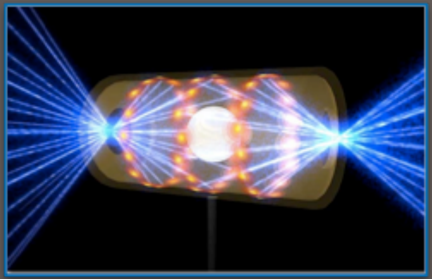
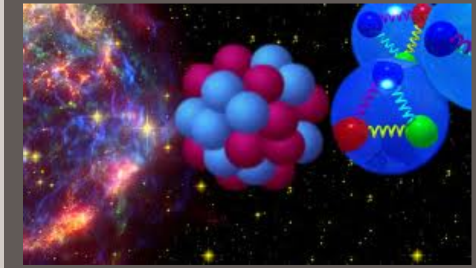
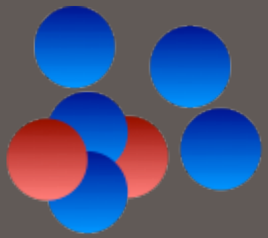
Ab initio many-body calculations of nuclear scattering and reactions



INT Workshop INT-13-53W
Nuclear Reactions from Lattice QCD
11th March 2013, Institute for Nuclear Theory



Petr Navratil | TRIUMF



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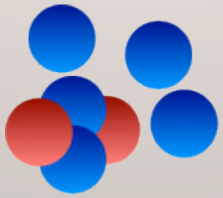
Outline

- Chiral forces
- No-core shell model
- Including the continuum with the resonating group method
  - NCSM/RGM
  - NCSMC
- ^{7}He resonances
- ^{7}Be(p,γ)^{8}B capture
- ^{3}H(d,n)^{4}He fusion
- Outlook



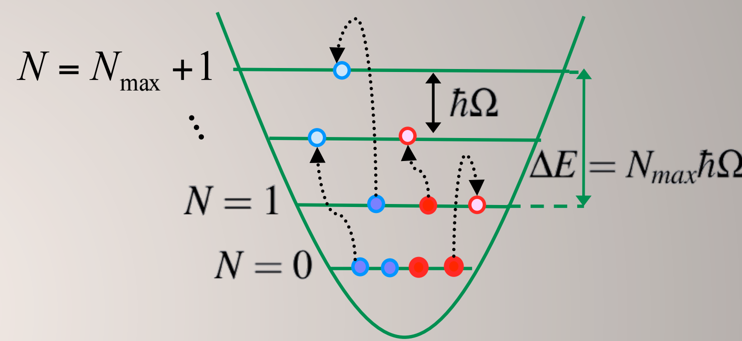
Chiral Effective Field Theory

- **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
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

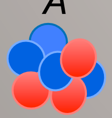
Λ_χ~1 GeV :
Chiral symmetry breaking scale

The *ab initio* no-core shell model (NCSM)

- The NCSM is a technique for the solution of the *A*-nucleon bound-state problem
- Realistic nuclear Hamiltonian
  - High-precision nucleon-nucleon potentials
  - Three-nucleon interactions
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
  - complete $N_{max}\hbar\Omega$ model space
- ***Effective interaction tailored to model-space truncation*** for NN(+NNN) potentials
  - Okubo-Lee-Suzuki unitary transformation
- Or a **sequence of unitary transformations in momentum space**:
  - Similarity-Renormalization-Group (SRG) evolved NN(+NNN) potential



A



$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

Convergence to exact solution with increasing $N_{\max}$ for bound states. No coupling to continuum.

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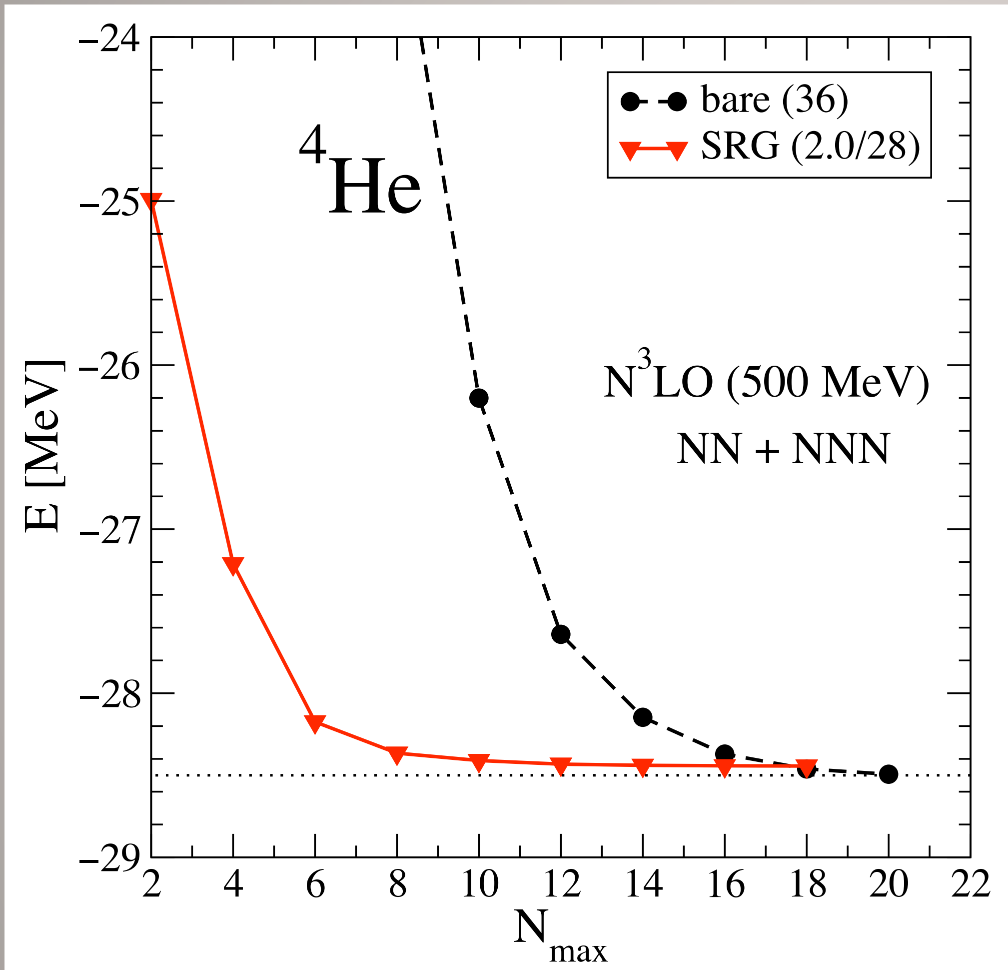
^{4}He from chiral EFT interactions: g.s. energy convergence



PRL **103**, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]

A=3 binding energy and half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

Chiral N^{3}LO NN plus N^{2}LO NNN potential

- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

$$\boxed{H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = \left[\left[T, H_\alpha\right], H_\alpha\right]} \quad \left(\alpha = 1/\lambda^4\right)$$

  - Two- plus *three*-body components, *four*-body omitted
  - Softens the interaction
    - Smaller basis sufficient

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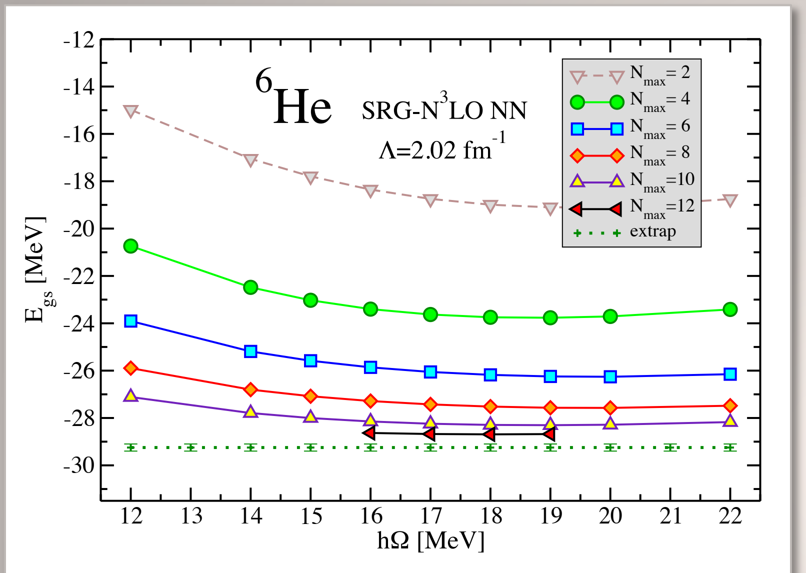
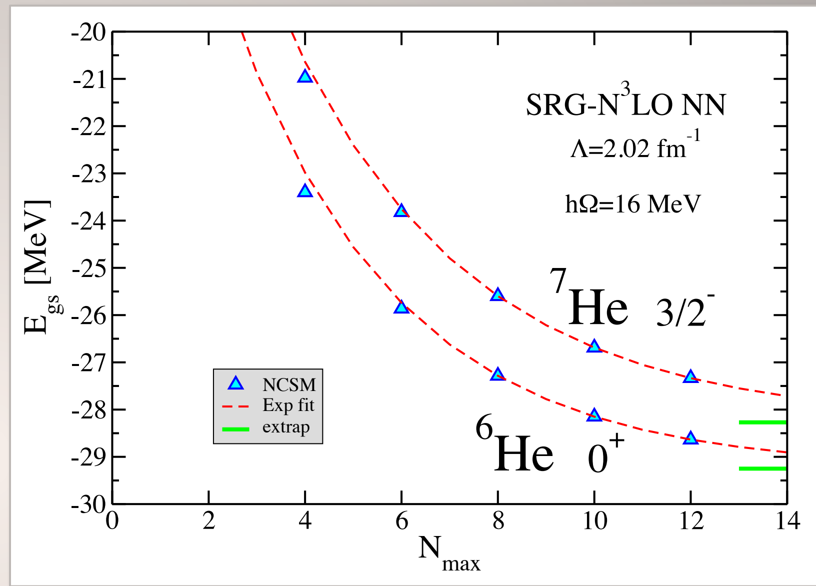
NCSM calculations of ^{6}He and ^{7}He g.s. energies

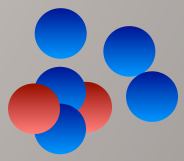




$E_{\mathrm{g.s.}}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible
  - ^{6}He: E_{gs}=-29.25(15) MeV (Expt. -29.269 MeV)
  - ^{7}He: E_{gs}=-28.27(25) MeV (Expt. -28.84(30) MeV)
- ^{7}He unbound (+0.430(3) MeV), width 0.182(5) MeV
  - **NCSM: no information about the width**

^{7}He



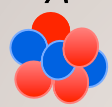
unbound

Extending no-core shell model beyond bound states

Include more many nucleon correlations…

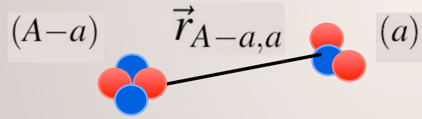
NCSM

A

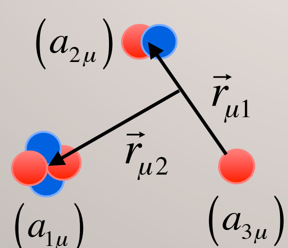


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

+



+



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

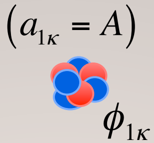
+

…

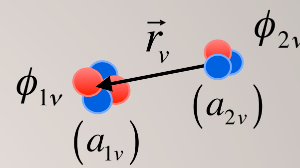
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



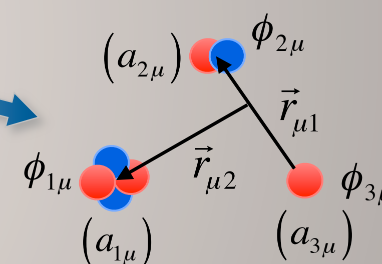
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

$$+ \cdots$$

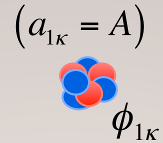


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

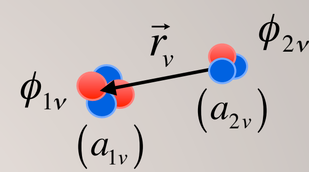
TRIUMF

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \boxed{\phi_{1\kappa}}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



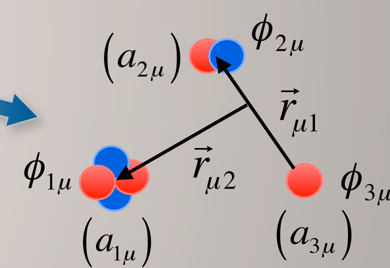
$$+\sum_{\nu} \hat{A}_{\nu} \boxed{\phi_{1\nu}}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \boxed{\phi_{2\nu}}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+\sum_{\mu} \hat{A}_{\mu} \boxed{\phi_{1\mu}}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \boxed{\phi_{2\mu}}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \boxed{\phi_{3\mu}}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

$$+ \cdots$$

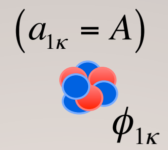


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

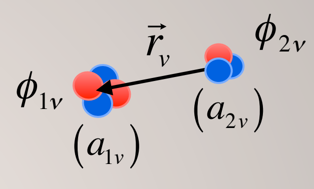
- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



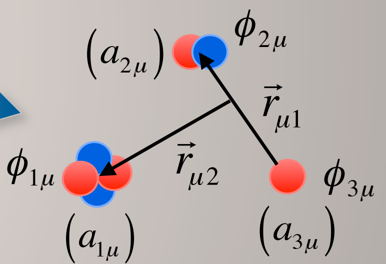
$$+ \sum_{\nu} \boxed{\hat{A}_\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \boxed{\hat{A}_\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_\mu(\vec{R}_{\mu 1}, \vec{R}_{\mu 2})$$

$$+ \cdots$$



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- $\boldsymbol{A_\nu}$, $\boldsymbol{A_\mu}$: intercluster antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

$$a_{1\nu} = A - 1,\ a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_\nu = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

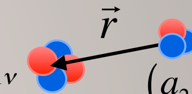
TRIUMF

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} \boxed{c_\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

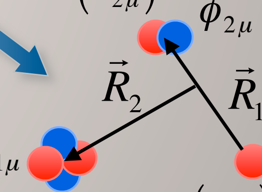
$$+ \sum_{\nu} \int \boxed{g_\nu(\vec{r}\,)}\, \hat{A}_\nu \left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) \delta(\vec{r} - \vec{r}_\nu) \right] d\vec{r}$$

$a_{1\nu} + a_{2\nu} = A$



$$+ \sum_{\mu} \iint \boxed{G_\mu(\vec{R}_1, \vec{R}_2)}\, \hat{A}_\mu \left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) \delta(\vec{R}_1 - \vec{R}_{\mu 1}) \delta(\vec{R}_2 - \vec{R}_{\mu 2}) \right] d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$

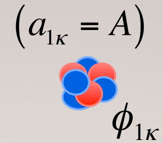


$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

- ***c***, ***g*** and ***G***: discrete and continuous linear variational amplitudes
  - Unknowns to be determined

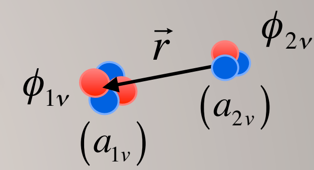
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \boxed{\phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)}$$



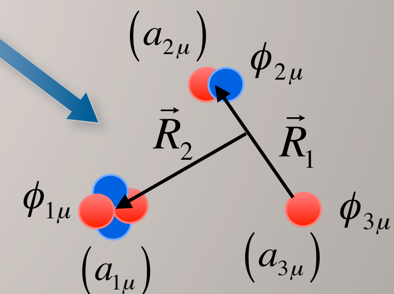
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\, \hat{A}_{\nu} \boxed{\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right]} d\vec{r}$$

$$a_{1\nu} + a_{2\nu} = A$$



$$+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1, \vec{R}_2)\, \hat{A}_{\mu} \boxed{\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right]} d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

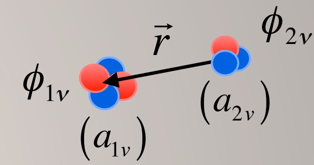
TRIUMF

Binary cluster wave function

$$\psi^{(A)} = \cancel{\sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)}$$

$$+ \sum_{\nu} \int g_\nu(\vec{r}\,)\ \hat{A}_\nu \left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r}-\vec{r}_\nu)\right] d\vec{r}$$

$$a_{1\nu} + a_{2\nu} = A$$



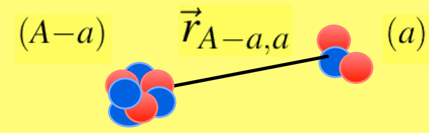
$$\cancel{+ \sum_{\mu} \iint G_\mu(\vec{R}_1,\vec{R}_2)\ \hat{A}_\mu \left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu 1})\delta(\vec{R}_2-\vec{R}_{\mu 2})\right] d\vec{R}_1 d\vec{R}_2}$$

$$+ \cdots$$

- In practice: function space limited by using relatively simple forms of Ψ chosen according to physical intuition and energetical arguments
  - Most common: expansion over binary-cluster basis

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

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

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

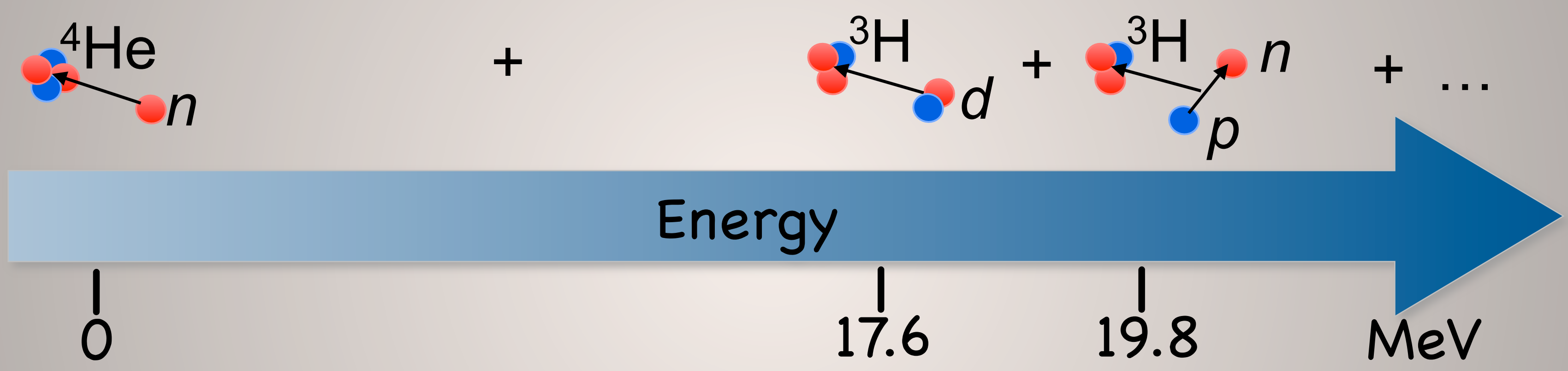
Hamiltonian kernel

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

Norm kernel

Example: the five-nucleon system

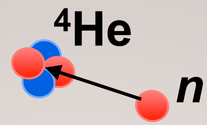
- Consider the T = ½ case: ^{5}He (^{5}Li)
  - Five-nucleon cluster unbound; ^{4}He tightly bound, not easy to deform

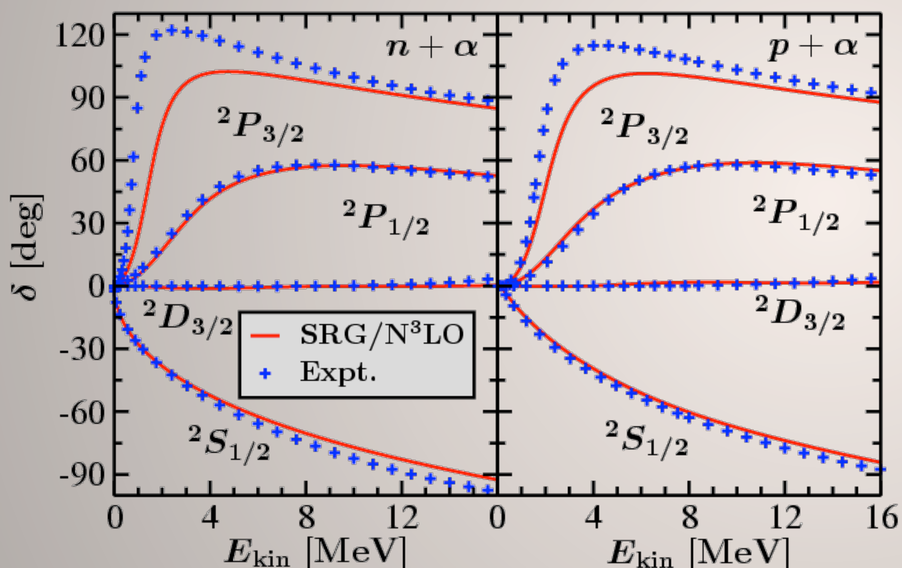


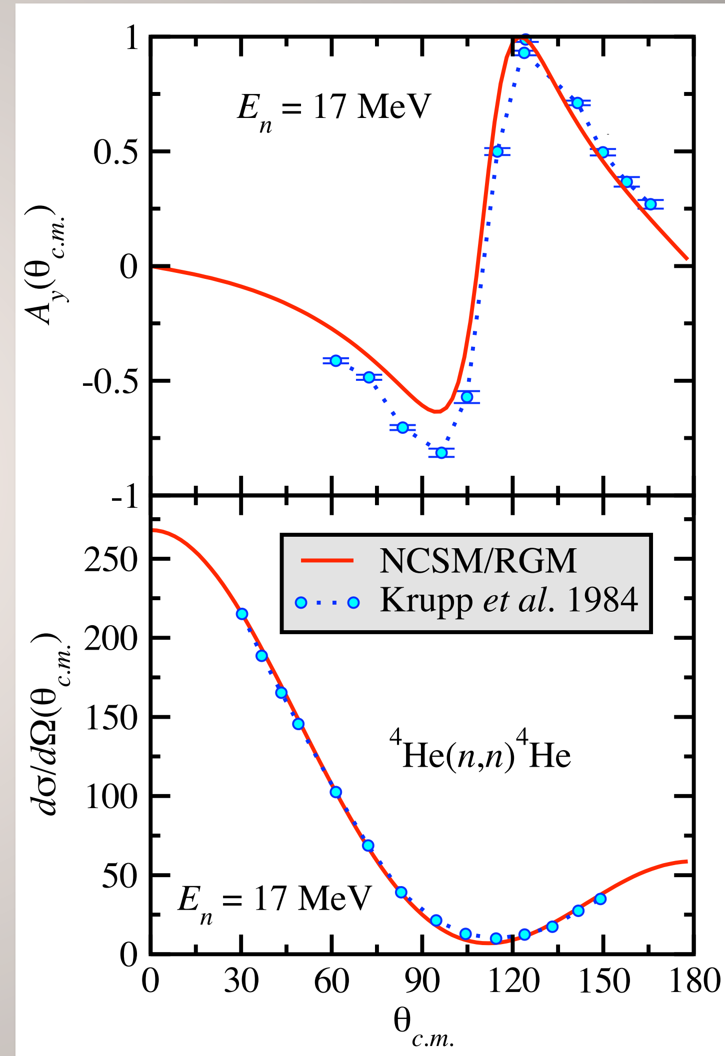
- Satisfactory description of n-^{4}He (p-^{4}He) scattering at low excitation energies within single-channel approximation
- However, both n(p) + ^{4}He and d + ^{3}H(^{3}He) channels needed to describe ^{3}H(d,n)^{4}He [^{3}He(d,p)^{4}He] fusion!

Unbound A=5 nuclei: ^{5}He→n+^{4}He, ^{5}Li→p+^{4}He

- NCSM/RGM calculations
  - SRG-N^{3}LO NN potential with Λ=2.02 fm^{-1}



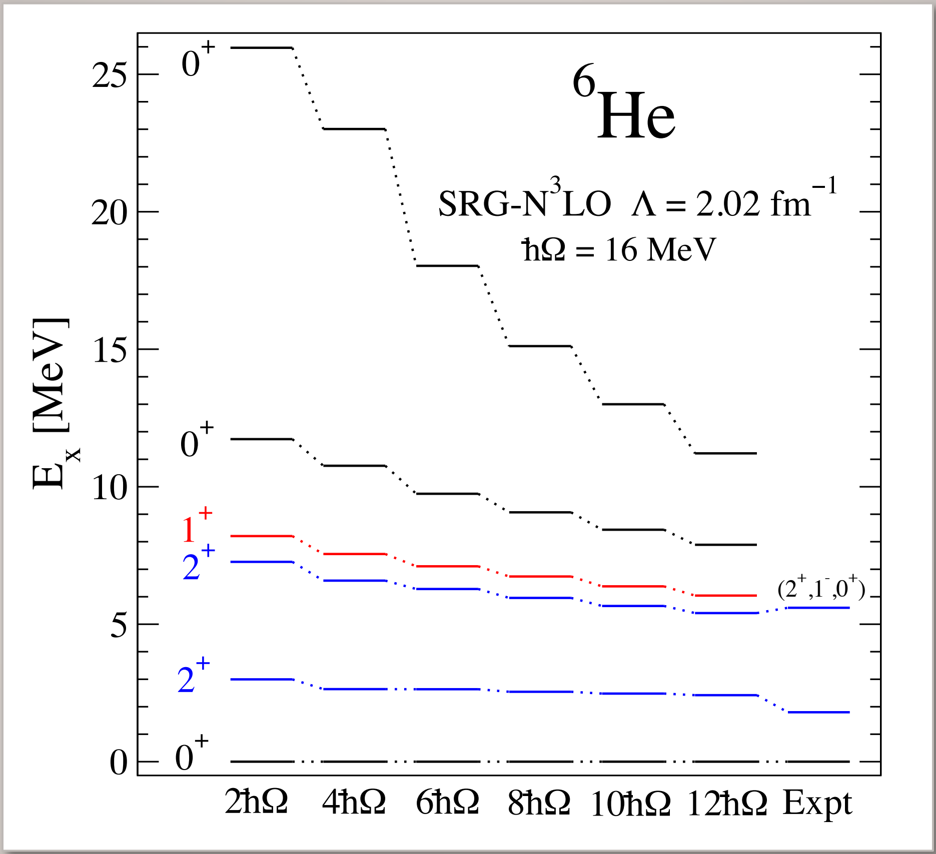




- Differential cross section and analyzing power @17 MeV neutron energy
  - Polarized neutron experiment at Karlsruhe

NNN and ^{4}He polarization missing: Good agreement only for energies beyond low-lying 3/2$^-$ resonance

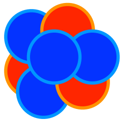
How about ^{7}He as n+^{6}He?



- All ^{6}He excited states above 2^+_1 broad resonances or states in continuum
- Convergence of the NCSM/RGM n+^{6}He calculation slow with number of ^{6}He states
  - Negative parity states also relevant
  - Technically not feasible to include more than ~ 5 states

New developments: NCSM with continuum

NCSM

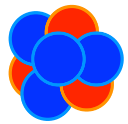


$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

TRIUMF

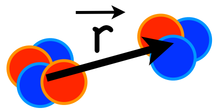
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

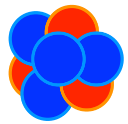
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$\boxed{(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}}$$

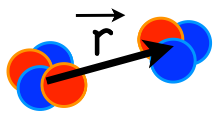
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



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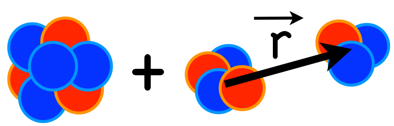
NCSMC



S. Baroni, P. N., and S. Quaglioni, PRL **110**, 022505 (2013); arXiv:1301.3450 [nucl-th] (submitted to PRC)

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle + \sum_\nu \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}\,' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r},\vec{r}\,') \bar{\chi}_{\nu'}(\vec{r}\,') \right) \hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

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

TRIUMF

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

NCSM sector:

$$(H_{NCSM})_{\lambda\lambda'} = \langle A\lambda J^\pi T|\hat{H}|A\lambda' J^\pi T\rangle = \varepsilon_\lambda^{J^\pi T}\delta_{\lambda\lambda'}$$

NCSM/RGM sector:

$$\overline{\mathcal{H}}_{\nu\nu'}(r,r') = \sum_{\mu\mu'} \int\int dy dy' y^2 y'^2 \mathcal{N}_{\nu\mu}^{-\frac{1}{2}}(r,y)\mathcal{H}_{\mu\mu'}(y,y')\mathcal{N}_{\mu'\nu'}^{-\frac{1}{2}}(y',r')$$

TRIUMF

How to calculate the NCSM/RGM kernels?

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \underbrace{\left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} \frac{\delta(r-r_{A-a,a})}{r r_{A-a,a}}}_{\left|\Phi_{\nu r}^{J^\pi T}\right\rangle} r^2 dr$$

(Jacobi) channel basis

- Since we are using NCSM wave functions, it is convenient to introduce Jacobi channel states in the HO space

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

  – The coordinate space channel states are given by

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

    - We used the closure properties of HO radial wave functions

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

  – Target and projectile wave functions are both translational invariant NCSM eigenstates calculated in the Jacobi coordinate basis

Norm kernel (Pauli principle)

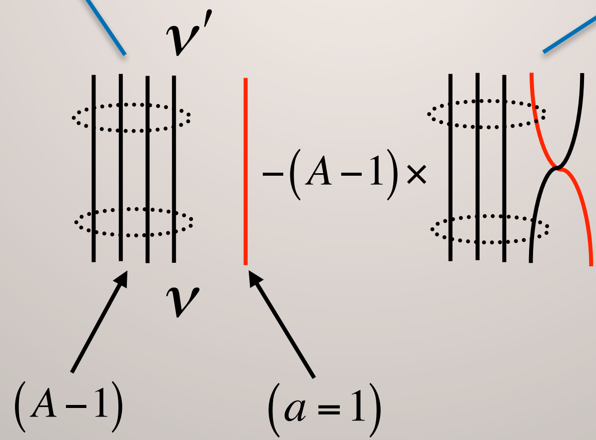
Single-nucleon projectile

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \; (A-1) \quad r' \quad (a'=1) \; \middle| \; 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \; \middle| \; (a=1) \quad r \quad (A-1) \; \right\rangle$$

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

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

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



Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

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

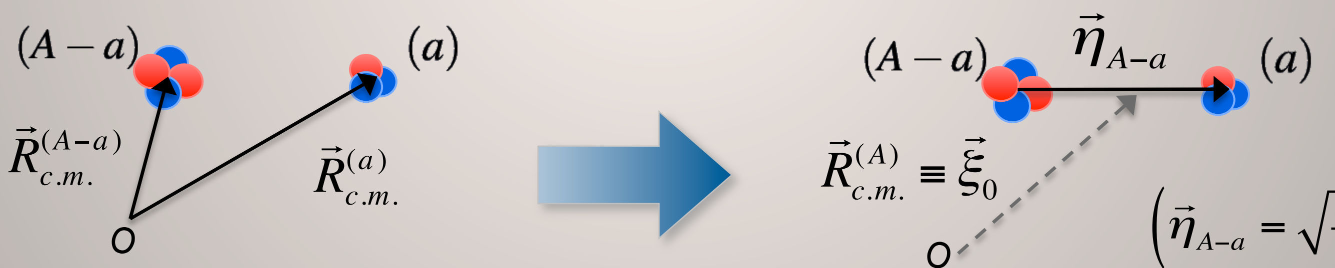
Introduce SD channel states in the HO space

- Define SD channel states in which the eigenstates of the heaviest of the two clusters (target) are described by a SD wave function:

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \left[\left(\underbrace{\left|A-a\;\alpha_1 I_1^{\pi_1}T_1\right\rangle_{SD}}_{\left|A-a\;\alpha_1 I_1^{\pi_1}T_1\right\rangle \varphi_{00}\left(\underbrace{\vec R^{(A-a)}_{c.m.}}\right)} \left|a\;\alpha_2 I_2^{\pi_2}T_2\right\rangle\right)^{(sT)} Y_\ell\left(\underbrace{\hat R^{(a)}_{c.m.}}\right)\right]^{(J^\pi T)} R_{n\ell}\left(\underbrace{R^{(a)}_{c.m.}}\right)$$

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

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



$$\left(\vec\eta_{A-a} = \sqrt{\frac{(A-a)a}{A}}\,\vec r_{A-a,a}\right)$$

$$\left(\varphi_{00}\left(\vec R^{(A-a)}_{c.m.}\right)\varphi_{n\ell}\left(\vec R^{(a)}_{c.m.}\right)\right)^{\ell} = \sum_{n_r\ell_r,NL} \left\langle 00,n\ell,\ell \middle| n_r\ell_r,NL,\ell\right\rangle_{d=\frac{a}{A-a}} \left(\varphi_{n_r\ell_r}\left(\vec\eta_{A-a}\right)\varphi_{NL}\left(\vec\xi_0\right)\right)^{\ell}$$

Translational invariant matrix elements from SD ones

- More in detail:

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

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

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

$$\boxed{\begin{aligned} &\times \sum_{NL} \hat{\ell}\hat{\ell}' \hat{J}_r^2 (-1)^{s+\ell-s'-\ell'} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \begin{Bmatrix} s' & \ell'_r & J_r \\ L & J & \ell' \end{Bmatrix} \\ &\times \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a}{A-a}} \langle 00, n'\ell', \ell' | n'_r \ell'_r, NL, \ell' \rangle_{d'=\frac{a'}{A-a'}} \end{aligned}}$$

Interested in this

Calculate these

Matrix that can be inverted

- Translational invariance preserved (exactly!) also with SD channels
- Transformation is general: same for different A's or different a's

TRIUMF

Is the SD channel basis advantageous?

- SD to Jacobi transformation is general and exact
- Can use powerful second quantization representation
  - Matrix elements of translational invariant operators can be expressed in terms of matrix elements of density operators on the target eigenstates
  - For example, for $a = a' = 1$

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

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

One-body density matrix elements

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

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

Coupling:

$$\bar{g}_{\lambda\nu}(r) = \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^\pi T | \hat{\mathcal{A}}_{\nu'} \Phi^{J^\pi T}_{\nu' r'} \rangle \, \mathcal{N}^{-\frac{1}{2}}_{\nu'\nu}(r', r)$$

$$\bar{h}_{\lambda\nu}(r) = \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^\pi T | \hat{H} \hat{\mathcal{A}}_{\nu'} | \Phi^{J^\pi T}_{\nu' r'} \rangle \, \mathcal{N}^{-\frac{1}{2}}_{\nu'\nu}(r', r)$$

Calculation of *g* from SD wave functions:

$$\begin{aligned} g_{\lambda\nu n} &= \langle A\lambda J^\pi T | \hat{\mathcal{A}}_\nu \Phi^{J^\pi T}_{\nu n} \rangle \\ &= \frac{1}{\langle n\ell 00, \ell | 00 n\ell, \ell \rangle_{\frac{1}{(A-1)}}} \; {}_{SD}\langle A\lambda J^\pi T | \hat{\mathcal{A}}_\nu \Phi^{J^\pi T}_{\nu n} \rangle_{SD} \\ &= \frac{1}{\langle n\ell 00, \ell | 00 n\ell, \ell \rangle_{\frac{1}{(A-1)}}} \frac{1}{\hat{J}\hat{T}} \sum_j (-1)^{I_1 + J + j} \hat{s}\hat{j} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} {}_{SD}\langle A\lambda J^\pi T ||| a^\dagger_{n\ell j \frac{1}{2}} ||| A-1 \alpha_1 I_1^{\pi_1} T_1 \rangle_{SD} \end{aligned}$$

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

$$N^{\lambda\lambda'}_{\nu r \nu' r'} = \begin{pmatrix} \delta_{\lambda\lambda'} & \bar{g}_{\lambda\nu'}(r') \\ \bar{g}_{\lambda'\nu}(r) & \delta_{\nu\nu'} \frac{\delta(r-r')}{rr'} \end{pmatrix}$$

Orthogonalization:

$$\overline{H} = N^{-\frac{1}{2}} \begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} N^{-\frac{1}{2}} \qquad \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = N^{+\frac{1}{2}} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

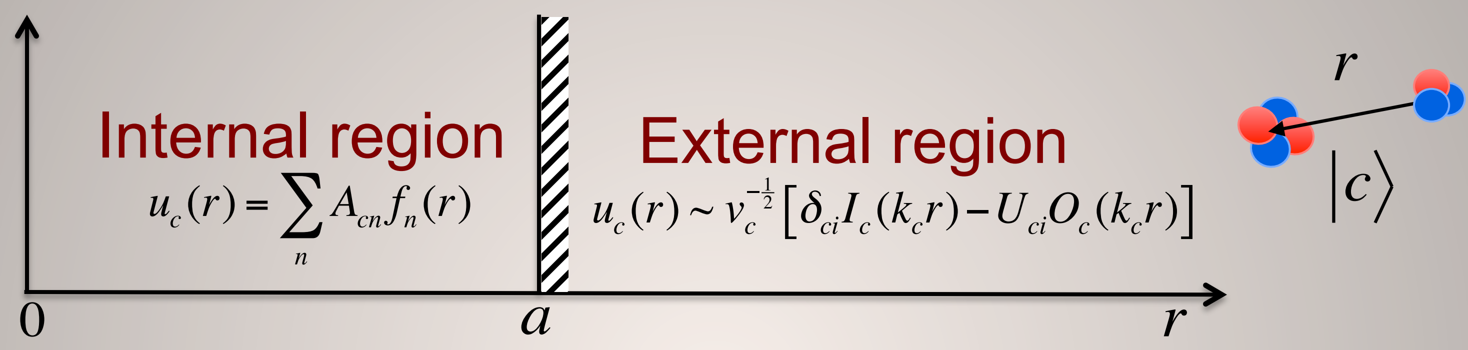
Solve with generalized microscopic R-matrix

$$(\hat{\overline{H}} + \hat{L} - E) \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = \hat{L} \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix}$$

Bloch operator $\longrightarrow$ $\hat{L}_\nu = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}\delta(r-a)(\frac{d}{dr} - \frac{B_\nu}{r}) \end{pmatrix}$

Microscopic R-matrix theory

- Separation into “internal” and “external” regions at the channel radius a



  - This is achieved through the Bloch operator: $L_c = \dfrac{\hbar^2}{2\mu_c}\delta(r-a)\left(\dfrac{d}{dr} - \dfrac{B_c}{r}\right)$
  - System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c)\right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

  - Internal region: expansion on square-integrable basis $\quad u_c(r) = \sum_n A_{cn} f_n(r)$
  - External region: asymptotic form for large r

$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$$

Scattering matrix

Bound state

Scattering state

TRIUMF

To find the Scattering matrix

- After projection on the basis $f_n(r)$:

$$\sum_{c'n'}\left[C_{cn,c'n'}-(E-E_c)\delta_{cn,c'n'}\right]A_{c'n'}=\frac{\hbar^2 k_c}{2\mu_c v_c^{1/2}}\left\langle f_n\middle|L_c\middle|I_c\delta_{ci}-U_{ci}O_c\right\rangle$$

$$\boxed{\left\langle f_n\middle|\hat{T}_{rel}(r)+L_c+\overline{V}_{Coul}(r)\middle|f_{n'}\right\rangle\delta_{cc'}+\left\langle f_n\middle|W_{cc'}(r,r')\middle|f_{n'}\right\rangle}$$

Lagrange basis associated with Lagrange mesh:

$$\{ax_n\in[0,a]\}$$

$$\int_0^1 g(x)dx\approx\sum_{n=1}^{N}\lambda_n g(x_n)$$

$$\int_0^a f_n(r)f_{n'}(r)dr\approx\delta_{nn'}$$

1. Solve for A_{cn}
2. Match internal and external solutions at channel radius, a

$$\sum_{c'}R_{cc'}\frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}}\left[I'_{c'}(k_{c'}a)\delta_{ci}-U_{c'i}O'_{c'}(k_{c'}a)\right]=\frac{1}{\sqrt{\mu_c v_c}}\left[I_c(k_c a)\delta_{ci}-U_{ci}O_c(k_c a)\right]$$

- In the process introduce *R*-matrix, projection of the Green's function operator on the channel-surface functions

$$R_{cc'}=\sum_{nn'}\frac{\hbar}{\sqrt{2\mu_c a}}f_n(a)\left[C-EI\right]^{-1}_{cn,c'n'}\frac{\hbar}{\sqrt{2\mu_{c'}a}}f_{n'}(a)$$

TRIUMF

To find the Scattering matrix

3. Solve equation with respect to the scattering matrix U

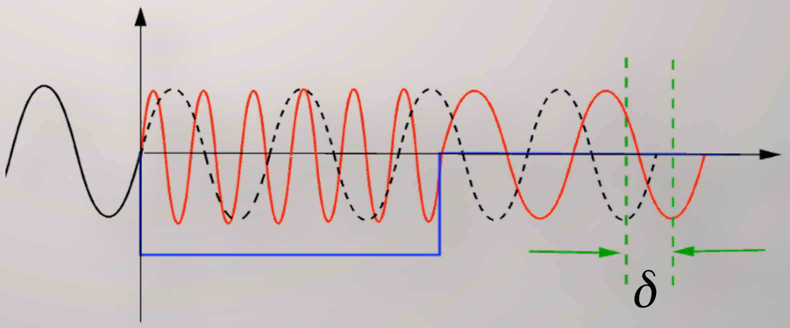
$$\sum_{c'} R_{cc'} \frac{k_{c'}a}{\sqrt{\mu_{c'} v_{c'}}} \left[I'_{c'}(k_{c'}a)\delta_{ci} - U_{c'i} O'_{c'}(k_{c'}a) \right] = \frac{1}{\sqrt{\mu_c v_c}} \left[I_c(k_c a)\delta_{ci} - U_{ci} O_c(k_c a) \right]$$

4. You can demonstrate that the solution is given by:

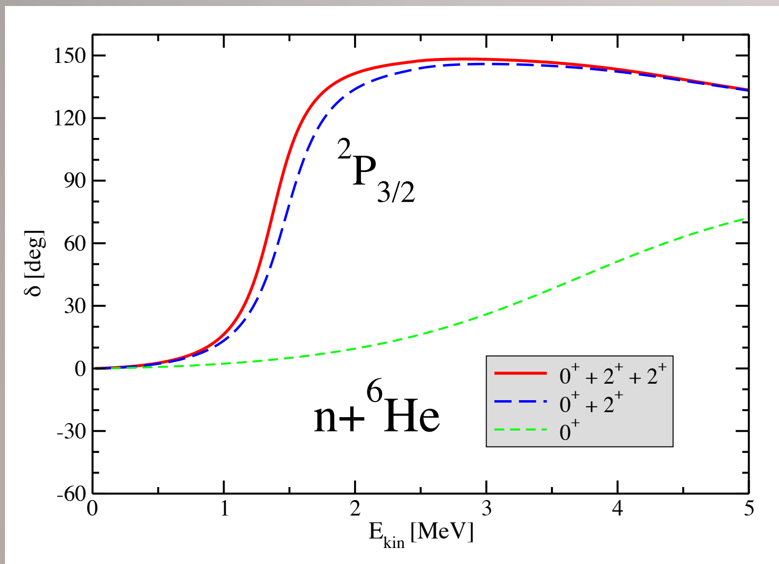
$$U = Z^{-1} Z^{*}, \qquad Z_{cc'} = \left(k_{c'}a\right)^{-1} \left[O_c(k_c a)\delta_{cc'} - k_{c'}a\, R_{cc'}\, O'_{c'}(k_{c'}a) \right]$$

- Scattering phase shifts are extracted from the scattering matrix elements

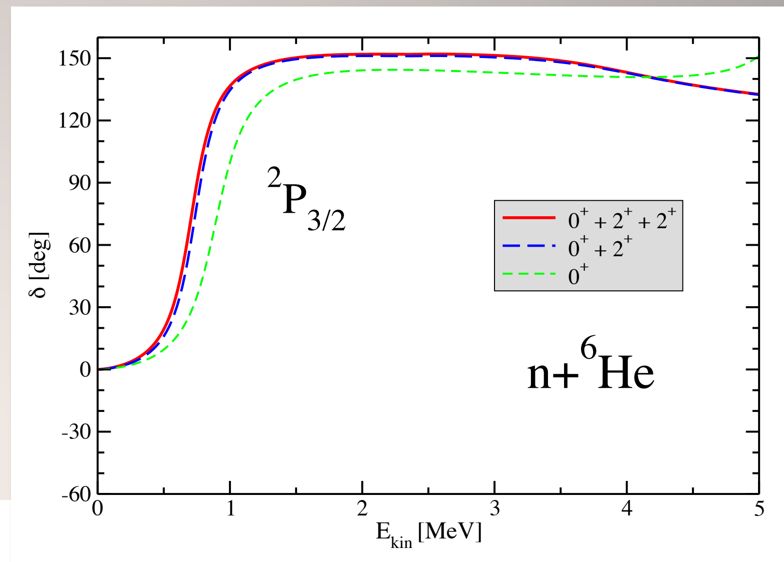
$$U = \exp(2i\delta)$$



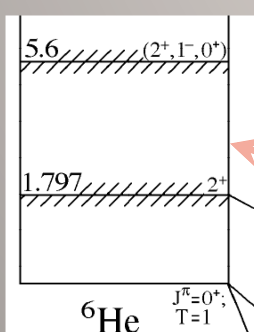
NCSM with continuum: ^{7}He ↔ ^{6}He+*n*



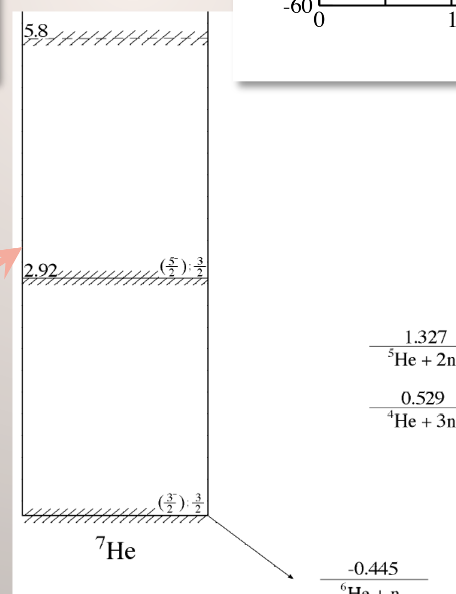
NCSM/RGM
with up to three ^{6}He states



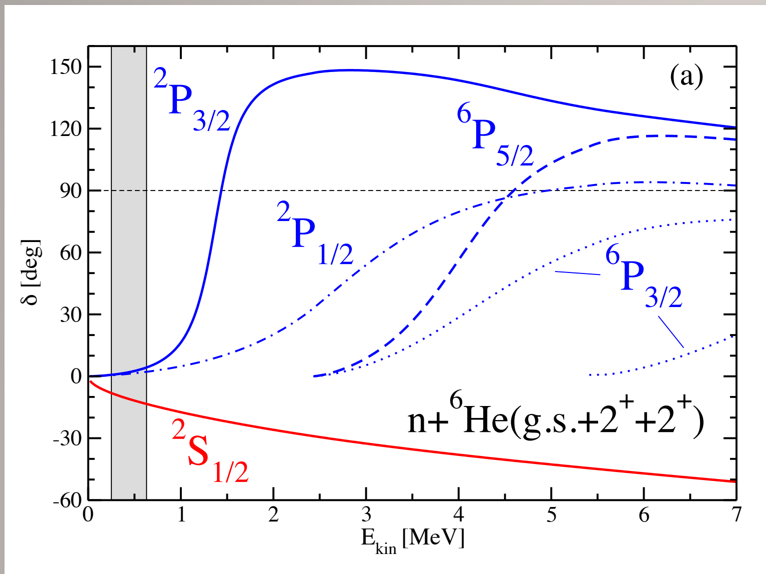
NCSMC
with up to three ^{6}He states
and four ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed

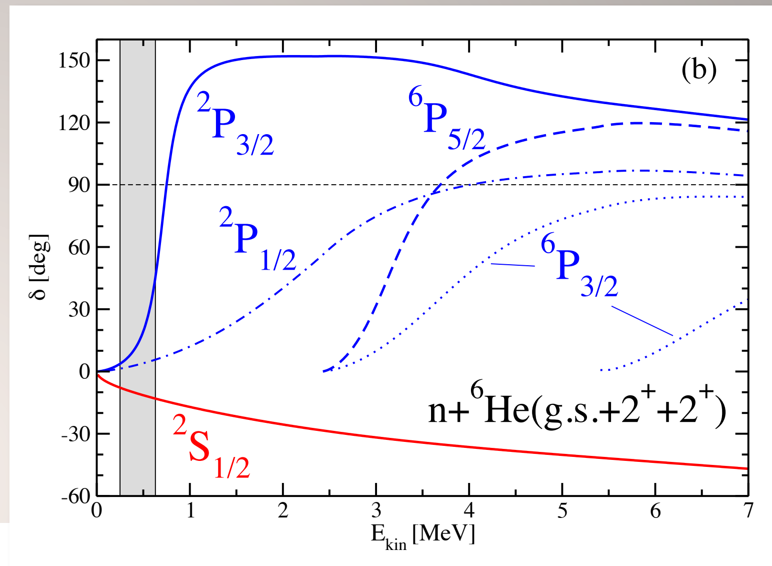


Expt.



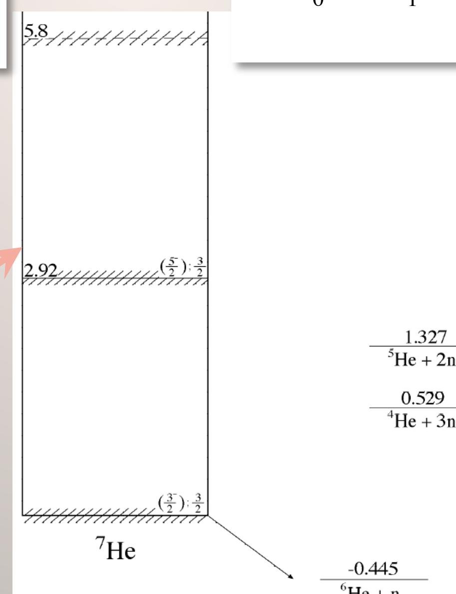
NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+*n*



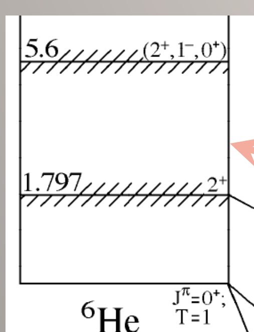


NCSM/RGM
with three ^{6}He states

NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed



Expt.



^{7}He: NCSMC vs. NCSM/RGM vs. NCSM

J^π	experiment			NCSMC		NCSM/RGM		NCSM
	E_R	Γ	Ref.	E_R	Γ	E_R	Γ	E_R
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30	1.39	0.46	1.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07	4.00	1.75	4.56
$1/2^-$	3.03(10)	2	[11]	2.39	2.89	2.66	3.02	3.26
	3.53	10	[15]					
	1.0(1)	0.75(8)	[5]					

[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

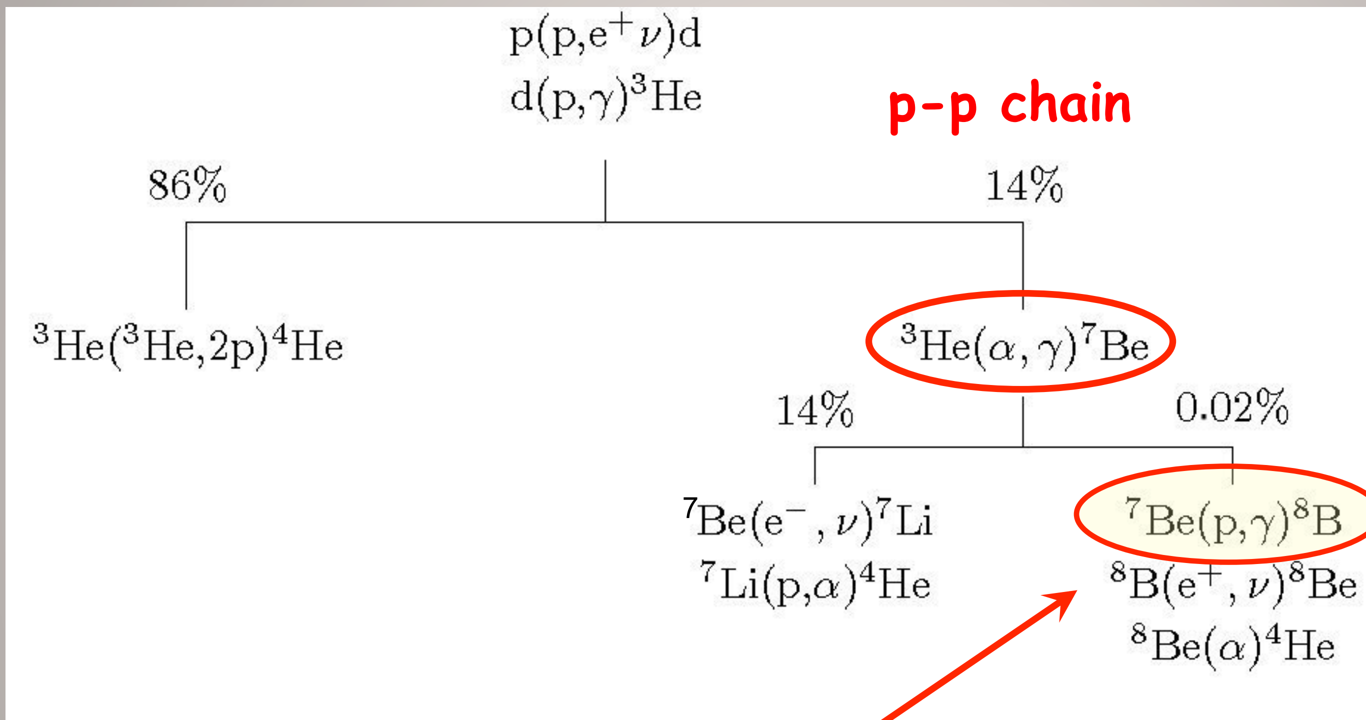
- NCSMC and NSCM/RGM energies where phase shift derivative maximal
- NCSMC and NSCM/RGM widths from the derivatives of phase shifts

$$\Gamma = \left.\frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\right|_{E_{kin}=E_R}$$

Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

Best agreement with the neutron pick-up and proton-removal reactions experiments [11]

Solar *p-p* chain



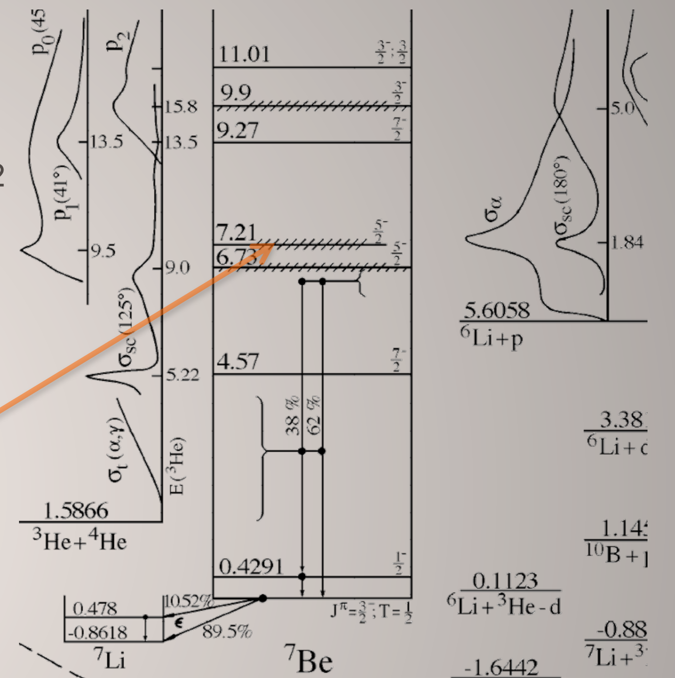
Solar neutrinos

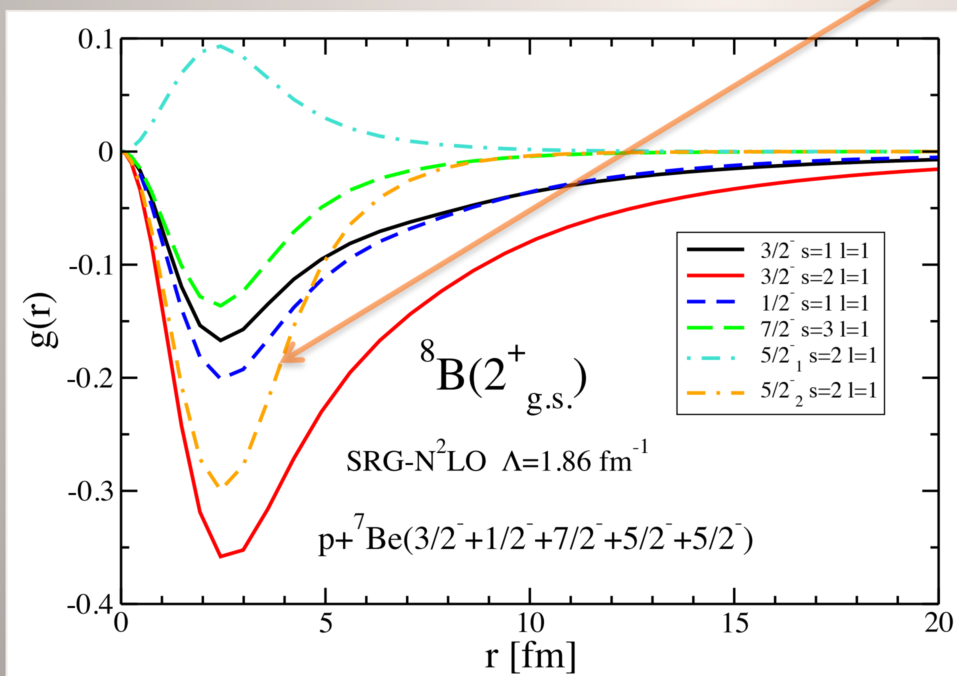
E_ν < 15 MeV

TRIUMF

Structure of the ^{8}B ground state

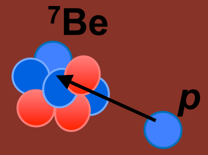
- NCSM/RGM *p*-^{7}Be calculation
  - five lowest ^{7}Be states: $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN SRG-N^{3}LO with Λ = 1.86 fm^{-1}
- ^{8}B 2$^+$ g.s. bound by 136 keV (Expt 137 keV)
  - Large *P*-wave $5/2^-_2$ component





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

TRIUMF



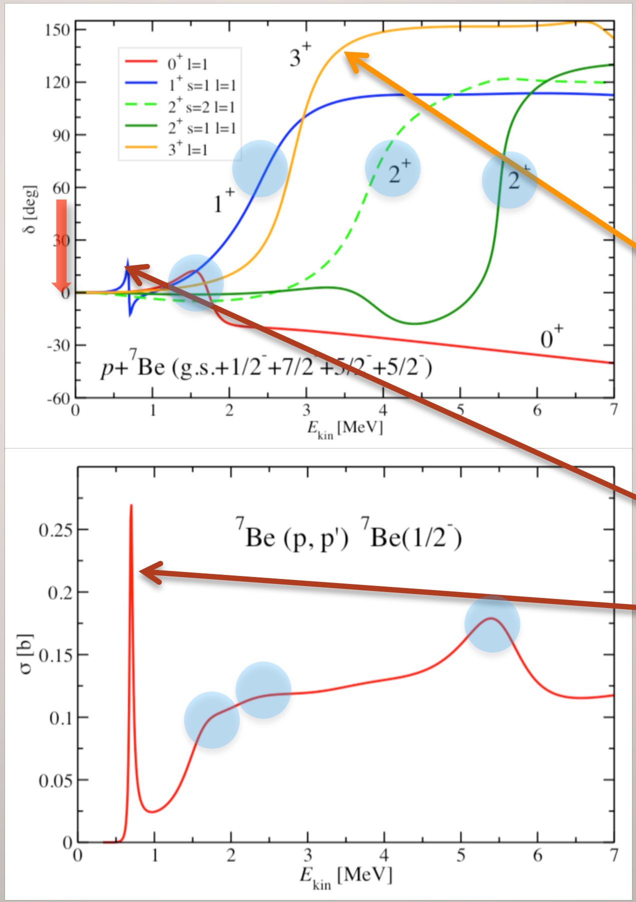
p-^{7}Be scattering

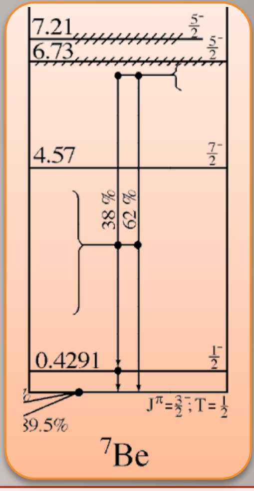
- NCSM/RGM calculation of *p*-^{7}Be scattering
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

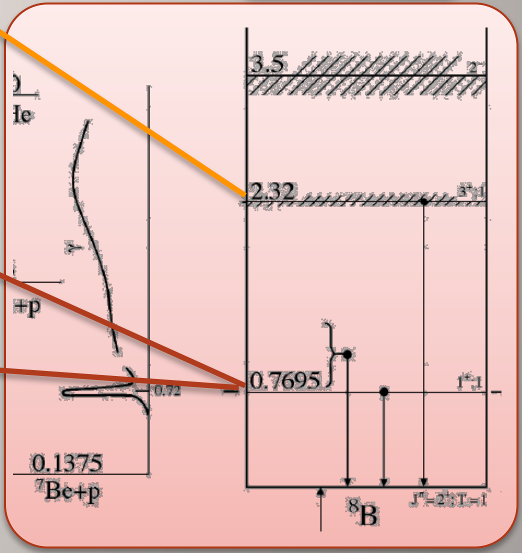
^{8}B 2^+ g.s. **bound** by 136 keV (expt. bound by 137 keV)

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

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







PRC **82**, 034609 (2010)
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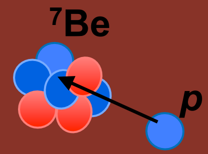
TRIUMF



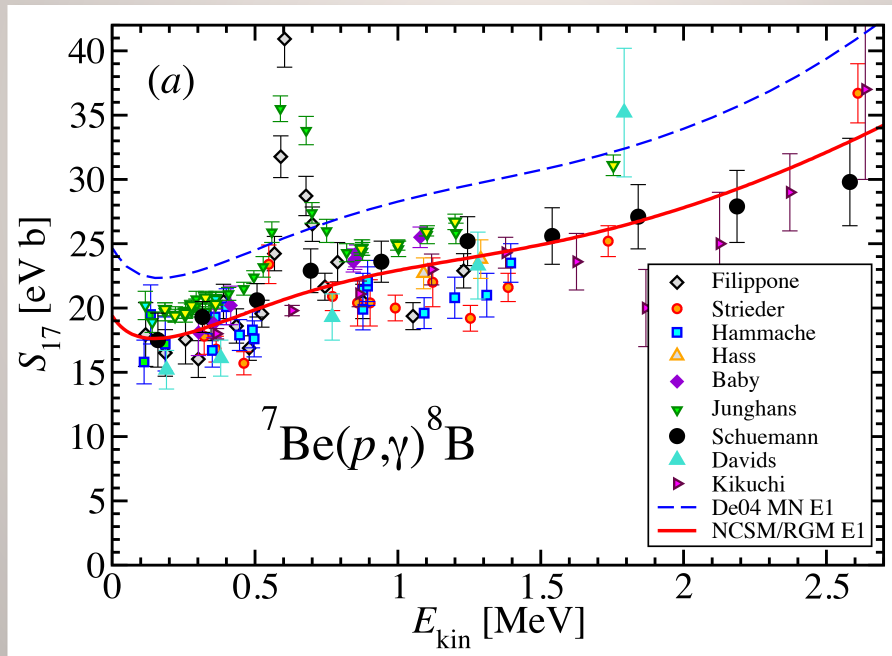
$^{7}Be(p,\gamma)^{8}B$ radiative capture

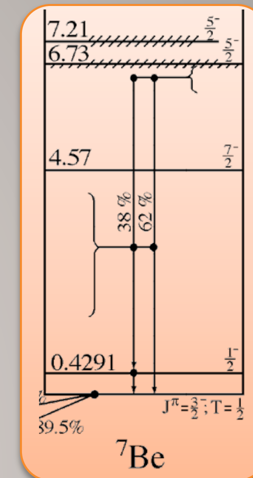
- NCSM/RGM calculation
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (chiral SRG-N^{3}LO with Λ = 1.86 fm^{-1})

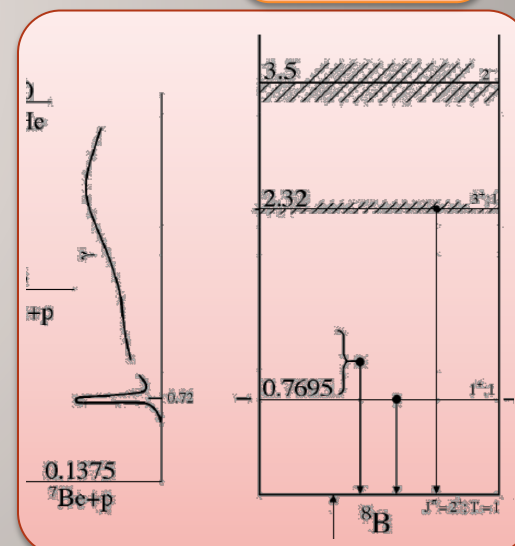
^{8}B 2^+ g.s. **bound** by 136 keV
(expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

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







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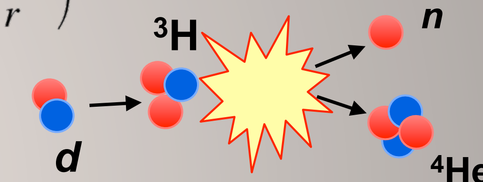
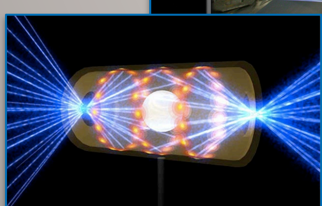
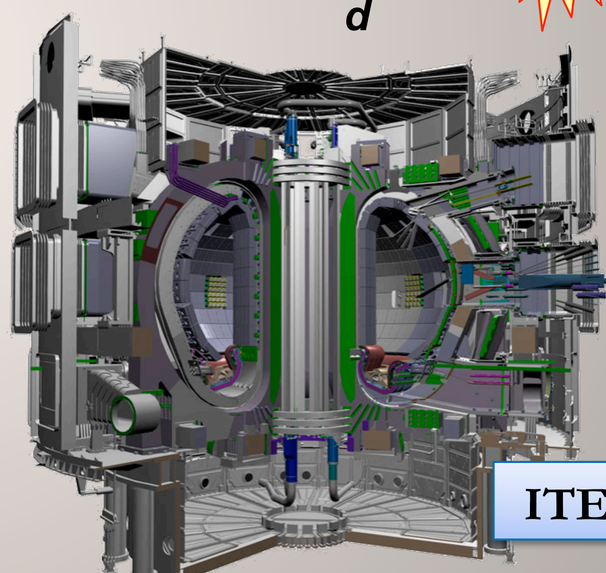
Ab initio calculation of the ^{3}H(d,n)^{4}He fusion

$$\int dr\, r^2 \begin{pmatrix} \left\langle {}^{r'}_{n}\ \alpha \right| \hat{A}_1 (H-E) \hat{A}_1 \left| \alpha\ {}^{r}_{n} \right\rangle & \left\langle {}^{r'}_{n}\ \alpha \right| \hat{A}_1 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\ {}^{r}_{d} \right\rangle \\ \left\langle {}^{r'}_{d}\ {}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_1 \left| \alpha\ {}^{r}_{n} \right\rangle & \left\langle {}^{r'}_{d}\ {}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\ {}^{r}_{d} \right\rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$





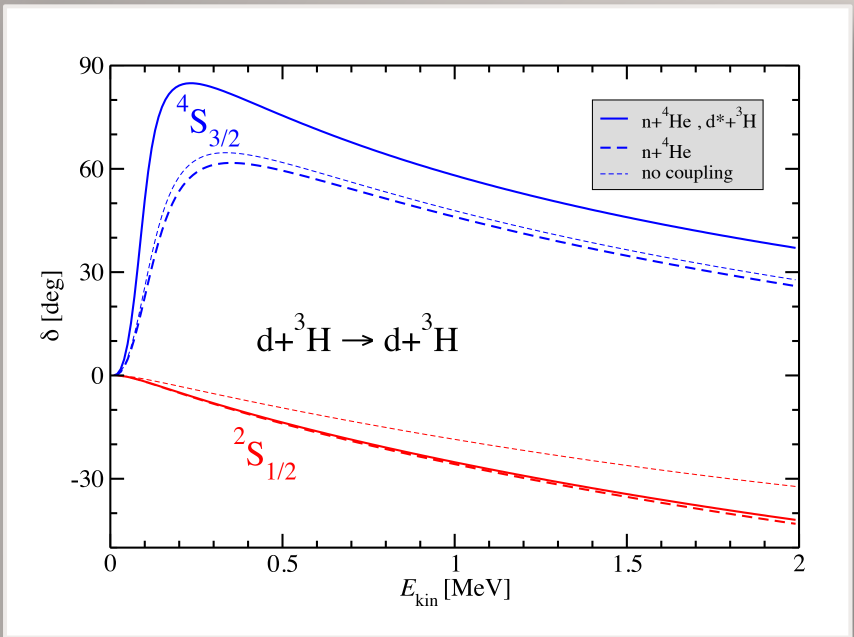
NIF

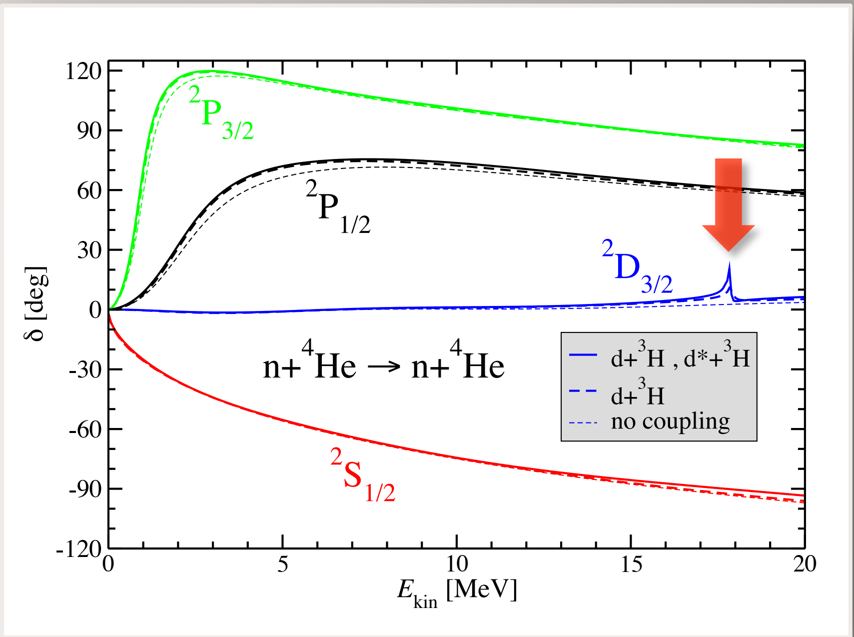


ITER

energy generation

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

d^* deuteron pseudo state in $^3S_1$-$^3D_1$ channel: deuteron polarization, virtual breakup

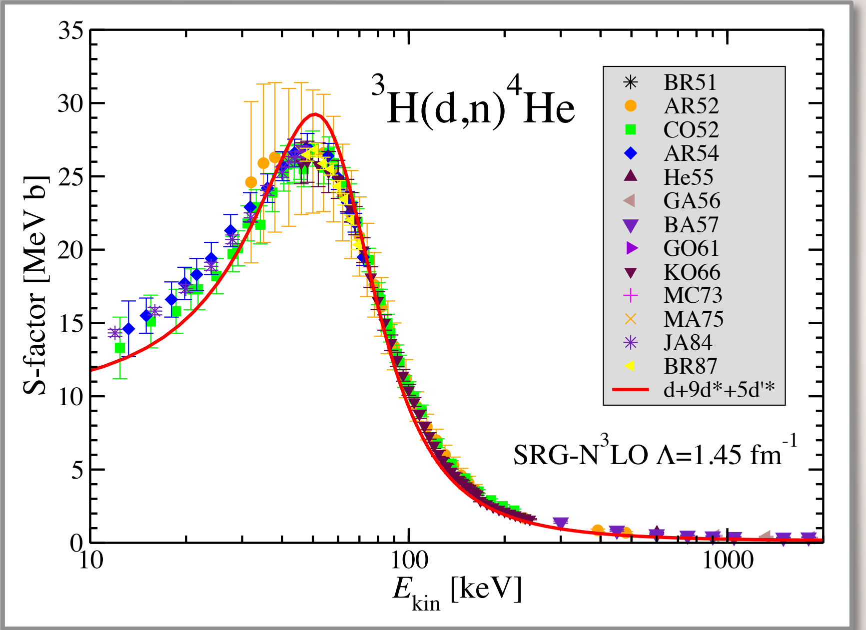
- n+^{4}He elastic phase shifts:
  - d+^{3}H channels produces slight increase of the P phase shifts
  - Appearance of resonance in the 3/2$^+$ D-wave, just above d-^{3}H threshold

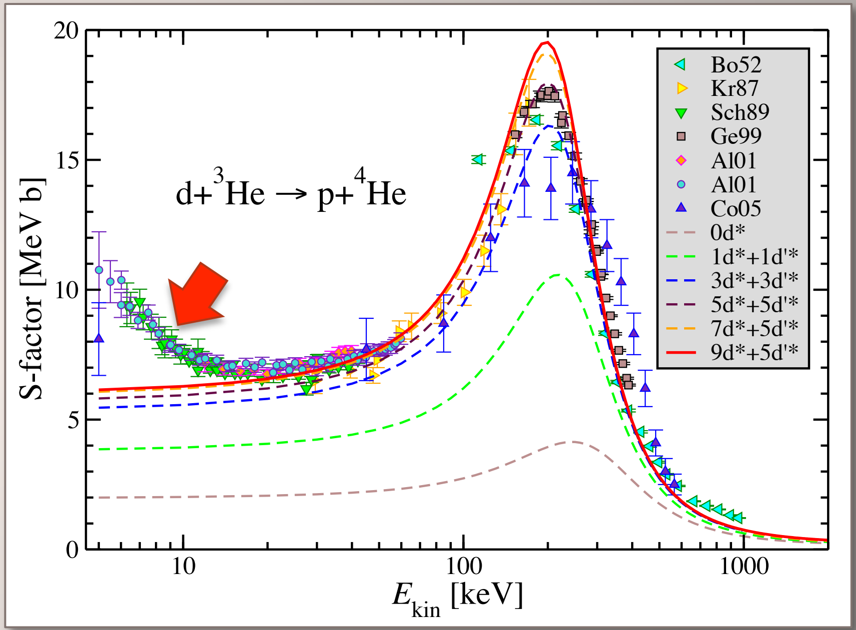
The d-^{3}H fusion takes place through a transition of d+^{3}H is S-wave to n+^{4}He in D-wave: Importance of the **tensor force**

TRIUMF

$^3H(d,n)^4He$ & $^3He(d,p)^4He$ fusion

- NCSM/RGM with *SRG-N^{3}LO NN* potentials





Potential to address unresolved fusion research related questions:
^{3}H(*d*,*n*)^{4}He fusion with polarized deuterium and/or tritium,
^{3}H(*d*,*n* γ)^{4}He bremsstrahlung,
Electron screening at very low energies …

P.N., S. Quaglioni,
PRL **108**, 042503 (2012)

Conclusions and Outlook

- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM

PRL **110**, 022505 (2013)

- We demonstrated its capabilities in calculations of ^{7}He resonances

- Successful NCSM/RGM applications to
  - ^{7}Be(p,γ)^{8}B radiative capture
  - ^{3}H(d,n)^{4}He and fusion

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PRL **108**, 042503 (2012)

- Outlook:
  - Inclusion of 3N interactions – first results available for n-^{4}He, p-^{4}He
  - Extension of the NCSMC formalism to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Extension of the formalism to coupling of three-body clusters (^{6}He ~ ^{4}He+n+n)

NCSMC and NCSM/RGM collaborators

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G. Hupin, M. Kruse (LLNL)

S. Baroni (ULB)

W. Horiuchi (Hokkaido)

Possible future benchmark: d-^{3}H fusion

- Calculation of the ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He using the NCSMC formalism and chiral NN+3N forces is within the reach
  - sensitive test of the chiral nuclear Hamiltonian
  - complex reaction mechanism
  - sensitive to the treatment of virtual excitations of the involved nuclei
    - many-nucleon dynamics in the continuum

- Benchmark with lattice QCD *ab initio* calculations beneficial for both the standard nuclear calculations and the lattice QCD many-nucleon calculations

- Physics issue:
  - Behavior of the d-^{3}H and n-^{4}He phase shifts at the resonance