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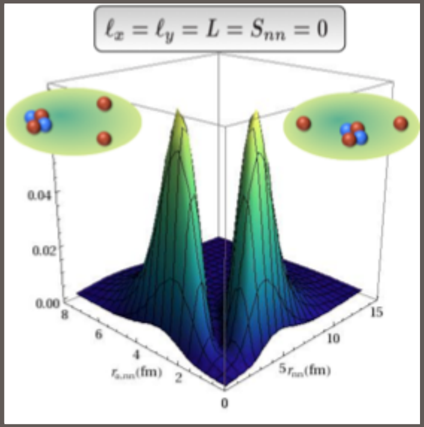
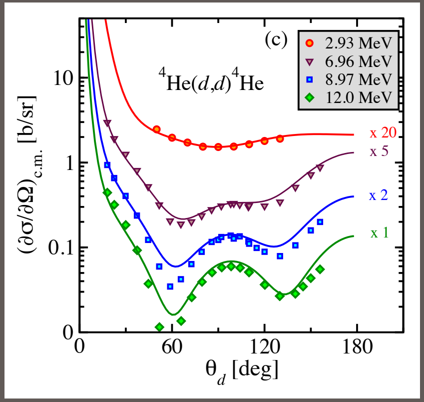
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

Ab Initio Unified Approach to Nuclear Structure and Reactions

INT Workshop INT 15-58W
Reactions and Structure of Exotic Nuclei
March 2 – March 13, 2015

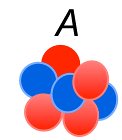
Petr Navratil | TRIUMF



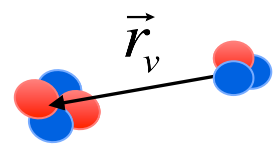


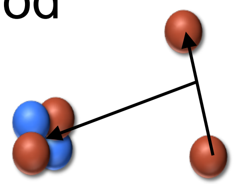
Outline

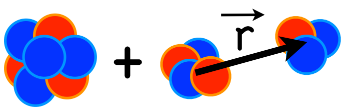
- What is meant by *ab initio* in nuclear physics
- Chiral nuclear forces
- Bound-state calculations: No-core shell model (NCSM)



- Including the continuum with the resonating group method
  - NCSM/RGM
  - NCSM with continuum







- Outlook

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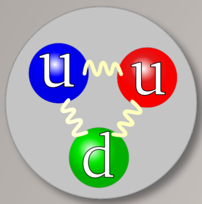
What is meant by *ab initio* in nuclear physics?

- **First principles for Nuclear Physics:**
  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future

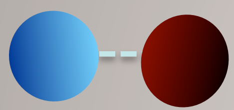
- Degrees of freedom: NUCLEONS
  - Nuclei made of nucleons
  - Interacting by nucleon-nucleon and three-nucleon potentials

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

From QCD to nuclei

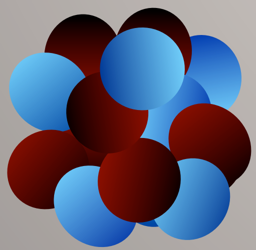


Low-energy QCD



NN+3N interactions
from chiral EFT

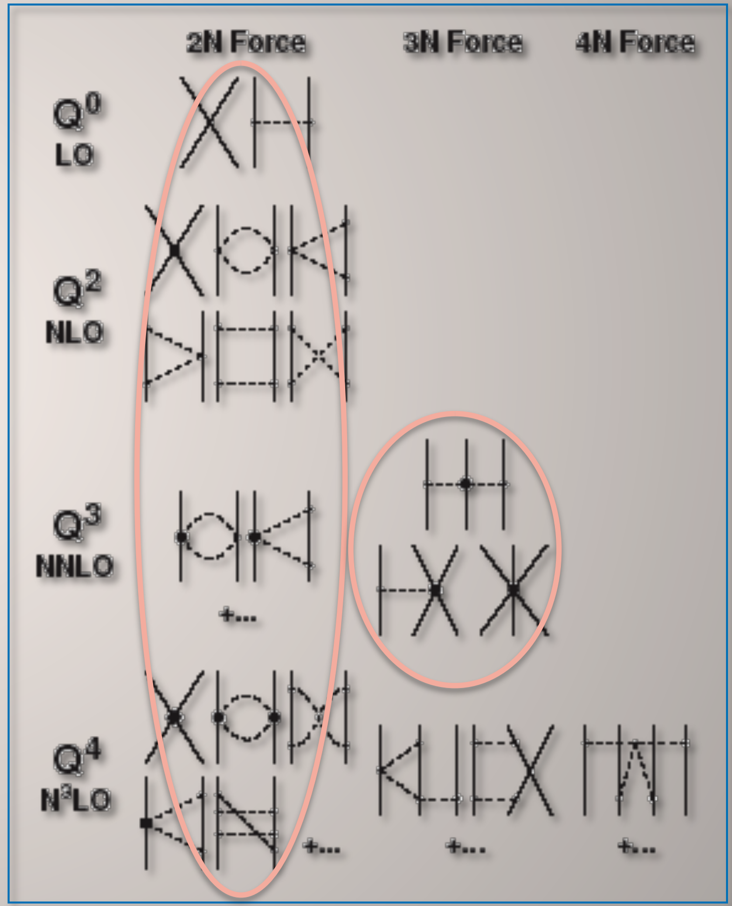
…or accurate
meson-exchange
potentials



Nuclear structure and reactions

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



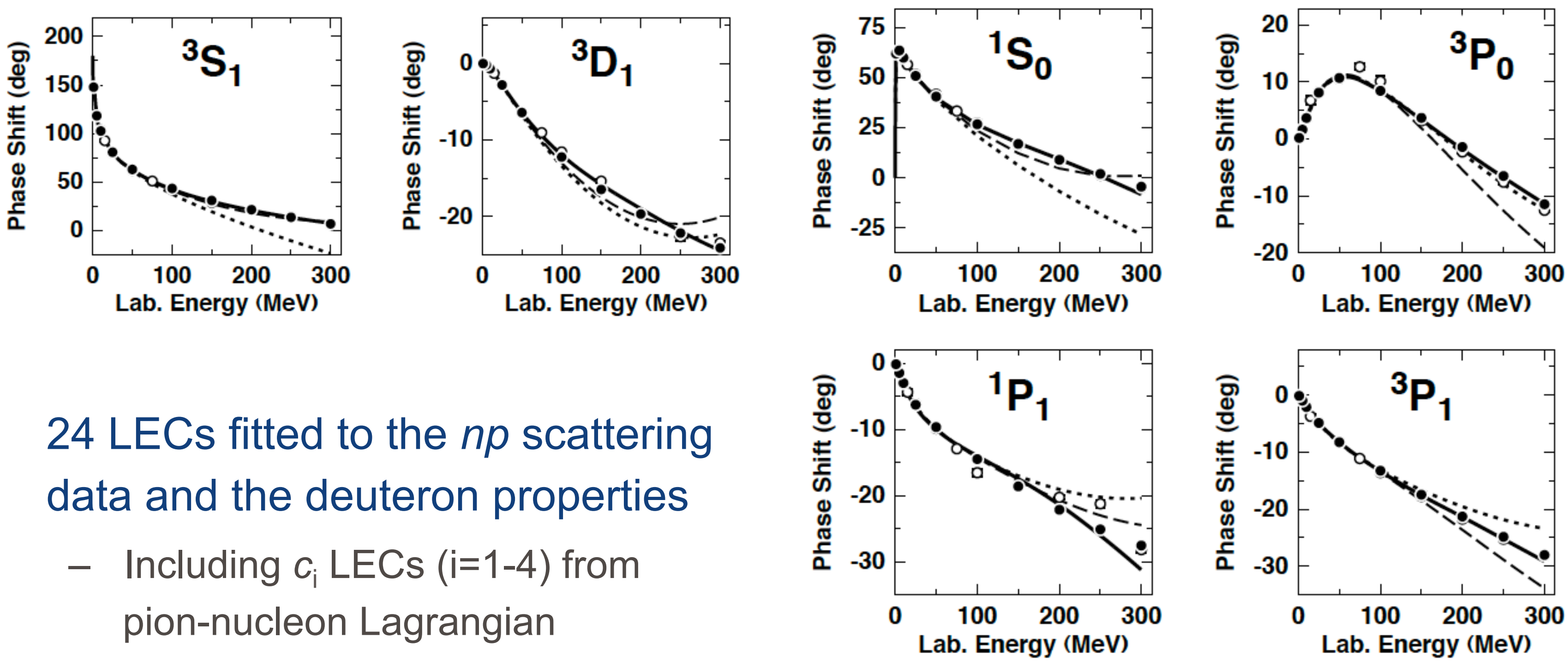
Λ_χ~1 GeV :
Chiral symmetry breaking scale

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

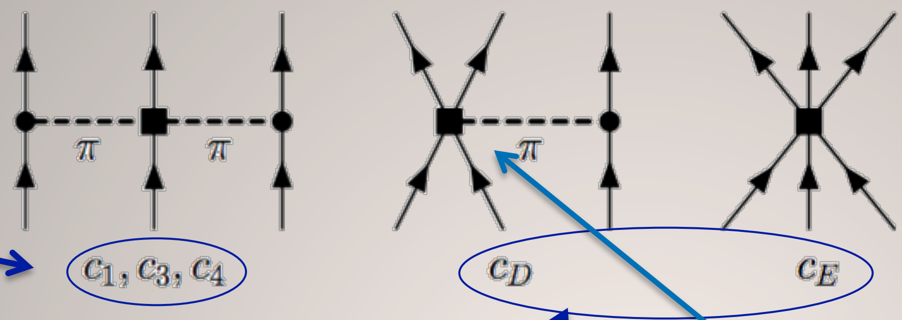
D. R. Entem[1,2,*] and R. Machleidt[1,†]



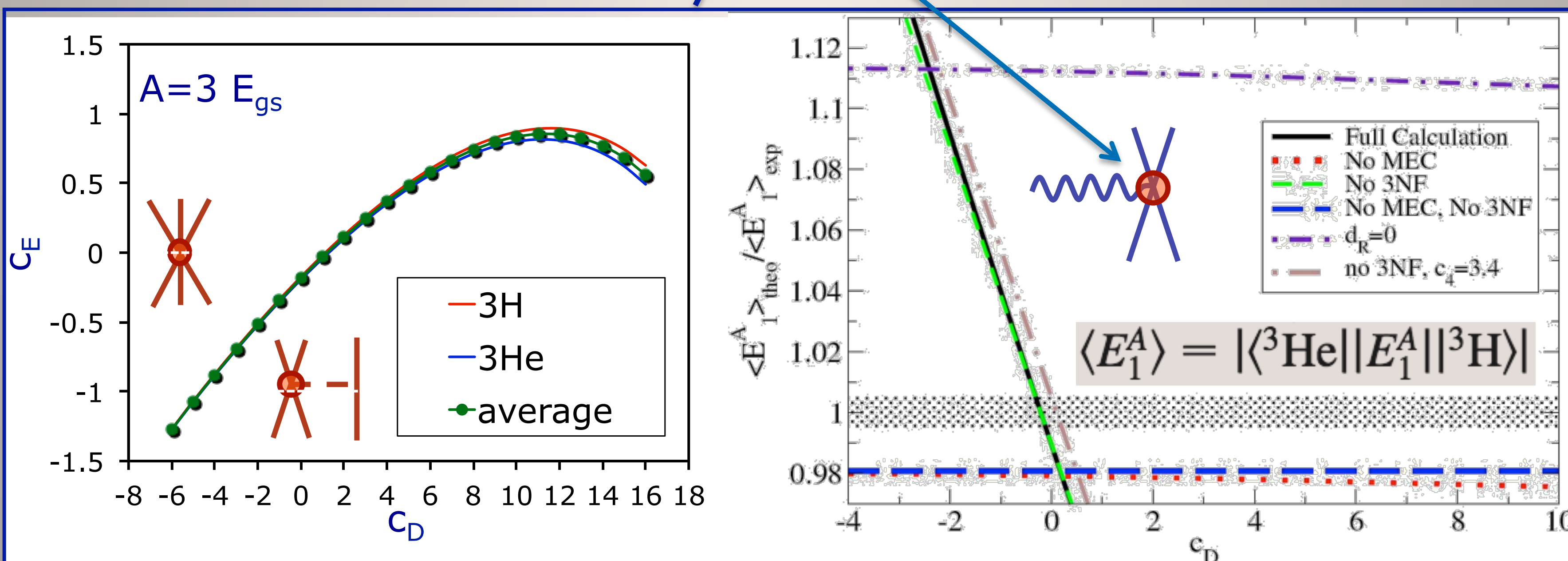
- 24 LECs fitted to the *np* scattering data and the deuteron properties
  - Including c_i LECs (i=1-4) from pion-nucleon Lagrangian

Leading terms of the chiral NNN force

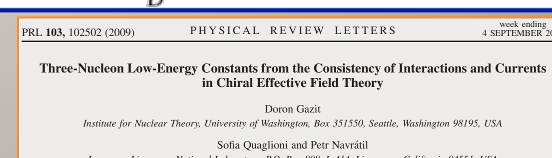
From NN & pion-nucleon scattering



Chiral EFT provides a link between the medium-range (c_D term) NNN force and the meson-exchange current appearing in nuclear beta decay



NNN parameters determined from the ^3H binding energy and half life


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

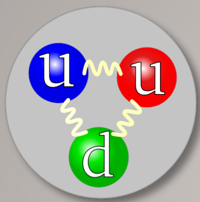
Doron Gazit

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

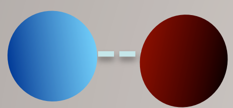
Sofia Quaglioni and Petr Navrátil

Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA

From QCD to nuclei



Low-energy QCD



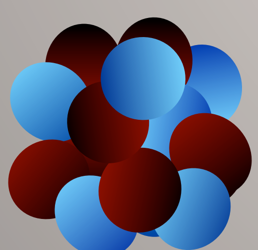
NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

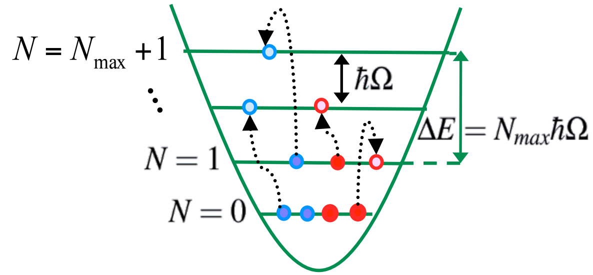
NCSM, NCSM/RGM, NCSMC, CCM, GFMC, HH, Nuclear Lattice EFT…



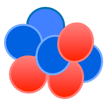
Nuclear structure and reactions

No-core shell model

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances



A



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

$$\Psi^{(A)} = \sum_\lambda c_\lambda \left| (A), \lambda \right\rangle$$

Unknowns

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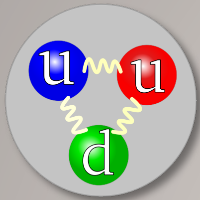
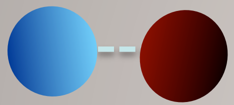
From QCD to nuclei



Low-energy QCD

↓



NN+3N interactions from chiral EFT

> …or accurate meson-exchange potentials

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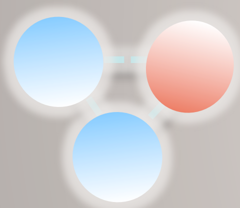


Unitary/similarity transformations

> Identity or SRG or OLS or UCOM … Softens NN, induces 3N

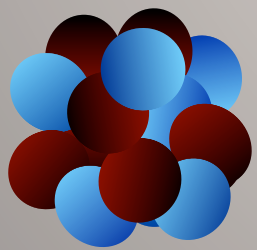
↓

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

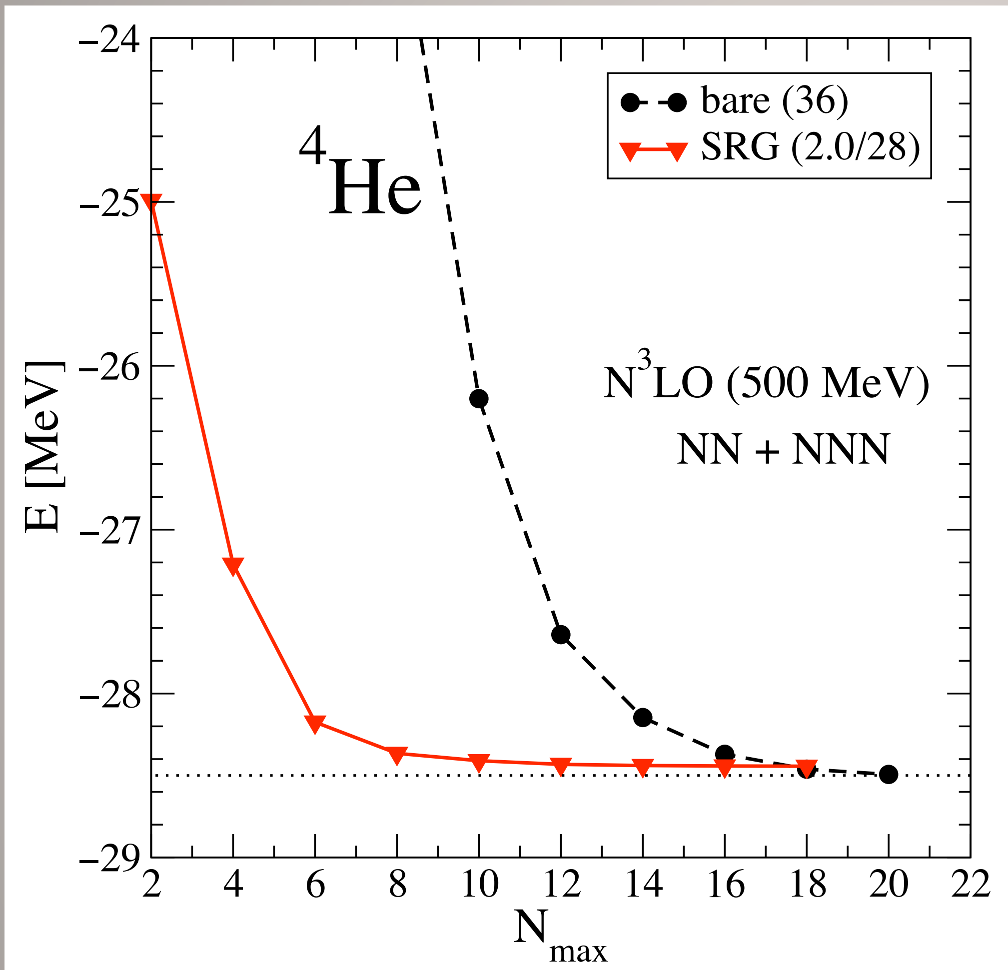
> NCSM, NCSM/RGM, CCM, GFMC, HH, Nuclear Lattice EFT…

↓



Nuclear structure and reactions

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

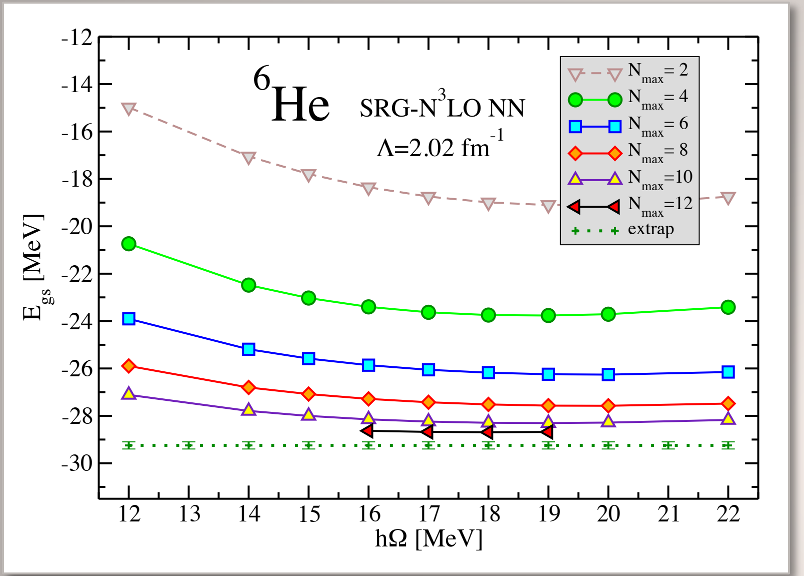
Chiral N^{3}LO NN plus N^{2}LO NNN potential

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

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

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

NCSM calculations of ^{6}He g.s. energy



Dependence on:

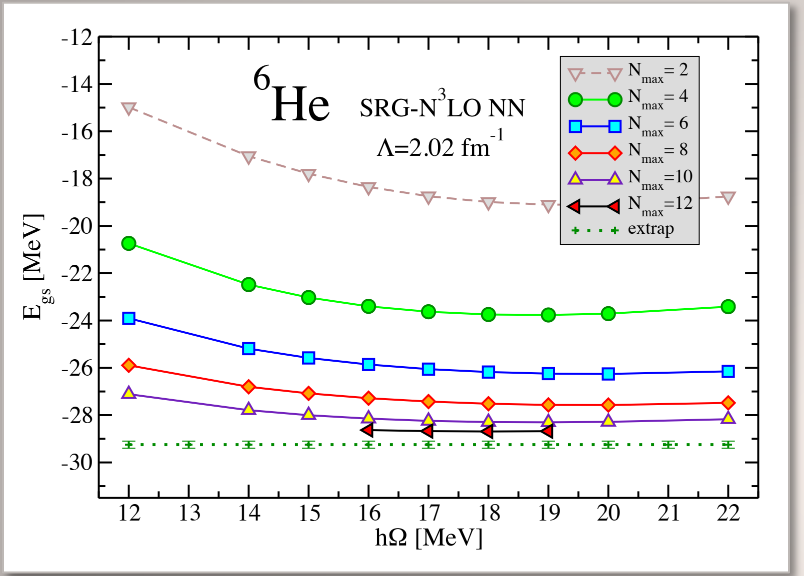
Basis size – N_{max}

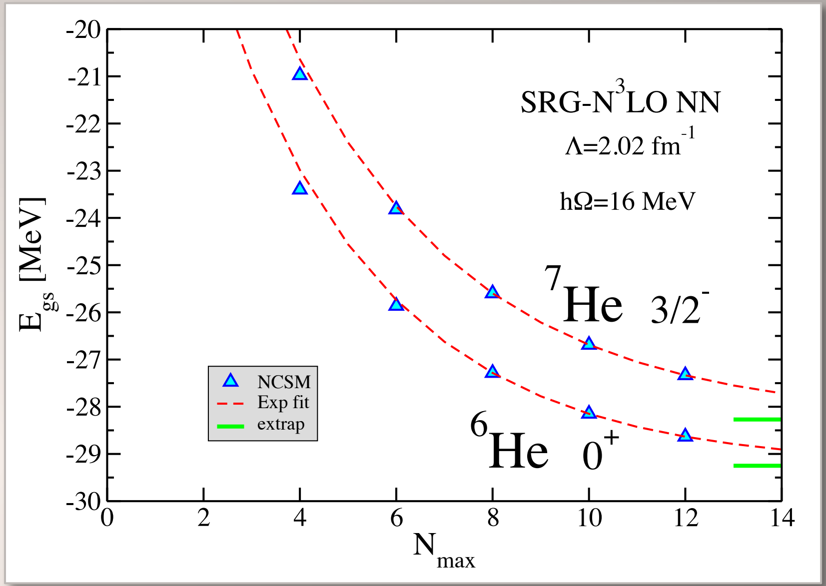
HO frequency – hΩ

- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

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

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

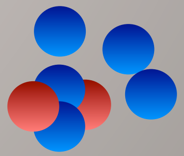




- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

$E_{g.s.}$ [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

- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM E_{th}≈ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**



^{7}He unbound

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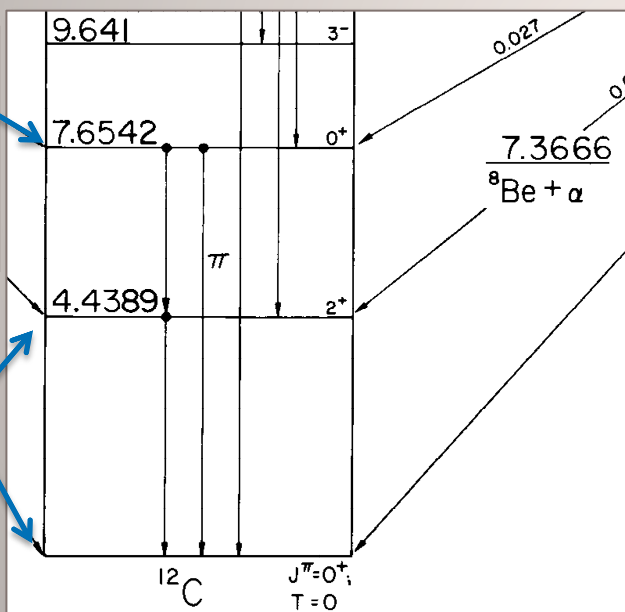
Light & medium mass nuclei from first principles

- Nuclear **structure** and **reaction** theory for light nuclei cannot be uncoupled
  - Well-bound nuclei, e.g. ^{12}C, have low-lying **cluster-dominated resonances**
  - Bound states of exotic nuclei, e.g. ^{11}Be, manifest **many-nucleon correlations**

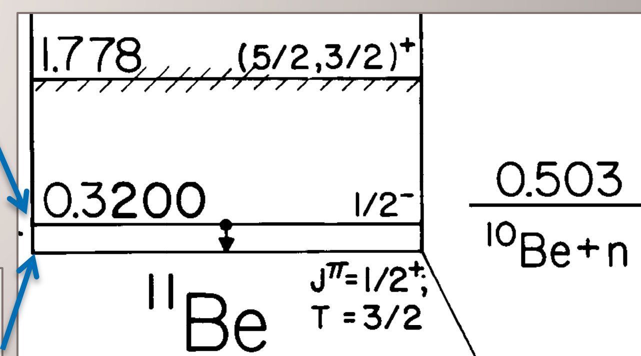
Hoyle state: α-cluster resonance with *p*-shell components

p-shell states



p-shell state with extended tail

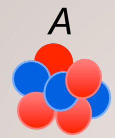
$^{10}Be_{gs}$ + (*l=0*) *n* with significant $^{10}Be^*$ components



Extending no-core shell model beyond bound states

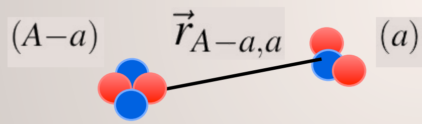
Include more many nucleon correlations…

NCSM →



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

+



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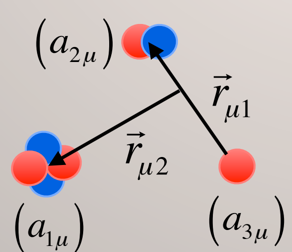


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

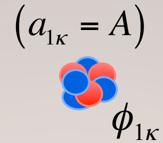
+

…

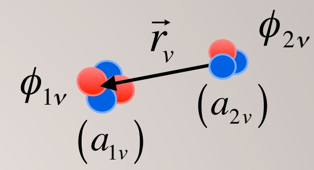
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

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



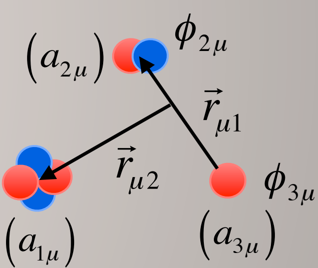
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

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

$$+ \cdots$$



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

Trial function: generalized cluster wave function

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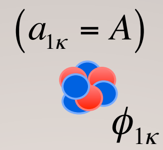
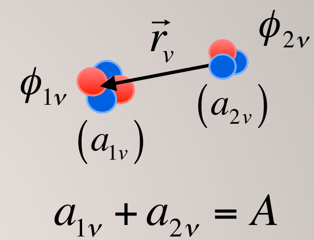
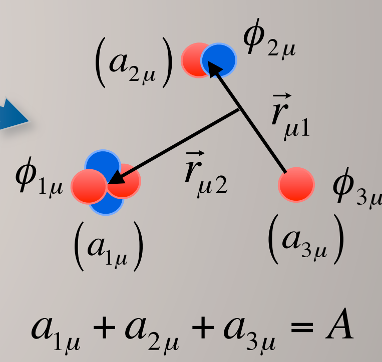


$$+ \sum_{\nu} \hat{A}_{\nu} \boxed{\phi_{1\nu}}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \boxed{\phi_{2\nu}}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

$$+ \cdots$$

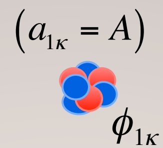


- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates

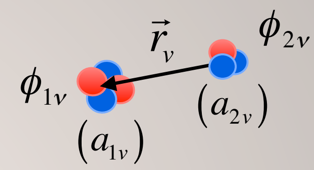
    (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

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



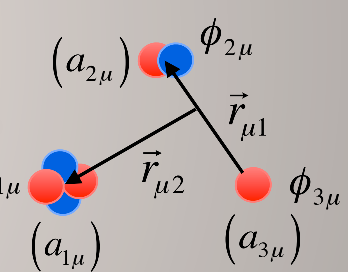
$$+ \sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



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

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

$$+ \cdots$$



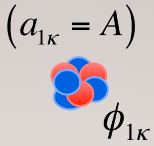
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

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

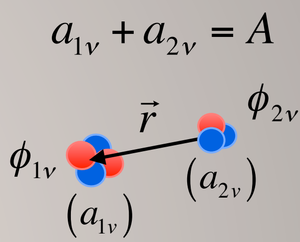
$$a_{1\nu} = A - 1,\; a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_\nu = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

Trial function: generalized cluster wave function

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

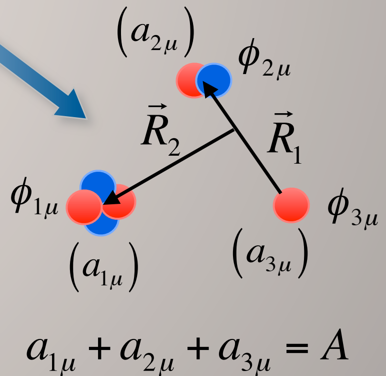


$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,) \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right]d\vec{r}$$



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

$$+ \cdots$$



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

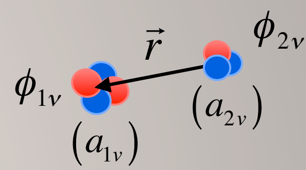
Trial function: generalized cluster wave function

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

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

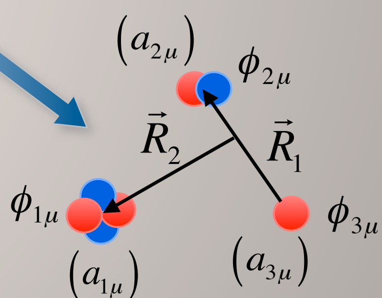
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right] d\vec{r}$$

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



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

$$+ \cdots$$

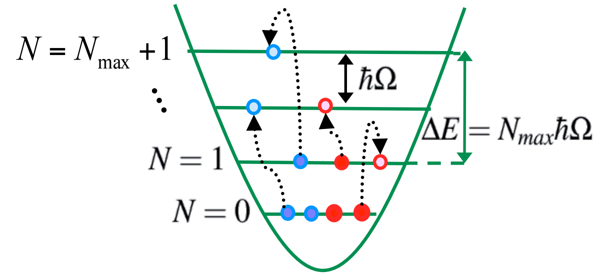


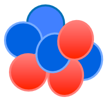
$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

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

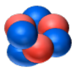
No-core shell model

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances





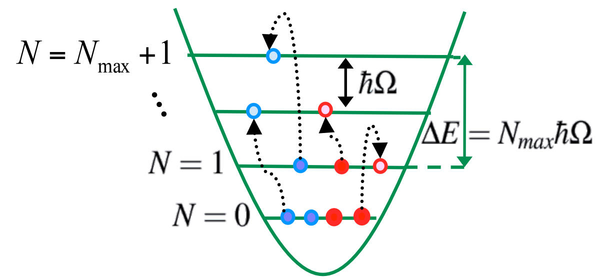
$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

$$\Psi^{(A)} = \sum_\lambda c_\lambda \left| {}^{(A)} \right.$$  $$\left. , \lambda \right\rangle$$

Unknowns

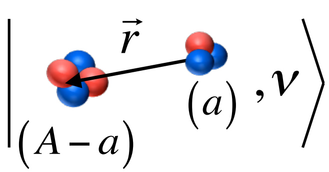
No-core shell model with RGM

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances



- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion
  - proper asymptotic behavior
  - long-range correlations

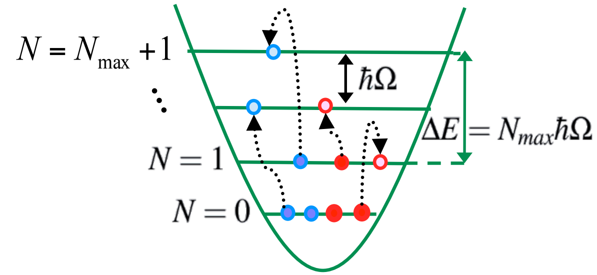
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| \; \right\rangle$$



Unknowns

No-core shell model with continuum

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances



- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion
  - proper asymptotic behavior
  - long-range correlations

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

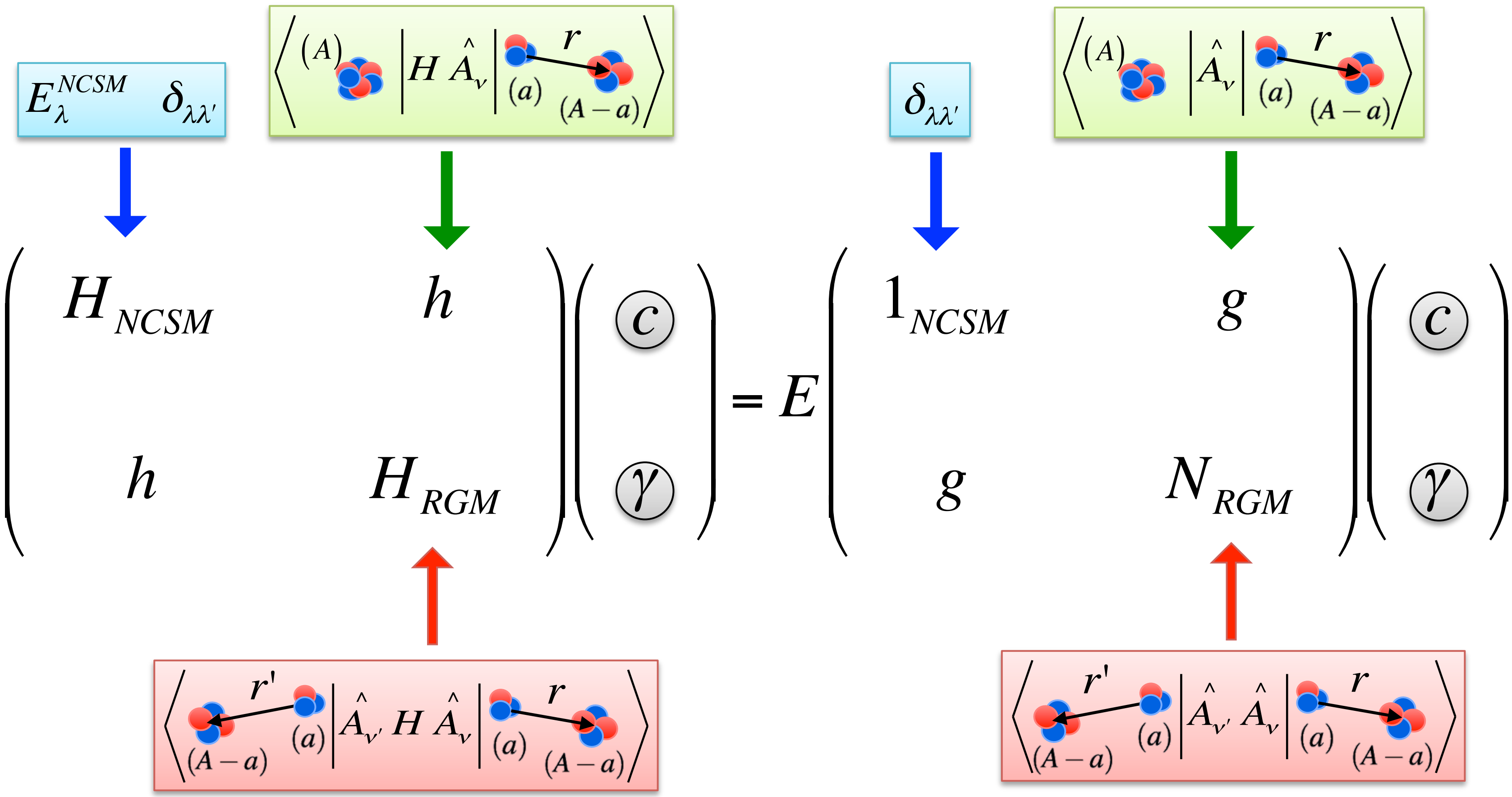
The most efficient:
No-Core Shell Model with Continuum (NCSMC)

NCSM eigenstates | **NCSM/RGM channel states**

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| {}_{(A-a)} \; \vec{r} \; {}_{(a)}, \nu \right\rangle$$

Unknowns: c_λ, $\gamma_\nu(\vec{r}\,)$

Coupled NCSMC equations



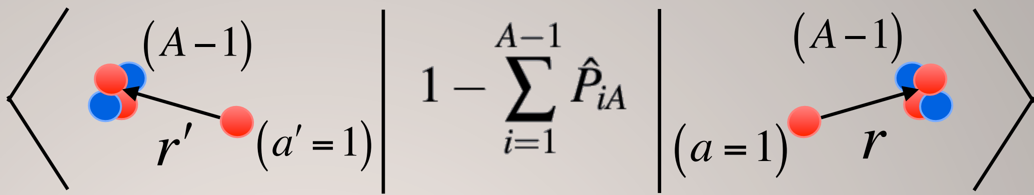
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh

Norm kernel (Pauli principle)

Single-nucleon projectile

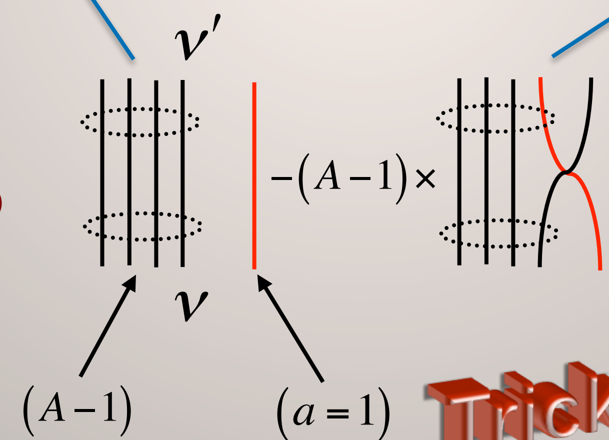
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



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

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

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



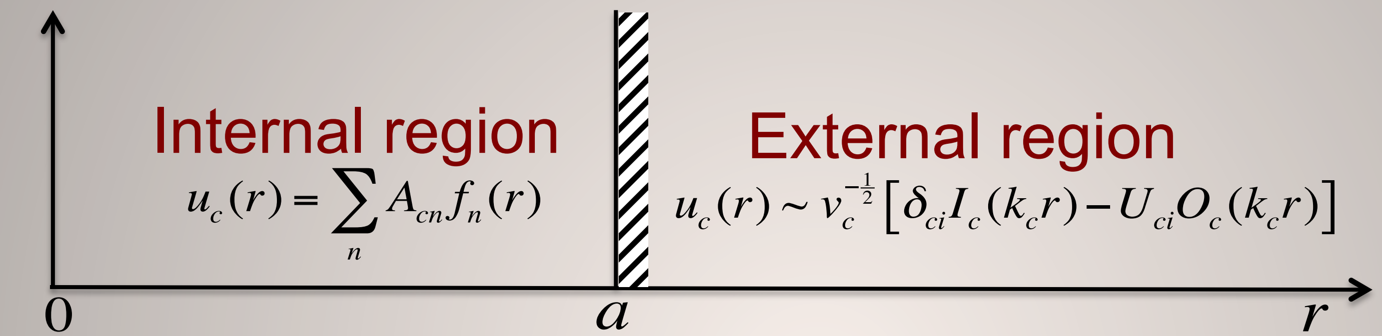
Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

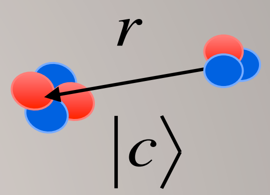
Trick #1 $$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Trick #2 Target wave functions expanded in the SD basis, the CM motion exactly removed

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
- External region: asymptotic form for large r

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

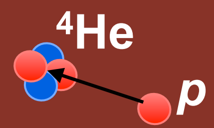
$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

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

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

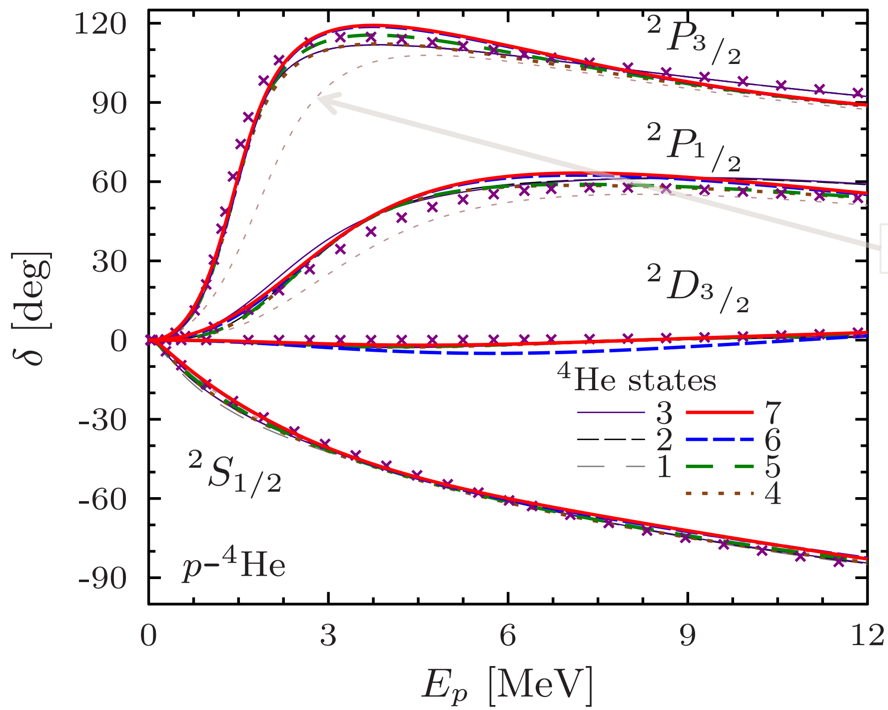
Bound state — Scattering state — Scattering matrix

TRIUMF

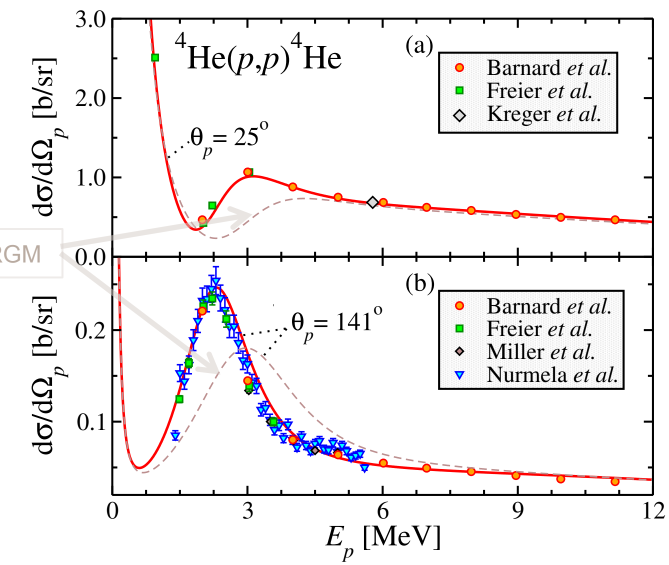


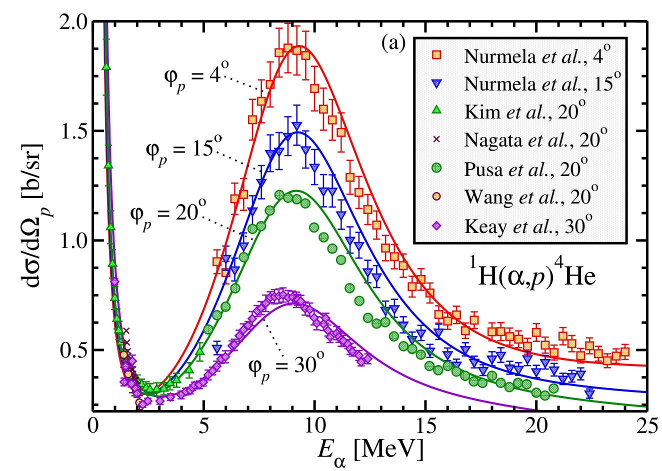
p-^{4}He scattering within NCSMC

p-^{4}He scattering phase-shifts for NN+3N potential: Convergence



Differential p-^{4}He cross section with NN+3N potentials





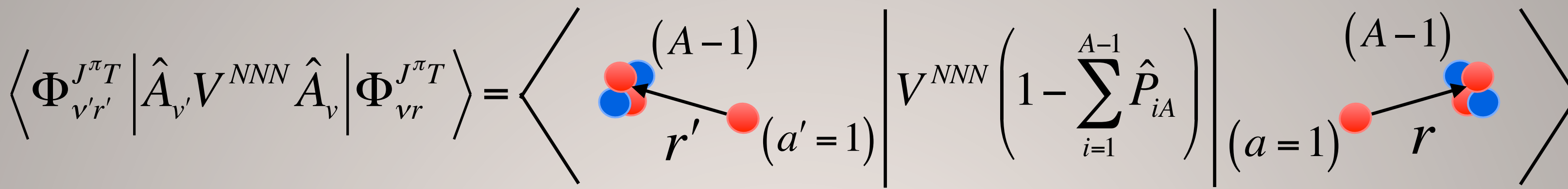
Predictive power in the 3/2$^-$ resonance region: Applications to material science

PHYSICAL REVIEW C **90**, 061601(R) (2014)

Predictive theory for elastic scattering and recoil of protons from ^{4}He

Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

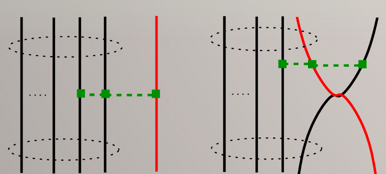
Including 3N interaction in the NCSM/RGM Single-nucleon projectile:



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

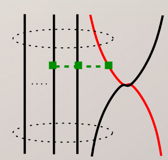
Direct potential: in the model space (interaction is localized!)

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



(a) (b)

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



(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*

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

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

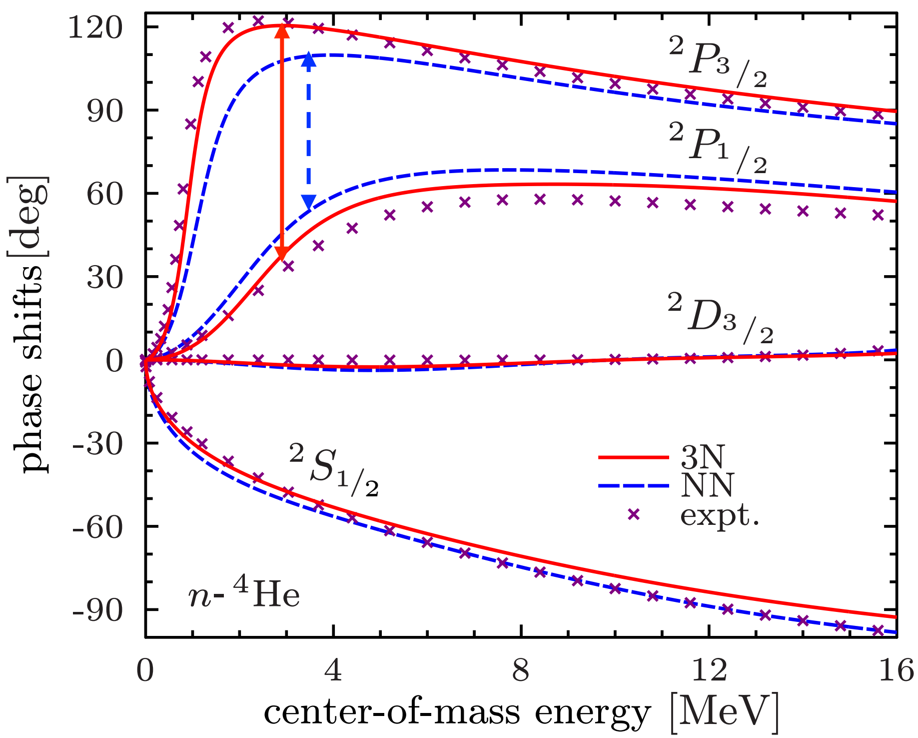
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,||] and Robert Roth[2,¶]

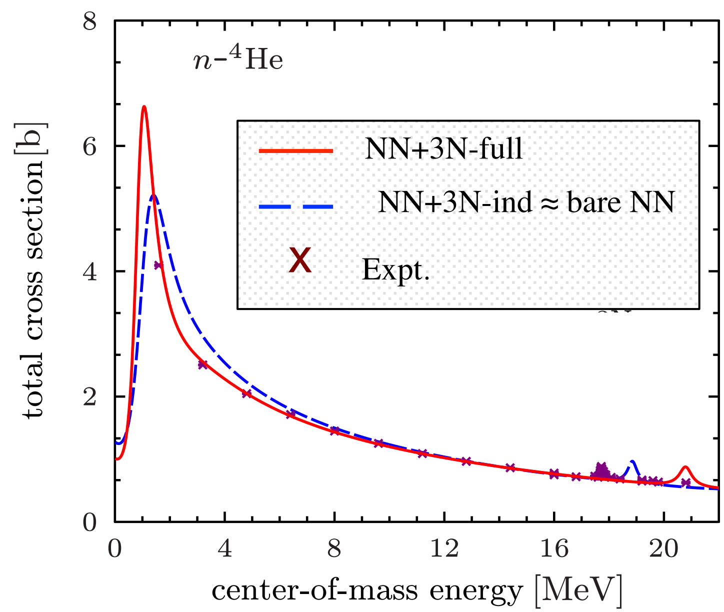
TRIUMF

n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N potential

Total n-^{4}He cross section with NN and NN+3N potentials





3N force enhances 1/2$^-$ ←→ 3/2$^-$ splitting: Essential at low energies!

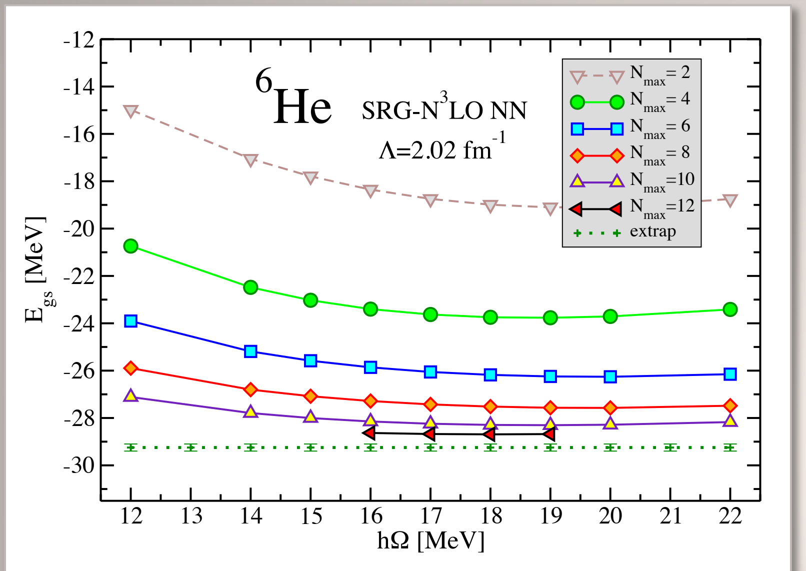
G. Hupin, S. Quaglioni and P. Navrátil

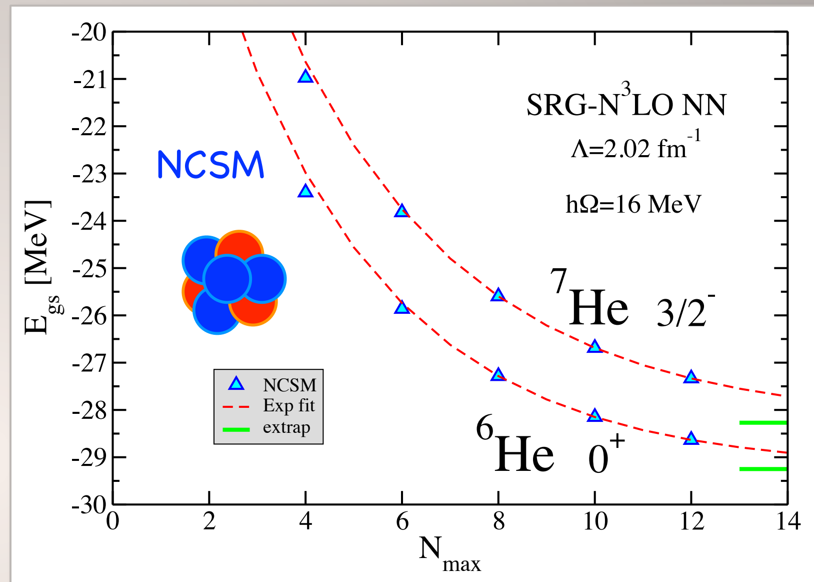
PHYSICAL REVIEW C **88**, 054622 (2013)

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,¶]

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

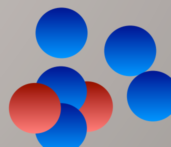




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

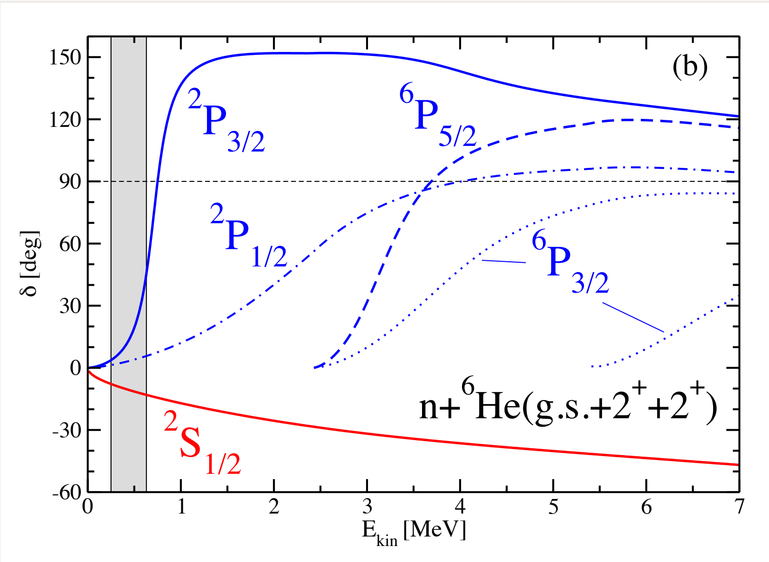
- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM E_{th}≈ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**

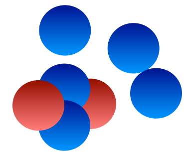


^{7}He unbound

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



^{7}He



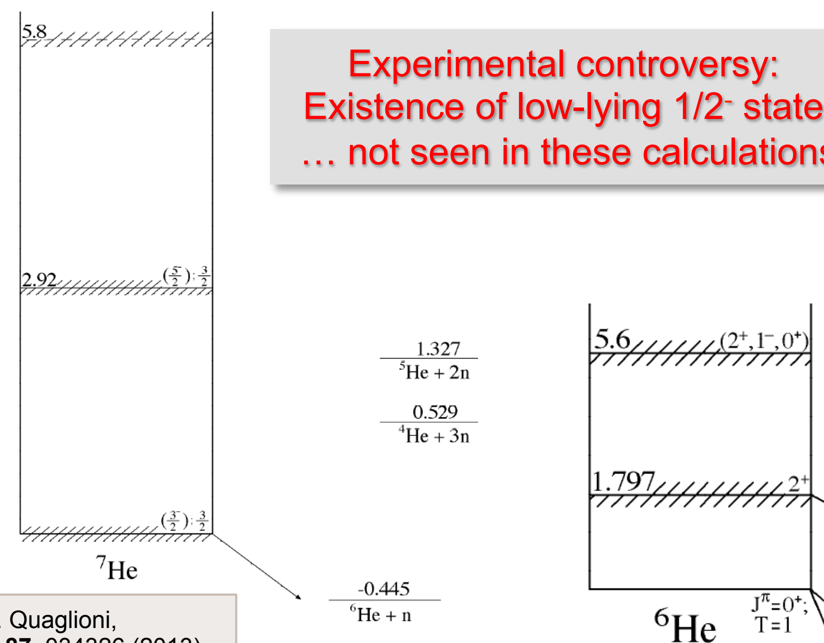
unbound

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).

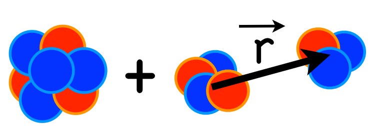
$$\Gamma = \left.\frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\right|_{E_{kin}=E_R}$$

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

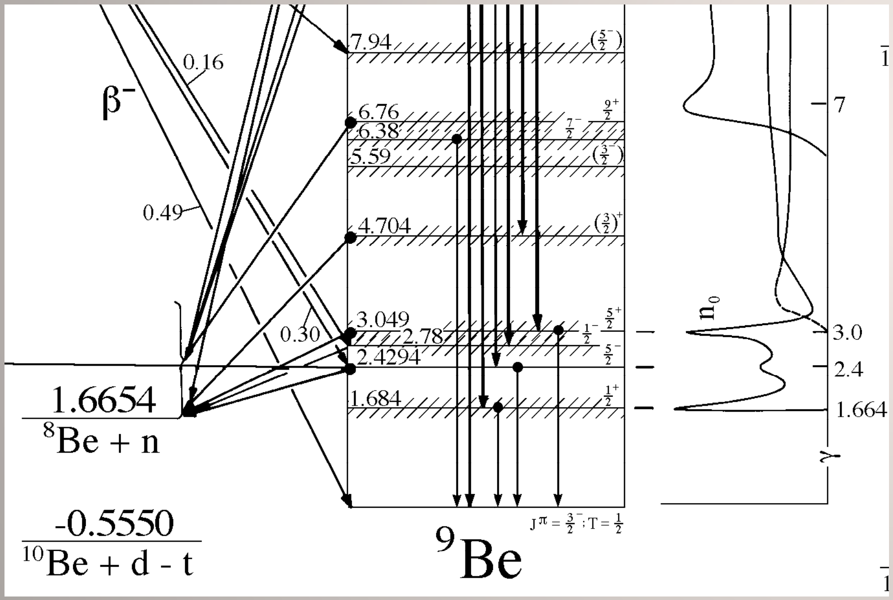
NCSMC



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

TRIUMF

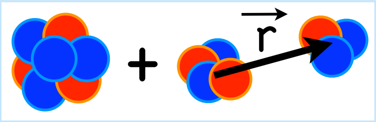
Structure of ^{9}Be



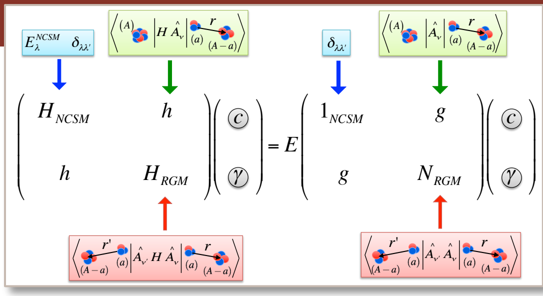
^{9}Be is a stable nucleus
… but all its excited states unbound
A proper description requires to include effects of continuum

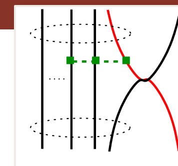
The lowest threshold: n-^{8}Be (n-α-α)

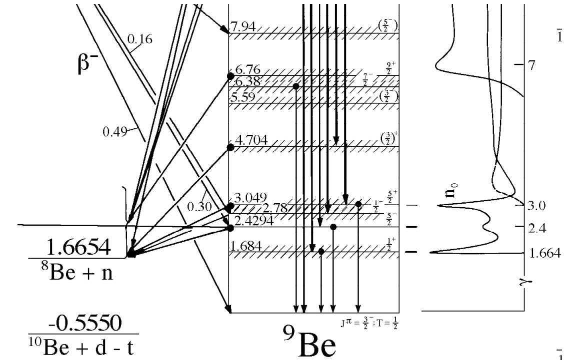
Optimal description:
Square-integrable ^{9}Be basis + n-^{8}Be clusters

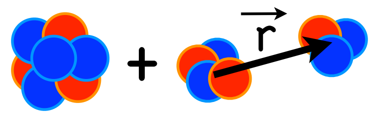


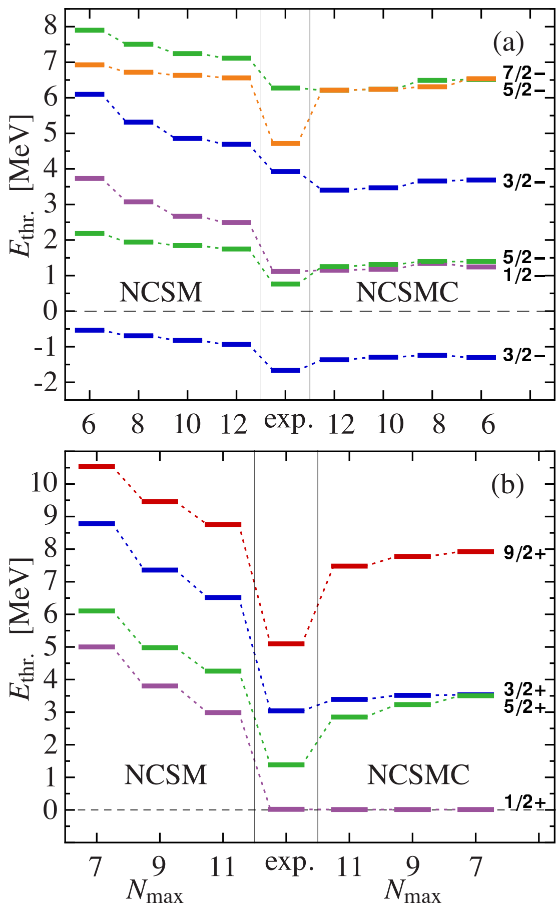
NCSMC with chiral NN+3N: Structure of ^{9}Be

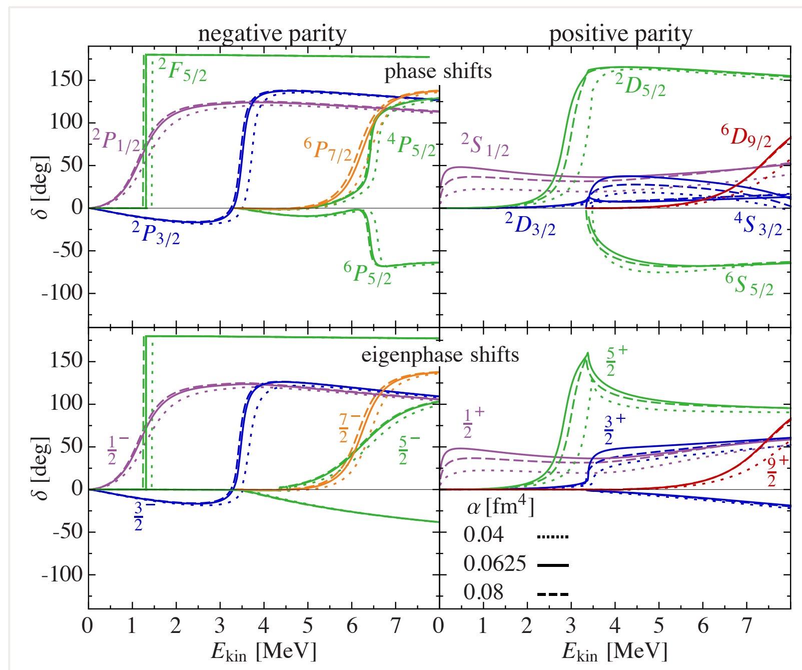


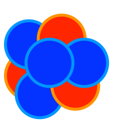










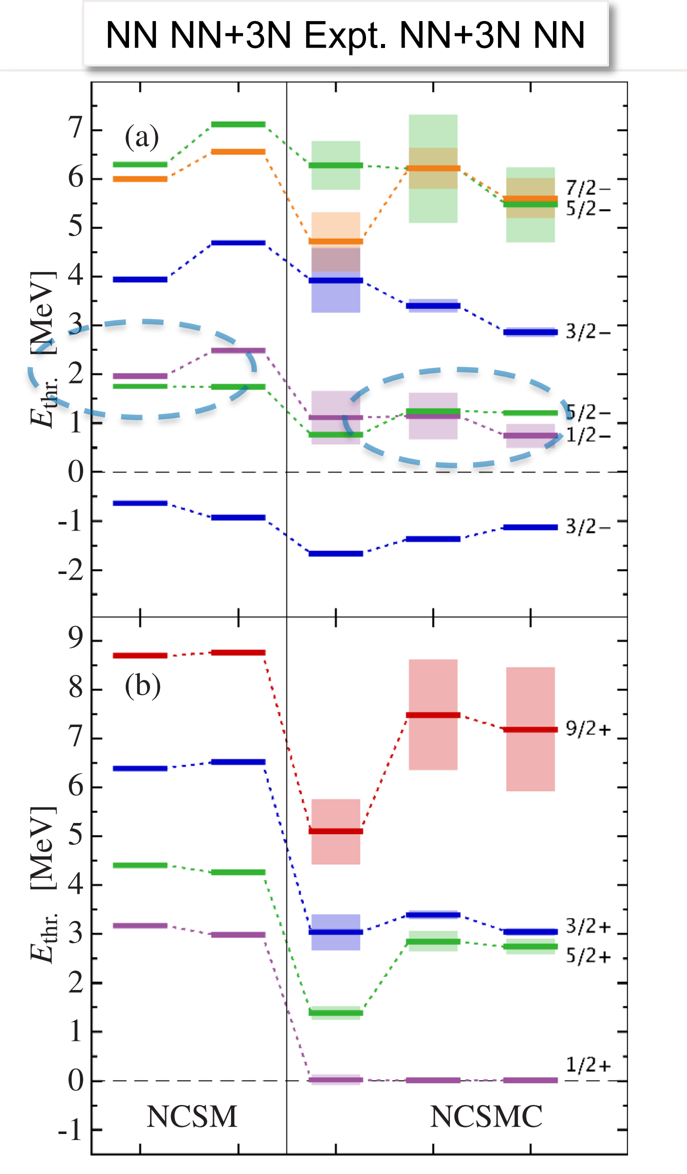


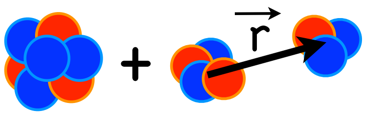
PHYSICAL REVIEW C **91**, 021301(R) (2015)

Continuum and three-nucleon force effects on ^{9}Be energy levels

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

NCSMC with chiral NN+3N: Structure of ^{9}Be

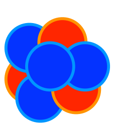




^{9}Be is a stable nucleus
… but all its excited states unbound
A proper description requires to include effects of continuum

Three-nucleon interaction *and* continuum improve agreement with experiment for negative parity states

Continuum crucial for the description of positive-parity states



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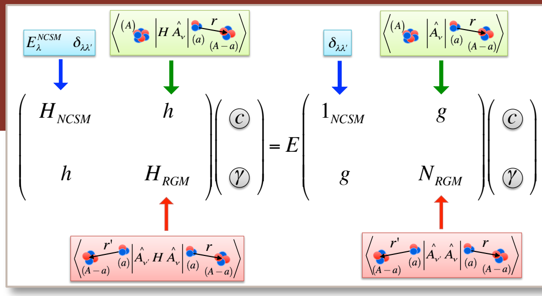
NCSMC wave function



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left|^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \left| \vec{r}\ \ _{(A-a)}\ \ (a) , \nu \right\rangle$$

$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{\lambda} |A\lambda J^\pi T\rangle \left[\sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda\lambda'} \bar{c}_{\lambda'} + \sum_{\nu'} \int dr'\, r'^2 (N^{-\frac{1}{2}})^{\lambda}_{\nu' r'} \frac{\bar{\chi}_{\nu'}(r')}{r'} \right]$$

$$+ \sum_{\nu\nu'} \int dr\, r^2 \int dr'\, r'^2 \hat{\mathcal{A}}_{\nu} |\Phi^{J^\pi T}_{\nu r}\rangle \mathcal{N}^{-\frac{1}{2}}_{\nu\nu'}(r, r') \left[\sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda'}_{\nu' r'} \bar{c}_{\lambda'} + \sum_{\nu''} \int dr''\, r''^2 (N^{-\frac{1}{2}})_{\nu' r' \nu'' r''} \frac{\bar{\chi}_{\nu''}(r'')}{r''} \right].$$

Asymptotic behavior $r \to \infty$:

$$\bar{\chi}_{\nu}(r) \sim C_{\nu} W(k_{\nu} r) \qquad \bar{\chi}_{\nu}(r) \sim \mathrm{v}_{\nu}^{-\frac{1}{2}} \left[\delta_{\nu i} I_{\nu}(k_{\nu} r) - U_{\nu i} O_{\nu}(k_{\nu} r) \right]$$

Bound state

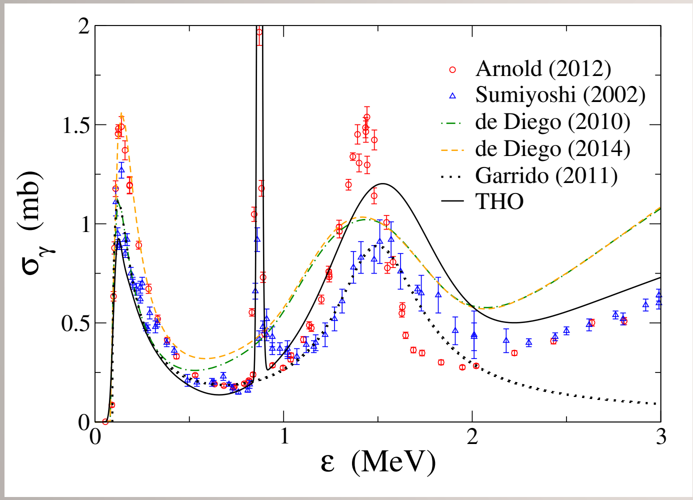
Scattering state

Scattering matrix

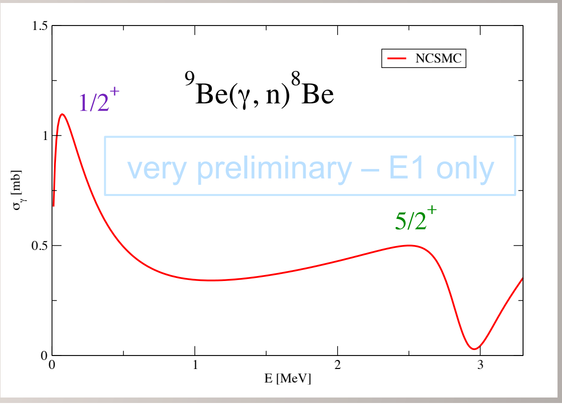
Photo-disassociation of ^{9}Be

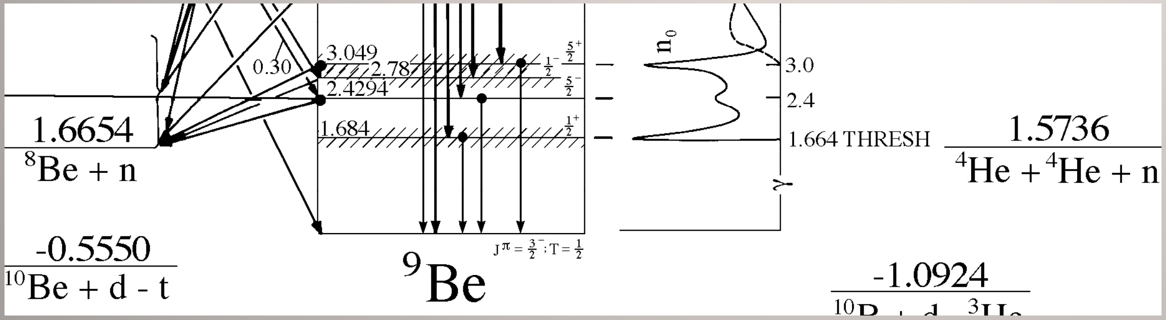
Reaction $\alpha(\alpha n,\gamma)^9\mathrm{Be}$ relevant for astrophysics: beginning of r-process

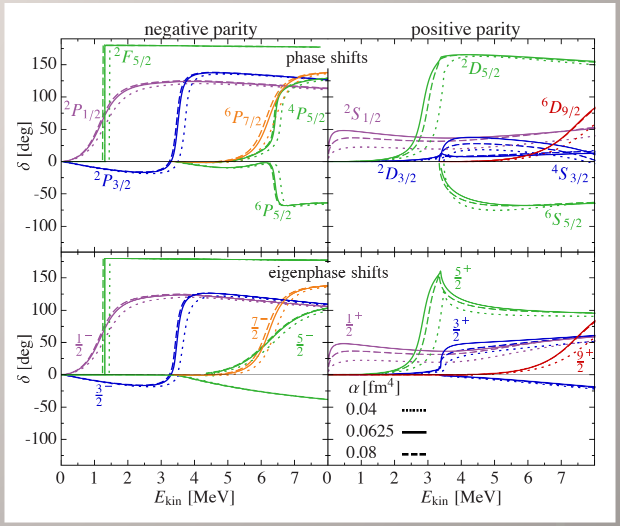
Inverse process ^{9}Be(γ,αn)α measured in laboratory

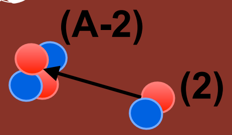


NCSMC

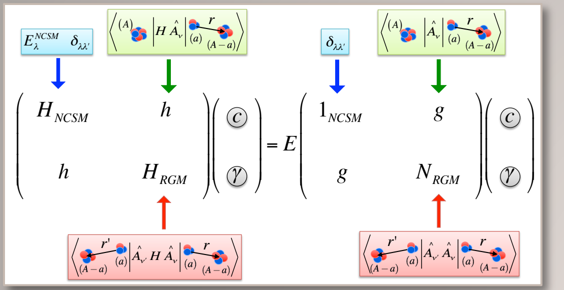


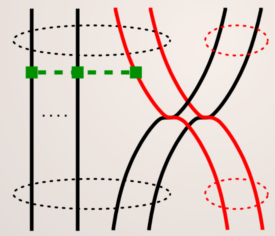






The deuteron-projectile formalism: Three-nucleon interaction





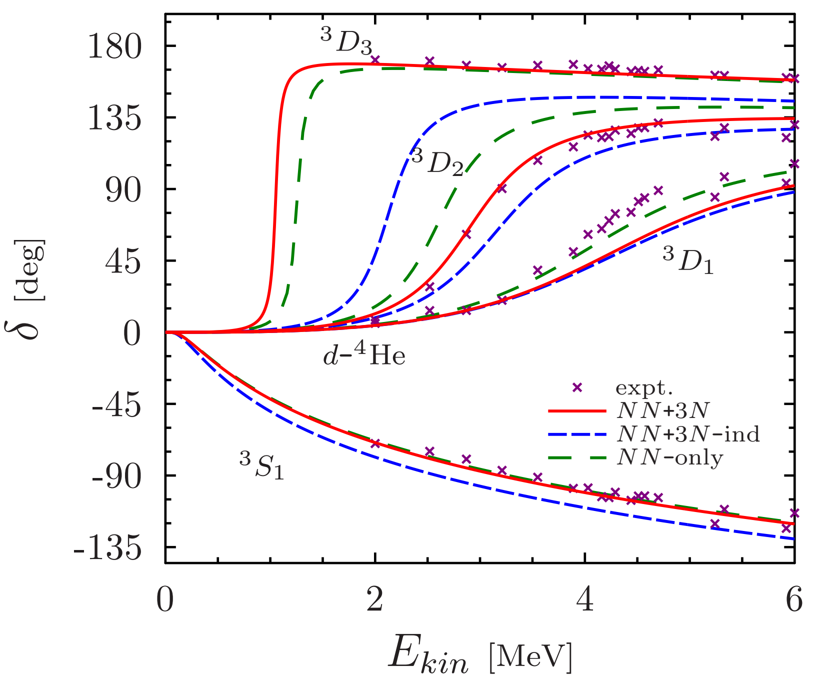
$$ {}_{\mathrm{SD}}\left\langle \psi^{(A-2)}_{\mu_1} \middle| a^+ a^+ a^+ a^+ a\, a\, a\, a \middle| \psi^{(A-2)}_{\nu_1} \right\rangle_{\mathrm{SD}} $$

For *A*=6 use completeness

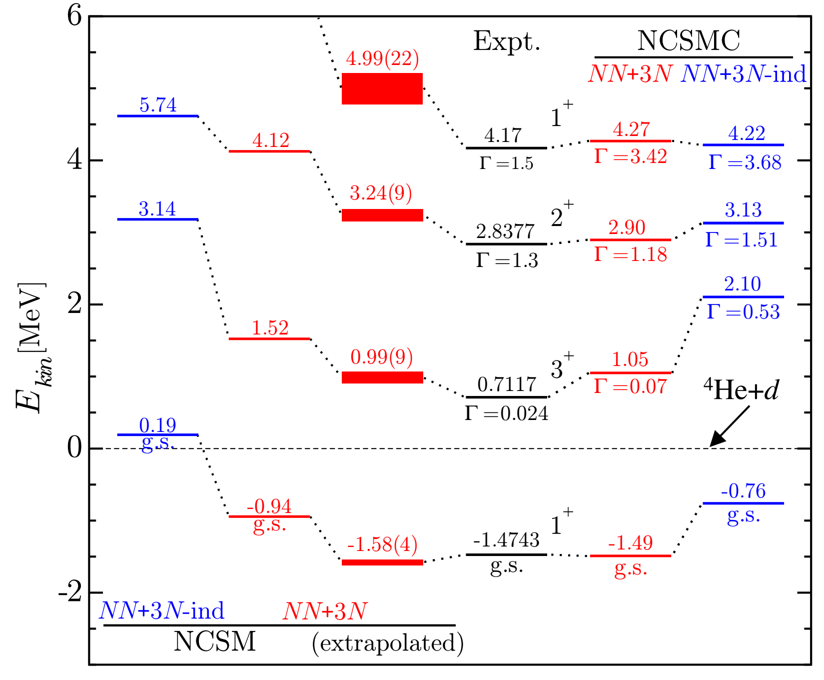
Unified description of ^{6}Li structure and d+^{4}He dynamics

- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li

d+^{4}He Scattering Phase Shifts

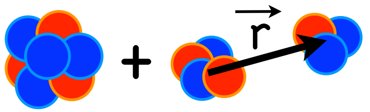


^{6}Li vs. (^{4}He+d)+^{6}Li calculation



G. Hupin, S. Quaglioni, and P. Navratil, arXiv:1412.4101 [nucl-th]

NCSMC



Unified description of ^{6}Li structure and d+^{4}He dynamics

- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li

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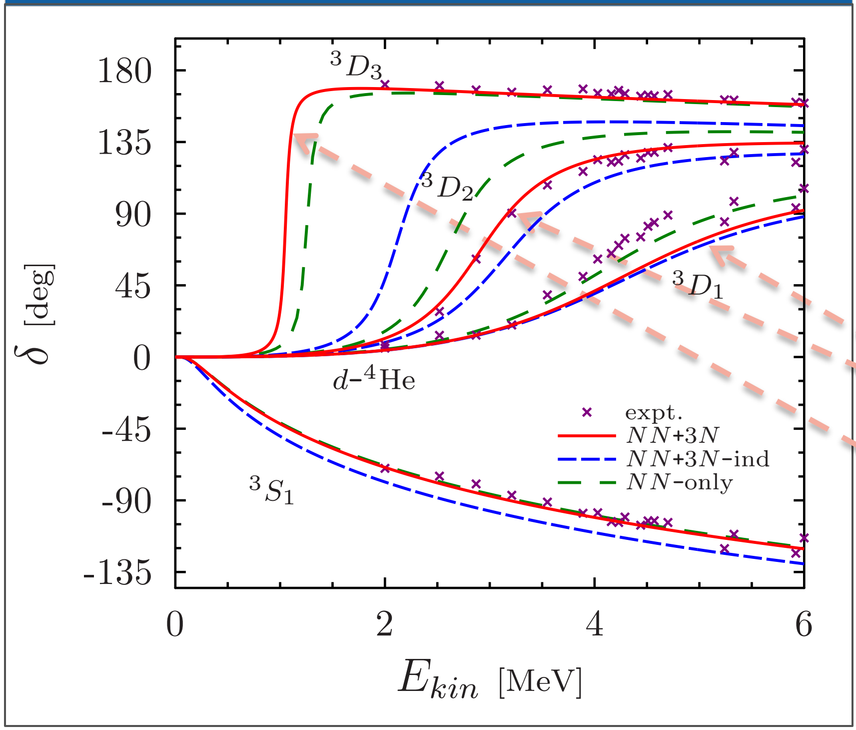

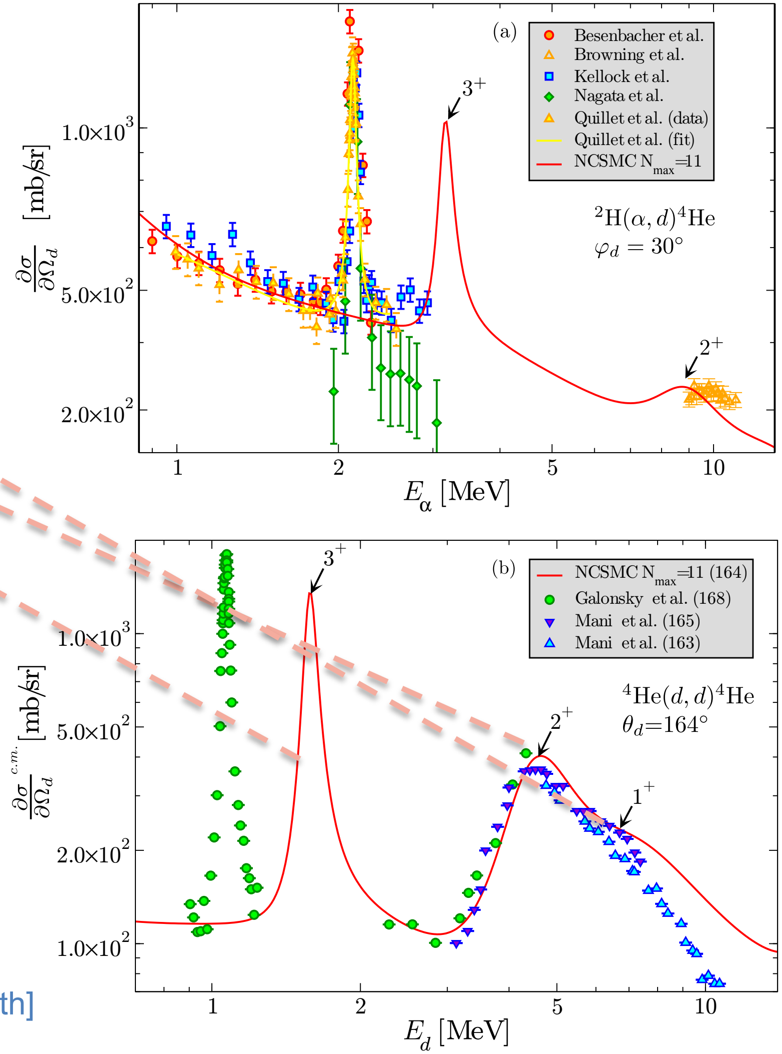

G. Hupin, S. Quaglioni, and P. Navratil, arXiv:1412.4101 [nucl-th]

Unified description of ^{6}Li structure and d+^{4}He dynamics

- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li

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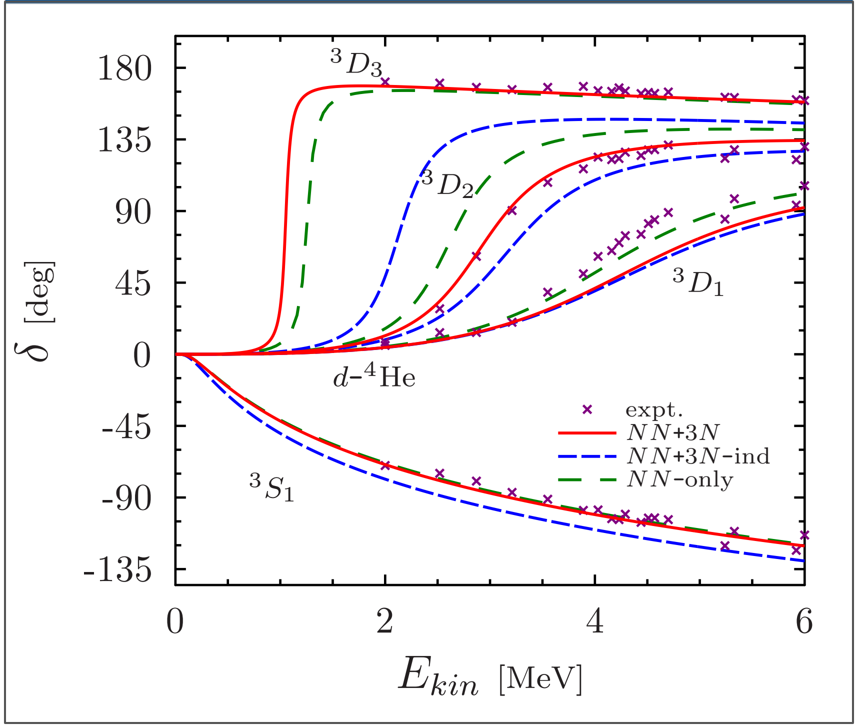
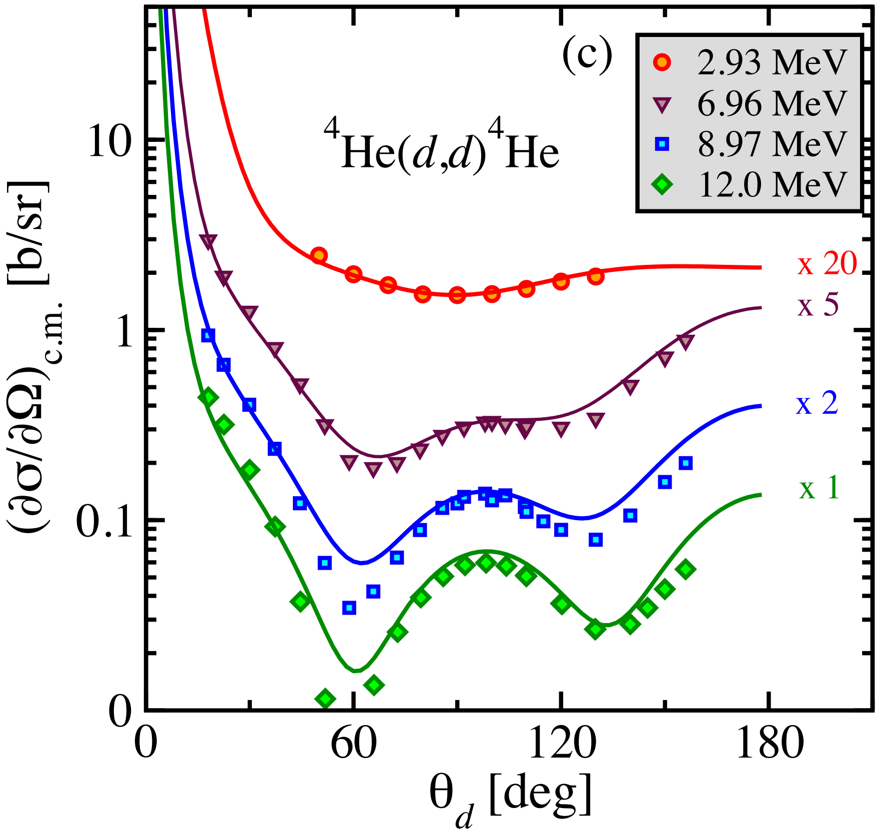




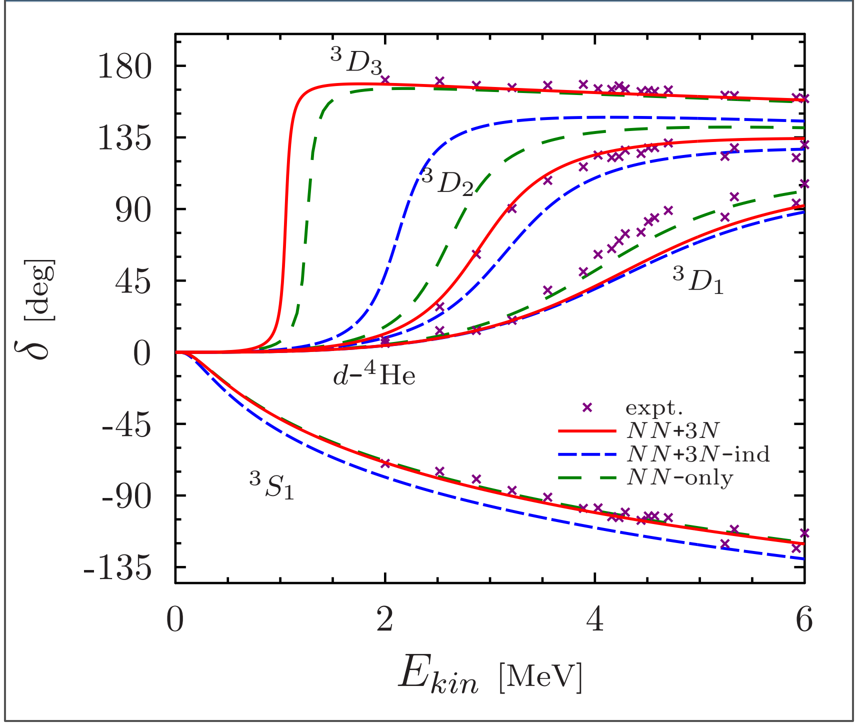
G. Hupin, S. Quaglioni, and P. Navratil, arXiv:1412.4101 [nucl-th]

TRIUMF

Unified description of ^{6}Li structure and d+^{4}He dynamics

- *S*- and *D*-wave asymptotic normalization constants

d+^{4}He Scattering Phase Shifts



	NCSMC	Experiment			
C_0 [fm$^{-1/2}$]	2.695	2.91(9)	[39]	2.93(15)	[38]
C_2 [fm$^{-1/2}$]	−0.074	−0.077(18)	[39]		
C_2/C_0	−0.027	−0.025(6)(10)	[39]	0.0003(9)	[41]

[38] L. D. Blokhintsev, V. I. Kukulin, A. A. Sakharuk, D. A. Savin, and E. V. Kuznetsova, Phys. Rev. C **48**, 2390 (1993).

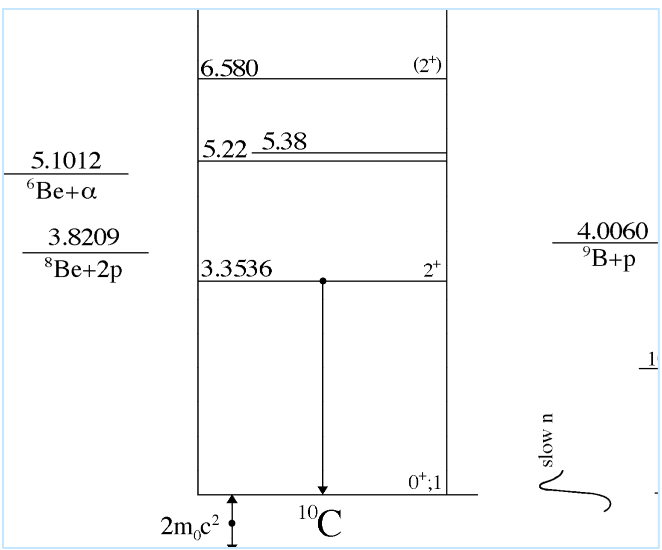
[39] E. A. George and L. D. Knutson, Phys. Rev. C **59**, 598 (1999).

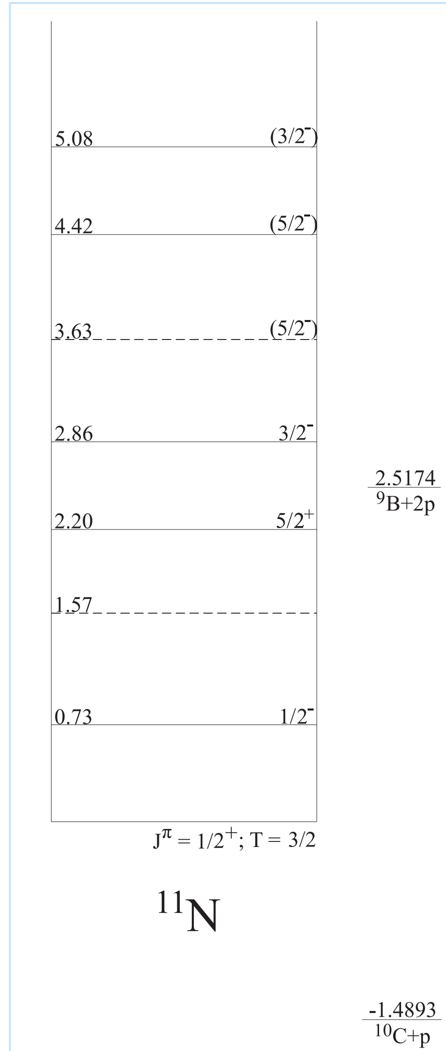
[41] K. D. Veal, C. R. Brune, W. H. Geist, H. J. Karwowski, E. J. Ludwig, A. J. Mendez, E. E. Bartosz, P. D. Cathers, T. L. Drummer, K. W. Kemper, A. M. Eiró, F. D. Santos, B. Kozlowska, H. J. Maier, and I. J. Thompson, Phys. Rev. Lett. **81**, 1187 (1998).

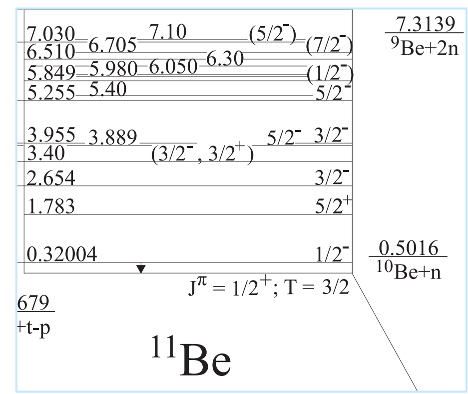
G. Hupin, S. Quaglioni, and P. Navratil, arXiv:1412.4101 [nucl-th]

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

- 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
- Importance of 3N force effects and continuum



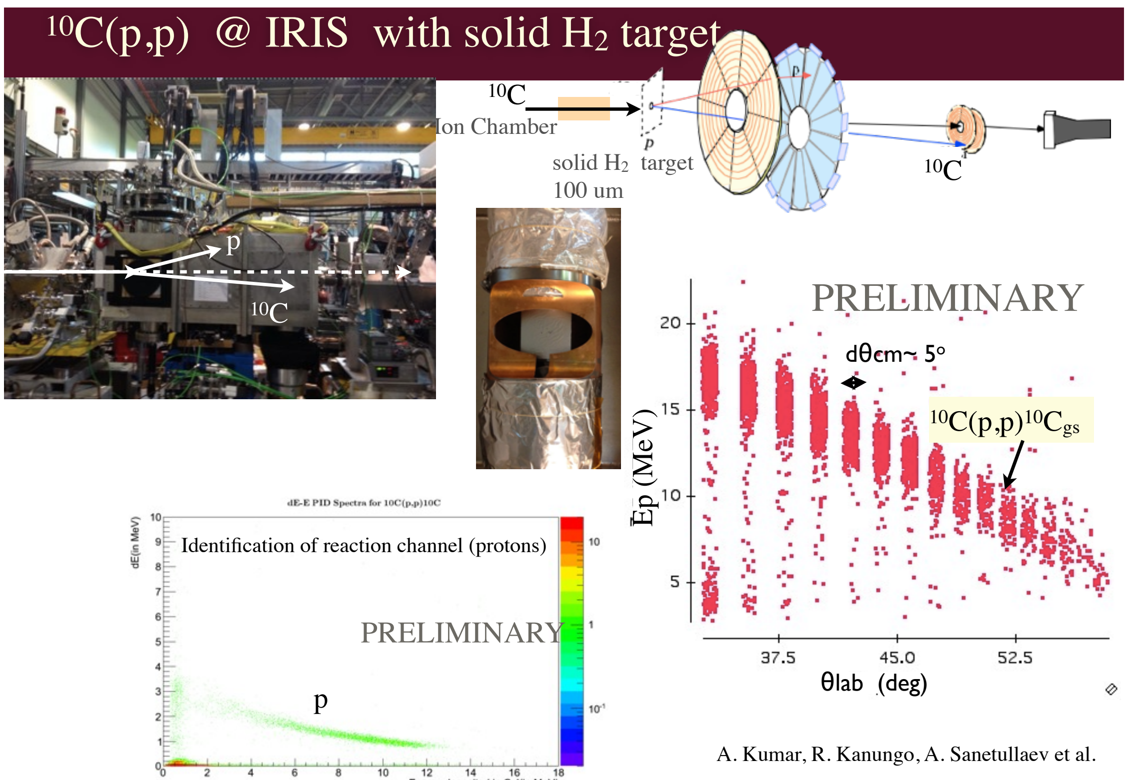




$^{10}C(p,p)$ @ IRIS with solid H_2 target

- 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
  - Data analysis under way

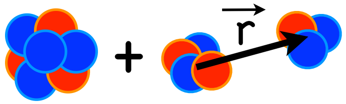
Talk by Ritu Kanungo on Friday



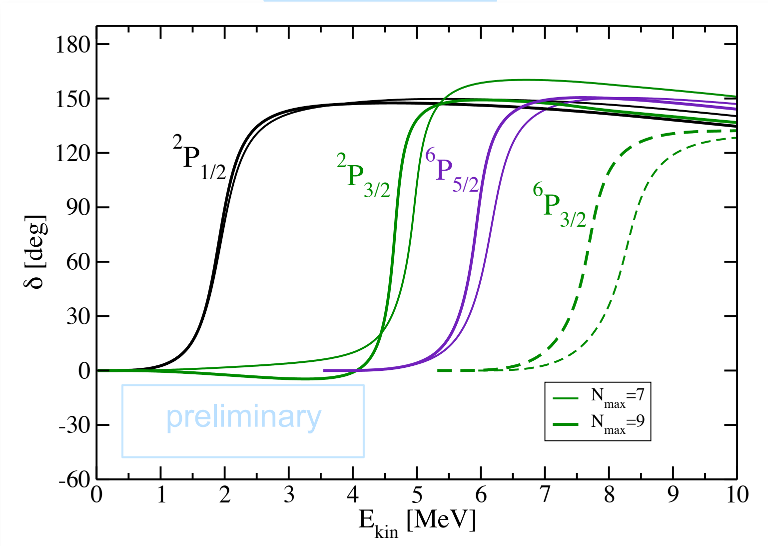
A. Kumar, R. Kanungo, A. Sanetullaev et al.

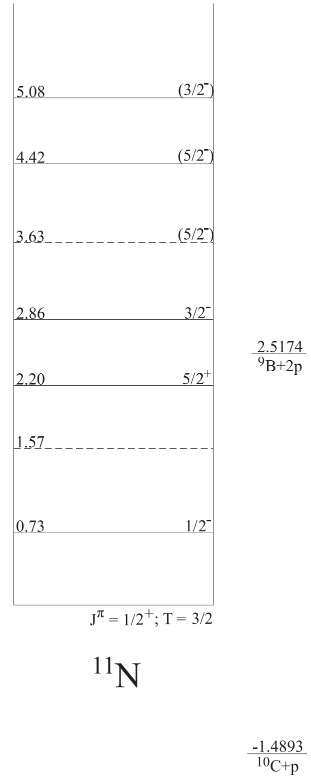
p+^{10}C scattering: structure of ^{11}N resonances

- NCSMC calculations **including chiral 3N** (N^3LO NN+N^2LO 3NF400)
  - p-^{10}C + ^{11}N
    - ^{10}C: 0^+, 2^+, 2^+ NCSM eigenstates
    - ^{11}N: 6 π = -1 and 3 π = +1 NCSM eigenstates



chiral NN+3N





J. Langhammer, P. N., G. Hupin, S. Quaglioni, A. Calci, R. Roth *et al*, in preparation

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

- NCSMC calculations **including chiral 3N** (N^{3}LO NN+N^{2}LO 3NF400)
  - p-^{10}C + ^{11}N
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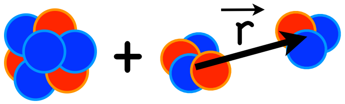
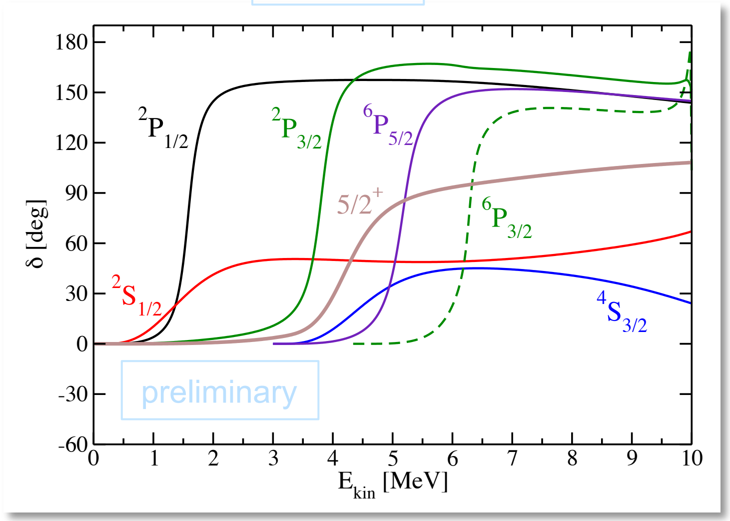
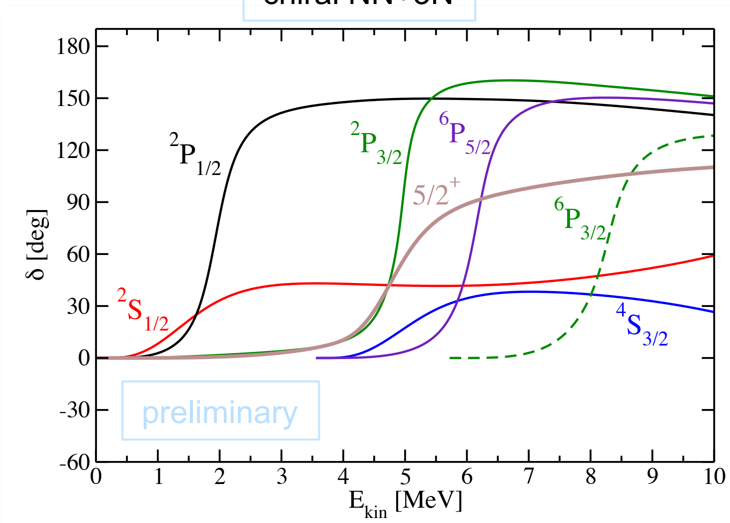
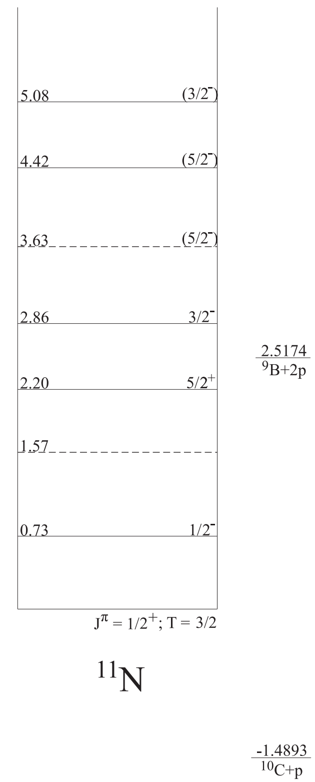


chiral NN



chiral NN+3N





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

TRIUMF

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

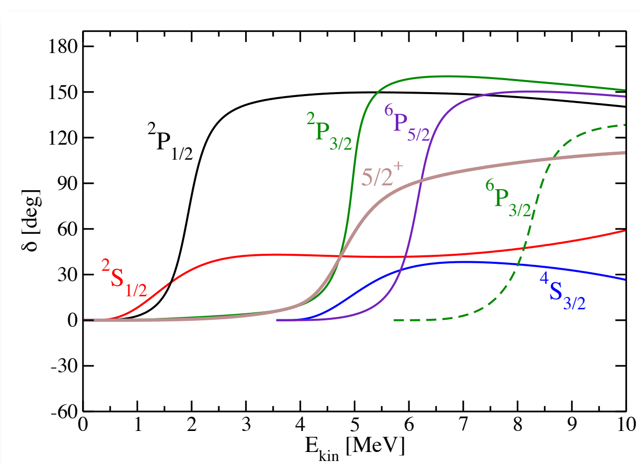
^{11}N from chiral NN+3N within NCSMC

– Preliminary

	J^π	T	E_{res} [MeV]	E_x [MeV]	Γ [keV]
	$1/2^+$	3/2	1.35	0	"4100"
✓	$1/2^-$	3/2	1.94	0.59	580
✓	$3/2^-$	3/2	4.69	3.34	280
	$5/2^+$	3/2	4.75	3.40	1790
	$3/2^+$	3/2	4.95	3.60	"4760"
	$5/2^-$	3/2	5.95	4.60	470
	$3/2^-$	3/2	7.68	6.33	620

^{11}N Expt. (TUNL evaluation)

$E_{\rm res}$ (MeV $\pm$ keV)	$E_{\rm x}$ (MeV $\pm$ keV)	$J^\pi; T$	Γ (keV)
1.49 ± 60	0	$\frac{1}{2}^+; \frac{3}{2}$	830 ± 30
2.22 ± 30	0.73 ± 70	$\frac{1}{2}^-$	600 ± 100
3.06 ± 80	(1.57 ± 80)		< 100
3.69 ± 30	2.20 ± 70	$\frac{5}{2}^+$	540 ± 40
4.35 ± 30	2.86 ± 70	$\frac{3}{2}^-$	340 ± 40
5.12 ± 80	(3.63 ± 100)	$(\frac{5}{2}^-)$	< 220
5.91 ± 30	4.42 ± 70	$(\frac{5}{2}^-)$	
6.57 ± 100	5.08 ± 120	$(\frac{3}{2}^-)$	100 ± 60



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

Negative parity 1/2$^-$ and 3/2$^-$ resonances in a good agreement with the current evaluation

Positive parity resonances too broad – N_{max} convergence

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

^{11}N from chiral NN+3N within NCSMC

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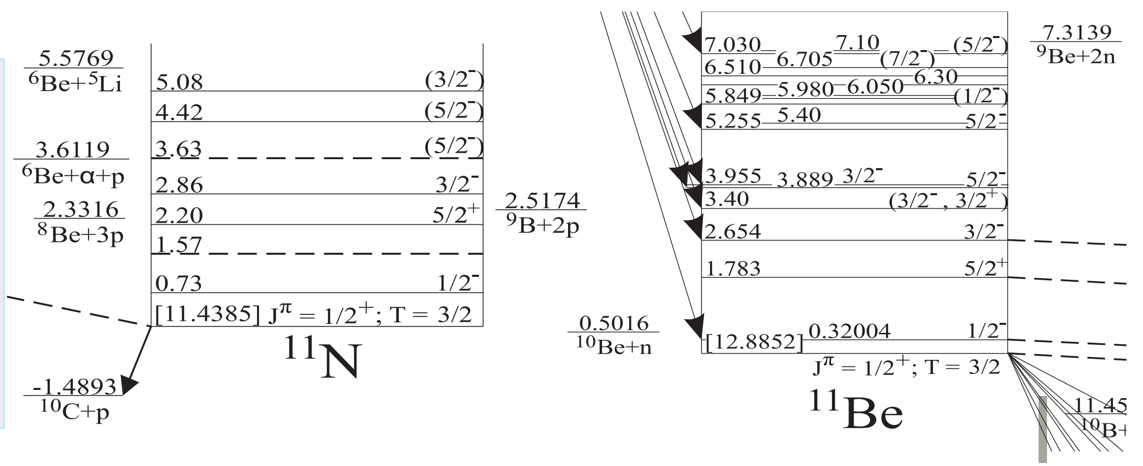
➔	5.91 ± 30	4.42 ± 70	$(\frac{5}{2}^-)$	
	6.57 ± 100	5.08 ± 120	$(\frac{3}{2}^-)$	100 ± 60

No candidate for 3.06 MeV resonance

We predict only one $5/2^-$ resonance below the $3/2^-_2$

Calculations suggest that either 5.12 MeV or 5.91 MeV resonance might be $3/2^+$ instead

NCSMC resonance predictions more in line with assignments in ^{11}Be

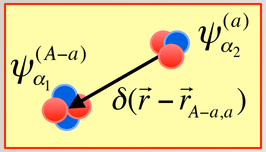


Three-body clusters in *ab initio* NCSM/RGM

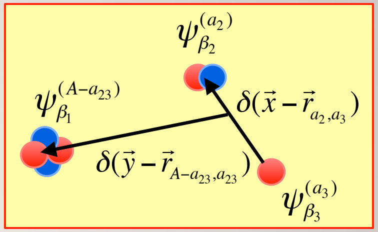
- Starts from:

$$\Psi^{(A)}_{RGM} = \sum_{\nu_2}\int g_{\nu_2}(\vec{r})\hat{A}_{\nu_2}\left|\phi_{\nu_2\vec{r}}\right\rangle d\vec{r} + \sum_{\nu_3}\iint G_{\nu_3}(\vec{x},\vec{y})\,\hat{A}_{\nu_3}\left|\Phi_{\nu_3\vec{x}\vec{y}}\right\rangle d\vec{x}d\vec{y}$$

2-body channels

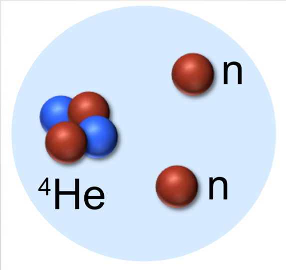


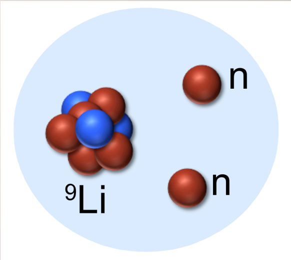
plus



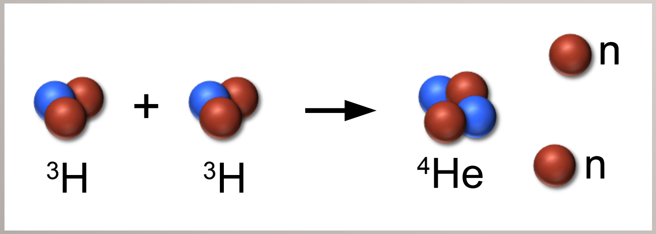
3-body channels

- Two-neutron halo nuclei





- Transfer reactions with three-body continuum final states



Three-body clusters in *ab initio* NCSM/RGM

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

Schrödinger equation

$$(\mathcal{H} - E)\,|\Psi^{J^\pi T}\rangle = 0$$

$$\sum_\nu \int dx dy x^2 y^2 \left[\mathcal{H}_{\nu'\nu}(x,y,x',y') - E\mathcal{N}_{\nu'\nu}(x,y,x',y')\right] G_\nu^{J^\pi T}(x,y) = 0$$

Hamiltonian Kernel

$$\langle\Phi^{J^\pi T}_{\nu' x' y'}|\hat{A}_{\nu'}\mathcal{H}\hat{A}_\nu|\Phi^{J^\pi T}_{\nu x y}\rangle$$

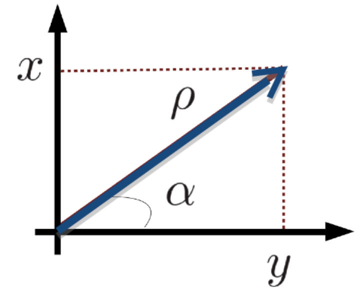
Norm kernel

$$\langle\Phi^{J^\pi T}_{\nu' x' y'}|\hat{A}^2|\Phi^{J^\pi T}_{\nu x y}\rangle$$

Three-body clusters in *ab initio* NCSM/RGM

Hyperspherical coordinates:

$$\rho = \sqrt{x^2 + y^2}, \quad \alpha = \arctan(x/y)$$



After changing to hyperspherical coordinates and integrating in α,α':

$$\sum_{\nu k} \int d\rho \rho^5 \left[\bar{\mathcal{H}}^{k'k}_{\nu'\nu}(\rho', \rho) - E \frac{\delta(\rho - \rho')}{\rho^5} \delta_{\nu'\nu} \delta_{k'k} \right] C^{J^\pi T}_{k\nu}(\rho) = 0$$

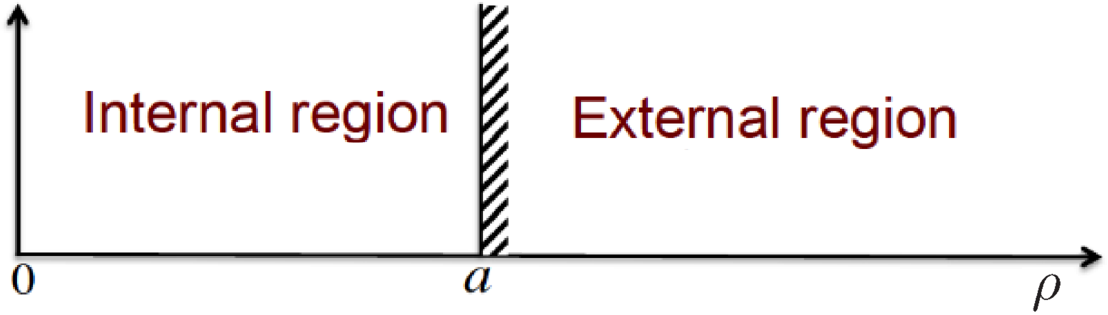
Coupled-channel microscopic R-matrix method on a Lagrange mesh*

*M. Hesse, J.-M. Sparenberg 1, E Van Raemdonck, D. Baye. Nuclear Physics A 640 (1998) 37-51

Three-body clusters in *ab initio* NCSM/RGM

Internal region: expansion on a basis ($\rho < a$)

$$C_{k\nu}(\rho) = \sum_i \beta_{k\nu i} f_i(\rho)$$



External region: known asymptotic behaviour ($\rho > a$)

* Bound state: $$C_{k\nu}(\rho) = A_{k\nu}\sqrt{\kappa\rho}K_{k+2}(\kappa\rho)$$

* Continuum state: $$C_{k\nu}(\rho) = A_{k\nu}\left[H_k^-(\kappa\rho)\delta_{\nu,\nu'}\delta_{k,k'} - S_{\nu k,\nu' k'}H_k^+(\kappa\rho)\right]$$

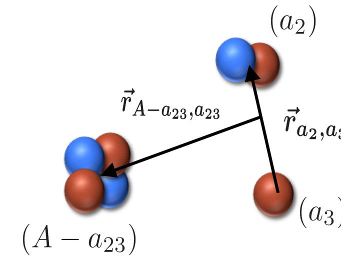
NCSM/RGM for three-body clusters: Structure of ^{6}He

^{4}He + *n* + *n*


PRL 113, 032503 (2014) PHYSICAL REVIEW LETTERS week ending 18 JULY 2014

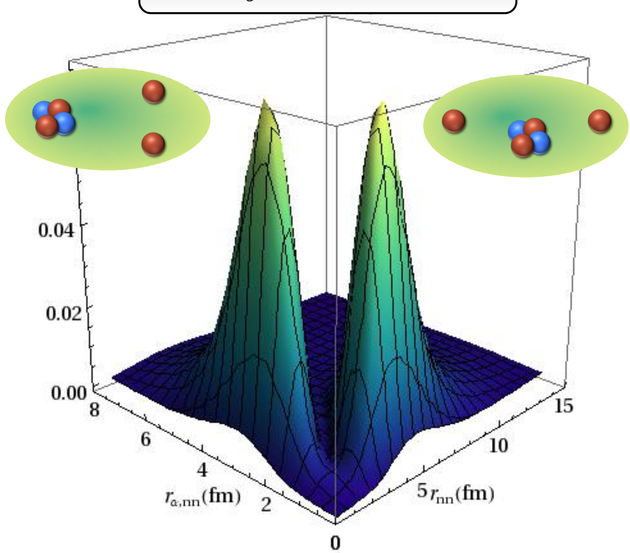
^{4}He + n + n Continuum within an *Ab initio* Framework

Carolina Romero-Redondo,[1,*] Sofia Quaglioni,[2,†] Petr Navrátil,[1,‡] and Guillaume Hupin[2,§]
[1]TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada
[2]Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA

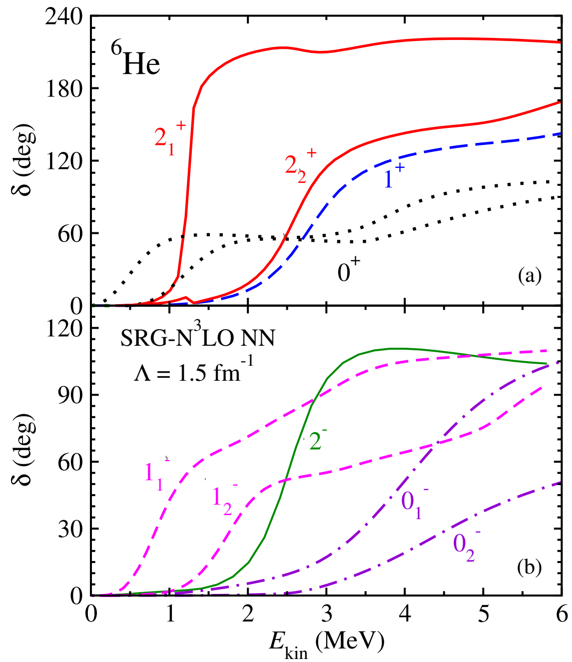


^{6}He bound 0^+ ground state

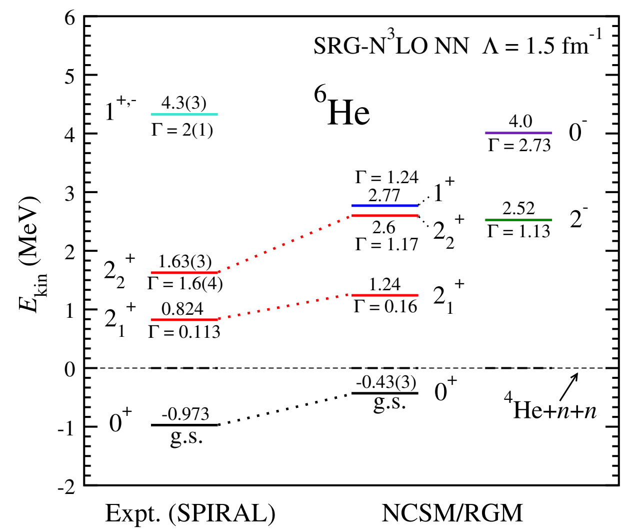
$\ell_x = \ell_y = L = S_{nn} = 0$



^{6}He resonances and continuum



Comparison to recent experiment



NCSMC implementation in progress…

^{5}H ≈ ^{4}He + *n* + *n* in progress

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*): NCSMC in progress

- Ongoing projects:
  - Transfer reactions: Talk by Francesco Raimondi on Tuesday
  - Applications to capture reactions important for astrophysics: Talk by Jeremy Dohet-Eraly on Friday
  - Bremsstrahlung: Talk by Jeremy Dohet-Eraly on Friday

- Outlook
  - Alpha-clustering (^{4}He projectile)
    - ^{12}C and Hoyle state: ^{8}Be+^{4}He
    - ^{16}O: ^{12}C+^{4}He

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