Weakly bound and unbound light nuclei from ab initio theory

INT Program INT 17-1a
Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart
March 16, 2017

Collaborators:
Sofia Quaglioni, Carolina Romero-Redondo (LLNL)
Guillaume Hupin (CEA/DAM)
Jeremy Dohet-Eraly, Angelo Calci, Peter Gysbers (TRIUMF)
Robert Roth (TU Darmstadt)
• New high precision chiral interactions
• No-Core Shell Model with Continuum (NCSMC) approach
• $^N{^4\text{He}}$ scattering
• $^{^{11}\text{Be}}$ parity inversion in low-lying states, photo-dissociation
• $^{^{11}\text{N}}$ and $^{^{10}\text{C}}(p,p)$ scattering
• $^{^{12}\text{N}}$ and $^{^{11}\text{C}}(p,p)$ scattering and $^{^{11}\text{C}}(p,\gamma)^{^{12}\text{N}}$
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

- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD $(m_u = m_d = 0)$, spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order $(Q/\Lambda_\chi)$
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

\[ \Lambda_\chi \approx 1 \text{ GeV} \]
Chiral symmetry breaking scale

N^2LO_{sat} NN+3N

N^4LO500 NN  N^3LO NN+N^2LO 3N
(NN+3N400, NN+3N500)
From QCD to nuclei

Low-energy QCD

NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials

Many-Body methods

NCSM, NCSM/RGM, NCSMC, CCM, SCGF, GFMC, HH, Nuclear Lattice EFT...

Nuclear structure and reactions

\[ H |\Psi\rangle = E |\Psi\rangle \]
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

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} |^{(A)} \rho \rho, \lambda \rangle \]
From QCD to nuclei

Low-energy QCD

NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials

Unitary/similarity transformations

Identity or SRG or OLS or UCOM ... Softens NN, induces 3N

Many-Body methods

NCSM, NCSM/RGM, CCM, SCGF, GFMC, HH, Nuclear Lattice EFT...

H |Ψ⟩ = E |Ψ⟩

Nuclear structure and reactions
Chiral EFT interactions up to N$^4$LO

- Systematic from LO to N$^4$LO
- High precision – $\chi^2$/datum = 1.15
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

Original EM 2003 N$^3$LO NN $E_{gs} = -25.39$ MeV

4He

LO-N$^4$LO500 NN

$E_{gs}$ [MeV] vs $N_{max}$

$E_{gs} = -26.61(2)$ MeV

4He

N$^4$LO500 NN

$E_{gs}$ [MeV] vs $N_{max}$
Chiral EFT interactions up to N$^4$LO

- Systematic from LO to N$^4$LO
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![Graph showing ground-state energies for 4He](image1)

Original EM 2003 N$^3$LO NN $E_{gs}=-25.39$ MeV

![Graph showing ground-state energies for 4He](image2)

Ground-State Energies in s-Shell

- N$^4$LO(500) NN seems to be softer!

Compared to standard N$^3$LO:

- N$^4$LO(500) NN seems to be softer!
Chiral EFT interactions up to N^4LO

- Systematic from LO to N^4LO
- High precision – \( \chi^2/\text{datum} = 1.15 \)
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

Determiniation of the \( c_D \) parameter relevant to chiral 3N force

\( c_D = 0.45 \) (3N repulsive)

Original EM 2003 N^3LO NN \( c_D = -0.2 \) (3N attractive)
Chiral EFT interactions up to $N^4$LO

- Systematic from LO to $N^4$LO
- High precision – $\chi^2$/datum = 1.15
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

Original EM 2003 $N^3$LO NN $E_{gs} = -28.0(5)\text{ MeV}$

$^6\text{Li}$ $N^4$LO500 NN

$E_{gs} = -29.5(2)\text{ MeV}$

$^{10}\text{B}$ $N^4$LO500 NN

$E_3^+ = -57.0(5)\text{ MeV}$

$E_1^+ = -58.0(5)\text{ MeV}$
Chiral EFT interactions up to $N^4$LO

- Systematic from LO to $N^4$LO
- High precision – $\chi^2$/datum = 1.15
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

Original EM 2003 $N^3$LO NN $E_{gs} = -77.2(3)$ MeV

$^{12}$C

$N^4$LO500 NN

$E_{gs} = -84.8(8)$ MeV

Original EM 2003 $N^3$LO NN $E_{gs} = -119.5(5)$ MeV

$^{16}$O

$N^4$LO500 NN

$E_{gs} = -131(1)$ MeV
Unified approach to bound & continuum states; to nuclear structure & reactions

- \textbf{\textit{Ab initio} no-core shell model}
  - Short- and medium range correlations
  - Bound-states, narrow resonances

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

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

Unknowns

NCSM

NCSM/RGM

Harmonic oscillator basis
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

- Most efficient: **ab initio** no-core shell model with continuum

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

Unknowns

NCSM eigenstates

NCSM/RGM channel states

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic $R$-matrix on Lagrange mesh
Predictive theory for elastic scattering and recoil of protons from $^4\text{He}$

Guillaume Hupin,1,4 Sofia Quaglioni,1,4 and Petr Navrátil2,1

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

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

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

NCSM/RGM
n-\(^4\)He scattering within NCSMC

\(n-\^4\)He scattering phase-shifts for chiral NN and NN+3N500 potential

Total n-\(^4\)He cross section with NN and NN+3N potentials

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

**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,\(^4\), Angelo Calci,\(^5\), and Robert Roth\(^6\)

*Invited Comment*

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil, Sofia Quaglioni, Guillaume Hupin, Carolina Romero-Rebollo, and Angelo Calci

*PHYSICAL REVIEW C 88, 054622 (2013)*
$n^{-4}\text{He}$ scattering within NCSMC

$n^{-4}\text{He}$ scattering phase-shifts for chiral NN and NN+3N500 potential

$n^{-4}\text{He}$ scattering phase-shifts for chiral $N^2\text{LO}_{\text{sat}}$ and NN+3N400 potentials

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

**Invited Comment**

*Unified ab initio approaches to nuclear structure and reactions*

Petr Navrátil, Sofia Quaglioni, Guillaume Hupin, Carolina Romero-Redondo and Angelo Calci

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

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

Guillaume Hupin, Joachim Langhammer, Petr Navrátil, Sofia Quaglioni, Angelo Calci and Robert Roth
$n^{-4}$He scattering within NCSMC

$n^{-4}$He scattering phase-shifts for chiral NN and NN+3N500 potential

$n^{-4}$He scattering phase-shifts for chiral N$^4$LO500 NN potential

3N force enhances $1/2^- \leftrightarrow 3/2^-$ splitting: Essential at low energies!
Neutron-rich halo nucleus $^{11}$Be

- $Z=4, \ N=7$
  - In the shell model picture g.s. expected to be $J^{\pi}=1/2^-$
    - $Z=6, \ N=7$ $^{13}$C and $Z=8, \ N=7$ $^{15}$O have $J^{\pi}=1/2^-$ g.s.
  - In reality, $^{11}$Be g.s. is $J^{\pi}=1/2^+$ - parity inversion
  - Very weakly bound: $E_{th}=-0.5$ MeV
    - Halo state – dominated by $^{10}$Be-n in the S-wave
    - The 1/2$^-$ state also bound – only by 180 keV

- Can we describe $^{11}$Be in $ab\ initio$ calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?
$^{10}\text{C}(p,p)$ @ IRIS with solid H$_2$ target

- New experiment at TRIUMF with the novel IRIS solid H$_2$ target
  - First re-accelerated $^{10}\text{C}$ beam at TRIUMF
  - $^{10}\text{C}(p,p)$ angular distributions measured at $E_{\text{CM}} \sim 4.16$ MeV and 4.4 MeV

IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev et al.
p\textsuperscript{10}\textsuperscript{C} scattering: structure of \textsuperscript{11}\textsuperscript{N} resonances

- NCSMC calculations with chiral NN+3N (N\textsuperscript{3}LO NN+N\textsuperscript{2}LO 3NF400, NNLOsat)
  - p\textsuperscript{-10}\textsuperscript{C} + \textsuperscript{11}\textsuperscript{N}
  - \textsuperscript{10}\textsuperscript{C}: 0\textsuperscript{+}, 2\textsuperscript{+}, 2\textsuperscript{+} NCSM eigenstates
  - \textsuperscript{11}\textsuperscript{N}: ≥4 π = -1 and ≥3 π = +1 NCSM eigenstates

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al with IRIS collaboration, submitted
p\(^+\)\(^{10}\)C scattering: structure of \(^{11}\)N resonances

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al with IRIS collaboration, submitted
\textbf{p}^{+10}\text{C} \text{ scattering: structure of }^{11}\text{N resonances}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figures}
\end{figure}

**IRIS collaboration:**
A. Kumar, R. Kanungo, A. Sanetullaev \textit{et al.}

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth \textit{et al} with IRIS collaboration, submitted
Structure of $^{11}\text{Be}$ from chiral NN+3N forces

- NCSMC calculations **including chiral 3N** ($N^3\text{LO NN}+N^2\text{LO 3NF}400$)
  - $n-^{10}\text{Be} + ^{11}\text{Be}$
  - $^{10}\text{Be}$: $0^+, 2^+, 2^+$ NCSM eigenstates
  - $^{11}\text{Be}$: $\geq 6\pi = -1$ and $\geq 3\pi = +1$ NCSM eigenstates

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![Diagram of energy levels and continuum effects](image-url)
$^{11}$Be within NCSMC: Discrimination among chiral nuclear forces

The graphs illustrate the comparison between experimental (exp.) and NCSM (NN) results for $n^{10}$Be states. The $n^{10}$Be($2^+$) and $n^{10}$Be($0^+$) levels are shown with their corresponding thresholds ($E_{\text{thr.}}$) in MeV. The NCSM results show much better convergence compared to the experimental data. NCSM tries to capture continuum effects via large $N_{\text{max}}$. A significant difference is observed for the $1/2^+$ state right at threshold.

References:
$^{11}\text{Be}$ within NCSMC: Discrimination among chiral nuclear forces

Discrimination among chiral nuclear forces

- **11Be within NCSMC:**

- **Parity inversion**

<table>
<thead>
<tr>
<th>Energy [MeV]</th>
<th>exp.</th>
<th>NN</th>
<th>NN+3N(400)</th>
<th>N²LO_{sat}</th>
<th>exp.</th>
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<tbody>
<tr>
<td>1/2^-</td>
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<td>1/2^+</td>
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<td>9/2^-</td>
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<td>9/2^+</td>
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</tbody>
</table>

- **Exp.:** $E = 0.0625 \text{ fm}^4$, $\hbar \Omega = 20 \text{ MeV}$, $E_{\text{max}} = 14$

- **Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)**

Discrimination among chiral nuclear forces

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

IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev et al.
\[ \Psi^{(A)} = \sum_{\lambda} c_\lambda \langle (A) c_\lambda, \lambda \rangle + \sum_{\nu} \int d\vec{r} \; \gamma_\nu(\vec{r}) \; \hat{A}_\nu \left( (A-a), \nu \right) \]

\[ |\Psi^{J^T}_A\rangle = \sum_\lambda |A\lambda J^T\rangle \left[ \sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda\lambda'} \tilde{c}_\lambda + \sum_{\nu'} \int dr' r'^2 (N^{-\frac{1}{2}})^{\lambda^\prime \nu^\prime^\prime} \frac{\tilde{\chi}_{\nu^\prime^\prime}(r^\prime)}{r^\prime} \right] \]

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

Asymptotic behavior \( r \to \infty \):

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

Bound state \quad Scattering state \quad \text{Scattering matrix}
E1 transitions in NCSMC

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} \langle (A), \lambda \rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}) \; \hat{A}_{\nu} \mid (A-a), \nu \rangle \]

\[ \vec{E}_1 = e \sum_{i=1}^{A-a} \left[ 1 + \frac{\tau_i^{(3)}}{2} \right] \left( \vec{r}_i - \vec{R}_{c.m.}(A-a) \right) \]

\[ + e \sum_{j=A-a+1}^{A} \left[ 1 + \frac{\tau_j^{(3)}}{2} \right] \left( \vec{r}_i - \vec{R}_{c.m.}(a) \right) \]

\[ + e \frac{Z_{(A-a)} a - Z_{(a)} (A-a)}{A} \frac{r_{A-a,a}}{A} \]

\[ M_{fi}^{E1} = \sum_{\lambda' \lambda} \langle A A' J_f \pi_f T_f || \vec{E}_1 || A \lambda J_i \pi_i T_i \rangle c_{\lambda} \]

\[ + \sum_{\lambda' \nu} \int dr r^2 c_{\lambda'}^{*} \langle A A' J_f \pi_f T_f || \vec{E}_1 \hat{A}_{\nu} || \Phi_{\nu r}^i \rangle \frac{\gamma_{\nu}^i(r)}{r} \]

\[ + \sum_{\lambda' \nu'} \int dr' r'^2 \frac{\gamma_{\nu'}^* (r')} {r'} \langle \Phi_{\nu r'}^f || \hat{A}_{\nu'} \vec{E}_1 \hat{A}_{\nu} || \Phi_{\nu r}^i \rangle \frac{\gamma_{\nu}^i(r)}{r} \]
Photo-disassociation of $^{11}\text{Be}$

<table>
<thead>
<tr>
<th>Bound to bound</th>
<th>NCSM</th>
<th>NCSMC-phenom</th>
<th>Expt.</th>
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<tr>
<td>$B(E1; 1/2^+ \rightarrow 1/2^-)$ [e$^2$ fm$^2$]</td>
<td>0.0005</td>
<td>0.117</td>
<td>0.102(2)</td>
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</table>
$E_{\lambda}^{NCSM}$ phenomenology

Cluster excitation energies treated as adjustable parameters

Cluster excitation energies set to experimental values

$E_{\lambda}^{NCSM}$ energies treated as adjustable parameters
Halo structure

Can \textit{Ab Initio} Theory Explain the Phenomenon of Parity Inversion in $^{11}$Be?

Angelo Calci, Petr Navrátil, Robert Roth, Jérémy Dohet-Eraly, Sofia Quaglioni, and Guillaume Hupin

PRL 117, 242501 (2016)

PHYSICAL REVIEW LETTERS

week ending 9 DECEMBER 2016

Boundary to bound

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Photo-disassociation of $^{11}\text{Be}$

### Bound to continuum

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Next: p+^{11}C scattering and ^{11}C(p,\gamma)^{12}N capture

- Measurement of ^{11}C(p,p) resonance scattering planned at TRIUMF
  - TUDA facility
  - ^{11}C beam of sufficient intensity produced

- NCSMC calculations of ^{11}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+^{11}C scattering and ^{11}C(p,\gamma)^{12}N capture

- ^{11}C(p,\gamma)^{12}N capture relevant in hot p-p chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture 

^4He(\alpha\alpha,\gamma)^{12}C

\[
\begin{align*}
\text{p-p chain} & \\
^{3}\text{He}(^{3}\text{He},2p)^{4}\text{He} & | & 86\% \\
^{3}\text{He}(\alpha,\gamma)^{7}\text{Be} & | & 14\% \\
\text{Be}(e^{-},\nu)^{7}\text{Li} & | & 14\% \\
^{7}\text{Li}(p,\alpha)^{4}\text{He} & | & 0.02\% \\
^{3}\text{He}(\alpha,\gamma)^{7}\text{Be} & | & 14\% \\
^{7}\text{Be}(p,\gamma)^{8}\text{B} & | & 0.02\% \\
^{7}\text{Li}(p,\alpha)^{4}\text{He} & | & 14\% \\
^{8}\text{Be}(e^{-},\nu)^{8}\text{Be} & | & 0.02\% \\
^{8}\text{Be}(\alpha)^{4}\text{He} & | & 0.02\% \\
^{3}\text{He}(\alpha,\gamma)^{7}\text{Be}(\alpha,\gamma)^{11}\text{C}(p,\gamma)^{12}N(p,\gamma)^{13}\text{O}(\beta^{+},\nu)^{13}N(p,\gamma)^{14}\text{O} \\
^{3}\text{He}(\alpha,\gamma)^{7}\text{Be}(\alpha,\gamma)^{11}\text{C}(p,\gamma)^{12}N(\beta^{+},\nu)^{12}\text{C}(p,\gamma)^{13}N(p,\gamma)^{14}\text{O} \\
^{11}\text{C}(\beta^{+},\nu)^{11}\text{B}(p,\alpha)^{8}\text{Be}(^{4}\text{He},^{4}\text{He})
\end{align*}
\]
Next: $p + ^{11}C$ scattering and $^{11}C(p,\gamma)^{12}N$ capture

- NCSMC calculations of $^{11}C(p,p)$ with chiral NN+3N under way
Next: $p^{+}{^{11}C}$ scattering and $^{11}C(p,\gamma)^{12}N$ capture

- NCSMC calculations of $^{11}C(p,p)$ with chiral NN+3N under way

NCSMC calculations to be validated by measured cross sections and applied to calculate the $^{11}C(p,\gamma)^{12}N$ capture
Next: $p + ^{11}C$ scattering and $^{11}C(p,\gamma)^{12}N$ capture

- NCSMC calculations of $^{11}C(p, p)$ with chiral NN+3N under way

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Figure 3: Elastic cross sections around the $^2_1\alpha$, $^1_1\alpha$ resonances (energy scan around the theoretically predicted resonance position) calculated using the NCSMC and the phenomenological calculation. Figures from Ref. [7].

The second $^{11}C + p$ experiment [17] was realized a few years later in form of a measurement campaign at two different facilities, namely at the Berkeley Experiments with Accelerated Radioactive Species (BEARS) coupled cyclotron system [18] and the Texas A&M University (TAMU) with the magnetic separator MARS [19]. This was done in order to cover the energy range from $E_x = 2.2$ MeV up to $E_x = 11.0$ MeV. The use of a gaseous target in comparison to a solid target opened up the opportunity to analyze the contribution of inelastic scattering in the solid target. In total 16 levels in $^{12}N$ were identified and the analysis of the excitation functions was performed based on an R-matrix framework. However, the choice of input parameters relied strongly on the properties of known levels in the mirror nucleus $^{12}B$, assuming a shift of 200 keV of the energy levels towards lower energies and allowing 500 keV variation. Further, the resonance widths for the levels in $^{12}B$ were utilized as initial parameters for the determination of all widths in the level structure of $^{12}N$. The data for resonance widths within the excitation energy of $E_x = 3.37$ MeV to 5.49 MeV in $^{12}B$ were based on the neutron decay to the ground state of $^{11}B$. Thus, the widths in $^{12}B$ had to be converted to $^{12}N$ widths by making use of a potential model (also employed in Ref. [20]) before the parameters were applied to describe the proton decay widths to the $^{11}C$ ground state.

The authors of Ref. [17] further state that any conclusions regarding potential resonance states above $E_x = 5.6$ MeV are merely speculative due to the uncertainties in the theoretical predictions resulting from the constrains of the shell model space. In addition, the cross sections generated from the R-matrix calculations were too large to be validated by measured cross sections and applied to calculate the $^{11}C(p,\gamma)^{12}N$ capture.
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 = \textbf{NCSMC}
  – Inclusion of three-nucleon interactions in reaction calculations for $A>5$ systems
  – Extension to three-body clusters ($^6\text{He} \sim ^4\text{He}+n+n$): NCSMC in progress

• Ongoing projects:
  – Transfer reactions
  – Applications to capture reactions important for astrophysics
  – Bremsstrahlung

• Outlook
  – Alpha-clustering ($^4\text{He}$ projectile)
    • $^{12}\text{C}$ and Hoyle state: $^8\text{Be}+^4\text{He}$
    • $^{16}\text{O}$: $^{12}\text{C}+^4\text{He}$
Chiral EFT interactions up to $N^4$LO

- Systematic from LO to $N^4$LO
- High precision – $\chi^2$/datum = 1.15
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

![Graph](image)
• Working in partial waves \( \nu = \{A-a \alpha_1 I_1^{\pi_1} T_1; a \alpha_2 I_2^{\pi_2} T_2; s \ell\} \)

\[
\psi^{J^T} = \sum_{\nu} \hat{A}_{\nu} \left[ \left( \langle A-a \alpha_1 I_1^{\pi_1} T_1 | a \alpha_2 I_2^{\pi_2} T_2 \rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^T)} \frac{g_{\nu}^{J^T}(r_{A-a,a})}{r_{A-a,a}}
\]

\( \hat{r}_{A-a,a} \) \( r \subseteq (A-a) \)

• Introduce a dummy variable \( \vec{r} \) with the help of the delta function

\[
\psi^{J^T} = \sum_{\nu} \int \frac{g_{\nu}^{J^T}(r)}{r} \hat{A}_{\nu} \left[ \left( \langle A-a \alpha_1 I_1^{\pi_1} T_1 | a \alpha_2 I_2^{\pi_2} T_2 \rangle \right)^{(sT)} Y_\ell(\hat{r}) \right]^{(J^T)} \delta(\vec{r} - \vec{r}_{A-a,a}) r^2 dr d\hat{r}
\]

– Allows to bring the wave function of the relative motion in front of the antisymmetrizer
Now introduce partial wave expansion of delta function

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

After integration in the solid angle one obtains:

\[
\left| \psi^{J^{sT}} \right> = \sum_v \int \frac{g_v^{J^{sT}}(r)}{r} \hat{A}_v \left[ \left| (A - a \alpha_1 I_1^{\pi_1} T_1) | a_2 I_2^{\pi_2} T_2 \right> \right]^{(sT)} Y_\ell (\hat{r}) \left]^{(J^{sT})} \right. \delta(\vec{r} - \vec{r}_{A-a,a}) \; r^2 dr \; d\hat{r}
\]

(Jacobi) channel basis
Binary cluster RGM equations

- Trial wave function:  
  \[ |\psi_{J^T}\rangle = \sum_{\nu} \int g_{\nu}^{J^T}(r) \hat{A}_\nu |\Phi_{\nu r}^{J^T}\rangle r^2 dr \]

- Projecting the Schrödinger equation on the channel basis yields:
  \[ \sum_{\nu} \int \left[ H_{\nu\nu}^{J^T}(r', r) - E N_{\nu\nu}^{J^T}(r', r) \right] \frac{g_{\nu}^{J^T}(r)}{r} r^2 dr = 0 \]

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

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

Note:

- The coordinate space channel states are given by

\[
\left| \Phi_{\nu r}^{J\pi T} \right> = \sum_n R_{n\ell}(r) \left| \Phi_{\nu n}^{J\pi T} \right>
\]

- 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
\[ \langle \Phi_{v'r'}^J | \hat{A}_v \hat{A}_v | \Phi_{vr}^{J\pi T} \rangle = \langle \Phi_{v'r'}^J \mid (A-1) \mid \left( a' = 1 \right) \left[ 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right] \mid (a = 1) \mid r \rangle \]

\[ N_{vv'}^{J\pi T} (r', r) = \delta_{vv'} \frac{\delta(r' - r)}{r'r} - (A - 1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \langle \Phi_{v'n'}^{J\pi T} \mid \hat{P}_{A-1,A} \mid \Phi_{vn}^{J\pi T} \rangle \]

**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:** Target wave functions expanded in the SD basis, the CM motion exactly removed.

\[ \frac{\delta(r - r_{A-a,a})}{rr_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a}) \]
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:

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

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

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

\[
u_c(r) \sim v_c^{\pm} \left[ \delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]
\]

Scattering matrix