Ab initio reaction theory for light nuclei

7th ANL/INT/JINA/MSU annual FRIB workshop

INT Program INT-11-2d: Interfaces between structure and reactions for rare isotopes and nuclear astrophysics

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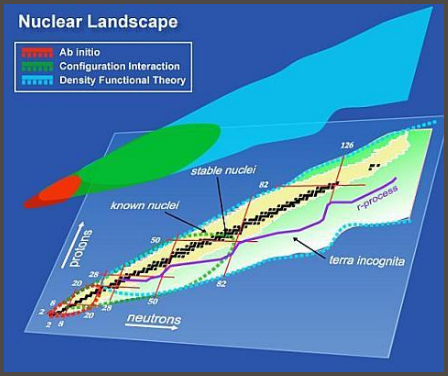
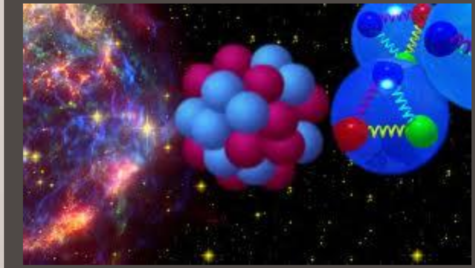
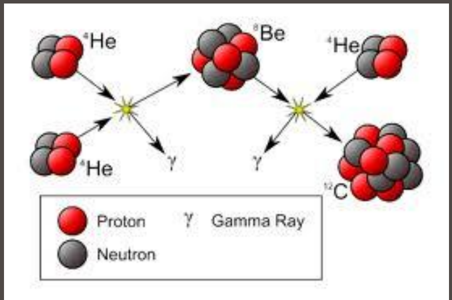
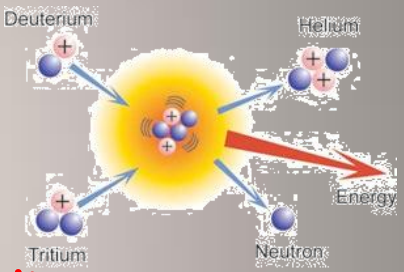






Light nuclei from first principles

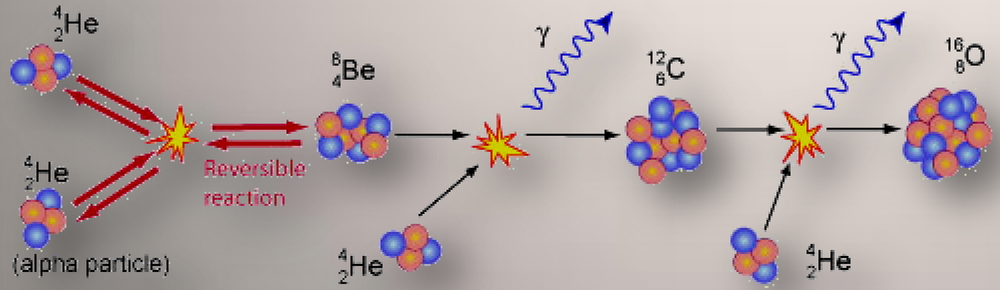
- **Goal**: Predictive theory of structure and reactions of light nuclei
- Needed for
  - Physics of exotic nuclei, tests of fundamental symmetries
  - **Understanding of nuclear reactions important for astrophysics**
  - Understanding of reactions important for energy generation

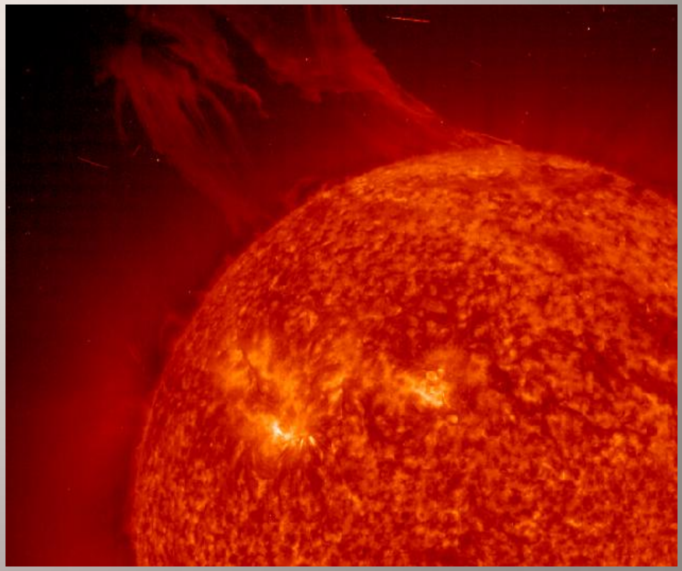


- **From first principles or *ab initio:***

✓ 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



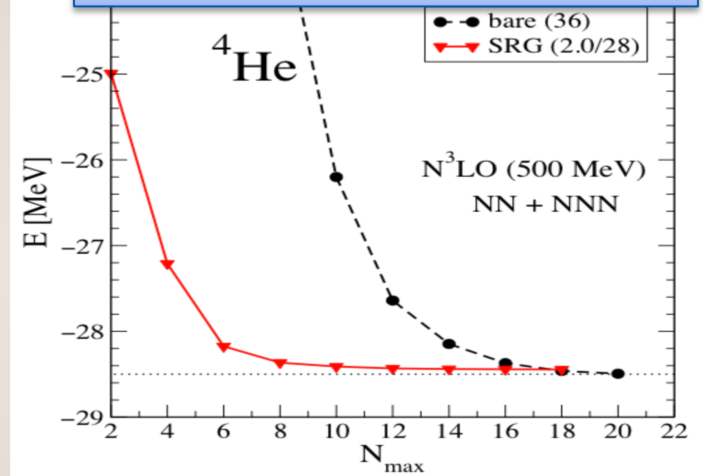


Our many-body technique:

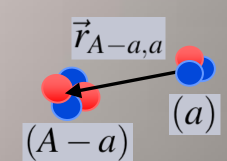
- **Combine** the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)

- **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

E. Jurgenson *et al.*, PRL 103, 082501 (2009)



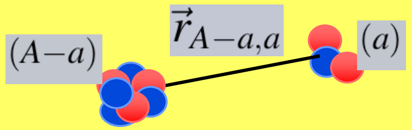
- **The RGM:** A microscopic approach to the A-nucleon scattering of clusters
  - Nuclear Hamiltonian may be simplistic
  - Cluster wave functions may be simplified and inconsistent with the nuclear Hamiltonian
  - Long range correlations, relative motion of clusters



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



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

eigenstates of $H_{(A\text{-}a)}$ 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

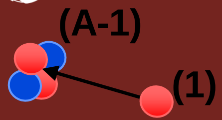
$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

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

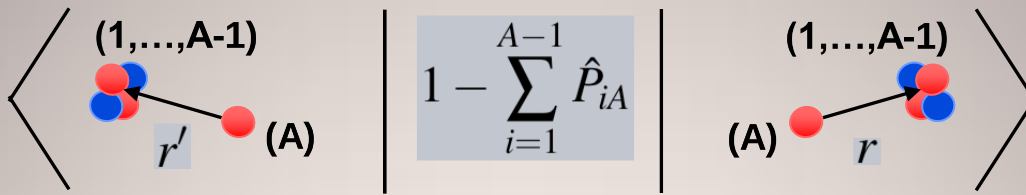
Hamiltonian kernel

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

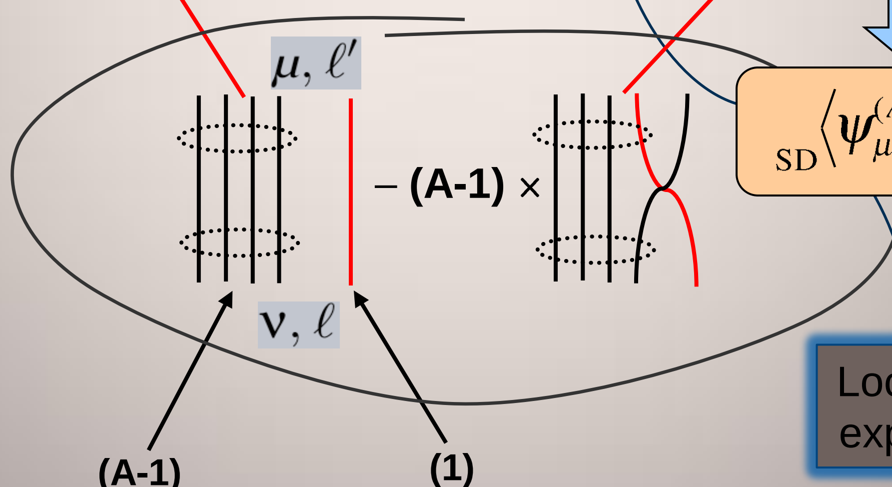
Norm kernel



Single-nucleon projectile: the norm kernel



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



$${}_{SD}\left\langle\psi^{(A-1)}_{\mu_1}\middle|a^+a\middle|\psi^{(A-1)}_{\nu_1}\right\rangle_{SD}$$

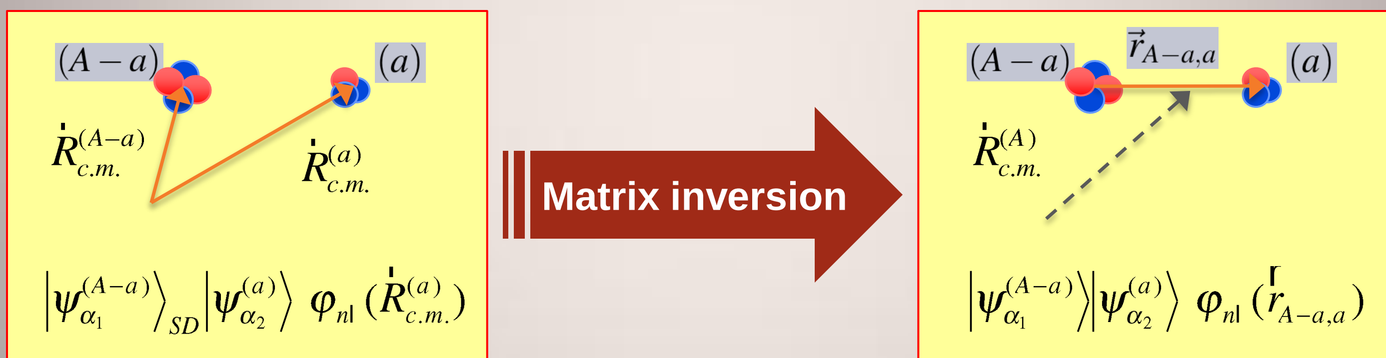
Localized parts of kernels expanded in the HO basis

Matrix elements of translationally invariant operators

- Translational invariance is preserved (exactly!) also with SD cluster basis

$$ {}_{SD}\left\langle \Phi^{(A-a',a')}_{f_{SD}} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{i_{SD}} \right\rangle_{SD} = \sum_{i_R f_R} M_{i_{SD} f_{SD}, i_R f_R} \left\langle \Phi^{(A-a',a')}_{f_R} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{i_R} \right\rangle $$

Calculate these **Interested in these**



- Advantage: can use powerful second quantization techniques

$$ {}_{SD}\left\langle \Phi^{(A-a',a')}_{\nu' n'} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{\nu n} \right\rangle_{SD} \propto {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \; {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a^+ a a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \ldots $$

Solving the RGM equations

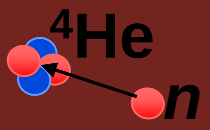
- The many-body problem has been reduced to a two-body problem!
  - Macroscopic degrees of freedom: nucleon clusters
  - Unknowns: relative wave function between the two clusters
- Non-local integral-differential coupled-channel equations:

$$\left[T_{rel}(r)+V_C(r)+E_{\alpha_1}^{(A-a)}+E_{\alpha_2}^{(a)}\right]u_\nu^{(A-a,a)}(r)+\sum_{a'\nu'}\int dr'r'\,W_{a\nu,a'\nu'}(r,r')u_{\nu'}^{(A-a',a')}(r')=0$$

- Solve with R-matrix theory on Lagrange mesh imposing
  - Bound state boundary conditions ➔ eigenenergy + eigenfunction
  - Scattering state boundary conditions ➔ Scattering matrix
    - Phase shifts
    - Cross sections
    - …

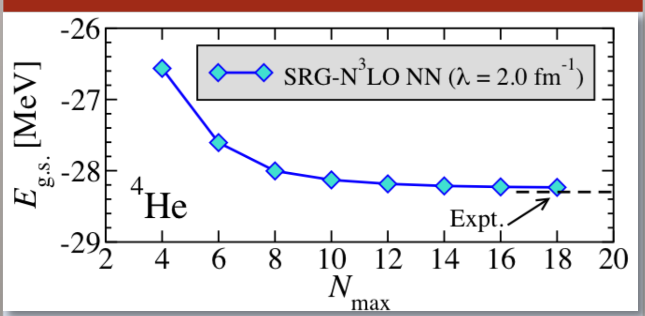
The R-matrix theory on Lagrange mesh is an elegant and powerful technique, particularly for calculations with non-local potentials

Convergence with respect to HO basis expansion

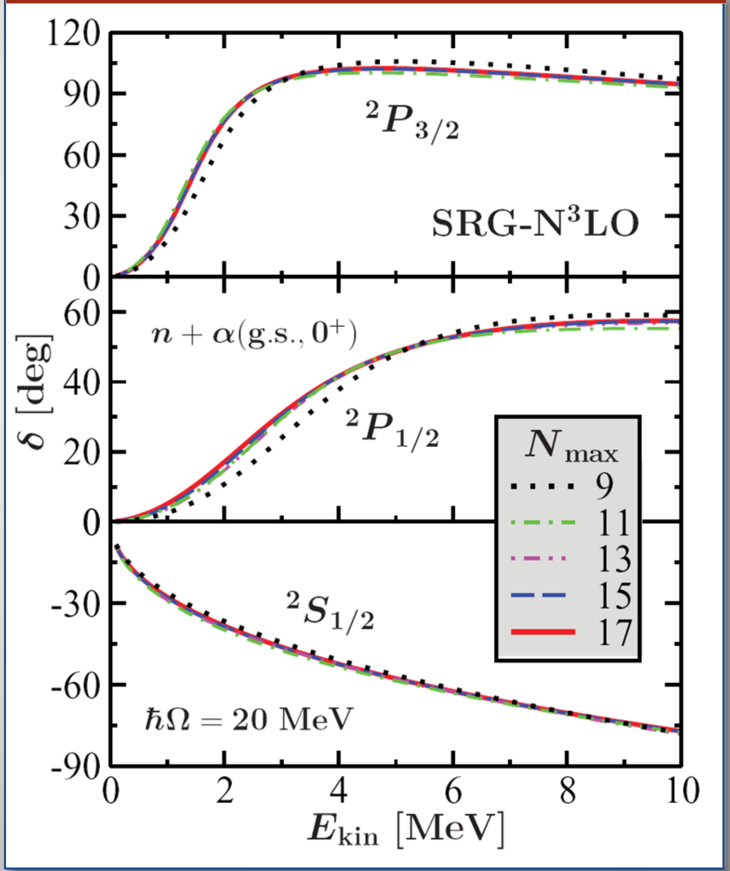


- Influenced by:
  1) Convergence of target and projectile wave functions
  2) Convergence of localized parts of the integration kernels
- Here:
  – n + 4He(g.s.,0$^+$) phase shifts
  – SRG-N^{3}LO NN potential (λ = 2 fm^{-1})

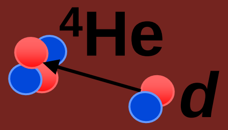
^{4}He ground-state energy



^{4}He(n,n)^{4}He phase shifts



Convergence with respect to RGM model space



- NCSM/RGM describes binary reactions (below three-body breakup threshold)
- If projectile (or target) can be easily deformed or broken apart
  - Need to account for virtual breakup
  - Approximate treatment:

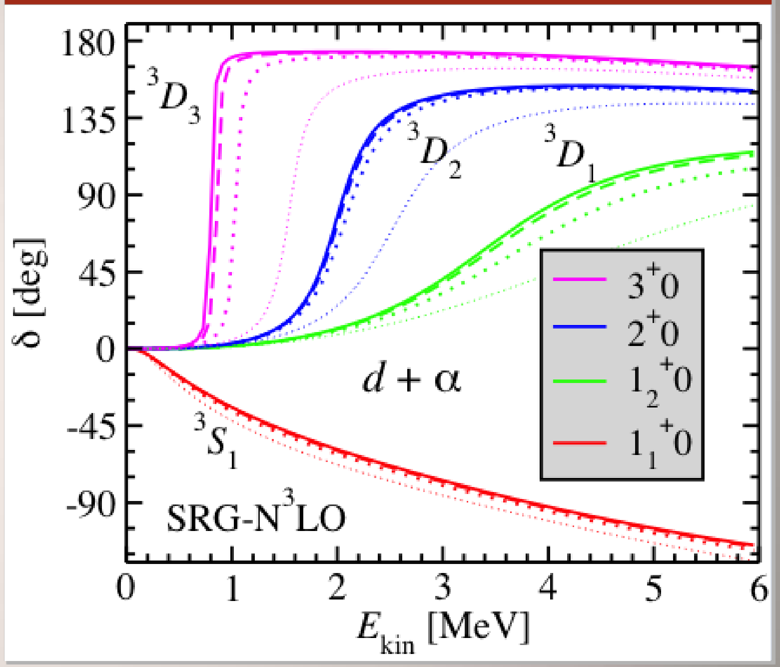
    Include multiple excited (pseudo-) states of the clusters
  - Exact treatment:

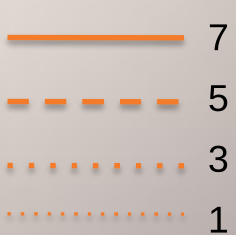
    1) Inclusion of three-body clusters

    2) Solution of three-body scattering

- Here:
  - d(g.s., ${}^3S_1$-${}^3D_1$, ${}^3D_2$, ${}^3D_3$-${}^3G_3$) + ^{4}He(g.s.)
  - SRG-N^{3}LO NN potential (λ = 1.5 fm^{-1})

^{4}He(d,d)^{4}He phase shifts

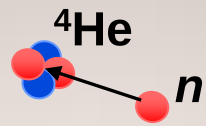


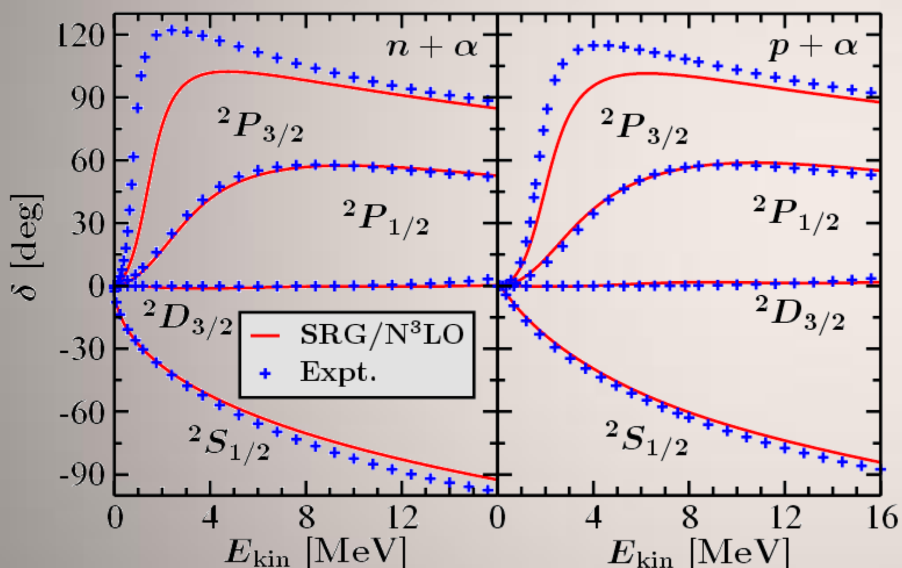


Pseudo-states in each channel

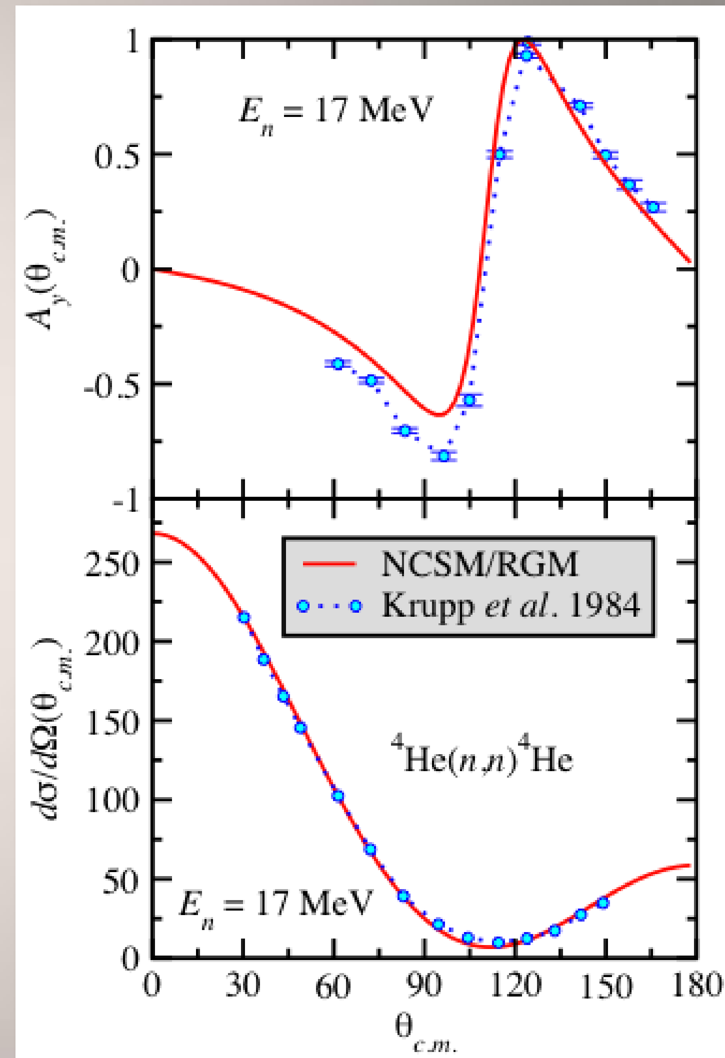
The best system to start with: $n+^4He$, $p+^4He$

- NCSM/RGM calculations with
  - $N + ^4He(g.s., 0^+0)$
  - 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

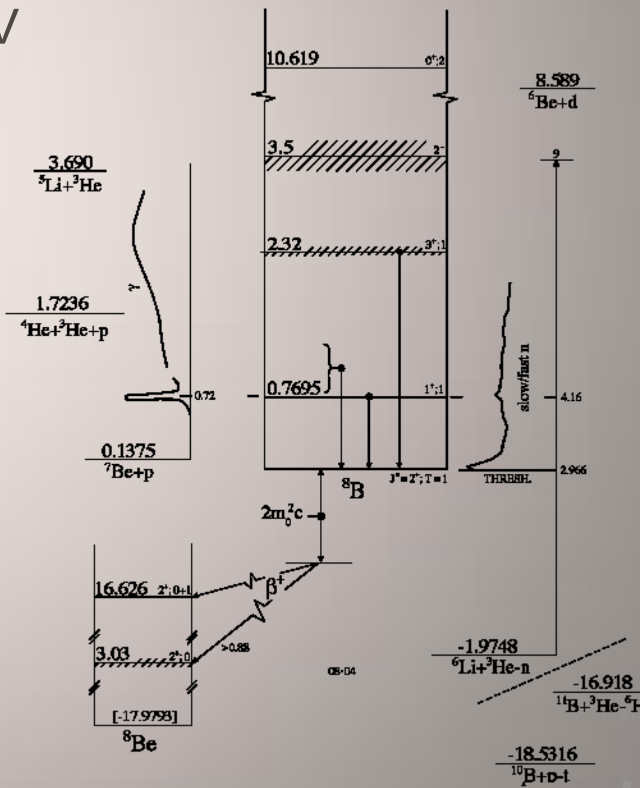
^{7}Be(p,γ)^{8}B S-factor

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

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

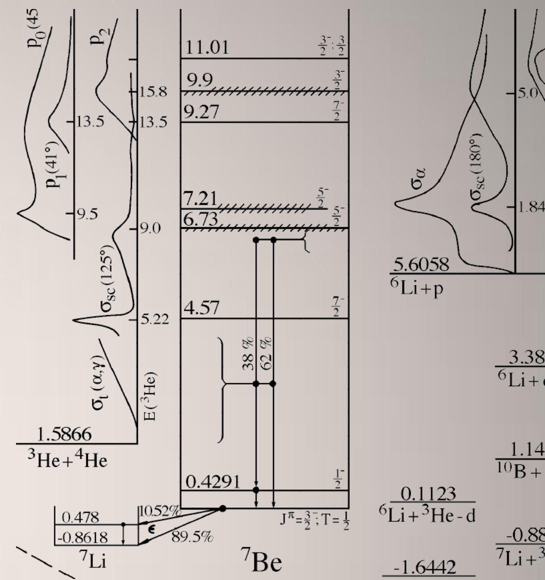
$$\eta(E) = Z_{A-a}Z_a e^2/\hbar v_{A-a,a}$$

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

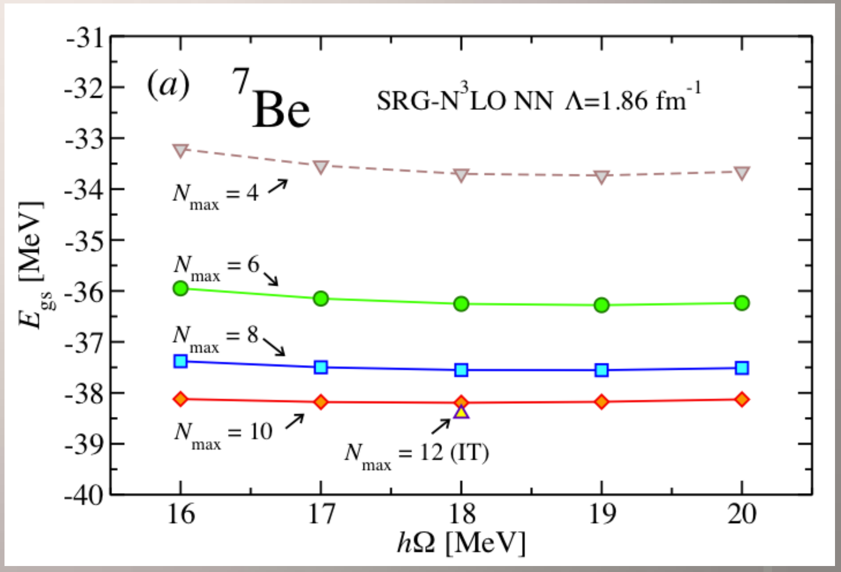


Input: *NN* interaction, ^{7}Be eigenstates

- Similarity-Renormalization-Group (SRG) evolved chiral N^{3}LO *NN* interaction
    - Accurate
    - Soft: Evolution parameter Λ
        - Study dependence on Λ

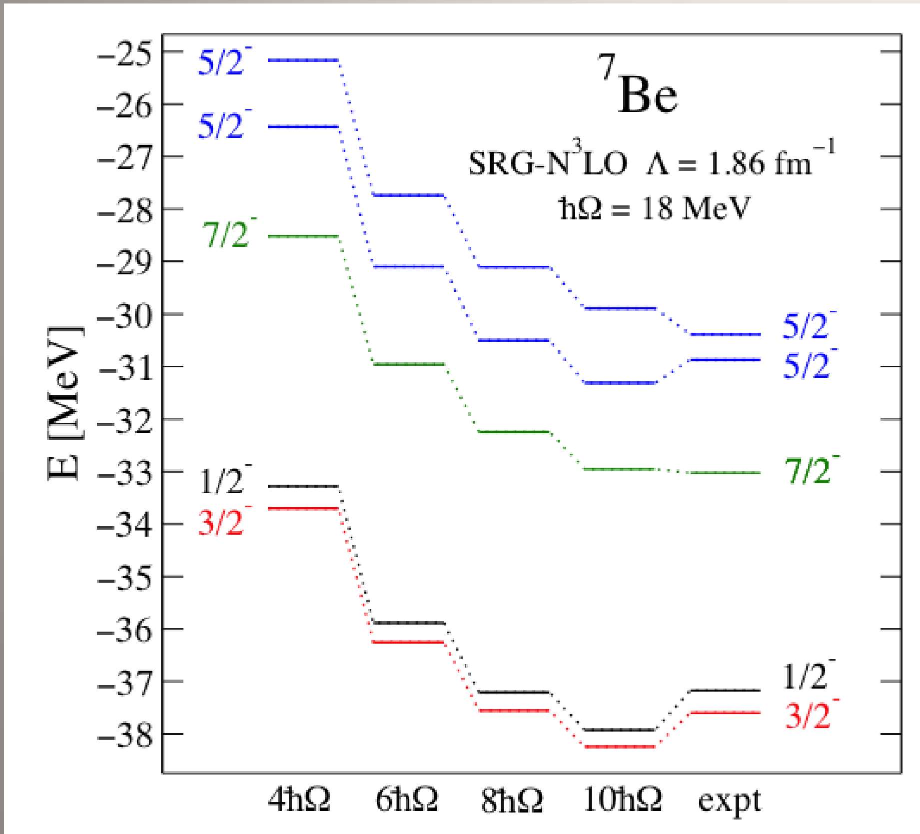


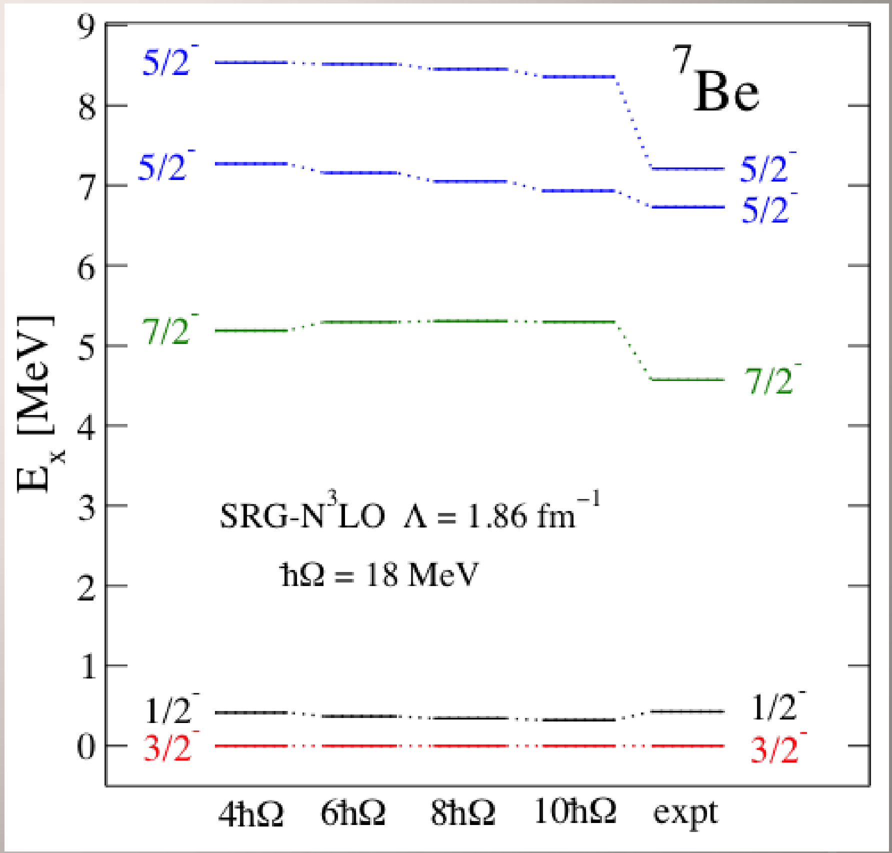
- ^{7}Be
    - NCSM up to N_{max}=10, Importance Truncated NCSM up to N_{max}=14
    - Variational calculation
        - optimal HO frequency from the ground-state minimum
        - For the selected NN potential with Λ=1.86 fm^{-1}: hΩ=18 MeV



Input: ^{7}Be eigenstates

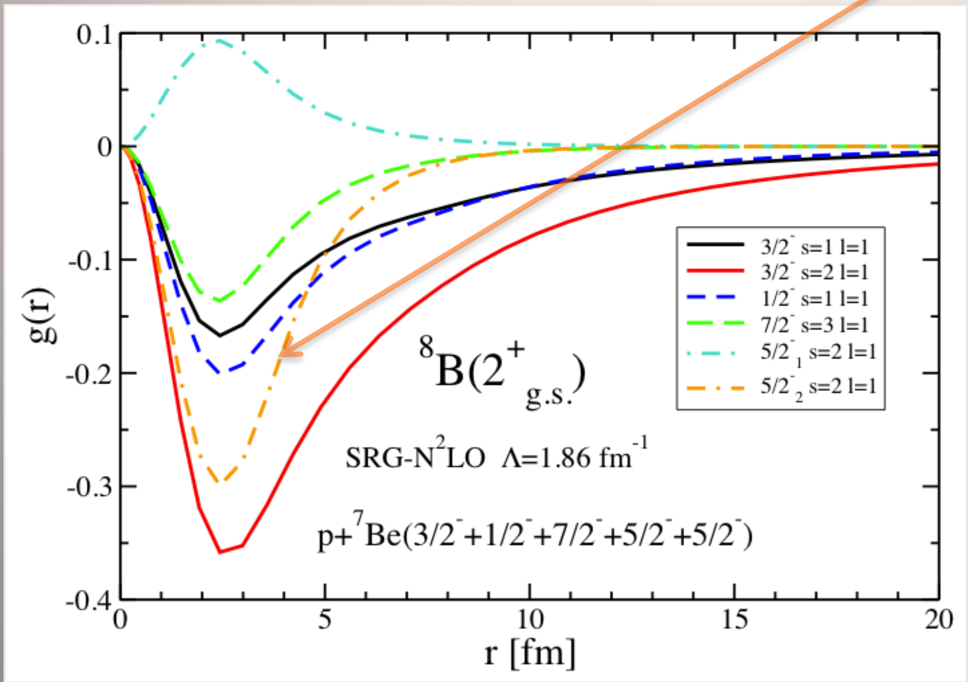
- Ground- and excited states at the optimal HO frequency, ħΩ=18 MeV

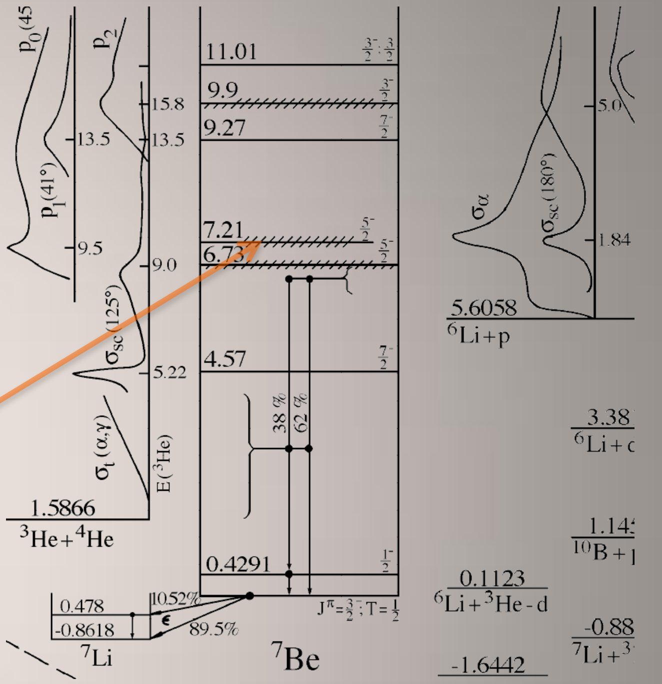




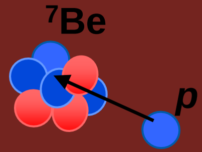
Structure of the ^{8}B ground state

- NCSM/RGM *p*-^{7}Be calculation
  - five lowest ^{7}Be states: $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN SRG-N^{3}LO with Λ = 1.86 fm^{-1}
- ^{8}B 2^+ g.s. bound by 136 keV (Expt 137 keV)
  - Large *P*-wave $5/2^-_2$ component





$5/2^-_2$ state of ^{7}Be should be included in ^{7}Be(p,γ)^{8}B calculations



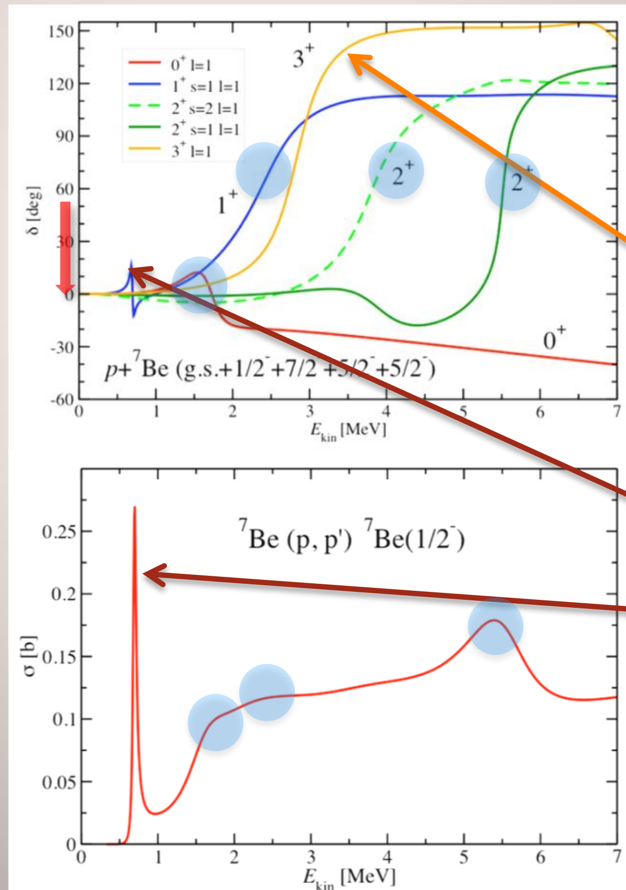
p-^{7}Be scattering

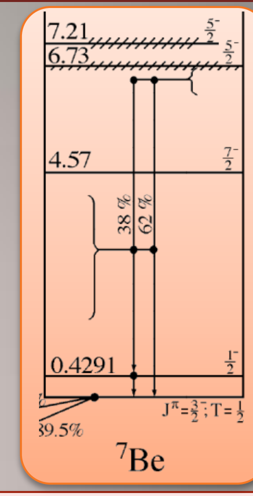
- NCSM/RGM calculation of p-^{7}Be scattering
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

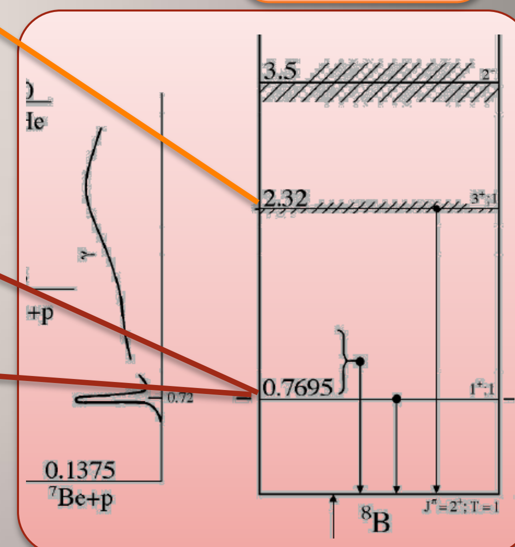
^{8}B 2^+ g.s. **bound** by 136 keV (expt. bound by 137 keV)

New 0^+, 1^+, and two 2^+ resonances **predicted**

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







P. Navratil et al., PRC **82**, 034609 (2010)

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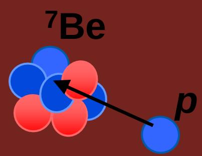


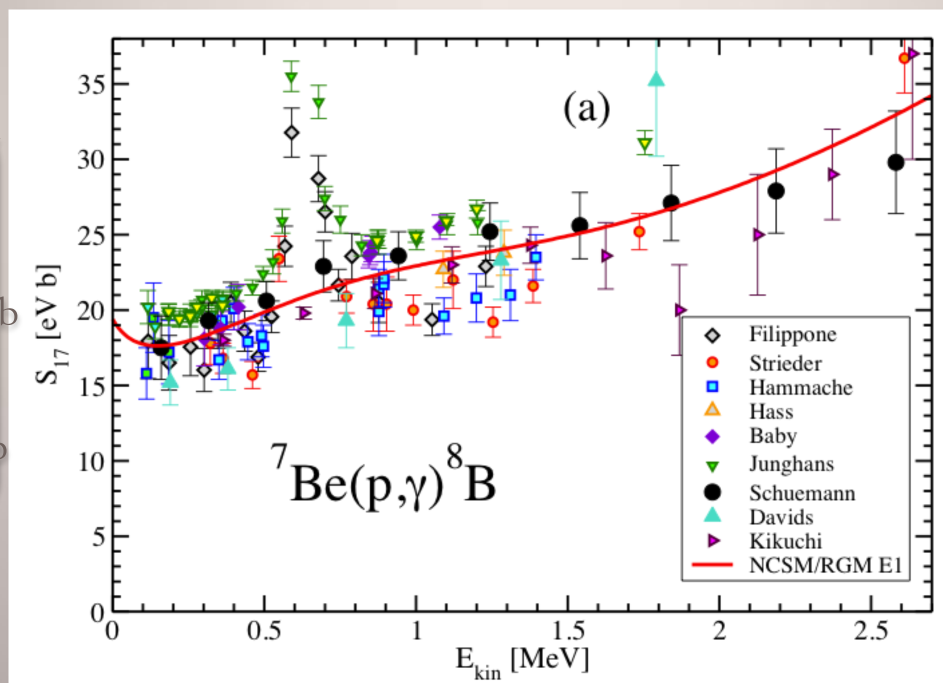
^{7}Be(p,γ)^{8}B radiative capture

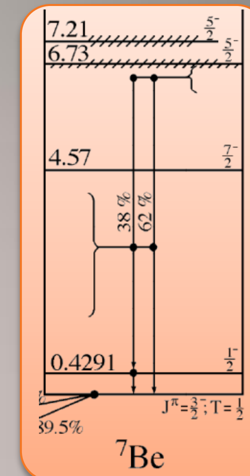
- NCSM/RGM calculation of ^{7}Be(p,γ)^{8}B radiative capture
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

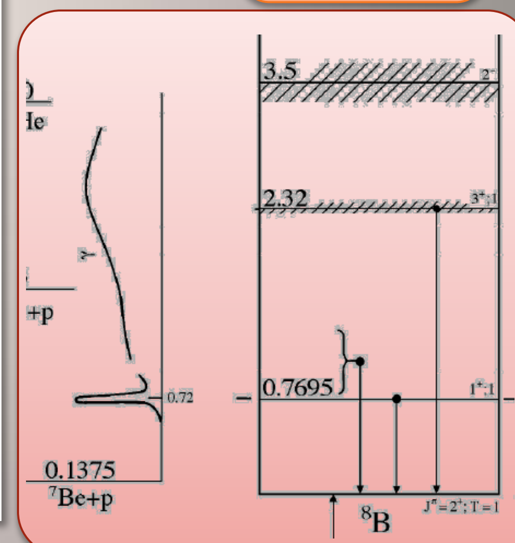
^{8}B 2^+ g.s. **bound** by 136 keV
(expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

Data evaluation:
S(0)=20.8(2.1) eV b







The first ever *ab initio* calculations of ^{7}Be(p,γ)^{8}B

arXiv:1105.5977 [nucl-th]

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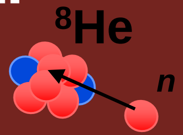
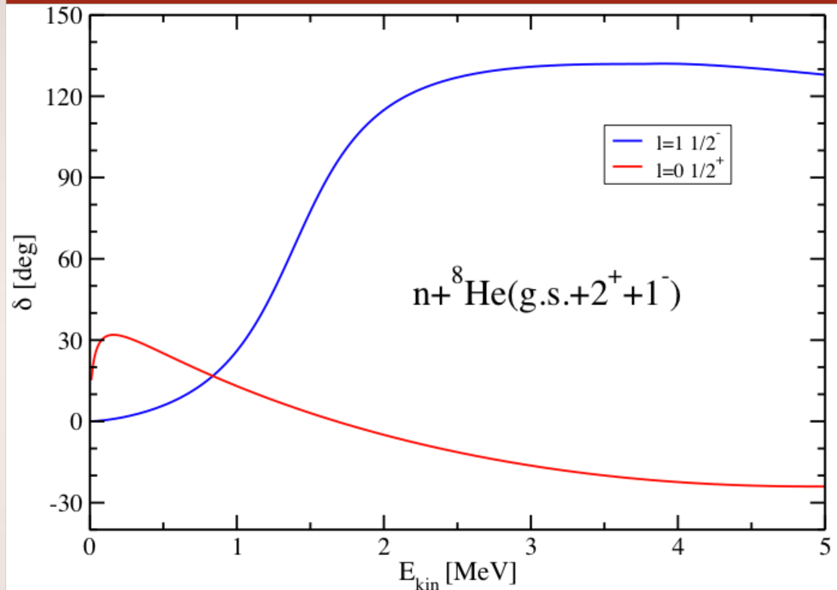


Structure of the unbound ^{9}He nucleus

- ^{9}He offers the opportunity to study the evolution of nuclear structure as a function of increasing number of neutrons
- Does the ground state of ^{9}He present the same parity inversion observed in the neighboring ^{11}Be and ^{10}Li ?
- Disappearance of the N = 8 magic number with increasing N/Z ratio
- Controversy on the nature of $S_{1/2}$ contribution to the ^{9}He spectrum
- Here:
  - n + ^{8}He(g.s.,2^{+},1^{-}), N_{max} = 13
  - SRG-N^{3}LO *NN* pot. (λ=2.02 fm^{-1})

n-^{8}He scattering phase shifts

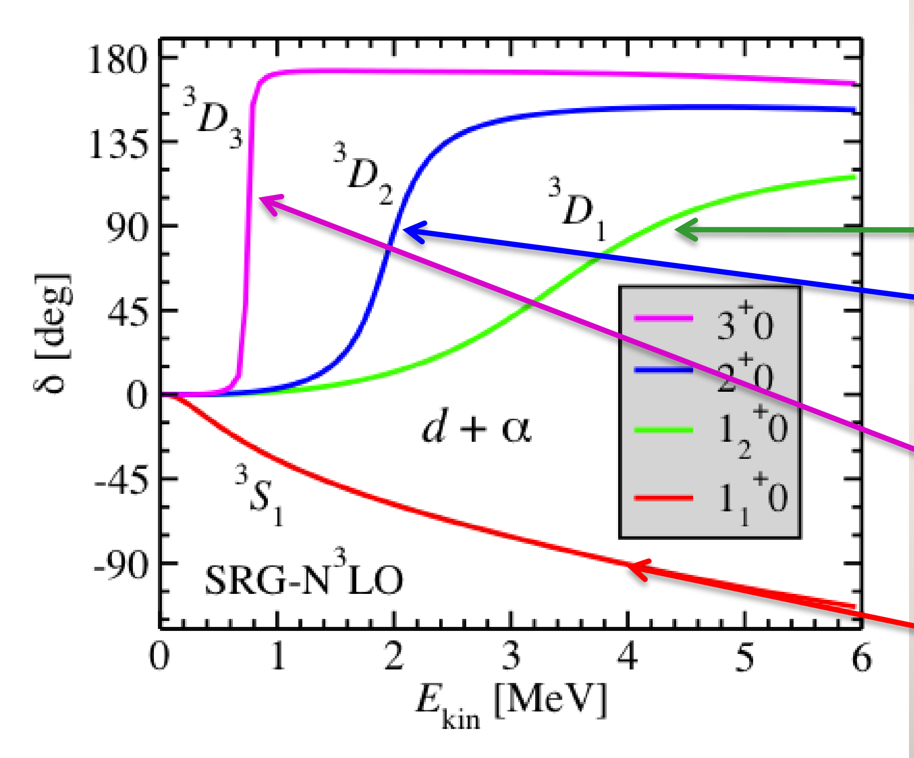


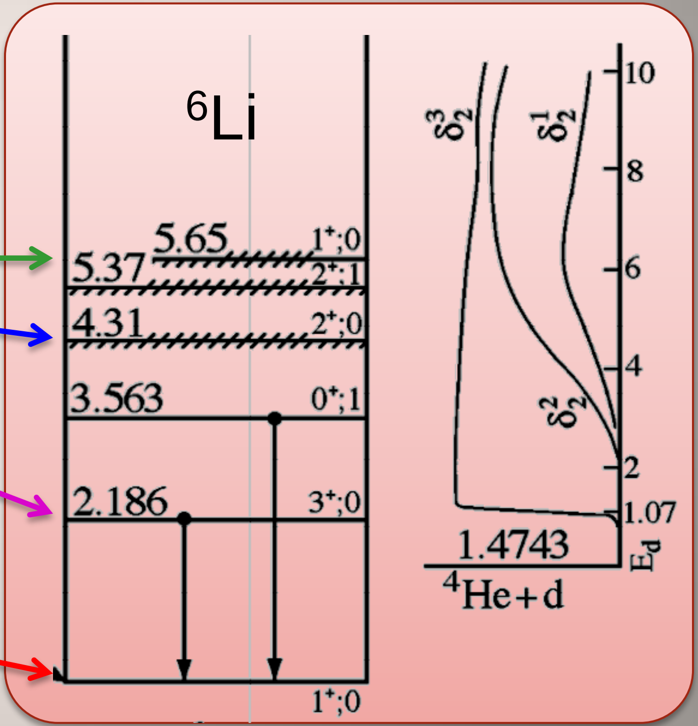
NCSM/RGM results for the *S*- and *P*-wave diagonal phase shifts. Need to study N_{max} dependence for an unambiguous answer.

g.s. parity inv. for exotic N=7 nuclei, well established in ^{11}Be and ^{10}Li, disappears for ^{9}He?

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

- NCSM/RGM calculation with d + ^{4}He(g.s.) up to N_{max} = 12
  - SRG-N^{3}LO potential with Λ = 1.5 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

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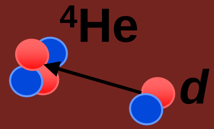
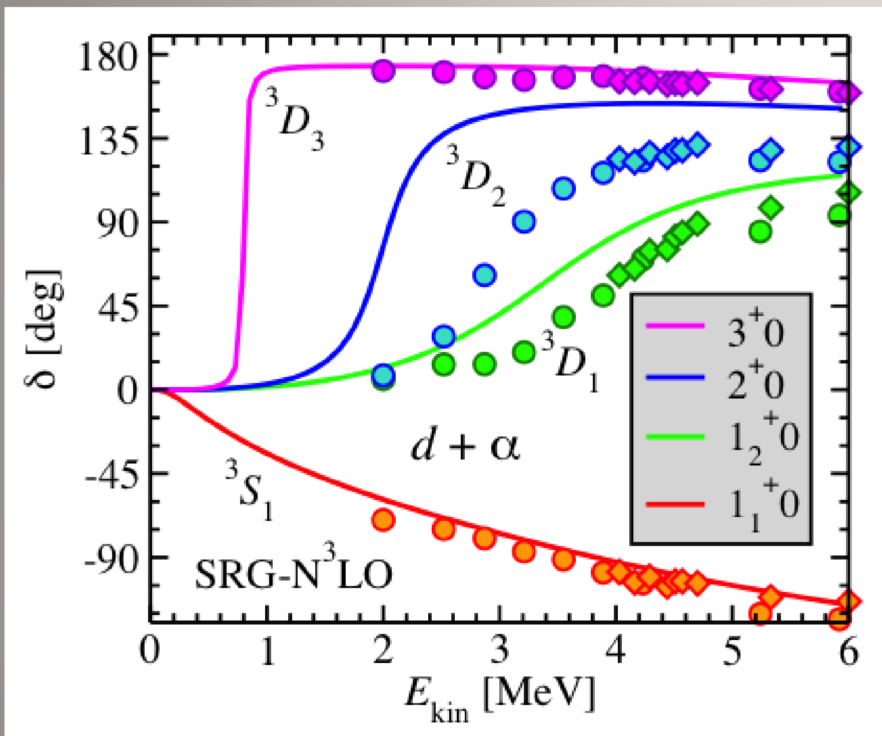
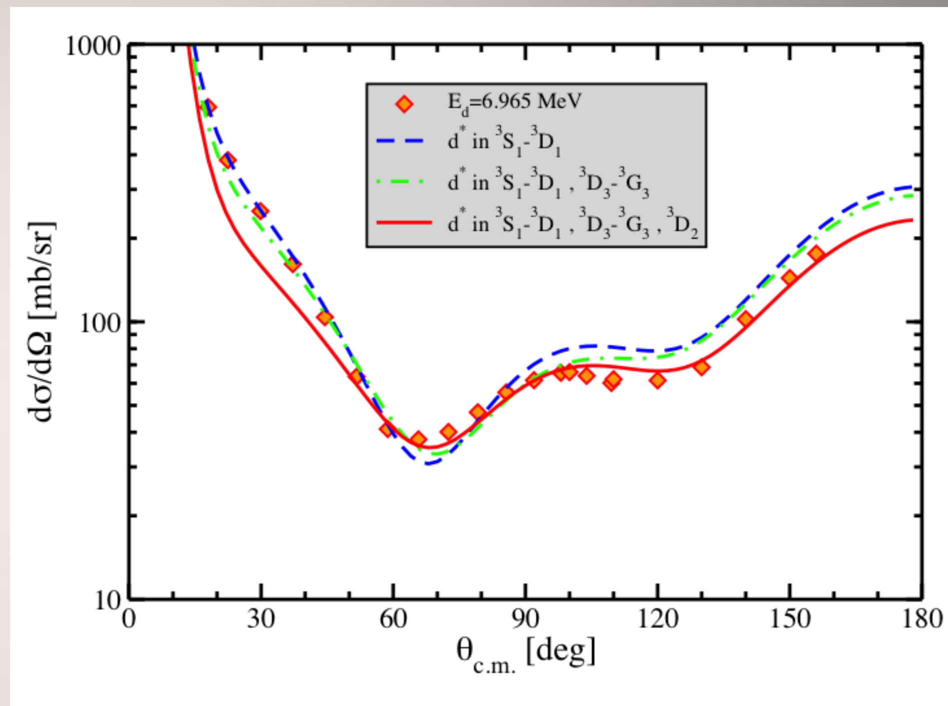


NCSM/RGM *ab initio* calculation of *d*-^{4}He scattering

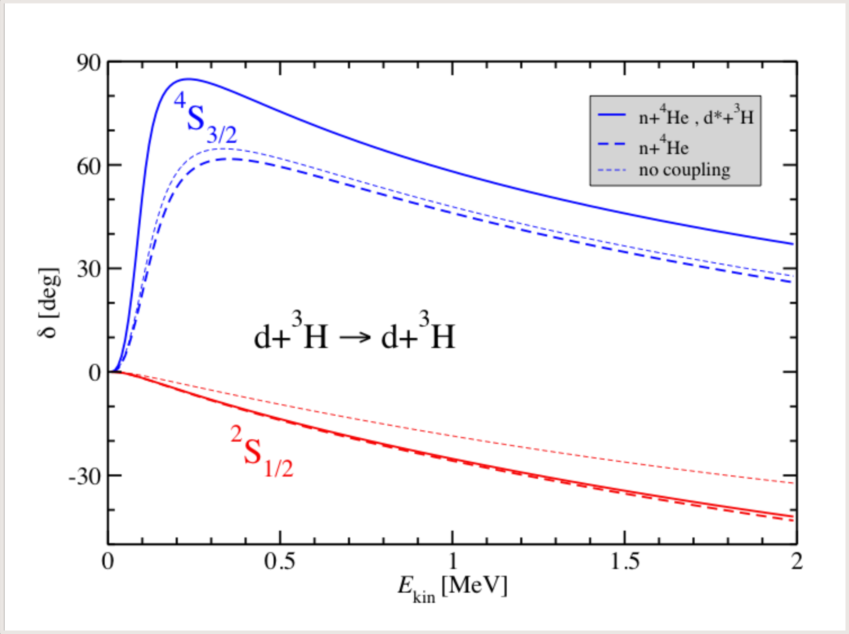
PHYS. REV. C **83**, 044609 (2011)

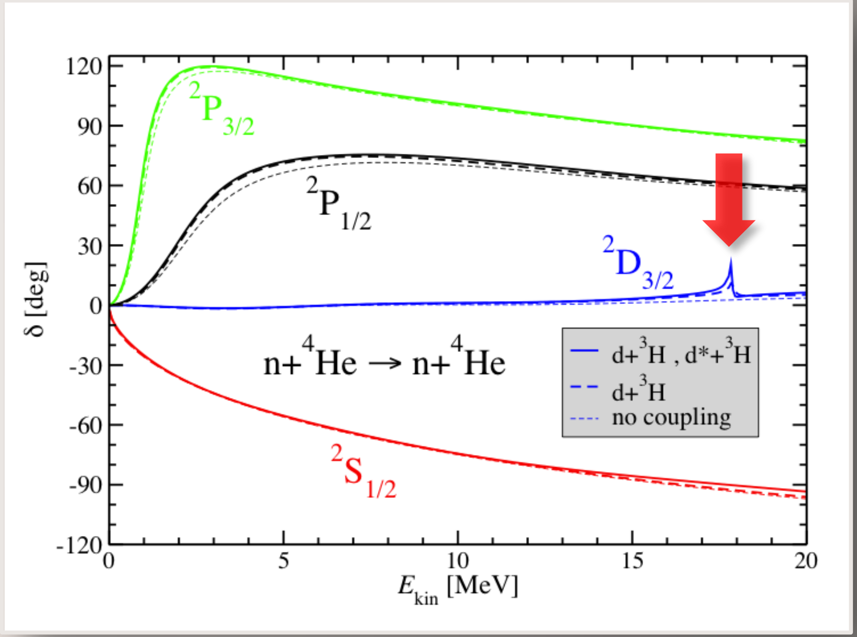




- NCSM/RGM a superior theory: Bound states, resonances, scattering
- NCSM efficiently accounts for many-nucleon correlations: **Coupling of the NCSM and the NCSM/RGM basis desirable**
- Scattering provides a strict test of NN and NNN forces

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

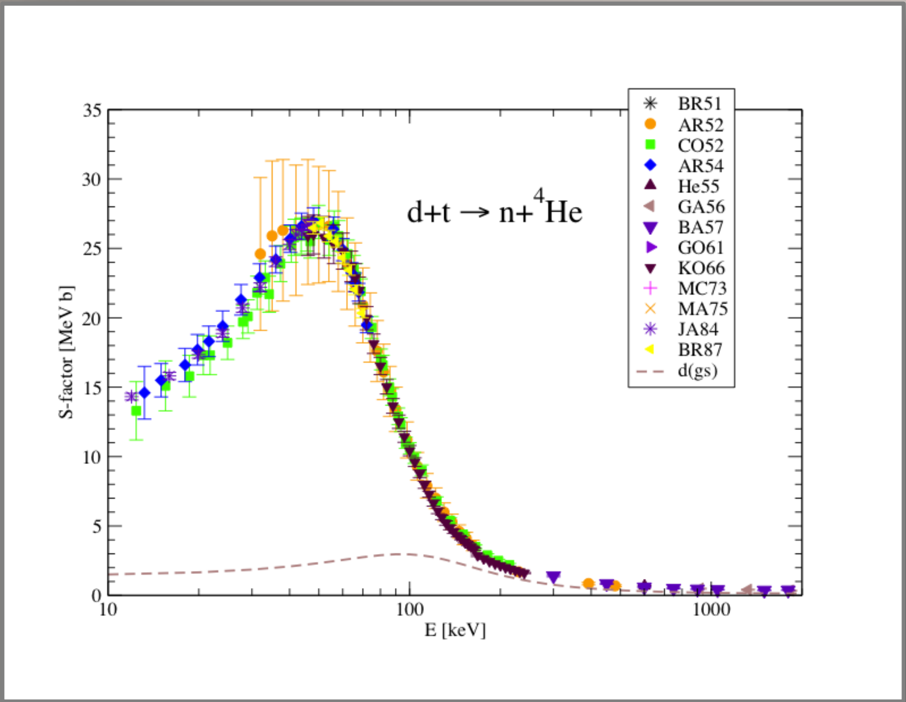


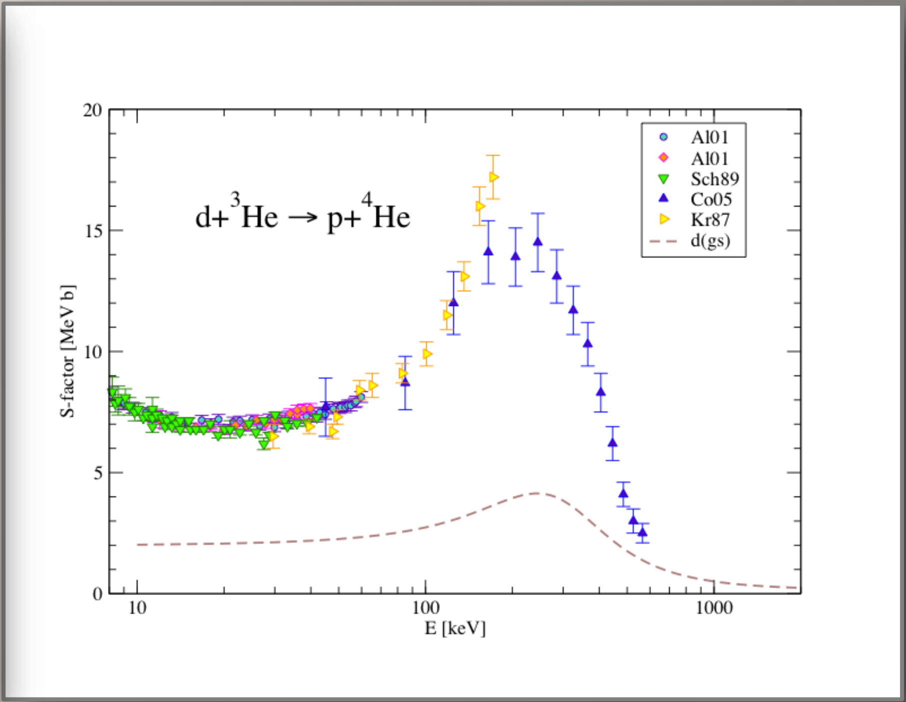


- *d*+^{3}H elastic phase shifts:
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel ➔ Pauli principle
- *n*+^{4}He elastic phase shifts:
  - *d*+^{3}H channels produces slight increase of the *P* phase shifts
  - Appearance of resonance in the $3/2^+$ *D*-wave,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

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

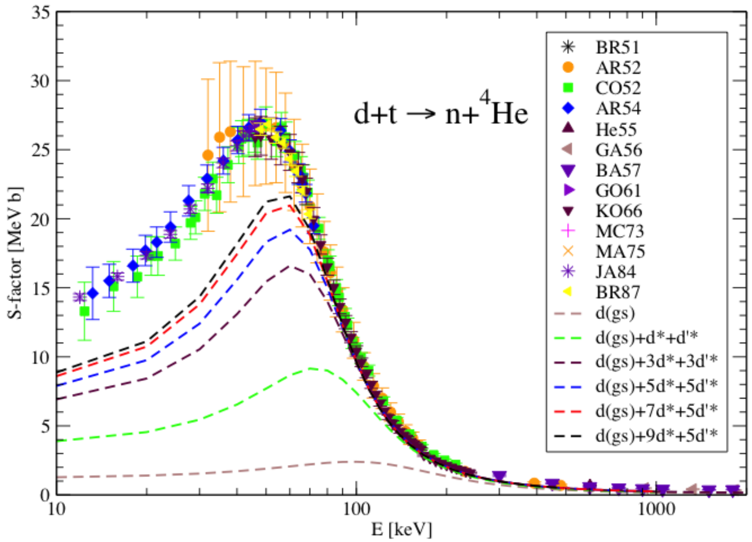


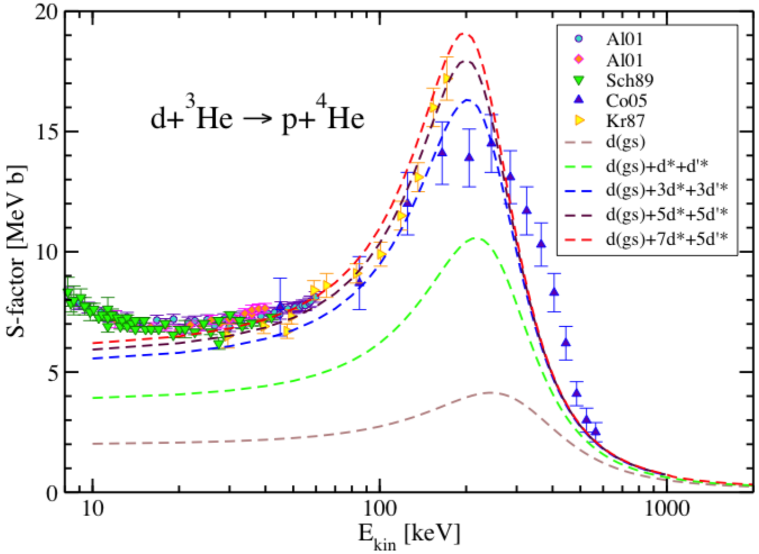


- NCSM/RGM:
  - N_{max}= 13
  - SRG-N^{3}LO NN (Λ=1.5 fm^{-1}) potential
  - NNN interaction interaction effects for *A*=3,4,5 partly included by the choice of Λ
  - Only **g.s.** of *d*, ^{3}H, ^{4}He included above

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

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



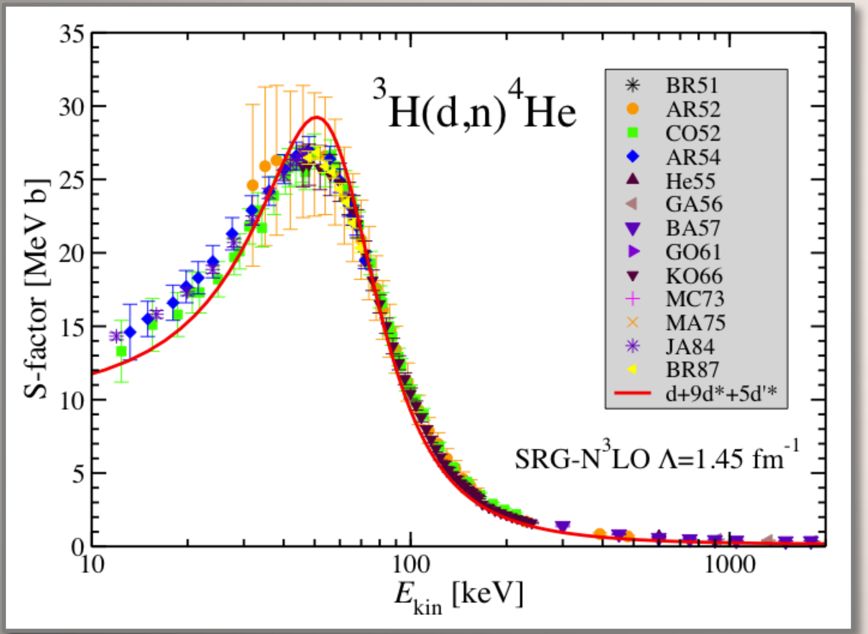


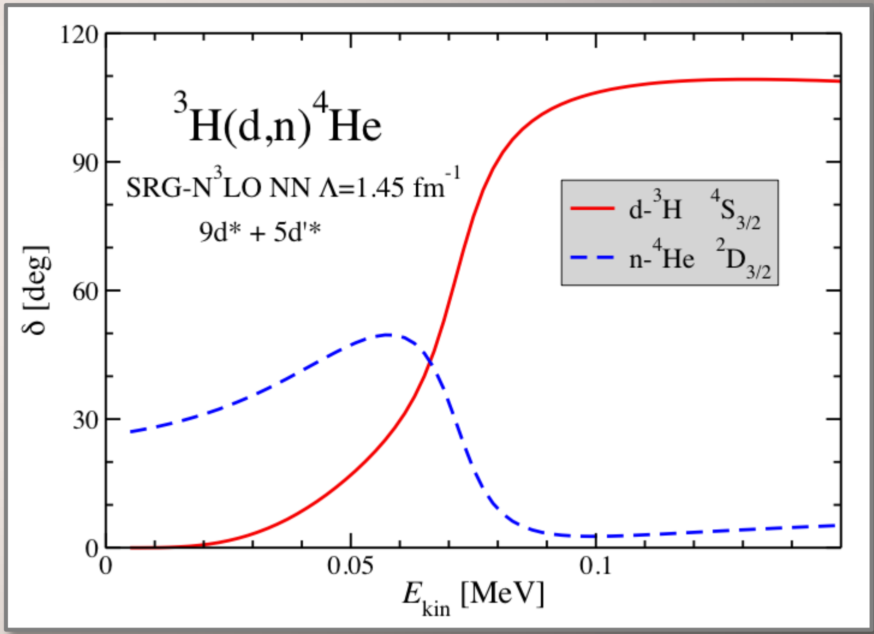
- The cross section improves with the inclusion of virtual breakup of the deuteron
  - Deuteron weakly bound: easily gets polarized and easily breaks
  - These effects included below the breakup threshold with continuum discretized by excited deuteron pseudo-states

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

$^3H(d,n)^4He$ cross section

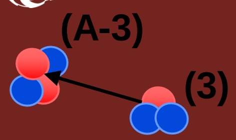
- SRG-N^{3}LO (Λ=1.45 fm^{-1}) NN potential
  - Position of the resonance matches experiment





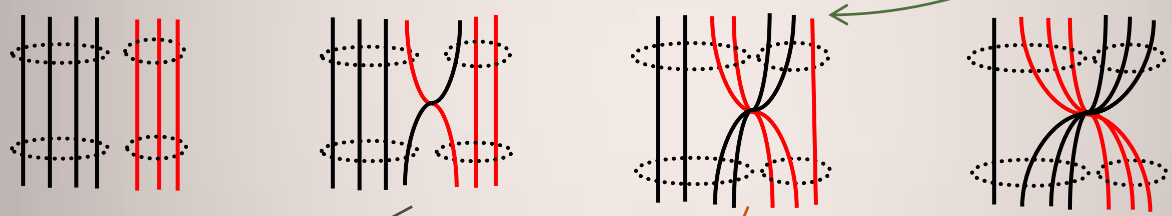
Narrower than the evaluation

Improvements:
Excitations of ^{4}He; n-p-^{3}H rather than d*, d'*
Polarization of ^{3}H; NNN interaction; Increase N_{max}(=15)



Towards an *ab initio* calculation of the ^{3}He+α scattering

$$\left\langle \begin{matrix}(1,\dots,A\text{-}3)\\ r' \;\; (A\text{-}2,A\text{-}1,A)\end{matrix} \right| 1-\sum_{i=1}^{A-3}\sum_{j=A-2}^{A}\hat{P}_{ij}+\tfrac{1}{2}\sum_{i\neq j=1}^{A-3}\left(\hat{P}_{i,A}\hat{P}_{j,A-1}+\hat{P}_{i,A}\hat{P}_{j,A-2}+\hat{P}_{i,A-1}\hat{P}_{j,A-2}\right) -\tfrac{1}{6}\sum_{i\neq j\neq k}\hat{P}_{i,A}\hat{P}_{j,A-1}\hat{P}_{k,A-2} \left| \begin{matrix}(1,\dots,A\text{-}3)\\ r \;\; (A\text{-}2,A\text{-}1,A)\end{matrix} \right\rangle$$



$${}_{\rm SD}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a \left|\psi^{(A-3)}_{\nu_1}\right\rangle_{\rm SD}$$

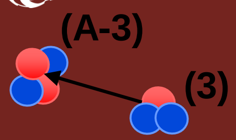
$${}_{\rm SD}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a^+ a\, a \left|\psi^{(A-3)}_{\nu_1}\right\rangle_{\rm SD}$$

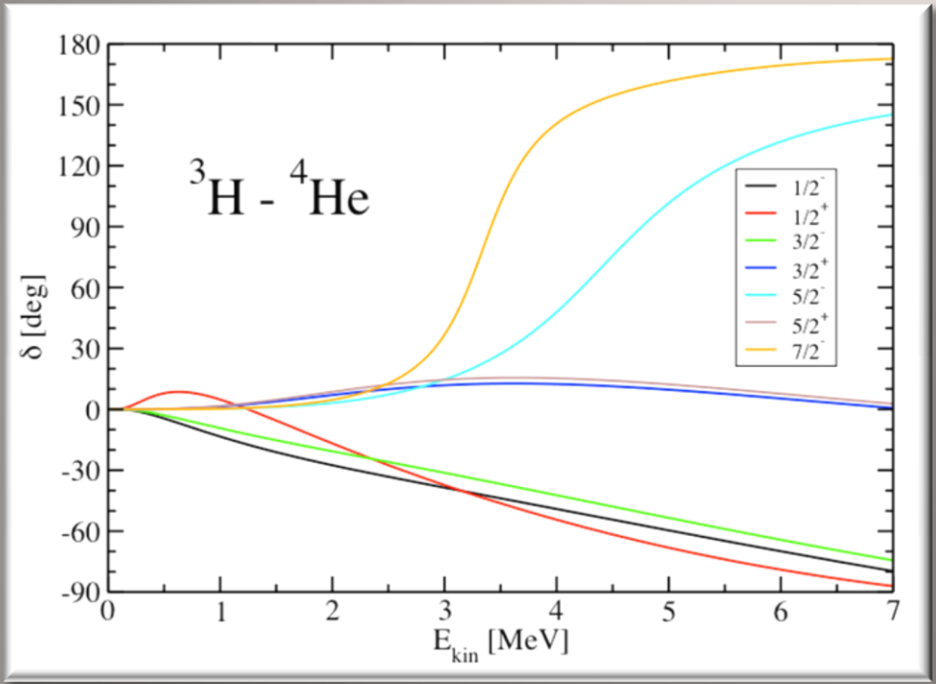
$${}_{\rm SD}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a^+ a^+ a\, a\, a \left|\psi^{(A-3)}_{\nu_1}\right\rangle_{\rm SD}$$

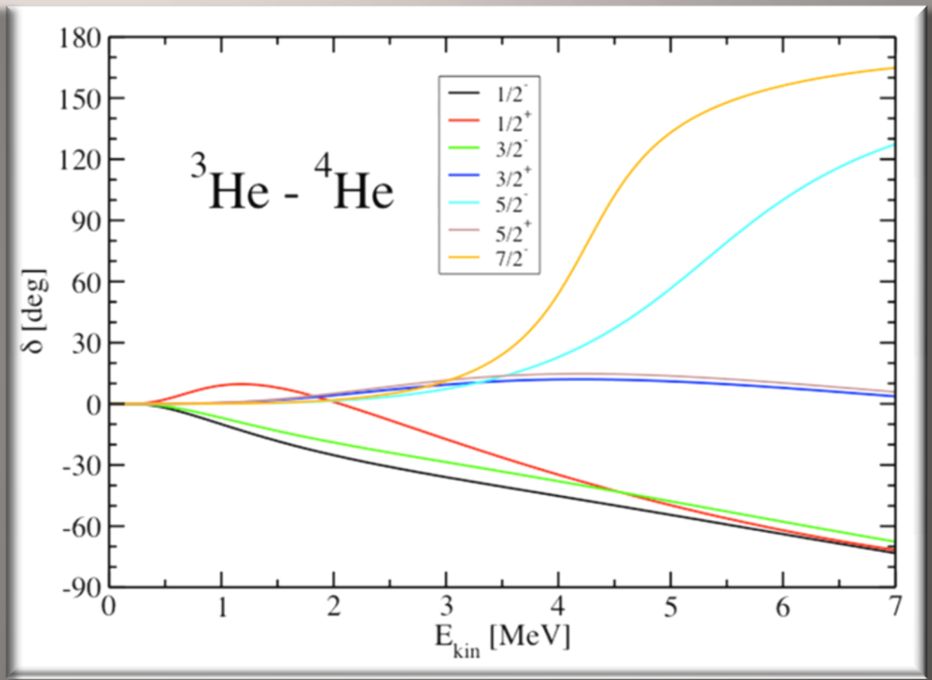
For *A*=7 use completeness

Calculations for *a*=3 projectile under way. Kernels completed…

Ab initio calculations of ^{3}H+α and ^{3}He+α scattering: First results (preliminary)







Calculations for *a*=3 projectile under way:
Soft SRG interactions (Λ=1.5 fm^{-1}), codes working up to N_{max}=11

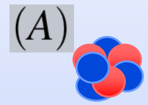
Addressing the program goals

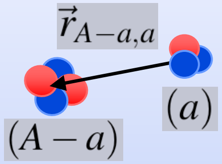
- Needs of reaction theory
  - More efficient coupling of the *ab initio* reaction theory with the *ab initio* structure calculations
    - No-core shell model with continuum (NCSMC)
  - Coupling of the *ab initio* reaction theory with traditional approaches
    - Breakup reactions on heavy targets (^{11}Be, ^{8}B …), fusion, … with the projectile described *ab initio*
  - Extension of *ab initio* reaction theory to heavier nuclei
    - Higher body-density calculations, *3N* interactions, importance truncation…

- Making codes available
  - Some of the codes developed at LLNL
    - Proper release procedure must be followed
  - Multiple codes involved, large-scale computation
  - Sharing the codes for collaborations possible now
  - Later a full release possible

Ab initio No-Core Shell Model with continuum

- Original idea:





$$\left|\Psi_A^J\right\rangle = \sum c_\lambda \left|A\lambda J\right\rangle + \sum \int d\vec{r} \int d\vec{r}\,' \hat{\mathcal{A}} \Phi_{\nu\vec{r}}^{(A-a,a)} \mathcal{N}_{\nu\nu'}^{-1/2}(\vec{r},\vec{r}\,') \chi_{\nu'}(\vec{r}\,')$$

- A better idea:

$$\begin{pmatrix} H & \bar{h} \\ \bar{h} & \mathcal{N}^{-1/2} \mathcal{H} \mathcal{N}^{-1/2} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

- Test case: ^{9}Li ⟷ ^{8}Li+*n*
  - SRG-N^{3}LO NN (Λ=1.9 fm^{-1}), ^{8}Li(2$^+$, 1$^+$, 3$^+$, 0$^+$), N_{max}=6
  - Ground state energy [MeV]:
    - ^{8}Li(2$^+$): (NCSM) -39.27; (Expt.) -41.28
    - ^{9}Li(3/2$^-$): (NCSM/RGM) -42.36; (NCSM) -43.03
      (NCSMC-HO) -43.27; (Expt.) -45.34

^{7}Be(3/2$^-$): (NCSM) -38.19; ^{8}B(2$^+$): (NCSM/RGM) -38.32; (NCSM) -38.27

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 $^{7}Be(p,\gamma)^{8}B$ *ab initio* S-factor calculation
  - Both the bound and the scattering states from first principles
  - SRG-N^{3}LO *NN* potential selected to match closely the experimental threshold ($\Lambda \approx 1.8 \sim 2$ fm^{-1})
  - No fit: Both normalization and shape predicted
  - Prediction of new ^{8}B resonances

arXiv:1105.5977 [nucl-th]

- New results with SRG-N^{3}LO *NN* potentials:
  - *d*-^{4}He scattering
  - Initial results for $^{3}H(d,n)^{4}He$ & $^{3}He(d,p)^{4}He$ fusion

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arXiv:1009.3965 [nucl-th]

- Under way:
  - ^{3}He+^{4}He scattering calculations
  - *Ab initio* NCSM with continuum (NCSMC)
  - Three-cluster NCSM/RGM and treatment of three-body continuum
- To do:
  - Inclusion of NNN force
  - Alpha clustering: ^{4}He projectile