Lawrence Livermore National Laboratory

Ab initio Theory for Light-ion Reactions and Nuclear Data Evaluations

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Outline

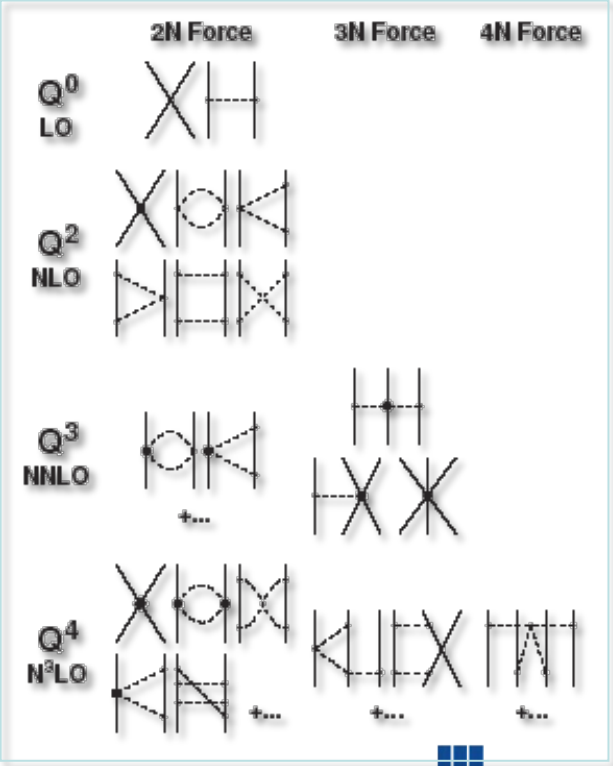
- Motivation
- Many-body technique:
  - *Ab initio* no-core shell model (NCSM) extended by the resonating group method (*ab initio* NCSM/RGM)
- Results
  - Nucleon-nucleus scattering
    - N-^{4}He
    - n-^{3}H, p-^{3}He
    - n-^{7}Li
  - d-T fusion
- Hybrid R-matrix approach
- Outlook

Light nuclei from first principles

- **Goal**: Predictive theory of structure and reactions of light nuclei
- Needed for our understanding of nuclear reactions important for astrophysics
- Needed for studies of exotic nuclei
- Needed for better understanding of nuclear reactions important for LLNL programs

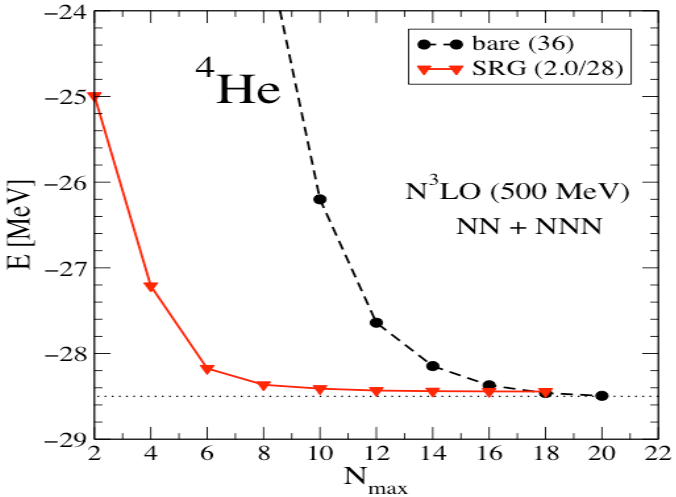
- ***Ab initio:***
- Nuclei as systems of point-like non-relativistic nucleons interacting by nucleon-nucleon (and three-nucleon) forces that describe accurately nucleon-nucleon (and three-nucleon) systems

- *Good place to start:*
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order

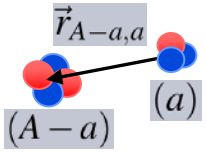


Our many-body technique:

- **Combine** the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)
- **The NCSM:** An approach to the solution of the *A*-nucleon bound-state problem
  - Accurate nuclear Hamiltonian
  - Finite harmonic oscillator (HO) basis
  - Complete $N_{max}\hbar\Omega$ model space
    - Relative or single-particle coordinates
  - Effective interaction due to the model space truncation
    - Similarity-Renormalization-Group evolved NN(+NNN) potential
  - Short & medium range correlations, no continuum
  - Description of single-particle degrees of freedom



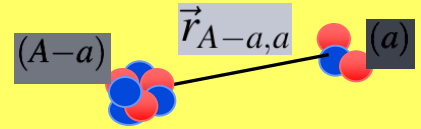
- **The RGM:** A microscopic approach to the *A*-nucleon scattering of clusters
  - Nuclear Hamiltonian may be simplistic
  - Cluster wave functions may be simplified and inconsistent with the nuclear Hamiltonian
  - Long range correlations
  - Description of clusters and their relative motion



***Ab initio* NCSM/RGM**: Combines the best of both approaches
Accurate nuclear Hamiltonian, consistent cluster wave functions
Coupling to continuum, Pauli principle and translational invariance

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$$



$$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

eigenstates of $H_{(A-a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

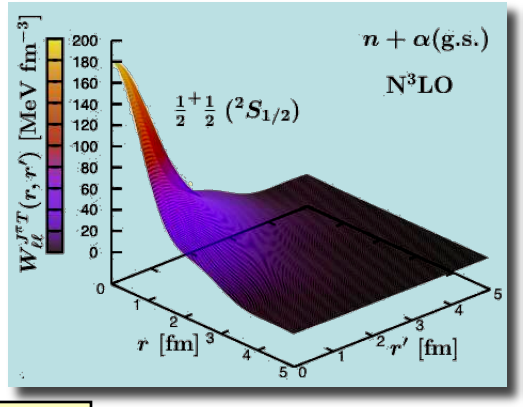
Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Norm kernel

- Non-local integro-differential coupled-channel equations:

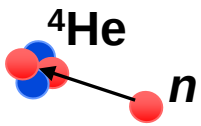
$$[\hat{T}_{\rm rel}(r) + \bar{V}_{\rm C}(r) - (E - E_\nu)]\, u_\nu(r) + \sum_{\nu} \int dr'\, r'\, W_{\nu\nu'}(r,r')\, u_\nu(r') = 0$$

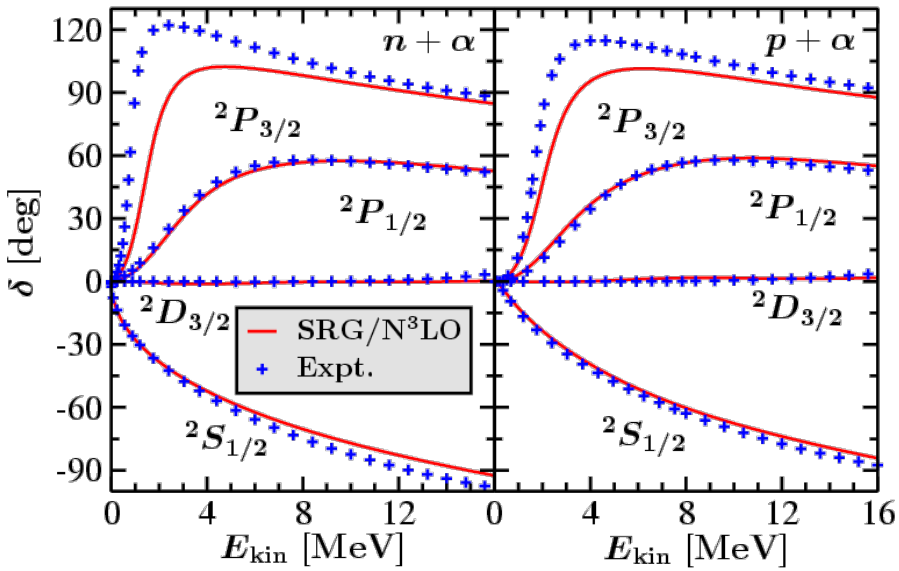


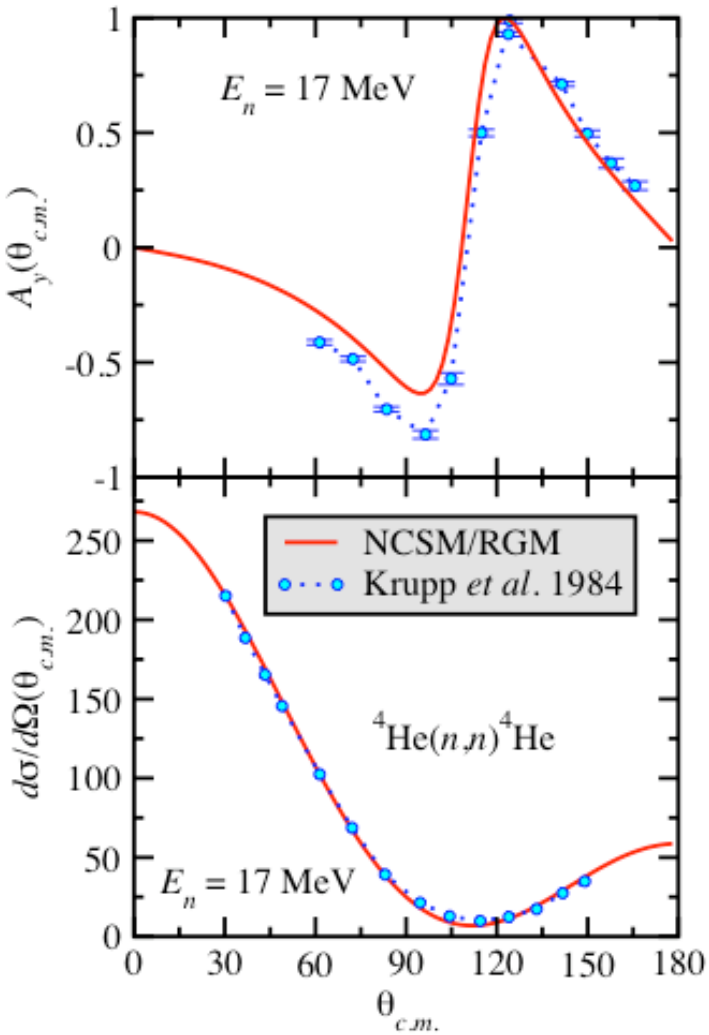
NCSM/RGM: NCSM microscopic wave functions for the clusters involved, and realistic (bare or derived NCSM effective) interactions among nucleons. Proper boundary conditions for scattering and/or bound states

n+^{4}He differential cross section and analyzing power

- NCSM/RGM calculations with
  - N + ^{4}He(g.s., 0^+0)
  - SRG-N^{3}LO NN potential with Λ=2.02 fm^{-1}



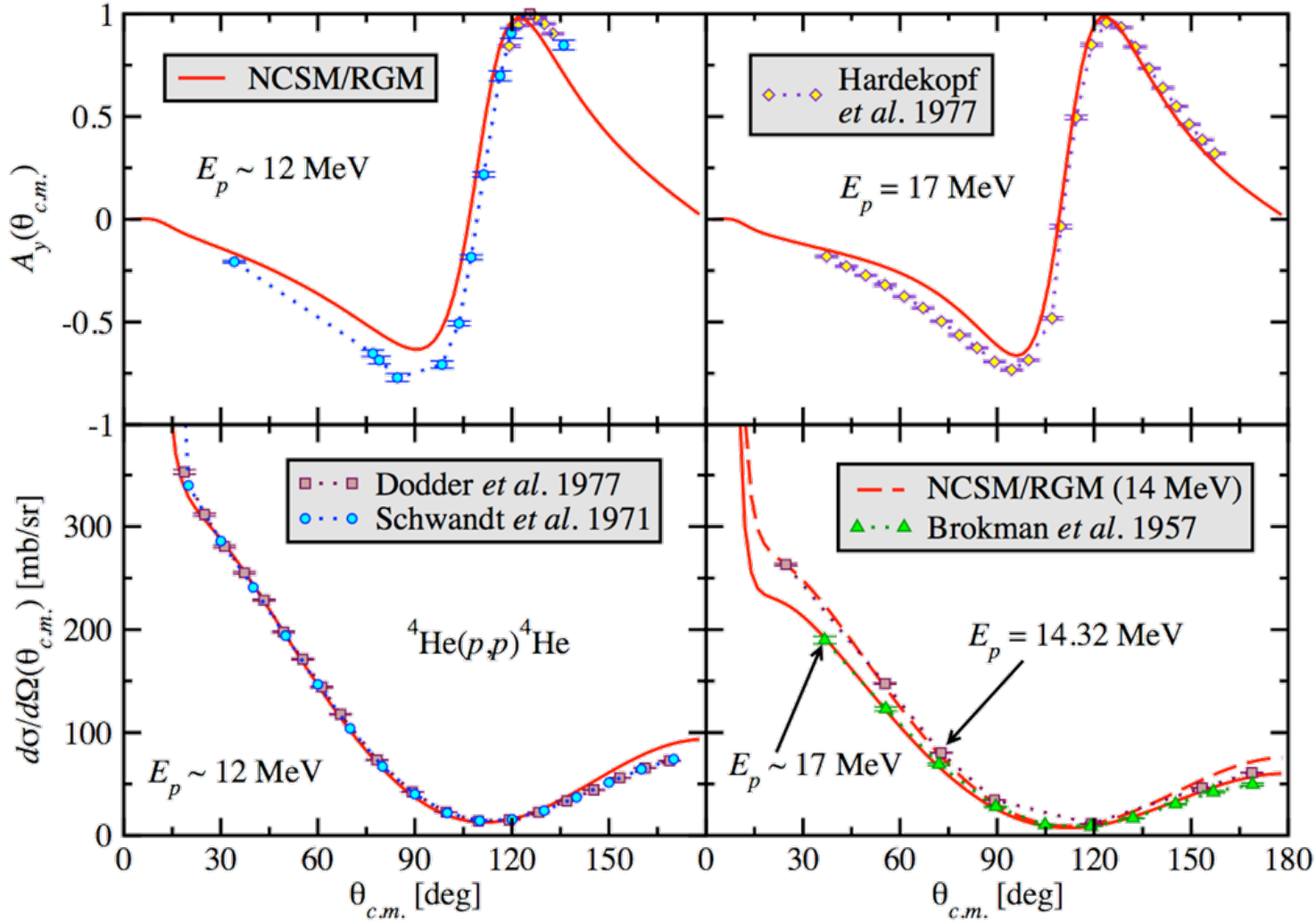




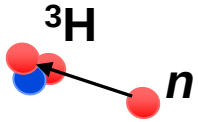
- Differential cross section and analyzing power @17 MeV neutron energy
  - Polarized neutron experiment at Karlsruhe

NNN missing: Good agreement only for energies beyond low-lying 3/2$^-$ resonance

p+^{4}He differential cross section and analyzing power



Neutron-triton elastic scattering at 14 MeV



- Important for NIF physics
  - deuteron-triton fusion generates 14 MeV neutrons
- Experimental situation confusing
- Good data for p+^{3}He elastic scattering

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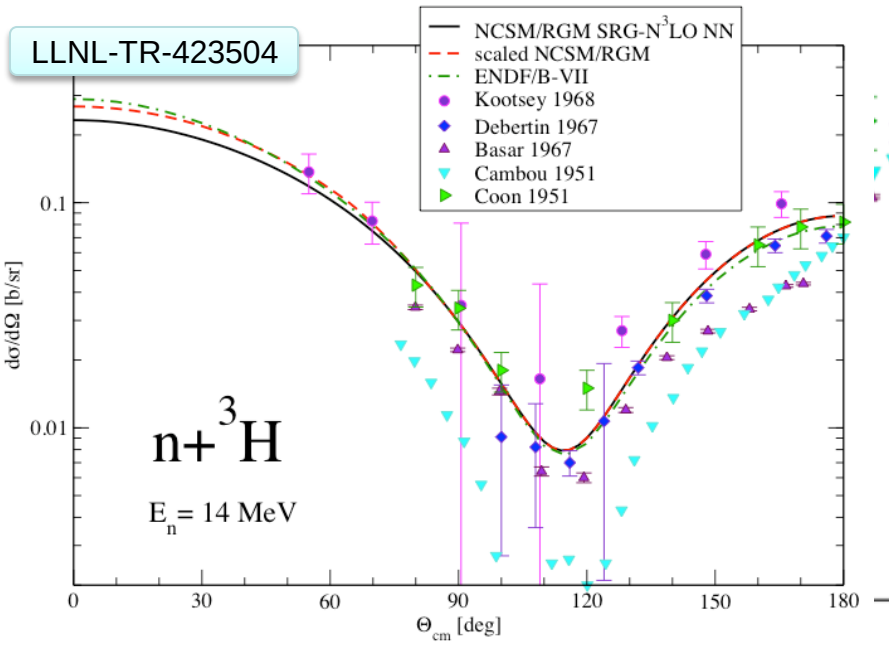
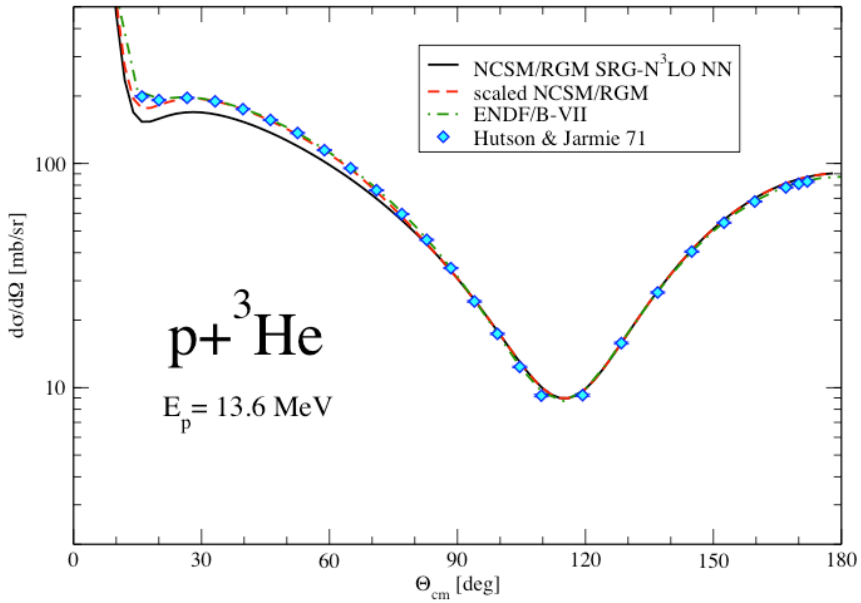
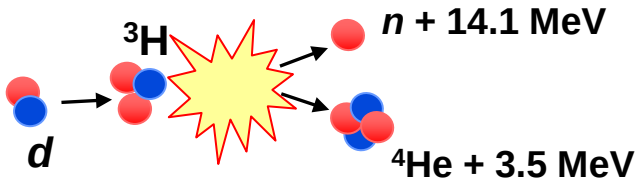


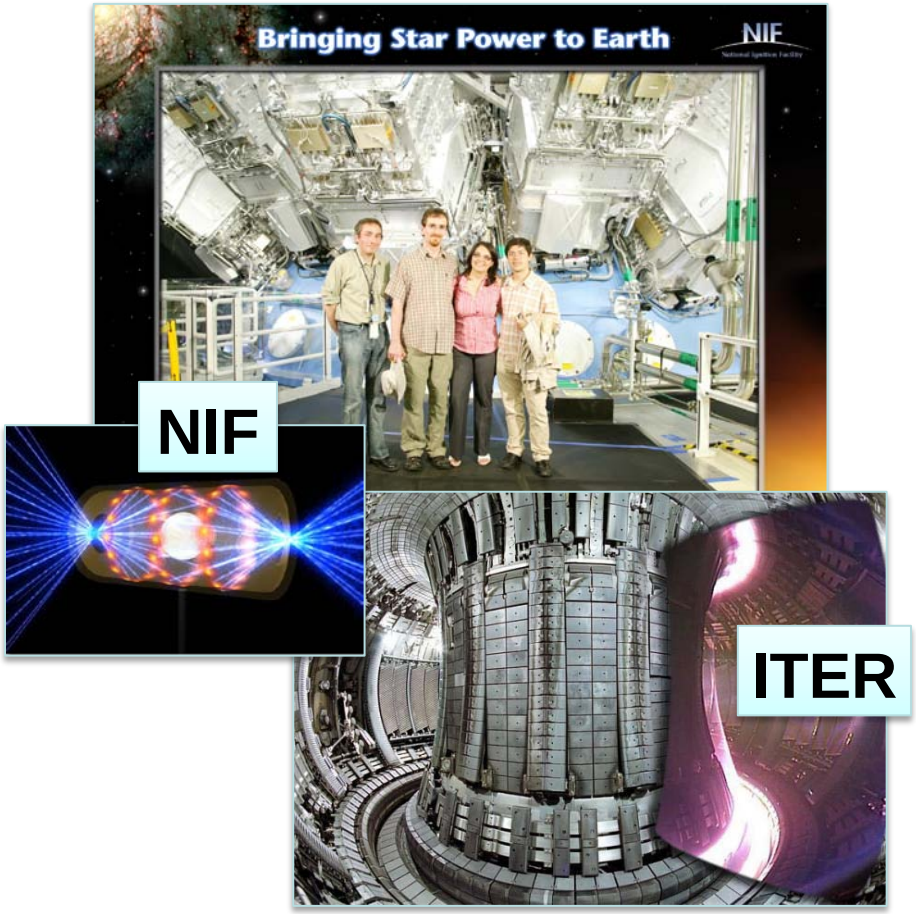


Use NCSM/RGM calculation to relate the two reactions and predict n+^{3}H cross section. Good agreement with the R-matrix analysis. Reduction of uncertainties.

Toward the first *ab initio* calculation of the Deuterium-Tritium fusion

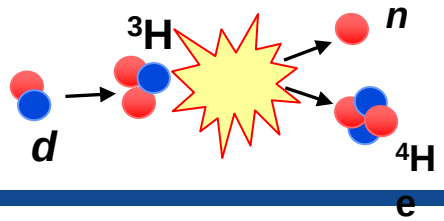


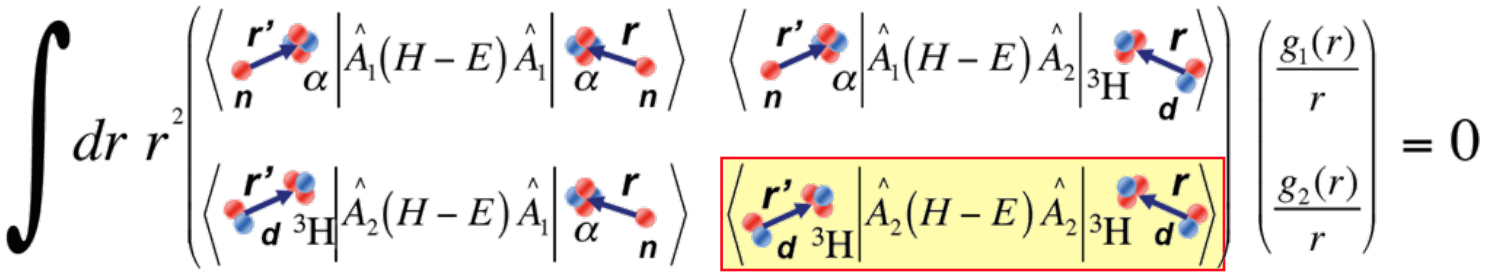
- The $d+^3\mathrm{H}\rightarrow n+^4\mathrm{He}$ reaction
  - The most promising for the production of fusion energy in the near future
  - Will be used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
- Unresolved issues remain
  - Cross section dependence on polarization of the *d* and ^{3}H nuclei not well known
  - Mirror reaction d-^{3}He also important, uncertainties larger



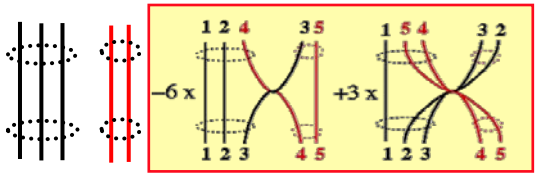
Ab initio theory can help shedding light on some of these issues: never attempted before!

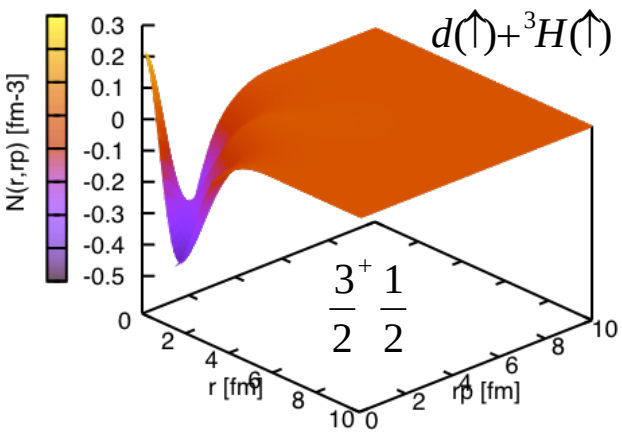
Toward the first *ab initio* calculation of the Deuterium-Tritium fusion

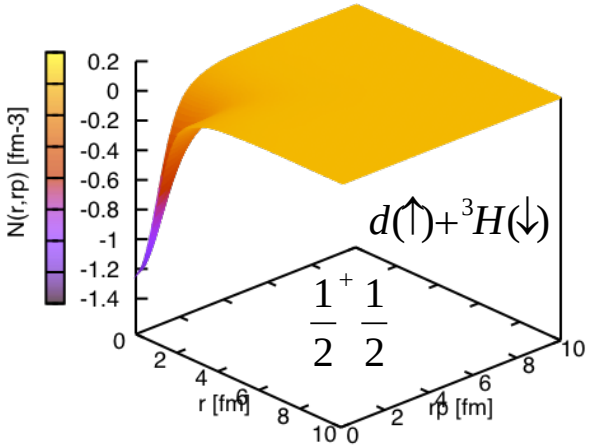


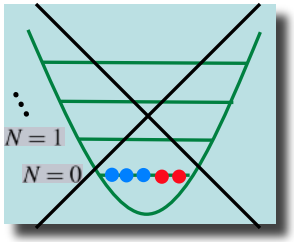


- d+^{3}H ➔ d+^{3}H *exchange* part of norm kern
  - *S*-wave channel: J=3/2$^+$,J=1/2$^+$

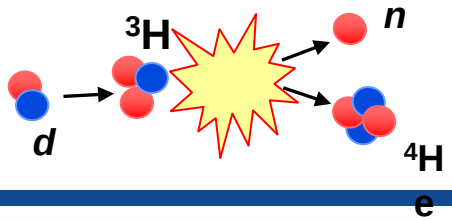


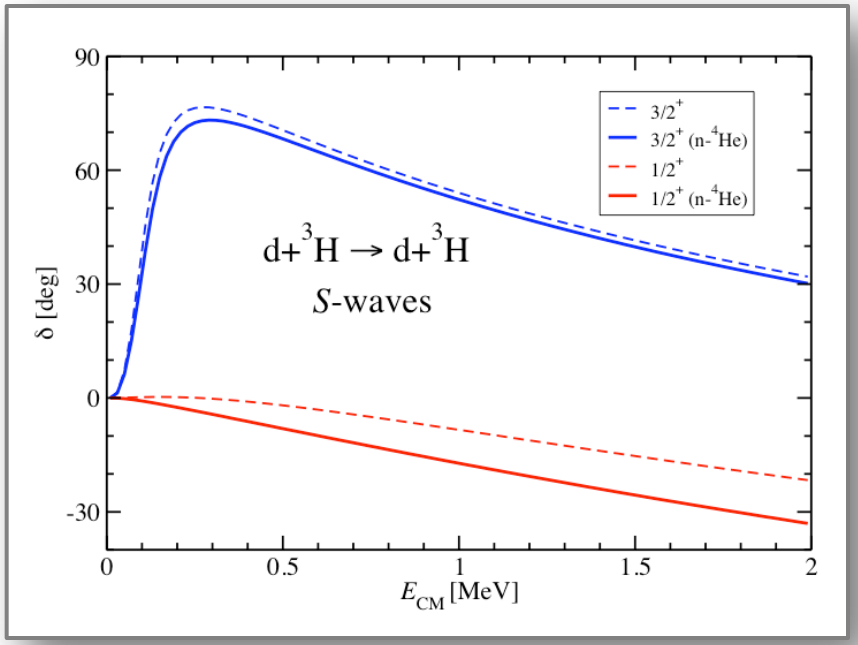


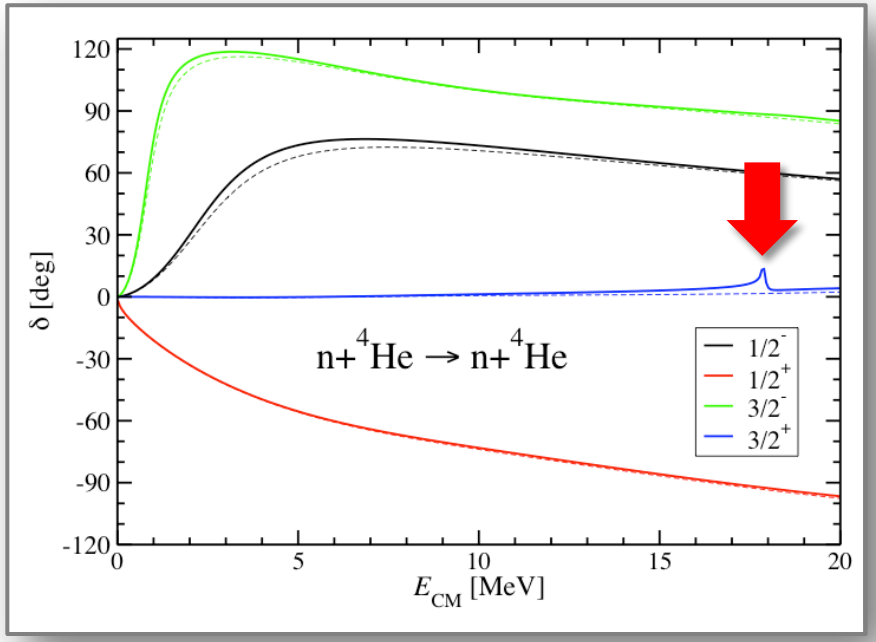




d+^{3}H and n+^{4}He elastic scattering: phase shifts



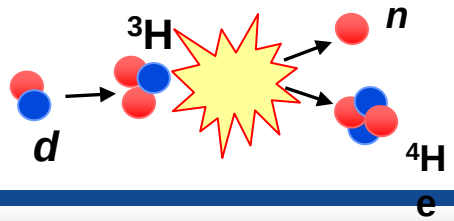


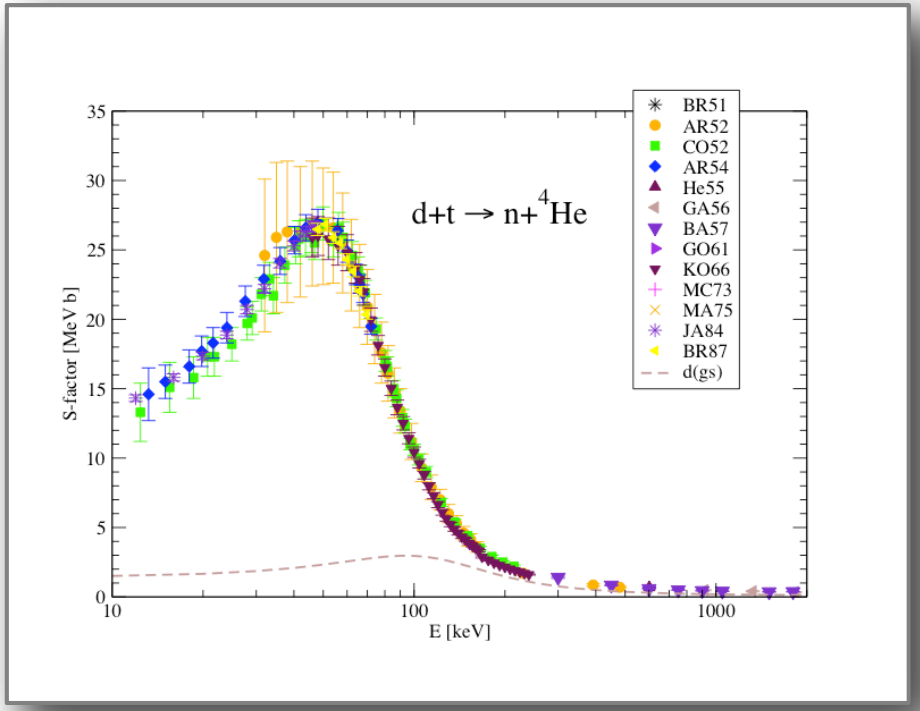


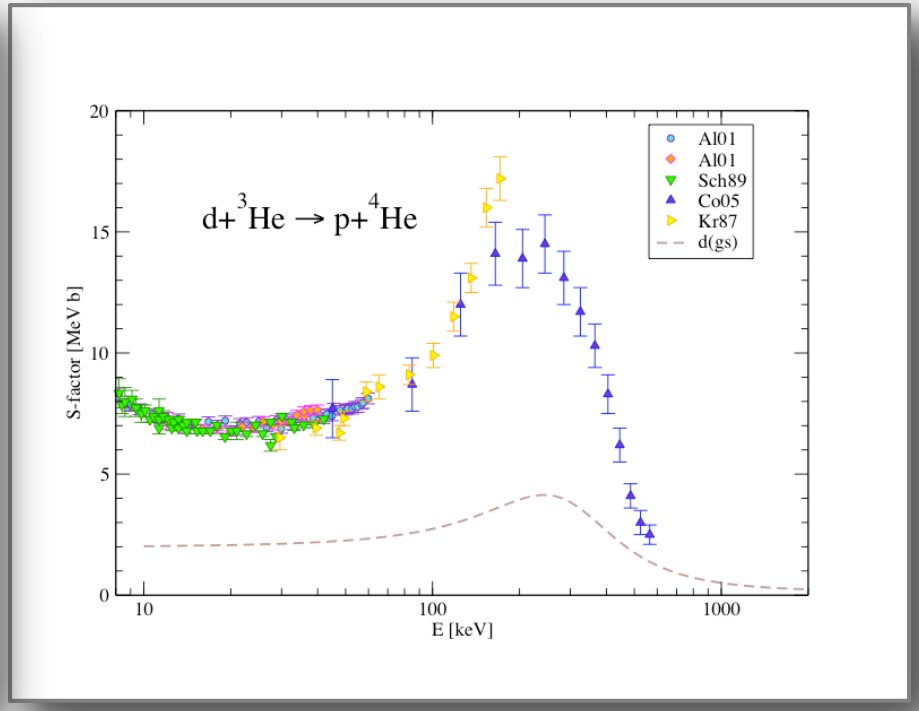
- d+^{3}H elastic phase shifts:
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel ➔ Pauli principle
- n+^{4}He elastic phase shifts:
  - d+^{3}H channels produces slight increase of the P phase shifts
  - Appearance of resonance in the $3/2^+$ D-wave, just above d-^{3}H threshold

The D-T fusion takes place through a transition of d+^{3}H is S-wave to n+^{4}He in D-wave

^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He cross sections





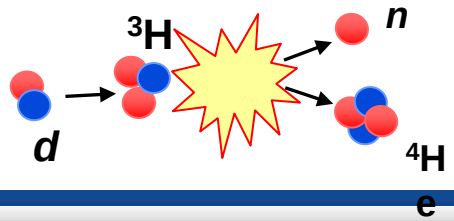


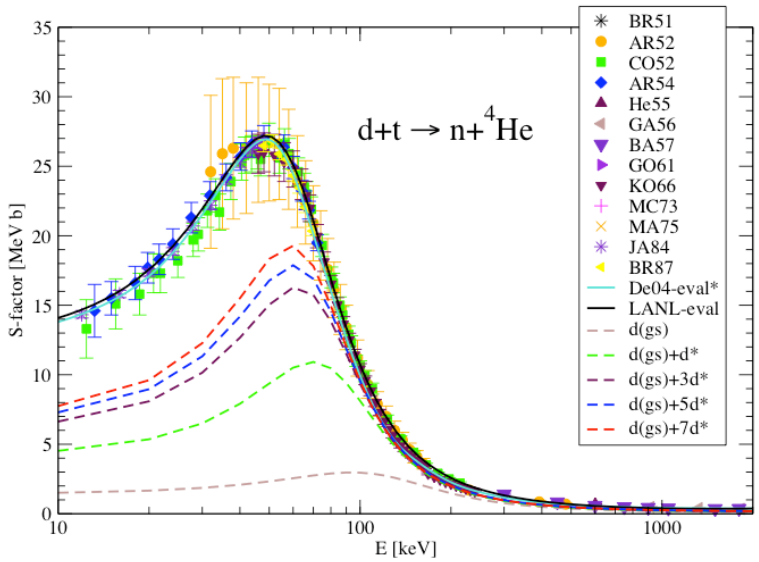
- The first results, still preliminary:
  - N_{max}= 11 (d-T), 13 (d-^{3}He)
  - SRG-N^{3}LO NN (Λ=1.5 fm^{-1}) potential
  - NNN interaction interaction effects for A=3,4,5 partly included by the choice of Λ
  - Only g.s . of d, ^{3}H, ^{4}He included above

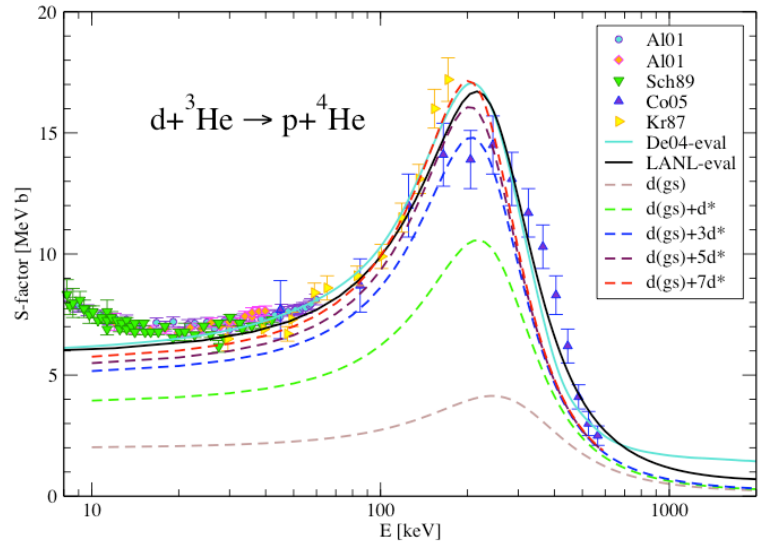
$$S(E) = E\sigma(E)\exp\left(\frac{2\pi\ Z_1 Z_2 e^2}{\hbar\sqrt{2mE}}\right)$$

Supported by PEM, LDRD

^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He cross sections





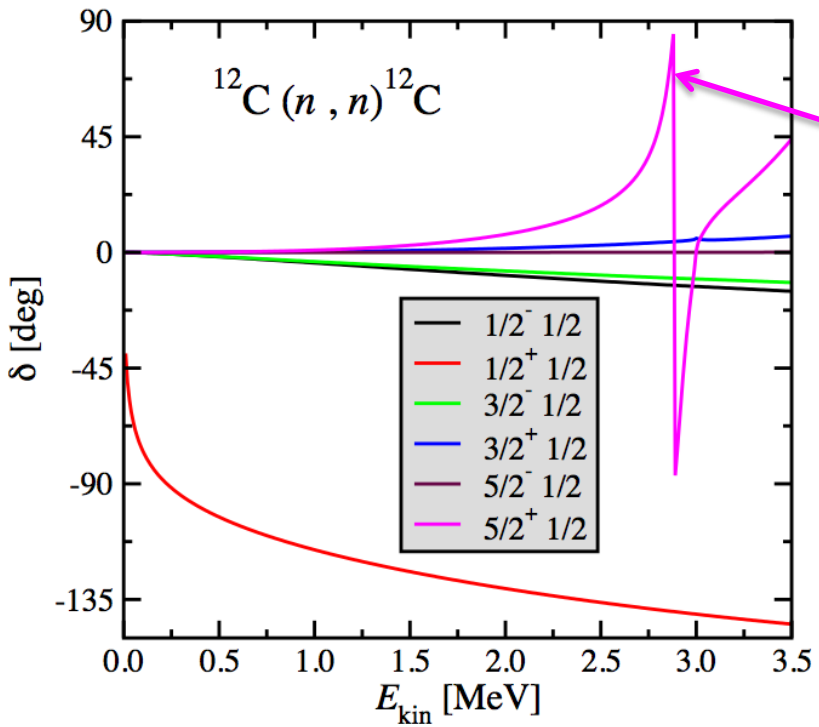


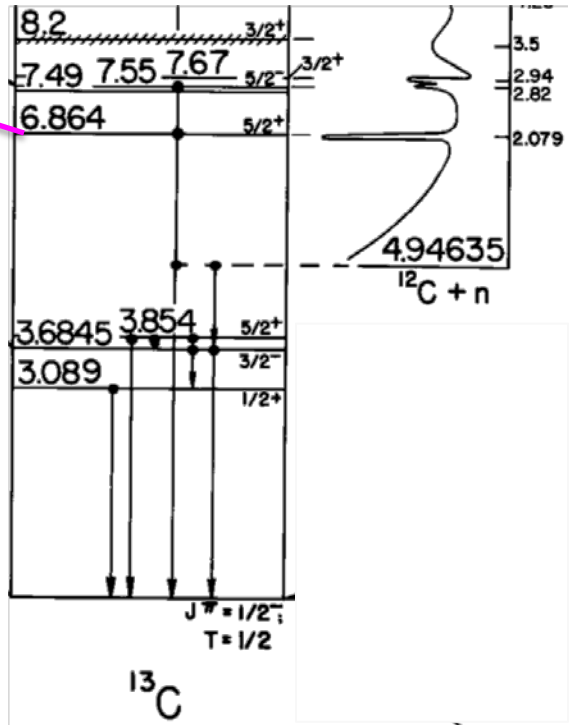
- The cross section improves with the inclusion of virtual breakup of the deuteron
  - Deuteron weakly bound: easily gets polarized and easily breaks
  - These effects included below the breakup threshold with continuum discretized by excited deuteron pseudo-states

First *ab initio* results for *d*-T and *d*-^{3}He fusion:
Very promising, correct physics, becoming competitive with fitted evaluations …

^{13}C bound states and n-^{12}C scattering

- N_{max} = 16 NCSM/RGM calculation with n + ^{12}C(g.s.,2^+_1)
- SRG-N^{3}LO NN potential with Λ = 2.02 fm^{-1}
  - Three ^{13}C bound states: $1/2^-$, $3/2^-$, $1/2^+$ ($5/2^+$ still unbound)
  - $5/2^+$ narrow resonance





Good start, but the (here missing) ^{9}Be + α (and other) channels are important!

Applications to heavier nuclei: Hybrid R-Matrix approach

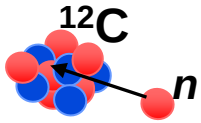
- In the NCSM/RGM the scattering equations are solved by means of the R-Matrix method on Lagrange mesh
  - Configuration space divided into "internal" and "external" regions separated by the "channel surface"
    - Internal region: expansion on Lagrange basis
    - External region: asymptotic form for large $\boldsymbol{r}$
  - *S*-Matrix calculated from microscopic R-Matrix

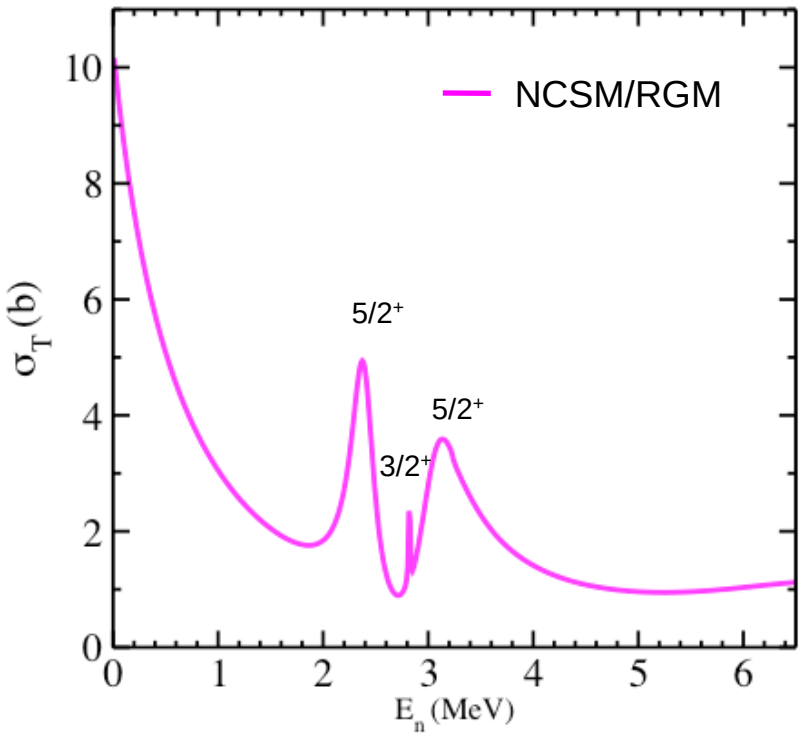
$$R_{cc'}(E) = \sum_{\lambda} \frac{\gamma_{\lambda}^{c}\gamma_{\lambda}^{c'}}{E_{\lambda} - E}$$

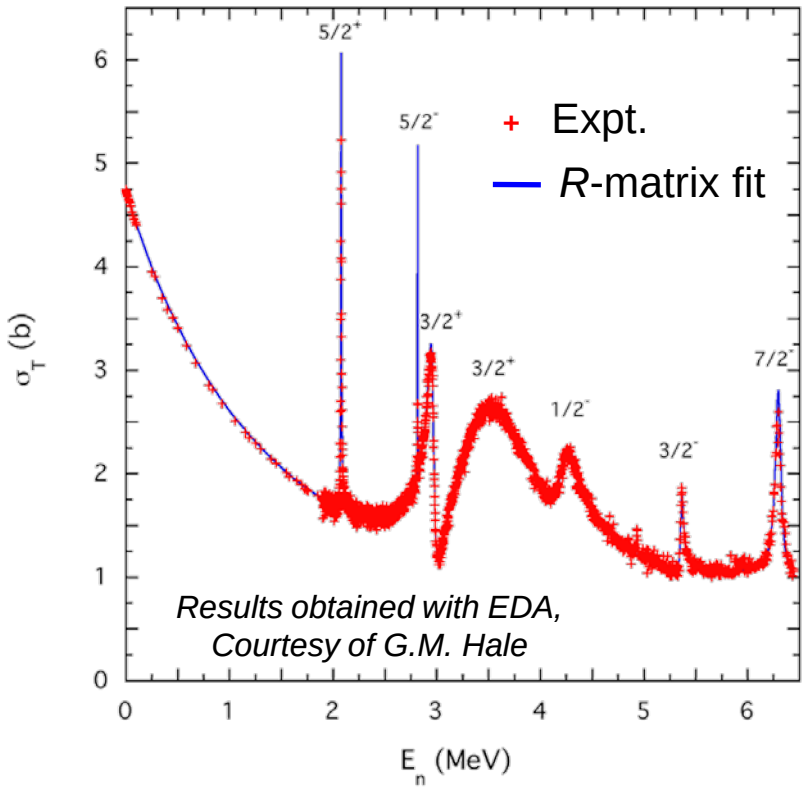
- The microscopic eigenenergies E_{λ} and real reduced-width amplitudes γ_{λ}^{c} obtained within the NCSM/RGM can be used as starting points for a traditional R-Matrix analysis

- Hybrid R-Matrix approach
  - *Ab initio* guided starting parameters for channels included (nucleon-nucleus, ...)
  - Traditional initial guess for channels not yet taken into account
  - Ongoing test on n+^{12}C reaction in collaboration with Gerry Hale (LANL)

n-^{12}C total elastic cross section



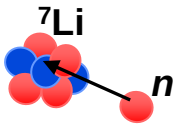




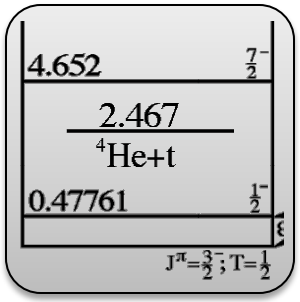
- N_{max} = 7 NCSM/RGM calculation with n + ^{12}C(g.s.,2^+_1)
  - $1/2^+$ state much less bound than in expt. ➔ large cross section at zero E_n
  - Need more ^{12}C excited states for higher resonances

Status: Input NCSM/RGM parameters into R-matrix code and reproduce the cross section. Ready to start fits.

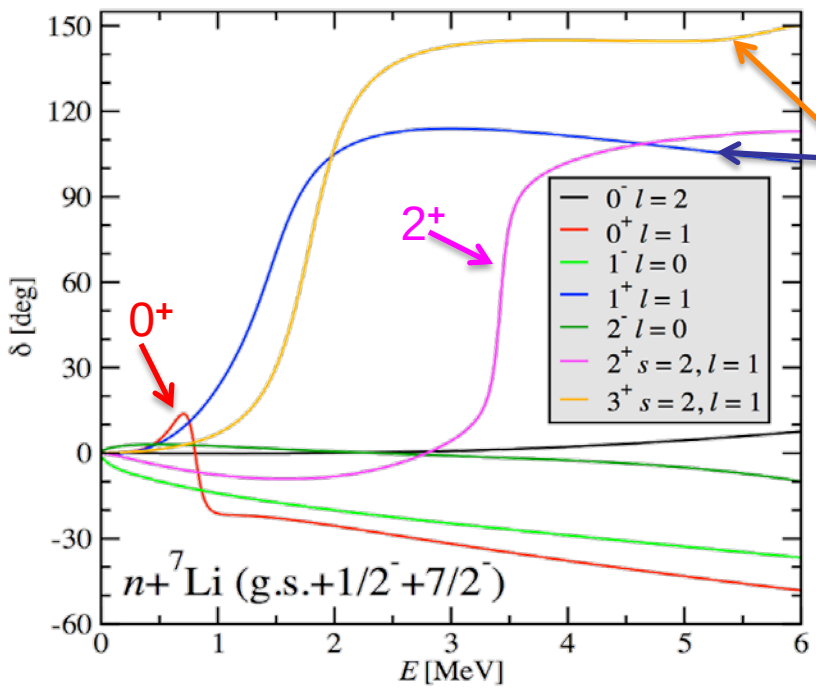
NCSM/RGM *ab initio* calculation of n+^{7}Li scattering

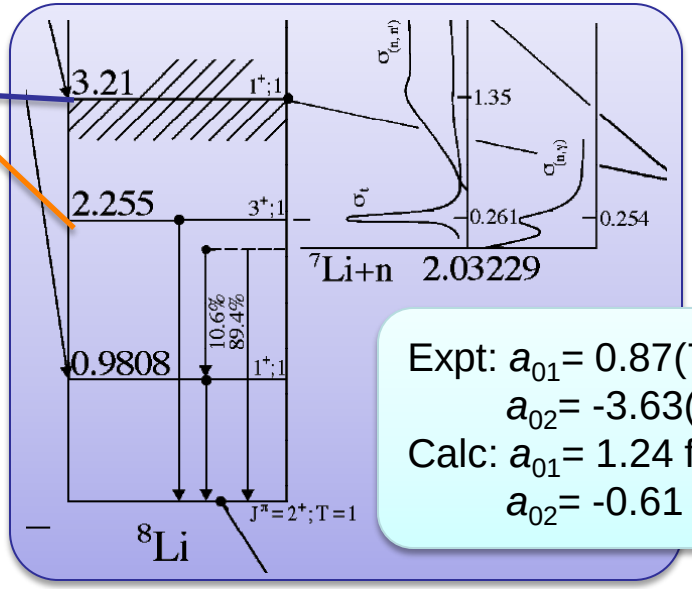


- N_{max} = 12 NCSM/RGM calculation with n + ^{7}Li(g.s.,1/2$^-$, 7/2$^-$)
- SRG-N^{3}LO NN potential with Λ = 2.02 fm^{-1}
  - ^{8}Li bound states: 2$^+$ and 1$^+$
  - Calculated broad 1$^+$ resonance
  - 3$^+$ resonance not seen when the 7/2$^-$ state of ^{7}Li is not included



^{7}Li

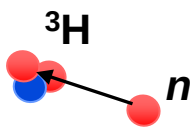


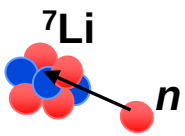


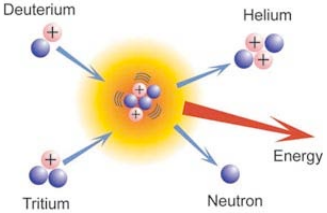
Expt: a_{01}= 0.87(7) fm
a_{02}= -3.63(5) fm
Calc: a_{01}= 1.24 fm
a_{02}= -0.61 fm

Predicted narrow 0$^+$ and 2$^+$ resonances seen at recent p+^{7}Be experiment at FSU

Conclusions and Outlook







- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
  - S. Quaglioni and P. N., PRL **101**, 092501 (2008), PRC **79**, 044606 (2009)
- Bring about the capability to perform modern evaluations based on *ab initio* theory and data
- First results for ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He
  - Complex transfer reaction, never calculated from first principles before
  - Soft accurate NN potential, virtual breakup through excited deuteron pseudo-states
  - Cross sections close to experimental data
  - Very promising approach…
- Formalism and code development for ^{3}H, ^{3}He projectiles
  - ^{3}H(^{3}H,2n)^{4}He reaction important for NIF experiments
- The microscopic eigenenergies E_λ and reduced-width amplitudes $\gamma_\lambda{}^c$ obtained within the NCSM/RGM can be used as starting points for a traditional R-Matrix analysis ➔ **Hybrid *R*-matrix approach**
- Guidance from *ab initio* valuable for data evaluations in particular if not enough accurate experimental data exist