

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 nuclear reactions important for astrophysics

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- Nuclear forces
  - chiral EFT, two-nucleon, three-nucleon
- Nuclear many-body calculations for bound states
  - No-core shell model (NCSM)
- Unitary transformations
  - Similarity Renormalization Group
- - NCSM with the Resonating Group Method (NCSM/RGM)
  - NCSM with continuum (NCSMC)
- Lecture 2
  - Ab initio calculations of nuclear reactions important for astrophysics
    - ${}^{7}\text{Be}(p,\gamma){}^{8}\text{B}$ ,  ${}^{3}\text{He}(\alpha,\gamma){}^{7}\text{Be}$ ,  ${}^{3}\text{H}(\alpha,\gamma){}^{7}\text{Li}$ ,  ${}^{3}\text{He}(d,p){}^{4}\text{He}$ ,  ${}^{3}\text{H}(d,n){}^{4}\text{He}$
    - Progress towards  ${}^{2}H(\alpha,\gamma){}^{6}Li$ ,  ${}^{4}He(nn,\gamma){}^{6}He$ ,  ${}^{11}C(p,\gamma){}^{12}N$



Outline







# Role of Nuclear Theory

#### Develop a unified theory of nuclei



Connecting to QCD

Connecting to Astrophysics



# Role of Nuclear Theory

Develop a unified theory of nuclei more specific questions...



Connecting to QCD

How does nuclear physics drive phenomena like the creation of elements and SN explosions?  How do nuclear forces give rise to nuclear structure? How do we explain reactions?

How do nuclear forces emerge from QCD?

Connecting to Astrophysics



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

# Why nuclei from first principles?

- <u>Goal</u>: Predictive theory of structure and reactions of nuclei
- Needed for
  - Physics of exotic nuclei, tests of fundamental symmetries
  - Understanding of nuclear reactions important for astrophysics
  - Understanding of reactions important for energy generation
  - Double beta decay nuclear matrix elements
  - Neutrino-nucleus cross sections



#### Understanding our Sun







# From QCD to nuclei





**Nuclear structure and reactions** 



# Nuclear forces



#### Nowadays: New vision of Effective Field Theory Links low energy physics to QCD in a systematic way

Nucleon-Nucleon force



Arise due to the effective nature of nuclear forces



Details of short distance physics not resolved, but captured in short range couplings should come from QCD but are now fit to experiment



# **Chiral Effective Field Theory**

- 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





### Chiral EFT NN interaction in the leading order (LO)

$$V^{\text{LO}} = -\frac{g_A^2}{4F_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \ \vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + M_\pi^2} + C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$\int \mathbf{r}_1 \cdot \mathbf{r}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \ \vec{\sigma}_2 \cdot \vec{q}}{\pi} + C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$\mathbf{r}_2 \cdot \mathbf{r}_3 \cdot \mathbf{r}_4 \cdot \mathbf{r}_4 \cdot \mathbf{r}_4 \cdot \mathbf{r}_5 \cdot$$

 $g_A$ =1.29 ...axial-vector coupling constant  $F_{\pi}$ =92.4 MeV ...pion decay constant  $\exp\left(-(k' / \Lambda)^{2n} - (k / \Lambda)^{2n}\right)$  $\Lambda \sim 500 \text{ MeV} << \Lambda_{\chi} \sim 1 \text{ GeV}$ 



# 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





### Three-nucleon forces why?



Two-pion exchange with virtual ∆ excitation – Fujita & Miyazawa (1957)

- Leading three-nucleon force terms
  - Long-range two-pion exchange
  - Medium-range one-pion exchange + two-nucleon contact
  - Short range three-nucleon contact

The question is not: Do three-body forces enter the description? The only question is: How large are three-body forces?



### Leading terms of the chiral NNN force





# From QCD to nuclei





### The nuclear many-body problem

• Start with the microscopic A-nucleon Hamiltonian

$$H^{(A)} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i< j=1}^{A} V^{2b}(\vec{r}_i - \vec{r}_j) + \left(\sum_{i< j< k=1}^{A} V^{3b}_{ijk}\right)$$

- Nucleons interact with two- and three-nucleon forces: this yields complicated quantum correlations
- Solve the many-body Schrödinger equation

$$H^{(A)}\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \dots \vec{r}_A) = E\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \dots \vec{r}_A)$$

- Negative energies (relative to a breakup threshold)— bound-state boundary conditions
  - Find eigenfunctions and eigenenergies
- Continuum of positive energies scattering boundary conditions
  - Find elements of the Scattering matrix

### The nuclear many-body wave function

A active nucleons – spatial, spin, and isospin degrees of freedom

$$\vec{r}_i \equiv \{\vec{r}_i, \vec{\sigma}_i, \vec{\tau}_i\}, i = 1, 2, \cdots, A$$

• Nucleons are fermions – wave function antisymmetric

$$\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \dots \vec{r}_k, \dots \vec{r}_j, \dots \vec{r}_A) = -\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \dots \vec{r}_j, \dots \vec{r}_k, \dots \vec{r}_A)$$

- Conserved total angular momentum J and parity  $\pi$ 
  - approximately conserved total isospin T
- We are not interested in the motion of the center of mass, but only in the intrinsic motion
  - Look for translationally invariant wave function. Two options:
    - Work with A 1 translational invariant coordinates known as Jacobi coordinates
    - Work with A single particle coordinates and aim at exact separation between intrinsic and center of mass motion

$$\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \dots \vec{r}_A) = \psi^{(A)}(\vec{\xi}_1, \vec{\xi}_2, \dots \vec{\xi}_{A-1}) \Psi_{CM}(\vec{R}_{CM})$$



• The nuclear wave function must factorize, e.g., for free c.m. motion

$$\Psi^{(A)} = \psi^{(A)} \exp\left(-i\frac{\vec{P}_{CM}\vec{R}_{CM}}{\hbar}\right) \qquad \qquad E = \varepsilon + \frac{P_{CM}^2}{2Am}$$

- First option: solve eigenvalue problem for the intrinsic Hamiltonian
  - <sup>©</sup> The c.m. motion is not present from the beginning
  - © Work with 3(A-1) spatial degrees of freedom (Jacobi relative coordinates)
  - Sacobi coordinates do not treat the nucleons in a symmetric manner

$$\hat{P}_{ij}\phi_{s,n}^{(A)}(\vec{\xi}_1,...\vec{\xi}_{A-1}) = \phi_{s,n}^{(A)}(\hat{P}_{ij}\vec{\xi}_1,...\hat{P}_{ij}\vec{\xi}_{A-1}) = \sum_{m=1}^N R_{nm}\phi_{s,m}^{(A)}(\vec{\xi}_1,...\vec{\xi}_{A-1})$$

$$\begin{cases} \vec{\xi}_1 = \frac{1}{\sqrt{2}} (\vec{r}_1 - \vec{r}_2) \\ \vec{\xi}_2 = \sqrt{\frac{2}{3}} \left[ \frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3 \right] \end{cases} \xrightarrow{\vec{\xi}_1} \vec{\xi}_2 \qquad 2 \iff 3 \qquad \begin{cases} \vec{\xi}_1' = \frac{1}{\sqrt{2}} (\vec{r}_1 - \vec{r}_3) \\ \vec{\xi}_2' = \sqrt{\frac{2}{3}} \left[ \frac{1}{2} (\vec{r}_1 + \vec{r}_3) - \vec{r}_2 \right] \xrightarrow{\vec{\xi}_1'} \vec{\xi}_1' \end{cases}$$

#### **RIUMF**

How to solve the many-body Schrödinger equation (for bound states)?

- Second option: tie the system to a fixed point  $H_{SM}^{(A)} = \sum_{i=1}^{A} \left( \frac{p_{i}^{2}}{2m} + U_{i}(r_{i}) \right) + \sum_{i < j=1}^{A} V^{2b}(\vec{r}_{i} - \vec{r}_{j}) - \sum_{i=1}^{A} U_{i}(r_{i}) \qquad \text{offp N=4} \\ \text{mean field} \qquad \text{residual interaction} \qquad \text{offp N=1} \\ \text{occ} \\ \text{$ 
  - <u>Antisymmetrized</u> product of single-particle wfs: use these as *A*-body basis states

$$\phi_{n}^{(A)} = \frac{1}{\sqrt{A!}} \begin{vmatrix} \varphi_{i}(\vec{r}_{1}) & \varphi_{i}(\vec{r}_{2}) & \dots & \varphi_{i}(\vec{r}_{A}) \\ \varphi_{j}(\vec{r}_{1}) & \varphi_{j}(\vec{r}_{2}) & \varphi_{j}(\vec{r}_{A}) \\ \vdots & \ddots & \vdots \\ \varphi_{l}(\vec{r}_{1}) & \varphi_{l}(\vec{r}_{2}) & \dots & \varphi_{l}(\vec{r}_{A}) \end{vmatrix}$$

- Slater Determinant (SD):
- Great to implement Pauli
   exclusion principle
- Very convenient, especially in second quantization formalism

#### **RIUMF**

How to solve the many-body Schrödinger equation for bound states?

- Single-particle shell-model states are very convenient basis states for expanding the many-body wave function
- However, the introduction of the mean-field potential U destroys the invariance of the system with respect to translations
- The c.m. motion is no longer separable and remains mixed to intrinsic motion, giving rise in general to spurious effects

$$\Psi_{SM}^{(A)} = \sum_{n} \psi_{n}^{(A)} \left( \left\{ \vec{\xi}_{i} \right\} \right) g_{n}(\vec{R}_{CM})$$

- Factorization for *H*<sub>int</sub> only when **complete convergence** reached (exact solution)
- Exception: harmonic oscillator (HO) potential is exactly separable

$$\sum_{i=1}^{A} \frac{1}{2} m \Omega^2 r_i^2 = \sum_{i < j=1}^{A} \frac{m \Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 + \frac{1}{2} A m \Omega^2 R_{CM}^2$$
$$= \sum_{i=1}^{A-1} \frac{1}{2} m \Omega^2 \xi_i^2 + \frac{1}{2} A m \Omega^2 R_{CM}^2$$

## Ab initio no-core shell model (NCSM)

- An *ab initio* approach to solve the many-body Schrödinger equation for bound states (narrow resonances) starting from
  - High-precision NN+NNN interactions

(coordinate/momentum space)

 Uses large (but finite!) expansions in HO many-body basis states

$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi_{Ni}^{HO}(\vec{r}_{1}, \vec{r}_{2}, \dots, \vec{r}_{A})$$



- Choice of either Jacobi relative or Cartesian single-particle coordinates according to the efficiency for the problem at hand
  - Translational invariance of the internal wave function is preserved also when single-particle Slater Determinant (SD) basis is used with N<sub>max</sub> truncation
- Convergence to exact result using effective interactions (obtained from unitary transformations of the bare interaction)

 $N_{\text{max}}$  ... maximal allowed HO excitation above the lowest possible A-nucleon configuration Full  $N_{\text{max}}$  space: All basis states with  $N \le N_{\text{max}}$  kept

### HO multi-particle states in Jacobi coordinates

- Build many-body basis by adding one particle at the time
- Antisymmetrized two-particle states

 $\left\langle \vec{\xi}_1 \vec{\sigma}_1 \vec{\sigma}_2 \vec{\tau}_1 \vec{\tau}_2 \middle| n_2 \ell_2 s_2 j_2 t_2 \right\rangle$ 

- Start with two-body basis states (LS coupled)

$$\vec{\xi}_1 = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2)$$

$$= R_{n_{2}\ell_{2}}(\xi_{1}) \left[ Y_{\ell_{2}}(\hat{\xi}_{1}) \otimes \left[ \chi_{\frac{1}{2}}^{S}(\vec{\sigma}_{1}) \otimes \chi_{\frac{1}{2}}^{S}(\vec{\sigma}_{2}) \right]^{s_{2}} \right]^{j_{2}} \left[ \chi_{\frac{1}{2}}^{T}(\vec{\tau}_{1}) \otimes \chi_{\frac{1}{2}}^{T}(\vec{\tau}_{2}) \right]^{t_{2}}$$

Now keep only antisymmetric ones, that is only those for which

$$\hat{P}_{12} \left| n_2 \ell_2 s_2 j_2 t_2 \right\rangle = - \left| n_2 \ell_2 s_2 j_2 t_2 \right\rangle \implies (-1)^{\ell_2 + s_2 + t_2} = -1$$

- Total energy

$$\varepsilon_N = (N + \frac{3}{2})\hbar\Omega \qquad \qquad N = 2n_2 + \ell_2$$

### HO three-particle states in Jacobi coordinates

Add one more body

$$\left\langle \vec{\xi}_{2}\vec{\sigma}_{3}\vec{\tau}_{3} \middle| N_{3}L_{3}J_{3} \right\rangle = R_{N_{3}L_{3}}(\xi_{2}) \left[ Y_{L_{3}}(\hat{\xi}_{2}) \otimes \chi_{\frac{1}{2}}^{S}(\vec{\sigma}_{3}) \right]^{J_{3}} \chi_{\frac{1}{2}}^{T}(\vec{\tau}_{3})$$

Three-body basis (JJ coupled)

$$\left\langle \vec{\xi}_1 \vec{\xi}_2 \vec{\sigma}_1 \vec{\sigma}_2 \vec{\sigma}_3 \vec{\tau}_1 \vec{\tau}_2 \vec{\tau}_3 \middle| \left[ n_2 \ell_2 s_2 j_2 t_2; N_3 L_3 J_3 \right] JT \right\rangle$$

Note: antisymmetric for exchange of particle 1 and 2, but not for exchange of partcles 1 and 3 or 2 and 3

$$\left| \left[ n_2 \ell_2 s_2 j_2 t_2; N_3 L_3 J_3 \right] JT \right\rangle$$

$$= \sum_{m_2, M_3} C_{j_2 m_2, J_3 M_3}^{JM} \sum_{m_2^t, M_3^t} C_{t_2 m_2^t, T_3 M_3^t}^{TM_T} \left| n_2 \ell_2 s_2 j_2 t_2 \right\rangle \left| N_3 L_3 J_3 \right\rangle$$

- Total energy:  $\varepsilon_N = (N+3)\hbar\Omega$  with  $N = 2n_2 + \ell_2 + 2N_3 + L_3$
- To find totally antisymmetric states, diagonalize:  $\hat{A} = \frac{1}{3}(1 \hat{P}_{13} \hat{P}_{23})$ 
  - Keep only antisymmetric eigenstates, that is those with eigenvalue 1

#### **RIUMF**

### HO single-particle wave functions

 Start with single-particle HO spatial wave function, defined by radial quantum number n, orbital angular momentum l, and z-projection μ

$$\varphi_{nl\mu}(\vec{r}) = R_{nl}(r)Y_{l\mu}(\hat{r}) \qquad \varepsilon_{nl} = \left(2n + l + \frac{3}{2}\right)\hbar\Omega$$

- Now include the spin and isospin wave functions:  $\chi^{S}_{\frac{1}{2}m_{s}}(\vec{\sigma}), \ \chi^{T}_{\frac{1}{2}m_{s}}(\vec{\tau})$ 
  - Uncoupled scheme

$$\varphi_{nl\mu\frac{1}{2}m_s\frac{1}{2}m_t}(\vec{r},\vec{\sigma},\vec{\tau}) = R_{nl}(r)Y_{l\mu}(\hat{r})\chi^S_{\frac{1}{2}m_s}(\vec{\sigma})\chi^T_{\frac{1}{2}m_t}(\vec{\tau})$$

- j-coupled scheme

$$\varphi_{nljm_{j}\frac{1}{2}m_{t}}(\vec{r},\vec{\sigma},\vec{\tau}) = R_{nl}(r) \Big[ Y_{l}(\hat{r}) \otimes \chi_{\frac{1}{2}}^{S}(\vec{\sigma}) \Big]_{m_{j}}^{J} \chi_{\frac{1}{2}m_{t}}^{T}(\vec{\tau}) \\ \Big[ Y_{l}(\hat{r}) \otimes \chi_{\frac{1}{2}}^{S}(\vec{\sigma}) \Big]_{m_{j}}^{j} = \sum_{\mu m_{s}} C_{l\mu,\frac{1}{2}m_{s}}^{j m_{j}} Y_{l\mu}(\hat{r}) \chi_{\frac{1}{2}m_{s}}^{S}(\vec{\sigma})$$

#### **RIUMF**

### Multi-particle states in the Slater Determinant basis

Many-body HO Slater determinants



- Antisymmetrization is trivial
- Good M,  $M_T$  and parity quantum numbers, but not J and T
  - Huge number of basis states



### **Second Quantization**

- One of the most useful representations in many-body theory
  - $|-|0\rangle$  : the state with no particles (the vacuum)
  - $-a_i^+$  : creation operator, creates a fermion in the state *i*
  - $-a_i$  : annihilation operator, annihilates a fermion in the state i  $a_i |i\rangle = |0\rangle$ ,  $a_i |0\rangle = 0$
  - Anticommutation relations:

$$\left\{a_i^+, a_j^+\right\} = \left\{a_i, a_j\right\} = 0, \qquad \left\{a_i^+, a_j\right\} = \left\{a_i, a_j^+\right\} = \delta_i$$
Pauli principle in  $a_i^+ a_j^+ = -a_j^+ a_i^+$ 
Pauli principle in  $a_i^+ a_j^+ = -a_j^+ a_i^+$ 

– So that the Slater determinant can be written as:

$$\phi_{n}^{(A)} = \frac{1}{\sqrt{A!}} \begin{vmatrix} \varphi_{i}(\vec{r}_{1}) & \varphi_{i}(\vec{r}_{2}) & \dots & \varphi_{i}(\vec{r}_{A}) \\ \varphi_{j}(\vec{r}_{1}) & \varphi_{j}(\vec{r}_{2}) & \varphi_{j}(\vec{r}_{A}) \\ \vdots & \ddots & \vdots \\ \varphi_{l}(\vec{r}_{1}) & \varphi_{l}(\vec{r}_{2}) & \dots & \varphi_{l}(\vec{r}_{A}) \end{vmatrix} = a_{l}^{+} \dots a_{j}^{+} a_{i}^{+} |0\rangle,$$

implicitly **assumes** we have **already** chosen the form of the **single-particle states**, (*i* = 1,2,3, ... *A*) as dictated by some mean-field potential

 $a_i^+|0\rangle = |i\rangle, \quad a_i^+|i\rangle = 0$ 



### **Basis states: occupation representation**

- How are Slater determinants actually represented in a computer program?
  - We are dealing with fermions, so a single-particle state is either occupied or empty, which in computer language translates to either 1's or 0's
  - A very useful approach is a bit representation known as M-scheme
    - If the mean-field is spherically symmetric, the single-particle states will have good j,  $m_i$

- A single integer represents a complicated slater determinant
- While the many-body states will have good M, they do not have good J. States of good J must be projected and will be a combination of Slater determinants. Same for T and  $M_T$ .

# RIVMF Getting the eigenvalues and wave functions

- Setup Hamiltonian matrix  $\langle \Phi_i | H | \Phi_i \rangle$  and diagonalize
- Lanczos algorithm
  - Bring matrix to tri-diagonal form ( $\mathbf{v}_1, \mathbf{v}_2 \dots$  orthonormal, H Hermitian)

 $H\mathbf{v}_{1} = \alpha_{1}\mathbf{v}_{1} + \beta_{1}\mathbf{v}_{2}$   $H\mathbf{v}_{2} = \beta_{1}\mathbf{v}_{1} + \alpha_{2}\mathbf{v}_{2} + \beta_{2}\mathbf{v}_{3}$   $H\mathbf{v}_{3} = \beta_{2}\mathbf{v}_{2} + \alpha_{3}\mathbf{v}_{3} + \beta_{3}\mathbf{v}_{4}$   $H\mathbf{v}_{4} = \beta_{3}\mathbf{v}_{3} + \alpha_{4}\mathbf{v}_{4} + \beta_{4}\mathbf{v}_{5}$ 

- n<sup>th</sup> iteration computes 2n<sup>th</sup> moment
- Eigenvalues converge to extreme (largest and smallest) values
- $\sim 100-200$  iterations needed for 10 eigenvalues (even for 10<sup>9</sup> states)
- Typically we use M-scheme:
  - Total  $M_J$ ,  $M_T = (Z-N)/2$  and parity conserved



- Repulsive core of nuclear force introduces coupling to high momenta
  - Very large model spaces are required to reach convergent solution of the nuclear many-body problem





# From QCD to nuclei





### <sup>4</sup>He from chiral EFT interactions: g.s. energy convergence





# Why similarity renormalization?



### Similarity Renormalization Group (SRG) evolution

- Continuous transformation driving Hamiltonian to band-diagonal form
  with respect to a chosen basis
- Unitary transformation  $H_{\alpha} = U_{\alpha} H U_{\alpha}^{+}$   $U_{\alpha} U_{\alpha}^{+} = U_{\alpha}^{+} U_{\alpha} = 1$  $\frac{dH_{\alpha}}{d\alpha} = \frac{dU_{\alpha}}{d\alpha} H U_{\alpha}^{+} + U_{\alpha} H \frac{dU_{\alpha}^{+}}{d\alpha} = \frac{dU_{\alpha}}{d\alpha} U_{\alpha}^{+} U_{\alpha} H U_{\alpha}^{+} + U_{\alpha} H U_{\alpha}^{+} U_{\alpha} \frac{dU_{\alpha}^{+}}{d\alpha}$   $= \frac{dU_{\alpha}}{d\alpha} U_{\alpha}^{+} H_{\alpha} + H_{\alpha} U_{\alpha} \frac{dU_{\alpha}^{+}}{d\alpha} = [\eta_{\alpha}, H_{\alpha}]$   $\eta_{\alpha} = \frac{dU_{\alpha}}{d\alpha} U_{\alpha}^{+} = -\eta_{\alpha}^{+}$  anti-Hermitian generator  $\frac{dH_{\alpha}}{d\alpha} = [[G_{\alpha}, H_{\alpha}], H_{\alpha}]$
- Customary choice in nuclear physics  $G_{\alpha} = T$  ...kinetic energy operator
  - band-diagonal in momentum space plane-wave basis
- Initial condition  $H_{\alpha=0} = H_{\lambda=\infty} = H$   $\lambda^2 = 1/\sqrt{\alpha}$



## SRG evolution in two-nucleon space





## SRG evolution in two-nucleon space



# SRG evolution in three-nucleon space



# SRG evolution in three-nucleon space

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# SRG evolution for A-nucleon system

• Evolution induces many-nucleon terms (up to A)

$$\tilde{H}_{\alpha} = \tilde{H}_{\alpha}^{[1]} + \tilde{H}_{\alpha}^{[2]} + \tilde{H}_{\alpha}^{[3]} + \tilde{H}_{\alpha}^{[4]} + \dots + \tilde{H}_{\alpha}^{[A]}$$

- In actual calculations so far only terms up to  $ilde{H}^{[3]}_{lpha}$  kept
- Three types of SRG-evolved Hamiltonians used
  - **NN only**: Start with initial T+V<sub>NN</sub> and keep  $\tilde{H}_{\alpha}^{[1]} + \tilde{H}_{\alpha}^{[2]}$
  - NN+3N-induced: Start with initial T+V<sub>NN</sub> and keep  $\tilde{H}_{\alpha}^{[1]} + \tilde{H}_{\alpha}^{[2]} + \tilde{H}_{\alpha}^{[3]}$
  - NN+3N-full: Start with initial T+V<sub>NN</sub>+V<sub>NNN</sub> and keep  $\tilde{H}_{\alpha}^{[1]} + \tilde{H}_{\alpha}^{[2]} + \tilde{H}_{\alpha}^{[3]}$

α variation (Λ variation) provides a diagnostic tool
 to asses the contribution of omitted many-body terms,
 tests the unitarity of the SRG transformation



#### SRG evolution: <sup>3</sup>H and <sup>4</sup>He



*Ab initio* calculations (NCSM, in this case) used also for SRG evolution of NNN force (in HO basis)



# NCSM calculations of <sup>6</sup>He g.s. energy



Dependence on: Basis size  $-N_{max}$ HO frequency  $-h\Omega$ 

- Soft SRG evolved NN potential
   N<sub>max</sub> convergence OK
   Extrapolation feasible
- $E_{\text{g.s.}}$  [MeV]<sup>4</sup>He<sup>6</sup>HeNCSM  $N_{\text{max}}$ =12-28.05-28.63NCSM extrap.-28.22(1)-29.25(15)Expt.-28.30-29.27



#### <sup>6</sup>Li from chiral EFT interactions: Ground-state & excitation energies



SRG with 2- plus 3-body: Good convergence, extrapolation to infinite basis space possible



### Light nuclei with SRG evolved interactions



- Fast convergence
- Significant 3N induced interaction
- No 4N induced interaction

#### 

# Heavier p-shell nuclei with SRG evolved interactions



#### **RIUMF**

## <sup>10</sup>B states very sensitive to 3N interaction



#### **RIUMF**

# 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



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

#### 

#### Light & medium mass nuclei from first principles

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





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

Include more many nucleon correlations...





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



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

•  $\phi$ : antisymmetric cluster wave functions

- {ε}: 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

#### 

# **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







### **Binary cluster Resonating Group Method**

• Working in partial waves  $(v = \{A - a \alpha_1 I_1^{\pi_1} T_1; a \alpha_2 I_2^{\pi_2} T_2; s\ell\})$ 

$$\left|\psi^{J^{\pi}T}\right\rangle = \sum_{v} \int \frac{g_{v}^{J^{\pi}T}(r)}{r} \hat{A}_{v} \left[ \left( \left| A - a \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \left| a \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right\rangle \right)^{(sT)} Y_{\ell}(\hat{r}) \right]^{(J^{\pi}T)} \delta(\vec{r} - \vec{r}_{A-a,a}) r^{2} dr d\hat{r}$$
Target
Projectile

Now introduce partial wave expansion of delta function

$$\delta(\vec{r} - \vec{r}_{A-a,a}) = \sum_{\lambda\mu} \frac{\delta(r - r_{A-a,a})}{rr_{A-a,a}} Y^*_{\lambda\mu}(\hat{r}) Y_{\lambda\mu}(\hat{r}_{A-a,a})$$

• After integration in the solid angle one obtains:

$$\left|\psi^{J^{\pi}T}\right\rangle = \sum_{v} \int \frac{g_{v}^{J^{\pi}T}(r)}{r} \hat{A}_{v} \left[ \left( \left| A - a \; \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \right| a \; \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right) \right]^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} r^{2} dr$$

$$\left| \Phi_{vr}^{J^{\pi}T} \right\rangle \quad \text{(Jacobi) channel basis}$$



#### **Binary cluster RGM equations**

- Trial wave function:  $|\psi^{J^{\pi}T}\rangle = \sum_{v} \int \frac{g_{v}^{J^{\pi}T}(r)}{r} \hat{A}_{v} |\Phi_{vr}^{J^{\pi}T}\rangle r^{2} dr$  (A-a)
- Projecting the Schrödinger equation on the channel basis yields:

$$\sum_{v} \int \left[ H_{v'v}^{J^{\pi}T}(r',r) - E N_{v'v}^{J^{\pi}T}(r',r) \right] \frac{g_{v}^{J^{\pi}T}(r)}{r} r^{2} dr = 0$$

$$\left\langle \Phi_{v'r'}^{J^{\pi}T} \left| \hat{A}_{v'} H \hat{A}_{v} \right| \Phi_{vr}^{J^{\pi}T} \right\rangle \qquad \left\langle \Phi_{v'r'}^{J^{\pi}T} \left| \hat{A}_{v'} \hat{A}_{v} \right| \Phi_{vr}^{J^{\pi}T} \right\rangle$$
Hamiltonian kernel
Overlap (or norm) kernel

- Breakdown of approach:
  - 1. Build channel basis states from input target and projectile wave functions
  - 2. Calculate Hamiltonian and norm kernels
  - 3. Solve RGM equations: find unknown relative motion wave functions
    - Bound-state / scattering boundary conditions



### How to calculate the RGM kernels?

• Since we are using NCSM wave functions, it is convenient to introduce Jacobi channel states in the HO space

$$\Phi_{vn}^{J^{\pi}T} \rangle = \left[ \left( \left| A - a \; \alpha_1 I_1^{\pi_1} T_1 \right\rangle \right| a \; \alpha_2 I_2^{\pi_2} T_2 \rangle \right)^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} R_{n\ell}(r_{A-a,a})$$

- Note :
  - The coordinate space channel states are given by

$$\left|\Phi_{vr}^{J^{\pi}T}\right\rangle = \sum_{n} R_{n\ell}(r) \left|\Phi_{vn}^{J^{\pi}T}\right\rangle$$

• We used the closure properties of HO radial wave functions



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

- We call them Jacobi channel states because they describe only the internal motion
  - Target and projectile wave functions are both translational invariant NCSM eigenstates calculated in the Jacobi coordinate basis

### 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)  

$$V' \qquad (A-1) \times (a=1)$$
Exchange term:  
Obtained in the model space!  
(Many-body correction due to  
the exchange part of the inter-  
cluster antisymmetrizer )  

$$\delta(r-r_{A-a,a}) = \sum_{n} R_{n\ell}(r)R_{n\ell}(r_{A-a,a})$$
Target wave functions expanded in the SD basis  
the CM motion exactly removed

#### 

### Solving the NCSM/RGM equations

- Other technical details
  - Because of the norm kernel, the radial wave functions solutions of the RGM equation are not Schrödinger wave functions
  - However, the RGM equations can be orthogonalized

$$\sum_{v'} \int dr' r'^2 \left[ N^{-\frac{1}{2}} H N^{-\frac{1}{2}} \right]_{vv'} (r,r') \frac{u_{v'}(r')}{r'} = E \frac{u_v(r)}{r}$$

- Explained, e.g., in Phys. Rev. C 79, 044606 (2009)
- In the end, a set of integral-differential coupled channel equations with a non-local potential of the type:

$$\left[T_{rel}(r) + \overline{V}_{Coul}(r) - (E - \varepsilon_{\alpha_1} - \varepsilon_{\alpha_2})\right] u_{\nu}(r) + \sum_{\nu'} \int dr' r' W_{\nu\nu'}(r, r') u_{\nu'}(r') = 0$$



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



W.f. matching 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:

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



### Microscopic *R*-matrix theory

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

$$\begin{array}{c|c}
 Internal region \\
 u_c(r) = \sum_n A_{cn} f_n(r) \\
 0 \\
 a \\
 \end{array}$$

$$\begin{array}{c}
 External region \\
 u_c(r) \sim v_c^{-\frac{1}{2}} \left[ \delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right] \\
 u_c(r) \sim v_c^{-\frac{1}{2}} \left[ \delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right] \\
 \hline
 \end{array}$$

- W.f. matching 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 basis
- External region: asymptotic form for large r

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

Scattering matrix

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

Bound state

Scattering state



### To find the Scattering matrix

Lagrange basis associated with Lagrange mesh:

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

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

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

• After projection on the basis  $f_n(r)$ :

$$\sum_{c'n'} \left[ C_{cn,c'n'} - (E - E_c) \delta_{cn,c'n'} \right] A_{c'n'} = \frac{\hbar^2 k_c}{2\mu_c v_c^{1/2}} \left\langle f_n | L_c | I_c \delta_{ci} - U_{ci} O_c \right\rangle$$

$$\left\langle f_n | \hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) | f_{n'} \right\rangle \delta_{cc'} + \left\langle f_n | W_{cc'}(r,r') | f_{n'} \right\rangle$$
1 Solve for  $A$ 

- 1. Solve for  $A_{cn}$
- 2. Match internal and external solutions at channel radius, a

$$\sum_{c'} R_{cc'} \frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}} \Big[ I'_{c'}(k_{c'}a)\delta_{ci} - U_{c'i}O'_{c'}(k_{c'}a) \Big] = \frac{1}{\sqrt{\mu_c v_c}} \Big[ I_c(k_ca)\delta_{ci} - U_{ci}O_c(k_ca) \Big]$$

• In the process introduce *R*-matrix, projection of the Green's function operator on the channel-surface functions

$$R_{cc'} = \sum_{nn'} \frac{\hbar}{\sqrt{2\mu_c a}} f_n(a) \left[ C - EI \right]_{cn,c'n'}^{-1} \frac{\hbar}{\sqrt{2\mu_c a}} f_{n'}(a)$$



### To find the Scattering matrix

3. Solve equation with respect to the scattering matrix U

$$\sum_{c'} R_{cc'} \frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}} \Big[ I'_{c'}(k_{c'}a)\delta_{ci} - U_{c'i}O'_{c'}(k_{c'}a) \Big] = \frac{1}{\sqrt{\mu_{c}v_{c}}} \Big[ I_{c}(k_{c}a)\delta_{ci} - U_{ci}O_{c}(k_{c}a) \Big]$$

4. You can demonstrate that the solution is given by:

$$U = Z^{-1}Z^*, \qquad Z_{cc'} = (k_{c'}a)^{-1} \Big[ O_c(k_ca) \delta_{cc'} - k_{c'}a R_{cc'} O_{c'}'(k_{c'}a) \Big]$$

Scattering phase shifts are extracted from the scattering matrix elements

$$U = \exp(2i\delta)$$



#### n-<sup>4</sup>He scattering within the NCSM/RGM



PHYSICAL REVIEW C 88, 054622 (2013)

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

Guillaume Hupin,<sup>1,\*</sup> Joachim Langhammer,<sup>2,†</sup> Petr Navrátil,<sup>3,‡</sup> Sofia Quaglioni,<sup>1,§</sup> Angelo Calci,<sup>2,∥</sup> and Robert Roth<sup>2,¶</sup>

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	
28.37 <u>2839 28.</u>	<u>64 28.67</u>	,2⁺,0 _0⁻,0
28.31	1+,0	1-,0
27.42	2+,0	
25,95	1-,1	
25.28	07,1	
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
1		

A larger splitting between the *P*-waves obtained with the chiral NN+NNN interaction

The 3/2<sup>-</sup> resonance still off: Interaction or **CONVERGENCE?** 



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

Include more many nucleon correlations...





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

Include more many nucleon correlations...



# Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



- ...with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



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





# **Coupled NCSMC equations**



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



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

*n*-<sup>4</sup>He scattering phase-shifts for chiral NN and NN+3N potential

Total *n*-<sup>4</sup>He cross section with NN and NN+3N potentials



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

Invited Comment

Petr Navrátil<sup>1</sup>, Sofia Quaglioni<sup>2</sup>, Guillaume Hupin<sup>3,4</sup> Carolina Romero-Redondo<sup>2</sup> and Angelo Calci<sup>1</sup>

Unified *ab initio* approaches to nuclear structure and reactions

PHYSICAL REVIEW C 88, 054622 (2013)

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

Guillaume Hupin,<sup>1,\*</sup> Joachim Langhammer,<sup>2,†</sup> Petr Navrátil,<sup>3,‡</sup> Sofia Quaglioni,<sup>1,§</sup> Angelo Calci,<sup>2,∥</sup> and Robert Roth<sup>2,¶</sup>



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

*p*-<sup>4</sup>He scattering phase-shifts for NN+3N potential: Convergence

Differential *p*-<sup>4</sup>He cross section with NN+3N potentials





# Neutron-rich halo nucleus <sup>11</sup>Be

#### • Z=4, N=7

- In the shell model picture g.s. expected to be  $J^{\pi}=1/2^{-1}$ 
  - Z=6, N=7 <sup>13</sup>C and Z=8, N=7 <sup>15</sup>O have  $J^{\pi}=1/2^{-}$  g.s.
- In reality, <sup>11</sup>Be g.s. is  $J^{\pi}=1/2^{+}$  parity inversion
- Very weakly bound: E<sub>th</sub>=-0.5 MeV
  - Halo state dominated by <sup>10</sup>Be-n in the S-wave
- The 1/2<sup>-</sup> state also bound only by 180 keV
- Can we describe <sup>11</sup>Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?



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1s<sub>1/2</sub> 0p<sub>1/2</sub>

0p<sub>3/2</sub> 0s<sub>1/2</sub>



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

- New experiment at TRIUMF with the novel IRIS solid H<sub>2</sub> target
  - First re-accelerated <sup>10</sup>C beam at TRIUMF
  - ${}^{10}C(p,p)$  angular distributions measured at  $E_{CM} \sim 4.16$  MeV and 4.4 MeV



#### TRIUMF

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

- NCSMC calculations with chiral NN+3N (N<sup>3</sup>LO NN+N<sup>2</sup>LO 3NF400, NNLOsat)
  - $p^{-10}C + {}^{11}N$ 
    - <sup>10</sup>C: 0<sup>+</sup>, 2<sup>+</sup>, 2<sup>+</sup> NCSM eigenstates



• <sup>11</sup>N:  $\geq 4 \pi = -1$  and  $\geq 3 \pi = +1$  NCSM eigenstates


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



**RIUMF** 

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al with IRIS collaboration, in preparation

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



TRIUMF

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



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#### 

### Structure of <sup>11</sup>Be from chiral NN+3N forces

- NCSMC calculations including chiral 3N (N<sup>3</sup>LO NN+N<sup>2</sup>LO 3NF400)
  - n-<sup>10</sup>Be + <sup>11</sup>Be

🤹 + 🤹 👘

- <sup>10</sup>Be: 0<sup>+</sup>, 2<sup>+</sup>, 2<sup>+</sup> NCSM eigenstates
- <sup>11</sup>Be:  $\geq 6 \pi = -1$  and  $\geq 3 \pi = +1$  NCSM eigenstates



# <sup>TRIUMF</sup> <sup>11</sup>Be within NCSMC: Discrimination among chiral nuclear forces



A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al., in preparation

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# <sup>TRIUMF</sup> Discrimination among chiral nuclear forces



A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al., in preparation

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# <sup>TRIUMF</sup> <sup>11</sup>Be within NCSMC: Discrimination among chiral nuclear forces



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



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



#### 

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





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 nuclear reactions important for astrophysics

NIC-XIV School 2016 Niigata University (Ikarashi Campus) Niigata, Japan June 13-17, 2016

#### Petr Navratil | TRIUMF





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### From QCD to nuclei



### 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



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \stackrel{(A)}{\textcircled{5}}, \lambda \right\rangle$$
  
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
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  - NCSM with Resonating Group Method (NCSM/RGM)
    - cluster expansion
    - proper asymptotic behavior
    - long-range correlations





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# No-core shell model with continuum

 $\sum_{v} \int d\vec{r} \gamma_{v}(\vec{r}) \hat{A}_{v}$ 

No-core shell model (NCSM)

RIUMF

- 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

 $\Psi^{(A)} = \sum$ 

proper asymptotic behavior

**NCSM** eigenstates

Unknowns

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/RGM channel states





### **NCSMC** wave function

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

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

Asymptotic behavior  $r \rightarrow \infty$ :

$$\overline{\chi}_{v}(r) \sim C_{v}W(k_{v}r) \qquad \overline{\chi}_{v}(r) \sim v_{v}^{-\frac{1}{2}} \Big[ \delta_{vi}I_{v}(k_{v}r) - U_{vi}O_{v}(k_{v}r) \Big]$$

Bound state

Scattering state

Scattering matrix



### E1 transitions in NCSMC

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

$$\vec{E1} = e \sum_{i=1}^{A-a} \frac{1 + \tau_i^{(3)}}{2} \left( \vec{r_i} - \vec{R}_{\text{c.m.}}^{(A-a)} \right) + e \sum_{j=A-a+1}^{A} \frac{1 + \tau_j^{(3)}}{2} \left( \vec{r_i} - \vec{R}_{\text{c.m.}}^{(a)} \right) + e \frac{Z_{(A-a)}a - Z_{(a)}(A-a)}{A} \vec{r}_{A-a,a}.$$

$$\begin{aligned} \mathcal{B}_{fi}^{E1} &= \sum_{\lambda\lambda'} c_{\lambda'}^{*f} \langle A\lambda' J_{f}^{\pi_{f}} T_{f} || \mathcal{M}_{1}^{E} || A\lambda J_{i}^{\pi_{i}} T_{i} \rangle c_{\lambda}^{i} \\ &+ \sum_{\lambda'\nu} \int dr r^{2} c_{\lambda'}^{*f} \langle A\lambda' J_{f}^{\pi_{f}} T_{f} || \mathcal{M}_{1}^{E} \hat{\mathcal{A}}_{\nu} || \Phi_{\nu r}^{i} \rangle \frac{\gamma_{\nu}^{i}(r)}{r} \\ &+ \sum_{\lambda\nu'} \int dr' r'^{2} \frac{\gamma_{\nu'}^{*f}(r')}{r'} \langle \Phi_{\nu'r'}^{f} || \hat{\mathcal{A}}_{\nu'} \mathcal{M}_{1}^{E} || A\lambda J_{i}^{\pi_{i}} T_{i} \rangle c_{\lambda}^{i} \\ &+ \sum_{\nu\nu'} \int dr' r'^{2} \int dr r^{2} \frac{\gamma_{\nu'}^{*f}(r')}{r'} \langle \Phi_{\nu'r'}^{f} || \hat{\mathcal{A}}_{\nu'} \mathcal{M}_{1}^{E} \hat{\mathcal{A}}_{\nu} || \Phi_{\nu r}^{i} \rangle \frac{\gamma_{\nu}^{i}(r)}{r} \end{aligned}$$

$$\mathcal{M}_{1\mu}^{E} = e \sum_{j=1}^{A} \frac{1 + \tau_{j}^{(3)}}{2} \left| \vec{r_{j}} - \vec{R}_{\text{c.m.}}^{(A)} \right| Y_{1\mu}(r_{j} - \vec{R}_{\text{c.m.}}^{(A)})$$

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## Photo-disassociation of <sup>11</sup>Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$ ) [ $e^2 \text{ fm}^2$ ]	5x10 <sup>-6</sup>	0.118	0.102(2)



### NCSMC phenomenology





## Photo-disassociation of <sup>11</sup>Be



### Next: p+<sup>11</sup>C scattering and <sup>11</sup>C(p,γ)<sup>12</sup>N capture

- Measurement of <sup>11</sup>C(p,p) resonance scattering planned at TRIUMF
  - TUDA facility
  - <sup>11</sup>C beam of sufficient intensity produced
- NCSMC calculations of <sup>11</sup>C(p,p) with chiral NN+3N under way
- Obtained wave functions will be used to calculate  ${}^{11}C(p,\gamma){}^{12}N$  capture relevant for astrophysics

### Next: p+<sup>11</sup>C scattering and <sup>11</sup>C(p,γ)<sup>12</sup>N capture

<sup>11</sup>C(p,γ)<sup>12</sup>N capture relevant in hot *p*-*p* chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture <sup>4</sup>He(αα,γ)<sup>12</sup>C



 ${}^{3}He(\alpha,\gamma)^{7}Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(p,\gamma)^{13}O(\beta^{+},\nu)^{13}N(p,\gamma)^{14}O$   ${}^{3}He(\alpha,\gamma)^{7}Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(\beta^{+},\nu)^{12}C(p,\gamma)^{13}N(p,\gamma)^{14}O$   ${}^{11}C(\beta^{+},\nu)^{11}B(p,\alpha)^{8}Be({}^{4}He,{}^{4}He)$ 

### Next: p+<sup>11</sup>C scattering and <sup>11</sup>C(p,γ)<sup>12</sup>N capture

NCSMC calculations of <sup>11</sup>C(p,p) with chiral NN+3N under way





### 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







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





NCSM/RGM p-<sup>7</sup>Be calculation

TRIUMF

<sup>7</sup>Be

- 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 scattering



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



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

 $7.21, \frac{5}{2}$ 

4.57

- 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>)





### **Big Bang nucleosythesis**



#### 

### **Deuterium-Tritium fusion: a future energy source**

- The  $d^{+3}H \rightarrow n^{+4}He$  reaction
  - The most promising for the production of fusion energy in the near future
  - Will be used to achieve inertial-confinement (laserinduced) fusion at NIF, and magnetic-confinement fusion at ITER
  - With its mirror reaction, <sup>3</sup>He(*d*,*p*)<sup>4</sup>He, important for Big Bang nucleosynthesis





Resonance at  $E_{cm}$  =48 keV ( $E_d$ =105 keV) in the J=3/2<sup>+</sup> channel Cross section at the peak: 4.88 b

17.64 MeV energy released: 14.1 MeV neutron and 3.5 MeV alpha



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

$$\int dr r^{2} \left( \left\langle \begin{array}{c} \mathbf{r}^{\prime} \mathbf{a}_{\alpha} \middle| \hat{A}_{1}(H-E) \hat{A}_{1} \middle| \begin{array}{c} \mathbf{a}_{\alpha} \middle| \mathbf{r}_{\alpha} \middle| \mathbf{a}_{\alpha} \middle| \mathbf{a}_{\alpha} \middle| \hat{A}_{1}(H-E) \hat{A}_{2} \middle|_{\mathbf{3}\mathbf{H}} \mathbf{a}_{\alpha} \right) \left\langle \begin{array}{c} \underline{g_{1}(r)} \\ \mathbf{r} \\ \mathbf{a}_{\alpha} \\ \mathbf{a}_{\alpha$$

### 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



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



## **Big Bang nucleosythesis**


## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

Continuum and three-nucleon force effects on d+<sup>4</sup>He and <sup>6</sup>Li



Unified Description of <sup>6</sup>Li Structure and Deuterium-<sup>4</sup>He Dynamics with Chiral Two- and Three-Nucleon Forces



Guillaume Hupin,1,\* Sofia Quaglioni,1,† and Petr Navrátil2,‡

## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

Continuum and three-nucleon force effects on d+<sup>4</sup>He and <sup>6</sup>Li



## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

• Continuum and three-nucleon force effects on d+<sup>4</sup>He and <sup>6</sup>Li



Guillaume Hupin,1,\* Sofia Quaglioni,1,† and Petr Navrátil2,‡

## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

Continuum and three-nucleon force effects on d+<sup>4</sup>He and <sup>6</sup>Li



## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

Continuum and three-nucleon force effects on d+<sup>4</sup>He and <sup>6</sup>Li



## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

 $C_{2}/C_{0}$ 

• S- and D-wave asymptotic normalization constants

week ending

29 MAY 2014



· ]		NCSMC	Experiment	
	$C_0 \; [{\rm fm}^{-1/2}]$	2.695	2.91(9) [ <b>39</b> ] $2.93(15)$	)
*	$C_2  [\mathrm{fm}^{-1/2}]$	-0.074	-0.077(18) [39]	

-0.027

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[39]

[38]

[41]

0.0003(9)

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Unified Description of <sup>6</sup>Li Structure and Deuterium-<sup>4</sup>He Dynamics with Chiral Two- and Three-Nucleon Forces

PRL 114, 212502 (2015)

Guillaume Hupin,1,\* Sofia Quaglioni,1,† and Petr Navrátil2,‡

PHYSICAL REVIEW LETTERS

## Unified description of <sup>6</sup>Li structure and d+<sup>4</sup>He dynamics

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



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







## Three nuclei in initial or final state

- Many astrophysics relevant reactions involve three nuclei in the initial or final state
  - <sup>3</sup>He(<sup>3</sup>He,2p)<sup>4</sup>He major pp chain reaction
  - Three-particle fusion may bridge the A=5, 8 gaps
  - Building blocks typically α, p, n
  - triple-alpha capture  ${}^{4}\text{He}(\alpha\alpha,\gamma){}^{12}\text{C}$
  - ${}^{4}\text{He}(\alpha n, \gamma){}^{9}\text{Be} \text{initiation of the r-process}$
  - ${}^{4}$ He(nn, $\gamma$ ) ${}^{6}$ He followed by  ${}^{6}$ He( $\alpha$ ,n) ${}^{9}$ Be could be an alternative to  ${}^{4}$ He( $\alpha$ n, $\gamma$ ) ${}^{9}$ Be in neutron rich environments
- Experimental investigation challenging



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

Include more many nucleon correlations...





## **NCSMC** for three-body clusters



$$\Psi^{(A)} = \sum_{\lambda} C_{\lambda} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \gamma_{\nu}(\vec{x}, \vec{y}) \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \hat{A}_{\nu} | \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \hat{A}_{\nu} | \langle \lambda \rangle + \sum_{\nu} \int d\vec{x} \, d\vec{y} \, \hat{A}_{\nu} | \hat{A}_$$



## **NCSMC** for three-body clusters

• Two-neutron halo nuclei



• Transfer reactions with three-body continuum final states



## NCSMC for three-body clusters



Solves:

$$\sum_{a_2a_3vK} \int d\rho \ \rho^5 \Big[ H_{a'v',av}^{K',K}(\rho',\rho) - E \ N_{a'v',av}^{K',K}(\rho',\rho) \Big] \ \rho^{-5/2} \chi_{vK}^{(A-a_{23},a_2,a_3)}(\rho) = 0$$

- Where the hyperspherical coordinates are given by:

$$\rho = \sqrt{x^2 + y^2}, \quad \alpha = \arctan\left(\frac{y}{x}\right) \qquad \left(x = \rho \cos \alpha, \quad y = \rho \sin \alpha\right)$$

# NCSMC for three-body clusters: <sup>6</sup>He ~ <sup>4</sup>He+n+n

TRIUMF

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066



# NCSMC for three-body clusters: <sup>6</sup>He ~ <sup>4</sup>He+n+n

TRIUMF

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066



\*D. Sääf, C. Forssén, PRC **89** 011303 (2014)

# NCSMC for three-body clusters: <sup>6</sup>He ~ <sup>4</sup>He+n+n

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066



The probability distribution of the <sup>6</sup>He ground state presents two peaks corresponding to the di-neutron and cigar configurations

## NCSMC for three-body clusters: <sup>6</sup>He ~ <sup>4</sup>He+n+n

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066



simultaneously consistent with experiment

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#### **R**TRIUMF

## NCSMC for three-body clusters: <sup>6</sup>He ~ <sup>4</sup>He+n+n





# Solar *p-p* chain





# **Big Bang nucleosythesis**





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







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



J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB 757, 430 (2016)

NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.15 fm<sup>-1</sup>)

<sup>3</sup>He, <sup>3</sup>H, <sup>4</sup>He ground state,  $8(\pi$ -) +  $6(\pi$ +) eigenstates of <sup>7</sup>Be and <sup>7</sup>Li

Preliminary:  $N_{max}$ =12, h $\Omega$ =20 MeV

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



TRIUMF

J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB 757, 430 (2016)

NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.15 fm<sup>-1</sup>)

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Preliminary:  $N_{max}$ =12, h $\Omega$ =20 MeV





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



J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB 757, 430 (2016)

NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.15 fm<sup>-1</sup>)

<sup>3</sup>He, <sup>3</sup>H, <sup>4</sup>He ground state,  $8(\pi$ -) +  $6(\pi$ +) eigenstates of <sup>7</sup>Be and <sup>7</sup>Li

Preliminary:  $N_{max}$ =12, h $\Omega$ =20 MeV

Theoretical calculations suggest that the most recent and precise 7Be and 7Li data are inconsistent





# <sup>3</sup>He-<sup>4</sup>He S-wave phase shifts



J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB 757, 430 (2016)

NCSMC calculations with chiral SRG-N<sup>3</sup>LO *NN* potential ( $\lambda$ =2.15 fm<sup>-1</sup>)

<sup>3</sup>He, <sup>3</sup>H, <sup>4</sup>He ground state,  $8(\pi$ -) +  $6(\pi$ +) eigenstates of <sup>7</sup>Be and <sup>7</sup>Li

Preliminary:  $N_{\text{max}}$ =12, h $\Omega$ =20 MeV

NCSMC calculations with chiral NN+3N forces in preparation



# From QCD to nuclei





### Nuclear Lattice Effective Field Theory Calculations E. Epelbaum, H. Krebs, T. Lahde, D. Lee, U.-G. Meissner

Discretized version of chiral EFT for nuclear dynamics

 $\left[\left(\sum_{i=1}^{A}\frac{-\vec{\nabla}_{i}^{2}}{2m_{N}}+\mathcal{O}(m_{N}^{-3})\right)+\underbrace{V_{2N}+V_{3N}+V_{4N}+\dots}\right]|\Psi\rangle=E|\Psi\rangle$ 





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Ground states of alpha nuclei from <sup>4</sup>He to <sup>28</sup>Si

Timo A. Lähde <sup>a,\*</sup>, Evgeny Epelbaum<sup>b</sup>, Hermann Krebs<sup>b</sup>, Dean Lee<sup>c</sup>, Ulf-G. Meißner<sup>a,d,e</sup>,

Gautam Rupak

### Nuclear Lattice Effective Field Theory Calculations E. Epelbaum, H. Krebs, T. Lahde, D. Lee, U.-G. Meissner





# **Conclusions and Outlook**

*Ab initio* calculations of nuclear structure and reactions with predictive power becoming feasible beyond the latest nuclei.

*Ab initio* structure calculations can even reach (selected) medium & medium-heavy mass nuclei

These calculations make the connection between the low-energy QCD, many-body systems, and **nuclear astrophysics**.

Thank you!



# **NCSMC and NCSM/RGM collaborators**

Sofia Quaglioni (LLNL)

Jeremy Dohet-Eraly, Angelo Calci (TRIUMF)

Guillaume Hupin (CEA/DAM)

Carolina Romero-Redondo (LLNL)

Francesco Raimondi (Surrey)

Wataru Horiuchi (Hokkaido)

Robert Roth (TU Darmstadt)



## Advertisement



28th Indian-Summer School of Physics

#### AB INITIO METHODS IN NUCLEAR PHYSICS

August 29 – September 2, 2016, Prague, Czech Republic

TOPICS:

Coupled Cluster Method No Core Shell Model and Its Resonating Group Method Extension Fermionic Molecular Dynamics Approach Self-consistent Green's Function Approach

LECTURERS: M. HJORTH-JENSEN (Univ. Oslo, Michigan State Univ.) P. MARIS (Iowa State Univ.) P. NAVRATIL (TRIUMF) T. NEFF (GSI) V. SOMA (CEA Saclay)

ORGANIZERS: F. Knapp (chairperson), P. Vesely (chairperson), J. Dolejsi, T. Dytrych, J. Hrtankova, M. Schaefer, D. Skoupil

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