Predictive Power of Chiral Interactions for Nuclear Structure and Reaction Calculations in the p-Shell

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Angelo Calci | TRIUMF
Introduction

The many-body eigenvalue problem for a given Hamiltonian $H$ is

$$\frac{\Psi_n}{\langle n |} = \frac{E_n}{\langle n |} \Psi_n$$

resonances & scattering states

Resonating Group Method (RGM)

Describing relative motion of clusters

Outline

ab initio description of nuclei

QCD-based interaction

realistic NN+3N interactions

Bound states & spectroscopy

NCSM

ab initio description of nuclear clusters

(IT-)NCSM

Ab-initio description of nuclear clusters

QCD-based interaction

realistic NN+3N interactions

Resonating Group Method (RGM)

Describing relative motion of clusters

NCSM with Continuum

continuum effects in spectroscopy

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Introduction

Many-body eigenvalue problem

\[
\frac{1}{\text{bare}} \Psi_n \rightarrow 1 = E_n \frac{1}{\text{bare}} \Psi_n \rightarrow 2
\]

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Outline

ab initio description of nuclei

QCD-based interaction
realistic NN+3N interactions
Chiral NN+3N Interactions

**standard interaction:**
- NN @ N³LO: Entem & Machleidt, 500MeV cutoff
- 3N @ N²LO: Navrátil, local, 500MeV cutoffs & modifications of the 3N force

**optimized N²LO interaction:**
- NN: Ekström et al., 500MeV cutoff, LECs fitted with POUNDerS
- 3N: Navrátil, local, 500MeV cutoff, fit to ⁴He & Triton

**EGM N²LO interaction:**
- NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
- 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard, ...
Chiral NN+3N Interactions

- **standard interaction:**
  - NN @ N^3LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N^2LO: Navrátil, local, 500MeV cutoffs & modifications of the 3N force

- **chiral interactions are not unique:**
  - chiral order
  - regularization
  - fit of low-energy constants (LECs)
  - (power counting)

- NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
- 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
Next Generation Interactions

- **standard interaction:**
  - NN @ N³LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N²LO: Navrátil, local cutoffs

- **N²LO_sat interaction:**
  - NN+3N: Ekström et al., nonlocal 450MeV cutoff, simultaneous fit to NN data and selected many-body observables

- **LENPIC interaction:**
  - NN up to N⁴LO: Epelbaum et al., semi-local cutoff
  - 3N up to N³LO: under construction

- **N⁴LO(500):**
  - NN @ N⁴LO: Machleidt et al., 500MeV cutoff
**Similarity Renormalization Group (SRG)**

*accelerate* convergence by *pre-diagonalizing* the Hamiltonian with respect to the many-body basis

- **unitary transformation** leads to evolution equation

\[
\frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha] = -\eta_\alpha^\dagger
\]

advantages of SRG: **flexibility** and **simplicity**

3B-Jacobi HO matrix elements

keep SRG induced contributions up to 3B level

\[
\langle E' i' | \tilde{H}_\alpha - T_{\text{int}} | E i \rangle
\]

\[J^\pi = \frac{1}{2}^+, \quad T = \frac{1}{2} \]

\[
h\Omega = 24 \text{ MeV}
\]
Introduction

Many-body eigenvalue problem

\[ \Psi_n \rightarrow 1 = E_n \Psi_n \rightarrow 1 \]

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Outline

Ab initio description of nuclei

QCD-based interaction
realistic NN+3N interactions

Bound states & spectroscopy

(NCSCM)

Ab initio description of nuclear clusters

(Importance Truncated)
No-Core Shell Model (NCSM)

- solving the eigenvalue problem:
  \[ H |\psi_n\rangle = E_n |\psi_n\rangle \]

- **model space:**
  spanned by Slater determinants with unperturbed excitation energy up to \( N_{\text{max}} \hbar \omega \)
No-Core Shell Model (NCSM)

- solving the eigenvalue problem:
  \[ H \left| \psi_n \right> = E_n \left| \psi_n \right> \]

- **model space:**
  spanned by Slater determinants with unperturbed excitation energy up to \( N_{\max} \hbar \Omega \)

---

**problem of NCSM**

enormous increase of model space with particle number \( A \)
No-Core Shell Model (NCSM)

- solving the eigenvalue problem:
  \[ H |\psi_n\rangle = E_n |\psi_n\rangle \]

- **model space:** spanned by Slater determinants with unperturbed excitation energy up to \( N_{\text{max}} \hbar \Omega \)

---

**Importance Truncated NCSM**

- a priori determination of relevant basis states via first-order perturbation theory

  \[ \kappa_{\nu} = - \frac{\langle \Phi_{\nu} | H_{\text{int}} | \psi_{\text{ref}} \rangle}{\epsilon_{\nu} - \epsilon_{\text{ref}}} \]

- **importance truncated space** spanned by basis states with \( |\kappa_{\nu}| \geq \kappa_{\text{min}} \)

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No-Core Shell Model (NCSM)

- solving the eigenvalue problem:
  \[ H \left| \psi_n \right> = E_n \left| \psi_n \right> \]

- model space:
  spanned by Slater determinants with unperturbed excitation energy up to \( N_{\text{max}} \hbar \Omega \)

**Importance Truncated NCSM**

- a priori determination of relevant basis states via first-order perturbation theory
- importance truncated space spanned by basis states with \( |\kappa_v| \geq \kappa_{\text{min}} \)

**Problem of NCSM**

enormous increase of model space with particle number \( A \)

**Extrapolation** of \( \kappa_{\text{min}} \to 0 \) recovers effect of omitted contributions
- IT-NCSM provides same results as full NCSM
- expands application range to larger \( A \)

**Importance Truncated NCSM**

- \( H |\psi_n\rangle = E_n |\psi_n\rangle \)

- model space: spanned by Slater determinants with unperturbed excitation energy up to \( N_{\text{max}} \hbar \Omega \)
Sensitivity on chiral 3N interactions

- analyze the sensitivity of spectra on **low-energy constants** ($c_i, c_D, c_E$) and **cutoff** ($\Lambda$) of the chiral 3N interaction at N$^2$LO
- why this is interesting:
  - **impact of N$^3$LO contributions**: some N$^3$LO diagrams can be absorbed into the N$^2$LO structure by shifting the $c_i$ constants
    \[
    \tilde{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64 \pi F_\pi^2}, \quad \tilde{c}_3 = c_3 + \frac{g_A^4 M_\pi}{16 \pi F_\pi^2}, \quad \tilde{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16 \pi F_\pi^2}
    \]
    (Bernard et al., Ishikawa, Robilotta)
  - **uncertainty propagation**: sizable variations of the $c_i$ from different extractions (also affects NN)
    \[
    c_1 = -1.23... - 0.76, \quad c_3 = -5.94... - 3.20, \quad c_4 = 3.40...5.40 \text{ [GeV}^{-1}\text{]}\]
  - **cutoff dependence**: does the cutoff choice in the 3N interaction affect nuclear structure observables?
Sensitivity on chiral 3N interactions

- analyze the sensitivity of spectra on **low-energy constants** \((c_i, c_D, c_E)\) and **cutoff** \((\Lambda)\) of the chiral 3N interaction at \(N^2\)LO

- why this is interesting:

  - **impact of \(N^3\)LO contributions**: some \(N^3\)LO diagrams can be absorbed into the \(N^2\)LO structure by shifting the \(c_i\) constants

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    \tilde{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64 \pi F_\pi^2}, \quad \tilde{c}_3 = c_3 + \frac{g_A^4 M_\pi}{16 \pi F_\pi^2}, \quad \tilde{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16 \pi F_\pi^2} \quad \text{(Bernard et al., Ishikawa, Robilotta)}
    \]

  - **uncertainty propagation**: sizable variation across different extractions (also affects NN)

    \[ c_1 = -1.23 \ldots - 0.76, \quad c_3 = -5.94 \ldots -3 \]

  - **cutoff dependence**: does the cutoff of \(\Lambda\) of the 3N interaction affect nuclear structure observables?

  - provide **constraints** for chiral Hamiltonians and quantify uncertainties
\[ ^{12}\text{C}: \text{Sensitivity to } c_i \]

- many states are rather \( c_i \) independent
- first \( 1^+ \) state shows strong \( c_3 \) dependence

\[ \hbar \Omega = 16 \text{ MeV} \]
\[ N_{\text{max}} = 8 \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\( ^{12}\text{C}: \text{Sensitivity to } c_D \text{ and cutoff} \)

- moderate dependence on \( c_D \),
- stronger dependence on \( \Lambda \)
- again first \( 1^+ \) state is most sensitive

**IT-NCSM**

\( \hbar \Omega = 16 \text{ MeV} \)
\( N_{\text{max}} = 8 \)
\( \alpha = 0.08 \text{ fm}^4 \)
Correlation Analysis: $^{12}\text{C}(1^+) \text{ vs. } ^{10}\text{B}(1^+)$

- correlation does not agree with experiment
- hints at problems with E&M NN interaction

**standard**
- $\hbar\Omega = 16 \text{ MeV}$
- $N_{max} = 8$
- $\alpha = 0.08 \text{ fm}^4$

$^{12}\text{C} : E(1^+) - E(0^+) \text{ [MeV]}$

$^{10}\text{B} : E(1^+) - E(3^+) \text{ [MeV]}$

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$^{12}$C: Cutoff Dependence

\[ E_x \text{ [MeV]} \]

- \( N^3\text{LO} \) & \( N^2\text{LO} \) standard
- \( N^2\text{LO} \) Opt.
- (450/500)
- (600/500)
- \( N^2\text{LO} \) EGM (550/600)
- (450/700)
- (600/700)
- EGM Bands

\[ IT-\text{NCSM} \]
\[ \hbar \Omega = 16 \text{ MeV} \]
\[ N_{\text{max}} = 10(8) \]
\[ \alpha = 0.08 \text{ fm}^4 \]
$^{12}\text{C}:\text{ Cutoff Dependence}$

- small cutoff dependence for NN+3N
10B: Cutoff Dependence

- complex system with compressed spectrum
- accurate predictions within large uncertainties
Correlation Analysis: $^{12}\text{C}(1^+) \text{ vs. } ^{10}\text{B}(1^+)$

- no obvious correlation for NN modifications

**standard**
- no 3N
- std 3N
- $c_i$ var
- $c_D$ var
- $\Lambda$ var

**EGM**
- no 3N (450,500)
- no 3N (600,500)
- no 3N (550,600)
- no 3N (450,700)
- 3N (450,500)
- 3N (600,500)
- 3N (550,600)
- 3N (450,700)

- $\hbar\Omega = 16 \text{ MeV}$
- $N_{\text{max}} = 8$
- $\alpha = 0.08 \text{ fm}^4$
Introduction

**Many-body eigenvalue problem**

\[
\frac{H}{\text{barex}} \Psi_n \rightarrow 1 = E_n \frac{\Psi_n}{\text{barex}}
\]

- **Resonances & scattering states**
- **Resonating Group Method (RGM)**
  - describing relative motion of clusters

**Outline**

- **ab initio description of nuclei**
  - QCD-based interaction
    - realistic NN+3N interactions
  - bound states & spectroscopy
  - (Importance Truncated) NCSM
    - ab initio description of nuclear clusters
  - resonances & scattering states
    - Resonating Group Method (RGM)
      - describing relative motion of clusters
  - NCSM with Continuum
    - continuum effects in spectroscopy
Can Ab Initio Theory Explain the Phenomenon of Parity Inversion in $^{11}\text{Be}$?

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

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Spectrum

- parity inversion
  - shell model predicts g.s. to be $J^\pi=1/2^-$
- Halo structure
  - weakly bound $J=1/2$ states
  - spectrum dominated by $n^{-10}\text{Be}$
Can Ab Initio Theory Explain the Phenomenon of Parity Inversion in $^{11}$Be?

Angelo Calci, Petr Navrátil, Giacomo Pallavicini, Cédrick Seligmann, Ilaria Meloni, and Guillaume Hupin

**Can ab initio theory describe this complicated system?**

### Example States in $^{11}$Be

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>Configuration</th>
<th>$J^\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.030</td>
<td>$9^+_{1/2}$</td>
<td></td>
</tr>
<tr>
<td>6.705</td>
<td>$9^+_{7/2}$</td>
<td></td>
</tr>
<tr>
<td>6.510</td>
<td>$9^+_{5/2}$</td>
<td></td>
</tr>
<tr>
<td>5.849</td>
<td>$9^+_{3/2}$</td>
<td></td>
</tr>
<tr>
<td>5.40</td>
<td>$9^+_{1/2}$</td>
<td></td>
</tr>
</tbody>
</table>

### $^{9}$Be States

- $^9$Be + 2n
  - $J^\pi = 1/2^+$; $T = 3/2$

### $^{10}$Be States

- $^{10}$Be(2$^+$)+n
  - $J^\pi = 3/2^-$

- $^{10}$Be(2$^+$)+n
  - $J^\pi = 5/2^-$

- $^{10}$Be(2$^+$)+n
  - $J^\pi = 3/2^-$

### Parity Inversion

- **Parity Inversion**
  - Shell model predicts g.s. to be $J^\pi = 1/2^-$

### Halo Structure

- **Halo structure**
  - Weakly bound $J = 1/2$ states
  - Spectrum dominated by n-$^{10}$Be
Can \textit{ab initio} Theory Explain the Phenomenon of Parity Inversion in $^{11}$Be?

Angelo Calci,\textsuperscript{1,*} Petr Naryshkin,\textsuperscript{2,3} Lorena Angeloni,\textsuperscript{3} and Guillaume Hupin\textsuperscript{4,5}

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\textsuperscript{2}Institut für Kernphysik, Technische Universität Darmstadt, Germany
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\textsuperscript{5}Institut de Physique Fondamentale, Université Paris Diderot, University Paris 7, CNRS/IN2P3, F-75005 Paris, France

Can \textit{ab initio} theory describe this complicated system?

- parity inversion
- shell model predicts $J^\pi = 1/2^-$, expected to be $J^\pi = 1/2^-$
- ground state (g.s.) is loosely $^{10}$Be $+$ n
- $^{10}$Be did not

\begin{tabular}{cccc}
7.030 & 6.705 & 7.10 & $^9$Be+$2n$ (5/2$^-$) (7/2$^-$) \hline
6.510 & 7.050 & 6.30 & (1/2$^-$) \hline
5.849 & 5.980 & 6.050 & \hline
5.255 & 5.40 & \hline
3.955 & 3.889 & \hline
3.40 & (3/2$^-$, 5/2$^-$) \hline
2.654 & \hline
1.783 & \hline
0.32004 & \hline
\end{tabular}

$J^\pi = 1/2^+$; $T = 0$

\[ Z=4 \quad N=7 \]

\[ 0p_{1/2} \quad 0p_{3/2} \quad 0s_{1/2} \]
Can ab initio theory describe this complicated system?

YES

BUT... huge challenge for interaction and many-body method

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

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

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4Institut de Physique Théorique, Ecole Polytechnique, CNRS, CEA, Palaiseau, France

Z=4 N=7

$^{11}$Be nucleus using the framework of Ab initio shell model predicts g.s. to be $J^\pi=1/2^-$.

$^{9}$Be+2n transition $E=0.5$ MeV is anticipated to be sensitive to the details of the nuclear force.

The weakly bound exotic $^{11}$Be did not have a role in the parity inversion.

The theoretical understanding of exotic neutron-rich nuclei and 2N systems often contradicts the regular shell structure.

The spectrum of $^{11}$Be is separated by only 320 keV from its parity-inverted partner.

With an increasing neutron to proton ratio, the next magic number ($Z=4$, $N=7$) was remeasured in 1983.

The spectrum dominated by n- $^{10}$Be is separated by only 320 keV from its parity-inverted state also bound – only by 180 keV.

Continuum must be included.

The weakly bound exotic $^{11}$Be is one of the best examples of the disappearance of the ground state (g.s.) is loosely bounded.

Ab initio calculations can provide an accurate description of the spectrum to the details of the three-nucleon force and demonstrate that only certain chiral interactions are capable of reproducing the parity inversion.

With such interactions, the extremely large $\Delta E$ is crucial. Moreover, the inclusion of three-nucleon (3N) effects has been found to be indispensable for an accurate description of nuclear systems.

An explicit treatment of continuum effects is found to be indispensable. We study the sensitivity of the spectrum to the details of the three-nucleon force and demonstrate that only certain chiral interactions are capable of reproducing the parity inversion. With such interactions, the extremely large $\Delta E$ is crucial. Moreover, the inclusion of three-nucleon (3N) effects has been found to be indispensable for an accurate description of nuclear systems.

Can ab initio theory explain the phenomenon of parity inversion in $^{11}$Be?
NCSM with Continuum (NCSMC)

• representing $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

\[
|\psi^{J\pi T}\rangle = \sum_{\lambda} c_\lambda |\Psi_A E\lambda J^{\pi T}\rangle + \sum_{\nu} \int dr^2 \frac{X_\nu(r)}{r} |\xi^{J\pi T}_{\nu r}\rangle
\]

expansion in A-body NCSM eigenstates

relative motion of clusters NCSM/RGM expansion

• leads to NCSMC equation

\[
\begin{pmatrix}
H_{NCSM} \\
h \\
\mathcal{H}
\end{pmatrix}
\begin{pmatrix}
c \\
\chi(r)/r
\end{pmatrix}
= E
\begin{pmatrix}
1 \\
g \\
1
\end{pmatrix}
\begin{pmatrix}
c \\
\chi(r)/r
\end{pmatrix}
\]

• with 3N contributions in $H_{NCSM}$

covered by NCSM

given by $\langle \Psi_A E\lambda J^{\pi T} | H |\xi^{J\pi T}_{\nu r}\rangle$

contains NCSM/RGM Hamiltonian kernel

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11Be: Ab initio NCSMC calculations

- **Halo structure**
  - spectrum dominated by n-10Be halo structure

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>State</th>
<th>Jπ</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.030</td>
<td>(5/2-)</td>
<td>1/2⁻</td>
</tr>
<tr>
<td>6.510</td>
<td>(7/2-)</td>
<td></td>
</tr>
<tr>
<td>5.849</td>
<td>(1/2-)</td>
<td></td>
</tr>
<tr>
<td>5.255</td>
<td>5/2⁺</td>
<td></td>
</tr>
<tr>
<td>3.955</td>
<td>5/2⁻</td>
<td></td>
</tr>
<tr>
<td>3.40</td>
<td>3/2⁻</td>
<td></td>
</tr>
<tr>
<td>2.654</td>
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</tr>
<tr>
<td>1.783</td>
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<td></td>
</tr>
<tr>
<td>0.32004</td>
<td>1/2⁻</td>
<td></td>
</tr>
</tbody>
</table>

- **NCSM input**
  - calculations use NCSM vectors and energies as input
  - include n-10Be continuum
    - (0⁺, 2⁺, 2⁺ states of 10Be)
  - include 11Be short-range correlations:
    - 4 negative parity (at least)
    - 3 positive parity states of 11Be

\[ J^π = 1/2⁺; T = 3/2 \]

11Be
11Be: Ab initio NCSMC calculations

- **Halo structure**
  - Spectrum dominated by n-\(^{10}\)Be halo structure

- **Presented NCSMC results are converged w.r.t. to NCSM input**

### NCSM input
- Calculations use NCSM vectors and energies as input
- Include n-\(^{10}\)Be continuum (0\(^+\), 2\(^+\), 2\(^+\) states of \(^{10}\)Be)
- Include \(^{11}\)Be short-range correlations:
  - 4 negative parity (at least)
  - 3 positive parity states of \(^{11}\)Be

\[
\begin{array}{c|c|c}
\text{Energy (MeV)} & \text{NCSM Input} & \text{NCSM Input} \\
7.030 & 7.10 & (5/2^-) (7/2^-) \\
6.510 & 6.705 & (5/2^-) (7/2^-) \\
5.849 & 5.980 & 6.30 (1/2^-) \\
5.255 & 5.40 & 5/2^- \\
3.955 & 3.889 & (3/2^-) (3/2^+) \\
3.40 & 3/2^- & 3/2^- \\
2.654 & 3/2^- & \\
1.783 & 5/2^+ & \\
0.32004 & 1/2^- & \\
\end{array}
\]

- J\(^\pi\) = 1/2^+ 
- \(^{9}\)Be+2n: 5.46 MeV
- \(^{10}\)Be(2^+)+n: 3.87 MeV
- \(^{10}\)Be(2^+)+n: 0.5016 MeV
$^{11}$Be excitation spectrum

NCSM  NCSM/RGM  NCSMC  exp.

$E_{\text{thr.}}$ [MeV]

$n^{+10}\text{Be}$

$\alpha = 0.0625 \text{ fm}^4$, $\hbar \Omega = 20 \text{ MeV}$, $E_{3\text{max}} = 14$

Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)
**11 Be excitation spectrum**

![Graph showing the excitation spectrum of 11 Be with various states and parity inversions.](image)

- **NCSM (N=5)**
- **NCSM/RGM (N=5)**
- **NCSMC**
- **Experiment (exp.)**

**Key Points**:

- **NN+3N(400)**
- **Parity inversion**
- **Probing chiral 3N forces**

**Other Details**:

- **E_{\text{thr.}} [MeV]**
- **N_{\text{max}}**
- **\alpha = 0.0625 \text{fm}^{-4}, \hbar \Omega = 20 \text{MeV}, E_{3\text{max}} = 14**

**References**:

Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)
Variation of 3N force

 parity inversion can be reproduced
**11Be: Photodisintegration process & E1 transition**

**B(E1:1/2⁻→1/2⁺) [e²fm²]**

<table>
<thead>
<tr>
<th></th>
<th>NCSM</th>
<th>NCSMC</th>
<th>NCSMC-pheno</th>
<th>exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NN+3N(400)</td>
<td>0.0005</td>
<td>-</td>
<td>0.146</td>
<td>0.102(2)*</td>
</tr>
<tr>
<td>N²LO_{SAT}</td>
<td>0.0005</td>
<td>0.127</td>
<td>0.117</td>
<td></td>
</tr>
</tbody>
</table>


- **strongest known E1** transition between low-lying states (attributed to halo structure)

- reproduced **only** with **continuum effects**

- **conflicting experimental measurements**

- ab initio results:
  - **discriminate** between measurements
  - **predict dip** at 3/2⁻ resonance energy

\[ \gamma^{11}\text{Be}(1/2^+) \rightarrow ^{10}\text{Be(g.s.)}+n \]
Mirror nuclei: $^{11}\text{Be}$ and $^{11}\text{N}$

Standard NN+3N(400)

- $n+^{10}\text{Be}$
- $p+^{10}\text{C}$

$N_{\text{max}} = 8,9$

$N_{\text{max}} = 6,7$

$E_{\text{kin}}$ [MeV]

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p$^{10}$C Scattering: Structure of $^{11}$N resonances

Mirror System
elastic scattering allows discrimination among chiral nuclear forces

IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev et al.

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al., with IRIS collaboration, in preparation
p+^{10}\text{C} Scattering: Structure of $^{11}\text{N}$ resonances

Mirror System
elastic scattering allows discrimination among chiral nuclear forces

scattering and transition observables enable interesting investigations

IRIS collaboration: A. Kumar, R. Kanungo, A. Sanetullaev et al.

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al, with IRIS collaboration, in preparation
Mirror System
elastic scattering allows discrimination among chiral nuclear forces

scattering and transition observables enable interesting investigations

BUT
also computational expensive

IRIS collaboration: A. Kumar, R. Kanungo, A. Sanetullaev et al.
A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al, with IRIS collaboration, in preparation
NCSMC with approximated 3N forces

with
P. Navrátil, R. Roth, E. Gebrerufael
NCSM with Continuum (NCSMC)

- representing $H |\psi^{\pi T}\rangle = E |\psi^{\pi T}\rangle$ using the over-complete basis

\[ |\psi^{\pi T}\rangle = \sum_\lambda c_\lambda |\Psi_A E_\pi^{\pi T}\rangle + \sum_\nu \int dr r^2 \frac{X_{\nu}(r)}{r} |\xi^{\pi^{\pi T}}_{\nu r}\rangle \]

expansion in A-body NCSM eigenstates

relative to NCSM/RGM expansion

- leads to NCSMC equation

\[
\begin{pmatrix}
H_{NCSM} & h \\
h & \mathcal{H}
\end{pmatrix}
\begin{pmatrix}
c \\ \chi(r)/r
\end{pmatrix}
= E \begin{pmatrix}
1 \\ g
\end{pmatrix}
\]

- with 3N contributions in $H_{NCSM}$

covered by NCSM

given by $\langle \Psi_A E_\pi^{\pi T} | H |\xi_{\nu r}^{\pi T}\rangle$

contains NCSM/RGM Hamiltonian Kernel

bottleneck: inclusion of 3N force

March 27 2017  Angelo Calci
Normal-ordering (NO) approximation

- standard tool to reduce particle rank
- generally NO can be considered as basis transformation
  \[ V_{3N} \approx \tilde{V}_0 + \tilde{V}_1 + \tilde{V}_2 + \tilde{V}_3 \]
  contain information of reference state and initial 3N force

- interested in direct description of open-shell systems
  - multi-reference normal ordering (MR-NO)
  - generalization of wicks theorem [Kutzelnigg, Mukherjee]

NCSM/RGM kernels with MR-NO contributions
- reduces computational costs tremendously
- impressively accurate approximation
Derive NCSM/RGM Kernels

0B kernel

dominant 0B kernel contribution included in target eigenstates
⇒ only MR-NO 1B and 2B kernels contribute

1B kernel

\[
SD < \epsilon_{\nu_n'}^{\mathcal{J}_T} | V_A | \epsilon_{\nu_n}^{\mathcal{J}_T} >_{SD} \\
= \sum_{M_1 m_1} \sum_{M_{T1} m_{T1}} \sum_{M_1' m_1'} \sum_{M_{T1}' m_{T1}'} \left( \begin{array}{c|c} I_1 & J \\ M_1 & m_1 \end{array} \right) \left( \begin{array}{c|c} T_1 & 1/2 \\ M_{T1} & m_{T1} \end{array} \right) \left( \begin{array}{c|c} I_1' & J' \\ M_1' & m_1' \end{array} \right) \left( \begin{array}{c|c} T_1' & 1/2 \\ M_{T1}' & m_{T1}' \end{array} \right)
\]

\times SD < \psi_{A-1}^{I_1 I_1'} E_1^{\pi_1} M_1 T_1 | \psi_{A-1}^{I_1 I_1'} E_1^{\pi_1} M_1 T_1 >_{SD}
\times < n' l' j' m_{l'} | V_A | n l j m_1 >

\[
-SD < \epsilon_{\nu_n'}^{\mathcal{J}_T} | V_A T_{A-1, A} | \epsilon_{\nu_n}^{\mathcal{J}_T} >_{SD} \\
= -\frac{1}{A-1} \sum_{M_1 m_1} \sum_{M_{T1} m_{T1}} \sum_{M_1' m_1'} \sum_{M_{T1}' m_{T1}'} \left( \begin{array}{c|c} I_1 & J \\ M_1 & m_1 \end{array} \right) \left( \begin{array}{c|c} T_1 & 1/2 \\ M_{T1} & m_{T1} \end{array} \right) \left( \begin{array}{c|c} I_1' & J' \\ M_1' & m_1' \end{array} \right) \left( \begin{array}{c|c} T_1' & 1/2 \\ M_{T1}' & m_{T1}' \end{array} \right)
\]

\times \sum_{\alpha A-1} SD < \psi_{A-1}^{I_1 I_1'} E_1^{\pi_1} M_1 T_1 | a_{n l j m_1}^{\dagger} a_{\alpha A-1}^{\dagger} | \psi_{A-1}^{I_1 I_1'} E_1^{\pi_1} M_1 T_1 >_{SD}
\times < n' l' j' m_{l'} | V_A | \alpha A-1 >

2B kernel

...
NCSMC: Impact of 3N in Kernels

![Graph showing the impact of 3N in kernels for n+4He and explicit 3N in NN+3N(500) using NCSMC and NCSMC with MR-NO(\textsuperscript{5}He).](image-url)
NCSMC: Impact of 3N in Kernels

impact of MR-NO approximation much smaller than effect of other incorporated truncations

\( \delta \) [deg]
\( \delta \) [deg]

\( E_{\text{kin}} \) [MeV]
\( E_{\text{kin}} \) [MeV]

\( N_{\text{max}}^\text{NCSMC} = 11 \)
\( N_{\text{max}}^\text{NCSM} \)

\( N_{\text{max}}^\text{NN+3N(400)} \)

\( P_{1/2}^2 \)
\( P_{3/2}^2 \)

\( P_{1/2}^4 \)
\( P_{5/2}^4 \)

\( P_{3/2}^6 \)
\( P_{5/2}^6 \)

\( P_{7/2}^6 \)

\( P_{5/2}^6 \)

\( P_{7/2}^6 \)

\( P_{5/2}^6 \)

\( P_{7/2}^6 \)

\( \alpha = 0.0625 \text{ fm}^4 \), \( h\Omega = 20 \text{ MeV} \), \( E_{3\text{max}} = 14 \)
First application: $^{12}\text{N}$

- ideal candidate
  - weakly bound J=1$^+$ state dominated by p-$^{11}\text{C}$

- some low lying resonances not measured precisely
- $^{11}\text{C}(p,\gamma)^{12}\text{N}$ can bypass triple-alpha process
- planned experiment at TUDA facility at TRIUMF

**ab initio NCSMC**

- include p-$^{11}\text{C}$ continuum 
  - (3/2$^-$, 1/2$^-$, 5/2$^-$, 3/2$^-$ states of $^{11}\text{C}$)
- include 4 negative and 6 positive parity states of $^{12}\text{N}$
- MR-NO with respect to $N_{\text{max}}=0$ eigenstate of $^{12}\text{N}$
$^{12}$N spectrum with continuum effects

![Diagram of $^{12}$N spectrum with continuum effects]

- NCSM
- NCSMC
- exp.
- NCSMC
- NCSM

$E_{\text{thr.}}$ [MeV] vs $N_{\text{max}}$

- $p^{+11}$C $(3/2)^-$
- $p^{+11}$C $(5/2)^-$
- $p^{+11}$C $(1/2)^-$
- $p^{-11}$C $(3/2)^-$

$NN+3N(400)$

$N^2L_O^{\text{SAT}}$

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

12N spectrum with continuum effects

Work in progress

- study incorporated truncations
- benchmark further chiral interactions

We need to improve our nuclear forces!

NCSM NCSMC exp. NCSMC NCSM

\[ 12\text{N spectrum with continuum effects} \]

\[ (a) \text{NCSM vs. NCSMC} \]

\[ (b) \text{NCSM vs. NCSMC} \]

\[ E_{\text{thr.}} \text{[MeV]} \]

\[ N_{\text{max}} \]

\[ a = 0.0625 \text{fm}^{4}, \hbar\omega = 20 \text{MeV}, E_{3\text{max}} = 14 \]

\[ 12\text{N} \]

\[ \text{N}^2\text{LO}_{\text{sat}} \]

\[ \text{NN+3N}(400) \]

\[ b : \text{NCSM vs. NCSMC} \]

\[ \text{NCSM shows much better } N_{\text{max}} \text{ convergence} \]

\[ \text{NCSM tries to capture continuum effects via large } N_{\text{max}} \]

\[ \text{dramatic difference for the } 1/2^+ \text{ state right at threshold} \]

\[ \text{negative parity} \]

\[ \text{positive parity} \]

-3 -2 -1 0 1 2 3 4 5 6 7 8 9 10 11 12

\[ E_{\text{thr.}} \text{[MeV]} \]

\[ N_{\text{max}} \]

\[ (a) \text{NCSM vs. NCSMC} \]

\[ (b) \text{NCSM vs. NCSMC} \]

\[ \text{NCSM vs. NCSMC} \]

\[ \text{NN+3N}(400) \]

\[ \text{N}^2\text{LO}_{\text{sat}} \]

\[ a = 0.0625 \text{fm}^{4}, \hbar\omega = 20 \text{MeV}, E_{3\text{max}} = 14 \]

\[ 12\text{N} \]

\[ \text{N}^2\text{LO}_{\text{sat}} \]

\[ \text{NN+3N}(400) \]

\[ E_{\text{thr.}} \text{[MeV]} \]

\[ N_{\text{max}} \]

\[ (a) \text{NCSM vs. NCSMC} \]

\[ (b) \text{NCSM vs. NCSMC} \]

\[ \text{NCSM vs. NCSMC} \]

\[ \text{NN+3N}(400) \]

\[ \text{N}^2\text{LO}_{\text{sat}} \]
Probe chiral interaction in light nuclear scattering
n-\textsuperscript{4}He: Standard interaction

\begin{itemize}
\item \textbf{Standard Interaction:}
  \begin{itemize}
  \item N\textsubscript{max} = 13
  \item NCSMC with MR-NO
  \item $\hbar \Omega = 20 \text{ MeV}$
  \item $\alpha = 0.0625 \text{ fm}^4$
  \item $E_{3max} = 14$
  \end{itemize}
\end{itemize}
Correlation Analysis:

\[ n^{-4}\text{He} \text{ vs. } B^{+} \text{ vs. } 10^{B} (1^{+} + 3^{+}) \text{ vs. } 10^{B} (1^{+} + 3^{+}) \text{ [MeV]} \]

- $P_{3/2} - P_{1/2}$ splitting sensitive to details of nuclear force
- under- or overestimated by NN+3N(400) or $N^2LO_{\text{SAT}}$ interaction

\[ \hbar \Omega = 20 \text{ MeV} \]
\[ \alpha = 0.0625 \text{ fm}^4 \]
\[ E_{3\text{max}} = 14 \]
n-^4^He with LENPIC interaction

- splitting underestimated without 3N interaction

LENPIC interaction
N^2^LO
R = 1.0 fm

N_{max} = 11

E_{kin} [MeV]

\[ \delta \text{ [deg]} \]

\[ n^+^4^He \]

\[ N_{CSMC} \text{ with MR-NO} \]

\[ \text{N}_{\text{max}} = 11 \]

\[ ^2P_{3/2} \]

\[ ^2P_{1/2} \]

\[ ^2D_{3/2} \]

\[ ^2S_{1/2} \]

\[ h\Omega = 24 \text{ MeV} \]

\[ \alpha = 0.08 \text{ fm}^4 \]

\[ E_{3_{\text{max}}} = 14 \]
n-\(^4\)He with LENPIC interaction

- splitting sensitive to \(c_D\)
- larger \(c_D\) values provide better reproduction

LENPIC interaction
\(N^2\text{LO}\)
\(R = 1.0\ \text{fm}\)

\[c_D = 2, 4, 6\]

\(c_E\) fitted to Triton g.s.

\[h\Omega = 24\ \text{MeV}\]
\[\alpha = 0.08\ \text{fm}^4\]

\(E_{3\text{max}} = 14\)
n-^4^He with N^4^LO(500) interaction

- promising splitting properties of N^4^LO(500) NN interaction
Angelo Calci

Outlook

• insufficient knowledge of nuclear force provides largest uncertainties in ab initio calculations

• p-shell spectra provide powerful testbed for chiral potential

• combination of NCSMC with MR-NO allows to include continuum effects at strongly reduced cost
  • enables heavier targets and complex projectiles
  • probe future interactions in weakly-bound system
  • splitting of $P_{3/2} - P_{1/2}$ phase shifts in n-$^4$He can be used to constrain 3N interaction
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