\rangle}_{NCSM} + \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\Phi_{\nu r}^{J\pi T}\rangle}_{NCSM/RGM}$$

$|A\lambda J^\pi T\rangle$ = approximate eigenstates of the A-nucleon Schrödinger equation obtained within the No-Core Shell Model.



$$|\Phi_{\nu r}^{J\pi T}\rangle = \left[\left(|A_1\alpha_1 I_1^{\pi_1} T_1\rangle |A_2\alpha_2 I_2^{\pi_2} T_2\rangle\right)^{IT} Y_\ell(\Omega_{12})\right] \frac{\delta(r - r_{12})}{r r_{12}}$$

= Cluster states where the clusters are approximate eigenstates (ground state and excited states) of the A_1- or A_2- nucleon Schrödinger equation within the No−Core Shell Model



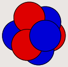
*S. Baroni, P. Navratil, and S. Quaglioni, Phys. Rev. Lett 110, 022505 (2013); Phys. Rev. C 87, 034326 (2013)

Describing scattering states

- In the NCSMC, the A-nucleon wave function is expanded as

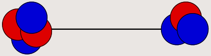
$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda \underbrace{|A\lambda J^\pi T\rangle}_{NCSM} + \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\Phi_{\nu r}^{J\pi T}\rangle}_{NCSM\,/\,RGM}$$

$|A\lambda J^\pi T\rangle$ = These states are essential to improve the quality of the wave function at short inter-cluster distances.



$$|\Phi_{\nu r}^{J\pi T}\rangle = \left[\left(|A_1\alpha_1 I_1^{\pi_1} T_1\rangle |A_2\alpha_2 I_2^{\pi_2} T_2\rangle\right)^{IT} Y_\ell(\Omega_{12})\right] \frac{\delta(r - r_{12})}{r r_{12}}$$

= Cluster states where the clusters are approximate eigenstates (ground state and excited states) of the A_1- or A_2- nucleon Schrödinger equation within the No−Core Shell Model



- NB:Linear dependence! *S. Baroni, P. Navratil, and S. Quaglioni, Phys. Rev. Lett 110, 022505 (2013); Phys. Rev. C 87, 034326 (2013)

TRIUMF

NCSMC equations

- Inserting the NCSMC expansion in the variational form of the Schrödinger equation (c_λ and the $\gamma_\nu^{J^\pi T}$ are the variational amplitudes)

$$\langle \delta\Psi_A^{J^\pi T} | H - E_T | \Psi_A^{J^\pi T} \rangle = 0,$$

leads to the NCSMC equations, schematically written as

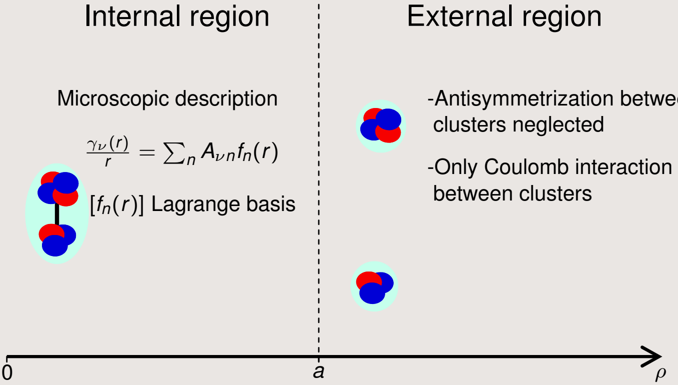
$$\begin{pmatrix} E_\lambda \delta_{\lambda\lambda'} & \langle A\lambda' J^\pi T | H \mathcal{A}_\nu | \Phi_{\nu r}^{J^\pi T} \rangle \\ \langle \Phi_{\nu' r'}^{J^\pi T} | \mathcal{A}_{\nu'} H | A\lambda J^\pi T \rangle & \langle \Phi_{\nu' r'}^{J^\pi T} | \mathcal{A}_{\nu'} H \mathcal{A}_\nu | \Phi_{\nu r}^{J^\pi T} \rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} =$$

$$E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle A\lambda' J^\pi T | \mathcal{A}_\nu | \Phi_{\nu r}^{J^\pi T} \rangle \\ \langle \Phi_{\nu' r'}^{J^\pi T} | \mathcal{A}_{\nu'} | A\lambda J^\pi T \rangle & \langle \Phi_{\nu' r'}^{J^\pi T} | \mathcal{A}_{\nu'} \mathcal{A}_\nu | \Phi_{\nu r}^{J^\pi T} \rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

- The most challenging (and time-consuming!) part is the calculation of these hamiltonian and norm kernels, mostly due to the inter-cluster antisymmetrization.
- The NCSMC equations are solved by the coupled-channel microscopic *R*-matrix method (MRM) on a Lagrange mesh*, which enables one to enforce the radial wave function $\gamma(r)$ to have the expected asymptotic behavior (as well for bound states as for scattering states).

*M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)

MRM on a Lagrange mesh



[D. Baye, P.-H. Heenen, and M. Libert-Heinemann, Nucl. Phys. A 291 (1977) 230]

[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]

- Choosing proper boundary conditions at the channel radius enables one to study boundstate or scattering wave functions

  $\Rightarrow$ ^{7}Be and ^{7}Li and $\alpha + ^3$He and $\alpha + ^3$H scattering can be studied within the same framework.

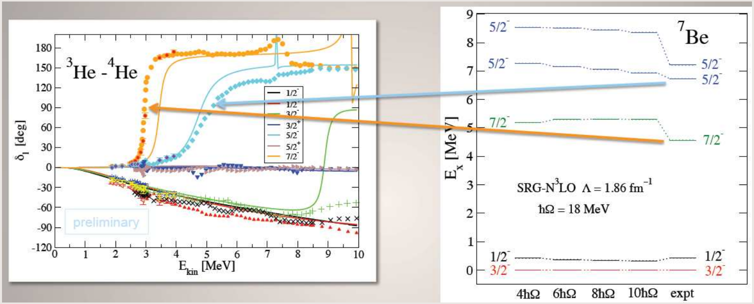
- From the electomagnetic matrix elements the $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ and $^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$ radiative captures can be studied.

- Only the inter-cluster part of the $E1$ operator, which should be dominant because these radiative captures are mostly external, is included now:

$$\vec{E1} \approx e\frac{Z_1 A_2 - Z_2 A_1}{A}\boldsymbol{r}_{12}$$

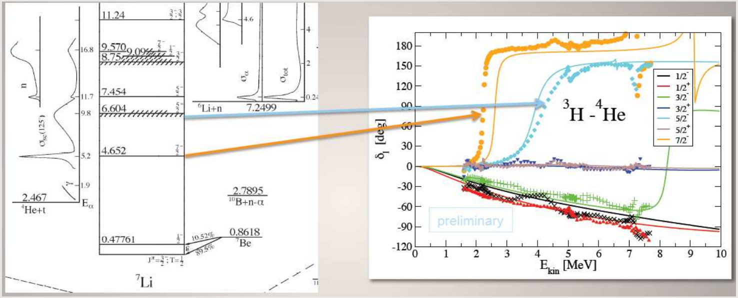
- NB: The NCSMC kernels of this approximate $E1$ operator can be written from the NCSMC norm kernels in a rather simple way, which makes relatively easy the evaluation of the $E1$ transitions.

$\alpha +^{3}$ He



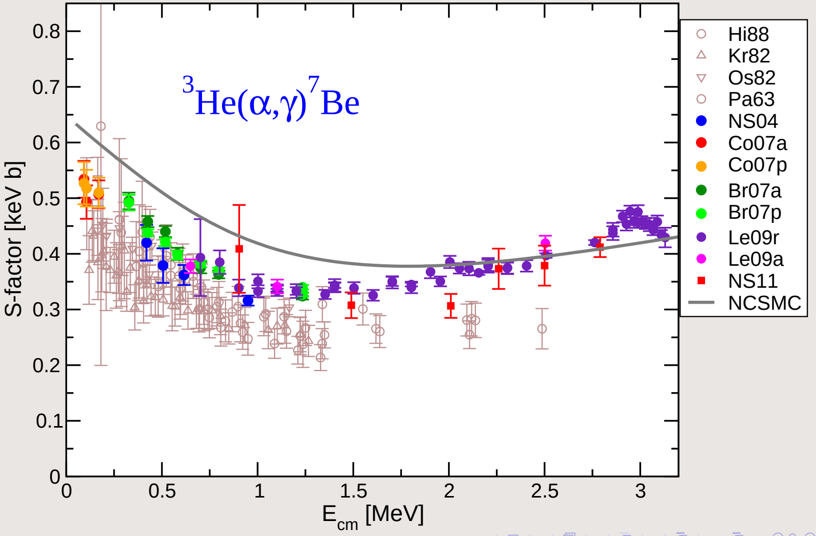
- NCSMC calculations with SRG N^{3}LO *NN* potenital ($\lambda = 2.1$ fm^{-1})
- Preliminary: $N_{max} = 12; \hbar\Omega = 20$ MeV
- ^{3}He, α ground state
- 8 eigenstates with negative parity of ^{7}Be
- 6 eigenstates with positive parity of ^{7}Be
- $E_{th}(^7\text{Be}) = -1.70$ MeV ; $E_{exp}(^7\text{Be}) = -1.59$ MeV

$\alpha +^3$ H

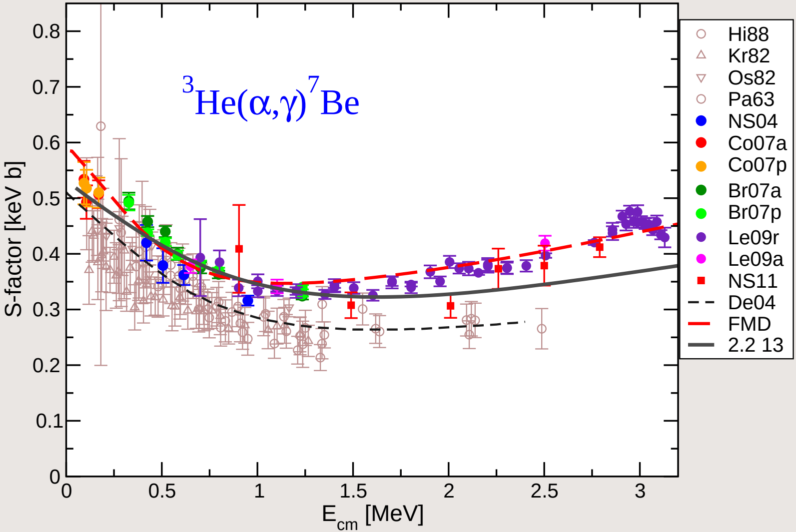


- NCSMC calculations with SRG N^{3}LO *NN* potenital ($\lambda = 2.1$ fm^{-1})
- Preliminary: $N_{max} = 12; \hbar\Omega = 20$ MeV
- ^{3}H, α ground state
- 8 eigenstates with negative parity of ^{7}Li
- 6 eigenstates with positive parity of ^{7}Li
- $E_{th}(^7\mathrm{Li}) = -2.62$ MeV ; $E_{exp}(^7\mathrm{Li}) = -2.47$ MeV

$^3He(\alpha,\gamma)^7Be$



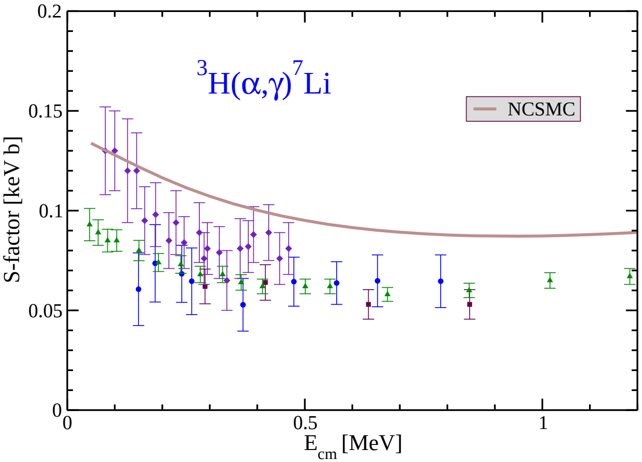
$^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$



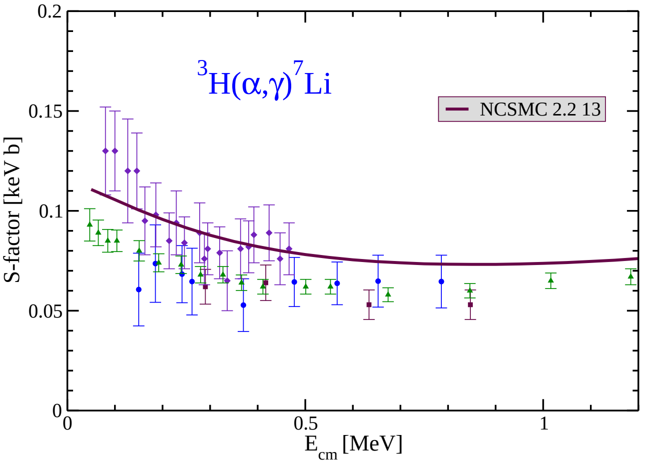
^{7}Be and ^{7}Li ground states

		E(MeV)	λ (fm^{-1})
^{7}Be	$3/2^-$	-1.70	2.1
		-1.33	2.2
		-1.59	exp
^{7}Li	$3/2^-$	-2.62	2.1
		-2.24	2.2
		-2.47	exp

$^{3}H(\alpha,\gamma)^{7}Li$



$^3H(\alpha,\gamma)^7Li$



Conclusion

- The NCSMC enables us to describe the boud states and the scattering states within the same framework.
- Hence, the radiative capture processes can be described in a rigorous way.
- The approach is applied to the 7-nucleon system:
  - the $^7\mathrm{Be}$ and $^7\mathrm{Li}$ ground states
  - the $\alpha +^3\mathrm{He}$ and $\alpha +^3\mathrm{H}$ elastic scattering
  - and the $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ and $^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$ radiative captures

  are studied.
- The results are qualitatively in agreement with the experiments.
- A quantitative comparison requires to increase the size of the NCSMC basis and to include three-nucleon forces.
- The accuracy could be improved by considering the full $E1$ operator (especially for the highest photon energies, which are considered).

Outline

- What?
- Why?

- How?

Ref: *G. Hupin, S. Quaglioni, P. Navrátil, Phys. Rev. C 90 (2014) 061601(R)*

Outline

- What? Elastic scattering: $\alpha + p$
- Why?
- How?

Ref: *G. Hupin, S. Quaglioni, P. Navrátil, Phys. Rev. C 90 (2014) 061601(R)*

Outline

- What? Elastic scattering: $\alpha + p$
- Why? Used to characterize $^{1}\mathrm{H}$ and $^{4}\mathrm{He}$ impurities in materials surfaces/Small enough for reaching convergence
- How?

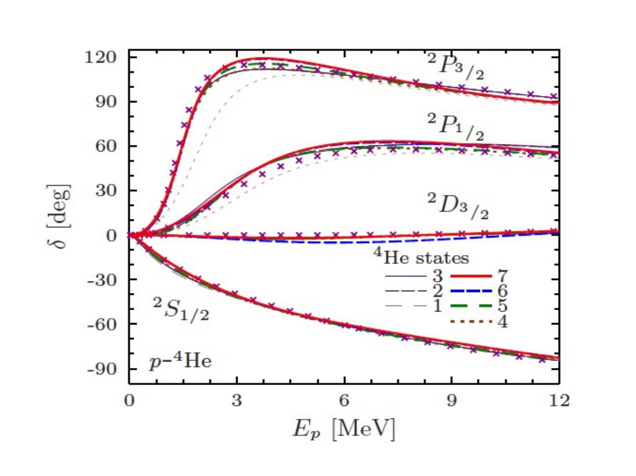
Ref: *G. Hupin, S. Quaglioni, P. Navrátil, Phys. Rev. C 90 (2014) 061601(R)*

Outline

- What? Elastic scattering: $\alpha + p$
- Why? Used to characterize $^{1}\mathrm{H}$ and $^{4}\mathrm{He}$ impurities in materials surfaces/Small enough for reaching convergence
- How? With the No-Core Shell Model with Continuum (NCSMC) approach

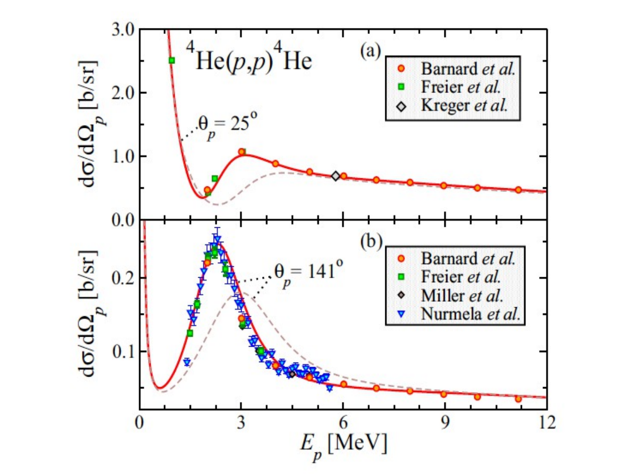
Ref: *G. Hupin, S. Quaglioni, P. Navrátil, Phys. Rev. C 90 (2014) 061601(R)*

$\alpha + p$ phase shifts



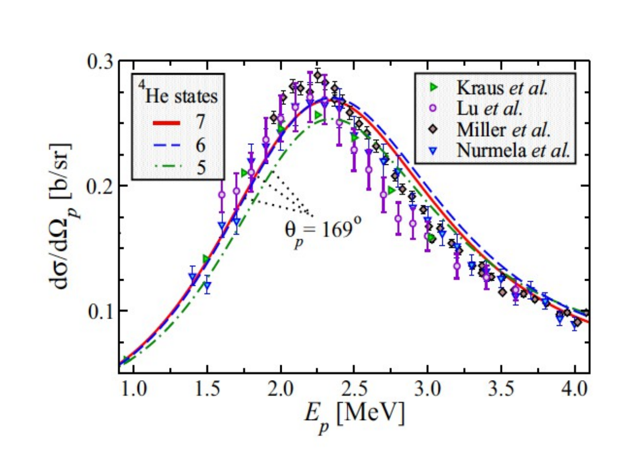
$N_{max} = 13$, $\hbar\Omega = 20$MeV, 14 ^{5}Li states, $\lambda = 2$ fm^{-1}

$\alpha + p$ phase shifts



$N_{max} = 13$, $\hbar\Omega = 20$MeV, 14 ^{5}Li states, $\lambda = 2$ fm^{-1}

$\alpha + p$ phase shifts



$N_{max} = 13$, $\hbar\Omega = 20$MeV, 14 ^{5}Li states, $\lambda = 2$ fm^{-1}

Conclusion

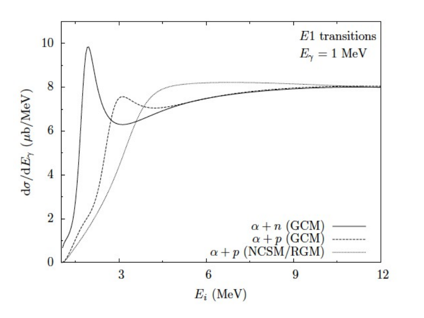
- Based on two- and three-nucleon forces, the NCSMC approach enables the first *ab initio* description of $\alpha + p$ scattering in good agreement with experimental data.

Prospect

- Using these wave functions to calculate the $\alpha + p$ bremsstrahlung (radiative transition between continuum states)

$$\alpha + p \rightarrow \alpha + p + \gamma$$

- Motivation: Preliminary work to the $t(d, \gamma n)\alpha$ (interesting for fusion experiments)



J. Dohet-Eraly, S. Quaglioni, P. Navrátil, G. Hupin, arXiv:1501.02744.

Thank you!
Merci

TRIUMF: Alberta | British Columbia | Calgary | Carleton | Guelph | Manitoba | McGill | McMaster | Montréal | Northern British Columbia | Queen's | Regina | Saint Mary's | Simon Fraser | Toronto | Victoria | Winnipeg | York

Canada Foundation for Innovation
Fondation canadienne pour l'innovation
Western Economic Diversification Canada
Diversification de l'économie de l'Ouest Canada
Natural Resources Canada
Ressources naturelles Canada