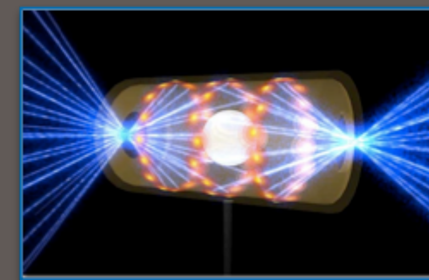
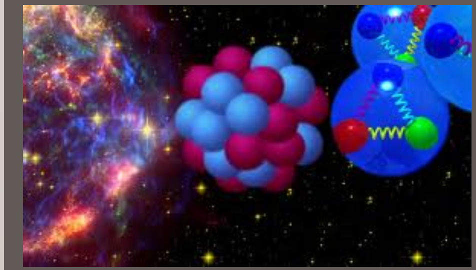
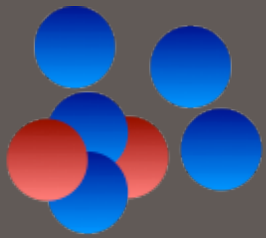
Ab initio description of the unbound ^{7}He

INT program INT-12-3
"Light nuclei from first principles"
15th October 2012, Institute for Nuclear Theory

Petr Navratil | TRIUMF

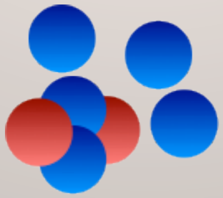






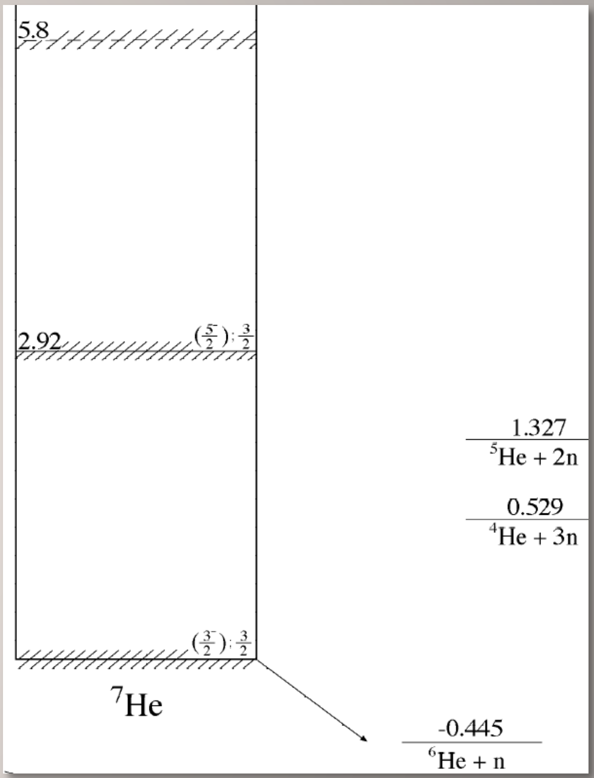
Outline

- Why ^{7}He?
- No-core shell model calculations for neutron rich He isotopes
- Introducing no-core shell model with continuum (NCSMC)
- ^{7}He calculations: Comparison of NCSM/RGM and NCSMC
- ^{7}He predictions and comparison to experiment
- Outlook



Unbound exotic ^{7}He

- Experimental situation
  - $3/2^-$ g.s. resonance at 0.43 MeV above *n* + ^{6}He
    - ^{6}He Borromean halo system
  - $5/2^-$ resonance established
  - Controversy about $1/2^-$ resonance
    - Low-lying narrow
    - Broad at 3 MeV
    - Extremely broad



Experiments very challenging: three-body background

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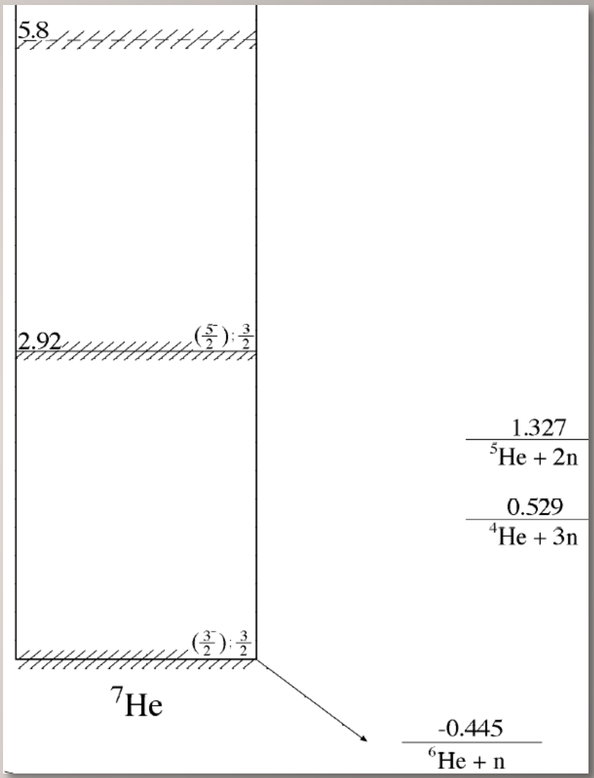
Unbound exotic ^{7}He

- Experimental situation
  - Controversy about 1/2$^-$ resonance
    - Low-lying narrow [^{8}He+^{12}C fragmentation]
    - Broad at 3 MeV [*d*(^{6}He,*p*)^{7}He,^{2}H(^{8}Li,^{3}He)^{7}He]
    - Extremely broad [*p*+^{6}He: isospin analog]

J^π	experiment		
	E_R	Γ	Ref.
$3/2^-$	0.430(3)	0.182(5)	[2]
$5/2^-$	3.35(10)	1.99(17)	[40]
$1/2^-$	3.03(10)	2	[11]
	3.53	10	[15]
	1.0(1)	0.75(8)	[5]



[5] M. Meister *et al.*, Phys. Rev. Lett. **88**, 102501 (2002).

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

[15] P. Boutachkov *et al.*, Phys. Rev. Lett. **95**, 132502 (2005).

Ab initio calculations based on bound-state techniques cannot give any insight

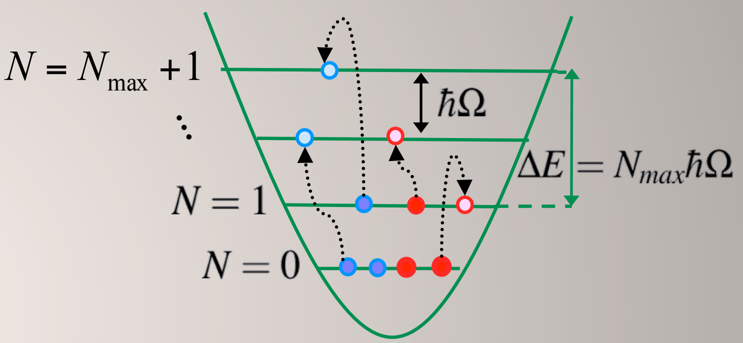
Chiral Effective Field Theory

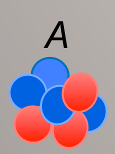
- **First principles for Nuclear Physics:**
  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future
- ***For now a good place to start*:**
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), 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

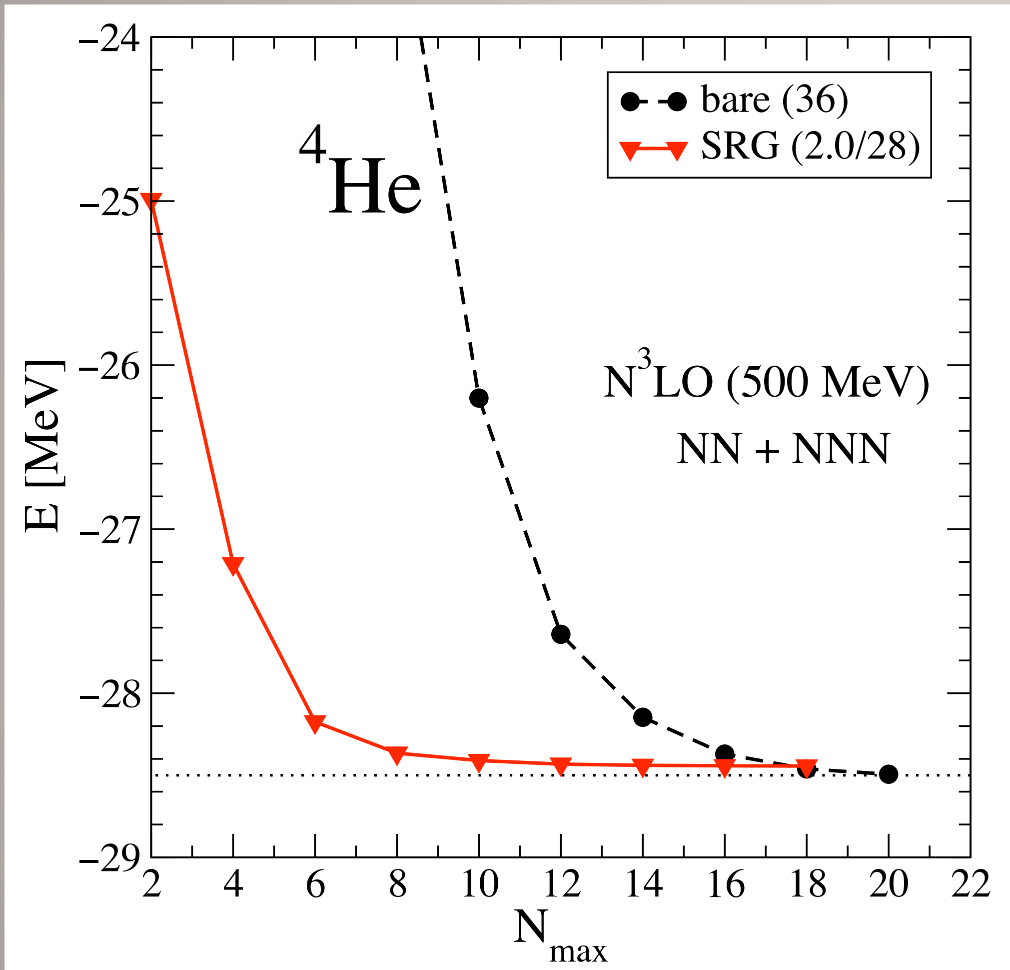




$$\Psi^A = \sum_{N=0}^{N_{max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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

^{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

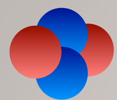
Chiral N^{3}LO NN plus N^{2}LO NNN potential

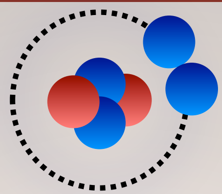
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

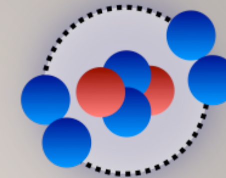
$$H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = [[T, H_\alpha], H_\alpha] \quad \left(\alpha = 1/\lambda^4\right)$$

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

NNN interaction effects in neutron rich nuclei: He isotopes

^{4}He 

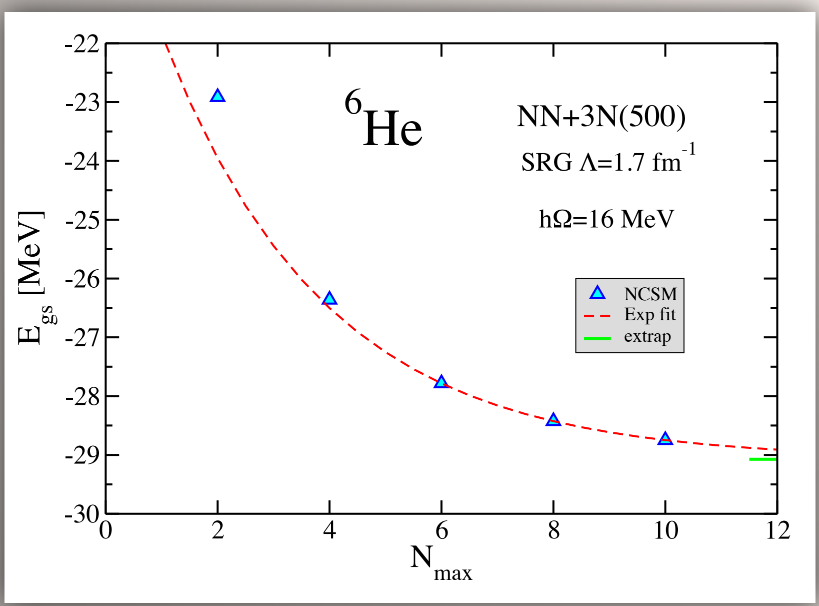
^{6}He 

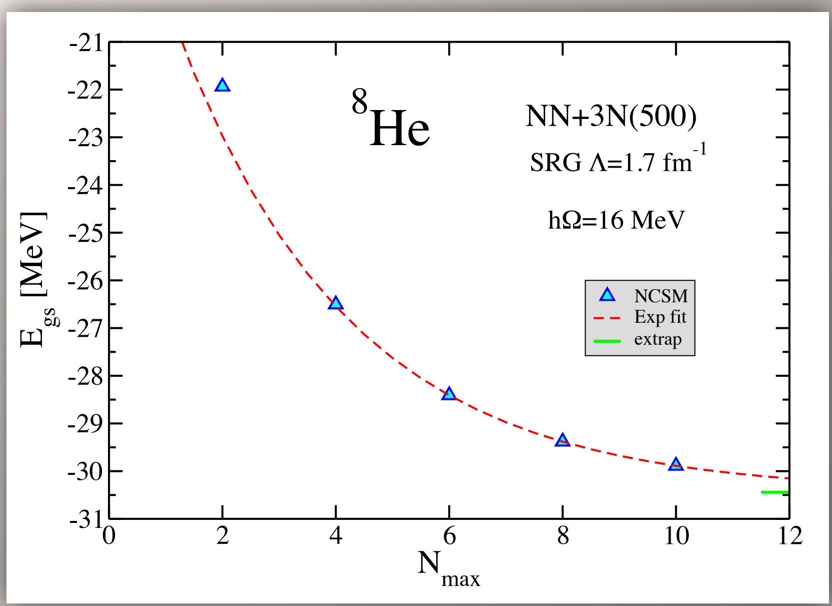
^{8}He 

^{6}He and ^{8}He with SRG-evolved chiral N^{3}LO NN + N^{2}LO NNN

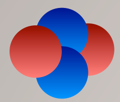
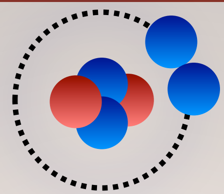
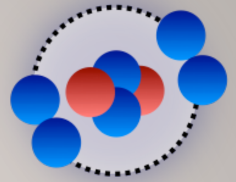
A=3 binding energy & half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

– 3N matrix elements in coupled-*J* single-particle basis:
  - Introduced and implemented by Robert Roth *et al.*
  - Now also in my codes: Jacobi-Slater-Determinant transformation & NCSD code
  - Example: ^{6}He, ^{8}He NCSM calculations up to N_{max}=10 done with moderate resources





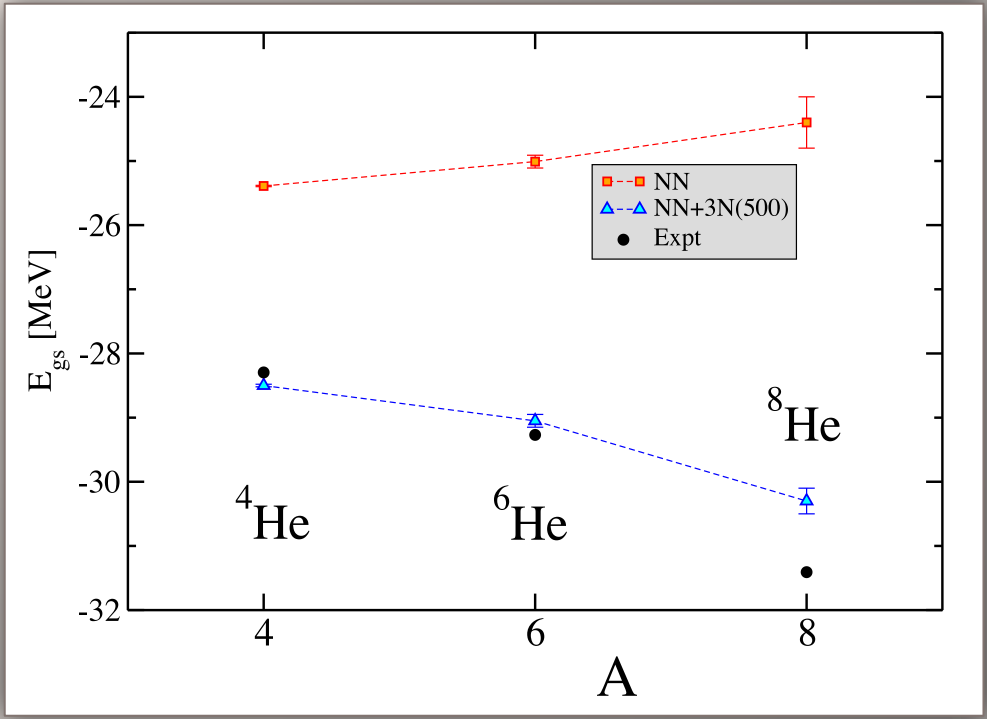
3N interaction effects in neutron rich nuclei: He isotopes

^{4}He  ^{6}He  ^{8}He 

- ^{6}He and ^{8}He with SRG-evolved chiral N^{3}LO NN + N^{2}LO 3N
  - chiral N^{3}LO NN: ^{4}He underbound, ^{6}He and ^{8}He unbound
  - chiral N^{3}LO NN + N^{2}LO 3N(500): ^{4}He OK, both ^{6}He and ^{8}He bound

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

NNN interaction important to bind neutron rich nuclei



3N interaction effects in neutron rich nuclei: He isotopes

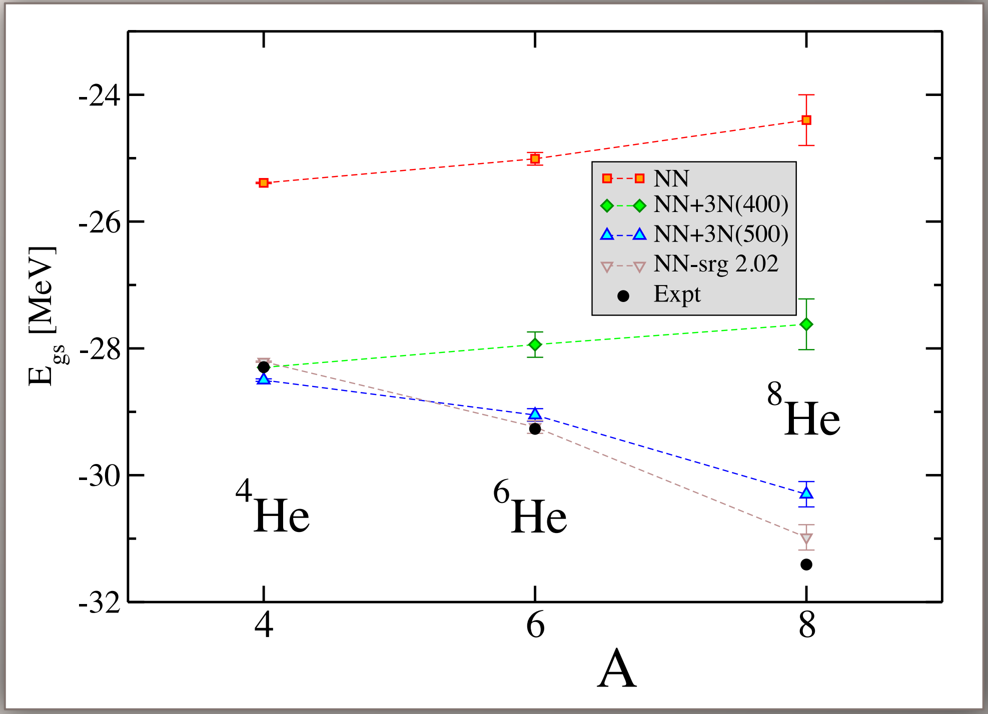
- ^{6}He and ^{8}He with SRG-evolved chiral N^{3}LO NN + N^{2}LO 3N
  - chiral N^{3}LO NN: ^{4}He underbound, ^{6}He and ^{8}He unbound
  - chiral N^{3}LO NN + N^{2}LO 3N(400): ^{4}He fitted, ^{6}He barely unbound, ^{8}He unbound
    - describes quite well binding energies of ^{12}C, ^{16}O, ^{40}Ca, ^{48}Ca
  - chiral N^{3}LO NN + N^{2}LO 3N(500): ^{4}He OK, both ^{6}He and ^{8}He bound
    - does well up to *A*=10, overbinds ^{12}C, ^{16}O, Ca isotopes
  - SRG-N^{3}LO NN Λ=2.02 fm^{-1}: ^{4}He OK, both ^{6}He and ^{8}He bound
    - ^{16}O, Ca strongly overbound

^{4}He binding energy & ^{3}H half life constraint
c_D=-0.2, c_E=+0.098, Λ=400 MeV

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

NNN interaction important to bind neutron rich nuclei

Our knowledge of the 3N interaction is incomplete



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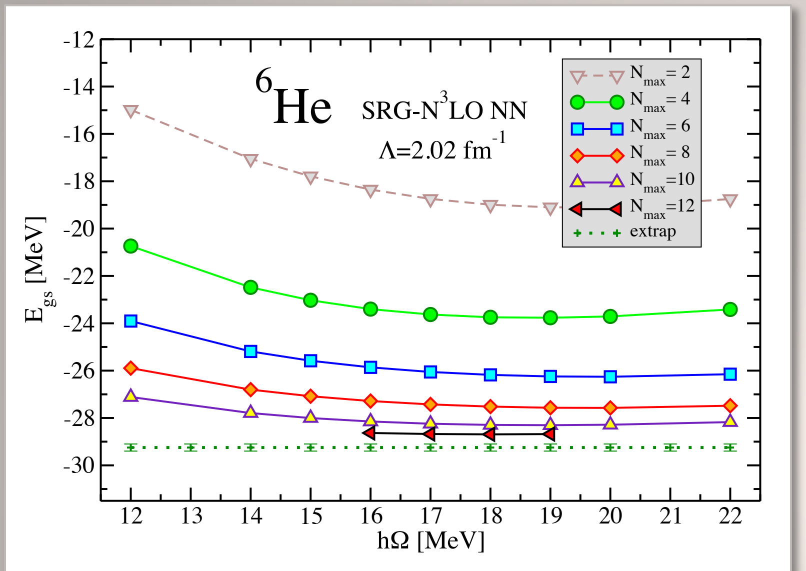
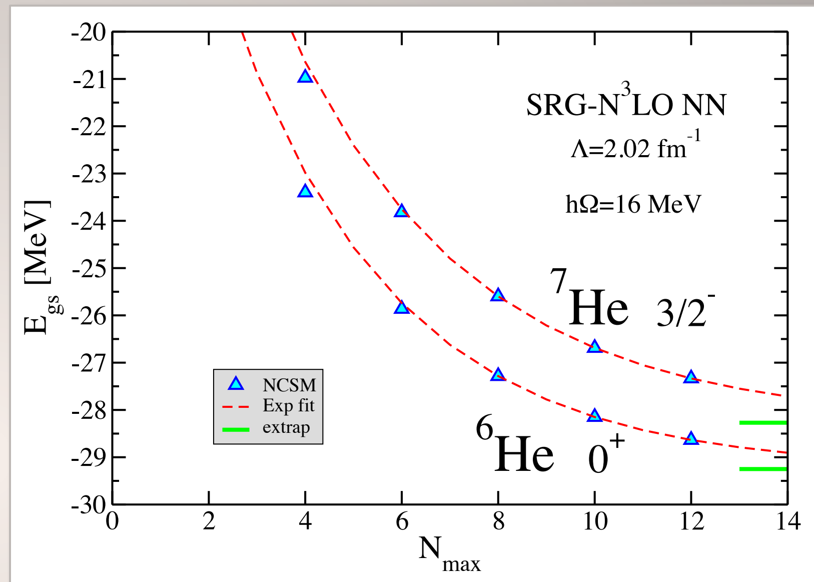
NCSM calculations of ^{6}He and ^{7}He g.s. energies

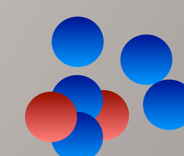




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ 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

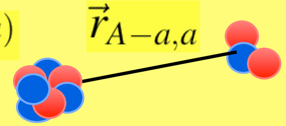


unbound

The *ab initio* NCSM/RGM in a snapshot

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

$(A-a)$ $\vec{r}_{A-a,a}$ (a)



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

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

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

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

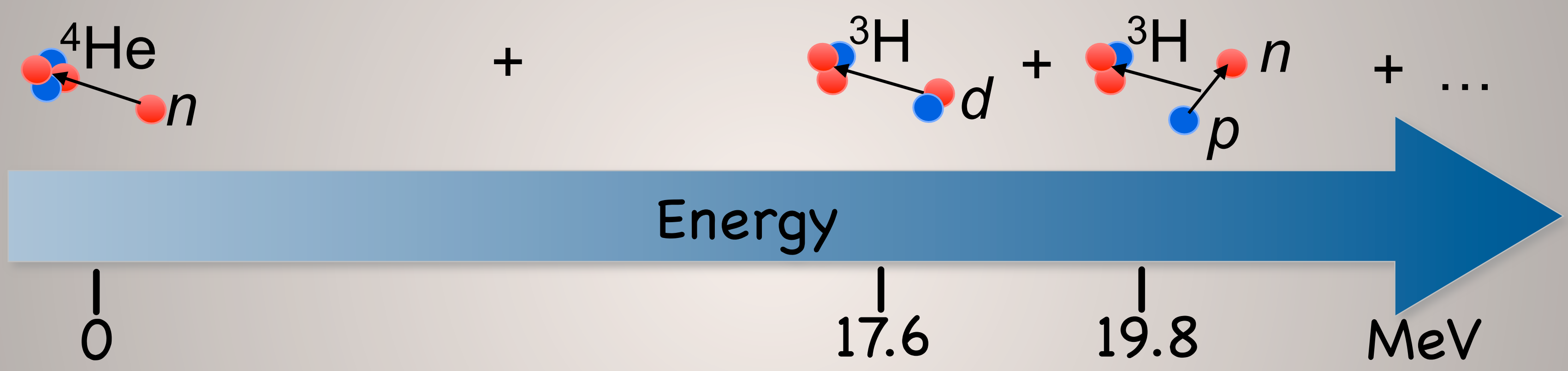
Hamiltonian kernel

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

Norm kernel

Example: the five-nucleon system

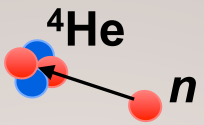
- Consider the T = ½ case: ^{5}He (^{5}Li)
  - Five-nucleon cluster unbound; ^{4}He tightly bound, not easy to deform

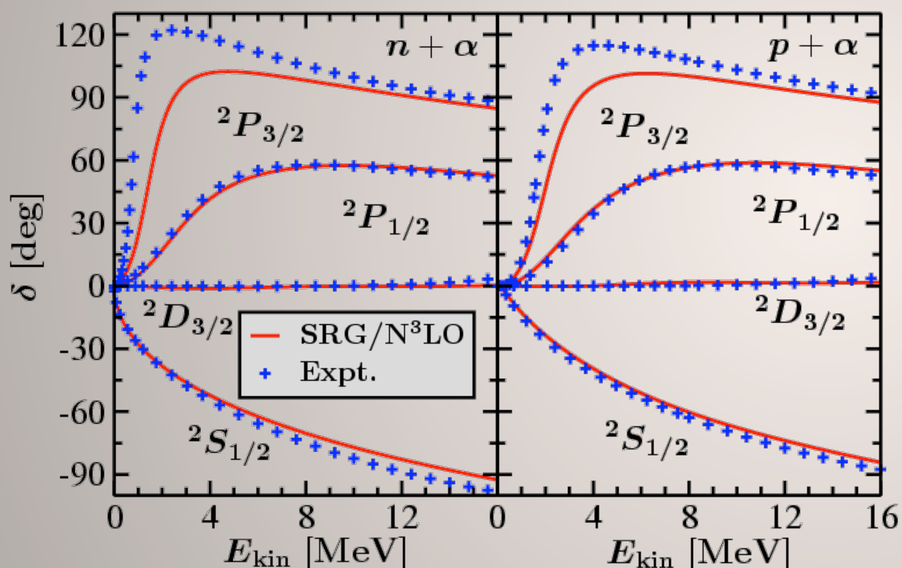


- Satisfactory description of *n*-^{4}He (*p*-^{4}He) scattering at low excitation energies within single-channel approximation
- However, both *n*(*p*) + ^{4}He and *d* + ^{3}H(^{3}He) channels needed to describe ^{3}H(*d*,*n*)^{4}He [^{3}He(*d*,*p*)^{4}He] fusion!

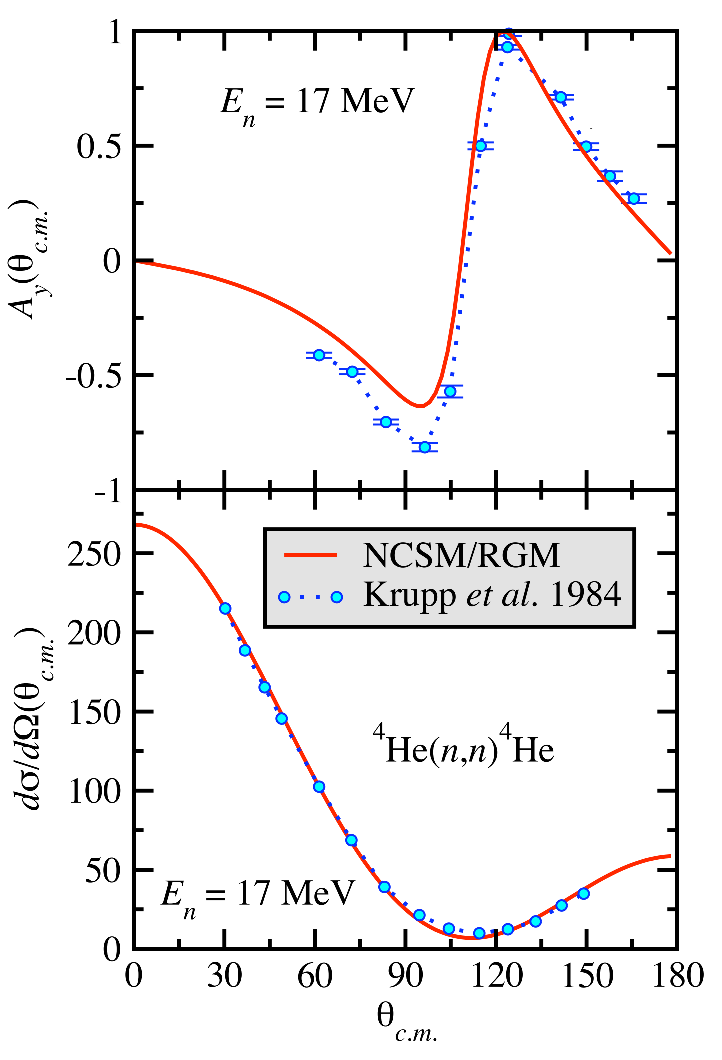
Unbound A=5 nuclei: ^{5}He→n+^{4}He, ^{5}Li→p+^{4}He

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



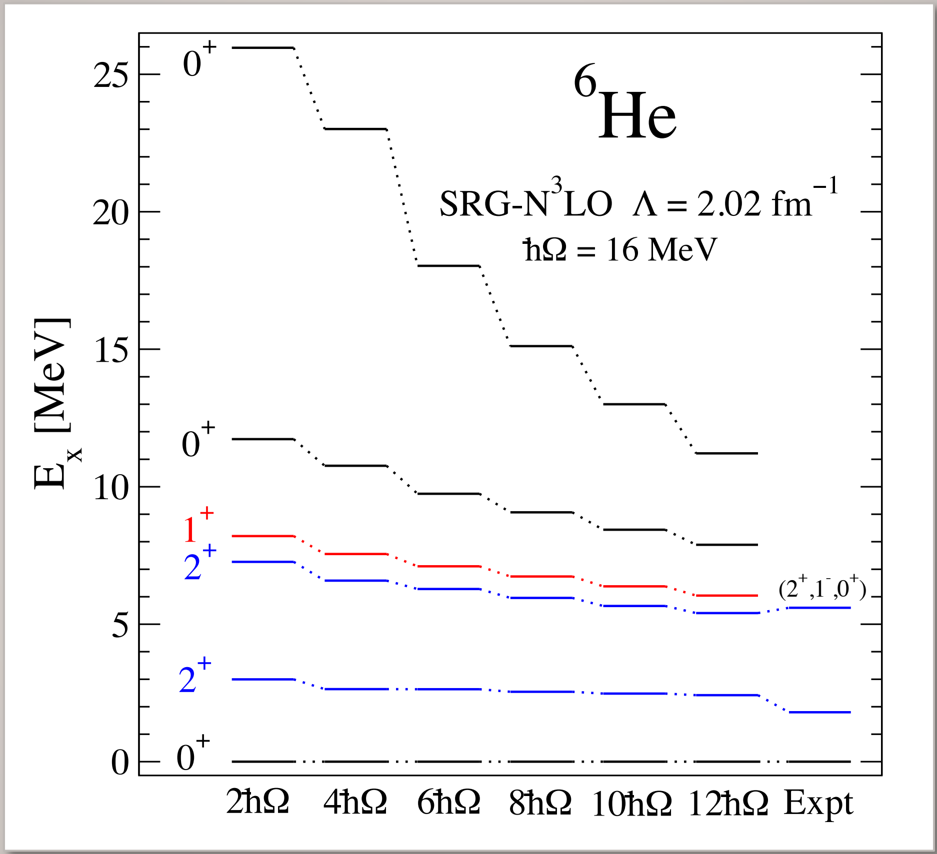


- Differential cross section and analyzing power @17 MeV neutron energy
  - Polarized neutron experiment at Karlsruhe



NNN 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

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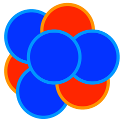
New approach: NCSM with continuum

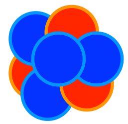
NCSM



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

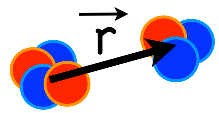
New developments: NCSM with continuum

NCSM



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

NCSM/RGM



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

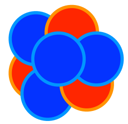
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

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

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

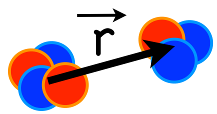
New developments: NCSM with continuum

NCSM



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

NCSM/RGM



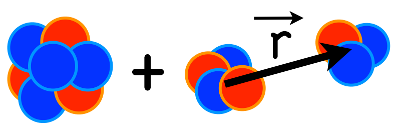
$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

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

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

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

NCSMC



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

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

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

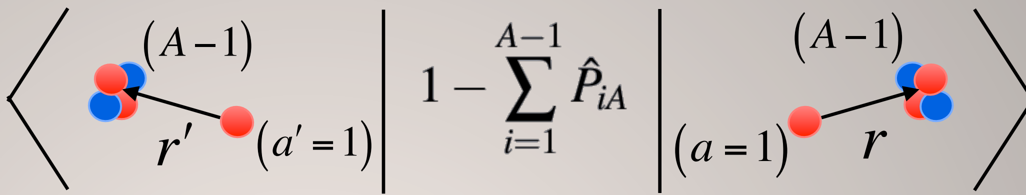
$$\delta(r-r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

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

Norm kernel (Pauli principle)

Single-nucleon projectile

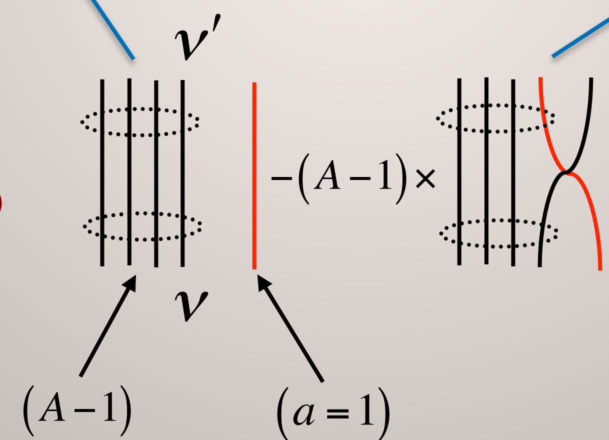
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



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

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

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

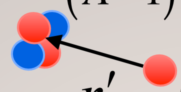
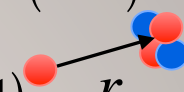


Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

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

Hamiltonian kernel (projectile-target potentials)

Single-nucleon projectile

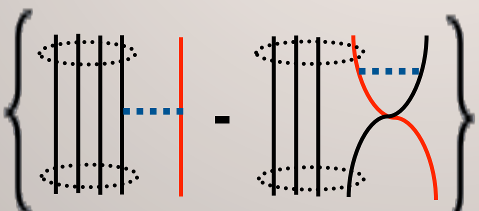
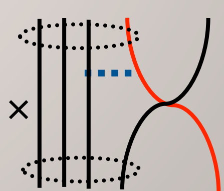



$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} H \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-1)\; r'\; (a'=1) \middle| H\left(1-\sum_{i=1}^{A-1}\hat{P}_{iA}\right) \middle| (a=1)\; r\; (A-1) \right\rangle$$

$$H^{J^\pi T}_{\nu'\nu}(r',r) = \left[T_{rel}(r) + \bar{V}_{Coul}(r) + \varepsilon^{I_1'^{\pi_1'} T_1'}_{\alpha_1'}\right] N^{J^\pi T}_{\nu'\nu}(r',r)$$

$$+ (A-1)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| V_{A-1,A}\left(1-\hat{P}_{A-1,A}\right) \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$$- (A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} V_{A-2,A-1} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$+(A-1)\times$  $-(A-1)(A-2)\times$ 

Direct potential: in the model space (interaction is localized!)

Exchange potential: in the model space

Introduce SD channel states in the HO space

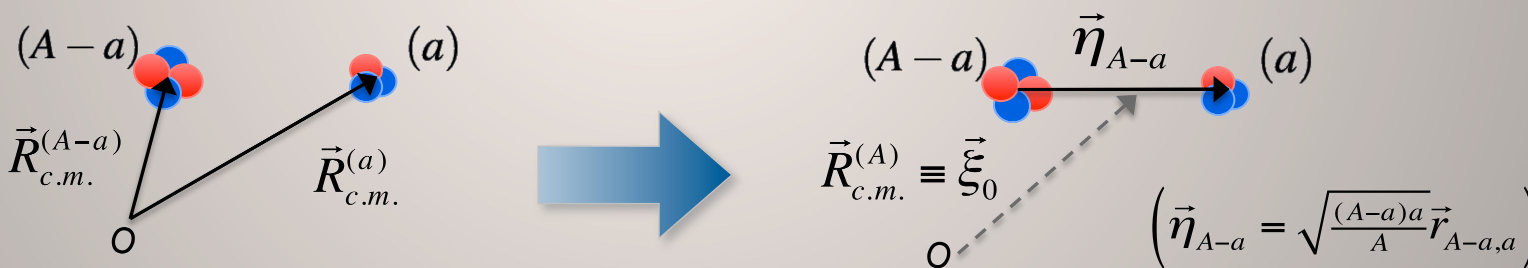
- Define SD channel states in which the eigenstates of the heaviest of the two clusters (target) are described by a SD wave function:

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

$$\left|A-a\;\alpha_1 I_1^{\pi_1}T_1\right\rangle \varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)$$

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

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



$$\left(\varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)\varphi_{n\ell}\left(\vec{R}^{(a)}_{c.m.}\right)\right)^{\ell} = \sum_{n_r\ell_r,NL}\left\langle 00,n\ell,\ell \middle| n_r\ell_r,NL,\ell\right\rangle_{d=\frac{a}{A-a}}\left(\varphi_{n_r\ell_r}\left(\vec{\eta}_{A-a}\right)\varphi_{NL}\left(\vec{\xi}_0\right)\right)^{\ell}$$

Translational invariant matrix elements from SD ones

- More in detail:

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

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

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

$$\times \sum_{NL} \hat{\ell}\hat{\ell}'\hat{J}_r^2 (-1)^{s+\ell-s'-\ell'} \left\{ \begin{array}{ccc} s & \ell_r & J_r \\ L & J & \ell \end{array} \right\} \left\{ \begin{array}{ccc} s' & \ell'_r & J_r \\ L & J & \ell' \end{array} \right\}$$

$$\times \langle 00,n\ell,\ell | n_r\ell_r,NL,\ell\rangle_{d=\frac{a}{A-a}} \langle 00,n'\ell',\ell' | n'_r\ell'_r,NL,\ell'\rangle_{d'=\frac{a'}{A-a'}}$$

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

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 $a = a' = 1$

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

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

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

One-body density matrix elements

TRIUMF

NCSMC formalism

Start from

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

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:

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

^{7}He spectroscopic factors

- Obtained as

$$S_{\lambda\nu} = \sum_n g^2_{\lambda\nu n}$$

- Not the final result to be compared to experiment, rather input in the NCSMC calculations

^{7}He J^{π}	^{6}He$-n(lj)$	NCSM	CK	VMC	GFMC	Exp.
$3/2^-_1$	$0^+ - p\frac{3}{2}$	0.56	0.59	0.53	0.565	0.512(18)[36]
						0.64(9) [50]
						0.37(7) [45]
$3/2^-_1$	$2^+_1 - p\frac{1}{2}$	0.001	0.06	0.006		
$3/2^-_1$	$2^+_1 - p\frac{3}{2}$	1.97	1.15	2.02		
$3/2^-_1$	$2^+_2 - p\frac{1}{2}$	0.12		0.09		
$3/2^-_1$	$2^+_2 - p\frac{3}{2}$	0.42		0.30		
$1/2^-$	$0^+ - p\frac{1}{2}$	0.94	0.69	0.91		
$1/2^-$	$2^+_1 - p\frac{3}{2}$	0.34	0.60	0.26		
$1/2^-$	$2^+_2 - p\frac{3}{2}$	0.93				
$5/2^-$	$2^+_1 - p\frac{1}{2}$	0.77	0.85	0.81		
$5/2^-$	$2^+_1 - p\frac{3}{2}$	0.49	0.52	0.37		
$5/2^-$	$2^+_2 - p\frac{1}{2}$	0.26				
$5/2^-$	$2^+_2 - p\frac{3}{2}$	1.30				
$3/2^-_2$	$0^+ - p\frac{3}{2}$	0.06	0.06	0.05		
$3/2^-_2$	$2^+_1 - p\frac{1}{2}$	1.10	1.05	1.07		
$3/2^-_2$	$2^+_1 - p\frac{3}{2}$	0.08	0.32	0.03		
$3/2^-_2$	$2^+_2 - p\frac{1}{2}$	0.03				
$3/2^-_2$	$2^+_2 - p\frac{3}{2}$	0.25				

NCSMC formalism

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

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

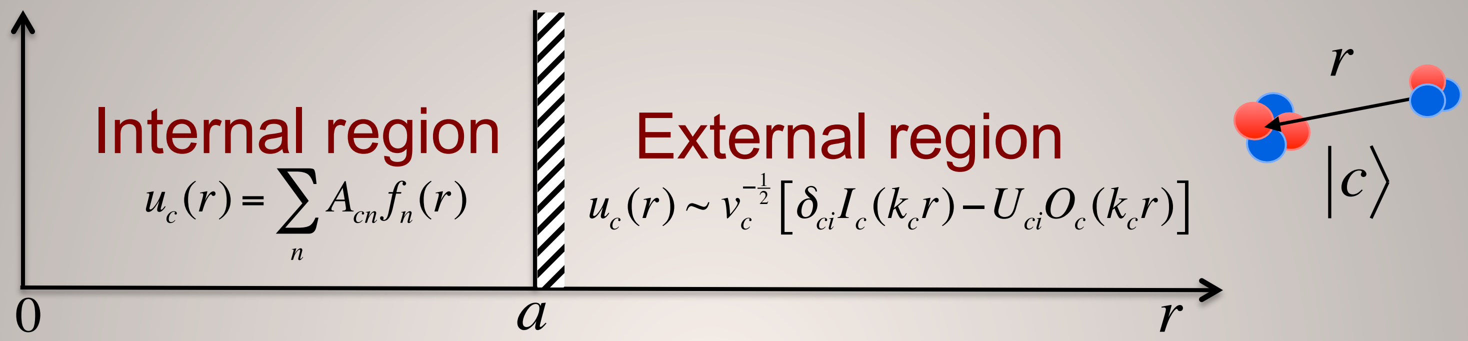
Orthogonalization:
$$\overline{H} = N^{-\frac{1}{2}} \begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} N^{-\frac{1}{2}} \qquad \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = N^{+\frac{1}{2}} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

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

Microscopic *R*-matrix theory

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



- This is achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$
- 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 $u_c(r) = \sum_n A_{cn} f_n(r)$
- External region: asymptotic form for large r

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

Bound state — Scattering state

Scattering matrix

TRIUMF

To find the Scattering matrix

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

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

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

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

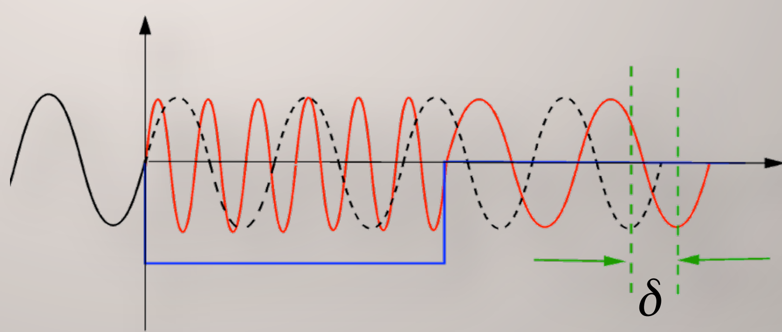
$$\sum_{c'} R_{cc'} \frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}}\left[I'_{c'}(k_{c'}a)\delta_{ci} - U_{c'i}O'_{c'}(k_{c'}a)\right] = \frac{1}{\sqrt{\mu_c v_c}}\left[I_c(k_c a)\delta_{ci} - U_{ci}O_c(k_c a)\right]$$

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

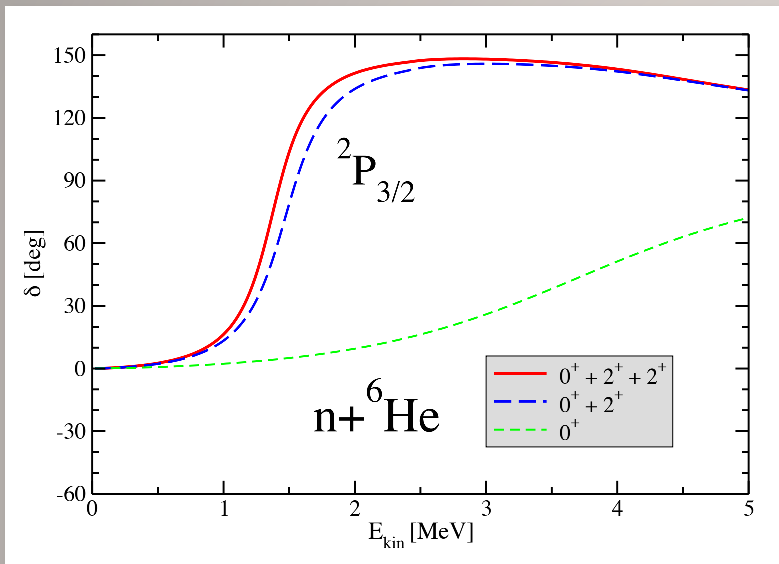
$$U = Z^{-1}Z^*, \qquad Z_{cc'} = \left(k_{c'}a\right)^{-1}\left[O_c(k_c a)\delta_{cc'} - k_{c'}a\, R_{cc'}\, O'_{c'}(k_{c'}a)\right]$$

- Scattering phase shifts are extracted from the scattering matrix elements

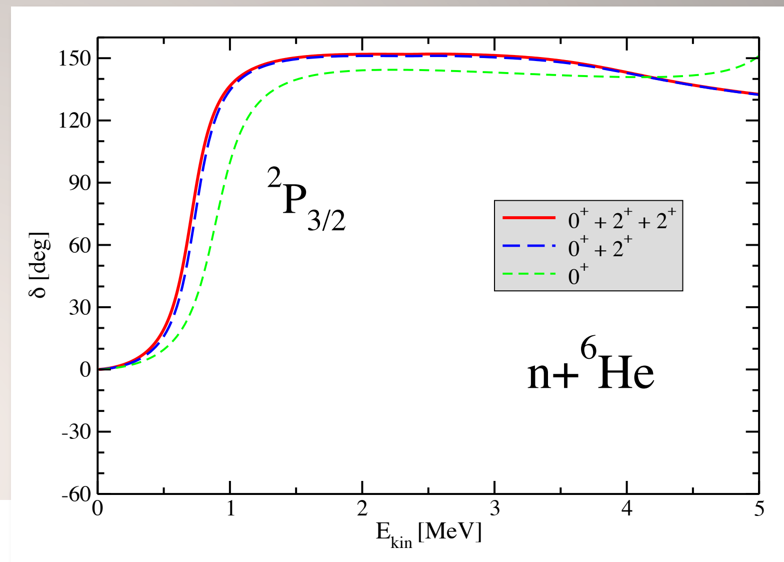
$$U = \exp(2i\delta)$$



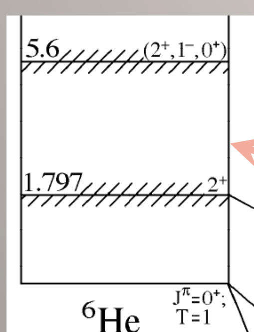
NCSM with continuum: ^{7}He ↔ ^{6}He+n



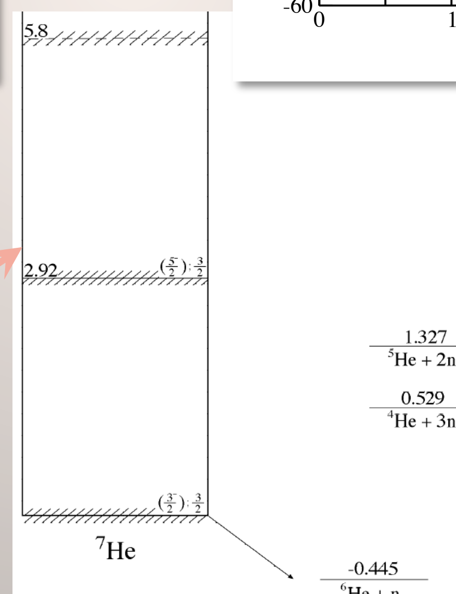
NCSM/RGM
with up to three ^{6}He states



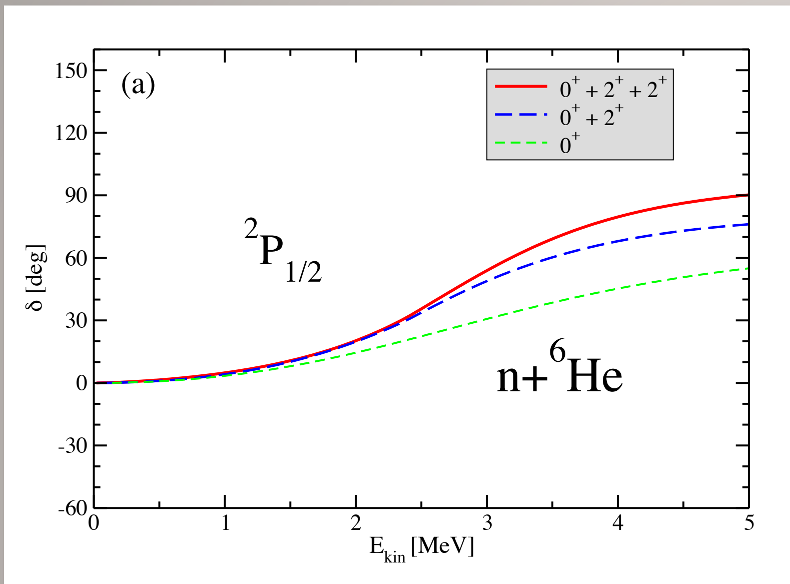
NCSMC
with up to three ^{6}He states
and four ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed



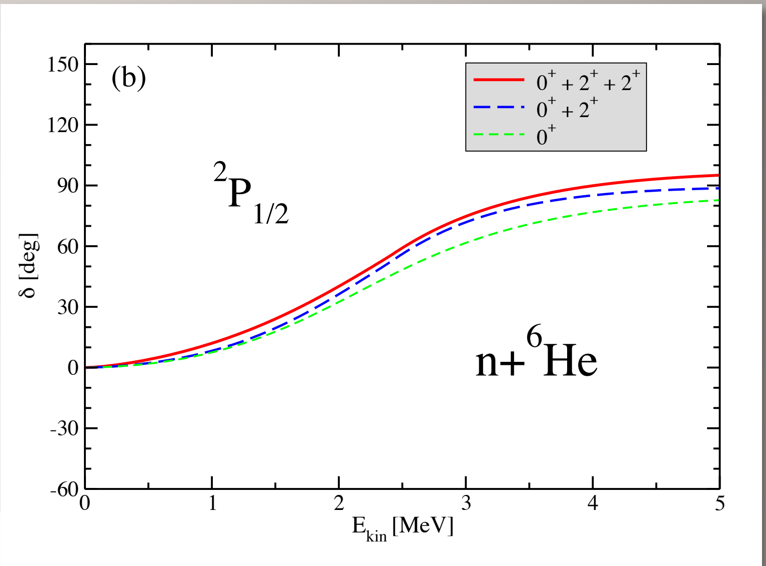
Expt.



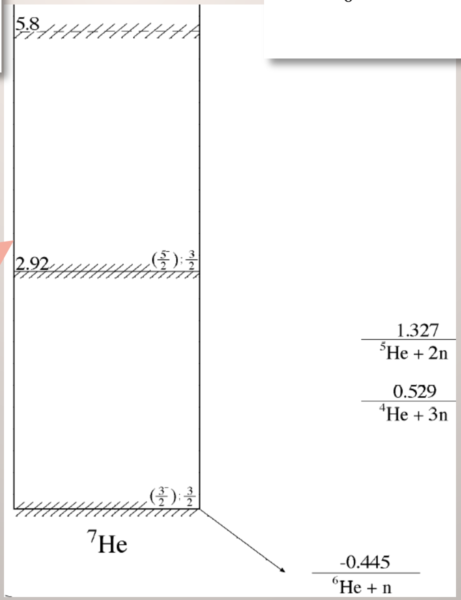
NCSM with continuum: ^{7}He ↔ ^{6}He+*n*

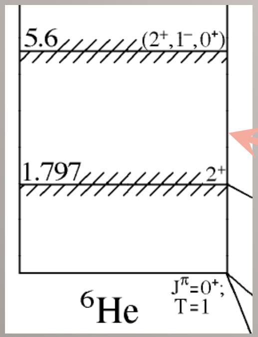


NCSM/RGM
with up to three ^{6}He states



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

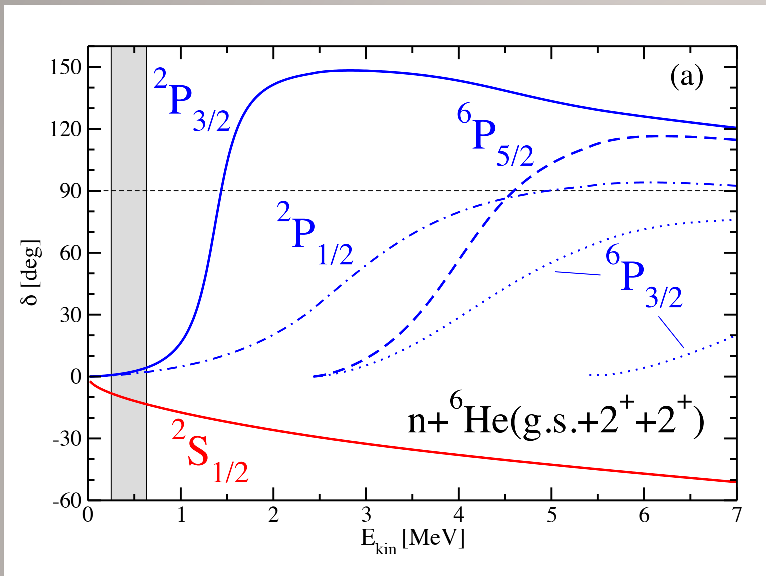




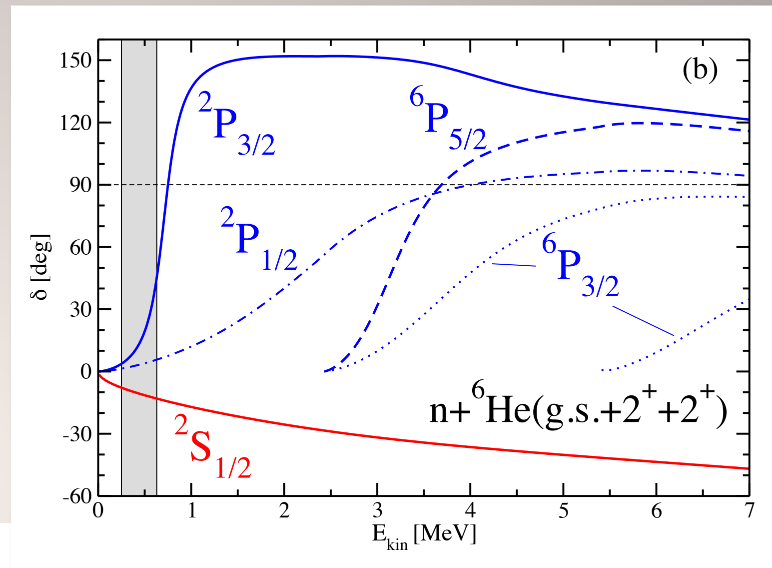
Expt.

TRIUMF

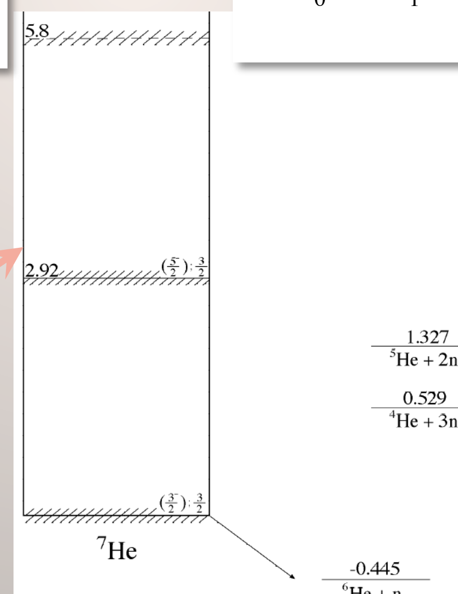
NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+n

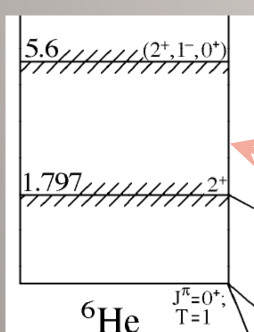


NCSM/RGM
with three ^{6}He states



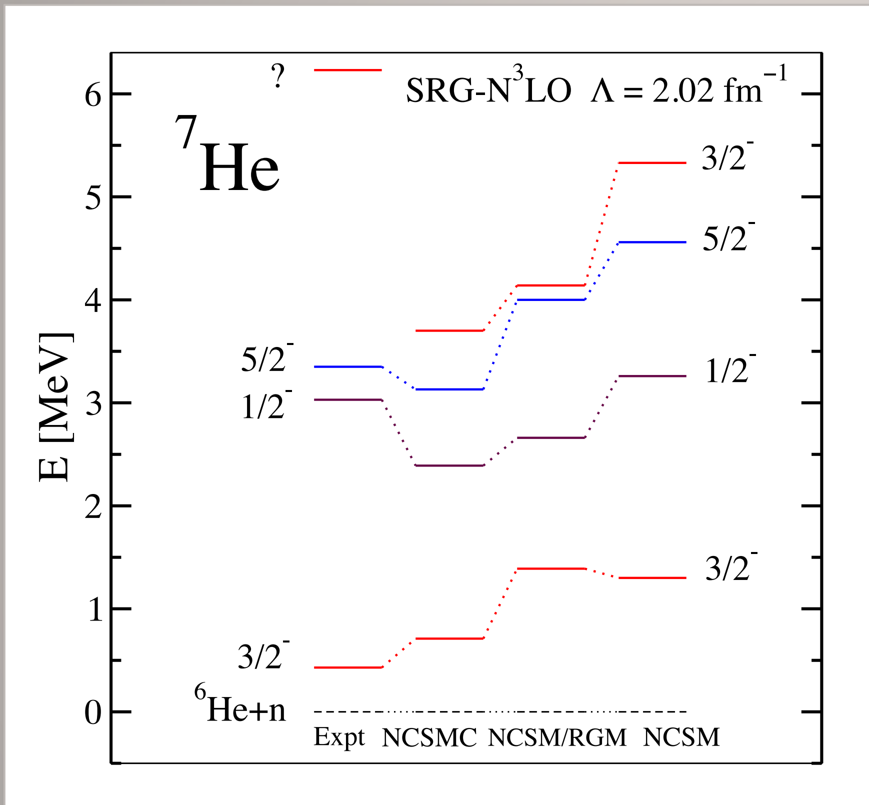
NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed





Expt.

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



J^π	experiment E_R	experiment Γ	experiment Ref.	NCSMC E_R	NCSMC Γ	NCSM/RGM E_R	NCSM/RGM Γ	NCSM 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

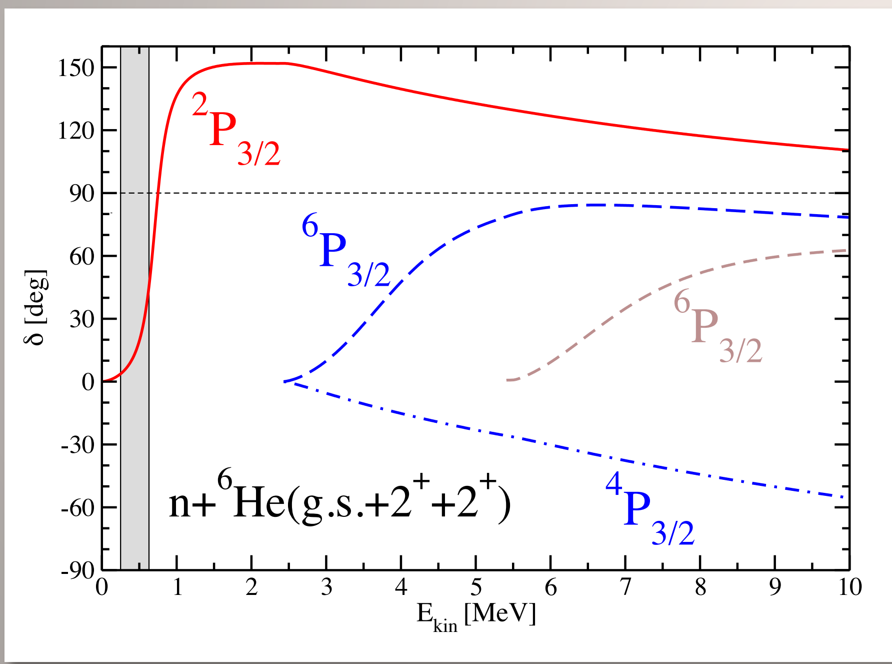
$$\Gamma = \left.\frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\right|_{E_{kin}=E_R}$$

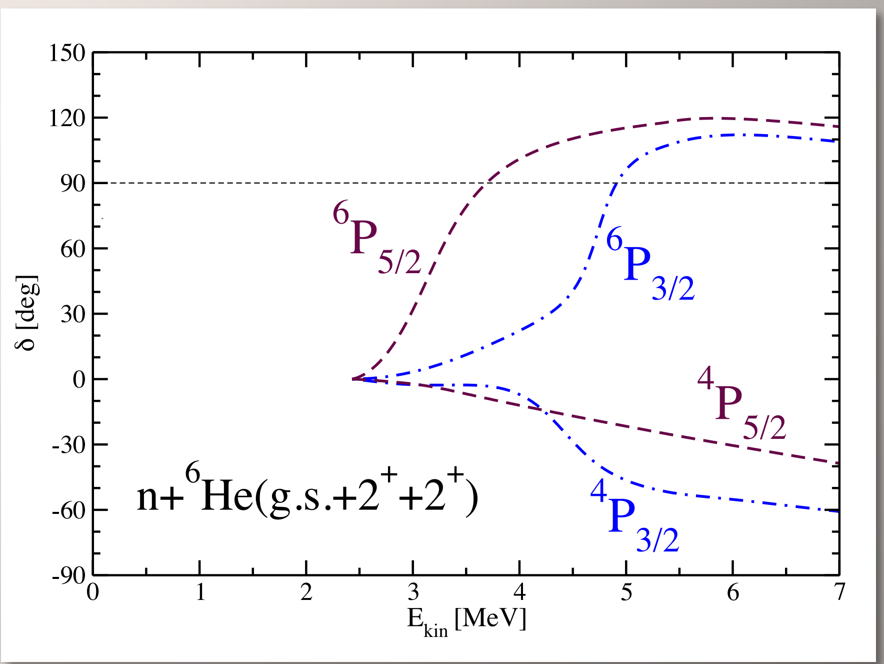
Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

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

Predictions of other resonances

- Two $3/2^-$ resonances predicted at about 3.7 MeV and 6.5 MeV with widths of 2.8 MeV and 4.3 MeV, respectively
  - Experiment: State of undetermined spin and parity at 6.2(3) MeV with the width of 4(1) MeV
- Considerable mixing of *P*-waves in $3/2^-_2$





NCSMC eigenphase shifts

NCSMC diagonal phase shifts

Conclusions and Outlook

- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NSM and the NCSM/RGM
- We demonstrated its capabilities in calculations of ^{7}He resonances
  - We find reasonable agreement with experiment for established $3/2^-$ and $5/2^-$ resonances
  - Our results do not support the existence of a low lying narrow 1/2- resonance
  - We predict two broad $3/2^-$ resonances

arXiv: 1210.1897

- Outlook:
  - Inclusion of 3N interactions
  - Extension of the formalism to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Extension of the formalism to coupling of three-body clusters

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