TRIUMF

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

## Ab initio calculations of light-ion reactions

Workshop on "Electron-Nucleus Scattering XII" June 25-29, 2012 Elba, Italy

Petr Navratil | TRIUMF

Collaborators: Sofia Quaglioni (LLNL), Robert Roth (TU Darmstadt), W. Horiuchi (RIKEN), C. Romero-Redondo (TRIUMF), M. Kruse (UA), S. Baroni (ULB), J. Langhammer (TU Darmstadt), G. Hupin (LLNL)

Accelerating Science for Canada Un accélérateur de la démarche scientifique canadienr

Owned and operated as a joint venture by a consortium of Canadian universities via a contribution through the National Research Council Canada Propriété d'un consortium d'universités canadiennes, géré en co-entreprise à partir d'une contribution administrée par le Conseil national de recherches Canada



Marciana Marina, Isola d'Elba, Italy.







### Outline



Connection to QCD

- Nuclear forces from chiral EFT
- Many-body techniques NCSM, NCSM/RGM
- Results for bound states, resonances, reactions

Connection to Astrophysics

## Nuclei from the first principles

#### 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
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order
  - Hierarchy

RIUMF

- Consistency
- Low energy constants (LEC)
  - Fitted to data
  - Can be calculated by lattice QCD





### 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<sup>1,†</sup>



Phase Shift (deg)

-10

-20

-30

0

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



# Determination of NNN LECs c<sub>D</sub> and c<sub>E</sub> from the triton binding energy and the half life

- **Chiral EFT**: *c*<sub>D</sub> also in the two-nucleon contact vertex with an external probe
- Calculate  $\langle E_1^A \rangle = |\langle^3 \text{He}||E_1^A||^3 \text{H} \rangle|$ 
  - Leading order GT
  - N<sup>2</sup>LO: one-pion exchange plus contact
- A=3 binding energy constraint:  $c_{\rm D}$ =-0.2±0.1  $c_{\rm E}$ =-0.205±0.015







### A=3,4 bound states

					-	-
	<sup>3</sup> H		<sup>3</sup> He		<sup>4</sup> He	
	$E_{\rm g.s.}$	$\langle r_p^2 \rangle^{1/2}$	$E_{\rm g.s}$	$\langle r_p^2  angle^{1/2}$	$E_{\rm g.s}$	$\langle r_p^2 \rangle^{1/2}$
NN	-7.852(4)	1.651(5)	-7.124(4)	1.847(5)	-25.39(1)	1.515(2)
NN + NNN	-8.473(4)	1.605(5)	-7.727(4)	1.786(5)	-28.50(2)	1.461(2)
Expt.	-8.482	1.60	-7.718	1.77	-28.296	1.467(13) [31]



#### Proton-<sup>3</sup>He elastic scattering with χEFT NN+NNN

- Variational calculations in hypherspherical-harmonics basis
  - M. Viviani, L. Girlanda, A. Kievski, L. E. Marcucci, and S. Rosati, arXiv:1004.1306
- A<sub>v</sub> puzzle resolved with the chiral N<sup>3</sup>LO NN plus local chiral N<sup>2</sup>LO NNN



Chiral NN+NNN Hamiltonian provides the best agreement with the cross section and analyzing power data and with the new TUNL PSA analysis

## No-core shell model combined with the resonating group method (NCSM/RGM)

- **The NCSM:** An approach to the solution of the *A*-nucleon bound-state problem
  - Accurate nuclear Hamiltonian
  - Finite harmonic oscillator (HO) basis
    - Complete  $N_{max} \hbar \Omega$  model space
  - Effective interaction due to the model space truncation
    - Similarity-Renormalization-Group evolved NN(+NNN) potential
  - Short & medium range correlations
  - No continuum

RIUMF

$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi^{A}_{Ni}$$



- **The RGM:** A microscopic approach to the A-nucleon scattering of clusters
  - Long range correlations, relative motion of clusters

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



Ab initio NCSM/RGM: Combines the best of both approaches Accurate nuclear Hamiltonian, consistent cluster wave functions Correct asymptotic expansion, Pauli principle and translational invariance

#### 

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

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

$$\sum_{n'n} \left\langle \psi_{\mu_{1}}^{(A-1)} \middle| a^{+}a \middle| \psi_{v_{1}}^{(A-1)} \right\rangle_{\text{SD}}$$

$$\sum_{n'n} \left\langle \psi_{\mu_{1}}^{(A-1)} \middle| a^{+}a \middle| \psi_{v_{1}}^{(A-1)} \right\rangle_{\text{SD}}$$

$$\sum_{n'n} \left\langle \psi_{\mu_{1}}^{(A-1)} \middle| a^{+}a \middle| \psi_{v_{1}}^{(A-1)} \right\rangle_{\text{SD}}$$

$$\sum_{n'n'} \left\langle \psi_{\mu_{1}}^{(A-1)} \middle| a^{+}a \middle| a^{+}a$$

#### Hamiltonian kernel (projectile-target potentials)

Single-nucleon projectile

$$\left\langle \Phi_{v'r'}^{I^{T}} \left| \hat{A}_{v} H \hat{A}_{v} \right| \Phi_{vr}^{J^{T}} \right\rangle = \left\langle \begin{array}{c} (A-1) \\ r' \\ r' \\ (a'=1) \end{array} \right| H \left( 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right) \left| \begin{array}{c} (A-1) \\ (a=1) \end{array} \right\rangle$$

$$H_{v'v}^{J^{T}T} (r',r) = \left[ T_{rel}(r) + \bar{V}_{Coul}(r) + \varepsilon_{\alpha_{1}}^{I^{T}T} \right] N_{v'v}^{J^{T}T} (r',r)$$

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

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

$$+ (A-1) \times \left\{ \left( \begin{array}{c} + 1 \\ + 1 \end{array} \right) \left( \begin{array}{c} + 1 \end{array} \right) \left( \begin{array}{c} + 1 \\ + 1 \end{array} \right) \left( \begin{array}{c} + 1 \end{array} \right) \left( \begin{array}{c}$$



### Solving the RGM equations

- Input: Realistic nuclear Hamiltonian, eigenfunctions of nucleon clusters
  - Macroscopic degrees of freedom: nucleon clusters
  - Unknowns: relative wave function between the two clusters
- Non-local integral-differential coupled-channel equations:

$$\left[T_{rel}(r) + V_C(r) + E_{\alpha_1}^{(A-a)} + E_{\alpha_2}^{(a)}\right] u_v^{(A-a,a)}(r) + \sum_{a'v'} \int dr'r' \ W_{av,a'v'}(r,r') u_{v'}^{(A-a',a')}(r') = 0$$

- Solve with R-matrix theory on Lagrange mesh imposing

  - − Scattering state boundary conditions → Scattering matrix
    - Phase shifts
    - Cross sections

• ...

The R-matrix theory on Lagrange mesh is an elegant and powerful technique, particularly for calculations with non-local potentials

#### 

### The best system to start with: *n*+<sup>4</sup>He, *p*+<sup>4</sup>He



NNN missing: Good agreement only for energies beyond low-lying 3/2<sup>-</sup> resonance

#### 

#### *p*+<sup>4</sup>He differential cross section and analyzing power



#### **®TRIUMF N-**<sup>4</sup>He scattering with NN+NNN interactions

G. Hupin, J. Langhammer, S. Quaglioni, P. Navratil, R. Roth, work in progress

 $n + {}^{4}\text{He}(g.s.)$ , SRG-(N<sup>3</sup>LO *NN* + N<sup>2</sup>LO NNN potential with ( $\lambda$ =2 fm<sup>-1</sup>).



Largest splitting between *P* waves obtained with NN+NNN. Need <sup>4</sup>He exited states and study with respect to SRG  $\lambda$ 



### Solar *p-p* chain





S

### <sup>7</sup>Be(*p*,γ)<sup>8</sup>B S-factor

- $S_{17}$  one of the main inputs for understanding the solar neutrino flux
  - Needs to be known with high precision
- Current evaluation has uncertainty ~ 10%
  - Theory needed for extrapolation to ~ 10 keV

$$\eta(E) = E\sigma(E) \exp[2\pi\eta(E)]$$
$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$

$$\left< {}^{8}\mathbf{B}_{g.s.} \left| E1 \right| {}^{7}\mathbf{Be}_{g.s.} + \mathbf{p} \right>$$



#### <sup>7</sup>Be(*p*,γ)<sup>8</sup>B radiative capture: Input - *NN* interaction, <sup>7</sup>Be eigenstates

- Similarity-Renormalization-Group (SRG) evolved chiral N<sup>3</sup>LO NN interaction
  - Accurate
  - Soft: Evolution parameter Λ
    - Study dependence on A

#### • <sup>7</sup>Be

RIUMF

- NCSM up to  $N_{max}$ =10, Importance Truncated NCSM up to  $N_{max}$ =14
- Variational calculation
  - optimal HO frequency from the ground-state minimum
  - For the selected NN potential with  $\Lambda$ =1.86 fm<sup>-1</sup>: h $\Omega$ =18 MeV







### Input: <sup>7</sup>Be eigenstates

• Excited states at the optimal HO frequency,  $\hbar\Omega$ =18 MeV





### 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>, 5/2<sup>-</sup>, 5/2<sup>-</sup>
  - 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







<sup>7</sup>Be

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







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

- NCSM/RGM calculation of <sup>7</sup>Be(p,γ)<sup>8</sup>B radiative capture
  - <sup>7</sup>Be states 3/2<sup>-</sup>, 1/2<sup>-</sup>, 7/2<sup>-</sup>, 5/2<sup>-</sup>, 5/2<sup>-</sup>, 5/2<sup>-</sup>
  - Soft NN potential (SRG-N<sup>3</sup>LO with  $\Lambda$  = 1.86 fm<sup>-1</sup>)



Physics Letters B 704 (2011) 379

7.21

4.57



#### NCSM/RGM *ab initio* calculation of *d*-<sup>4</sup>He scattering

- NCSM/RGM calculation with  $d + {}^{4}\text{He}(g.s.)$  up to  $N_{\text{max}} = 12$ 
  - SRG-N<sup>3</sup>LO potential with  $\Lambda$  = 1.5 fm<sup>-1</sup>
  - Deuteron breakup effects included by continuum discretized by pseudo states in  ${}^{3}S_{1}$ - ${}^{3}D_{1}$ ,  ${}^{3}D_{2}$  and  ${}^{3}D_{3}$ - ${}^{3}G_{3}$  channels



• The 1<sup>+</sup>0 ground state bound by 1.9 MeV (expt. 1.47 MeV)

• Calculated T=0 resonances: 3<sup>+</sup>, 2<sup>+</sup> and 1<sup>+</sup> in correct order close to expt. energies



#### NCSM/RGM *ab initio* calculation of *d*-<sup>4</sup>He scattering

PHYS. REV. C 83, 044609 (2011)



Scattering provides a strict test of NN and NNN forces Important to include 6-nucleon correlations – deuteron (virtual) breakup ...

#### 

#### Ab initio calculation of the ${}^{3}H(d,n){}^{4}He$ fusion

$$\int dr r^{2} \left\{ \begin{pmatrix} r \\ n \\ n \end{pmatrix} \left| \hat{A}_{1}(H-E) \hat{A}_{1} \right| \left| \frac{r}{\alpha} \right| n \\ \langle r \\ d^{2} d$$

#### **RIUMF**

#### d+<sup>3</sup>H and n+<sup>4</sup>He elastic scattering: phase shifts



- d+<sup>3</sup>H elastic phase shifts:
  - Resonance in the <sup>4</sup>S<sub>3/2</sub> channel
  - Repulsive behavior in the <sup>2</sup>S<sub>1/2</sub>
     channel → Pauli principle
  - $d^*$  deuteron pseudo state in  ${}^3S_1 {}^3D_1$  channel: deuteron polarization, virtual breakup



- *n*+<sup>4</sup>He elastic phase shifts:
  - d+<sup>3</sup>H channels produces slight increase of the *P* phase shifts
  - Appearance of resonance in the 3/2<sup>+</sup> *D*-wave, just above *d*-<sup>3</sup>H threshold

The  $d^{-3}$ H fusion takes place through a transition of  $d^{+3}$ H is *S*-wave to  $n^{+4}$ He in *D*-wave: Importance of the **tensor force** 

#### 

### ${}^{3}H(d,n){}^{4}He \& {}^{3}He(d,p){}^{4}He$ fusion

NCSM/RGM with SRG-N<sup>3</sup>LO NN potentials



Potential to address unresolved fusion research related questions:

 ${}^{3}\text{H}(d,n){}^{4}\text{He}$  fusion with polarized deuterium and/or tritium,  ${}^{3}\text{H}(d,n \gamma){}^{4}\text{He}$  bremsstrahlung,

Electron screening at very low energies ...

P.N., S. Quaglioni, PRL **108**, 042503 (2012)



#### Borromean halo nuclei: He isotopes



- <sup>6</sup>He and <sup>8</sup>He with chiral N<sup>3</sup>LO NN + N<sup>2</sup>LO 3N
  - chiral N<sup>3</sup>LO NN: <sup>4</sup>He underbound, <sup>6</sup>He and <sup>8</sup>He unbound
  - chiral N<sup>3</sup>LO NN + N<sup>2</sup>LO 3N(500): <sup>4</sup>He OK, both <sup>6</sup>He and <sup>8</sup>He bound



#### 

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

• Starts from:



Transfer reactions with three-body continuum final states





#### Norm kernel for *n*+*n*+<sup>4</sup>He





#### *Ab initio* calculations of <sup>3</sup>He+α scattering: First results (preliminary, incomplete)



Calculations for *a*=3 projectile under way: Soft SRG interactions ( $\Lambda$ =1.5 fm<sup>-1</sup>,  $\Lambda$ =1.86 fm<sup>-1</sup>) Virtual breakup of <sup>3</sup>He included by pseudostates (in 1/2<sup>+</sup>, 5/2<sup>+</sup> channels so far)



#### 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





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





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



### **Conclusions and Outlook**

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
- The first  ${}^{7}Be(p,\gamma){}^{8}B$  ab initio S-factor calculation

PLB 704 (2011) 379

- Deuteron-projectile results with SRG-N<sup>3</sup>LO *NN* potentials:
  - d-<sup>4</sup>He scattering
  - First *ab initio* study of  ${}^{3}H(d,n){}^{4}He \& {}^{3}He(d,p){}^{4}He$  fusion
- Under way:
  - *n*-<sup>8</sup>He scattering and <sup>9</sup>He structure
  - <sup>3</sup>He-<sup>4</sup>He and <sup>3</sup>He-<sup>3</sup>He scattering calculations
  - Ab initio NCSM with continuum (NCSMC)
  - Three-cluster NCSM/RGM and treatment of three-body continuum
  - Inclusion of NNN force
- To do:
  - Alpha clustering: <sup>4</sup>He projectile

PRL 108, 042503 (2012)

PRC 83, 044609 (2011)

