Ab initio many-body calculations of nucleon-nucleus scattering

Petr Navratil and Sofia Quaglioni
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Ab initio approach to light-ion reactions

- Combining the ab initio no-core shell model (NCSM) with the resonating group method (RGM)

  \[ \Rightarrow \text{ab initio NCSM/RGM} \]

  - NCSM - single-particle degrees of freedom
  - RGM - clusters and their relative motion

\[ H \Psi^{(A)} = E \Psi^{(A)} \sum_v \int d\vec{r} \left[ H^{(A-a,a)}_{\mu \nu}(\vec{r}', \vec{r}) - E N^{(A-a,a)}_{\mu \nu}(\vec{r}', \vec{r}) \right] \Phi_v(\vec{r}) = 0 \]

- Non-local integro-differential coupled-channel equations:

  \[ [T_c + \tilde{V}_C(r) - (E - \varepsilon_c)]u_c(r) + \sum_{c'} \int dr' r'^2 W_{cc'}(r, r') u_{c'}(r') = 0 \]

Fully implemented and tested for the case of a single-nucleon projectile (nucleon-nucleus system). Capability to calculate bound states, scattering matrix, phase shifts, cross sections.
Single-nucleon projectile: the norm kernel

\[ \mathcal{N}_{\mu \ell', \nu \ell}^{(A-1,1)}(r', r) = \delta_{\mu \nu} \delta_{\ell \ell'} \frac{\delta(r' - r)}{r' r} - (A - 1) \sum_{n'n} R_{n'n'}(r') \langle \Phi_{\mu \ell' n' \ell'}^{(A-1,1)JT} | P_{A,A-1} | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n \ell}(r) \]

\[ - (A-1) \times \langle \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{\nu_1}^{(A-1)} \rangle_{SD} \]
Single-nucleon projectile basis: the Hamiltonian kernel

\[ \langle (1, \ldots, A-1) \mid H \left( 1 - \sum_{j=1}^{A-1} P_{jA} \right) \mid (1, \ldots, A-1) \rangle \]

\[ H_{\mu \ell', \nu \ell}^{(A-1, 1)}(r', r) = (E_{A-1} + T_{\text{rel}}) \mathcal{N}_{\mu \ell', \nu \ell}^{(A-1, 1)}(r', r) \]

\[ + (A - 1) \sum_{n'n} R_{n'\ell'}(r') \langle \Phi_{\mu n' \ell'}^{(A-1, 1)JT} | V_{A-1,A} (1 - P_{A-1,A}) | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n\ell}(r) \]

\[ - (A - 1)(A - 2) \sum_{n'n} R_{n'\ell'}(r') \langle \Phi_{\mu n' \ell'}^{(A-1,1)JT} | V_{A-2,A} P_{A,A-1} | \Phi_{\nu n \ell}^{(A-1,1)JT} \rangle R_{n\ell}(r) \]

\[ + \text{ terms containing NNN potential} \]

SD \[ \langle \psi^{(A-1)}_{\mu_1} \mid a^+ a \psi^{(A-1)}_{\nu_1} \rangle \]

SD \[ \langle \psi^{(A-1)}_{\mu_1} \mid a^+ a a \psi^{(A-1)}_{\nu_1} \rangle \]

\( (A-1) \times \{ \ldots \} \]

\( (A-1)(A-2) \times \{ \ldots \} \]

"direct potential"  "exchange potential"
\( n^{-4}\text{He} \) phase shifts with mSSC V8’ NN interaction

- NCSM/RGM calculation:
  - mSSC V8’ NN potential
  - two-body effective interaction
    \( N_{max} = 17 @ \hbar \Omega = 22 \text{ MeV} \)
    - Dotted lines \( N_{max} = 15 \)
  - \( ^4\text{He} \) states: g.s. + 0\(^+\)0
- \( p^+4\text{He} \) calculated as well

| 24.25  | 1\(^-\)0 |
| 23.64  | 1\(^-\)1 |
| 23.33  | 2\(^-\)1 |
| 21.84  | 2\(^-\)0 |
| 21.01  | 0\(^+\)0 |
| 20.21  | 0\(^+\)0 |

Done with the NN potential used for UNEDF benchmarks. Other resonances still should be included: 0\(^-\) 0, 1\(^-\) 0, 2\(^-\) 0. To be compared to GFMC calculations.
Parity-inverted ground state of $^{11}\text{Be}$

- $^{11}\text{Be}$
  - Disappearance of $N=8$ magic number with increasing $N/Z$ ratio
  - Ground state $1/2^+$ instead of the $p$-shell expected $1/2^-$

- Large-scale *ab initio* NCSM calculations with several accurate NN potentials do not explain the parity inversion
  - PRC 71, 043312 (2005)

- Problem:
  - Extended $n+^{10}\text{Be}$ configurations suppressed
n-\(^{10}\)Be phase shifts with CD-Bonn NN interaction

- NCSM/RGM calculation:
  - CD-Bonn 2000 NN potential
  - two-body effective interaction
    \(N_{\text{max}} = 7 \ @ \ \hbar \Omega = 13 \ \text{MeV}\)
  - \(^{10}\)Be states:
    - g.s., \(2_1^+, 2_2^+, 1_1^+\)
    - g.s., \(2_1^+, 2_2^+\)
    - g.s., \(2_1^+\)
    - g.s.

- Dramatic increase of \(^{11}\)Be 1/2\(^+\) binding energy
- Inversion between 1/2\(^-\) and 1/2\(^+\) states reproduced
\textit{n-}^{10}\text{Be} \& \text{parity-inverted ground state of} \; ^{11}\text{Be}

- What happens?
  - \textit{n-}^{10}\text{Be} \text{ wave function extends to large distances}
  - Relative kinetic and potential energies decrease in absolute values
  - The kinetic energy more dramatically
    - Net effect: \textbf{Gain in binding energy}

\begin{tabular}{|l|c|c|c|c|}
\hline
\text{NCSM} / \text{RGM} & \text{T}_{\text{rel}} & \text{V}_{\text{rel}} & \text{E}_{10\text{Be}} & \text{E}_{\text{tot}} \\
\hline
\text{Model-space} & 16.65 & -15.02 & -56.66 & -55.03 \\
\hline
\text{Full} & 6.56 & -7.39 & -57.02 & -57.85 \\
\hline
\end{tabular}

The proper description of extended \textit{n-}^{10}\text{Be} \text{ configurations leads to parity-inverted} \; ^{11}\text{Be} \text{ g.s.}
$n^{-12}\text{C}$ scattering with mSSC V8’ NN interaction

- NCSM $^{12}\text{C}$ benchmark calculation: $E_{gs} = -86(2)$ MeV
- NCSM $^{13}\text{C}$ calculation:
  - $1/2^+, 5/2^+$ states too high, unbound
- NCSM/RGM $^{13}\text{C}$ calculation:
  - two-body effective interaction
    - $N_{max} = 7 @ h \Omega = 14$ MeV
  - $^{12}\text{C}$ states: g.s., $2^+_1$
    - $1/2^+$ state bound
    - $1/2^-, 3/2^-$ and $5/2^+$ bound

<table>
<thead>
<tr>
<th></th>
<th>$^{12}\text{C}$</th>
<th>$^{13}\text{C}$: $^1 \frac{1}{2}^-$</th>
<th>$^3 \frac{2}{2}^-$</th>
<th>$^1 \frac{3}{2}^+$</th>
<th>$^3 \frac{5}{2}^+$</th>
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</thead>
<tbody>
<tr>
<td>$E_{gs}$ (MeV)</td>
<td>-86</td>
<td>-101.18</td>
<td>-8.59</td>
<td>-7.11</td>
<td>0.08</td>
</tr>
<tr>
<td>$E_{th}$ (MeV)</td>
<td>-92.59</td>
<td>-7.13</td>
<td>-5.35</td>
<td>-2.85</td>
<td>-0.62</td>
</tr>
</tbody>
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*Expt.*

- NCSM $6h \Omega / 7h \Omega$
- NCSM/RGM
- Expt.
\( n^{12}\text{C} \) scattering with mSSC V8’ NN interaction

- NCSM/RGM  \( n^{+12}\text{C} \) total cross section dominated by \( d \)-wave resonances:
  - 5/2\(^+\), 3/2\(^+\) states in \( ^{13}\text{C} \)
  - 1/2\(^-\), 3/2\(^-\), 1/2\(^+\) and 5/2\(^+\) states bound
  - 5/2\(^+\), 3/2\(^+\) and 5/2\(^-\) narrow resonances
  - 3/2\(^+\) broad resonance

- Scattering calculation a much stricter test of NN (+NNN) interactions than the discrete state calculation alone
\(-^{16}\text{O} \text{ scattering with SRG-N}^3\text{LO NN potential}\)

- \(^{16}\text{O} \) ground state calculated within importance-truncated NCSM
  - in collaboration with R. Roth (TU Darmstadt)
  - 4p-4h up to \(N_{\text{max}}=14\) (\(N_{\text{max}}=18\) possible!?), \(h\Omega=20\) MeV
  - SRG-N\(^3\)LO with \(\Lambda=2.66\) fm\(^{-1}\)
    - Less overbinding
  - Benchmarking with full NCSM
    - \(^{16}\text{O} \) binding energy up to \(N_{\text{max}}=8\)
    - Perfect agreement

- \(^{17}\text{O} \) within \textit{ab initio} NCSM/RGM
  - \(1/2^+\) bound: \(E_b=-0.87\) MeV wrt \(^{16}\text{O}\)
  - \(5/2^+\) bound: \(E_b=-0.40\) MeV wrt \(^{16}\text{O}\)
    - \(N_{\text{max}}=15\), \(h\Omega=20\) MeV
    - Only \(^{16}\text{O} \) ground-state included

\[2p-2h\]
\[4p-4h\]
\[4p-4h + Davidson\]
$n^{-16}\text{O}$ scattering with SRG-$N^3\text{LO}$ NN potential

- Phase-shift convergence reasonable
- Essential to use large $N_{\text{max}}$
  - Target wave function
  - Expansion of short-range parts of kernels
  - IT NCSM for the target makes it possible
- Need to include $^{16}\text{O}$ excited states (1p-1h...)
  - IT NCSM for excited states under way

Combining the ab initio NCSM/RGM with the importance-truncated NCSM highly promising. Access to medium mass nuclei.

$N_{\text{max}} = 14$
**$n^{-16}\text{O}$ scattering with SRG-N$^3$LO NN potential**

- Orthogonalized NCSM/RGM equations:
  - Non-local nucleon-nucleus potential
    - Channel dependent
  - Wave functions

Direct connection to phenomenological reaction theory: Comparison of coupling potentials, wave functions
Computational issues

- The most computationally intensive:
  - NCSM/RGM with the target wave function expanded in Slater determinant basis ($A>3$)
    - Target wave functions calculations
      - Limit: Dimensions up to $10^8$
      - Antoine
      - Codes developed from “Arizona” version of the MFD; MPI; up to 512 processors
    - One- and two-body transition densities from the target wave functions
      - TRDENS; MPI; up to 512 processors
      - Memory intensive: many combinations of operators in multi-shell HO basis (especially for eigenstates with $J>0$)
      - The kernel calculations from the densities is less challenging
  - NCSM/RGM with the target wave function expanded in Jacobi basis ($A=3-5$)
    - The kernel calculations
      - Sofia’s code; MPI; up to 256 processors

- CS assistance sought for the TRDENS development and optimization
Past year publications citing UNEDF

Ab Initio Study of $^{40}$Ca with an Importance-Truncated No-Core Shell Model

R. Roth
Institut für Kernphysik, TU Darmstadt, Schloßgartenstr. 9, 64289 Darmstadt, Germany

P. Navrátil
Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA
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We propose an importance truncation scheme for no-core shell model or configuration interaction approaches, which enables converged calculations for nuclei well beyond the $p$ shell. It is based on an apriori measure for the importance of individual basis states constructed by means of many-body perturbation theory. Only the physically relevant states of the no-core model space are considered, which leads to a dramatic reduction of the basis dimension. We analyze the validity and efficiency of this truncation scheme using different realistic nuclear-nucleon interactions and compare to conventional no-core shell model calculations for $^4$He and $^{40}$Ca. Then, we present first converged calculations for the ground state of $^{40}$Ca within no-core model spaces including up to $16\hbar^2$ excitations using realistic low-momentum interactions. The scheme is universal and can be easily applied to other quantum many-body problems.

Nuclear Electric Dipole Moment of $^3$He

I. Stetcu a, C.-P. Liu a,b,c, J. L. Friar a, A. C. Hayes a, P. Navrátil d

a Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.
b Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, U.S.A.
c Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.
d Lawrence Livermore National Laboratory, P.O. Box 808, L-414, CA 94551, USA.

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Local three-nucleon interaction from chiral effective field theory

P. Navrátil
Lawrence Livermore National Laboratory, Livermore, CA, USA

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Abstract The three-nucleon (NNN) interaction derived within the chiral effective field theory at the next-to-next-to-leading order (N3LO) is regulated with a function depending on the magnitude of the momentum transfer. The regulated NNN interaction is then local in the coordinate space, which is advantageous for some many-body techniques. Matrix elements of the local chiral NNN interaction are evaluated in a three-nucleon basis. Using the ab initio no-core shell model (NCSM) the NNN matrix elements are employed in $^3$H and $^4$He bound-state calculations.

Ab Initio Many-Body Calculations of $n-^3$H, $n-^4$He, $p-^3$He, and $n-^{10}$Be Scattering

Sofia Quaglioni and Petr Navrátil
Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, CA 94551, USA
(Dated: April 9, 2008)

arXiv:0804.1560; submitted to PRL
Past year accomplishments and future plans

- Benchmark calculations for $^7\text{Li}$, $^9\text{Be}$ and $^{12}\text{C}$ with mSSC V8’ NN potential
- Development of \textit{ab initio} many-body reaction theory by merging the NCSM and the RGM
  - Results with NN potentials used by UNEDF collaboration
    - $n^{-4}\text{He}$ ($p^{-4}\text{He}$) with SRG-N$^3\text{LO}$, SRC-AV18, mSSC V8’
    - $n^{-12}\text{C}$ with mSSC V8’
    - $n^{-16}\text{O}$ with SRG-N$^3\text{LO}$ using the importance-truncated NCSM
    - Calculation of nucleon-nucleus non-local potentials
  - Bottleneck: Target wave-function and two-body density calc.
- $^{40}\text{Ca}$ with 4p-4h IT NCSM
- Development of the TRDENS transition density code
  - Used for the NCSM/RGM (one- and two-body) and other
  - MPI, memory intensive, CS assistance welcome
- LLNL Grand Challenge Award: 25 kCPU hours per week
- Year 2: Further work on non-local densities
- Year 3: Deuteron projectile within NCSM/RGM; nucleon scattering on medium-mass nuclei including excited states (IT NCSM); $A=12$ nuclei with chiral EFT NN+NNN
- Year 4,5: Realistic non-local potentials for nucleon-nucleus, deuteron-nucleus, connection to phenomenological reaction theory
- High-profile science: Capture reactions - $^3\text{He}(\alpha,\gamma)^7\text{Be}$, alpha-clustering