

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 treatment of nuclear reactions

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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-4He, <sup>3</sup>He(d,p)<sup>4</sup>He, <sup>7</sup>Be(p,γ)<sup>8</sup>B
  - NCSMC: <sup>5,7</sup>He, <sup>3</sup>He-<sup>4</sup>He, <sup>3</sup>He(α,γ)<sup>7</sup>Be, <sup>11</sup>N (*p*-<sup>10</sup>C)
  - Three-body cluster dynamics: <sup>6</sup>He
- Outlook









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### Ab initio Nuclear Structure & Reaction approaches

#### Ab initio

- $\diamond$  All nucleons are active
- ♦ Exact Pauli principle
- $\diamond$  Realistic inter-nucleon interactions
  - Accurate description of NN (and 3N) data
- $\diamond$  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  $(Q/\Lambda_x)$
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD



 $\Lambda_{\chi}$ ~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



- Acceleration of convergence by a sequence of unitary transformations in momentum space
  - Similarity-Renormalization-Group (SRG) evolved NN(+NNN) potential



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



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# NCSM calculations of <sup>6</sup>He and <sup>7</sup>He g.s. energies





Soft SRG evolved NN potential
 N<sub>max</sub> convergence OK
 Extrapolation feasible

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

- <sup>7</sup>He unbound
  - Expt. *E*<sub>th</sub>=+0.430(3) MeV: NCSM *E*<sub>th</sub>≈ +1 MeV
  - Expt. width 0.182(5) MeV: NCSM no information about the width



<sup>7</sup>He unbound



### Extending no-core shell model beyond bound states

Include more many nucleon correlations...





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



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

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

$$\phi_{1\kappa}$$

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

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

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

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

•  $\phi$ : antisymmetric cluster wave functions

- {ξ}: Translationally invariant internal coordinates

(Jacobi relative coordinates)

- These are known, they are an input



$$\begin{split} \psi^{(A)} &= \sum_{\kappa} c_{\kappa} \phi_{1\kappa} \left( \left\{ \vec{\xi}_{1\kappa} \right\} \right) & (a_{1\kappa} = A) \\ & \phi_{1\kappa} \\ &+ \sum_{\nu} \widehat{A}_{\nu} \phi_{1\nu} \left( \left\{ \vec{\xi}_{1\nu} \right\} \right) \phi_{2\nu} \left( \left\{ \vec{\xi}_{2\nu} \right\} \right) g_{\nu}(\vec{r}_{\nu}) & \phi_{1\nu} (a_{2\nu}) \\ & a_{1\nu} + a_{2\nu} = A \\ &+ \sum_{\mu} \widehat{A}_{\mu} \phi_{1\mu} \left( \left\{ \vec{\xi}_{1\mu} \right\} \right) \phi_{2\mu} \left( \left\{ \vec{\xi}_{2\mu} \right\} \right) \phi_{3\mu} \left( \left\{ \vec{\xi}_{3\mu} \right\} \right) G_{\mu}(\vec{R}_{\mu 1}, \vec{R}_{\mu 2}) & (a_{2\mu}) (a_{2\mu$$

•  $A_{\nu}, A_{\mu}$ : intercluster antisymmetrizers

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

Antisymmetrize the wave function for exchanges of nucleons between clusters

Example:  

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



• >

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





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





### **Binary cluster wave function**

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

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

a,a)  

$$(A-a) \overrightarrow{r}_{A-a,a} (a)$$
eigenstates of  
 $H_{(A-a)}$  and  $H_{(a)}$   
in the *ab initio*  
NCSM basis

Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$\downarrow$$

$$\sum_{v} \int d\vec{r} \left[ \mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}',\vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}',\vec{r}) \right] \phi_{v}(\vec{r}) = 0$$
realistic nuclear Hamiltonian
$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}'} | \hat{\mathcal{A}}H\hat{\mathcal{A}} | \Phi^{(A-a,a)}_{v\vec{r}} \rangle$$
Hamiltonian kernel
Norm kernel
Norm kernel

## Norm kernel (Pauli principle) Single-nucleon projectile

$$N_{v'v}^{J^{\pi}T}(r',r) = \delta_{v'v} \frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')R_{n\ell}(r) \left\langle \Phi_{v'n'}^{J^{\pi}T} \middle| \hat{P}_{A-1,A} \middle| \Phi_{vn}^{J^{\pi}T} \right\rangle$$
Direct term:  
Treated exactly!  
(in the full space)
$$V'$$

$$-(A-1) \times \left(a=1\right)$$

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

# Microscopic *R*-matrix on a Lagrange mesh

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



– This is achieved through the Bloch operator:

$$L_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left(\frac{d}{dr} - \frac{B_c}{r}\right)$$

- System of Bloch-Schrödinger equations:

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

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

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

Bound state

TRIUMF

Scattering state

Scattering matrix

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

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

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

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



### n-<sup>4</sup>He scattering: NN vs. NN+NNN interactions



PHYSICAL REVIEW C 88, 054622 (2013)

*Ab initio* many-body calculations of nucleon-<sup>4</sup>He scattering with three-nucleon forces

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chiral NN+NNN(500) chiral NN+NNN-induced SRG  $\lambda$ =2 fm<sup>-1</sup> HO N<sub>max</sub>=13, hΩ=20 MeV

#### <sup>4</sup>He g.s. and 6 excited states

29.89	2+,0	
<u>28.37 <b>28</b>39 28.64</u>	28.67	2 <sup>+,0</sup>
28.31	1+,0	1-,0
27.42	2+,0	
25, <del>9</del> 5	1-,1	
25,28	0~,1	
24.25	17,0	
23.64	1-,1	
23.33	27,1	
21.84	27,0	
21.01	0.0	
20.21	0,0	p(1

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





## New developments: NCSM with continuum



## RIUMF Building blocks of the NCSMC equations



#### **RIUMF**

# *n*-<sup>4</sup>He & *p*-<sup>4</sup>He scattering within NCSMC

#### Study of the convergence with respect to the # of <sup>4</sup>He low-lying NCSM states

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



 $\lambda$ =2.0 fm<sup>-1</sup> and 8 low-lying NCSM states of <sup>5</sup>He.



#### **RIUMF**

# **NCSM/RGM** calculations of transfer reactions

$$\int dr r^{2} \left[ \begin{pmatrix} \mathbf{r} \\ \mathbf{n} \\ \mathbf{n}$$

Straightforward to couple different mass partitions in the NCSM/RGM formalism

Applications to (d,p) and (d,n) reactions Example: <sup>3</sup>He(d,p)<sup>4</sup>He

Work in progress: <sup>7</sup>Li(d,p)<sup>8</sup>Li & <sup>8</sup>Li(d,p)<sup>9</sup>Li Technical issue: Calculation of kernels with three-body densities for systems with A>5



Ab Initio Many-Body Calculations of the  ${}^{3}H(d, n){}^{4}He$  and  ${}^{3}He(d, p){}^{4}He$  Fusion Reactions

Petr Navrátil<sup>1,2</sup> and Sofia Quaglioni<sup>2</sup>



# Solar *p-p* chain





# Structure of the <sup>8</sup>B ground state

- NCSM/RGM p-<sup>7</sup>Be calculation
  - five lowest <sup>7</sup>Be states: 3/2<sup>-</sup>, 1/2<sup>-</sup>, 7/2<sup>-</sup>, 5/2<sup>-</sup><sub>1</sub>, 5/2<sup>-</sup><sub>2</sub>
  - Soft NN SRG-N<sup>3</sup>LO with  $\lambda$  = 1.86 fm<sup>-1</sup>
- <sup>8</sup>B 2<sup>+</sup> g.s. bound by 136 keV (Expt 137 keV)
  - Large *P*-wave 5/2<sup>-</sup><sub>2</sub> component







# p

<sup>7</sup>Be

# *p*-<sup>7</sup>Be scattering







# <sup>7</sup>Be(*p*,γ)<sup>8</sup>B radiative capture



Petr Navrátil<sup>a,b,\*</sup>, Robert Roth<sup>c</sup>, Sofia Quaglioni<sup>b</sup>



# <sup>3</sup>He-<sup>4</sup>He and <sup>3</sup>H-<sup>4</sup>He scattering



NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.1 fm<sup>-1</sup>) <sup>3</sup>He, <sup>3</sup>H, <sup>4</sup>He ground state, 8( $\pi$ -) + 8( $\pi$ +) eigenstates of <sup>7</sup>Be and <sup>7</sup>Li Preliminary: N<sub>max</sub>=10, hΩ=20 MeV E<sub>th</sub>(<sup>7</sup>Be)=-1.32 MeV (Expt. -1.59 MeV) E<sub>th</sub>(<sup>7</sup>Li) = -2.20 MeV (Expt. -2.47 MeV)

Goal: Calculations of <sup>3</sup>He(<sup>4</sup>He,γ)<sup>7</sup>Be & <sup>3</sup>H(<sup>4</sup>He,γ)<sup>7</sup>Li capture







NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.1 fm<sup>-1</sup>) <sup>3</sup>He, <sup>3</sup>H, <sup>4</sup>He ground state, 8( $\pi$ -) + 8( $\pi$ +) eigenstates of <sup>7</sup>Be and <sup>7</sup>Li Preliminary: N<sub>max</sub>=10, hΩ=20 MeV E<sub>th</sub>(<sup>7</sup>Be)=-1.32 MeV (Expt. -1.59 MeV) E<sub>th</sub>(<sup>7</sup>Li) = -2.20 MeV (Expt. -2.47 MeV)

Goal: Calculations of <sup>3</sup>He(<sup>4</sup>He,γ)<sup>7</sup>Be & <sup>3</sup>H(<sup>4</sup>He,γ)<sup>7</sup>Li capture



# NCSM with continuum: <sup>7</sup>He $\leftrightarrow$ <sup>6</sup>He+*n*



#### **TRIUMF**

# p+<sup>10</sup>C scattering: structure of <sup>11</sup>N resonances

- Limited information about the structure of proton rich <sup>11</sup>N – mirror nucleus of <sup>11</sup>Be halo nucleus
- Incomplete knowledge of <sup>10</sup>C unbound excited states
- Importance of 3N force effects and continuum





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# <sup>10</sup>C(p,p) @ IRIS with solid H<sub>2</sub> target

- New experiment at ISAC TRIUMF with reaccelerated <sup>10</sup>C
  - The first ever <sup>10</sup>C beam at TRIUMF
  - Angular distributions measured at  $E_{\rm CM}$  ~ 4.1 MeV and 4.4 MeV
  - Data analysis under way



# p+<sup>10</sup>C scattering: structure of <sup>11</sup>N resonances

🜔 + 🚰 🗲

 $(3/2^{-})$ 

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NCSMC calculations including chiral 3N

 $- p^{-10}C + {}^{11}N$ 

TRIUMF

- <sup>10</sup>C: 0<sup>+</sup>, 2<sup>+</sup>, 2<sup>+</sup> NCSM eigenstates
- <sup>11</sup>N: 6  $\pi$  = -1 and 3  $\pi$  = +1 NCSM eigenstates
- $N_{\text{max}}$ = 7,  $N_{\text{max}}$ =9 under way



With the 3N the <sup>2</sup>P<sub>1/2</sub> and <sup>2</sup>P<sub>3/2</sub> resonances broader and shifted to higher energy in a better agreement with experiment

# RIUMF p+<sup>10</sup>C scattering: Elastic differential cross section



Significant difference in angular distributions in the experimentally explored energy range due to the shift of the  ${}^{2}P_{3/2}$  resonance

<sup>10</sup>C+p

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#### **ETRIUMF**

# <sup>10</sup>C(p,p')<sup>10</sup>C(2<sup>+</sup><sub>1</sub>) scattering: Differential cross section



Significant difference in the shape of the inelastic differential g.s. to  $2^+_1$  cross section around  $E_{kin} \sim 5$  MeV The shape determined by an interference of 5/2<sup>+</sup> and 3/2<sup>-</sup> resonances

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### NCSM/RGM for three-body clusters: Structure of <sup>6</sup>He



#### **RIUMF**

### NCSM/RGM for three-body clusters: Structure of <sup>6</sup>He





# **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 ( $^{6}\text{He} \sim {}^{4}\text{He}+n+n$ )
  - Applications to capture reactions important for astrophysics

#### • Outlook:

- Extension to composite projectiles (deuteron, <sup>3</sup>H, <sup>3</sup>He)
- Transfer reactions
- Bremsstrahlung
- Alpha-clustering (<sup>4</sup>He projectile)
  - <sup>12</sup>C and Hoyle state: <sup>8</sup>Be+<sup>4</sup>He
  - <sup>16</sup>O: <sup>12</sup>C+<sup>4</sup>He



# **NCSMC and NCSM/RGM collaborators**

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