Towards a fundamental understanding of light nuclei and their low-energy reactions

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Effective Field Theories and the Many-Body Problem
INT 09-1, Seattle, March 24, 2009
The advancement in the determination of the inter-nucleon interactions strives on the progress of the ab initio description of nuclei and vice versa

Outline

Part I
- Three-nucleon low-energy constants from the consistency of interactions and currents in chiral effective field theory
  - in collaboration with Doron Gazit and Petr Navratil

Part II
- *Ab initio* many-body calculations of nucleon-nucleus scattering
  - in collaboration with Petr Navratil
A new generation of nuclear interactions (and currents)

- Nuclear forces are governed by quantum chromodynamics (QCD)
  - QCD non-perturbative at low energies
- Chiral effective field theory ($\chi$EFT)
  - Retains all symmetries of QCD
  - Explicit degrees of freedom: $\pi$, $N$
- Perturbative expansion in positive powers of $Q/\Lambda_\chi \ll 1$ ($\Lambda_\chi \sim 1$ GeV)
  - Nuclear interactions
  - Nuclear currents
- Chiral symmetry dictates operator structure
- Low-energy constants (LECs) absorb short-range physics
  - Some day all from lattice QCD
  - Now constrained by experiment

Challenge and necessity: apply $\chi$EFT forces to nuclei

Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...
**χEFT NN + NNN interactions and currents**

- A high precision fit to NN data is reached at order $N^3LO$ in the chiral expansion
  - $N^3LO$ NN [Entem&Machleidt, PRC 68, 041001 (2003); Epelbaum et al., NPA 747, 362 (2005)]
- Nuclear current [Park et al., PRC 67, 055206 (2003); Gazit, PLB 666, 472 (2008)]
  - LO: standard single-nucleon terms
  - $N^2LO$: first appearance of meson-exchange current (MEC)
- Up to $N^3LO$ both potential and current are fully constrained by the parameters defining the NN interaction, with the exception of two “new” LECs, $c_E$ and $c_D$

**Diagram:**
- NNN force
- $N^2LO$ “new” LECs
- MEC
- $d_R \propto c_D$
- $c_E$ contact
- $c_D$ contact
- 1-$\pi$ exchange + contact
- Must be determined in $A \geq 3$

**Link between medium-range NNN force ($c_D$ term) and MEC in nuclear $\beta$-decay**
Triton half life

- The $^3$H is an unstable nucleus, which undergoes $\beta$-decay
  - Simpson, PRC 35, 752 (1987); Schiavilla et al., PRC 58, 1263 (1998)

\[
(fT_{1/2})_t = \frac{K / G_V^2}{(1 - \delta_c) + 3\pi \frac{f_A}{f_V} \left\langle E_1^A \right\rangle^2}
\]

Small difference in statistical rate functions

kinematical factor over vector coupling constant

“comparative” half life
\[(fT_{1/2})_t = 1129.6 \pm 3 \text{ s}\]

PLB 610, 45 (2005)

\[\left\langle \frac{3\text{He}}{F} \left\| ^3H \right\| \right\rangle^2\]
\[\delta_c = 0.13\% \text{ effect of isospin-breaking}\]

N.B.: $E_1^A_{LO} \propto GT$

- Extract the phenomenological value of $\left\langle E_1^A \right\rangle_{\text{exp,}t} = 0.6848 \pm 0.0011$
The *ab initio* no-core shell model (NCSM) in brief

The NCSM is a technique for the solution of the $A$-nucleon bound-state problem

- **Hamiltonian**
  - “realistic” (= reproduce NN data with high precision) NN potentials:
    - coordinate space: Argonne ...
    - momentum space: CD-Bonn, $\chi$EFT $N^3$LO, ...
  - NNN interactions:
    - Tucson-Melbourne TM’, $\chi$EFT $N^2$LO

- **Finite harmonic oscillator (HO) basis**
  - $A$-nucleon HO basis states
    - Jacobi relative or Cartesian single-particle coordinates
  - complete $N_{\text{max}} \hbar \Omega$ model space
    - translational invariance preserved even with Slater-determinant (SD) basis

- Constructs effective interaction tailored to model-space truncation
  - unitary transformation in a $n$-body cluster approximation ($n=2,3$)

**Convergence to exact solution with increasing $N_{\text{max}}$**
Fit $c_D, c_E$ to experimental binding energy of $^3\text{H}$ ($^3\text{He}$)

- NCSM calculations in Jacobi coordinates
  - $N^3\text{LO NN}$ (Entem & Machleidt),
    (two-body effective interaction)
  - $N^2\text{LO NNN}$ (bare)

There is an infinite number of $c_D$-$c_E$ combinations that fit the $A=3$ b.e.

Next: determine for which $c_D$ along the trajectory the calculated $\langle E_1^A \rangle$ reproduces $\langle E_1^A \rangle_{\text{expt}}$
$E_1^A$ reduced matrix element from $\chi$EFT

- LO: $E_1^A|_{LO} \propto GT$

- $N^2$LO: MEC
  - One (charged) pion exchange term
  - contact term

\[ d_R = \frac{M_N}{\Lambda_{\chi g_A}} c_D + \frac{M_N}{3} (c_3 + 2c_4) + \frac{1}{3} \]

- NCSM calculation in Jacobi coordinates: $N^3$LO NN (Entem&Machleidt) + $N^2$LO NNN
  - MEC essential (especially contact term!)
  - weak sensitivity to NNN force
  - somewhat sensitive to $c_3$ and $c_4$


The half-life of Triton is a robust 2nd constraint!
Conclusions

- **Chiral symmetry of QCD**: link between electroweak processes and NNN-force
  - $\chi$EFT: $c_D$ both in NN-$\pi$-N part of NNN force and contact term of MEC (Hanhart et al., Gårdestig & Phillips)
- **Triton $\beta$-decay** could be used to fix the NNN force (Gårdestig & Phillips)
- *Ab initio* NCSM calculations with $N^3$LO NN (Entem & Machleidt) + $N^2$LO NNN
  - we have shown that the Triton half-life is a robust second constraint
- **Point of view of many-body theory:**
  - Treat $N^3$LO NN (Entem & Machleidt) as phenomenological model
  - we have constrained the “corresponding” $N^2$LO NNN force
- **Point of view of chiral effective filed theory:**
  - To do: study cutoff dependence, clarify role of $c_3$ and $c_4$
  - more work ahead: determination of $c_D$, $c_E$ not yet conclusive
- **Work underway**: *ab initio* NCSM calculations with $N^3$LO NN (Epelbaum *et al.*)
  - study cutoff dependence; clarify role of $c_3$ and $c_4
The advancement in the determination of the inter-nucleon interactions strives on the progress of the ab initio description of nuclei and vice versa

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Nuclear foundations of astrophysics, experimental research on exotic nuclei, ... formidable challenges to nuclear theory

- Astrophysics needs detailed and accurate nuclear physics inputs
  - low-energy reactions very difficult or impossible to measure
    - low rates due to Coulomb repulsion
    - energies relevant to astrophysics hard to reach in laboratory
    - electron screening can be large
  - extrapolations into regions in which experimental data are absent have uncertainties that are not quantifiable

- Exotic nuclei bring new phenomena to the forefront
  - weak binding, coupling to the continuum, extreme isospin
  - nucleon halos and skins, clustering
  - vanishing of magic numbers, abnormal spin-parity of ground states

\[
\sigma(E) = \frac{S(E)}{E} \exp \left( -\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}} \right)
\]

"Nuclear theory has to go beyond its empirical roots, and arrive at a fundamental understanding of nuclear properties from a unified theoretical standpoint rooted in the fundamental forces among nucleons" RIA Theory Bluebook, 2005
Our goal is to develop an *ab initio* approach to light nuclei and their low-energy reactions

- *Ab initio*, literally “from the beginning”, meaning:
  - non-relativistic quantum mechanics
  - \( A \) (active) point-like nucleons
  - realistic two- and three-nucleon forces (NN+NNN)

- A great deal of progress in *ab initio* nuclear structure
  - nuclei up to \( A=16 \) and beyond (mostly well-bound)
  - provide insight on the role of the NNN force

- Now we need to extend the *ab initio* effort to describe
  - Nuclear reactions
    - many-body quantum-mechanical problem in the continuum. Even more challenging!
      - accurate nuclear reaction calculations for \( A=3,4 \)
      - many-body scattering calculations for \( A>4 \) only now under development
  - weakly-bound systems
    - need coupling of structure and reaction mechanisms
Combining the *ab initio* no-core shell model (NCSM) and the resonating-group method (RGM) - *ab initio* NCSM/RGM

- **NCSM** - single-particle degrees of freedom
  - a successful *ab initio* approach to nuclear structure
  - for $A>4$, the only capable of employing QCD-based NN and NNN interactions derived within effective-field theory
  - incorrect description of wave function asymptotic ($r>5$ fm)
  - lack of coupling to the continuum

- **RGM** - clusters and their relative motion
  - a successful microscopic-cluster technique
  - preserves Pauli principle
  - describes reactions and clustering in light nuclei
  - simplified NN interactions and internal description of clusters
  - no link to fundamental interactions among nucleons

- **NCSM/RGM** - RGM + realistic interactions + consistent description of clusters
  - *ab initio* description of both bound and scattering states in light nuclei

\[ N = N_{\text{max}} + 1 \]
\[ \Delta E = N_{\text{max}} \hbar \Omega \]

The Hoyle state is missing!
The \textit{ab initio} NCSM/RGM in a snapshot

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

- Many-body Schrödinger equation:

\[
H \Psi^{(A)} = E \Psi^{(A)}
\]

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

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

\[
[\hat{T}_{\text{rel}}(r) + \hat{V}_C(r) - (E - E_\nu)] u_\nu(r) + \sum_{\nu} \int d\vec{r}' r W_{\nu \nu'}(r, r') u_\nu(r') = 0
\]

Fully implemented and tested for \textbf{single-nucleon projectile} (nucleon-nucleus) basis
Single-nucleon projectile: the norm kernel

\[
\left< (1, \ldots, A-1) r' \begin{array}{l}(A) \end{array} \right| 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \left| (1, \ldots, A-1) r \begin{array}{l}(A) \end{array} \right>
\]

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

\[
\left< \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{\nu_1}^{(A-1)} \right>_{SD}
\]
Single-nucleon projectile basis: the Hamiltonian kernel

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

\[ \mathcal{H}_{\mu_1, \nu_1}^{(A-1,1)}(r, r') = \left[ \hat{T}_{\text{rel}}(r') + \hat{V}_{\text{Coul}}(r') + E_{\mu_1} \right] \mathcal{N}_{\mu_1, \nu_1}^{(A-1,1)}(r', r) \]

\[ + (A - 1) \sum_{n'n} R_{n'n'}(r') \Phi_{\mu_1, \nu_1}^{(A-1,1)JT} | V_{A-1,A} (1 - P_{A-1,A}) | \Phi_{\nu_1}^{(A-1,1)JT} \rangle \langle \Phi_{\nu_1}^{(A-1,1)JT} | R_{n'n}(r) \]

\[ - (A - 1)(A - 2) \sum_{n'n} R_{n'n'}(r') \Phi_{\mu_1, \nu_1}^{(A-1,1)JT} | V_{A-2,A} P_{A,A-1} | \Phi_{\nu_1}^{(A-1,1)JT} \rangle \langle \Phi_{\nu_1}^{(A-1,1)JT} | R_{n'n}(r) \]

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

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

\[ \langle \psi^{(A-1)}_{\mu_1} | a^+ a \langle \psi^{(A-1)}_{\nu_1} \rangle \]
The RGM kernels in the single-nucleon projectile basis

\[ \delta_{\mu \nu} \delta_{\nu' \ell} \frac{\delta(x)}{x'} \]

\[ N^{(A-1,1)}_{\mu \nu \ell, \nu \ell} (r', r) = \]

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

“direct potential”

“exchange potential”
NCSM/RGM \textit{ab initio} calculation of $n$-$^4$He phase shifts

- NCSM/RGM calculations with $n+^4$H(g.s.)
- Low-momentum $V_{\text{low } k}$ NN potential: convergence reached with bare interaction
- $\chi$EFT N$^3$LO NN potential: convergence reached with two-body effective interaction

<table>
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<tr>
<th>$N_{\text{max}}$</th>
<th>$^4$He</th>
<th>$\frac{E_{\text{g.s.}}}{^4}\text{He}$</th>
<th>$\frac{3}{2}^- (^2P_{3/2})$</th>
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<td>15</td>
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Fully \textit{ab initio}. No fit. No free parameters. Convergence in $N_{\text{max}}$ under control.

Is everything else under control? ... need verification against independent \textit{ab initio} approach!
NCSM/RGM ab initio calculation of $n^{-3}H$ and $p^{-3}He$ phase shifts

- NCSM/RGM calculations with $n^{+3}H$ (g.s.) and $p^{+3}He$ (g.s.), respectively.
- $\chi$EFT N$^3$LO NN potential: convergence reached with two-body effective interaction
- Benchmark with Alt, Grassberger and Sandhas (AGS) results [PRC75, 014005(2007)]
  - What is missing? - $n^{+3}H$ (ex), $2n+d$, $p^{-3}He$ (ex), $2p+d$ configurations

The omission of three-nucleon partial waves with $1/2 < J \leq 5/2$ leads to effects of comparable magnitude on the AGS results. Need to include target excited states!
$n$-$^4\text{He}$ phase shifts with $\chi$EFT N$^3$LO NN interaction

- NCSM/RGM calculation with $n^+^4\text{He}(\text{ex})$
- $\chi$EFT N$^3$LO NN potential: convergence reached with two-body effective interaction

very mild effects of $0^+0$ on $^2S_{1/2}$

the negative-parity states have larger effects on $^2P_{1/2}$ and $^2P_{3/2}$
- $0^-, 1^-0$ and $1^-1$ affect $^2P_{1/2}$
- $2^-0$ and $2^-1$ affect $^2P_{3/2}$

The resonances are sensitive to the inclusion of the first six excited states of $^4\text{He}$. 
Nucleon-\(\alpha\) phase-shifts with \(\chi\)EFT N\(^3\)LO NN interaction

- NCSM/RGM calculation with \(N^+^4\text{He}(\text{g.s., } 0^+0, 0^-0, 1, 1^-0, 2^-0, 2^-1)\)
- \(\chi\)EFT N\(^3\)LO NN potential: convergence reached with two-body effective interaction
- \(^2S_{1/2}\) in agreement with Expt. (dominated by \(N-\alpha\) repulsion induced by Pauli principle)
- Insufficient spin-orbit splitting between \(^2P_{1/2}\) and \(^2P_{3/2}\) (sensitive to interaction model)

The first \(n-^4\text{He}\) and \(p-^4\text{He}\) phase shifts calculation within the NCSM/RGM approach. Fully \textit{ab initio}, very promising results. The resonances are sensitive to NNN interaction.
$n + ^4\text{He}$ differential cross section and analyzing power

- Neutron energy of 17 MeV
  - beyond low-lying resonances
- Polarized neutron experiment at Karlsruhe
- NCSM/RGM calculations
  - $n + ^4\text{He}(\text{g.s},0^+0)$
  - SRG-evolved N$^3$LO NN potential
- Good agreement for angular distribution
- Differences for analyzing power
  - $A_y$ puzzle for $A=5$?

First ever \textit{ab initio} calculation of $A_y$ in for a $A=5$ system. \textit{Strict test of inter-nucleon interactions.}
\( ^{11}\text{Be} \) bound states and \( n-^{10}\text{Be} \) phase shifts

- \( ^{11}\text{Be} \): 1/2\(^+\) g.s. instead of \( p\)-shell expected 1/2\(^-\)
  - disappearance of \( N=8 \) magic number with increasing \( N/Z \) ratio
  - several realistic NN potentials
  - do not explain parity inversion
$^{11}$Be bound states and $n$-$^{10}$Be phase shifts

- $^{11}$Be: $1/2^+$ g.s. instead of $p$-shell expected $1/2^-$
  - disappearance of $N=8$ magic number with increasing $N/Z$ ratio

  - several realistic NN potentials
  - do not explain parity inversion

  - $n+^{10}$Be(g.s.,$2_1^+,$$2_2^+,$$1_1^+)$
  - realistic CD-Bonn NN potential
  - reproduce parity inversion

<table>
<thead>
<tr>
<th></th>
<th>$^{10}$Be</th>
<th>$^{11}$Be($\frac{1}{2}^-$)</th>
<th>$^{11}$Be($\frac{1}{2}^+$)</th>
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<tr>
<td></td>
<td>$N_{\text{max}}$</td>
<td>$E_{\text{g.s.}}$</td>
<td>$E$</td>
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<tr>
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<td>NCSM</td>
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<td>NCSM/ RGM</td>
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<tr>
<td>Expt.</td>
<td></td>
<td>-64.98</td>
<td>-65.16</td>
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**11Be bound states and n-10Be phase shifts**

- **What happens?**
  - The \(n-\)10Be w.f. has a large extension
  - When the Whittaker tail is recovered, the w.f. internal region is rescaled
  - Relative kinetic and potential energies decrease in absolute value
    - kinetic energy more dramatically
  - **Net effect:** gain in binding energy

<table>
<thead>
<tr>
<th>NCSM/RGM</th>
<th>(\langle T_{rel} \rangle)</th>
<th>(\langle W \rangle)</th>
<th>(E^{10})Be(g.s., ex.)</th>
<th>(E_{\text{tot}})</th>
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</thead>
<tbody>
<tr>
<td>Model Space</td>
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<tr>
<td>Full</td>
<td>6.56</td>
<td>-7.39</td>
<td>-57.02</td>
<td>-57.85</td>
</tr>
</tbody>
</table>

Only when an approach is capable of describing the 11Be halo can one obtain a meaningful insight on the parity-inversion of its ground state.
Conclusions and outlook

- With the NCSM/RGM approach we are extending the \textit{ab initio} effort to describe low-energy reactions and weakly-bound systems

  - $n$-$^3$H, $n$-$^4$He, $n$-$^{10}$Be and $p$-$^3,^4$He scattering phase-shifts with realistic NN potentials
  - study of the parity-inverted ground state of $^{11}$Be

- More work ahead!
  - Inclusion of NNN force
  - Binary cluster basis with $d$, $^3$H, $^3$He, $^4$He projectiles
  - Need three-body cluster basis
    - three-body breakup
    - two-nucleon halos
  - New model space spanned by NCSM + NCSM/RGM bases

\[ \Psi_A' = \sum c_\lambda |A\lambda J\rangle + \sum \int d\vec{r} \varphi_v(\vec{r}) \hat{A} \Phi_{v\vec{r}}(A-a,a) \]

\[ \begin{pmatrix} H & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix} = E \begin{pmatrix} 1 & g \\ g & \mathcal{N} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix} \]