Minimally nonlocal nucleon-nucleon potentials with chiral two-pion exchange including Δ resonances

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https://arxiv.org/abs/1606.06335
Nuclear $\chi$EFT Approach:


- $\chi$EFT uses the chiral-symmetry to constrain the interactions of $\pi$’s among themselves or with baryons ($N$ and $\Delta$-isobar)

- $\pi$’s couple by powers of its momentum $Q$, and the Lagrangian ($L_{\text{eff}}$) can be expanded systematically in powers of $Q/\Lambda$; ($Q \ll \Lambda \sim 1 \text{ GeV}$ is the chiral-symmetry breaking scale and $Q \sim m_\pi$)

\[
L_{\text{eff}} = L^{(0)} + L^{(1)} + L^{(2)} + \ldots
\]

- $\chi$EFT allows for a perturbative treatment in terms of powers of $Q$

- The unknown coefficients of the perturbative expansion are called LEC’s and are determined fitting the experimental data

- The $\chi$-expansion gives rise to potentials and external currents can be naturally incorporated
The derivation of nuclear forces from $\chi$EFT has been a topic of active interest for the past 25 years

Previous work:

Recent work:
Motivations:

**WHY?**
Many of the available versions of chiral potentials are strongly non-local

- Non-localities due to contact interactions
- Non-localities due to regulator functions

Non-local interactions hard (but not impossible; see A. Roggero et al. PRL 112, 221103 (2014)) handle in for example Quantum Monte Carlo (QMC) methods

**GOAL:**
Construct a local $\chi$EFT NN potential with chiral TPE including $\Delta$-isobar:

- Minimize the number of non-localities due to contact interactions and remove those due to the regulator functions
  
  M. Piarulli et al. PRC 91, 024003 (2015)
  
  Minimally nonlocal nucleon-nucleon potentials with chiral two-pion exchange including $\Delta$’s

- The LECs multiplying these non-localities are now absent
  
  M. Piarulli et al. arXiv/1606.06335
  
  Local chiral $NN$ potentials and the structure of light nuclei
Local chiral $NN$ Potentials:

\[ v_{12} = v_{12}^{\text{EM}} + v_{12}^L + v_{12}^S \]

- $v_{12}^{\text{EM}}$: EM interaction component
- $v_{12}^L$: long-range component

\[ k = p' - p \]

- Dependence on $g_A$, $F_\pi$ and $h_A = 3 \frac{g_A}{\sqrt{2}}$

$Q^0$ : LO

$Q^2$ : NLO

$Q^3$ : N2LO

\[ c_1, c_2, c_3, c_4 \ (L_{\pi N}^{(2)}) \]

\[ b_3 + b_8 \ (L_{\pi N\Delta}^{(2)}) \]

*taken from $\pi$-N scattering*

\( \nu_{12}^S \): short range component

NLO: \( Q^2 \)

N3LO: \( Q^4 \)

- \( K = \frac{1}{2}(p + p') \)
- \( k = p' - p \)

In the NLO and N3LO contact interactions terms proportional to \( K^2 \) and \( K^4 \) have been removed by Fierz rearrangements:

\[
\langle f | O | i \rangle = - \langle f | P^{\text{exc}} O | i \rangle
\]

\[
P^{\text{exc}} = \frac{1 + \sigma_1 \cdot \sigma_2}{2} \frac{1 + \tau_1 \cdot \tau_2}{2} P_{\text{space}} \quad k \rightarrow -2K \text{ and } K \rightarrow -1/2k
\]

\[
K^m \rightarrow - \frac{1 + \tau_1 \cdot \tau_2}{2} \frac{1 + \sigma_1 \cdot \sigma_2}{2} k^m \quad \text{with } m=2 \text{ or } 4
\]

Fierz rearrangement is effective in completely removing non-localities at NLO (see A. Gezerlis et al. PRC 90, 054323 (2014), M. Piarulli et al. PRC 91, 024003 (2015)), but it cannot do so at N3LO.

Of course mixed terms as \( k^2 K^2 \) or \( K \times k \) can not Fierz-transformed away

\[
k^2 K^2 \rightarrow - \frac{1 + \tau_1 \cdot \tau_2}{2} \frac{1 + \sigma_1 \cdot \sigma_2}{2} K^2 k^2
\]
Coordinate-space $v_{12}^L$: 

$$v_{12}^L = \left[ \sum_{l=1}^{6} v_l^L (r) O_{12}^l \right] + v_L^{\sigma T} (r) O_{12}^{\sigma T} + v_L^{tT} (r) O_{12}^{tT}$$

- $O_{12}^{l=1,...,6} = [1, \sigma_1 \cdot \sigma_2, S_{12}] \otimes [1, \tau_1 \cdot \tau_2]$
- $O_{12}^{\sigma T} = \sigma_1 \cdot \sigma_2 T_{12}$
- $O_{12}^{tT} = S_{12} T_{12}$
- $T_{12} = 3 \tau_1 \tau_2 - \tau_1 \cdot \tau_2$

CIB terms

- $v_L^l (r) \quad v_L^{\sigma T} (r) \quad v_L^{tT} (r)$ divergencies of type $1/r^n, 1 \leq n \leq 6$

$$C_{R_L} (r) = 1 - \frac{1}{(r/R_L)^6 e^{(r-R_L)/a_L} + 1}$$

- $R_L = (0.8, 1.0, 1.2) \text{ fm}$
- $a_L = R_L/2$
Coordinate-space $v_{12}^S$:

\[ v_{12}^S = \sum_{l=1}^{16} v_l^S(r) O_{12}^l \]

- $O_{12}^{l=1,...,6} = [1, \sigma_1 \cdot \sigma_2, S_{12}] \otimes [1, \tau_1 \cdot \tau_2]$
- $O_{12}^{l=7,...,11} = L \cdot S, L \cdot S \tau_1 \cdot \tau_2, (L \cdot S)^2, L^2, L^2 \sigma_1 \cdot \sigma_2$
- $O_{12}^{l=12,...,16} = T_{12}, (\tau_1^z + \tau_2^z), \sigma_1 \cdot \sigma_2 T_{12}, S_{12} T_{12}, L \cdot S T_{12}$

- In this parametrization we removed
  \[ \{ v_p^S(r) + v_p^{p\sigma}(r) \sigma_1 \cdot \sigma_2 + v_{pt}^S(r) S_{12} + v_{pt\tau}^S(r) S_{12} \tau_1 \cdot \tau_2, p^2 \} \]
  and also we considered CD terms

- For the short-range terms the regularization is achieved by employing a local regulator

\[ \widetilde{C}_{RS}(k) = e^{-R^2_s k^2/4} \rightarrow C_{RS}(r) = \frac{1}{\pi^{3/2} R^3_s} e^{-\left(r/R_S\right)^2} \]

- In combination with $R_L = (0.8, 1.0, 1.2)$ fm $\rightarrow R_S = (0.6, 0.7, 0.8)$ fm
  \[ \Lambda_S = 2/R_S \ (700, 600, 500) \text{ MeV} \]
Fitting Procedure I:

In this work the LECs are fixed by fitting the pp and np Granada database up to laboratory frame energies $E_{\text{lab}} = 125$ MeV and $E_{\text{lab}} = 200$ MeV, the deuteron binding energy and the nn scattering length

- $3\sigma$-criterion to remove inconsistencies in the database [1]
- There are 2493 exp data up to 125MeV (3476 data up to 200 MeV)
- There are $N$ sets each one corresponding to a different experiment
- Each data set contains measurements at fixed energy and different scattering angle (except total cross sections)

We fit first phase shifts and then refine the fit by minimizing the $\chi^2$ obtained from a direct comparison with the database

http://www.ugr.es/ amaro/nndatabase/
Fitting Procedure II:
To minimize the total $\chi^2$, we use the Practical Optimization Using No Derivatives (for Squares), POUNDerS (with the help of J. Sarich and S. Wild)
M. Kortelainen, PRC 82, 024313 (2010)

Model a: $(R_L, R_S) = (1.2, 0.8)$
Model b: $(R_L, R_S) = (1.0, 0.7)$
Model c: $(R_L, R_S) = (0.8, 0.6)$

<table>
<thead>
<tr>
<th>model</th>
<th>order</th>
<th>$R_L$ (fm)</th>
<th>$R_S$ (fm)</th>
<th>$E_{LAB}$ (MeV)</th>
<th>$\chi^2$/datum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model b</td>
<td>LO</td>
<td>1.0</td>
<td>0.7</td>
<td>125</td>
<td>59.88</td>
</tr>
<tr>
<td>Model b</td>
<td>NLO</td>
<td>1.0</td>
<td>0.7</td>
<td>125</td>
<td>2.18</td>
</tr>
<tr>
<td>Model b</td>
<td>N2LO</td>
<td>1.0</td>
<td>0.7</td>
<td>125</td>
<td>2.32</td>
</tr>
<tr>
<td>Model b</td>
<td>N3LO</td>
<td>1.0</td>
<td>0.7</td>
<td>125</td>
<td>1.07</td>
</tr>
<tr>
<td>Model a</td>
<td>N3LO</td>
<td>1.2</td>
<td>0.8</td>
<td>125</td>
<td>1.05</td>
</tr>
<tr>
<td>Model c</td>
<td>N3LO</td>
<td>0.8</td>
<td>0.6</td>
<td>125</td>
<td>1.11</td>
</tr>
<tr>
<td>Model $\tilde{a}$</td>
<td>N3LO</td>
<td>1.2</td>
<td>0.8</td>
<td>200</td>
<td>1.37</td>
</tr>
<tr>
<td>Model $\tilde{b}$</td>
<td>N3LO</td>
<td>1.0</td>
<td>0.7</td>
<td>200</td>
<td>1.37</td>
</tr>
<tr>
<td>Model $\tilde{c}$</td>
<td>N3LO</td>
<td>0.8</td>
<td>0.6</td>
<td>200</td>
<td>1.40</td>
</tr>
</tbody>
</table>
Phase shifts model b up to 125 MeV (order by order):

![Graphs showing phase shifts for different partial waves and orders](image)
Phase shifts model b up to 125 MeV (order by order):

\( np \quad T=0 \)
Phase shifts: np T=1
Phase shifts: pp $T=1$

\begin{align*}
1S_0 & \\
3P_1 & \\
1D_2 & \\
3P_0 & \\
3P_2 & \\
\varepsilon_2 & \\
\end{align*}

Lab. Energy [MeV]
Nuclear Many-Body Problem:

- Few- and many-body systems provide a laboratory to study nuclear forces with a variety of numerical and computational techniques.

\[
H \Psi(R; s_1, \ldots, s_A; t_1, \ldots, t_A) = E \Psi(R; s_1, \ldots, s_A; t_1, \ldots, t_A)
\]

\[
H = -\frac{\hbar^2}{2m} \sum_i \nabla^2_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}
\]

- HH method (A. Kievsky et al., NPA 577, 511 (1994); A. Kievsky et al., FBS 22, 1 (1997); M. Viviani et al., PRC 71, 024006 (2005); A. Kievsky et al., JPG: NPP 35, 063101 (2008)) is used to calculate the ground-state energies of \(^3\)H and \(^4\)He: provide a benchmark for the corresponding QMC calculations.

- QMC methods (J. Carlson et al., RMP 87, 1067 (2015)) are then applied to compute BE and rms radii of the \(^3\)He ground state, of the \(^6\)Li and \(^6\)He ground and excited states.
Variational Monte Carlo (VMC):

Minimize the expectation value of $H$:

$$
E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0
$$

Trial wave function (involves variational parameters):

$$
|\Psi_T\rangle = \left[ S \prod_{i<j}^A (1 + U_{ij}) \right] |\Psi_J\rangle
$$

- $|\Psi_J\rangle = \left[ \prod_{i<j} f_c(r_{ij}) \right] |\Phi(JMTT_z)\rangle$ (s-shell nuclei): Jastrow wave function, fully antisymmetric
- $S \prod_{i<j}$ represents a symmetrized product
- pair correlation operators $U_{ij} = \sum_{p=2,6} u_p(r_{ij}) O^p_{ij}
- pair correlation obtained by solving the (two-body) Euler-Lagrange equations (in spin $S$ and isospin $T$ channels)

The search in parameter space is made using COBYLA (Constrained Optimization BY Linear Approximations) algorithm available in the NLopt library

http://ab-initio.mit.edu/wiki/index.php/NLopt
Green’s Function Monte Carlo (GFMC):

Projects out lowest energy state from the best variational $\Psi_T$:

$$\lim_{\tau \to \infty} |\Psi_0\rangle = \lim_{\tau \to \infty} \frac{|\Psi(\tau)\rangle}{e^{-(H-E_0)\tau}} |\Psi_T\rangle$$

$$|\Psi(\tau = 0)\rangle = |\Psi_T\rangle$$

- the imaginary-time evolution operator is computed for small time steps $\Delta\tau$ ($\tau = n \Delta\tau$)

Propagator does not contain $p^2, L^2, (L \cdot S)^2$:
- it is carried out with a simplified version $H'$ of the full Hamiltonian $H$;
  $H'$ contains a charge independent eight-operator projection:

$$[1, \sigma_1 \cdot \sigma_2, S_{12}, L \cdot S] \otimes [1, \tau_1 \cdot \tau_2]$$

Fermion sign problem limits maximum $\tau$:

- limits the initial propagation to regions where the propagated $|\Psi(\tau)\rangle$ and trial $|\Psi_T\rangle$ wave functions have a positive overlap and discards those configurations that instead have a small or vanishing overlap
- small number of unconstrained time steps $n_{uc} \sim 20$ are used when evaluating the expectation values
## Results for binding energies: HH vs QMC

The $^3$H ground-state energies $E_0$ (MeV) and rms proton radii $r_p$ (fm)

<table>
<thead>
<tr>
<th>Method</th>
<th>Model a</th>
<th>Model $\tilde{a}$</th>
<th>Model b</th>
<th>Model $\tilde{b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_0$</td>
<td>$\sqrt{\langle r_p^2 \rangle}$</td>
<td>$E_0$</td>
<td>$\sqrt{\langle r_p^2 \rangle}$</td>
</tr>
<tr>
<td>VMC</td>
<td>-7.592(6)</td>
<td>1.65</td>
<td>-7.691(6)</td>
<td>1.62</td>
</tr>
<tr>
<td>GFMC</td>
<td>-7.818(8)</td>
<td>1.62</td>
<td>-7.917(10)</td>
<td>1.60</td>
</tr>
<tr>
<td>HH</td>
<td>-7.818</td>
<td>-7.949</td>
<td>-7.599</td>
<td>-7.866</td>
</tr>
</tbody>
</table>

The $^4$He ground-state energies $E_0$ (MeV) and rms proton radii $r_p$ (fm)

<table>
<thead>
<tr>
<th>Method</th>
<th>Model a</th>
<th>Model $\tilde{a}$</th>
<th>Model b</th>
<th>Model $\tilde{b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_0$</td>
<td>$\sqrt{\langle r_p^2 \rangle}$</td>
<td>$E_0$</td>
<td>$\sqrt{\langle r_p^2 \rangle}$</td>
</tr>
<tr>
<td>VMC</td>
<td>-24.38(1)</td>
<td>1.51</td>
<td>-25.03(1)</td>
<td>1.49</td>
</tr>
<tr>
<td>GFMC</td>
<td>-25.13(5)</td>
<td>1.49</td>
<td>-25.71(3)</td>
<td>1.50</td>
</tr>
<tr>
<td>HH</td>
<td>-25.15</td>
<td>-25.80</td>
<td>-23.96</td>
<td>-25.28</td>
</tr>
</tbody>
</table>
Results for binding energies:

The $^3\text{H}$, $^3\text{He}$, $^4\text{He}$, $^6\text{He}$, and $^6\text{Li}$ ground- and excited-state energies in MeV and proton rms radii $r_p$ in fm with model $\tilde{b}$ compared with the corresponding GFMC results obtained with the AV18.

<table>
<thead>
<tr>
<th>$^A!^Z(J^{\pi}; T)$</th>
<th>VMC</th>
<th>GFMC</th>
<th>GFMC(AV18)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_0$</td>
<td>$\sqrt{\langle r_p^2 \rangle}$</td>
<td>$E_0$</td>
</tr>
<tr>
<td>$^3\text{H}(\frac{1}{2}^+; \frac{1}{2})$</td>
<td>$-7.643(5)$</td>
<td>$1.63$</td>
<td>$-7.863(8)$</td>
</tr>
<tr>
<td>$^3\text{He}(\frac{1}{2}^+; \frac{1}{2})$</td>
<td>$-6.907(5)$</td>
<td>$1.84$</td>
<td>$-7.115(9)$</td>
</tr>
<tr>
<td>$^4\text{He}(0^+; 0)$</td>
<td>$-24.46(2)$</td>
<td>$1.49$</td>
<td>$-25.21(4)$</td>
</tr>
<tr>
<td>$^6\text{He}(0^+; 1)$</td>
<td>$-22.58(3)$</td>
<td>$2.05$</td>
<td>$-24.53(6)$</td>
</tr>
<tr>
<td>$^6\text{He}(2^+; 1)$</td>
<td>$-20.94(2)$</td>
<td>$2.06$</td>
<td>$-22.87(6)$</td>
</tr>
<tr>
<td>$^6\text{Li}(1^+; 0)$</td>
<td>$-25.86(3)$</td>
<td>$2.58$</td>
<td>$-27.71(8)$</td>
</tr>
<tr>
<td>$^6\text{Li}(3^+; 0)$</td>
<td>$-22.73(3)$</td>
<td>$2.59$</td>
<td>$-24.56(8)$</td>
</tr>
<tr>
<td>$^6\text{Li}(2^+; 0)$</td>
<td>$-21.42(3)$</td>
<td>$2.61$</td>
<td>$-24.04(9)$</td>
</tr>
<tr>
<td>$^6\text{Li}(1^+; 0, 3^D[2])$</td>
<td>$-20.42(3)$</td>
<td>$2.58$</td>
<td>$-23.09(11)$</td>
</tr>
</tbody>
</table>
Conclusions:
We constructed a family of local NN potential with chiral TPE including \(\Delta\)-isobar up to N2LO \((Q^3)\) and contact interactions up to N3LO \((Q^4)\).

Three versions of this chiral potential for three different cutoffs have been developed with fits to np and pp data up to \(E_{\text{lab}} = 125\) MeV and 200 MeV, deuteron binding energy and nn scattering length.

A subset of the potentials—\(a, \tilde{a}, b, \text{ and } \tilde{b}\)—have been used in HH, VMC, and GFMC calculations of binding energies and proton rms radii of nuclei with \(A = 2–6\).

Plans:
The next stage in the program of studies of light nuclei structure with chiral interactions will be the inclusion of a 3N potential.

A chiral version of it at leading order, including \(\Delta\)-isobar intermediate states, has been developed, and is currently being constrained by reproducing observables in the \(A = 3\) systems.
Phase Shifts: 125 and 200 MeV
The $S$-wave and $D$-wave components of the deuteron wave function corresponding to models a (dashed lines), b (dotted-dashed lines) and c (dotted-dashed-dotted lines) are compared with those corresponding to the AV18 (solid lines).