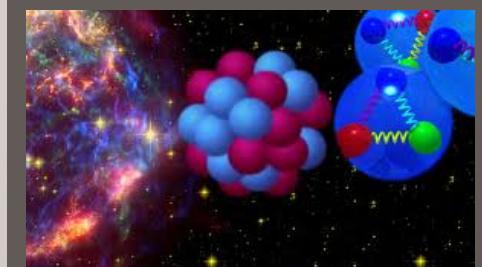
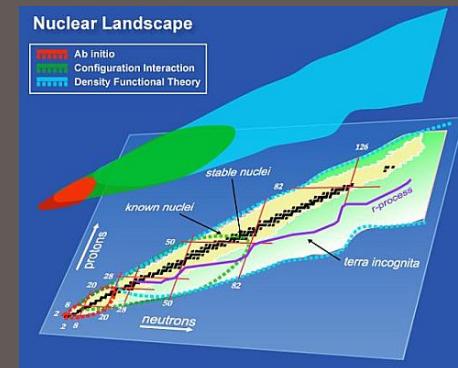


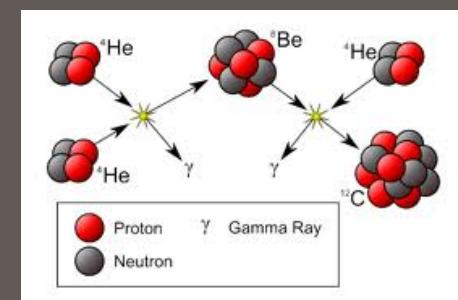
Unifying nuclear structure and reactions within the NCSM/RGM

Perspectives of the *Ab Initio* No-Core Shell Model

TRIUMF, February 10-12, 2011



Petr Navratil | TRIUMF

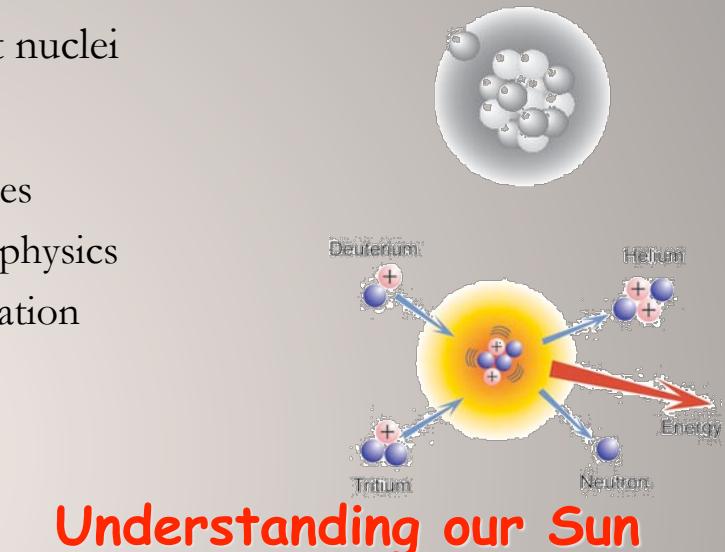
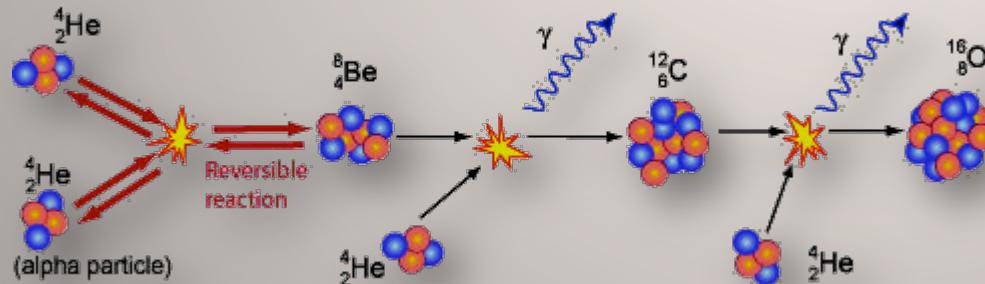


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 Un accélérateur de la démarche scientifique canadienne

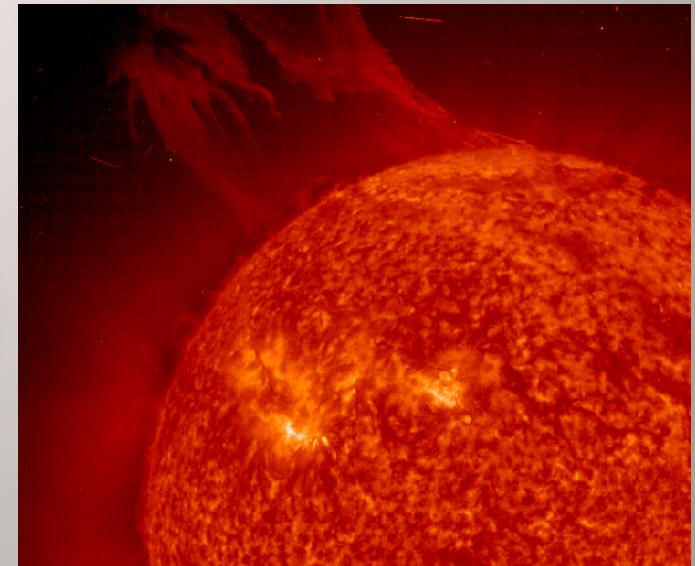
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Light nuclei from first principles

- **Goal:** Predictive theory of structure and reactions of light nuclei
- Needed for
 - Physics of exotic nuclei, tests of fundamental symmetries
 - Understanding of nuclear reactions important for astrophysics
 - Understanding of reactions important for energy generation
- **From first principles or *ab initio*:**
 - ✓ Nuclei as systems of nucleons interacting by nucleon-nucleon (and three-nucleon) forces that describe accurately nucleon-nucleon (and three-nucleon) systems

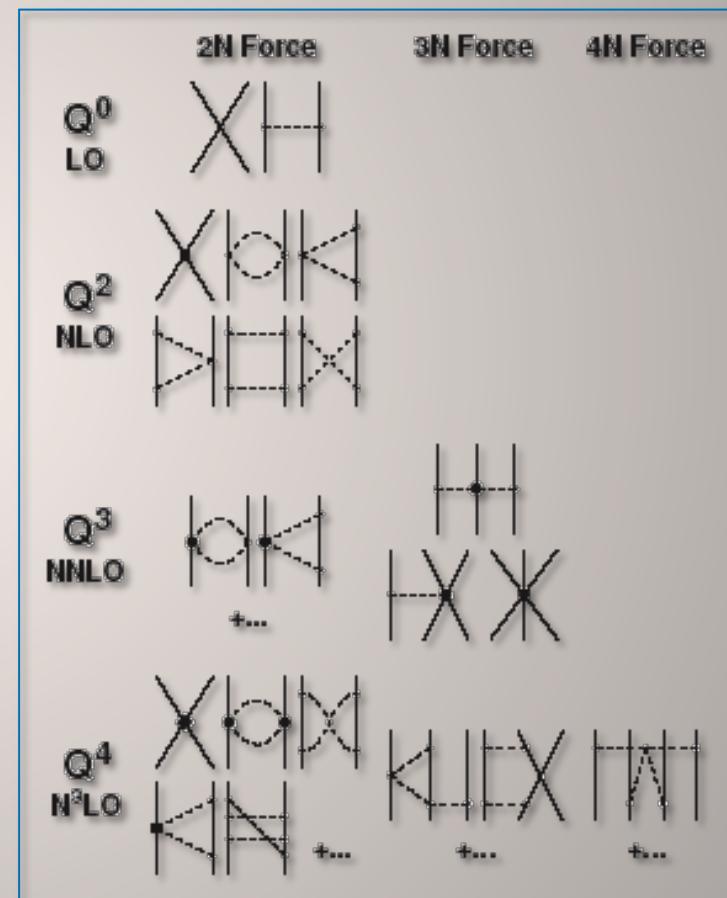


Understanding our Sun



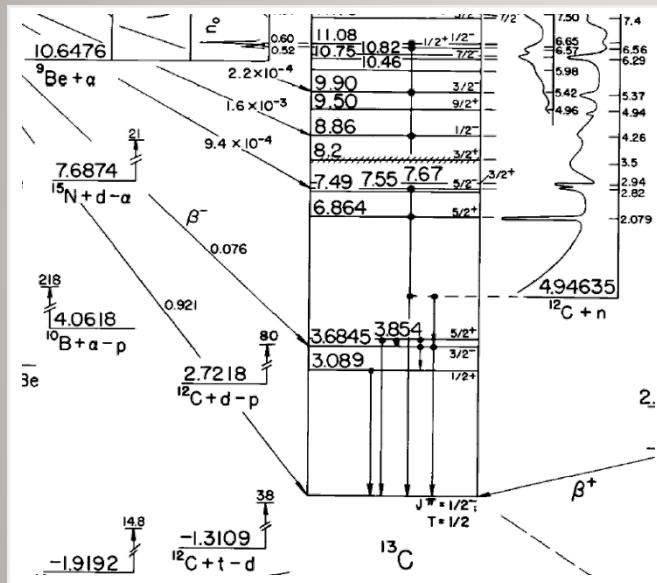
Light nuclei from the first principles

- First principles for Nuclear Physics:
- QCD
 - Non-perturbative at low energies
 - Lattice QCD in the future
- *For now a 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
 - Hierarchy
 - Consistency
 - Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD



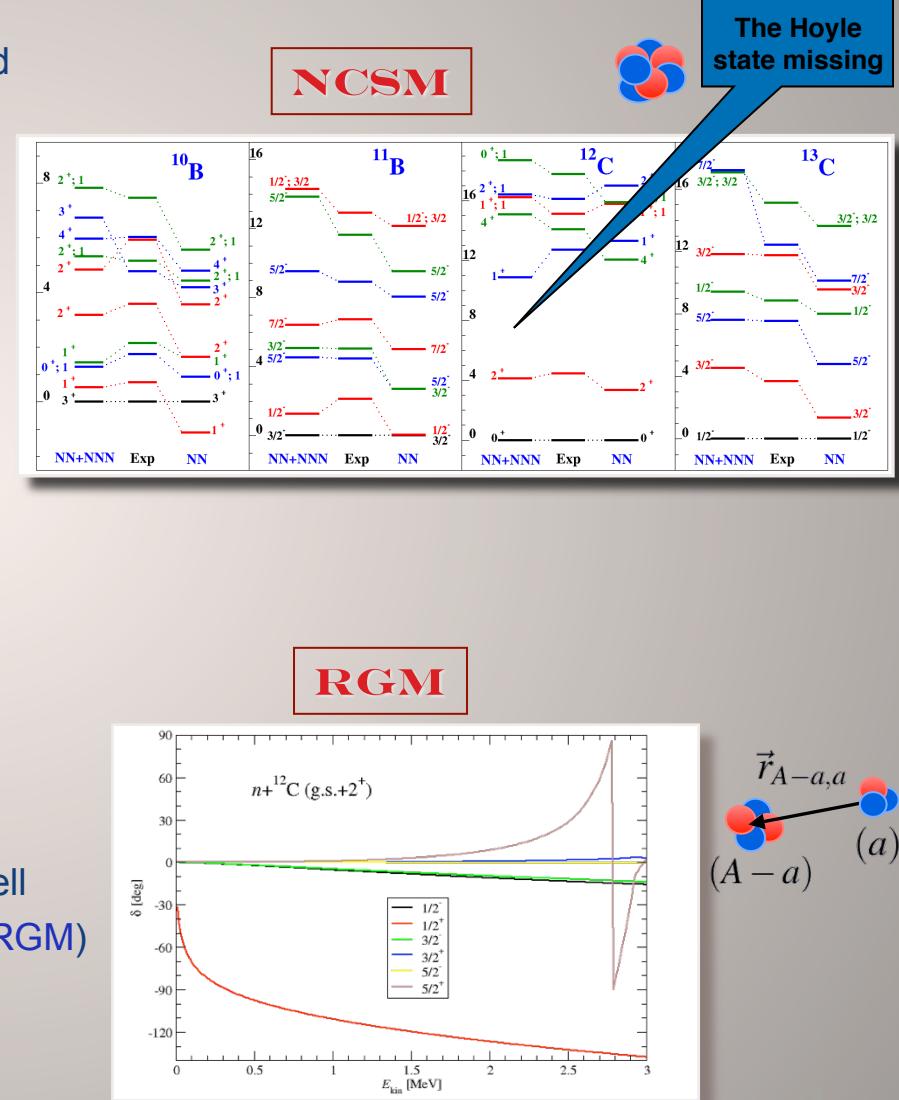
Predictive *ab initio* theory must provide a unified description of structure and reactions of light nuclei

- Nuclei are quantum many-body systems with bound states, resonances, scattering states
 - Bound-state techniques not sufficient



- Our approach** - combining the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)

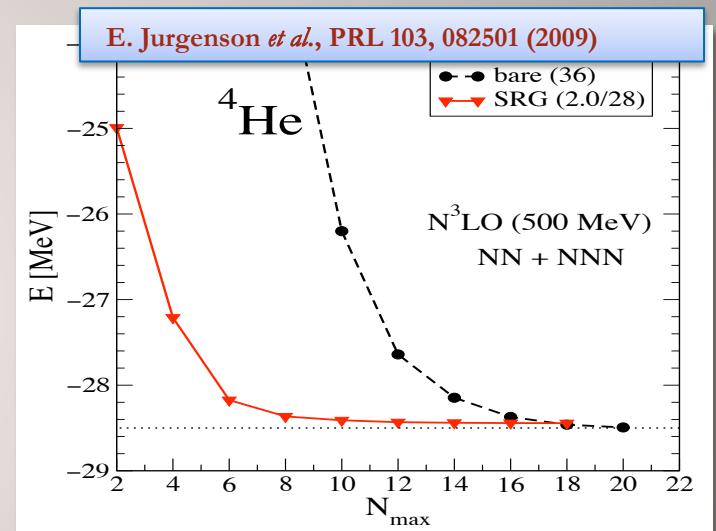
 \Rightarrow ***ab initio* NCSM/RGM**
 - NCSM - single-particle degrees of freedom
 - RGM - clusters and their relative motion



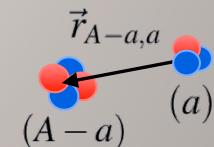
Our many-body technique:

- **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
- Effective interaction due to the model space truncation
 - Similarity-Renormalization-Group evolved NN(+NNN) potential
- Short & medium range correlations
- No continuum



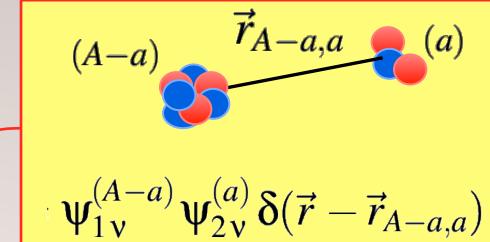
- **The RGM:** A microscopic approach to the A -nucleon scattering of clusters
 - Nuclear Hamiltonian may be simplistic
 - Cluster wave functions may be simplified and inconsistent with the nuclear Hamiltonian
 - Long range correlations, relative motion of clusters



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

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_v \int d\vec{r} \varphi_v(\vec{r}) \hat{\mathcal{A}} \Phi_{v\vec{r}}^{(A-a,a)}$
- Many-body Schrödinger equation:



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

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

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

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

realistic nuclear Hamiltonian

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

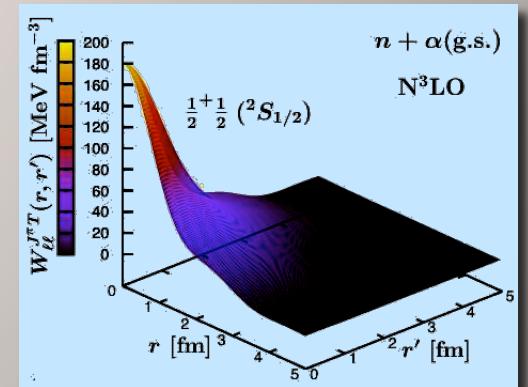
Hamiltonian kernel

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

Norm kernel

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

$$[\hat{T}_{\text{rel}}(r) + \bar{V}_{\text{C}}(r) - (E - E_v)] u_v(r) + \sum_v \int dr' r' W_{vv'}(r, r') u_{v'}(r') = 0$$



(A-1)
(1)

Single-nucleon projectile: the norm kernel

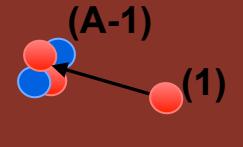
$$\left\langle \begin{array}{c} (1, \dots, A-1) \\ \text{---} \\ \text{---} \end{array} \right| \left| 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right| \left| \begin{array}{c} (1, \dots, A-1) \\ \text{---} \\ \text{---} \end{array} \right\rangle_{(A)} \quad r' \quad r$$

$$\mathcal{N}_{\mu\ell',\nu\ell}^{(A-1,1)}(\mathbf{r}', \mathbf{r}) = \delta_{\mu\nu} \delta_{\ell'\ell} \frac{\delta(\mathbf{r}' - \mathbf{r})}{\mathbf{r}' \cdot \mathbf{r}} - (A-1) \sum_{n'n} R_{n'\ell'}(\mathbf{r}') \langle \Phi_{\mu n' \ell'}^{(A-1,1)JT} | \mathbf{P}_{A,A-1} | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n\ell}(\mathbf{r})$$

Diagram illustrating the localized parts of kernels expanded in the HO basis:

The diagram shows two sets of vertical lines representing harmonic oscillator basis states. The left set is labeled μ, ℓ' and the right set is labeled ν, ℓ . A red oval encloses the left set, and a blue oval encloses the right set. A red bracket labeled $-(A-1) \times$ connects the two ovals. A blue arrow points from the right side of the diagram to a box containing the expression $\text{SD} \langle \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{\nu_1}^{(A-1)} \rangle_{\text{SD}}$. A blue box at the bottom right contains the text "Localized parts of kernels expanded in the HO basis".

Single-nucleon projectile basis: the Hamiltonian kernel



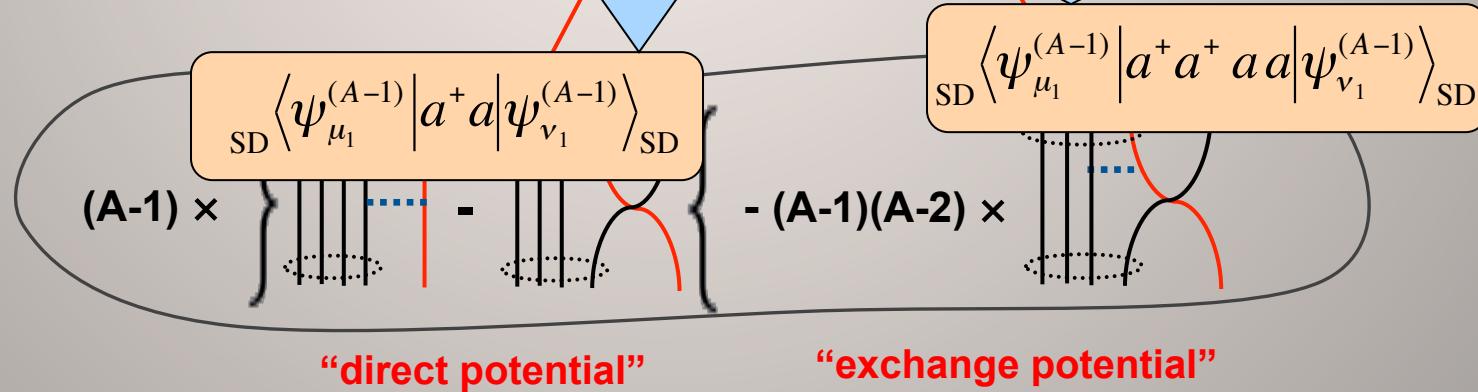
$$\left\langle \begin{array}{c} (1,\dots,A-1) \\ \text{---} \\ \text{(A)} \end{array} \right| H \left(1 - \sum_{j=1}^{A-1} P_{jA} \right) \left| \begin{array}{c} (1,\dots,A-1) \\ \text{---} \\ (\text{A}) \end{array} \right\rangle$$

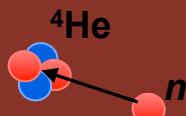
$$\mathcal{H}_{\mu\ell',\nu\ell}^{(A-1,1)}(\mathbf{r}', \mathbf{r}) = (E_{A-1} + T_{rel}) \mathcal{N}_{\mu\ell',\nu\ell}^{(A-1,1)}(\mathbf{r}', \mathbf{r})$$

$$+ (A-1) \sum_{n'n} R_{n'\ell'}(r') \langle \Phi_{\mu n' \ell'}^{(A-1,1)JT} | V_{A-1,A} (1 - P_{A-1,A}) | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n\ell}(r)$$

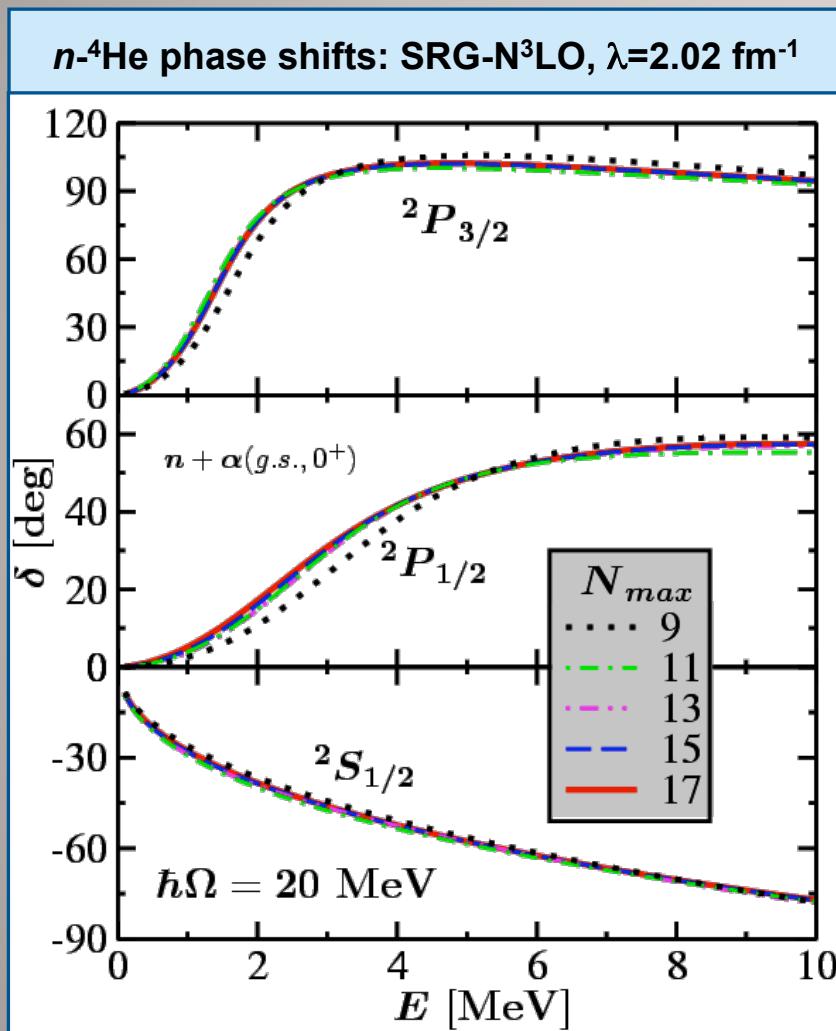
$$- (A-1)(A-2) \sum_{n'n} R_{n'\ell'}(r') \langle \Phi_{\mu n' \ell'}^{(A-1,1)JT} | V_{A-2,A} P_{A,A-1} | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n\ell}(r)$$

+ terms containing NNN potential

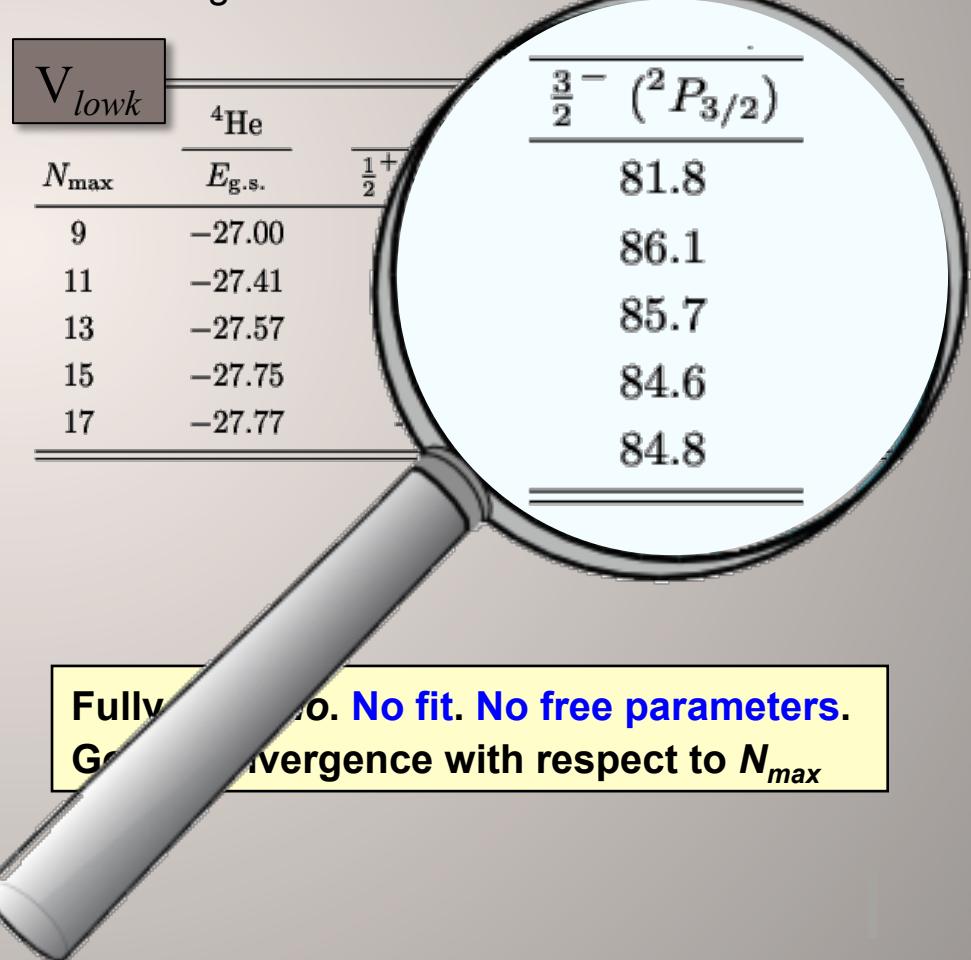




Convergence of the *ab initio* NCSM/RGM: $n\text{-}{}^4\text{He}$ phase shifts

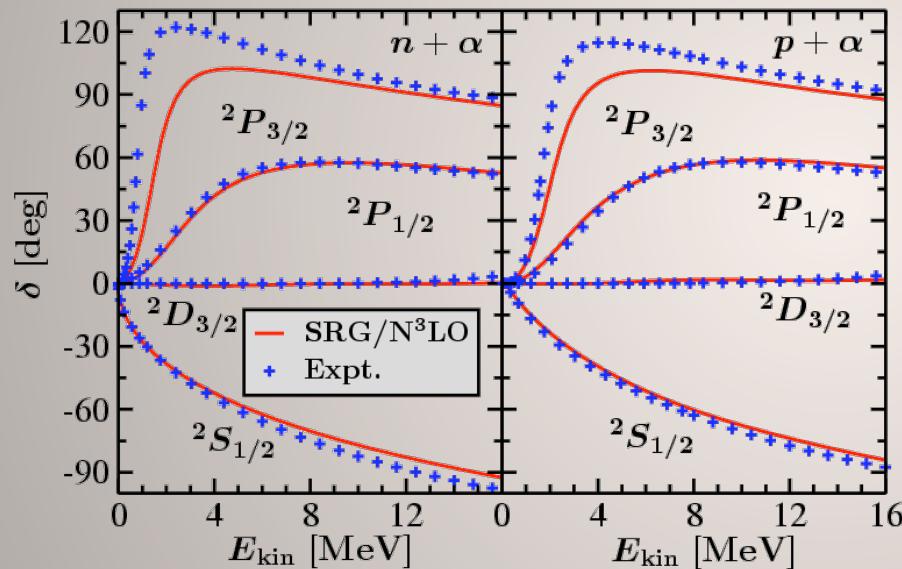


- Similarity-renormalization-group (SRG) evolved chiral N³LO NN interaction
- Low-momentum V_{lowk} NN potential
- convergence reached with **bare** interaction

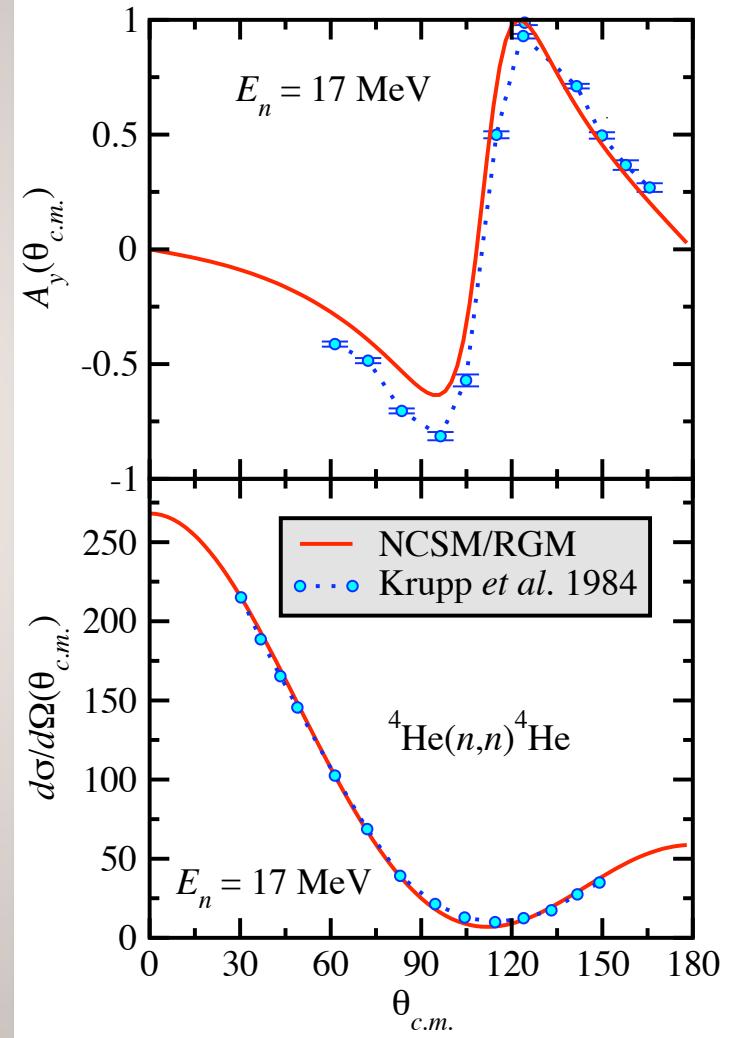
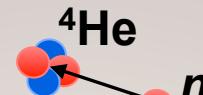


The best system to start with: $n+{}^4\text{He}$, $p+{}^4\text{He}$

- NCSM/RGM calculations with
 - $N + {}^4\text{He}(\text{g.s.}, 0^+0)$
 - SRG-N³LO NN potential with $\Lambda=2.02 \text{ fm}^{-1}$

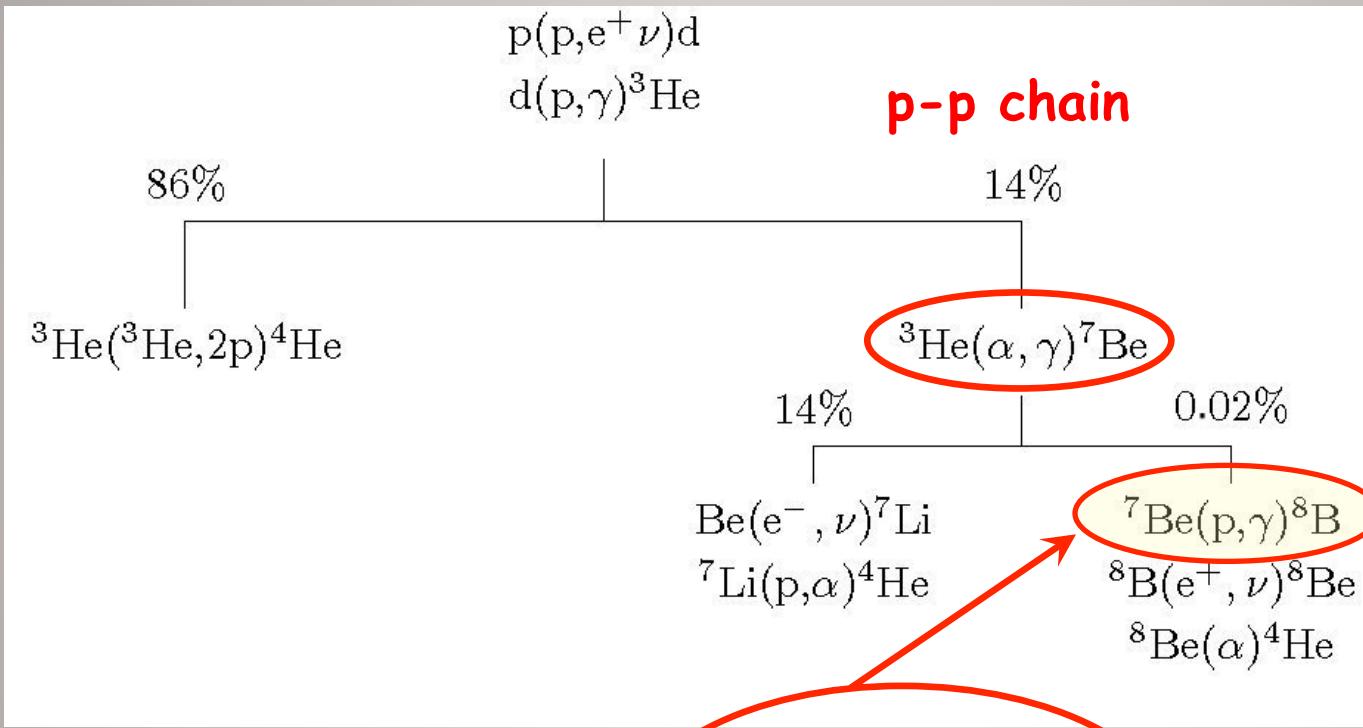


- Differential cross section and analyzing power @17 MeV neutron energy
 - Polarized neutron experiment at Karlsruhe



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

Solar p - p chain



$^{7}\text{Be}(\text{p},\gamma)^{8}\text{B}$ S-factor

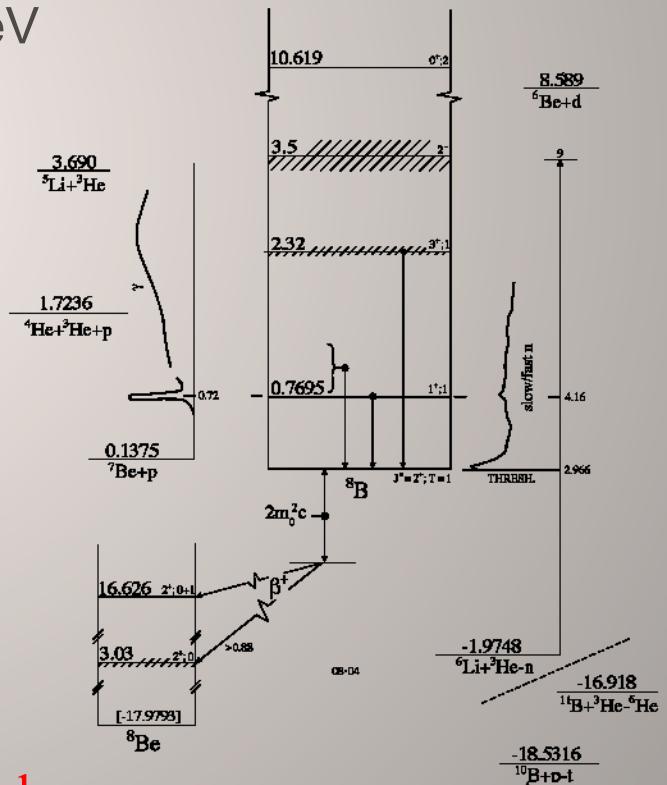
- S_{17} one of the main inputs in solar neutrino problem
 - Needs to be known with a precision better than 9 %
- Current evaluation has uncertainty >10%
 - Theory needed for extrapolation to ~ 10 keV

$$S(E) = E \sigma(E) \exp[2\pi\eta(E)]$$

$$\eta(E) = Z_{A-a} Z_a e^2 / \hbar v_{A-a,a}$$

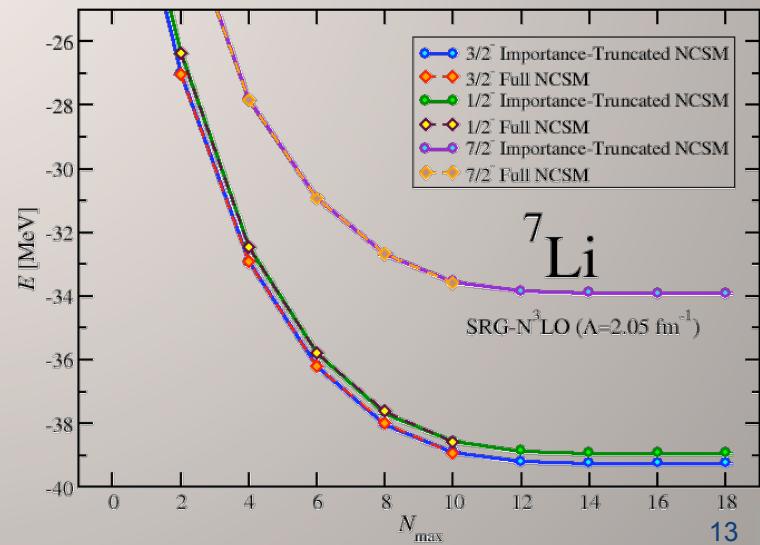
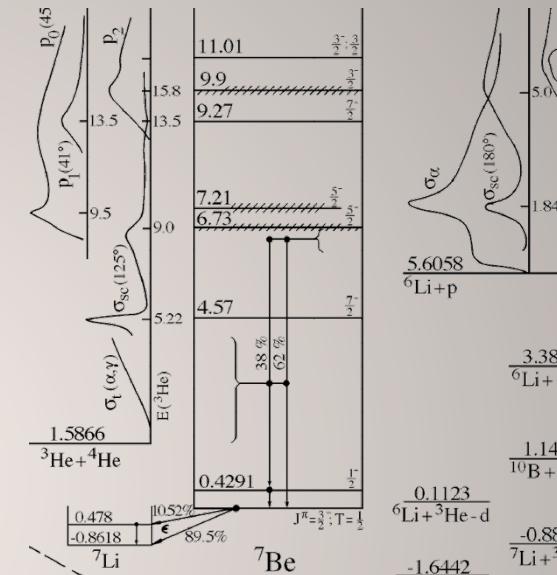
$$\left\langle {}^8\text{B}_{\text{g.s.}} \left| E1 \right| {}^7\text{Be}_{\text{g.s.}} + \text{p} \right\rangle$$

Many theoretical calculations in the past...
 ...now something new: Starting from first principles



Input: NN interaction, ${}^7\text{Be}$ eigenstates

- Similarity-Renormalization-Group (SRG) evolved chiral N³LO NN interaction
 - Accurate
 - Soft: Evolution parameter Λ
- ${}^7\text{Be}$ (${}^7\text{Li}$)
 - NCSM up to $N_{\max}=10$ possible
 - Importance Truncated NCSM up to $N_{\max}=18$
 - R. Roth & P. N., PRL **99**, 092501 (2007)
 - large N_{\max} needed for convergence of
 - Target eigenstates
 - Localized parts of integration kernels



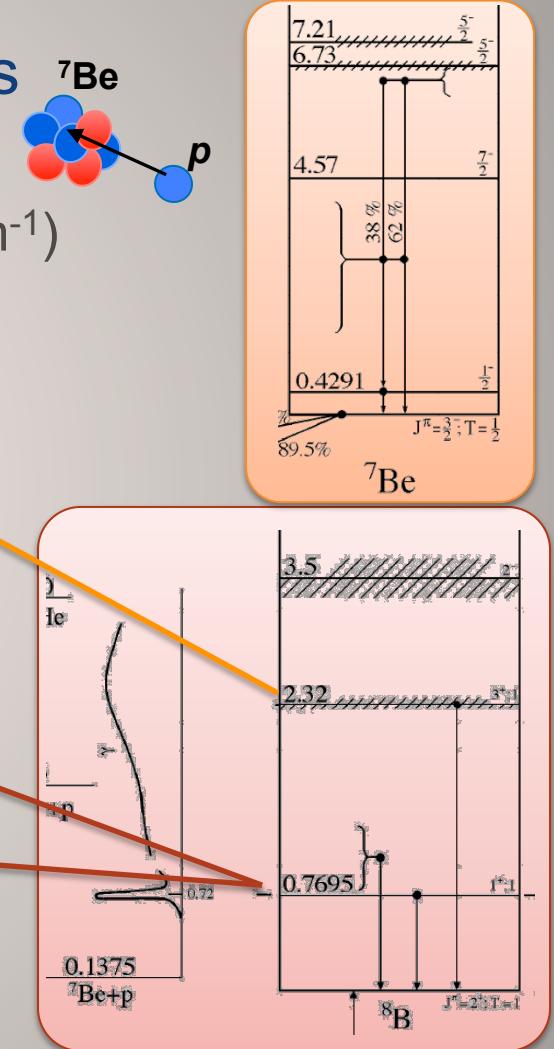
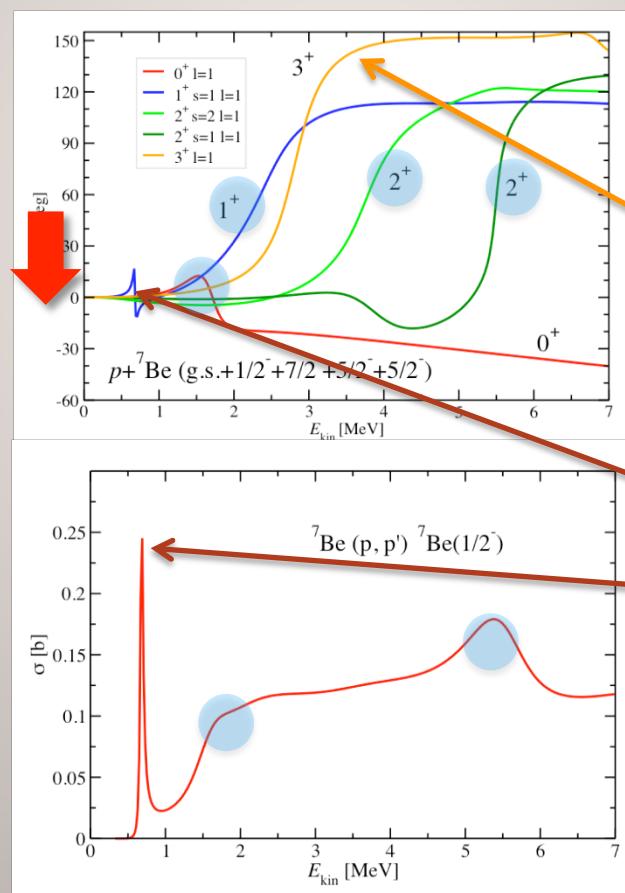
$p\text{-}{}^7\text{Be}$ scattering: Impact of $5/2^-$ states

- NCSM/RGM coupled channel calculations
 - ${}^7\text{Be}$ states $3/2^-, 1/2^-, 7/2^-, 5/2_1^-, 5/2_2^-$
 - Soft NN potential (SRG-N³LO with $\Lambda = 1.86 \text{ fm}^{-1}$)

${}^8\text{B}$ 2^+ g.s. bound by 135 keV
(expt. bound by 137 keV)

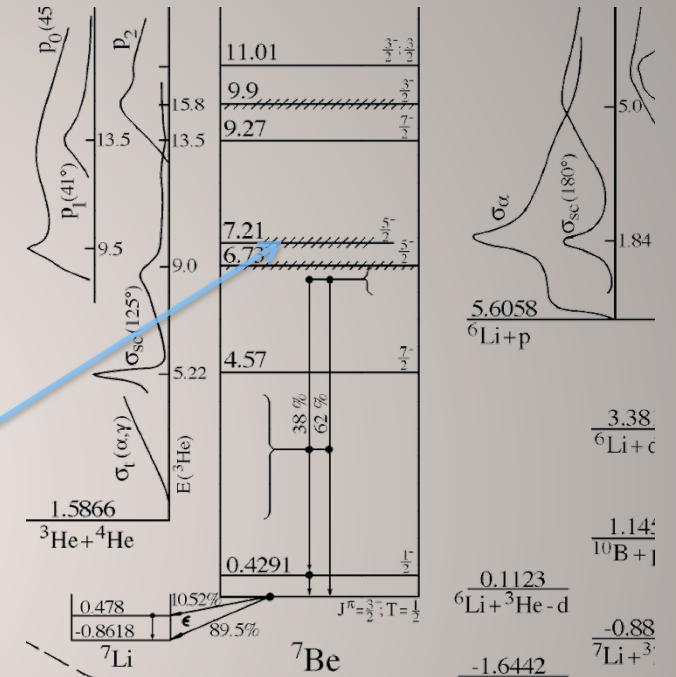
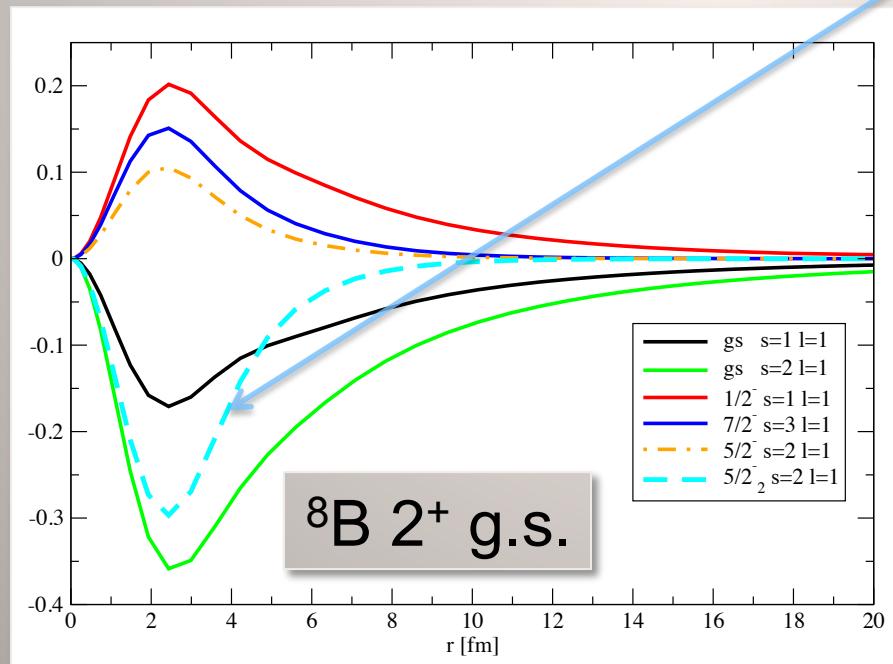
New $0^+, 1^+, \text{two } 2^+$ resonances predicted

$s=1 \ l=1 \ 2^+$ clearly visible
in (p,p') cross sections



Impact of higher excited states of ${}^7\text{Be}$

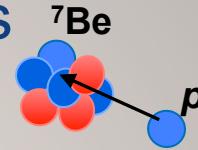
- NCSM/RGM p - ${}^7\text{Be}$ calculation with more excited states
 - $1/2^-$, $7/2^-$, $5/2_-^1$, $5/2_-^2$
- ${}^8\text{B}$ 2⁺ g.s.
 - Large P -wave $5/2_-^2$ component



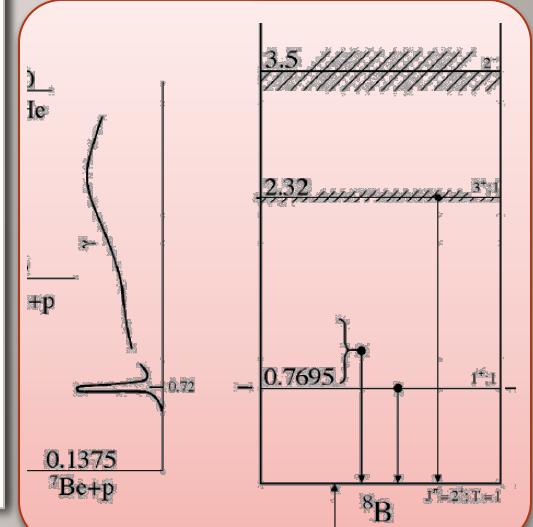
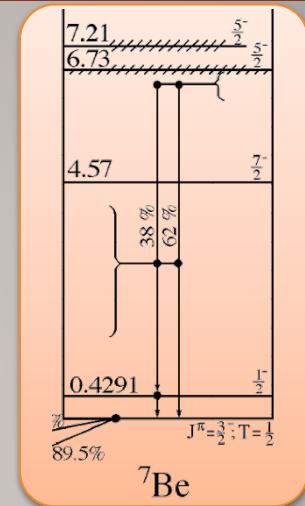
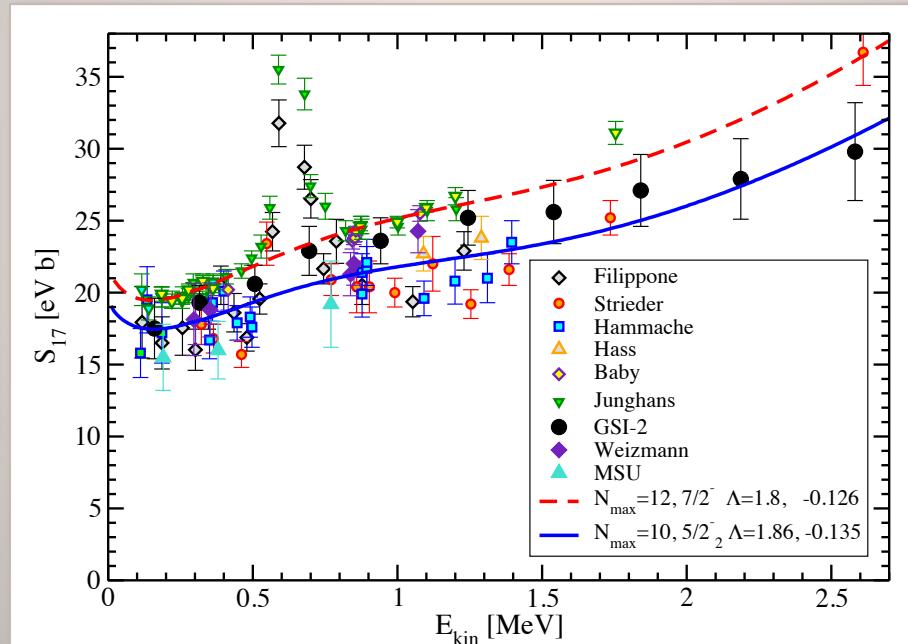
5/2₂⁻ state of ${}^7\text{Be}$
should be included
in ${}^7\text{Be}(p, \gamma){}^8\text{B}$
calculations

$^{7}\text{Be}(p,\gamma)^{8}\text{B}$: Impact of $5/2^{-}$ states

- NCSM/RGM coupled channel calculations
 - ^{7}Be states $3/2^{-}, 1/2^{-}, 7/2^{-}, 5/2_{-1}, 5/2_{-2}$
 - Soft NN potential (SRG-N³LO with $\Lambda = 1.86 \text{ fm}^{-1}$)



^{8}B 2^{+} g.s. bound by
 135 keV
 (expt. 137 keV)
 $S(0) \sim 20 \text{ eV b}$
 (preliminary)
 Data evaluation:
 $S(0)=20.8(2.1) \text{ eV b}$

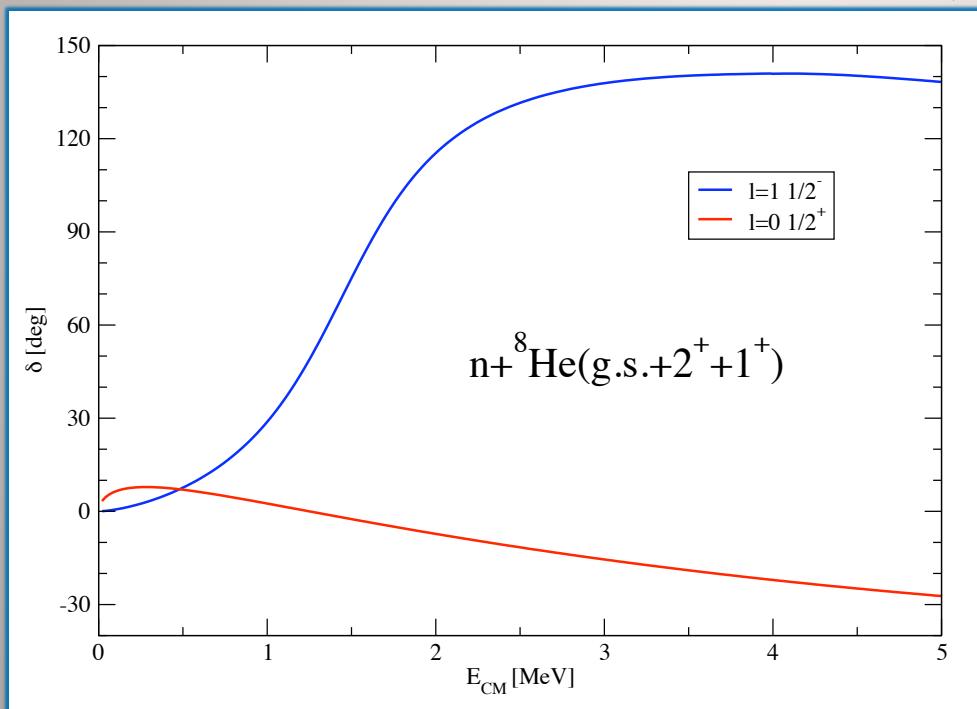
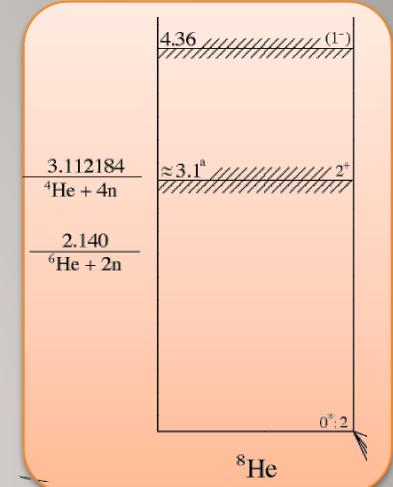


The $5/2_{-2}^{-}$ state improves $^{7}\text{Be}(p,\gamma)^{8}\text{B}$ S-factor energy dependence for $E > 0.4 \text{ MeV}$

Is ${}^9\text{He}$ bound? What is its ground state?

- NCSM/RGM calculation of $n+{}^8\text{He}$
 - SRG-N³LO NN potential with $\Lambda = 2.02 \text{ fm}^{-1}$
 - ${}^8\text{He}$ 0^+ g.s. and $2^+, 1^+$ excited states included
 - Up to $N_{\max} = 8$

exotic nuclei

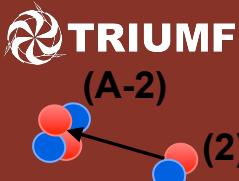


No bound state

P -wave resonance at $\sim 1.7 \text{ MeV}$
Expt. $\sim 1.27(10) \text{ MeV}$ (Bohlen *et al.*)

Weak attraction in the S -wave, $a_0 \sim -2 \text{ fm}$
Expt. $a_0 \sim -10 \text{ fm}$ (Chen *et al.*)
 $a_0 \sim -3 \text{ fm}$ (Al Falou, *et al.*)

Calculation suggests $1/2^+$ g.s.?
More ${}^8\text{He}$ excited states needed



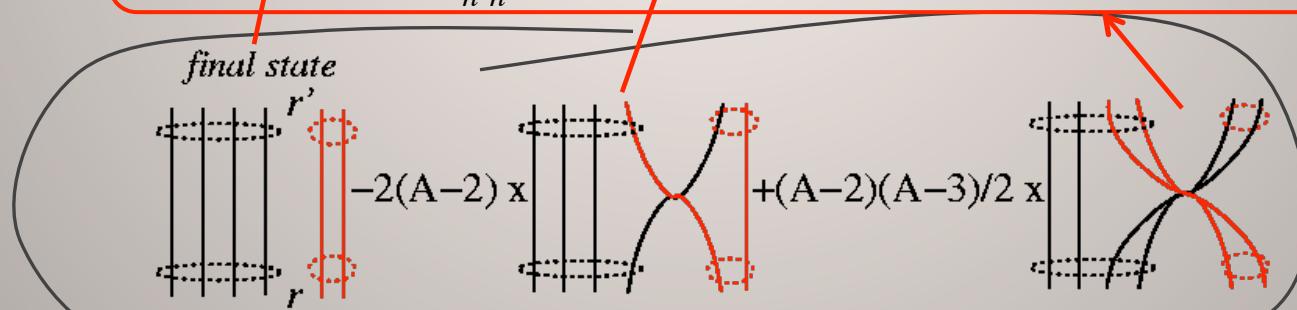
The deuteron-projectile formalism: norm kernel

$$\left\langle \begin{array}{c} (1,\dots,A-2) \\ \text{---} \\ \text{---} \end{array} r' \begin{array}{c} (A-1,A) \end{array} \right| 1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^A \hat{P}_{ij} + \sum_{i < j=1}^{A-2} \hat{P}_{i,A} \hat{P}_{j,A-1} \left| \begin{array}{c} (1,\dots,A-2) \\ \text{---} \\ \text{---} \end{array} r \begin{array}{c} (A-1,A) \end{array} \right\rangle$$

$$N_{\mu\ell', v\ell}^{(A-2,2)}(r', r) = \delta_{\mu\nu} \delta_{\ell'\ell} \frac{\delta(r' - r)}{r' r}$$

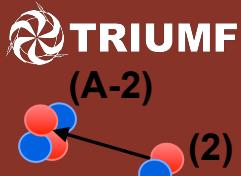
$$-2(A-2) \sum_{n'n} R_{n'\ell'}(r') \left\langle \Phi_{\mu n'\ell'}^{(A-2,2)JT} \middle| P_{A-2,A-1} \middle| \Phi_{vn\ell}^{(A-2,2)JT} \right\rangle R_{n\ell}(r)$$

$$+ \frac{(A-2)(A-3)}{2} \sum_{n'n} R_{n'\ell'}(r') \left\langle \Phi_{\mu n'\ell'}^{(A-2,2)JT} \middle| P_{A-2,A-1} P_{A-3,A} \middle| \Phi_{vn\ell}^{(A-2,2)JT} \right\rangle R_{n\ell}(r)$$

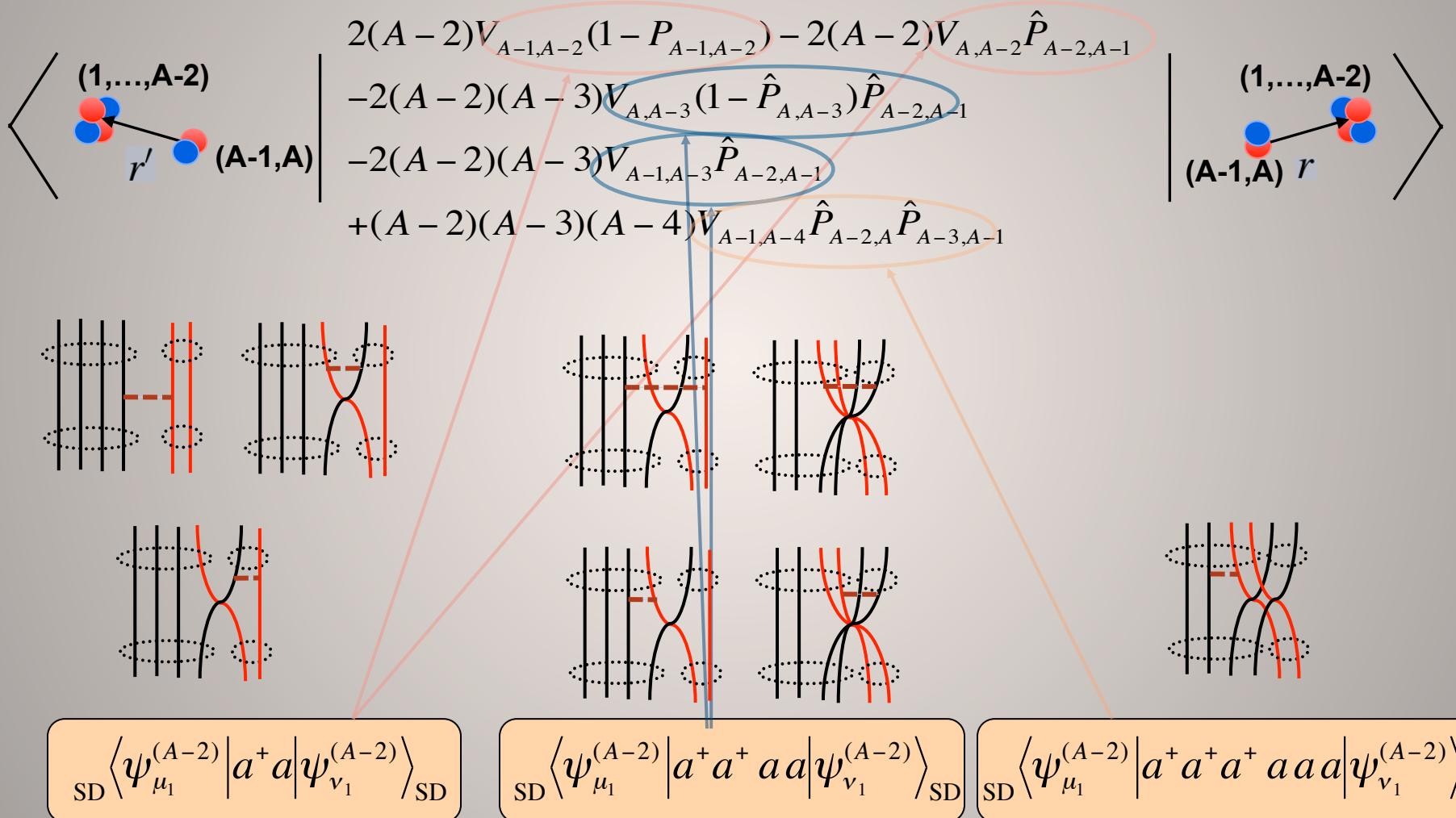


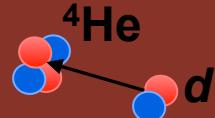
$$SD \left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a \middle| \psi_{v_1}^{(A-2)} \right\rangle_{SD}$$

$$SD \left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a^+ a a \middle| \psi_{v_1}^{(A-2)} \right\rangle_{SD}$$



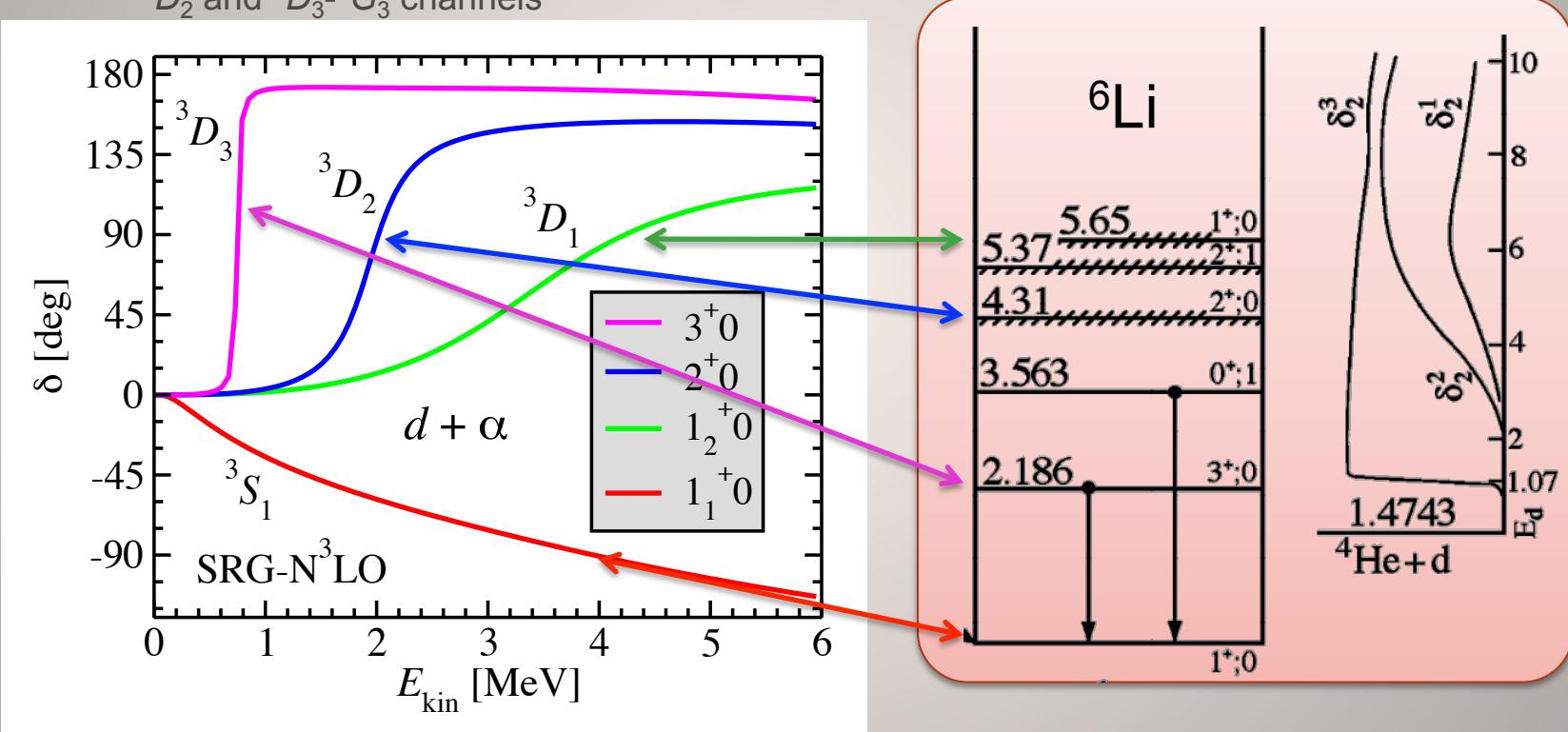
The deuteron projectile: Hamiltonian kernel



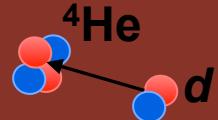


NCSM/RGM *ab initio* calculation of d - ${}^4\text{He}$ scattering

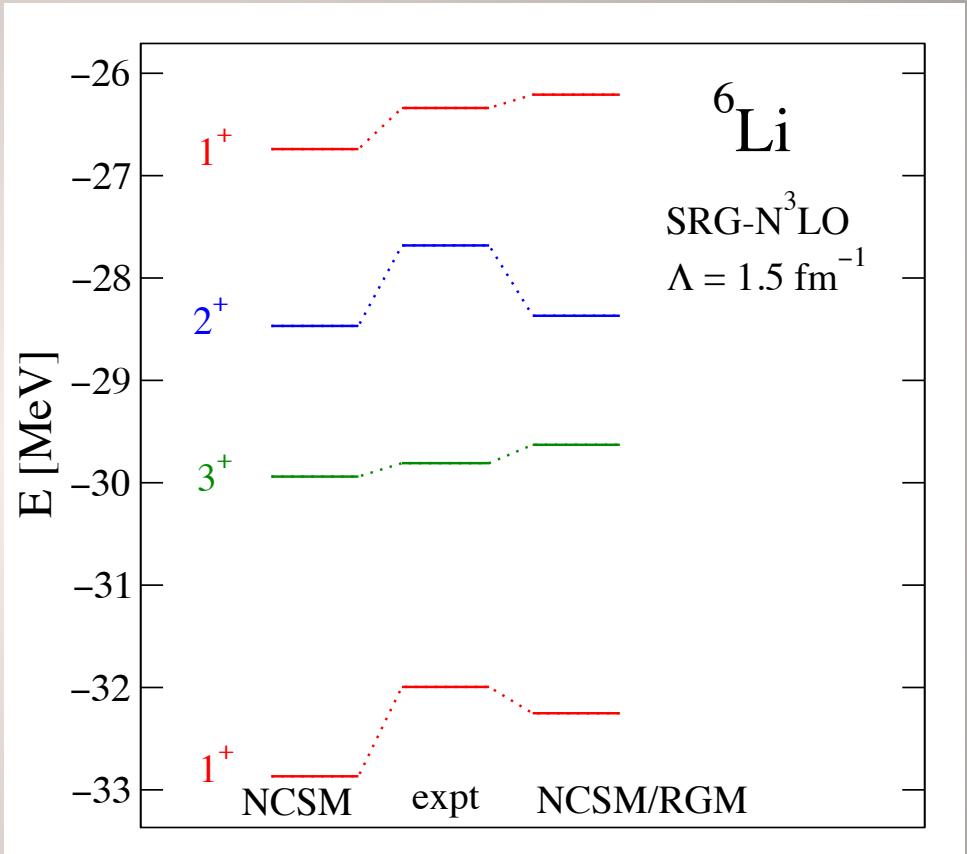
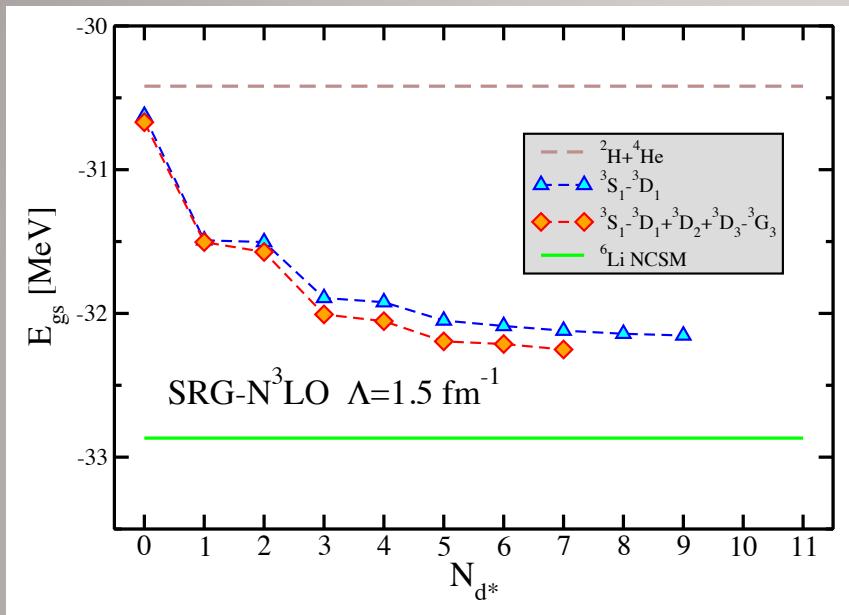
- NCSM/RGM calculation with $d + {}^4\text{He}(\text{g.s.})$ up to $N_{\text{max}} = 12$
 - SRG-N³LO potential with $\Lambda = 1.5 \text{ fm}^{-1}$
 - Deuteron breakup effects included by continuum discretized by pseudo states in 3S_1 - 3D_1 , 3D_2 and 3D_3 - 3G_3 channels



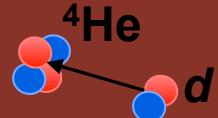
- The 1^+0 ground state bound by 1.9 MeV (expt. 1.47 MeV)
- Calculated T=0 resonances: 3^+ , 2^+ and 1^+ in correct order close to expt. energies



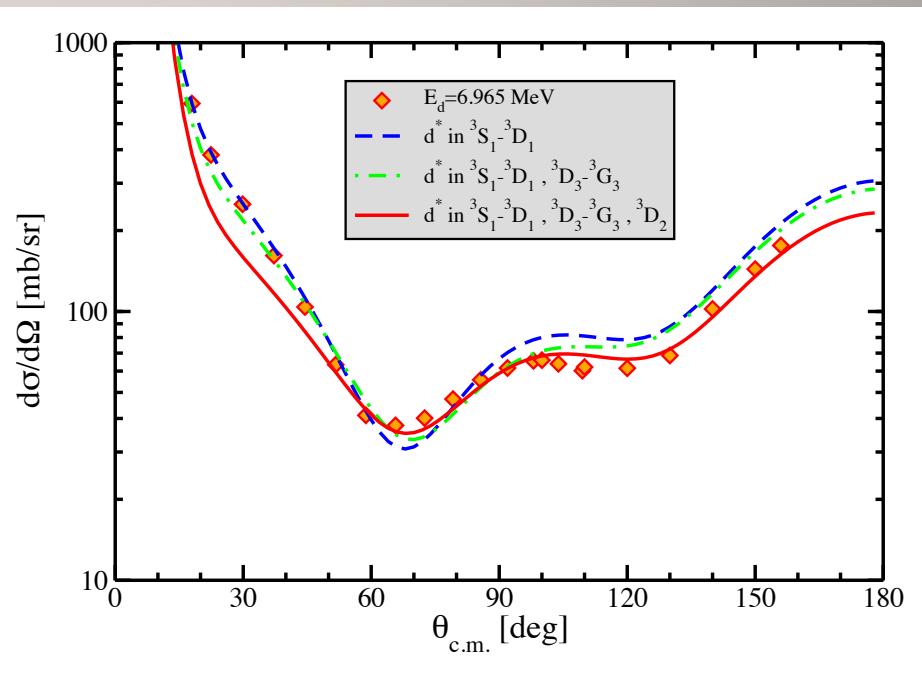
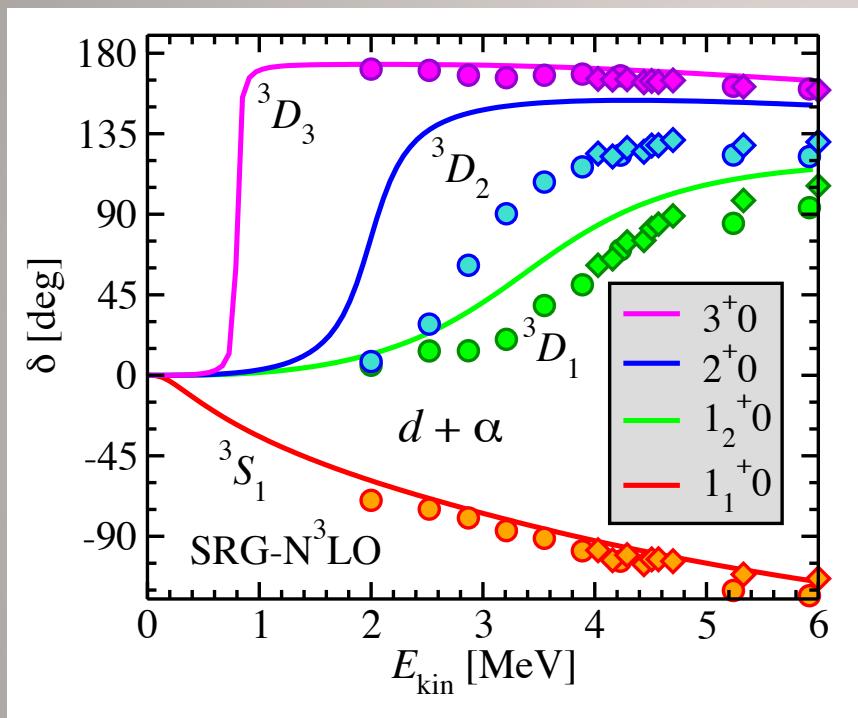
NCSM/RGM *ab initio* calculation of $d\text{-}{}^4\text{He}$ scattering



- The deuteron polarization and virtual break up must be taken into account
- NCSM/RGM calculates bound states as well as excited states...

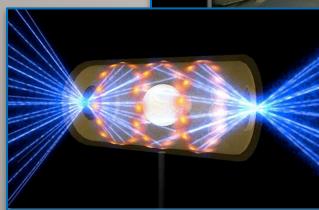
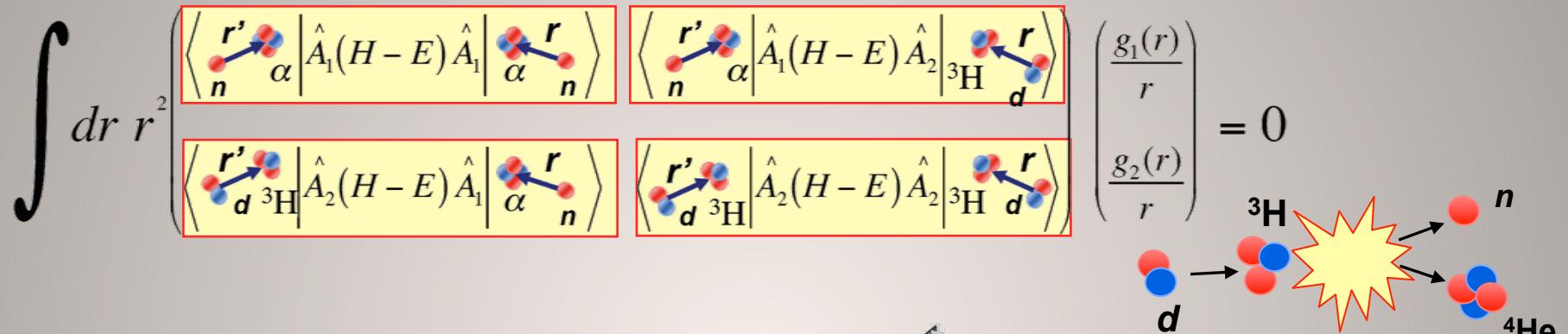
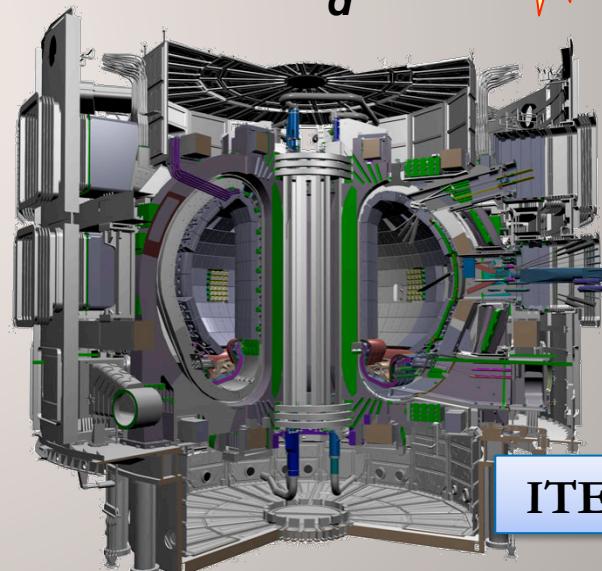


NCSM/RGM *ab initio* calculation of d - ${}^4\text{He}$ scattering

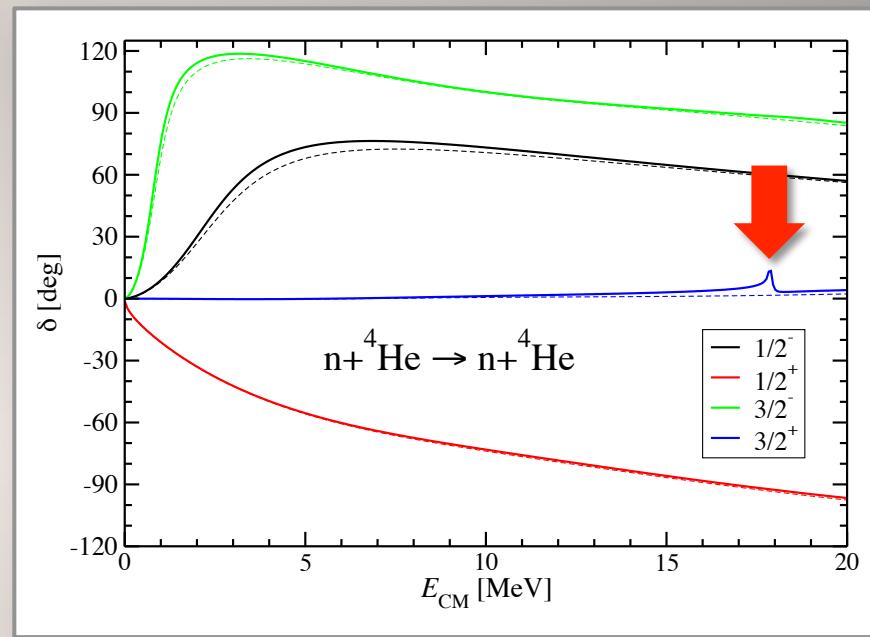
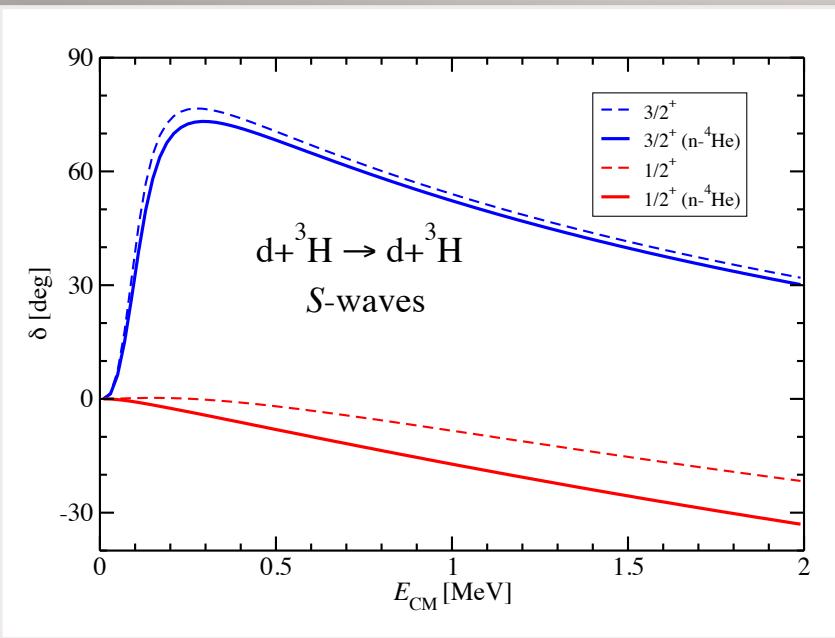


- NCSM/RGM a superior theory: Bound states, resonances, scattering
- NCSM efficiently accounts for many-nucleon correlations: **Coupling of the NCSM and the NCSM/RGM basis desirable**
- Scattering provides a strict test of NN and NNN forces

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


NIF
energy generation

ITER

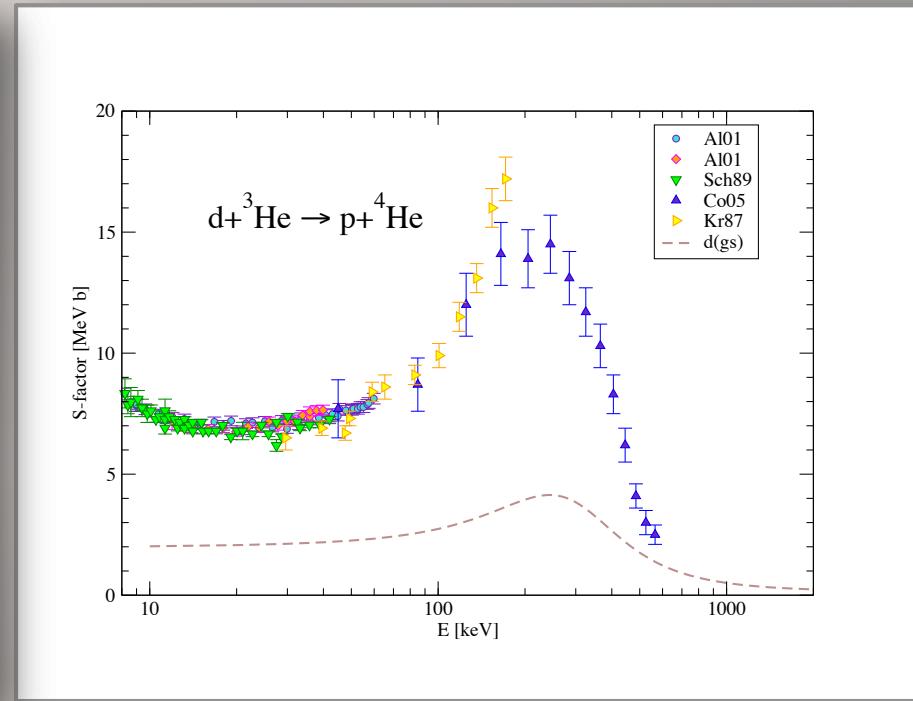
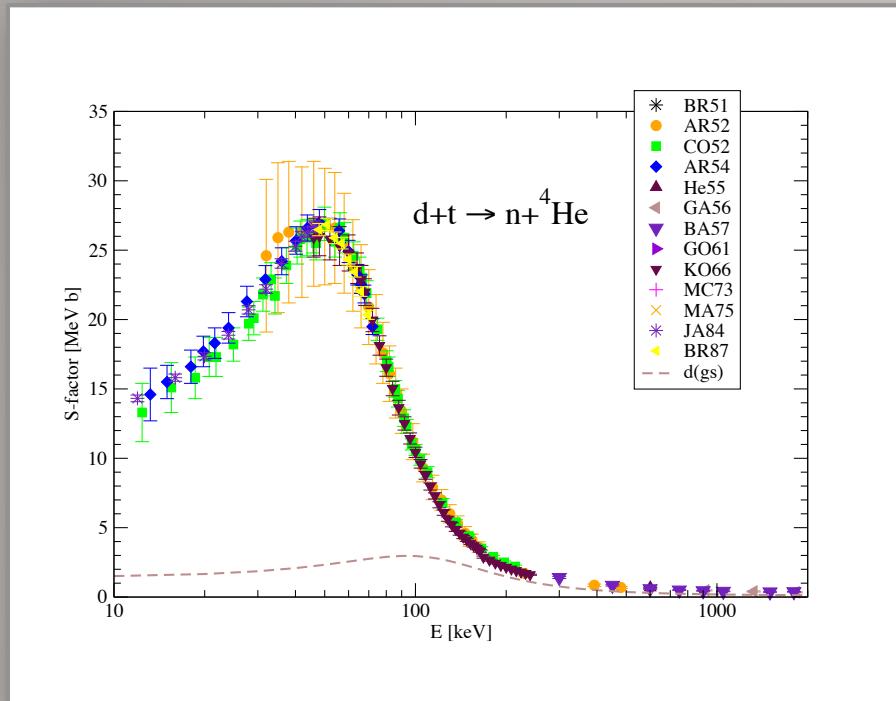
$d+^3\text{H}$ and $n+^4\text{He}$ elastic scattering: phase shifts



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

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

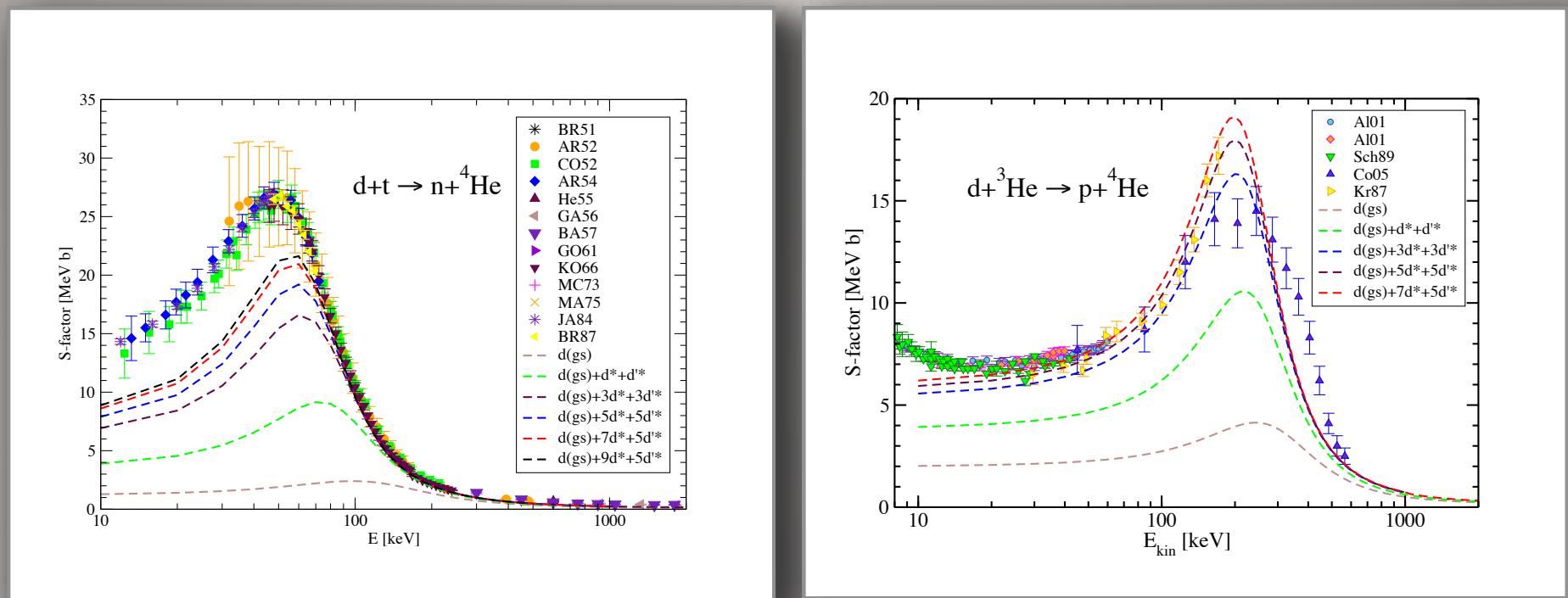
$^3\text{H}(d,n)^4\text{He}$ and $^3\text{He}(d,p)^4\text{He}$ cross sections



- The first results, still preliminary:
 - $N_{\max} = 13$
 - SRG-N³LO NN ($\Lambda = 1.5 \text{ fm}^{-1}$) potential
 - NNN interaction interaction effects for $A=3,4,5$ partly included by the choice of Λ
 - Only **g.s.** of d , ^3H , ^4He included above

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

$^3\text{H}(d,n)^4\text{He}$ and $^3\text{He}(d,p)^4\text{He}$ 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 - ^3He fusion:

Very promising, correct physics, can become competitive with fitted evaluations ...

Conclusions and Outlook

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
- The first ${}^7\text{Be}(p,\gamma){}^8\text{B}$ *ab initio* S-factor calculation
 - Both the bound and the scattering states from first principles
 - No fit
 - SRG-N³LO *NN* potential selected to match closely the experimental threshold ($\Lambda \approx 1.8 \sim 2 \text{ fm}^{-1}$)
 - Prediction of new ${}^8\text{B}$ resonances
- New results with SRG-N³LO *NN* potentials:
 - Initial results for ${}^3\text{H}(d,n){}^4\text{He}$ & ${}^3\text{He}(d,p){}^4\text{He}$ fusion and d - ${}^4\text{He}$ scattering
 - First steps towards ${}^3\text{He}+{}^4\text{He}$ scattering
 - Wataru Horiuchi
- To do:
 - Inclusion of **NNN** force
 - Alpha clustering: ${}^4\text{He}$ projectile
 - NCSM with continuum (**NCSMC**)
 - Three-cluster NCSM/RGM and treatment of three-body continuum

(A)  $(A-a)$ 

$$\left| \Psi_A^J \right\rangle = \sum c_\lambda |A\lambda J\rangle + \sum \int d\vec{r} \varphi_v(\vec{r}) \hat{\mathcal{A}} \Phi_{v\vec{r}}^{(A-a,a)}$$

\rightarrow

$$\begin{pmatrix} H & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix} = E \begin{pmatrix} 1 & g \\ g & \mathcal{N} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix}$$

Collaborators

Sofia Quaglioni (LLNL)

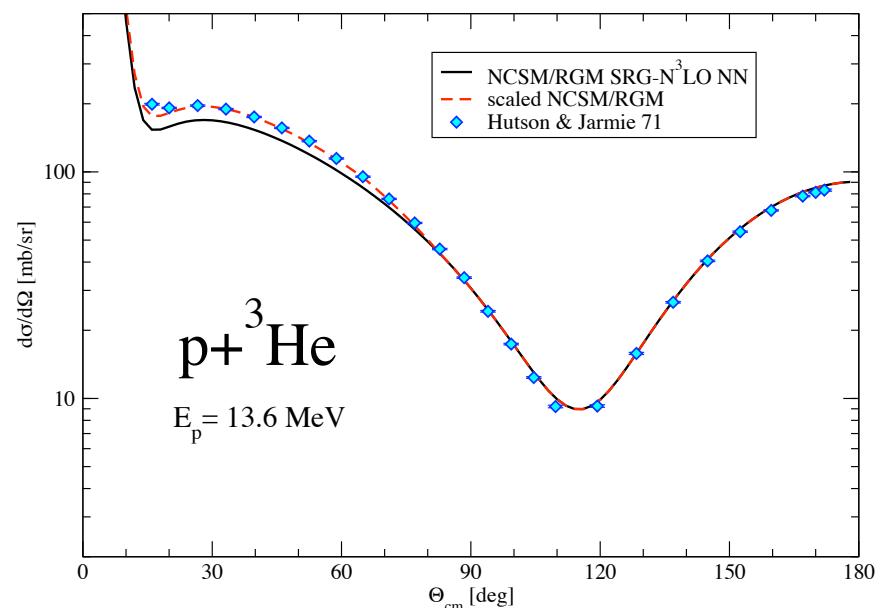
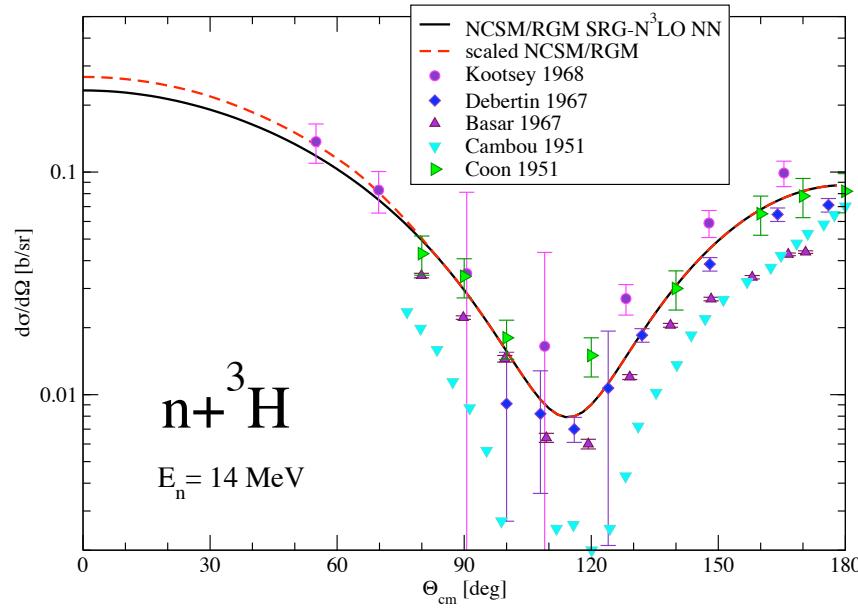
Robert Roth (TU Darmstadt)

E. Jurgenson (LLNL), Dick Furnstahl (OSU)

**V. Gueorguiev (UC Merced), J. P. Vary (ISU),
W. E. Ormand (LLNL), A. Nogga (Julich)**

Connection to the real world: neutron-triton elastic scattering at 14 MeV

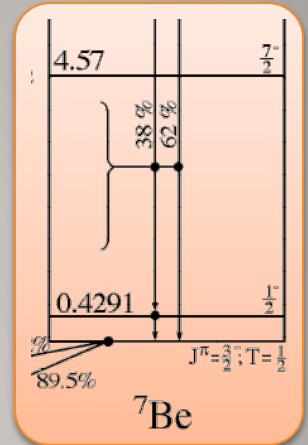
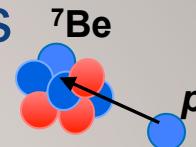
- Important for the National Ignition Facility physics
 - deuteron-triton fusion generates 14 MeV neutrons
- Experimental situation confusing
- Good data for $p+^3\text{He}$ elastic scattering



Use NCSM/RGM calculation to relate the two reactions and predict $n+{}^3\text{H}$ cross section

$p\text{-}{}^7\text{Be}$ scattering

- NCSM/RGM coupled channel calculations
 - ${}^7\text{Be}$ states $3/2^-$, $1/2^-$, $7/2^-$
 - Soft NN potential (SRG-N³LO with $\Lambda = 1.8 \text{ fm}^{-1}$)

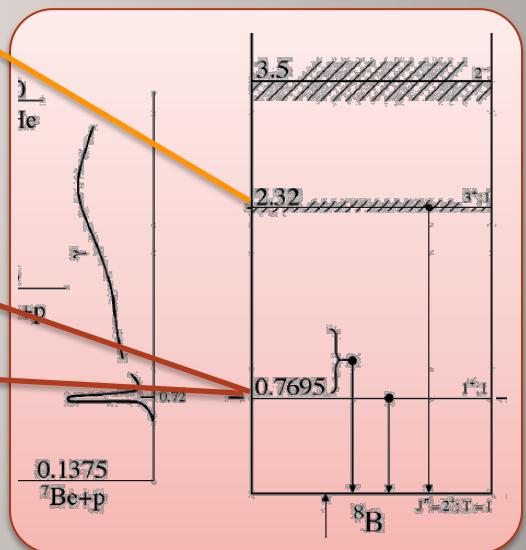
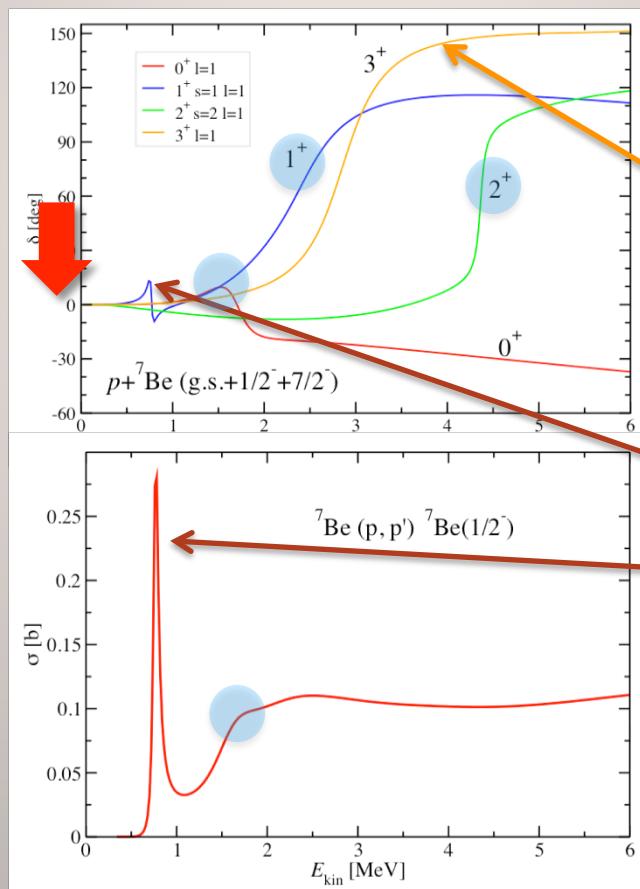


${}^8\text{B}$ 2^+ g.s. bound by 126 keV
(expt. bound by 137 keV)

New 0^+ , 1^+ , 2^+ resonances predicted

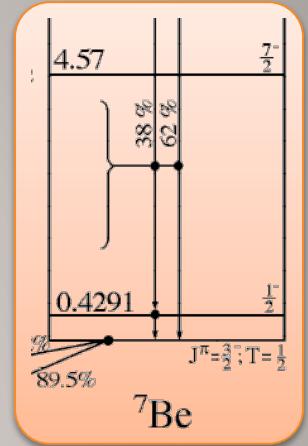
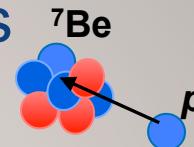
Scattering length:
Expt: $a_{02} = -7(3) \text{ fm}$
Calc: $a_{02} = -10.2 \text{ fm}$
($\Lambda = 2.02 \text{ fm}^{-1}$)

P. N., R. Roth, S. Quaglioni,
PRC **82**, 034609 (2010)

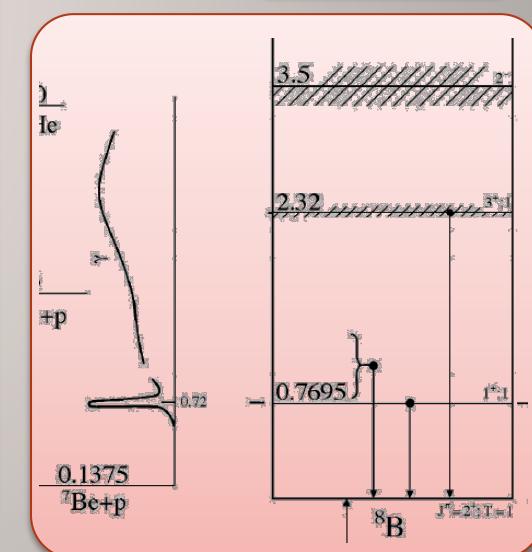
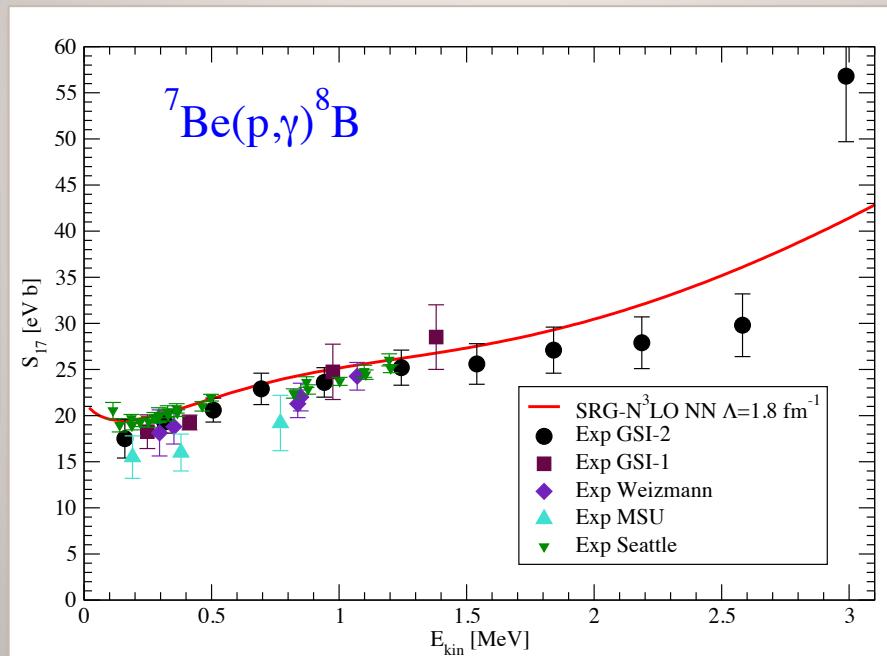


$^7\text{Be}(p,\gamma)^8\text{B}$ radiative capture S-factor

- NCSM/RGM coupled channel calculations
 - ^7Be states $3/2^-$, $1/2^-$, $7/2^-$
 - Soft NN potential (SRG-N³LO with $\Lambda = 1.8 \text{ fm}^{-1}$)

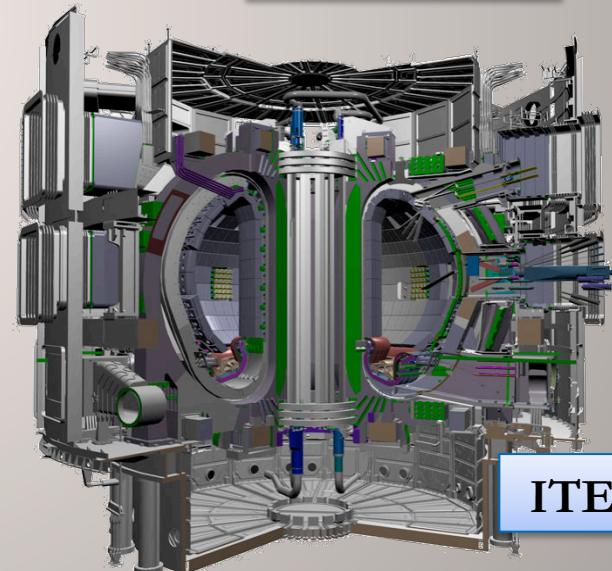
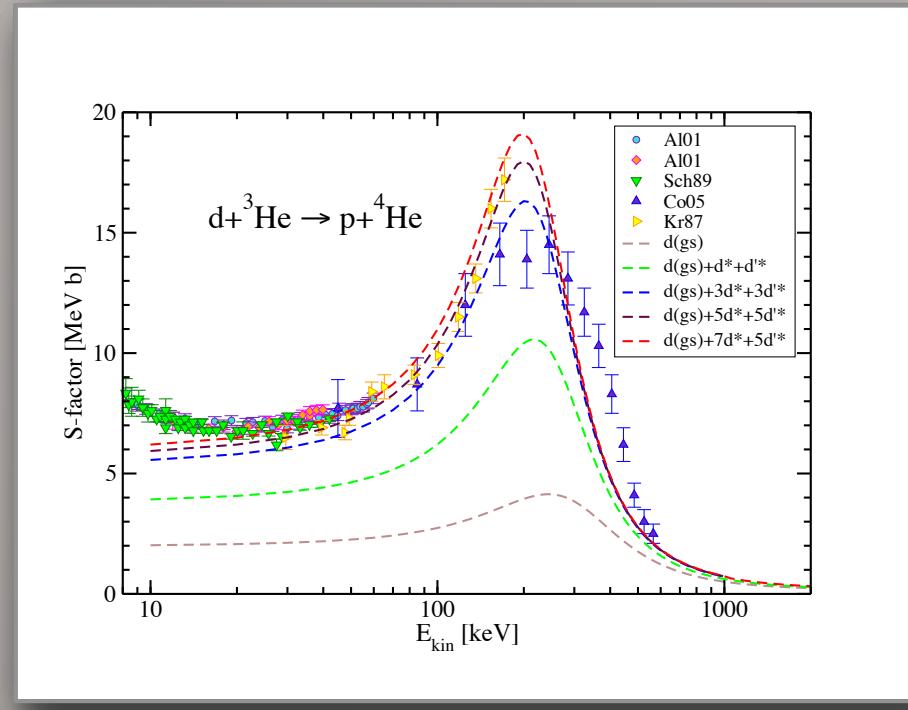
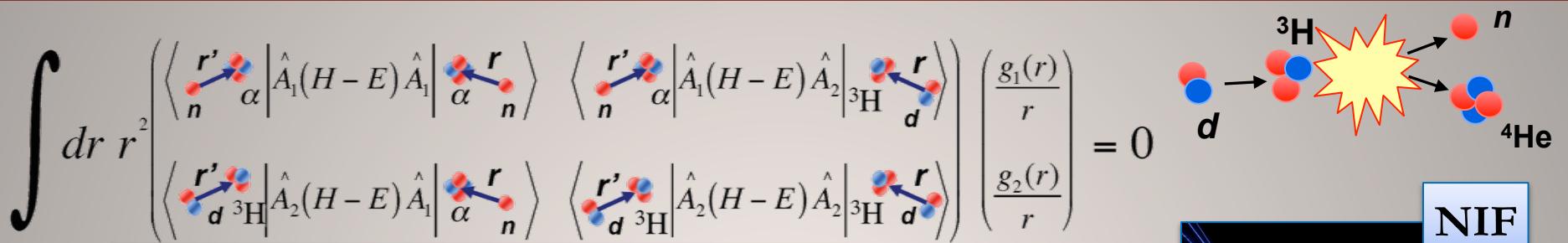


${}^8\text{B}$ 2⁺ g.s. bound by
126 keV
(expt. 137 keV)
 $S(0) \sim 21.5 \text{ eV b}$



The first ever *ab initio* calculations of ${}^7\text{Be}(p, \gamma){}^8\text{B}$ (still preliminary)

Toward the first *ab initio* calculation of the Deuterium-Tritium and $d\text{-}{}^3\text{He}$ fusion



Predictive theory useful
 Low energy: Electron screening problem. Resonance energy: Shape of the peak

P. Navratil et al.,
 arXiv:1009.3965