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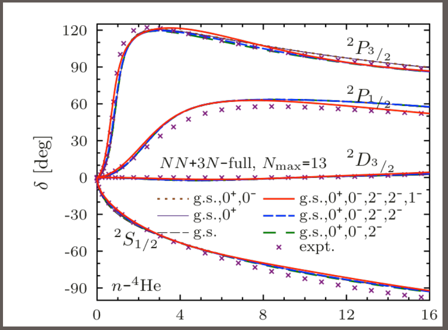
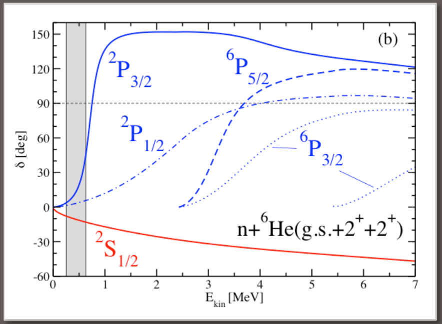
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

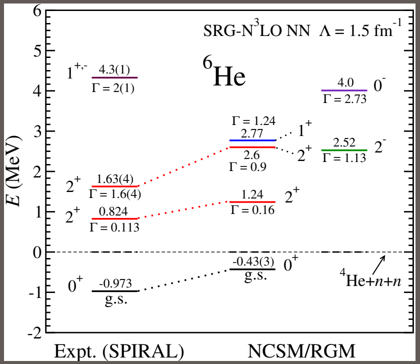
Ab initio many-body calculations of nuclear scattering and reactions

FUSTIPEN Topical Meeting
«Understanding Nuclear Structure and Reactions Microscopically, including the Continuum»
March 17-21, 2014, GANIL, Caen, France

Petr Navratil | TRIUMF







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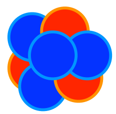
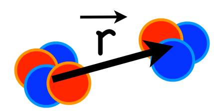
Outline

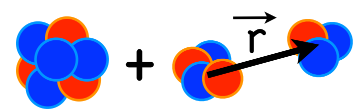
- *Ab initio* calculations in nuclear physics
  - Chiral NN and 3N interactions
- No-core shell model



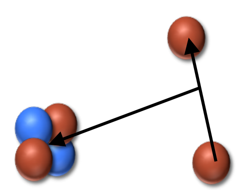
- Including the continuum with the resonating group method
  - NCSM/RGM: *N*-^{4}He



  - NCSMC: ^{5,7}He, ^{9}Be, ^{11}N (*p*-^{10}C), ^{17}C(n-^{16}C)



  - Three-body cluster dynamics: ^{6}He



- Outlook

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Ab initio Nuclear Structure & Reaction approaches

Ab initio

- ✧ All nucleons are active
- ✧ Exact Pauli principle
- ✧ Realistic inter-nucleon interactions
  - ✧ Accurate description of NN (and 3N) data
- ✧ Controllable approximations

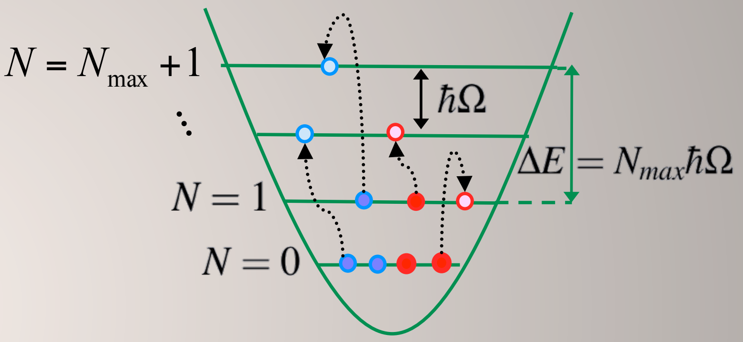
Chiral Effective Field Theory

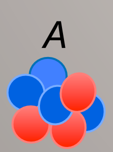
- **First principles for Nuclear Physics:**
  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future
- ***For now a good place to start*:**
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx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

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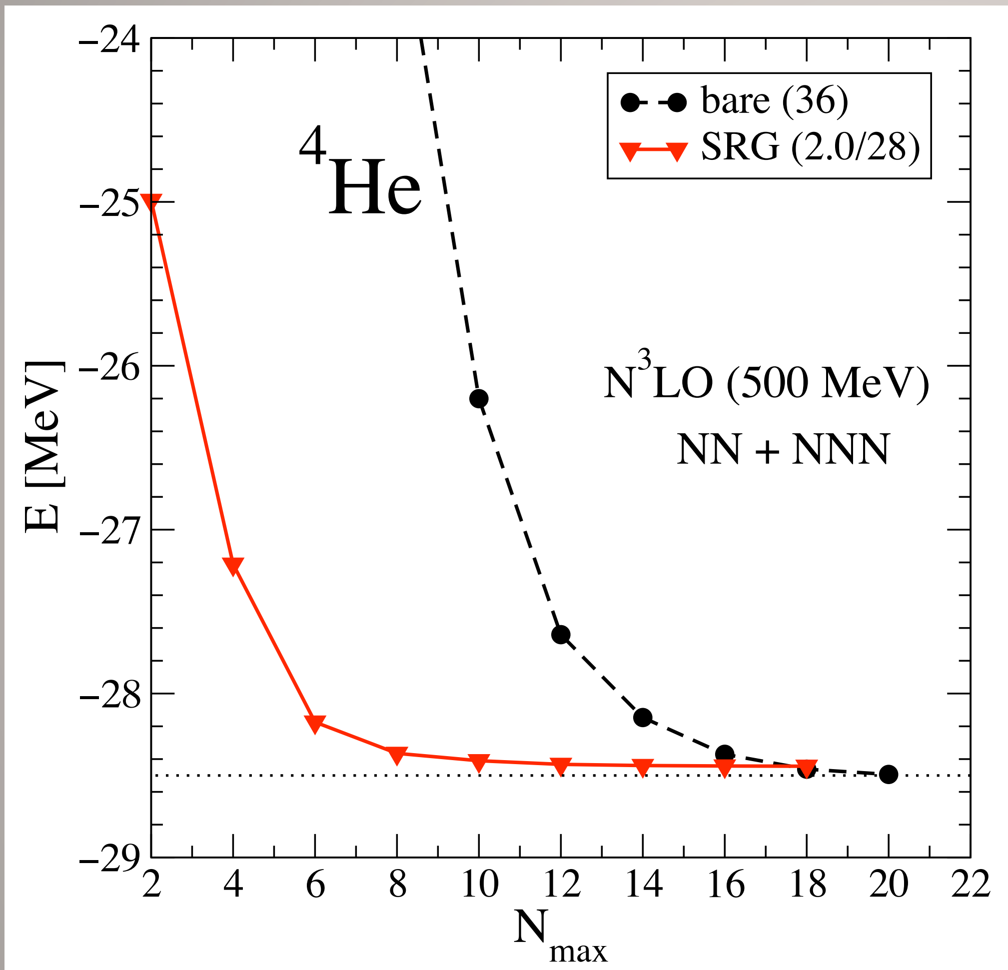
Calculations with chiral 3N: SRG renormalization needed



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

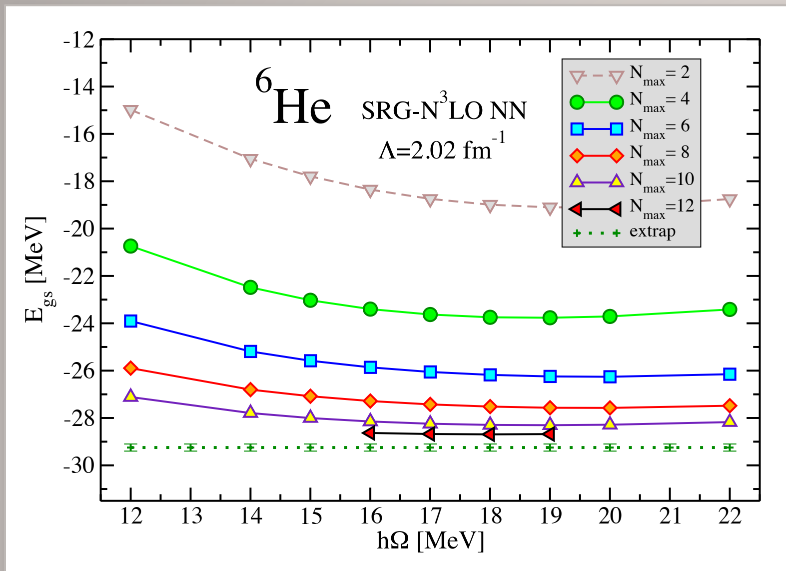
Chiral N^{3}LO NN plus N^{2}LO NNN potential

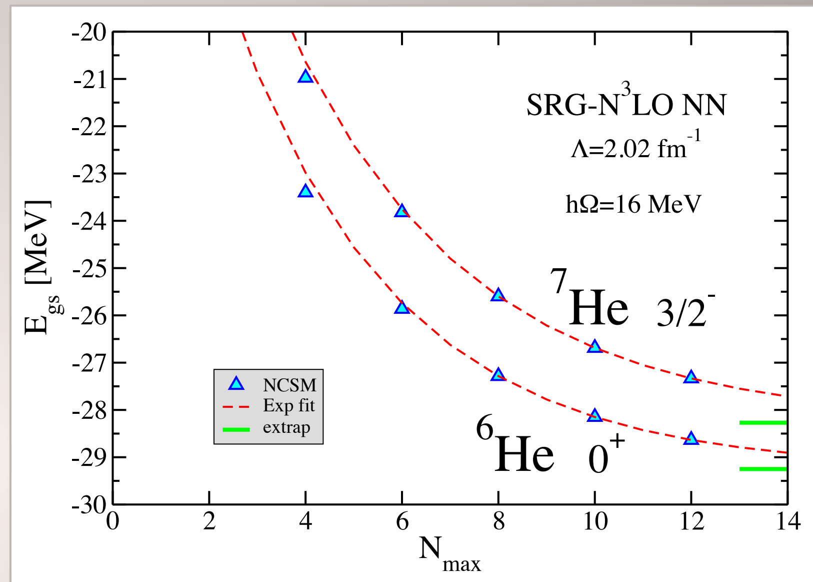
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

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

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

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

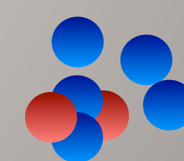




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ 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

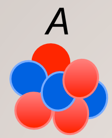


unbound

Extending no-core shell model beyond bound states

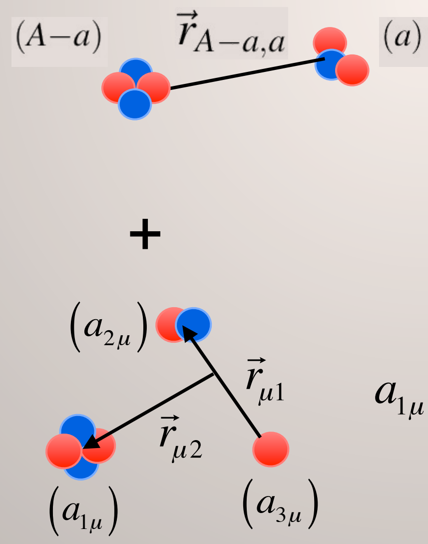
Include more many nucleon correlations…

NCSM →



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

+



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

+

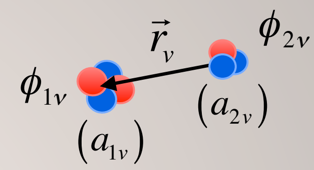
…

…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

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

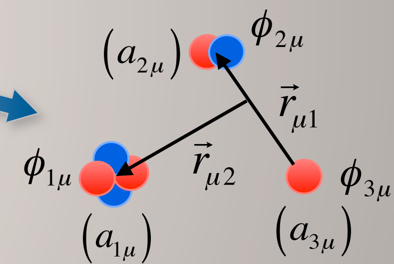
$$+\sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



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

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

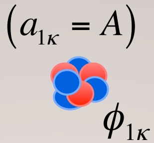
$$+ \cdots$$



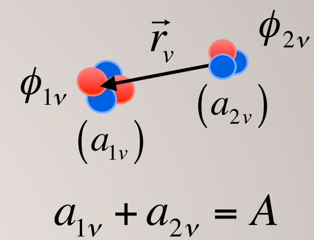
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

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

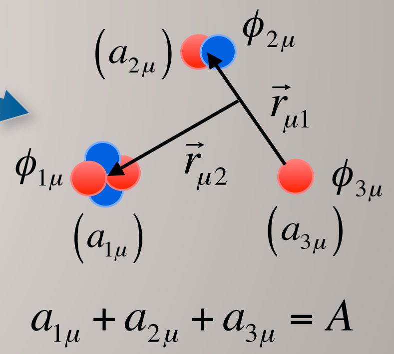


$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

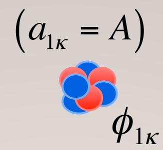
$$+ \cdots$$



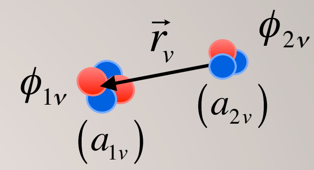
- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

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



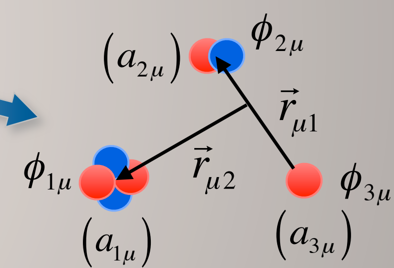
$$+\sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



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

$$+\sum_{\mu} \hat{A}_\mu \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_\mu(\vec{R}_{\mu1}, \vec{R}_{\mu2})$$

$$+ \cdots$$



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

- ***A_ν, A_μ*** : intercluster antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

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

Trial function: generalized cluster wave function

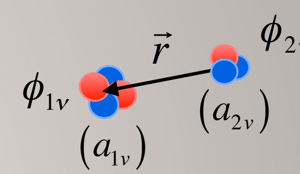
$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$(a_{1\kappa} = A)$

$\phi_{1\kappa}$

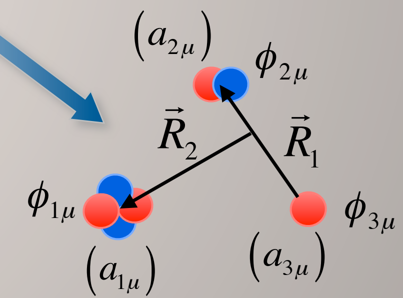
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\, \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right] d\vec{r}$$

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



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

$$+ \cdots$$



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

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

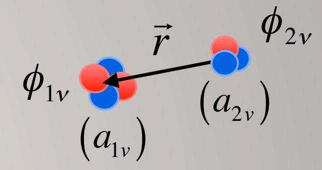
Trial function: generalized cluster wave function

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

$(a_{1\kappa} = A)$

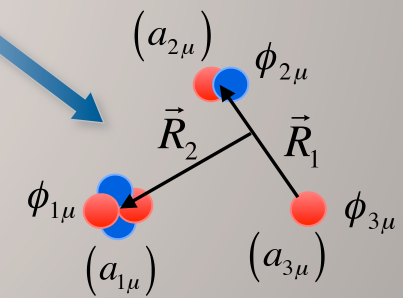
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\, \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right] d\vec{r}$$

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



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

$$+ \cdots$$



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

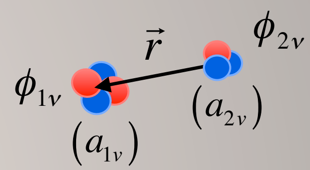
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

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

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

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



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

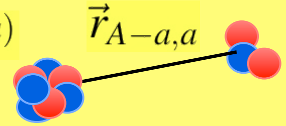
$$+ \cdots$$

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

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

Norm kernel (Pauli principle)

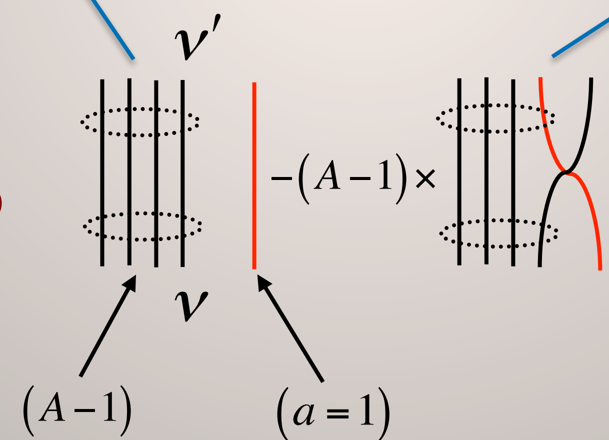
Single-nucleon projectile

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

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

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

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)

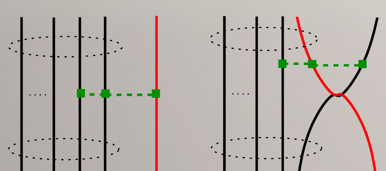
$$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Including 3N interaction in the NCSM/RGM Single-nucleon projectile:

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

$$\mathcal{V}^{NNN}_{\nu'\nu}(r,r') = \sum R_{n'l'}(r') R_{nl}(r) \left[\frac{(A-1)(A-2)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | V_{A-2A-1A}(1-2P_{A-1A}) | \Phi^{J^\pi T}_{\nu n} \rangle - \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | P_{A-1A} V_{A-3A-2A-1} | \Phi^{J^\pi T}_{\nu n} \rangle \right] .$$

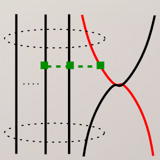
Direct potential: in the model space (interaction is localized!)



(a) (b)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a_i^+ a_j^+ a_l a_k \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

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



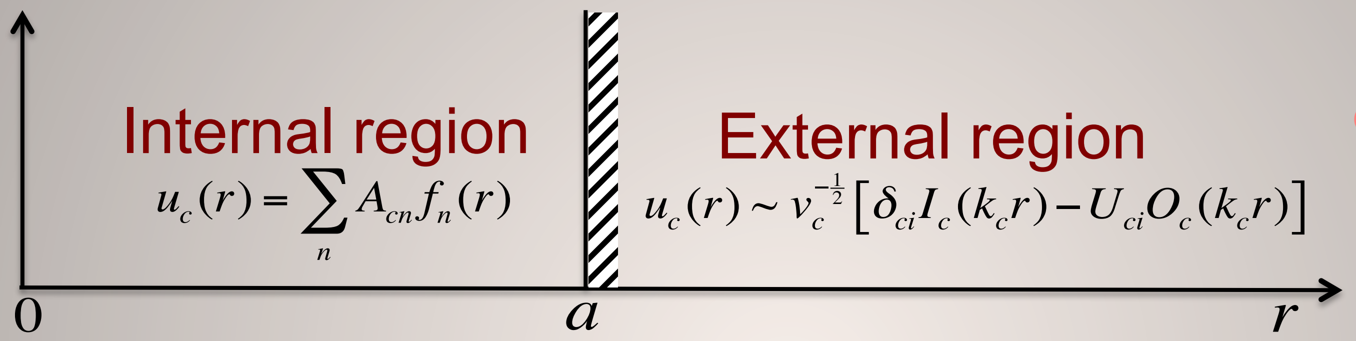
(c)

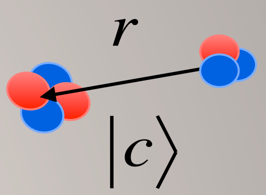
$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a_h^+ a_i^+ a_j^+ a_m a_l a_k \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

Including 3N interaction challenging: more than *2 body density required*

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

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

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

- Internal region: expansion on square-integrable Lagrange mesh basis
- External region: asymptotic form for large r

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

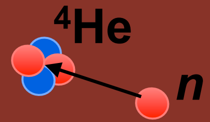
$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

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

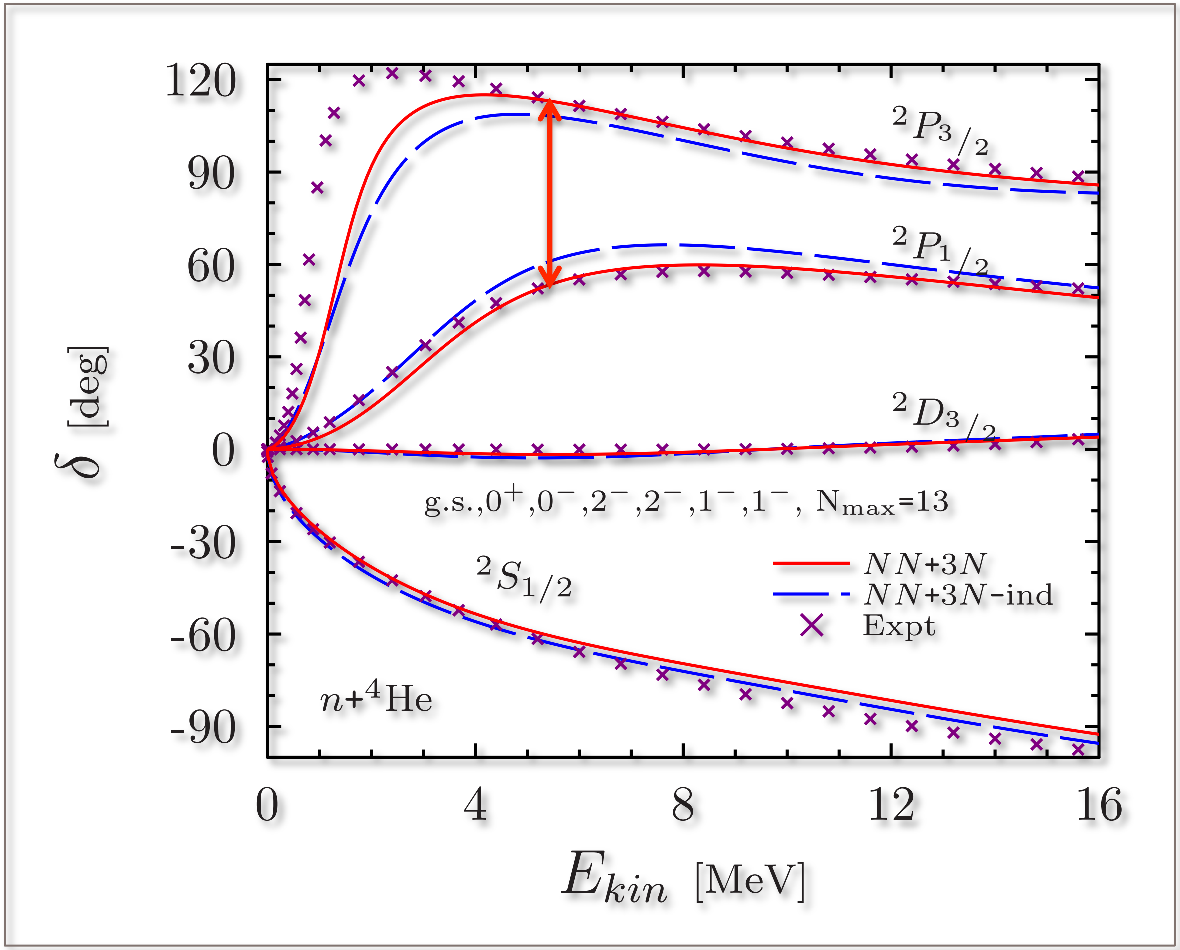
$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$$

Bound state — Scattering state — Scattering matrix

TRIUMF



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



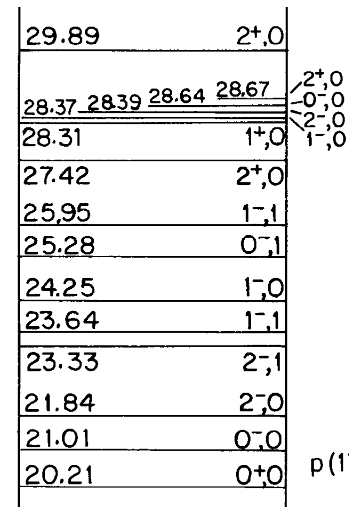
PHYSICAL REVIEW C **88**, 054622 (2013)

Ab initio **many-body calculations of nucleon-^{4}He scattering with three-nucleon forces**

Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]

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

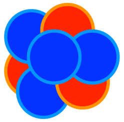
^{4}He g.s. and 6 excited states



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

New developments: NCSM with continuum

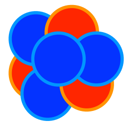
NCSM



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

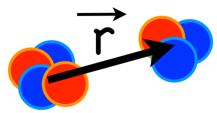
New developments: NCSM with continuum

NCSM



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

NCSM/RGM



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

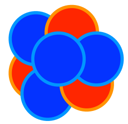
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

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

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

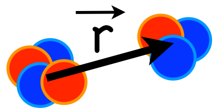
New developments: NCSM with continuum

NCSM



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

NCSM/RGM

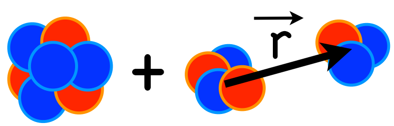


$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r}\,\chi_\nu(\vec{r})\hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

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

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

NCSMC



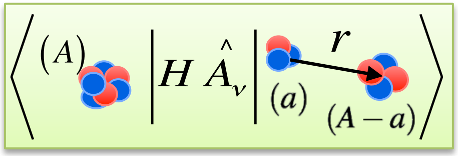
S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

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

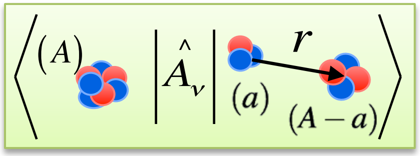
$$\boxed{\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix}}$$

Building blocks of the NCSMC equations

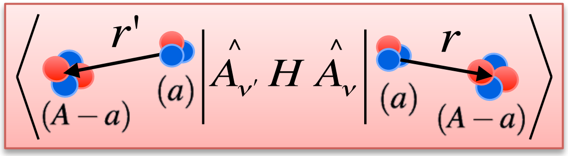
$E_\lambda^{NCSM} \quad \delta_{\lambda\lambda'}$

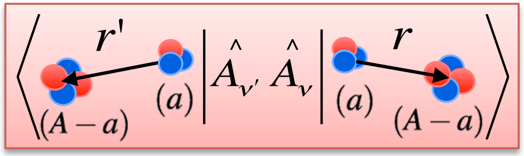


$\delta_{\lambda\lambda'}$



$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

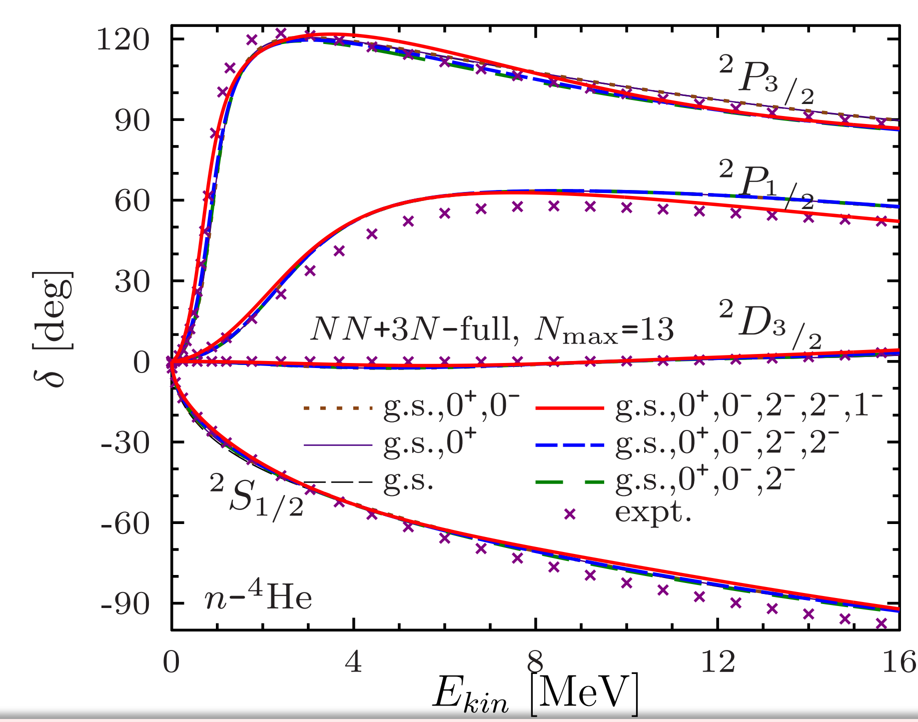




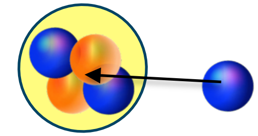
n-^{4}He scattering with NCSMC

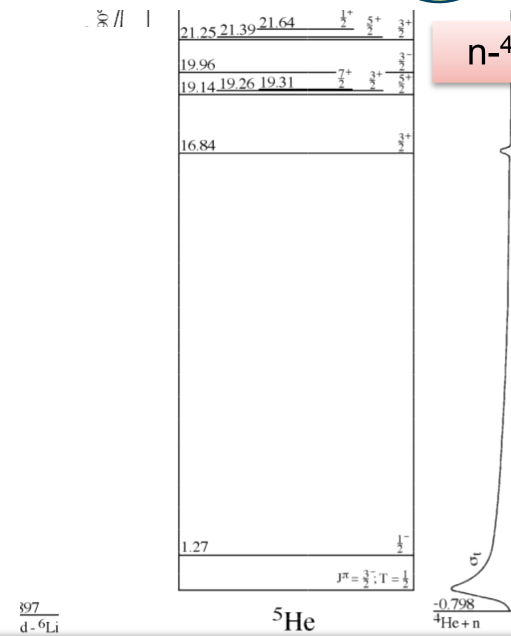
G. Hupin, S. Quaglioni and P. Navrátil, work in progress

Study of the convergence with respect to the # of ^{4}He low-lying states



n-^{4}He scattering phase-shifts for NN+NNN potential with λ=2.0 fm^{-1} and 8 low-lying state of ^{5}He.



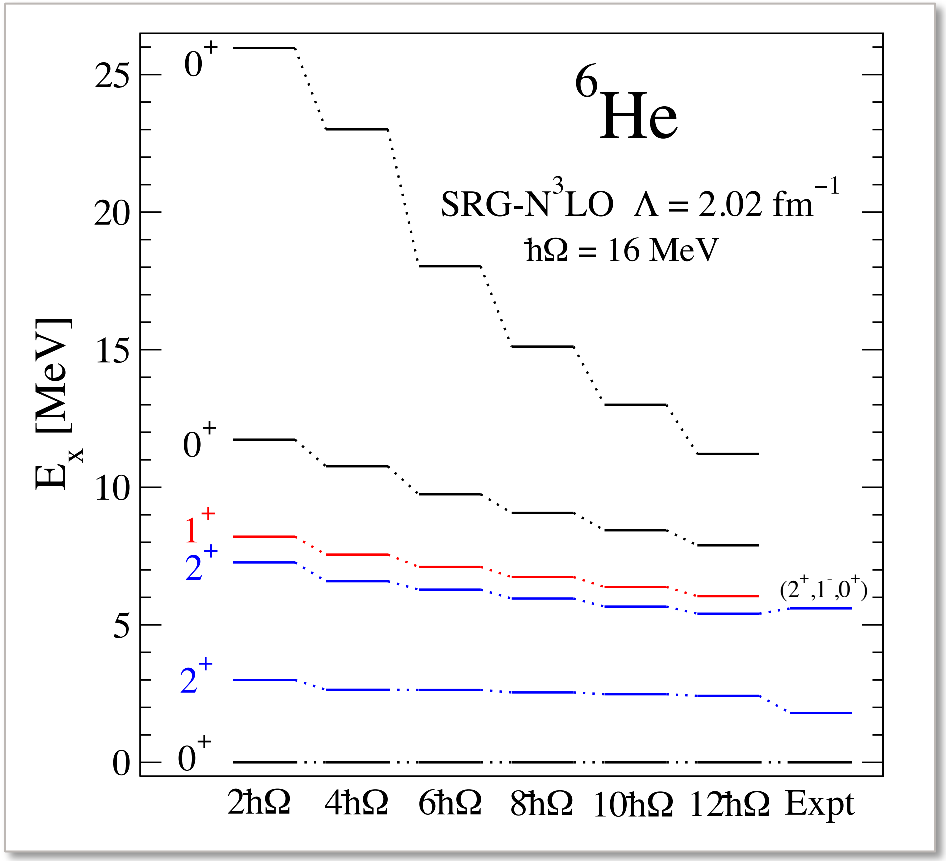


n-^{4}He scattering

Experimental low-lying states of the A=5 nucleon systems.

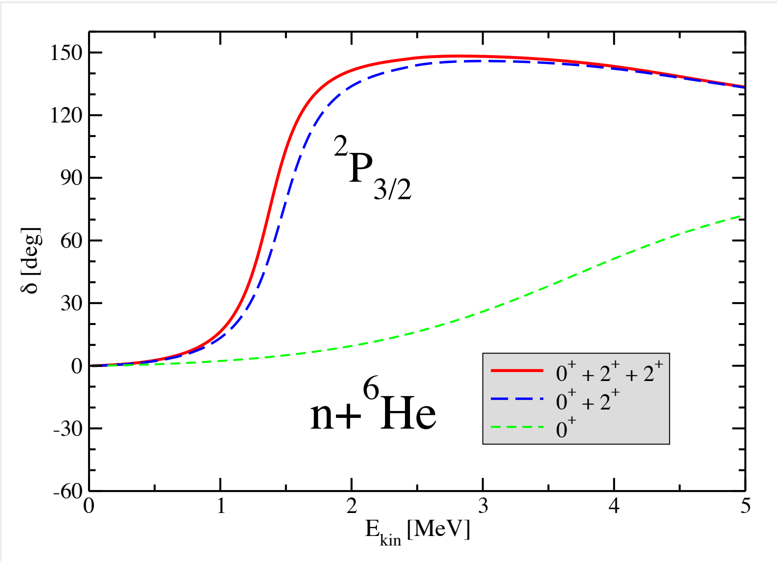
- The convergence pattern looks good.
- The experimental phase-shifts are well reproduced.

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

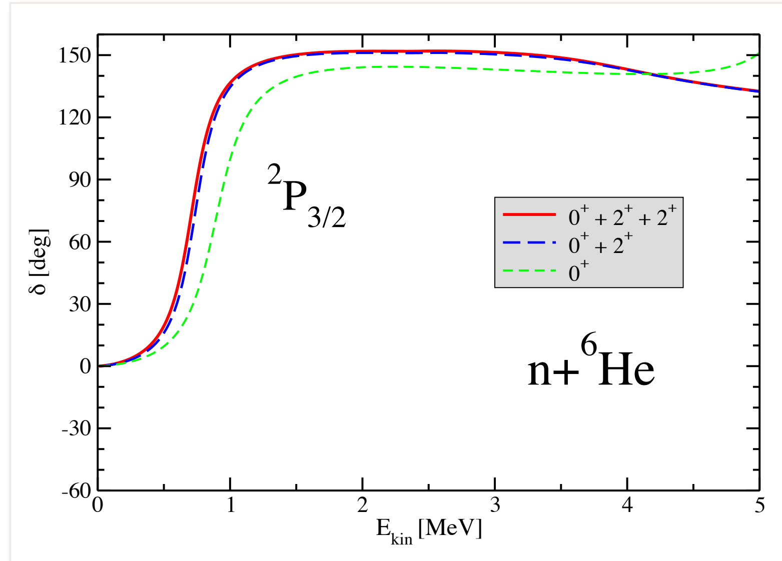


- All ^{6}He excited states above 2^+_1 broad resonances or states in continuum
- Convergence of the NCSM/RGM n+^{6}He calculation slow with number of ^{6}He states
  - Negative parity states also relevant
  - Technically not feasible to include more than ~ 5 states

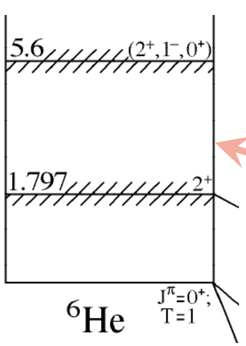
NCSM with continuum: ^{7}He ↔ ^{6}He+n



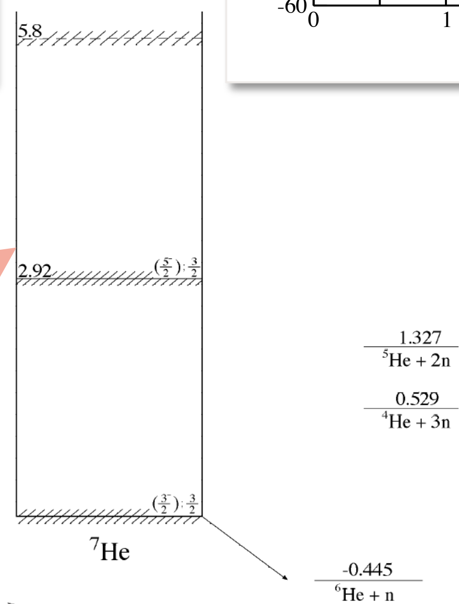
NCSM/RGM
with up to three ^{6}He states



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

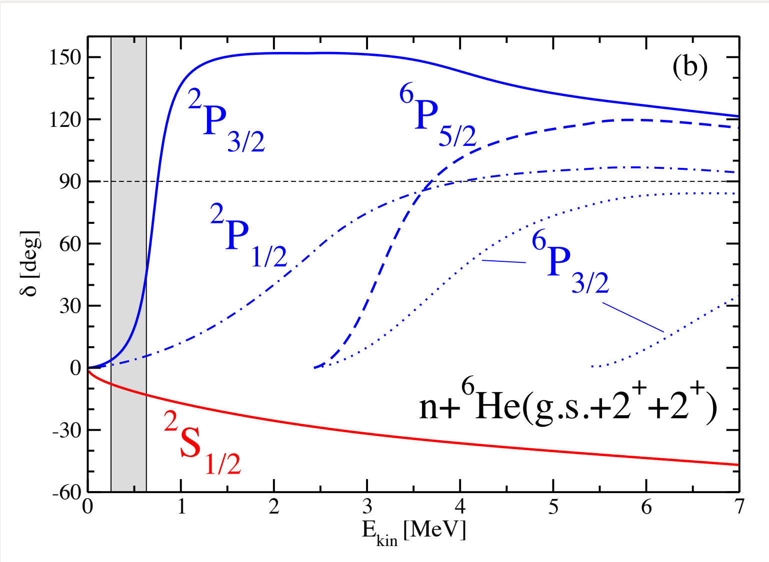


Expt.

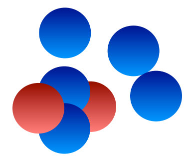


TRIUMF

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



^{7}He



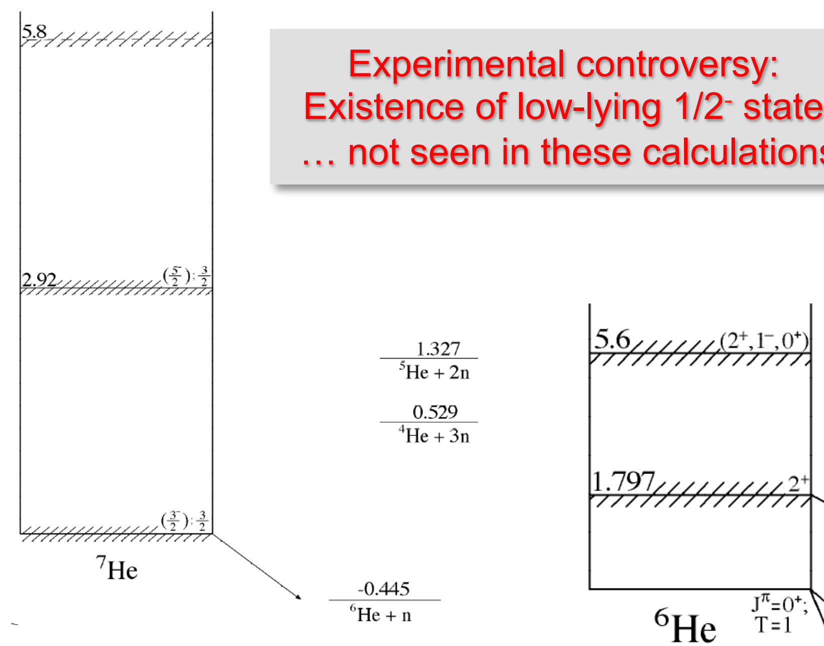
unbound

J^π	experiment			NCSMC	
	E_R	Γ	Ref.	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]		

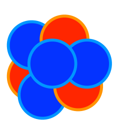
[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

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

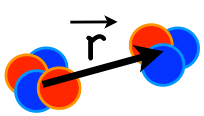
Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations



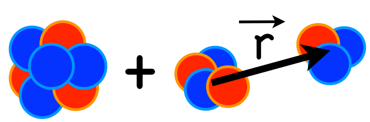
NCSM



NCSM/RGM



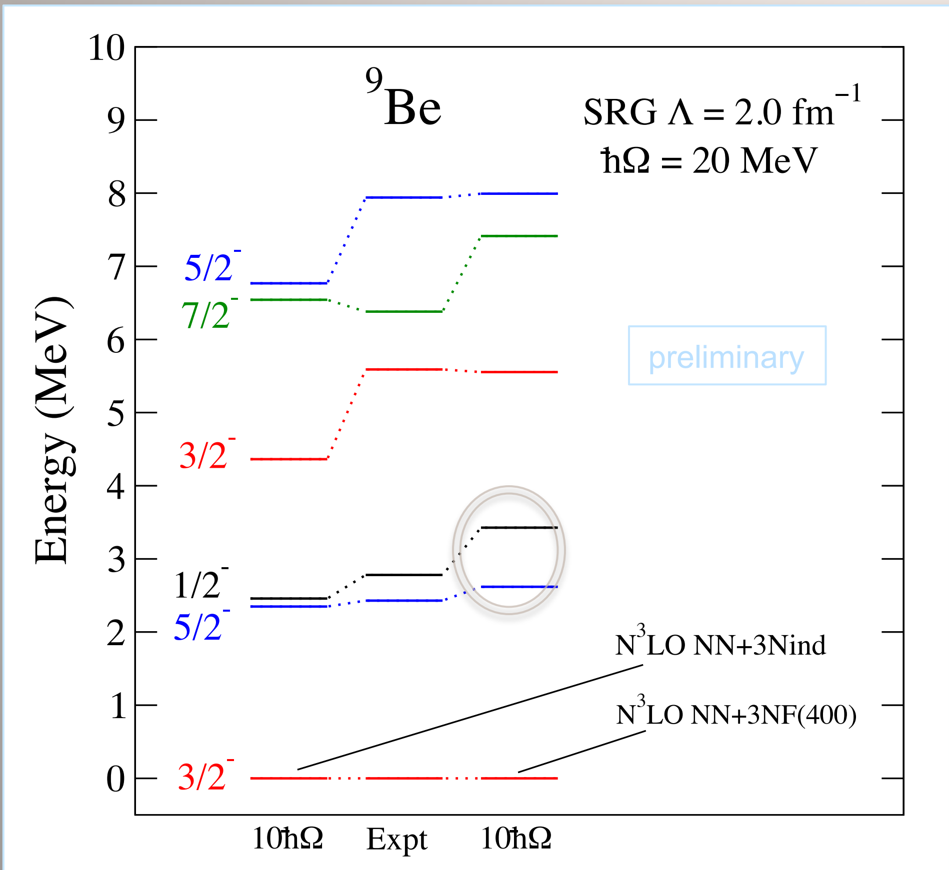
NCSMC



Structure of ^{9}Be

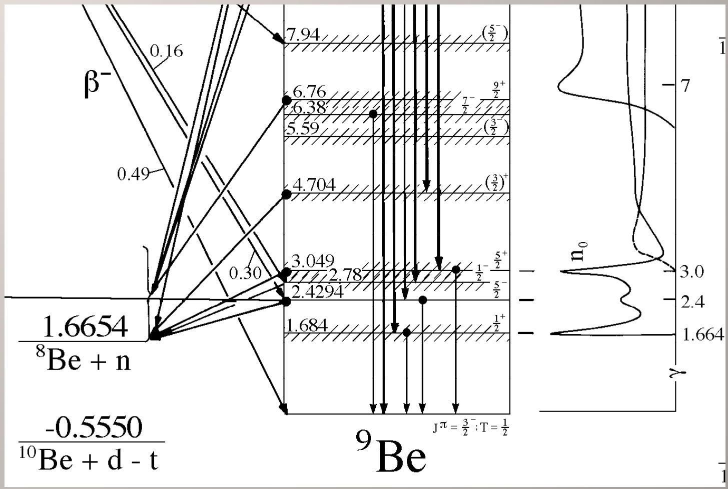
in collaboration with Joachim Langhammer et al.

- 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?

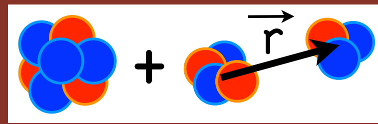


1/2$^-$ state moved to high energy by the 3N interaction

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



TRIUMF



Structure of ^{9}Be

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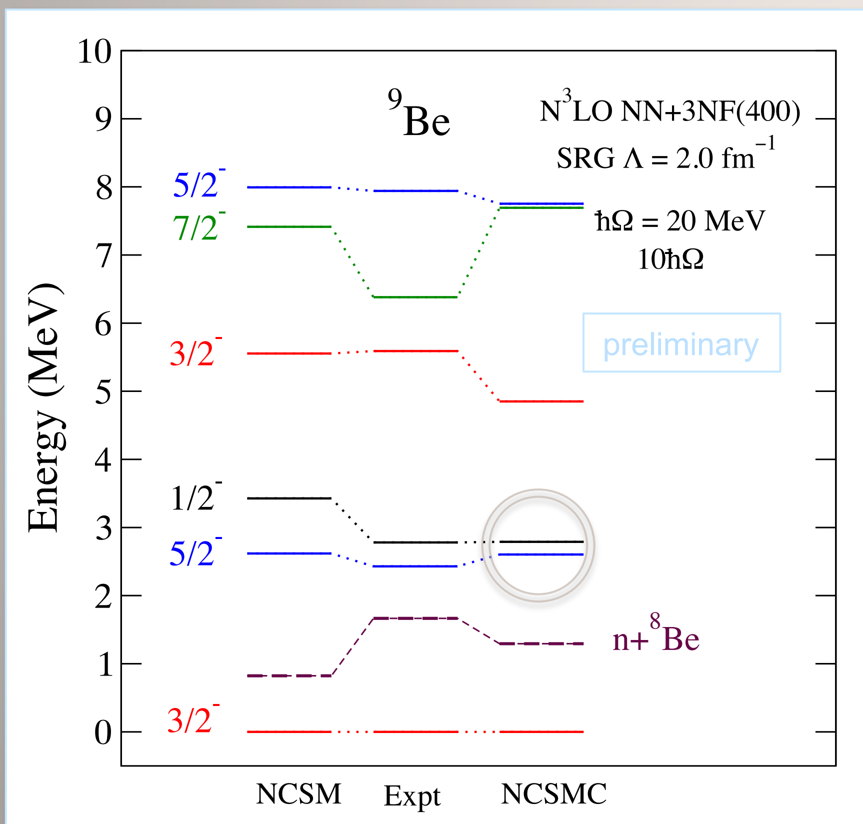


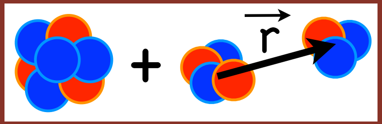
NCSMC
n-^{8}Be(0^{+},2^{+}) + ^{9}Be

NCSMC with the 3N under way

Preliminary results
in N_{max}=10 space:

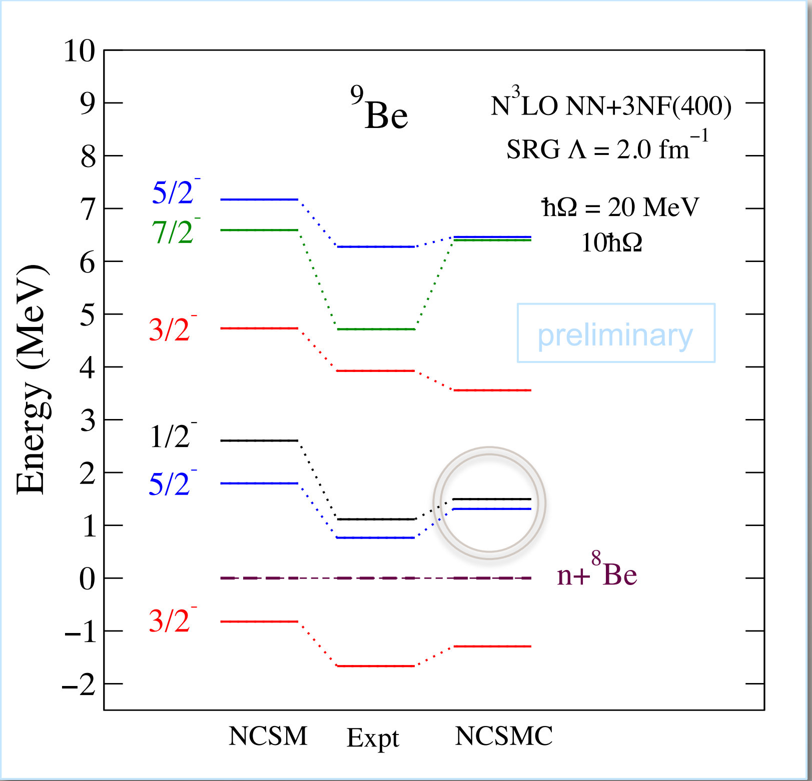
$5/2^{-}$ a very narrow *F*-wave resonance – no shift

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

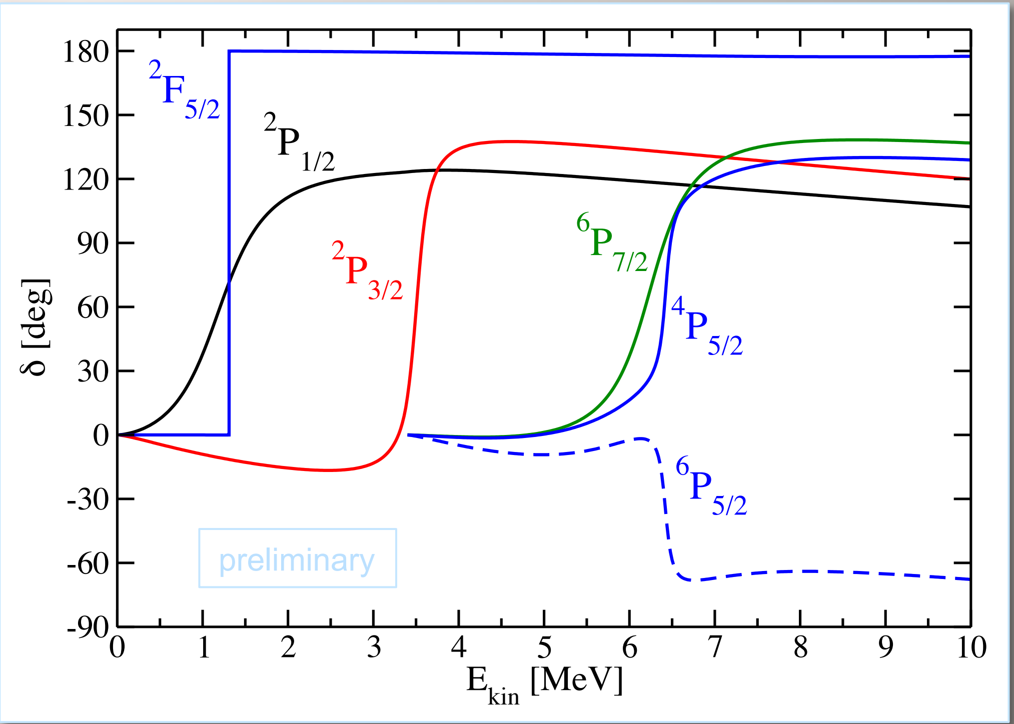


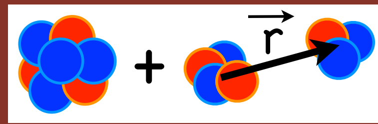
Structure of ^{9}Be

- 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

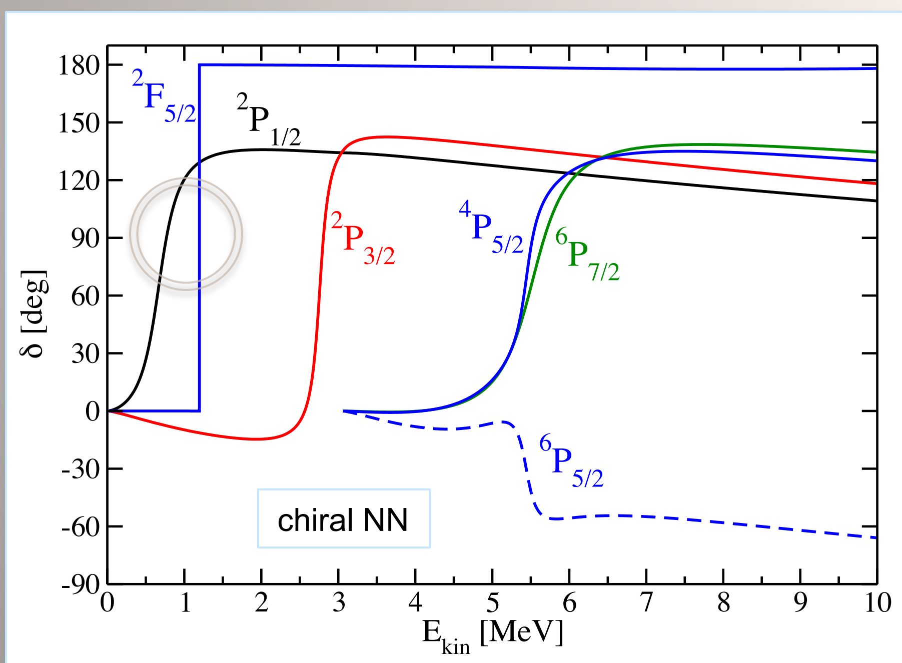


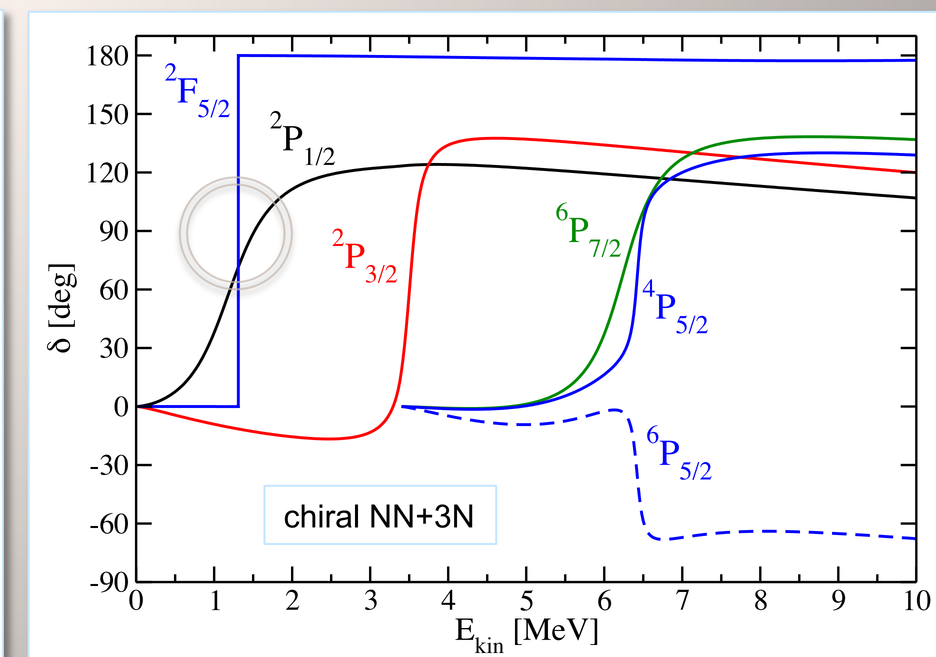


Structure of ^{9}Be

- The 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!**
- Without the 3N the 5/2^{-} and 1/2^{-} resonances reversed!

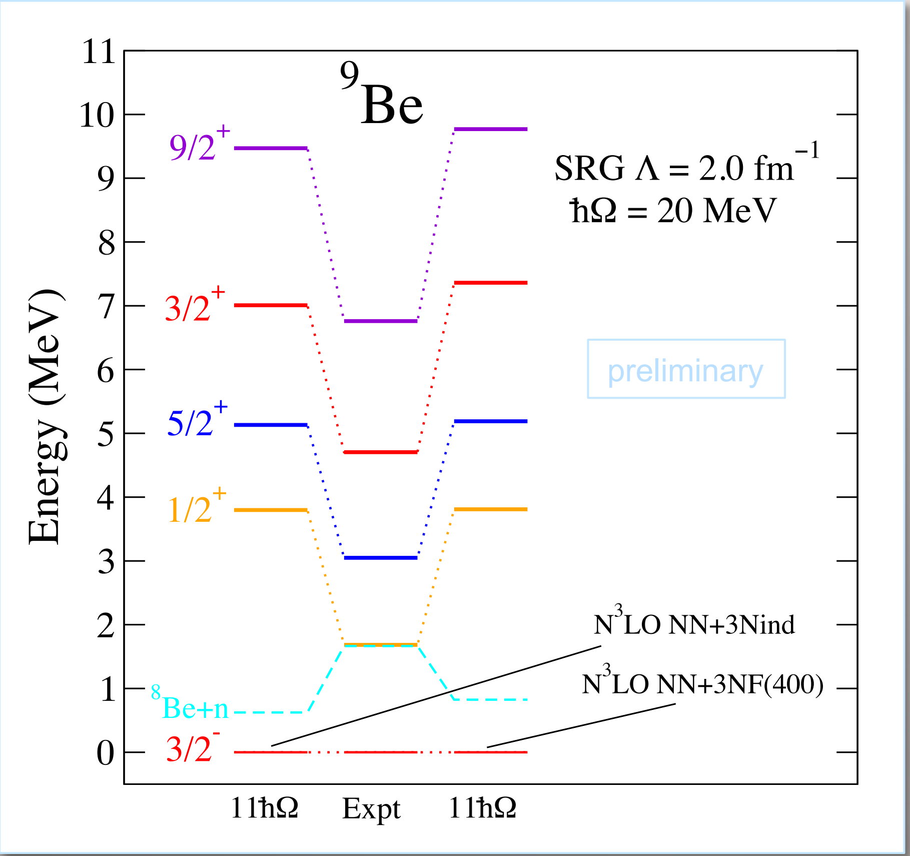
NCSMC
n-^{8}Be(0^{+},2^{+}) + ^{9}Be





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?

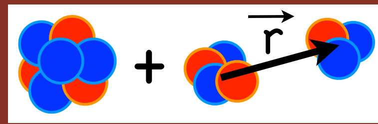


Bad with any interaction

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

But…

TRIUMF

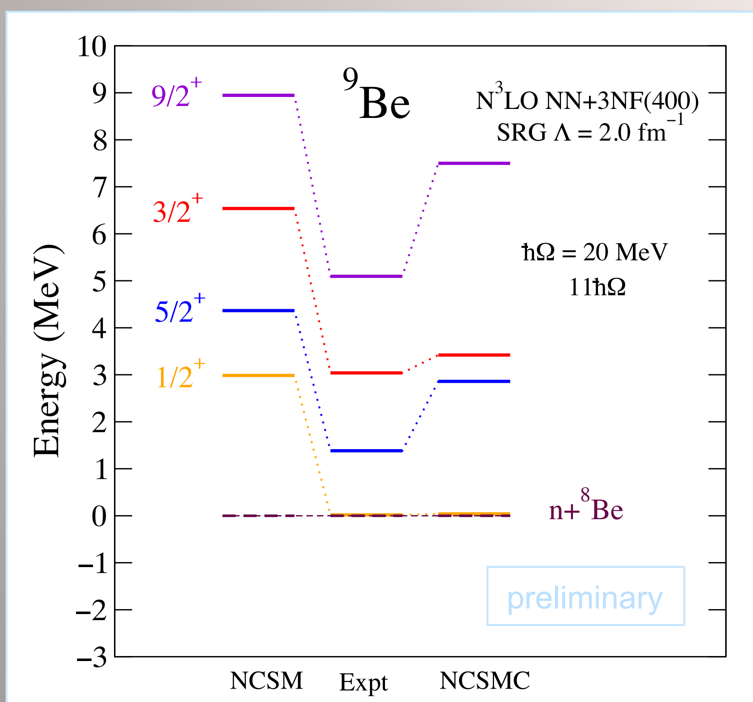


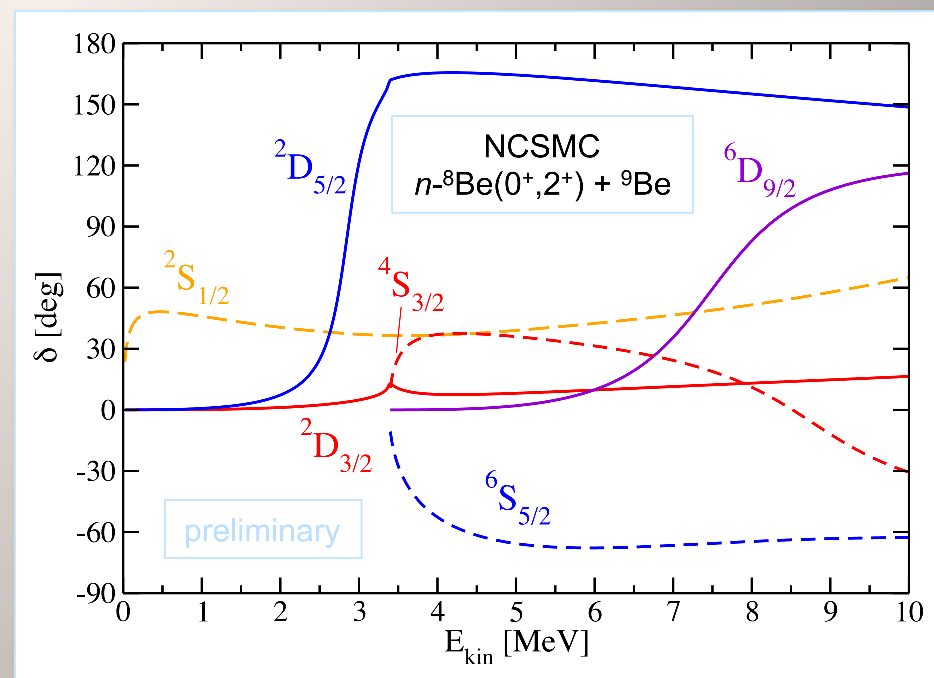
Structure of ^{9}Be

- 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

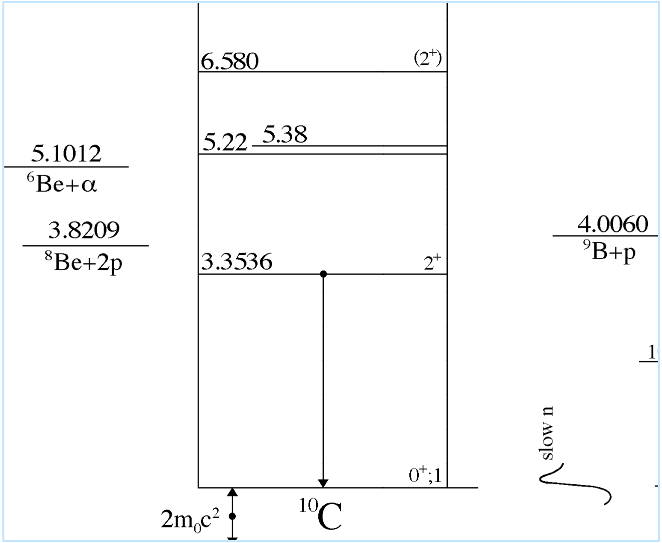


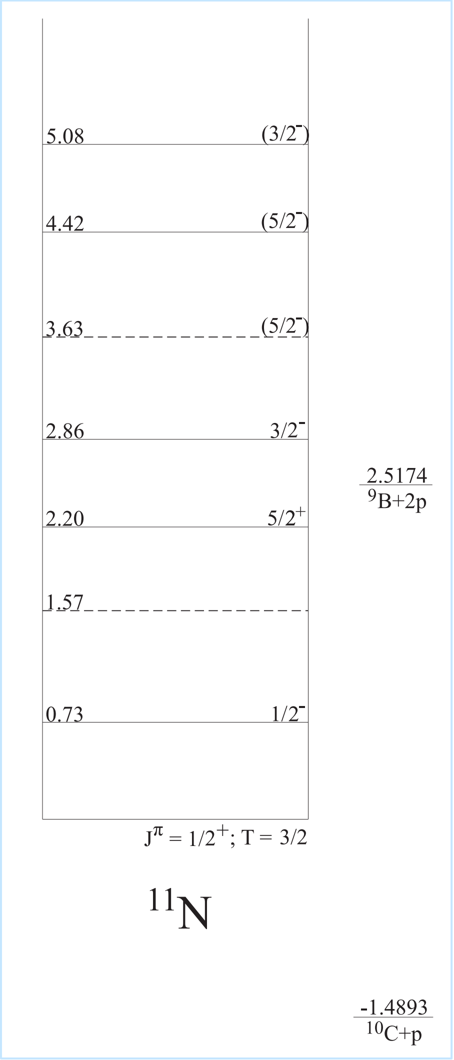


p+^{10}C scattering: structure of ^{11}N resonances

in collaboration with Joachim Langhammer et al.

- Limited information about the structure of proton rich ^{11}N – mirror nucleus of ^{11}Be halo nucleus
- Incomplete knowledge of ^{10}C unbound excited states

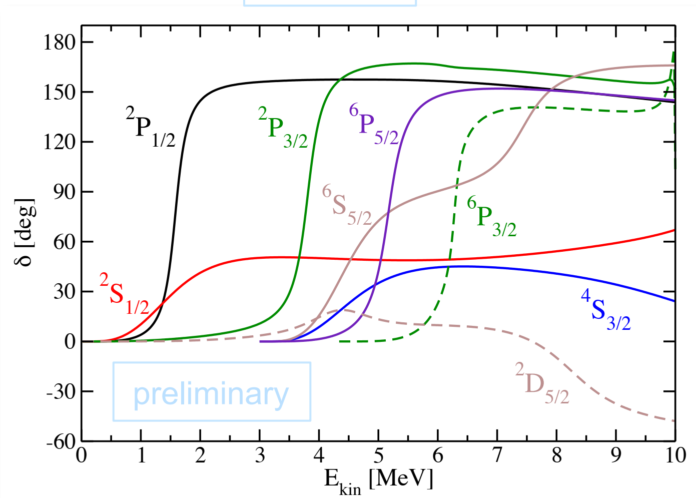




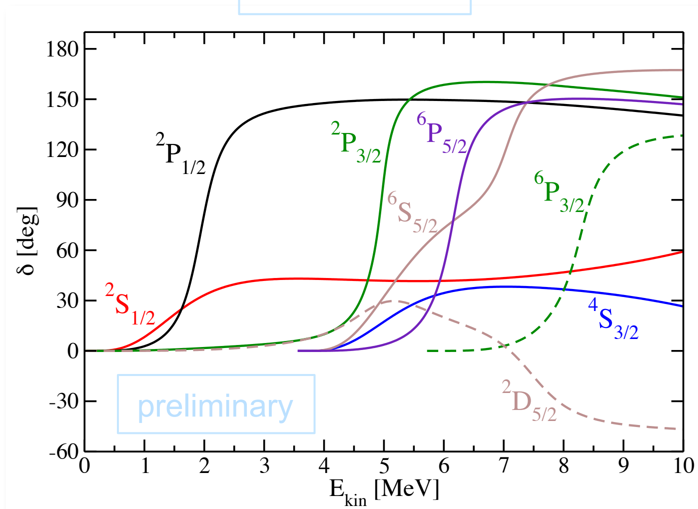
p+^{10}C scattering: structure of ^{11}N resonances

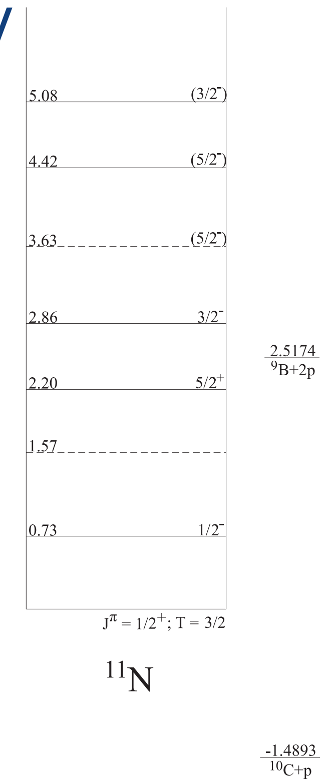
- New experiment at ISAC TRIUMF with reaccelerated ^{10}C
  - The first ever ^{10}C beam at TRIUMF
  - Angular distributions measured at E_{CM} ~ 4.1 MeV and 4.4 MeV
- NCSMC calculations including chiral 3N under way
  - p-^{10}C(0^+,2^+,2^+)+^{11}N (N_{max}= 7 so far)

chiral NN



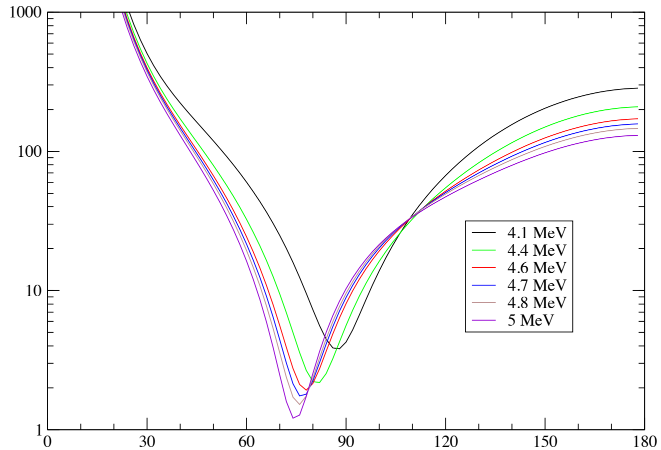
chiral NN+3N



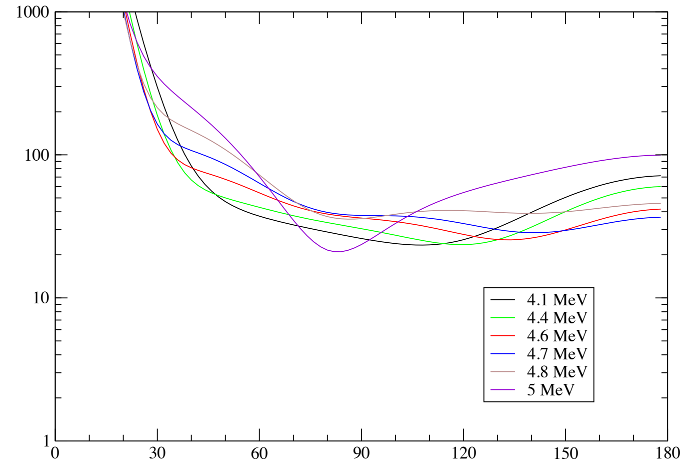


With the 3N the $^2P_{1/2}$ and $^2P_{3/2}$ resonances broader and shifted to higher energy in a better agreement with experiment

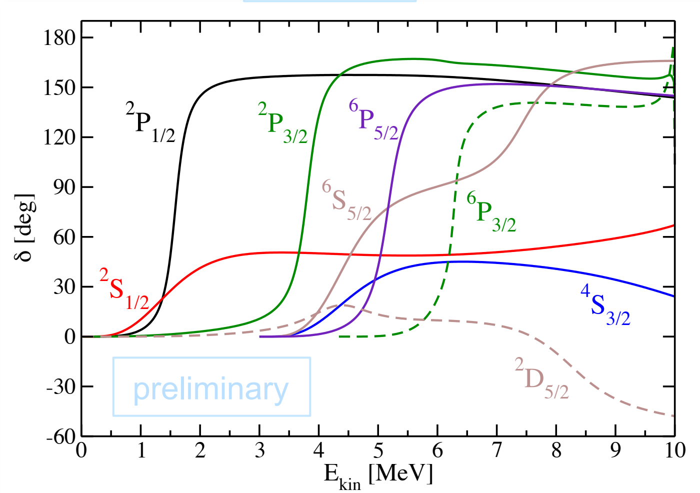
$p+{}^{10}C$ scattering: structure of ${}^{11}N$ resonances

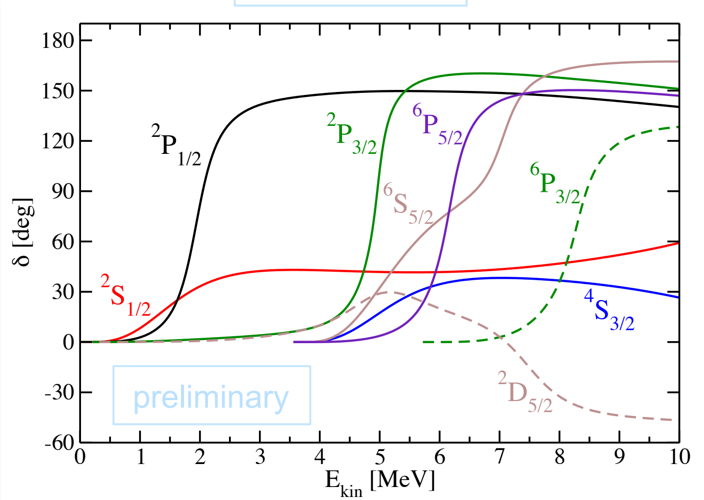


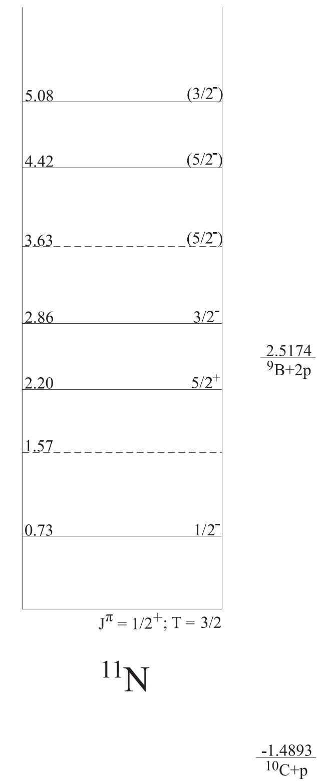
chiral NN



chiral NN+3N



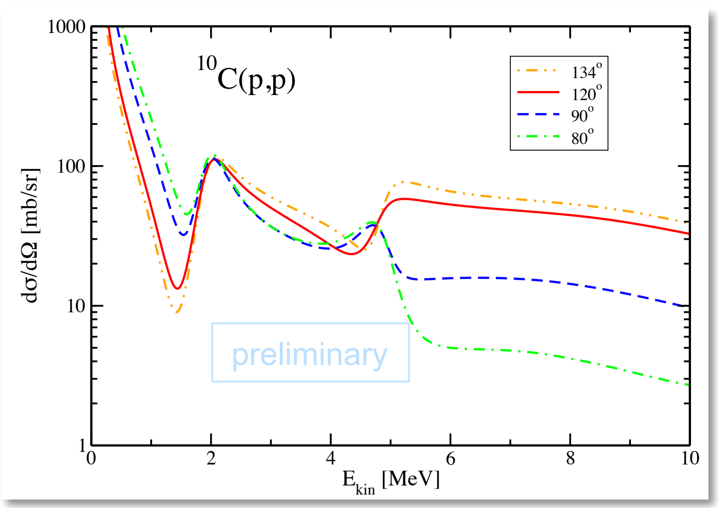


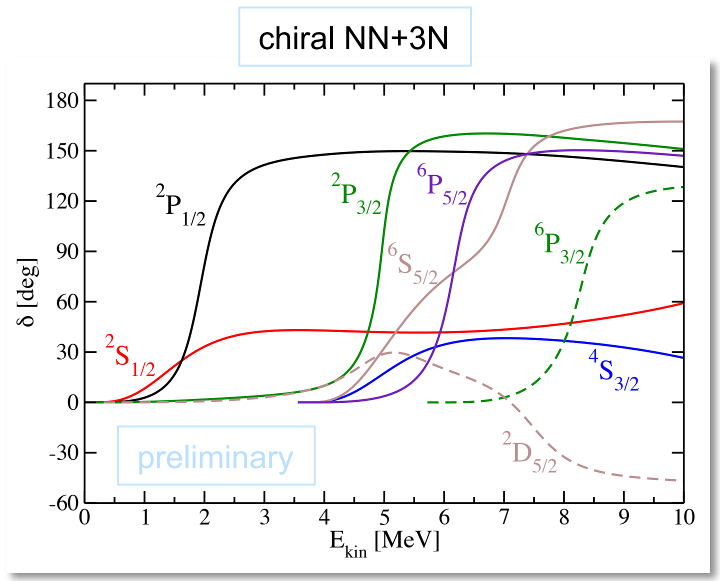


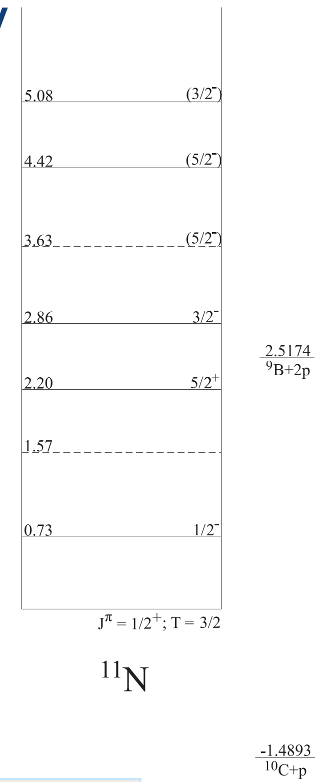
Significant difference in angular distributions in the experimentally explored energy range

p+^{10}C scattering: structure of ^{11}N resonances

- New experiment at ISAC TRIUMF with reaccelerated ^{10}C
  - The first ever ^{10}C beam at TRIUMF
  - Angular distributions measured at E_{CM} ~ 4.1 MeV and 4.4 MeV
- NCSMC calculations including chiral 3N under way
  - p-^{10}C(0^+,2^+,2^+)+^{11}N







Strong variations in angular distributions associated with the $^2P_{1/2}$ and $^2P_{3/2}$ resonances

p+^{10}C scattering: structure of ^{11}N resonances

- New experiment at ISAC TRIUMF with reaccelerated ^{10}C
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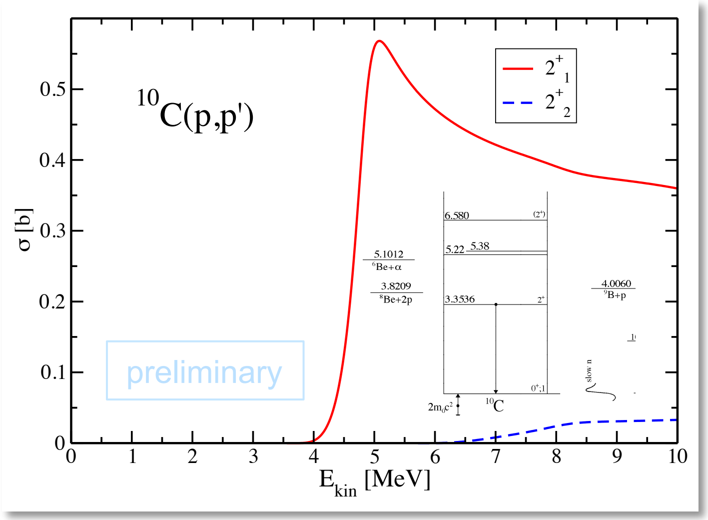
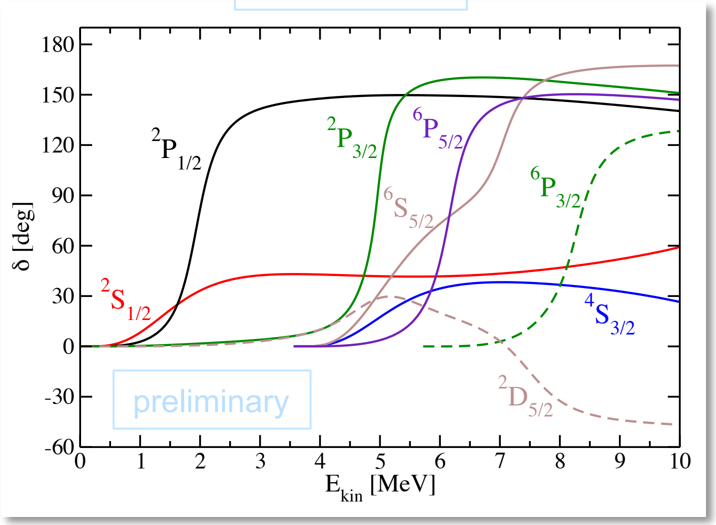
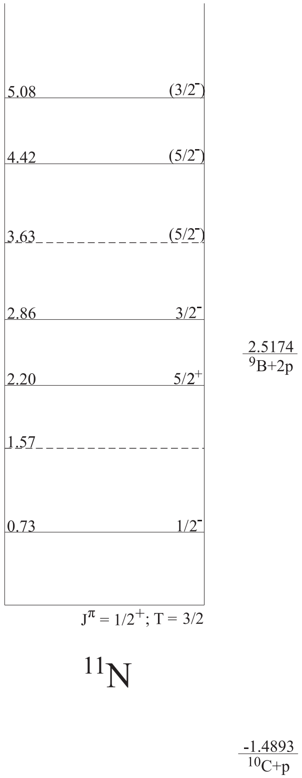


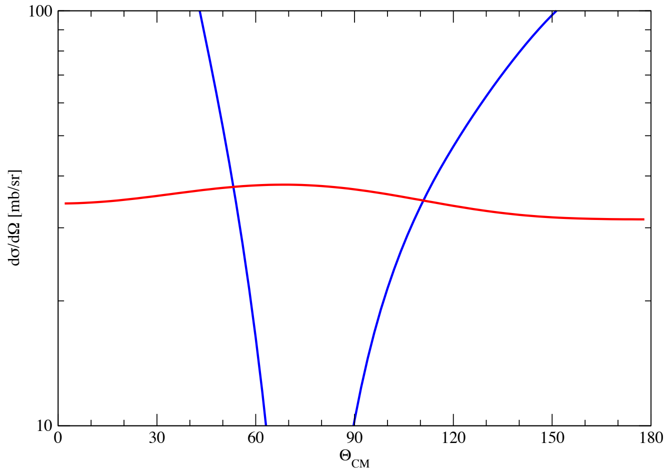
chiral NN+3N



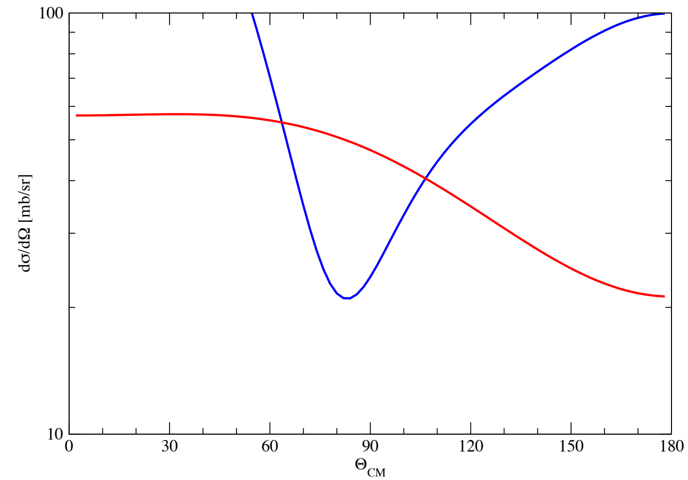


Inelastic cross section enhanced by the $5/2^+$ resonance

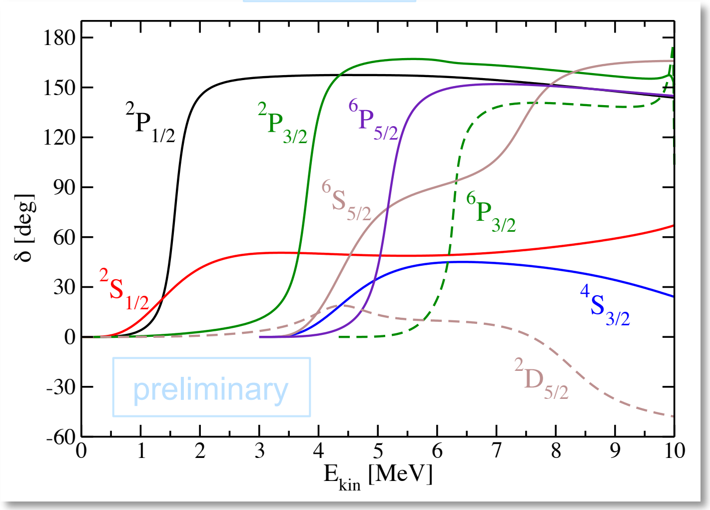
$p+^{10}$C scattering: structure of ^{11}N resonances

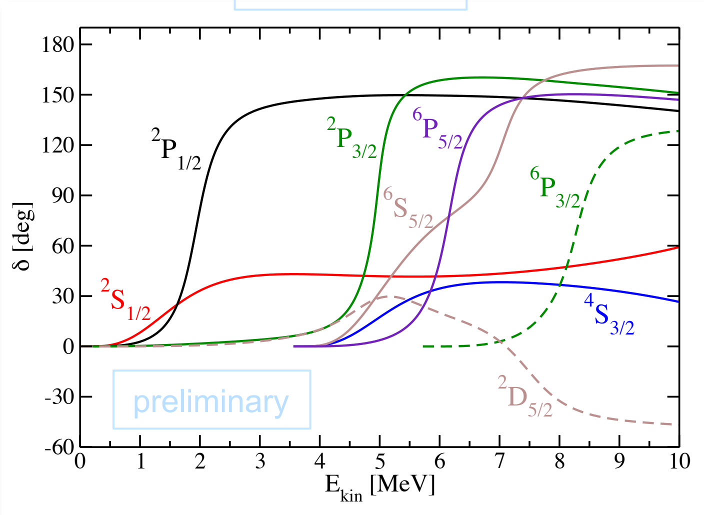


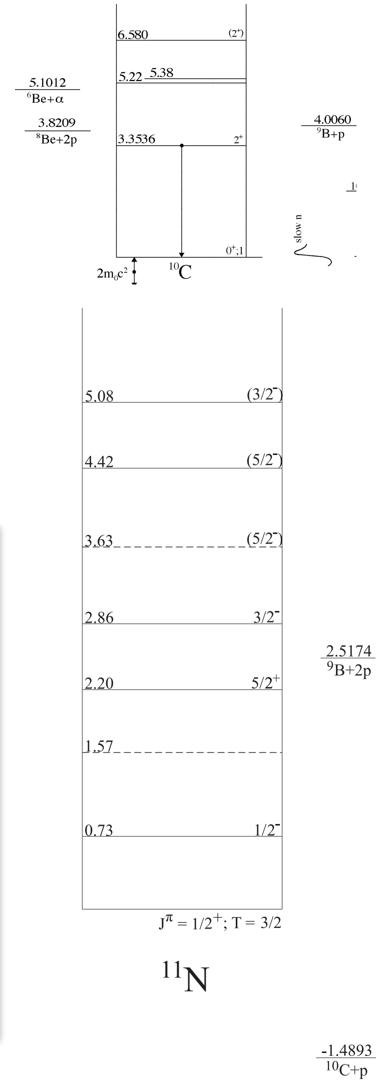
chiral NN



chiral NN+3N



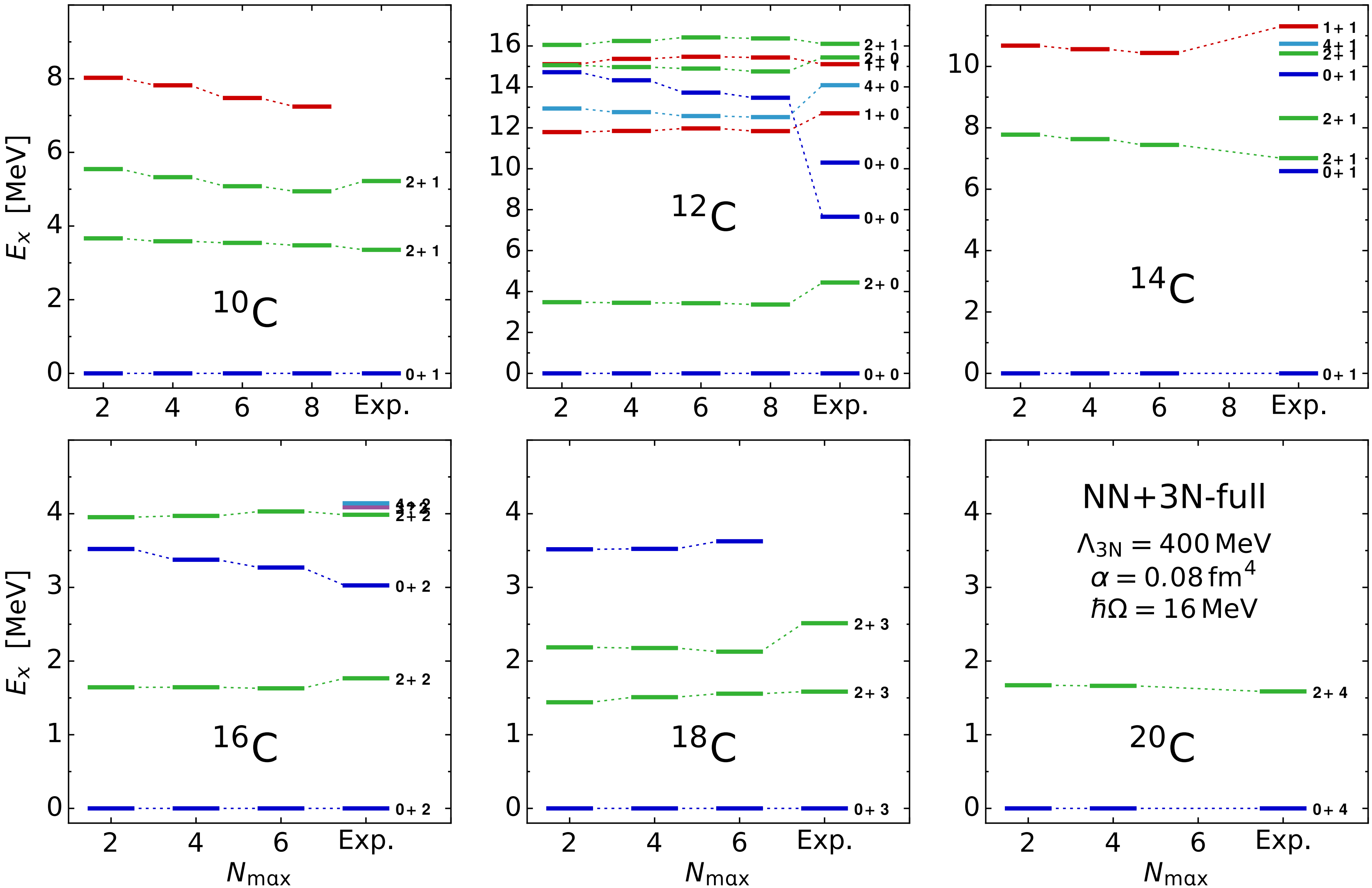




Significant difference in the shape of the inelastic differential cross section g.s. to 2^+_1 around E_{kin} ~ 5 MeV

TRIUMF

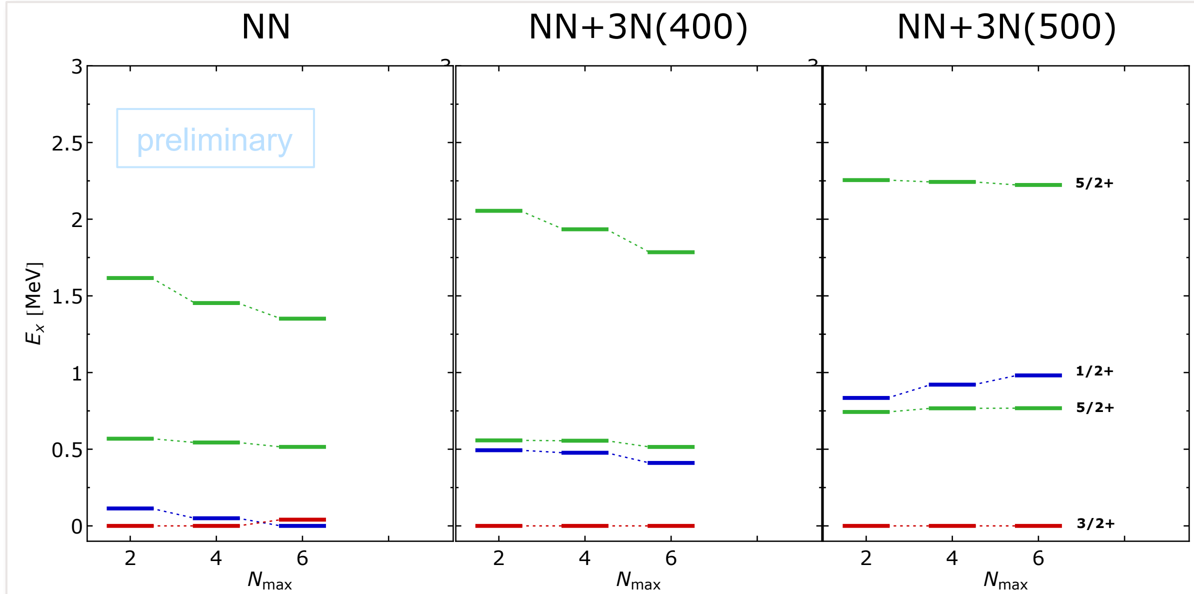
Neutron rich Carbon isotopes from chiral NN+NNN interactions (IT-NCSM, R. Roth *et al.*)



Neutron rich Carbon isotopes from chiral NN+NNN interactions (IT-NCSM, R. Roth *et al.*)

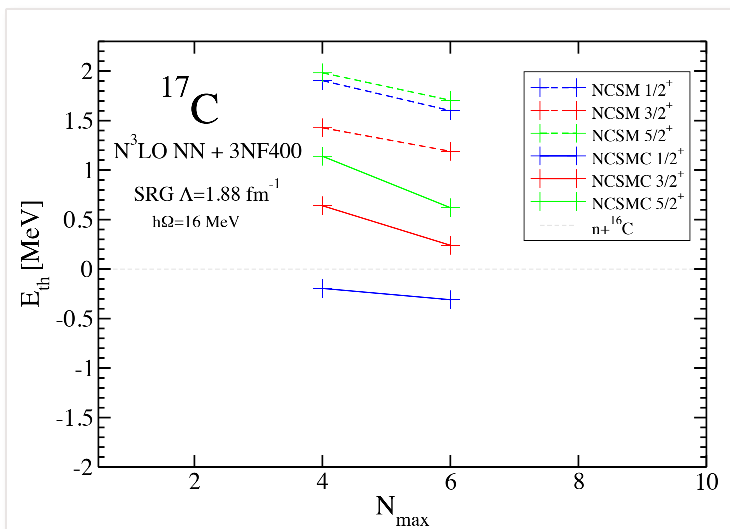
^{17}C

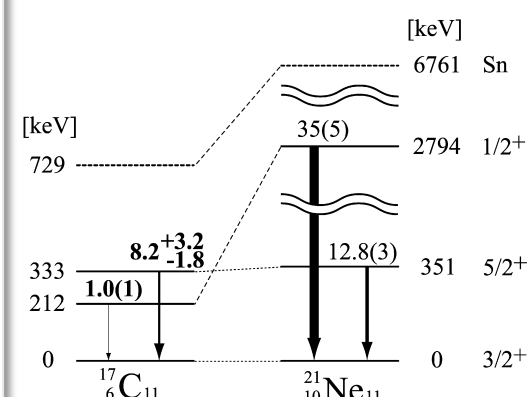
Strong sensitivity of excitation energies and even the ground state spin to the 3N interaction



What is the impact of continuum?

NN+3NF400:
NCSM states unbound
NCSMC binds $1/2^+$, lowers $3/2^+$ and $5/2^+$





Neutron rich Carbon isotopes from chiral NN+NNN interactions (IT-NCSM, R. Roth *et al.*)

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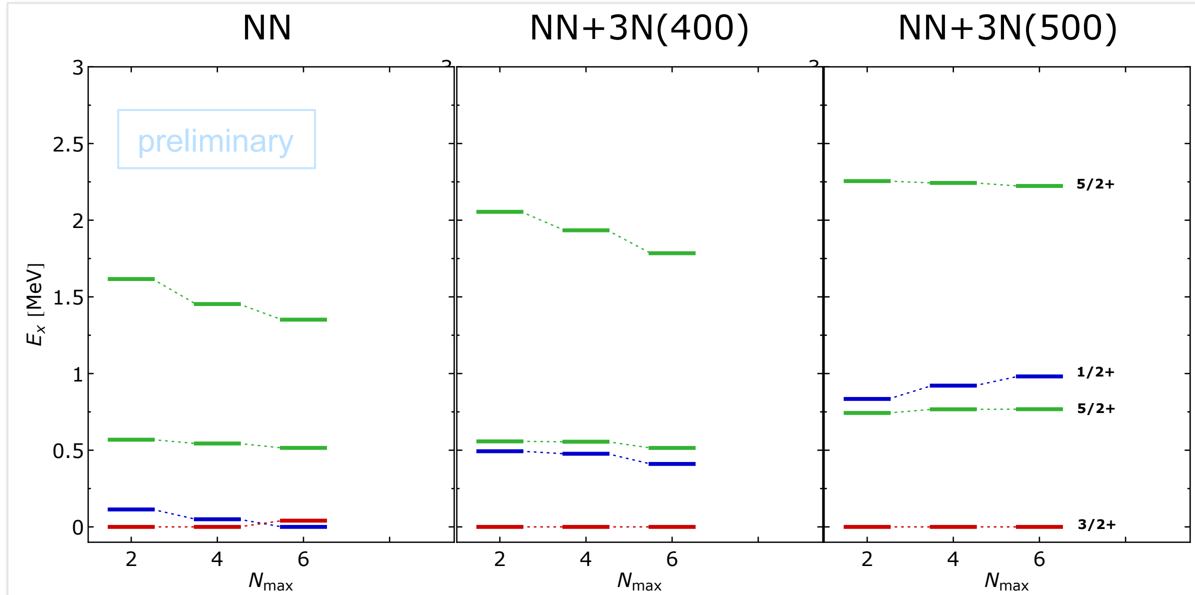
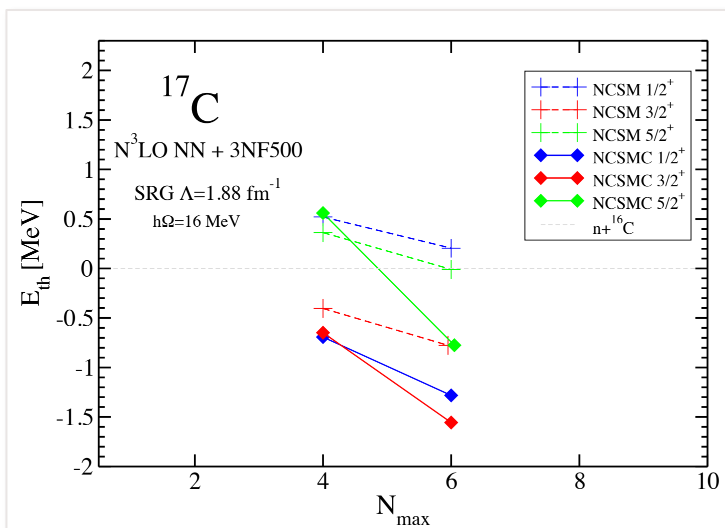
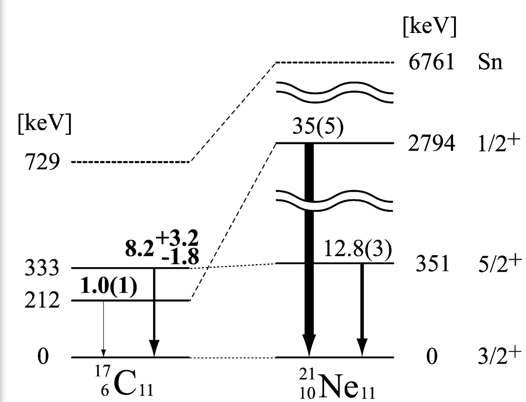


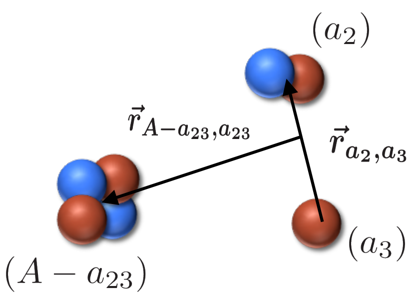
What is the impact of continuum?

NN+3NF500:
NCSM $3/2^+$, $5/2^+$ states bound, $1/2^+$ unbound
NCSMC binds all





NCSM/RGM for three-body clusters: Structure of ^{6}He

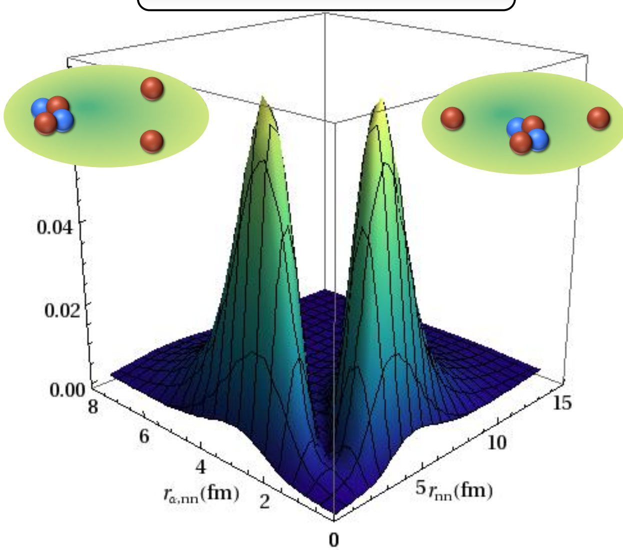


$$|\Phi^{J^\pi T}_{\nu r}\rangle \sim \underbrace{\Psi^{A-a_{23}}_{\alpha_1} \; \Psi^{a_2}_{\alpha_2} \; \Psi^{a_3}_{\alpha_3}}_{\text{NCSM}}$$

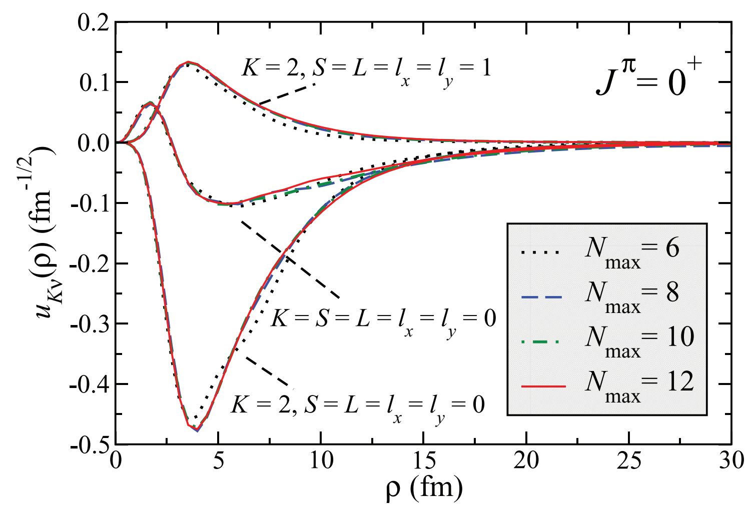
$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx\, x^2 \int dy\, y^2 G^{J^\pi T}_\nu(x,y) \hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle$$

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

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



^{6}He ground state calculation with proper asymptotic conditions



PHYSICAL REVIEW C **88**, 034320 (2013)

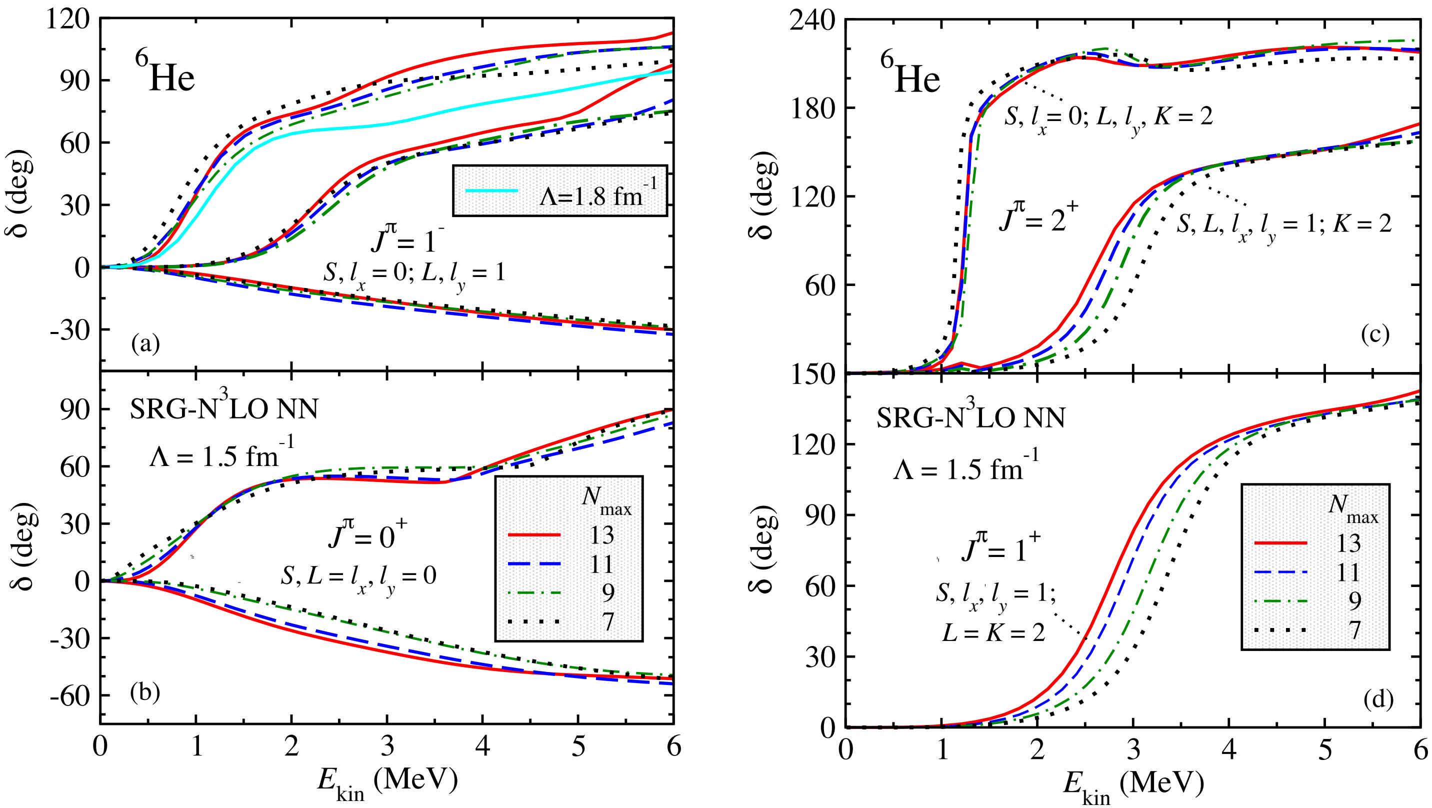
Three-cluster dynamics within an *ab initio* framework

Sofia Quaglioni,[1,*] Carolina Romero-Redondo,[2,†] and Petr Navrátil[2,‡]

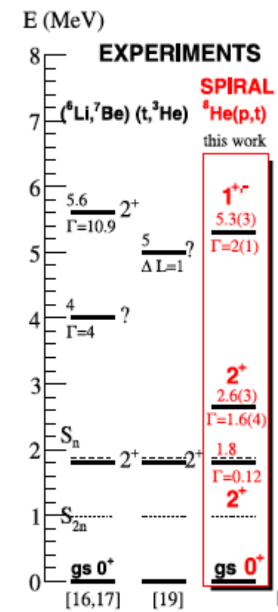
NCSM/RGM for three-body clusters: Structure of ^{6}He

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

Soft SRG-evolved chiral N^{3}LO NN potential, λ=1.5 fm^{-1}



Recent experiment:
PLB 718 (2012) 441



Narrow 2$^+$ resonance

A second low-lying broader 2$^+$ resonance: Found in recent GANIL experiment

1$^+$ resonance

0$^+$ and 1$^-$ very broad

NCSM/RGM for three-body clusters: Structure of ^{6}He

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

Soft SRG-evolved chiral N^{3}LO NN potential, λ=1.5 fm^{-1}

Recent experiment:
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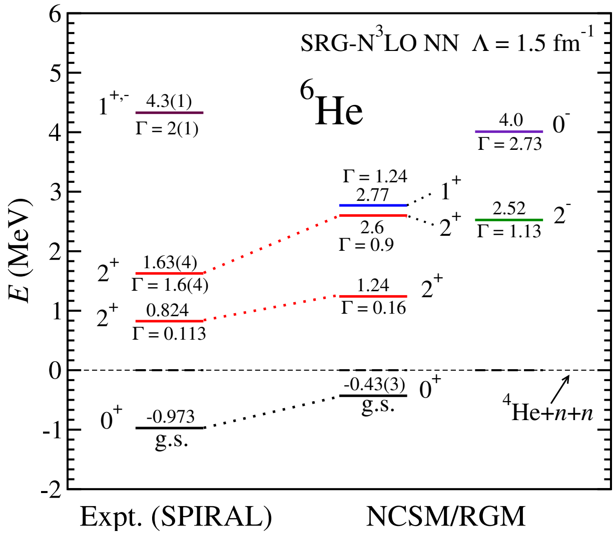
preliminary



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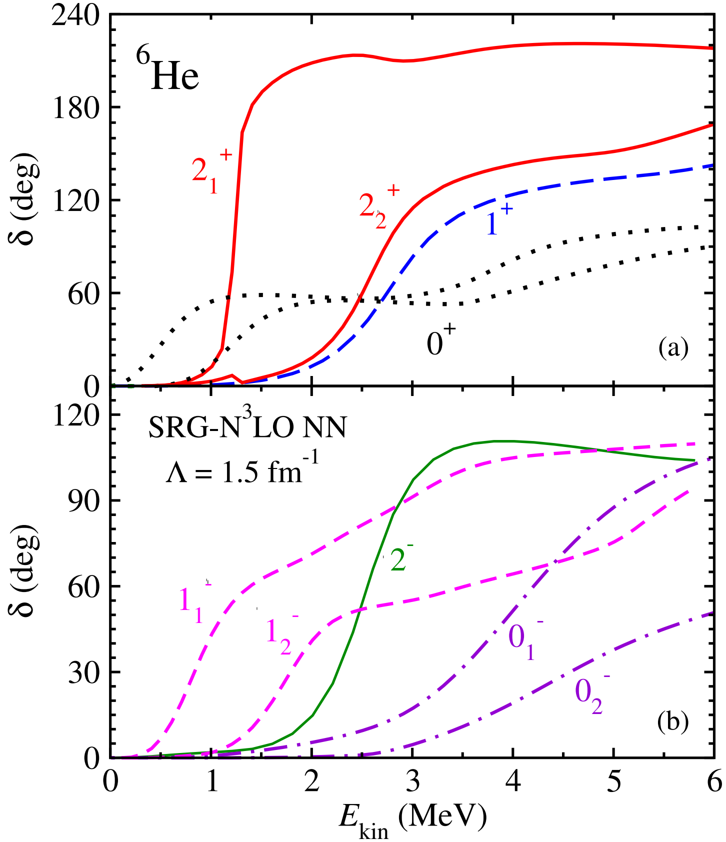

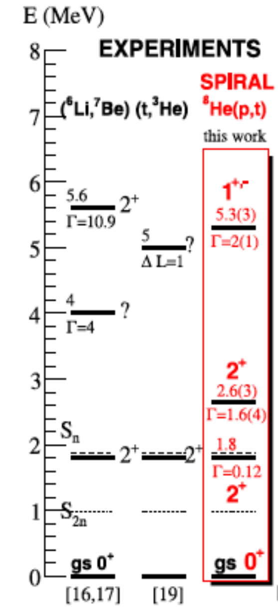

Narrow 2$^+$ resonance

A second low-lying broader 2$^+$ resonance:
Found in recent GANIL experiment

2$^-$, 1$^+$ and 0$^-$ resonances

0$^+$ and 1$^-$ very broad

TRIUMF

Conclusions and Outlook

- *Ab initio* calculations of nuclear structure and reactions is a dynamic field with significant advances

- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM = **NCSMC**
  - Inclusion of three-nucleon interactions in reaction calculations for A>5 systems
  - Extension to three-body clusters (^{6}He ~ ^{4}He+n+n)

- Outlook:
  - Extension to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Composite-projectile reactions on targets heavier than ^{4}He
  - Transfer reactions
  - Bremsstrahlung and capture reactions

NCSMC and NCSM/RGM collaborators

Sofia Quaglioni (LLNL)

Joachim Langhammer, Angelo Calci, Robert Roth (TU Darmstadt)

Carolina Romero-Redondo, Francesco Raimondi, Jeremy Dohet-Eraly (TRIUMF)

Guillaume Hupin, Michael Kruse (LLNL)

Simone Baroni (ULB)