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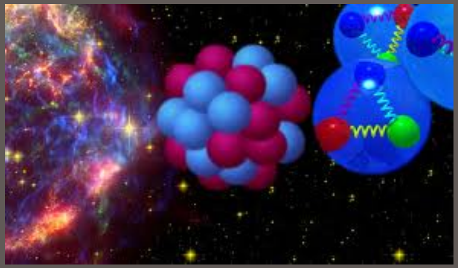
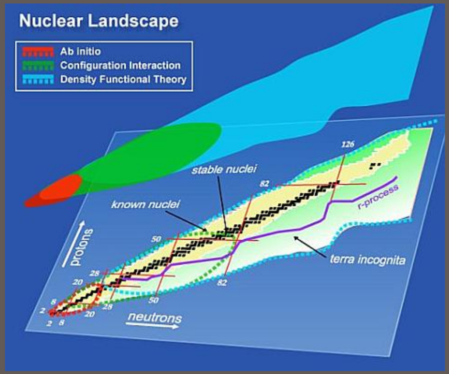
Canada’s national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

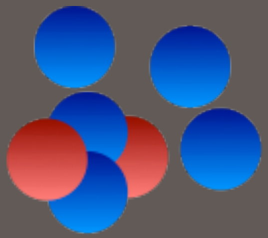
Ab initio calculations of bound and unbound states

From Few-Nucleon Forces to Many-Nucleon Structure
ECT* Workshop, Trento
12th June 2013

Petr Navratil | TRIUMF

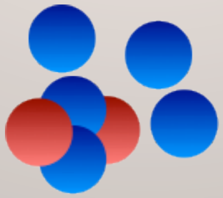






Outline

- Chiral forces
  - Exploratory calculations with the new $NNLO_{opt}$ NN
- Including the continuum with the resonating group method
  - NCSM/RGM
  - NCSMC
- ^{7}He resonances
- ^{9}Be structure
- ^{6}He as ^{4}He-n-n
- 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

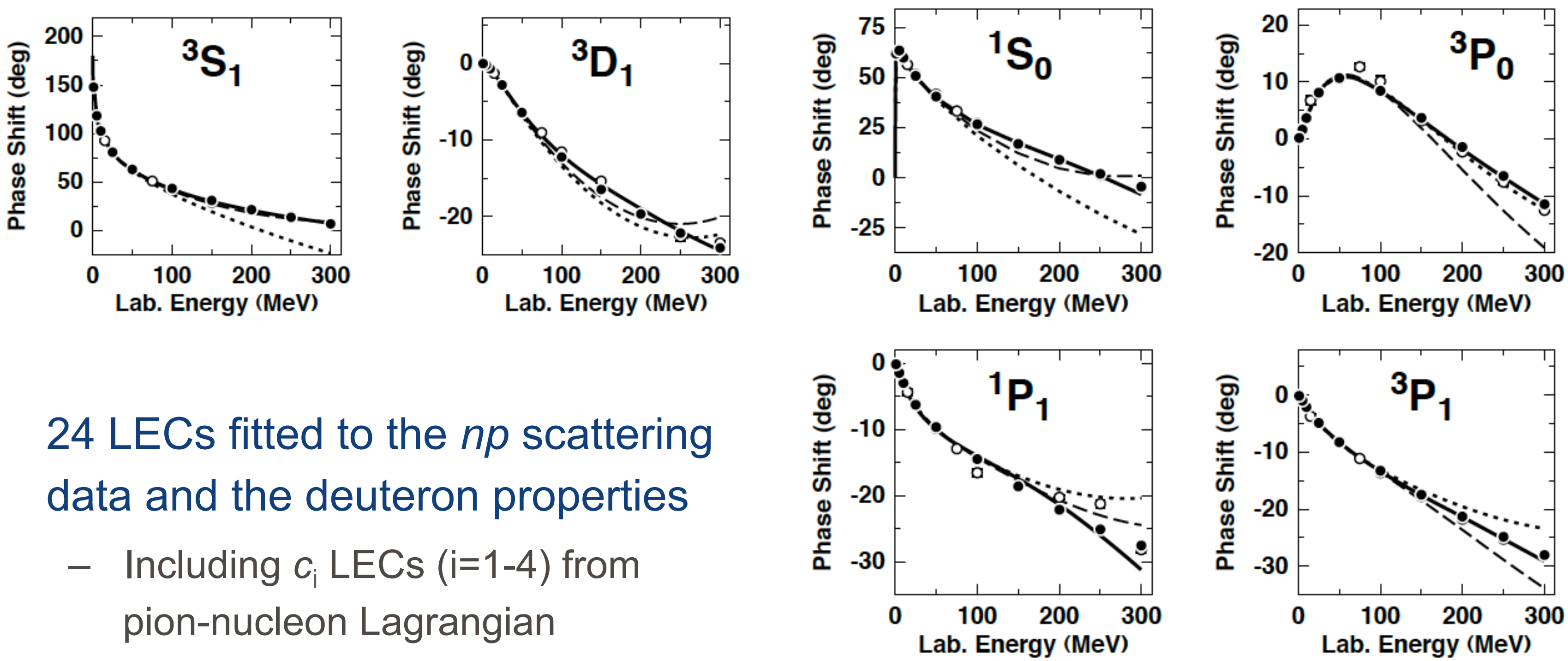
Λ_χ~1 GeV :
Chiral symmetry breaking scale

The NN interaction from chiral EFT

PHYSICAL REVIEW C **68**, 041001(R) (2003)

Accurate charge-dependent nucleon-nucleon potential at fourth order of chiral perturbation theory

D. R. Entem[1,2,*] and R. Machleidt[1,†]



- 24 LECs fitted to the *np* scattering data and the deuteron properties
  - Including c_i LECs (i=1-4) from pion-nucleon Lagrangian

New developments: NNLO(POUNDerS) NN interaction

PRL **110,** 192502 (2013) PHYSICAL REVIEW LETTERS week ending 10 MAY 2013

Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström,[1,2] G. Baardsen,[1] C. Forssén,[3] G. Hagen,[4,5] M. Hjorth-Jensen,[1,2,6] G. R. Jansen,[4,5] R. Machleidt,[7] W. Nazarewicz,[5,4,8] T. Papenbrock,[5,4] J. Sarich,[9] and S. M. Wild[9]

- Improved χ^2 fit
  - Excellent at energies up to 125 MeV
- *A*=3,4 nuclei more bound (closer to experiment)
- Better description of *p*-shell nuclei and O isotopes
- Code available for general use
  - implemented in the NCSM codes

TABLE IV. Ground-state energies (in MeV) and point proton radii (in fm) for ^{3}H, ^{3}He, and ^{4}He using the NNLO$_{\text{opt}}$ with and without the NNLO 3NF interaction for $c_D = -0.20$ and $c_E = -0.36$.

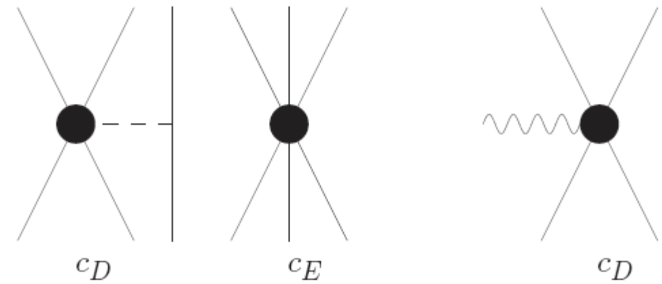
	$E(^3\text{H})$	$E(^3\text{He})$	$E(^4\text{He})$	$r_p(^4\text{He})$
NNLO	−8.249 ✓	−7.501 ✓	−27.759 ✗	1.43(8)
NNLO+NNN	−8.469 ✓	−7.722 ✓	−28.417 ✗	1.43(8)
Experiment	−8.482	−7.717	−28.296	1.467(13)

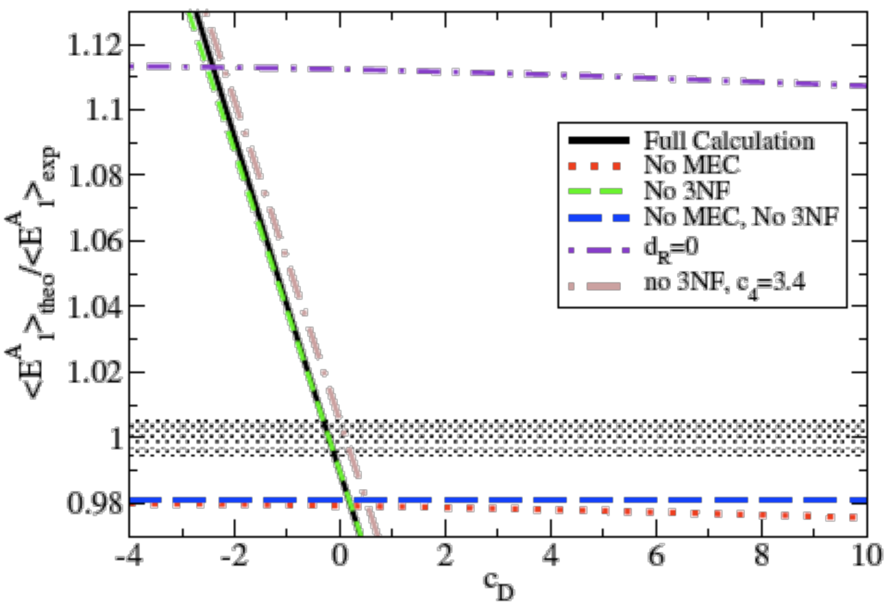
NCSM
^{4}He with NNLO$_{\text{opt}}$
E_{gs}=-27.590(1) MeV
(EM N^{3}LO NN: -25.38 MeV)
^{4}He with NNLO$_{\text{opt}}$+3N
E_{gs}=-28.38(1) MeV

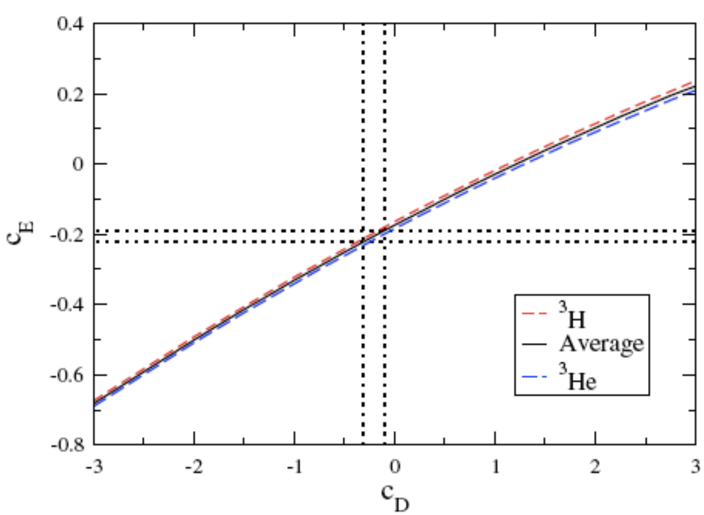
Determination of NNN constants c_D and c_E from the triton binding energy and the half life

- **Chiral EFT**: c_D also in the two-nucleon contact vertex with an external probe
- Calculate $\langle E_1^A \rangle = |\langle ^3\mathrm{He} || E_1^A || ^3\mathrm{H} \rangle|$
  - Leading order GT
  - N^{2}LO: one-pion exchange plus contact
- *A*=3 binding energy constraint:

c_D=-0.2±0.1 c_E =-0.205±0.015







PRL **103,** 102502 (2009) PHYSICAL REVIEW LETTERS week ending 4 SEPTEMBER 2009

Three-Nucleon Low-Energy Constants from the Consistency of Interactions and Currents in Chiral Effective Field Theory

Doron Gazit
Institute for Nuclear Theory, University of Washington, Box 351550, Seattle, Washington 98195, USA

Sofia Quaglioni and Petr Navrátil
Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA

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NNLO(POUNDerS) NN with local N^{2}LO 3N

- c_D-c_E fit to ^{3}H/^{3}He binding energy and ^{3}H half life (performed with Sofia Quaglioni)
- N^{2}LO 3N Λ=500 MeV
  - c_D = -0.39 +/- 0.07, c_E = -0.398 +0.015/-0.016

^{4}He E_{gs}= -28.47(1) MeV
$\langle V_{3N-2\pi} \rangle$ = -6.76 MeV $\langle V_{3N-D} \rangle$ = -1.31 MeV $\langle V_{3N-E} \rangle$ = 5.72 MeV

E-term stronger

^{4}He with EM N^{3}LO+3NF(500) E_{gs}= -28.50(2) MeV
$\langle V_{3N-2\pi} \rangle$ = -5.88 MeV $\langle V_{3N-D} \rangle$ = -0.22 MeV $\langle V_{3N-E} \rangle$ = 1.27 MeV

- N^{2}LO 3N Λ=400 MeV (Λ=500 MeV in the current)
  - c_D = -0.40 +0.06/-0.07, c_E = -0.212 +/-0.015

^{4}He E_{gs}= -29.06(1) MeV
$\langle V_{3N-2\pi} \rangle$ = -3.19 MeV $\langle V_{3N-D} \rangle$ = -1.02 MeV $\langle V_{3N-E} \rangle$ = 2.35 MeV

c_E re-fit to ^{4}He b.e. useful

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NNLO(POUNDerS) NN with local N^{2}LO 3N

- c_D-c_E fit to ^{3}H/^{3}He binding energy and ^{3}H half life (performed with Sofia Quaglioni)
- N^{2}LO 3N Λ=400 MeV (Λ=500 MeV in the current)
  - c_D = -0.40 +0.06/-0.07, c_E = -0.212 +/-0.015

^{4}He E_{gs}= -29.06(1) MeV
$\langle V_{3N\text{-}2\pi} \rangle$ = -3.19 MeV $\langle V_{3N\text{-}D} \rangle$ = -1.02 MeV $\langle V_{3N\text{-}E} \rangle$ = 2.35 MeV

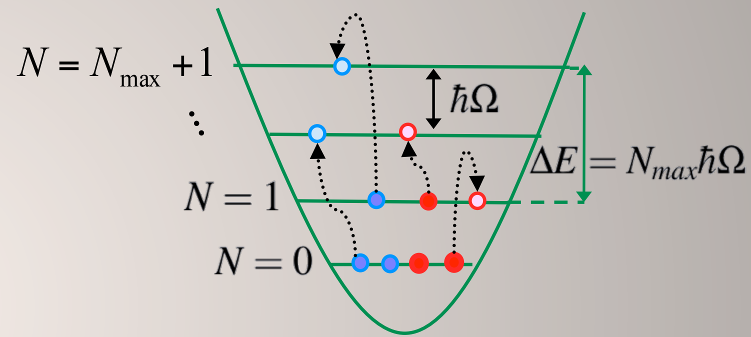
- Re-fit of c_E to ^{4}He binding energy:
  - c_D=-0.4, c_E=-0.2812

^{4}He E_{gs}= -28.296 MeV
$\langle V_{3N\text{-}2\pi} \rangle$ = -2.99 MeV $\langle V_{3N\text{-}D} \rangle$ = -0.96 MeV $\langle V_{3N\text{-}E} \rangle$ = 2.96 MeV

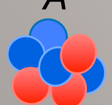
Unlike the N^{3}LO NN +3NF400, where all 3N terms attractive

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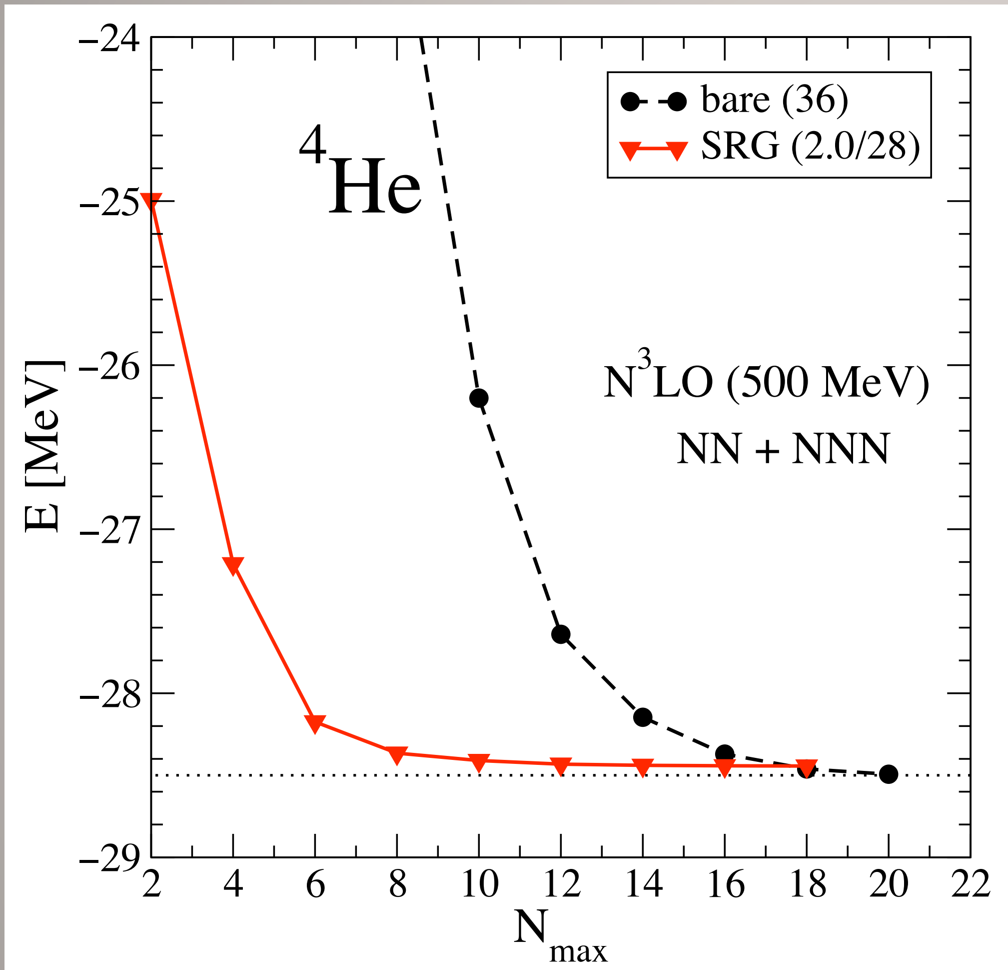
^{4}He from chiral EFT interactions: g.s. energy convergence



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

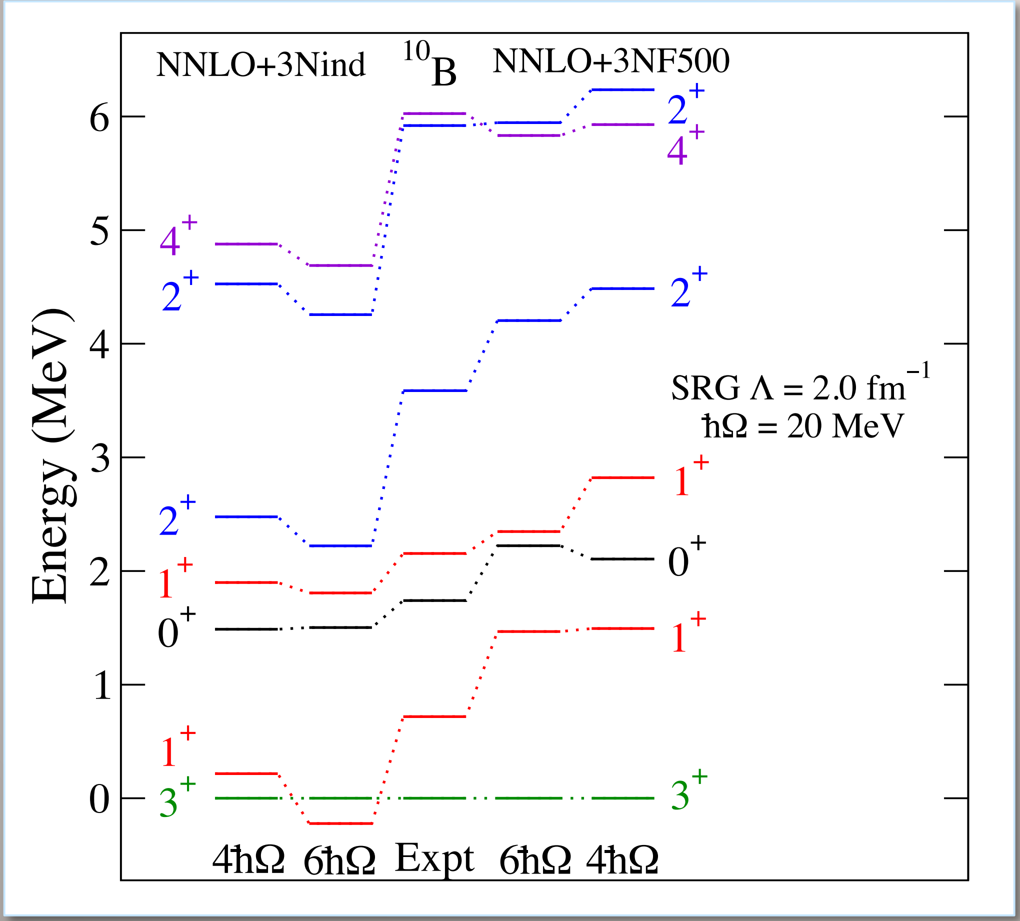
– SRG evolved effective interaction (red line)
  - Unitary transformation

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

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

^{10}B with the NNLO$_{opt}$ NN potential

- Does an improved NN potential fit at NNLO imply a better description of *p*-shell nuclei?



Yes
…but 3N still needed.

The NNLO$_{opt}$ NN predicts (most likely) the 1^+ g.s. in ^{10}B

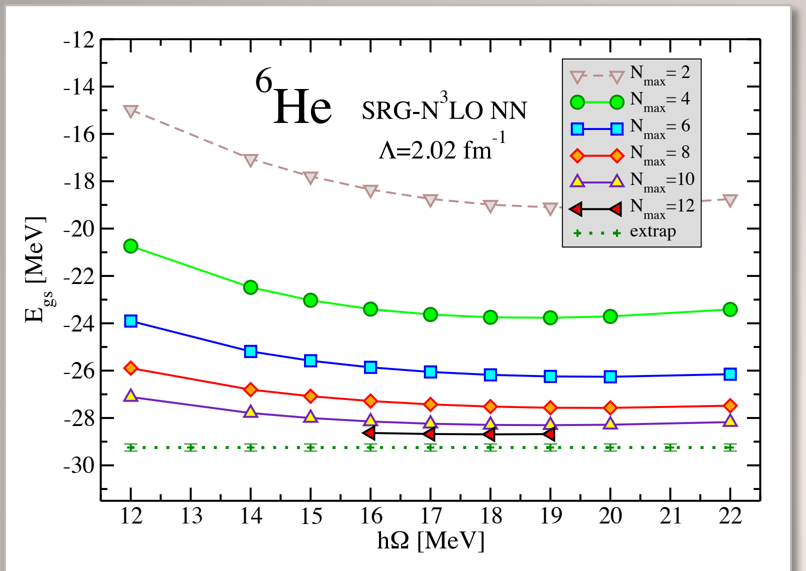
The N^{2}LO 3N(500) appear rather strong: The two lowest 1^+ states may be reversed

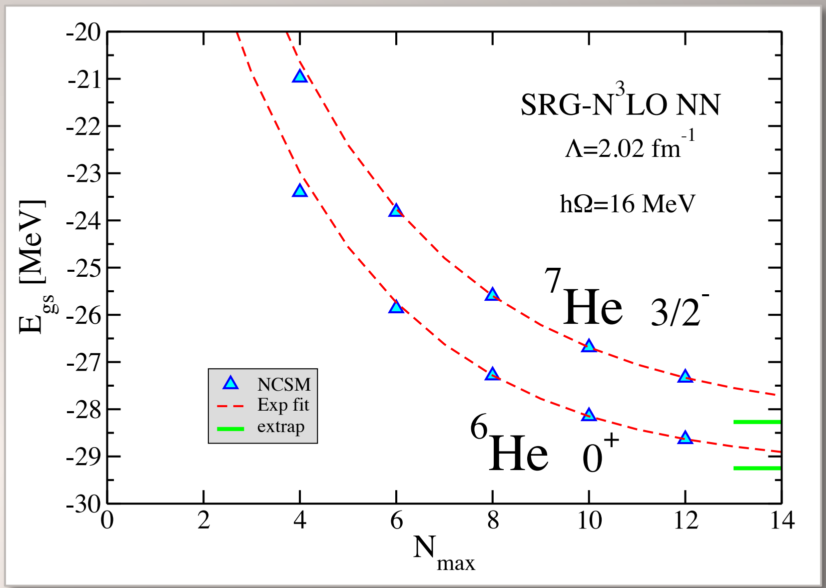
Next:
Test the N^{2}LO 3N(400)

Overall very encouraging development!

The extension of the fit to N^{3}LO NN very important.

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

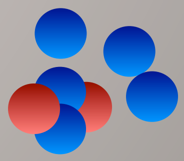




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ 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

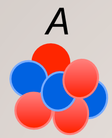


unbound

Extending no-core shell model beyond bound states

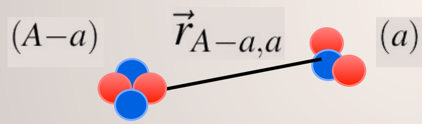
Include more many nucleon correlations…

NCSM

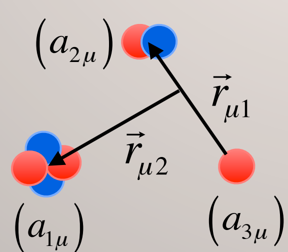


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

+



+



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

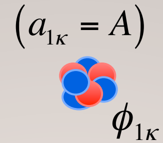
+

…

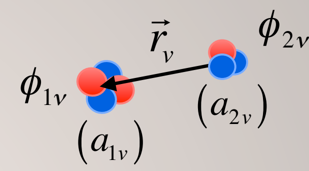
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

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



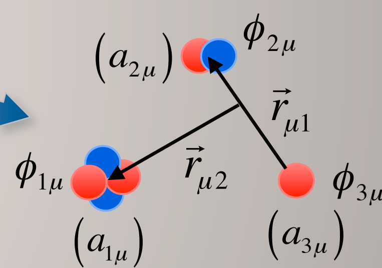
$$+ \sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



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

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

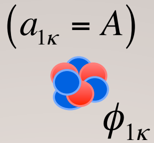
$$+ \cdots$$



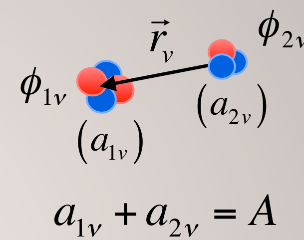
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

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

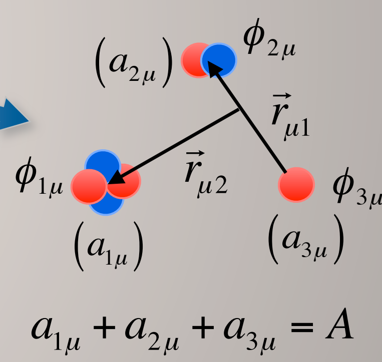


$$+ \sum_{\nu} \hat{A}_{\nu} \boxed{\phi_{1\nu}} \left(\left\{ \vec{\xi}_{1\nu} \right\} \right) \boxed{\phi_{2\nu}} \left(\left\{ \vec{\xi}_{2\nu} \right\} \right) g_{\nu}(\vec{r}_{\nu})$$



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

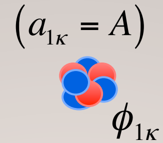
$$+ \cdots$$



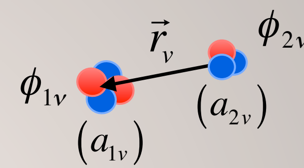
- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

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



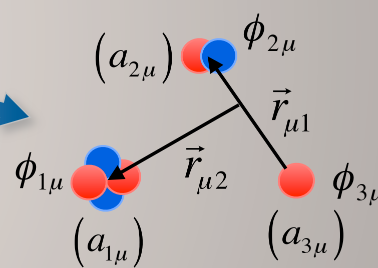
$$+ \sum_{\nu} \boxed{\hat{A}_{\nu}} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

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

$$+ \cdots$$



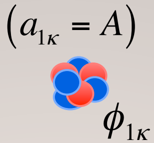
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

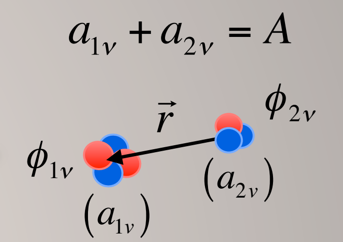
- $\boldsymbol{A_{\nu}}$, $\boldsymbol{A_{\mu}}$: interclusters antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

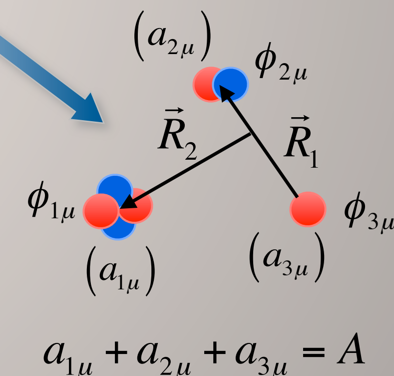
$$a_{1\nu} = A - 1,\ a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_{\nu} = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

Trial function: generalized cluster wave function

$$
\begin{aligned}
\psi^{(A)} = {} & \sum_{\kappa} \boxed{c_{\kappa}} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right) \\
& + \sum_{\nu} \int \boxed{g_{\nu}(\vec{r}\,)} \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r}-\vec{r}_{\nu})\right]d\vec{r} \\
& + \sum_{\mu} \iint \boxed{G_{\mu}(\vec{R}_1,\vec{R}_2)} \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu 1})\delta(\vec{R}_2-\vec{R}_{\mu 2})\right]d\vec{R}_1 d\vec{R}_2 \\
& + \cdots
\end{aligned}
$$







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

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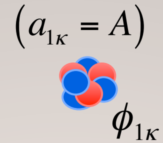
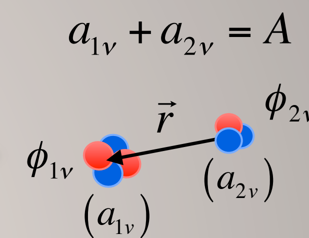
Trial function: generalized cluster wave function

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

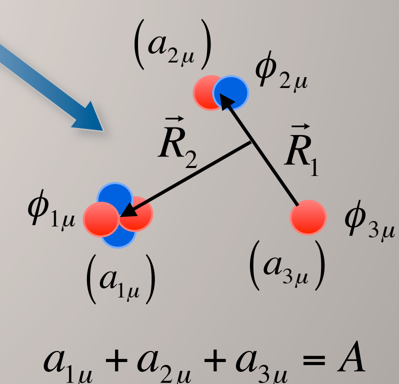


$$+\sum_{\nu} \int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \boxed{\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r}-\vec{r}_{\nu})\right]} d\vec{r}$$



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

$$+\ \cdots$$



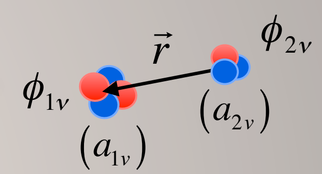
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

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

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

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



$$\cancel{+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1,\vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu1})\delta(\vec{R}_2-\vec{R}_{\mu2})\right]d\vec{R}_1 d\vec{R}_2}$$

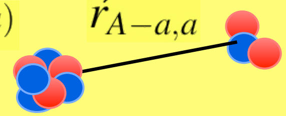
$$+ \cdots$$

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

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

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

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

Trick #1

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

TRIUMF

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:

Trick #2

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

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

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

$$\left(\vec{\eta}_{A-a} = \sqrt{\tfrac{(A-a)a}{A}}\,\vec{r}_{A-a,a}\right)$$

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

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

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

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

Interested in this

Calculate these

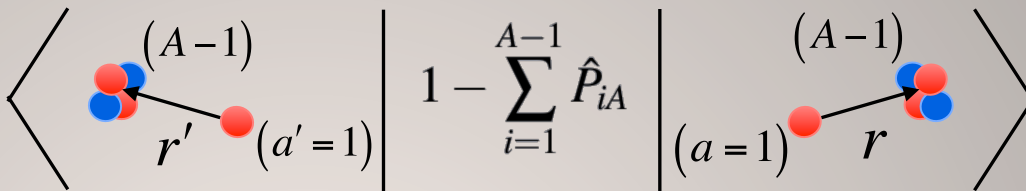
Matrix that can be inverted

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

Norm kernel (Pauli principle)

Single-nucleon projectile

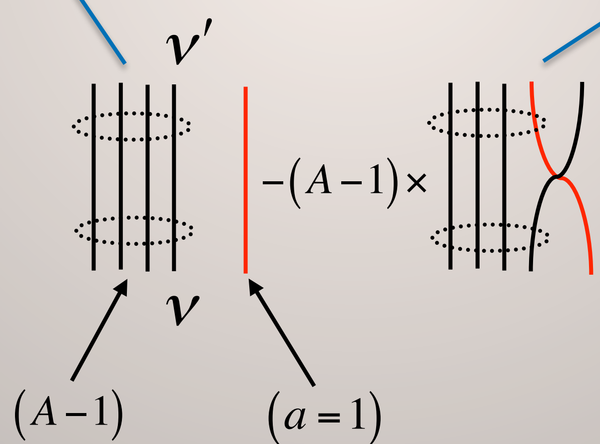
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



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

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

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

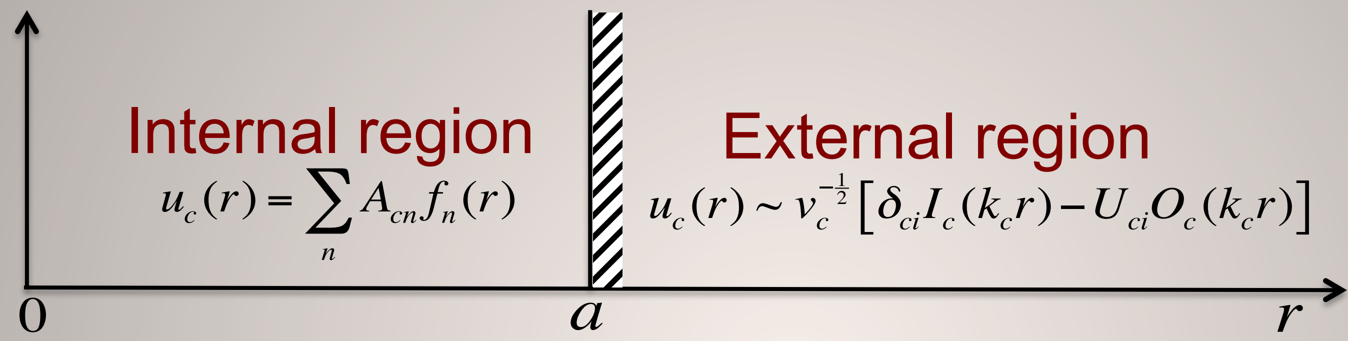


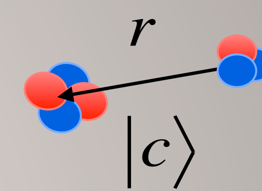
Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

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

Microscopic *R*-matrix on a Lagrange mesh

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:

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

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

- Internal region: expansion on square-integrable Lagrange mesh basis

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

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

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

- External region: asymptotic form for large r

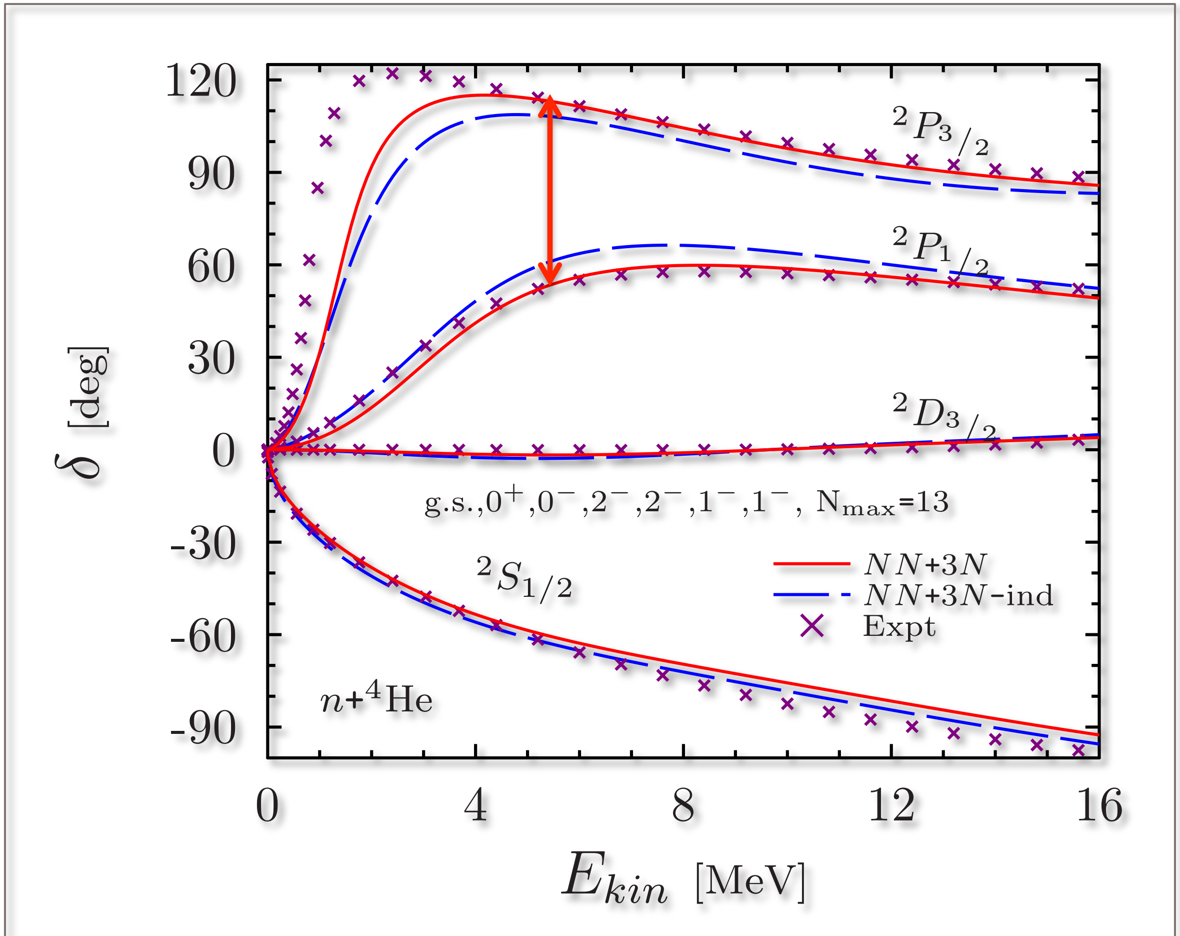
$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r)\right]$$

Bound state

Scattering state

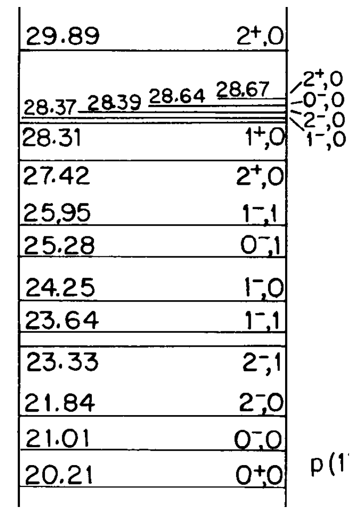
Scattering matrix

n-^{4}He scattering: NN vs. NN+NNN interactions



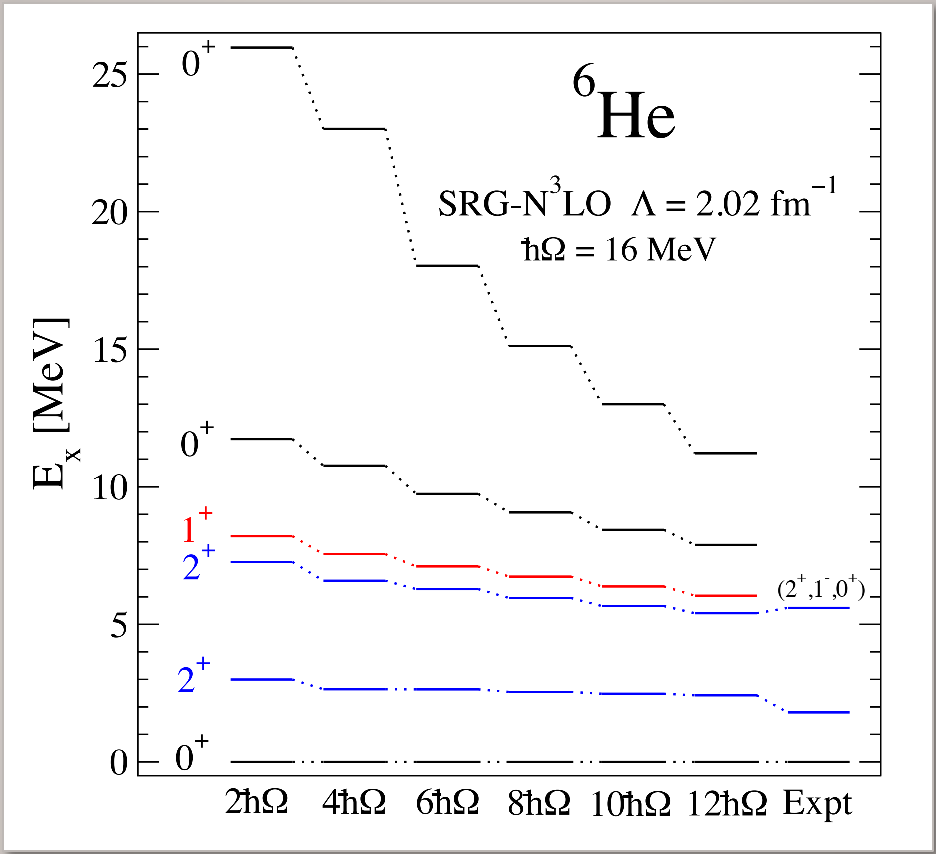
chiral NN+NNN(500)
chiral NN+NNN-induced
SRG λ=2 fm^{-1}
HO N$_{max}$=13, hΩ=20 MeV

^{4}He g.s. and 6 excited states



The largest splitting between the P-waves obtained with the chiral NN+NNN interaction

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

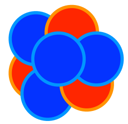


- All ^{6}He excited states above 2^+_1 broad resonances or states in continuum
- Convergence of the NCSM/RGM n+^{6}He calculation slow with number of ^{6}He states
  - Negative parity states also relevant
  - Technically not feasible to include more than ~ 5 states

TRIUMF

New developments: NCSM with continuum

NCSM

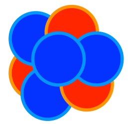


$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

TRIUMF

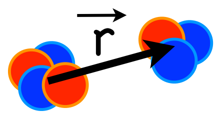
New developments: NCSM with continuum

NCSM



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

NCSM/RGM



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

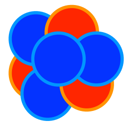
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

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

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

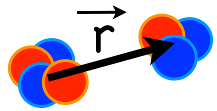
New developments: NCSM with continuum

NCSM



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

NCSM/RGM

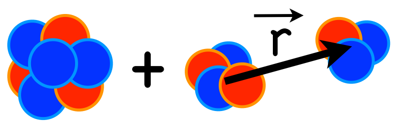


$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r}\,\chi_\nu(\vec{r})\hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

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

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

NCSMC



S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

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

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

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

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:

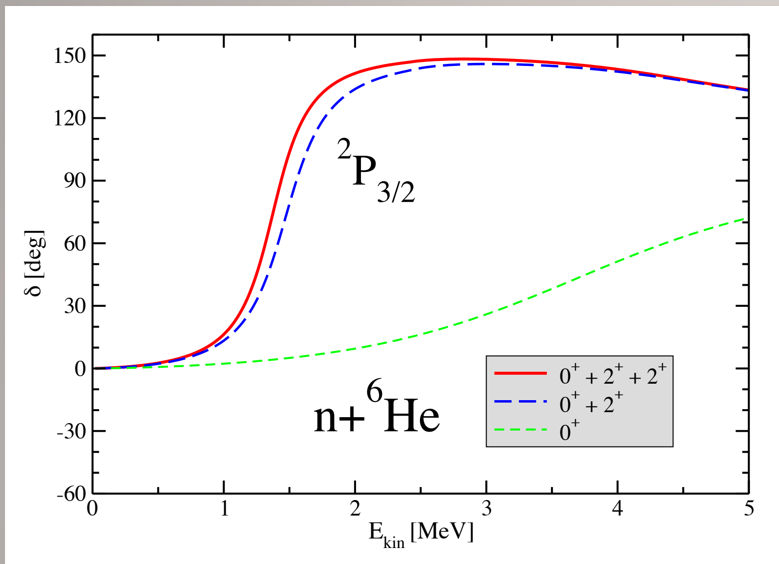
$$\overline{H} = N^{-\frac{1}{2}} \begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} N^{-\frac{1}{2}} \qquad \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = N^{+\frac{1}{2}} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

Solve with generalized microscopic R-matrix

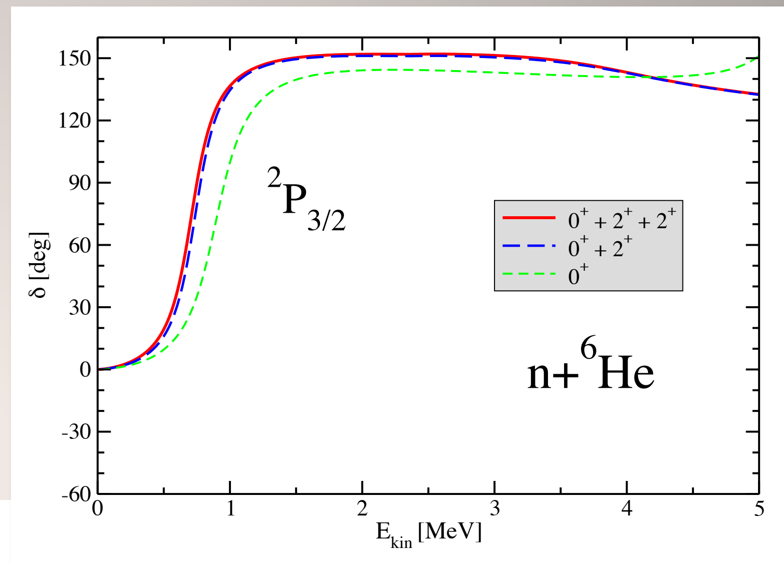
$$(\hat{\overline{H}} + \hat{L} - E) \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = \hat{L} \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix}$$

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

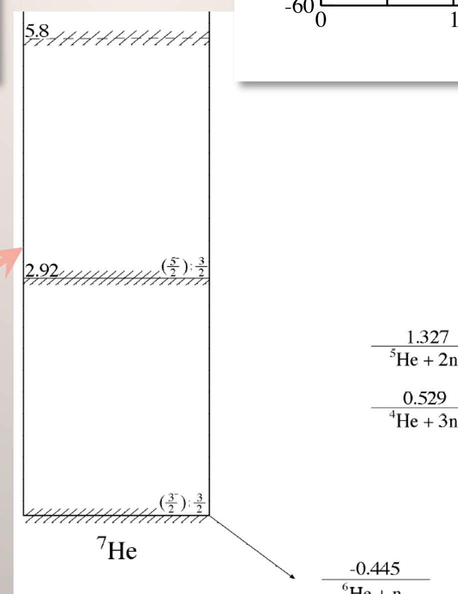
NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+n

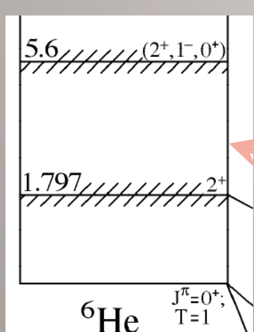


NCSM/RGM
with up to three ^{6}He states



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

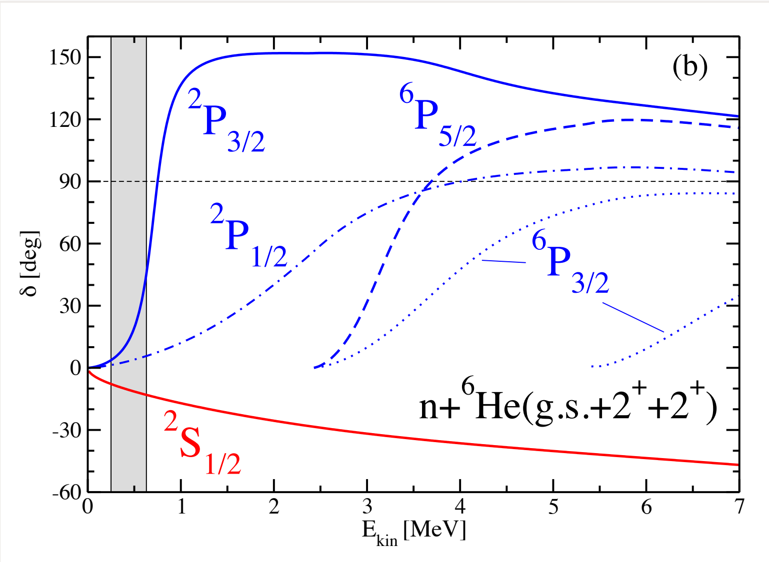




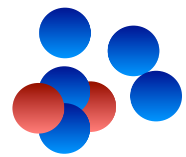
Expt.

TRIUMF

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



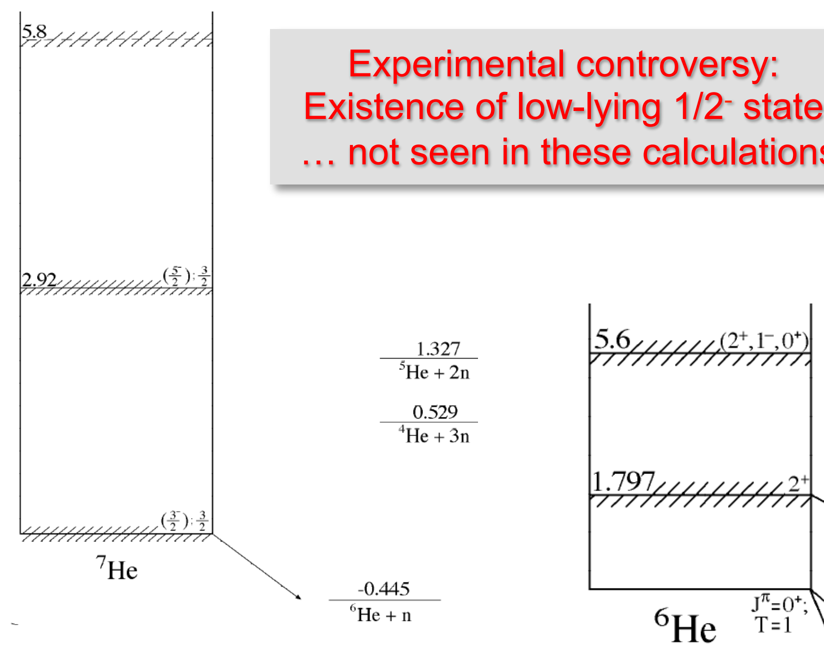
^{7}He



unbound

J^π	experiment E_R	Γ	Ref.	NCSMC E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

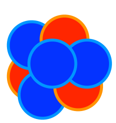
[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).



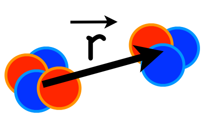
Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

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

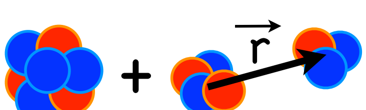
NCSM



NCSM/RGM

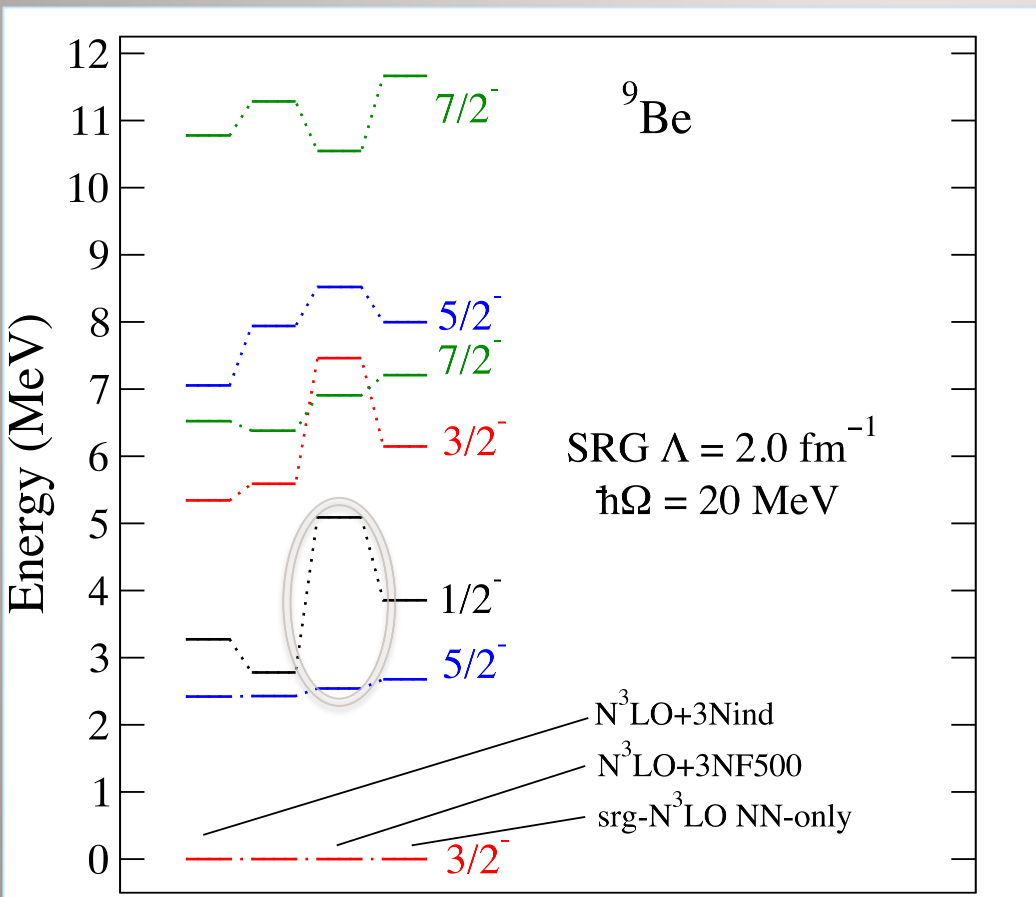


NCSMC



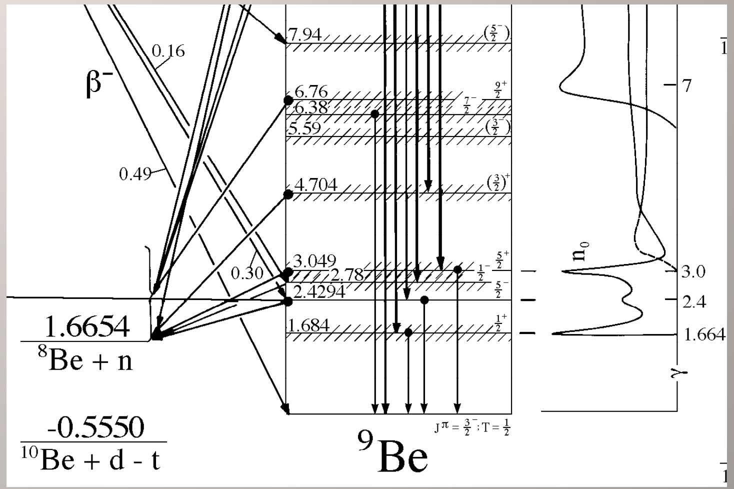
Structure of ^{9}Be

- The lightest nucleus where the 3N interaction appear to make the description of low lying states worse: Does this suggest our 3N interaction models are wrong?



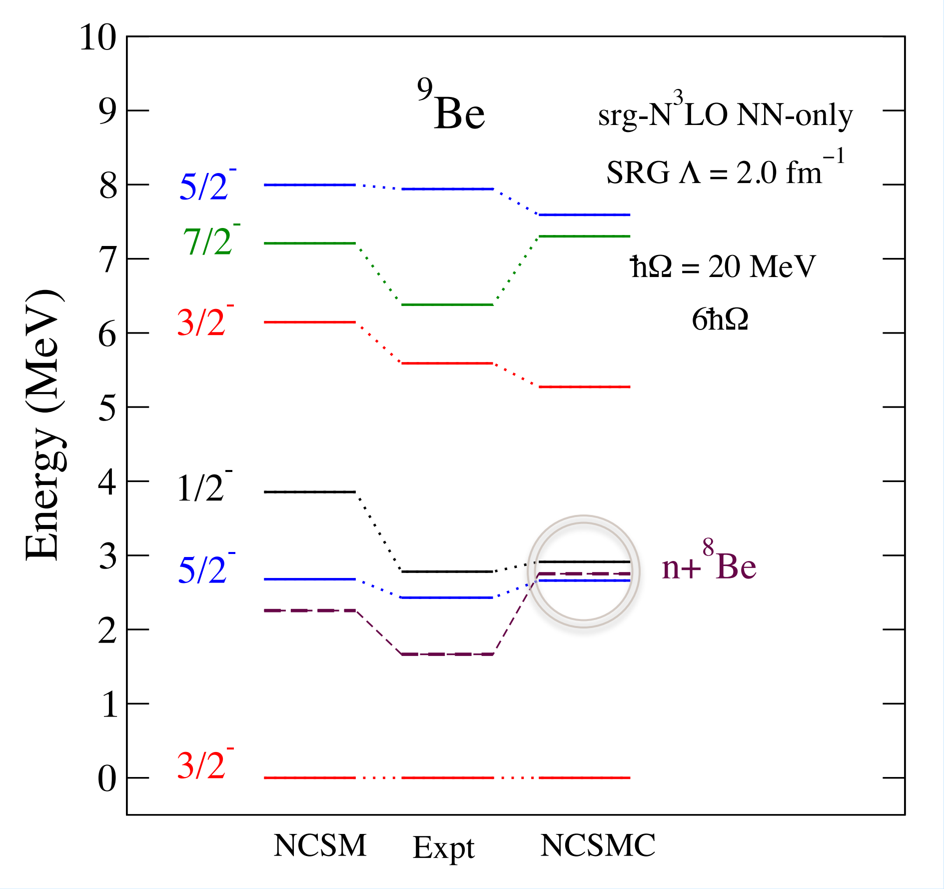
1/2^{-} state moved to high energy by the 3N interaction

However, all excited states are resonances. What is the effect of the continuum?



Structure of ^{9}Be

- The lightest nucleus where the 3N interaction appear to make the description of low lying states worse: Does this suggest our 3N interaction models are wrong?



NCSMC with the 3N under way

For now, we analyze this with the srg-N^{3}LO NN-only:

5/2$^-$ a very narrow (or bound) *F*-wave – no shift

1/2$^-$ a broader *P*-wave – a large shift due to the continuum

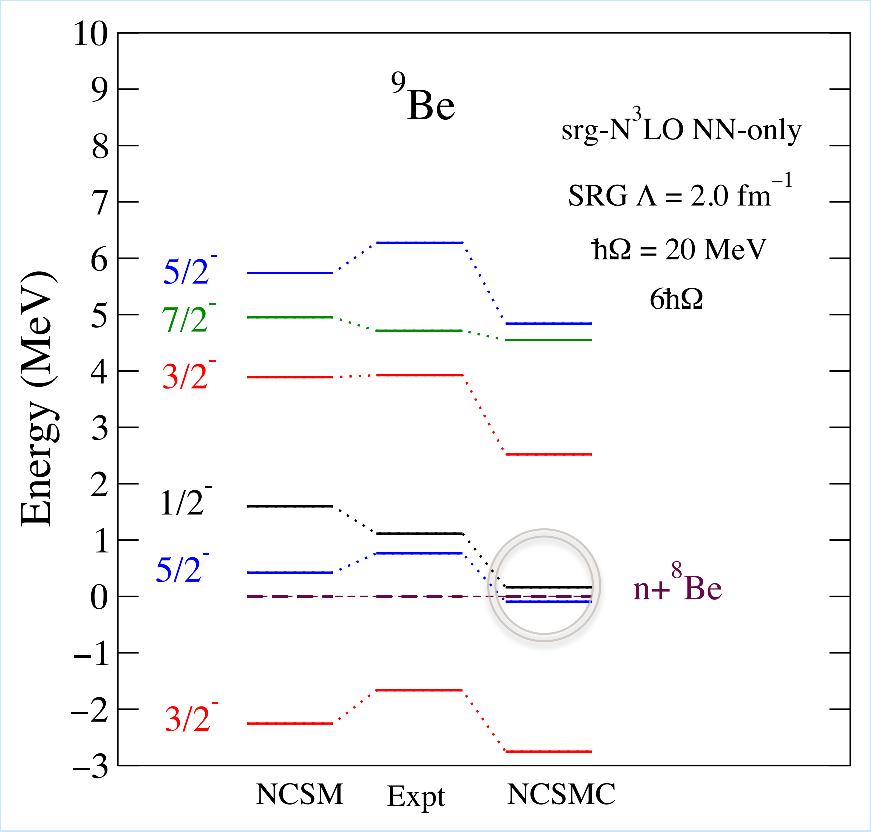
Structure of ^{9}Be

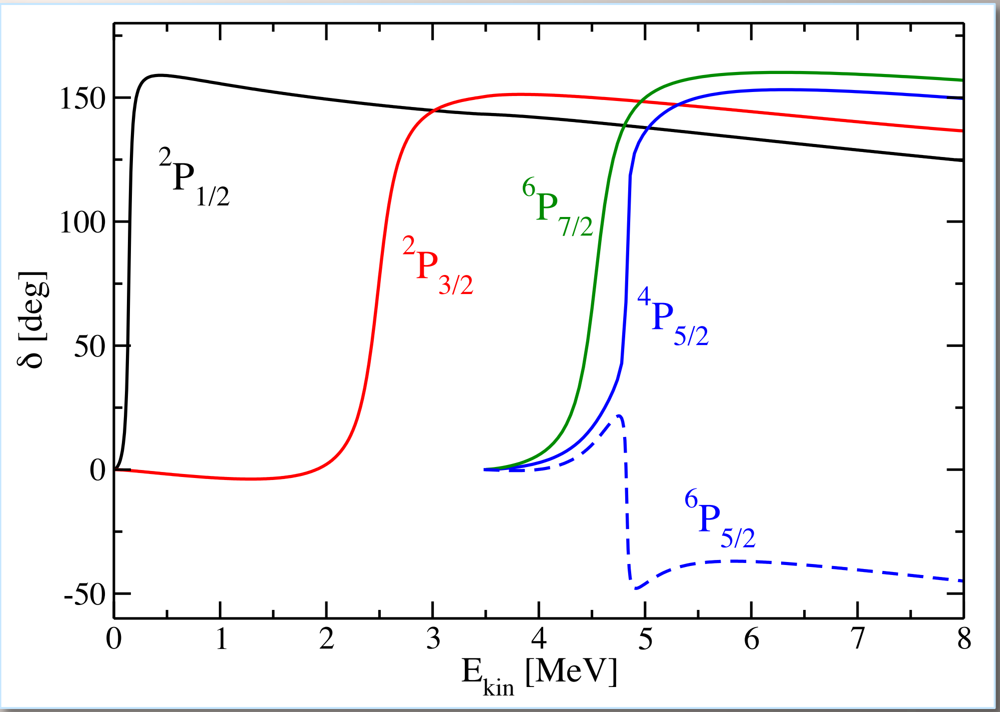
- The lightest nucleus where the 3N interaction appear to make the description of low lying states worse: Does this suggest our 3N interaction models are wrong?

No!

NCSMC

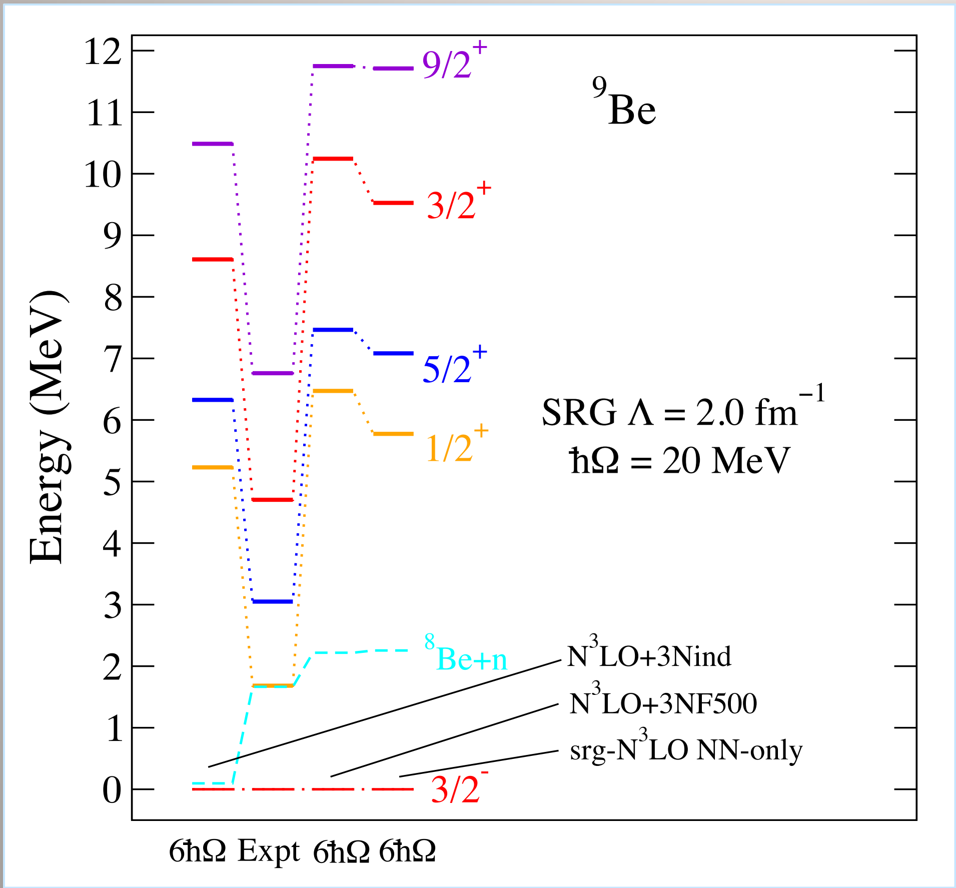
n-^{8}Be(0^{+},2^{+}) + ^{9}Be





Structure of ^{9}Be

- The unnatural parity states are predicted too high in the NCSM calculations. Is this a HO basis size problem? Is this an interaction dependent problem?



Bad with any interaction

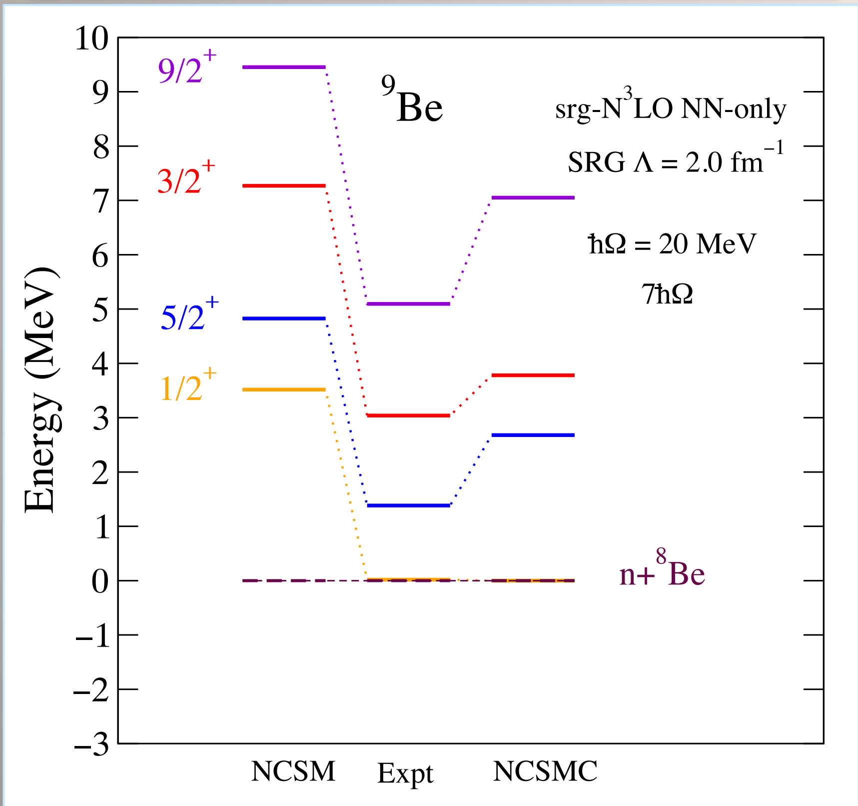
Large HO basis size (N_{max}) definitely helps.

But…

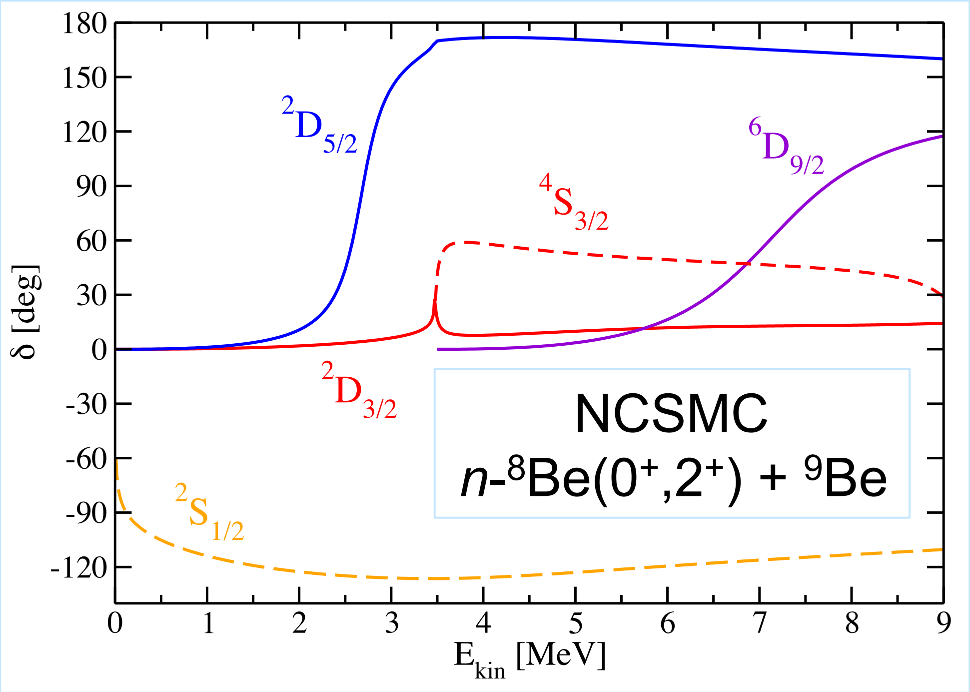
Structure of ^{9}Be

- The unnatural parity states are predicted too high in the NCSM calculations. Is this a HO basis size problem? Is this an interaction dependent problem?

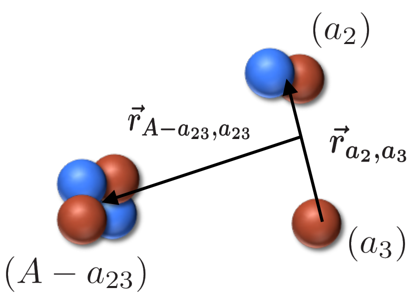
Need to switch to NCSMC!



Breakup thresholds impact *S*-waves
Continuum important for other waves as well



NCSM/RGM for three-body clusters



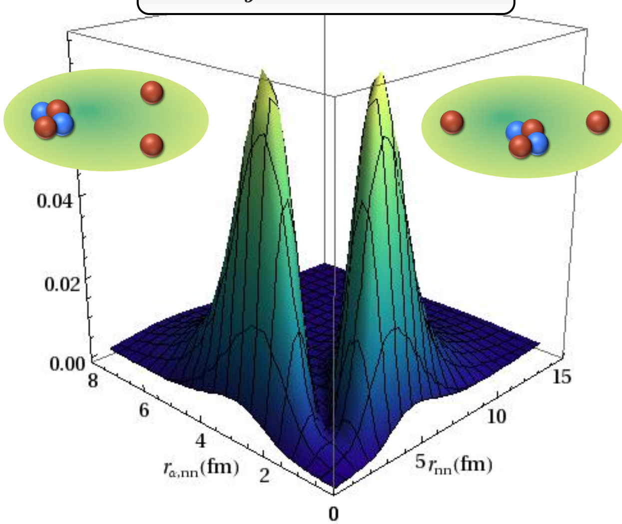
$$|\Phi^{J^\pi T}_{\nu r}\rangle \sim \underbrace{\Psi^{A-a_{23}}_{\alpha_1}\ \Psi^{a_2}_{\alpha_2}\ \Psi^{a_3}_{\alpha_3}}_{\text{NCSM}}$$

$$\boxed{|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 G^{J^\pi T}_\nu(x,y)\hat{A}_\nu |\Phi^{J^\pi T}_{\nu xy}\rangle}$$

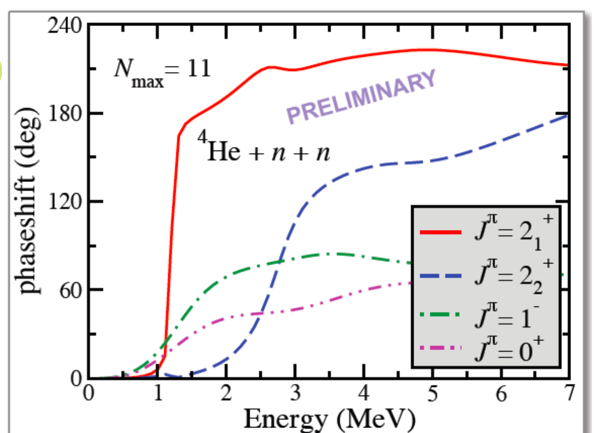
NCSM

^{4}He(g.s.)+n+n

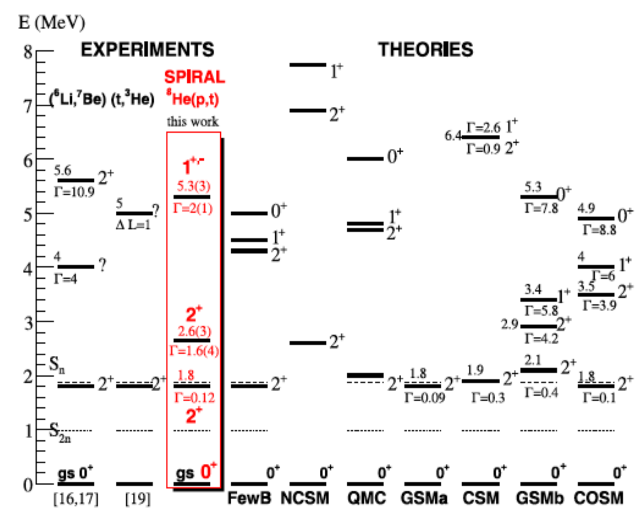
$$\ell_x = \ell_y = L = S_{nn} = 0$$



Phaseshifts (preliminary results)



Recent exp.: Phys. Lett. B 718 (2012) 441



INCITE Award – Titan

TRIUMF

Conclusions and Outlook

- Exploratory calculations with the new $NNLO_{opt}$ NN
  - Fits of the 3N LECs
  - Structure of ^{10}B
- 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
- First NCSMC applications to the structure of ^{9}Be
  - One of the goals: $^{8}Be(n,\gamma)^{9}Be$ radiative capture
- 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 ($^{6}He \sim {}^{4}He+n+n$)

NCSMC and NCSM/RGM collaborators

Sofia Quaglioni (LLNL)

Joachim Langhammer, Robert Roth (TU Darmstadt)

C. Romero-Redondo, F. Raimondi (TRIUMF)

G. Hupin, M. Kruse (LLNL)

S. Baroni (ULB)

W. Horiuchi (Hokkaido)