Chiral 2N and 3N interactions and quantum Monte Carlo applications

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Abstract. Chiral Effective Field Theory (EFT) two- and three-nucleon forces are now widely employed. Since they were originally formulated in momentum space, these interactions were non-local, making them inaccessible to Quantum Monte Carlo (QMC) methods. We have recently derived a local version of chiral EFT nucleon-nucleon and three-nucleon interactions, which we also used in QMC calculations for neutron matter and light nuclei. In this contribution I go over the basics of local chiral EFT and then summarize recent results.

1 Introduction

Chiral EFT nuclear forces were designed to provide a connection with the symmetries of QCD [1–3]. Such interactions contain pion exchanges as well as shorter-range phenomenological terms. These include consistently predicted three-nucleon (3N) forces, which first enter at next-to-next-to-leading order (N²LO) [4, 5]. (The expansion parameter here is \( Q/\Lambda_b \) where \( Q \) is the soft scale—typically a nucleon momentum or the pion mass—and \( \Lambda_b \sim M_\rho \) is the hard scale where the chiral EFT expansion breaks down.) These interactions are critical for neutron and nuclear matter [6–14].

While the rest of the nuclear many-body community adopted chiral EFT interactions as input in their calculations, Quantum Monte Carlo methods (namely Green’s function Monte Carlo (GFMC) [15–17] and Auxiliary-Field Diffusion Monte carlo (AFDMC) [18]), did not. Given the accuracy and precision of QMC calculations for strongly interacting systems [19, 20], this state of affairs was problematic, a direct consequence of chiral EFT potentials being non-local. (It’s worth noting that Monte Carlo methods have, however, been used to study neutron matter based on lattice techniques [21] and with momentum-space QMC approaches [22, 23].) The main reason for chiral EFT interactions being non-local was that they are naturally formulated in momentum space, so they were historically constructed without considering their locality or non-locality.

Recently, we have been constructing local chiral potentials, at the NN and 3N level, and using them to calculate properties of neutron matter and light nuclei. [24–28] Here we briefly summarize basic aspects of local chiral EFT, before discussing NN+3N results for neutron matter and light nuclei.

2 Local chiral NN interactions

There are two major sources of non-locality in standard chiral EFT up to N²LO: a) the subleading contact terms in the NN sector, and b) the choice of regulator.
At next-to-leading (NLO) order, there are 14 contact terms that are allowed by symmetries. In momentum-space chiral potentials, only 7 (independent terms) were used, as the other 7 can be produced by antisymmetrizing. These 7 were selected by treating on an equal basis the momentum transfer $q$ and the momentum transfer in the exchange channel $k$. In Refs. [24, 25], instead, the choice was made to favor terms containing $q$ (and isospin):

$$V_{\text{cont}}^{(2)} = C_1 q^2 + C_2 q^2 \tau_1 \cdot \tau_2 + (C_3 q^2 + C_4 q^2 \tau_1 \cdot \tau_2) \sigma_1 \cdot \sigma_2$$

$$+ i \frac{C_5}{2} (\sigma_1 + \sigma_2) \cdot q \times k + C_6 (\sigma_1 \cdot q)(\sigma_2 \cdot q) + C_7 (\sigma_1 \cdot q)(\sigma_2 \cdot q) \tau_1 \cdot \tau_2,$$

which are local except for the $k$-dependent spin-orbit interaction ($C_5$).

Turning to the regulator, which (in principle) is just a technical aspect of producing nuclear interactions, Refs. [24, 25] regulate directly in coordinate space, by multiplying the long-range pion-exchange terms with a regulator function:

$$V_{\text{long}}(r) \rightarrow V_{\text{long}}(r)(1 - e^{-r/R_0})^4,$$

thereby ensuring that short-distance parts of the long-range potentials at $r < R_0$ are smoothly cut off. The short-range terms like those in Eq. (1) were regulated via a local regulator $f_{\text{local}}(q^2)$, which smears out the $\delta$-function by introducing the same exponential factor as for the long-range regulator:

$$\delta(r) \rightarrow \delta_{R_0}(r) = \alpha e^{-r/R_0},$$

We also note that the removal of the second source of non-locality discussed here (in the regulator) has since led to a new (semi-local) generation of chiral EFT potentials, see Ref. [29].

### 3 Local chiral 3N interactions

The contributions to the $N^2$LO chiral 3N potential are shown in Fig. 1 and are, in momentum space, given by [4, 5]

$$V_C = \frac{1}{2} \left( \frac{g_A}{2f_\pi} \right)^2 \sum_{\pi(ijk)} \frac{\sigma_i \cdot q_j \sigma_k \cdot q_k}{(q_i^2 + m_\pi^2)(q_j^2 + m_\pi^2)} F_{ijk}^{\alpha \beta} \tau_i^\alpha \tau_k^\beta,$$

$$V_D = -\frac{g_A}{8f_\pi^2} \frac{c_D}{f_\pi^2 A_\chi} \sum_{\pi(ijk)} \frac{\sigma_k \cdot q_k \sigma_i \cdot q_k}{q_k^2 + m_\pi^2} \tau_i \cdot \tau_k,$$

$$V_E = \frac{c_E}{2f_\pi^4 A_\chi} \sum_{\pi(ijk)} \tau_i \cdot \tau_k.$$
Here, as in the NN sector discussed in the previous section, \( q_i = p'_i - p_i \) is the momentum transfer of particle \( i \), while and \( F^{\alpha \beta}_{ijk} \) includes the \( c_i \) contributions:

\[
F^{\alpha \beta}_{ijk} = \delta^{\alpha \beta} \left[ -\frac{4c_1 m_n^2}{f_n^2} + \frac{2c_3}{f_n^2} \mathbf{q}_i \cdot \mathbf{q}_k \right] + \sum_{\gamma} \frac{c_4}{f_n^2} \varepsilon^{\alpha \beta \gamma \delta} \mathbf{r}_j \cdot (\mathbf{q}_i \times \mathbf{q}_k) .
\]

Since local chiral EFT is used in coordinate space, one needs to Fourier transform these expressions. \[27\] Doing so gives, for the \( V_E \) 3N contact contribution:

\[
V_{ij}^{ijk} = \frac{c_E}{2f_n^2 \Lambda_n} \sum_{n(ijk)} \mathbf{r}_i \cdot \mathbf{r}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) .
\]

Similarly, Fourier transforming the one-pion-exchange–contact \( V_D \) 3N interaction gives:

\[
V_{ij}^{ijk} = \frac{c_D^{DA}}{24f_n^2 \Lambda_n} \sum_{n(ijk)} \mathbf{r}_i \cdot \mathbf{r}_k \left[ \frac{m_n^2}{4\pi} \delta(\mathbf{r}_{ij})X_{ik}(\mathbf{r}_{kj}) - \mathbf{r}_i \cdot \mathbf{r}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right] .
\]

which can be seen to contain not only a one-pion-exchange–contact part, but also a contact–contact part. Finally, the two-pion-exchange \( V_C \) part leads to the following three contributions:

\[
V_{ij}^{ijk} = \frac{c_1 m_n^2 f_n^2}{2f_n^2 (4\pi)^2} \sum_{n(ijk)} \mathbf{r}_i \cdot \mathbf{r}_k \mathbf{r}_{ij} \cdot \mathbf{r}_{kj} \times U(\mathbf{r}_{ij})Y(\mathbf{r}_{ij})U(\mathbf{r}_{kj})Y(\mathbf{r}_{kj}) .
\]

and

\[
V_{ij}^{ijk} = \frac{c_3 g_n^2}{36f_n^4} \sum_{n(ijk)} \mathbf{r}_i \cdot \mathbf{r}_k \times \mathbf{r}_{ij} \times \mathbf{r}_{kj}
\]

\[
\times \left[ \frac{m_n^4}{(4\pi)^2} X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj}) - \frac{m_n^2}{4\pi} X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj}) - \frac{m_n^2}{4\pi} X_{ik}(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij}) + \mathbf{r}_i \cdot \mathbf{r}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right] .
\]

and

\[
V_{ij}^{ijk} = \frac{c_4 g_n^2}{72f_n^4} \sum_{n(ijk)} \mathbf{r}_i \cdot (\mathbf{r}_k \times \mathbf{r}_j)
\]

\[
\times \left[ \frac{m_n^4}{2i(4\pi)^2} [X_{ij}(\mathbf{r}_{ij}), X_{kj}(\mathbf{r}_{kj})] - \frac{m_n^2}{4\pi} \mathbf{r}_i \cdot (\mathbf{r}_k \times \mathbf{r}_j)(1 - T(\mathbf{r}_{ij}))Y(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij})
\]

\[- \frac{m_n^2}{4\pi} \mathbf{r}_i \cdot (\mathbf{r}_k \times \mathbf{r}_j)(1 - T(\mathbf{r}_{kj}))Y(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj}) - \frac{3m_n^2}{4\pi} \mathbf{r}_i \times (\mathbf{r}_k \times \mathbf{r}_j)T(\mathbf{r}_{ij}))Y(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij})
\]

\[- \frac{3m_n^2}{4\pi} \mathbf{r}_k \cdot (\mathbf{r}_i \times (\mathbf{r}_k \times \mathbf{r}_j)T(\mathbf{r}_{ij}))Y(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij}) + \mathbf{r}_i \cdot (\mathbf{r}_k \times \mathbf{r}_j)\delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right] .
\]

Note that while the Feynman diagram for \( V_C \), in accordance with its physical interpretation, implies that two-pion exchange part is long-range, the Fourier transformation also leads to terms that are short-range and intermediate-range: these do not contain 3N low-energy couplings.

Similarly to the NN regularization scheme discussed above, the local 3N forces are regulated by smearing out delta functions as follows:

\[
\delta(\mathbf{r}) \rightarrow \delta_{R3N}(\mathbf{r}) = \frac{1}{\pi \Gamma(3/4) R_{3N}^3} e^{-r/R_{3N}} ,
\]

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where $R_{3N}$ is the three-nucleon cutoff. Again, consistent with what was done in the NN sector, for the long-range pion-exchange contributions we multiply the Yukawa functions with a long-range regulator $f_{\text{long}}$:

$$Y(r) \rightarrow Y(r)\left(1 - e^{-r/R_{3N}}\right).$$

(13)

The question, then, arises of what is the range over which the 3N cutoff should be varied. The NN cutoff was varied between $R_0 = 1.0 - 1.2$ fm: for smaller values spurious bound states appear, while for larger values too large a part of the (physically significant) pion exchanges is cut off.

### 4 Local chiral EFT in neutron matter

In neutron matter (NM), the isospin structure of the 3N interaction is simplified considerably. Specifically, the short-range and intermediate-range parts of $V_C$, as well as the $V_E$ and $V_D$ contributions, vanish in NM for $R_{3N} \to 0$ (i.e. for infinite momentum-space cutoffs). Thus, their contribution in NM for finite cutoffs is only a regulator effect which (one hopes) will be removed at higher orders. Consistently with the NN cutoff $R_0 = 1.0 - 1.2$ fm, we have varied the 3N cutoff in this range, $R_{3N} = 1.0 - 1.2$ fm (so there will still be regulator effects from the shorter-range terms).

In Fig. 2 I show AFDMC results from Ref. [27] on the equation of state of neutron matter using chiral NN and the $V_C$ 3N force at $N^2$LO. These results are for an NN cutoff $R_0 = 1.0 - 1.2$ fm and $R_{3N}$ in the same range. Note that for the softer NN potential ($R_0 = 1.2$ fm, lower lines) the energy per particle is $12.3 - 12.5$ MeV at saturation density for different 3N cutoffs. This is to be compared with the NN-only energy ($11.4$ MeV), so the 3N $V_C$ has an impact of $\approx 1$ MeV. On the other hand, for the harder NN potential ($R_0 = 1.0$ fm, upper lines) the energy per particle is $15.5 - 15.6$ MeV (to be compared to $14.1$ MeV for an NN-only calculation). Here, the impact of the 3N $V_C$ is $\approx 1.5$ MeV. Note also that the variation of the total energy with the 3N cutoff is $\approx 0.2$ MeV, considerably smaller than the variation with the NN cutoff (in absolute terms). The magnitude of the local 3N two-pion-exchange $V_C$ forces (at most about $1.5$ MeV at saturation density), is smaller than a typical contribution of $4$ MeV [6] in momentum space with nonlocal regulators. This difference is probably due to the present local regulators. This is similar to findings with coupled cluster theory [11].
5 Local chiral EFT in light nuclei

Having probed the effects of the two-pion exchange (parameter-free) $V_C$ term in neutron matter, the natural next step is to study the impact of the other two terms ($V_D$ and $V_E$) in light nuclei and neutron matter. Before such a study, the values of the two couplings ($c_D$ and $c_E$) have to be fit to specified quantities. These are often selected to be properties of $A = 3$ and $A = 4$ systems. In ongoing work [28] we have opted, instead, to fit these 3N low-energy couplings to the binding energy of $^4$He and $n - \alpha$ scattering $P$-wave phase shifts. These were chosen due to the fact that the $P$-wave and the $T = 3/2$ components of the three-nucleon force enter our observables more directly.

In Fig. 3 I show ground-state energies and point-proton radii for nuclei with $A = 3, 4$ at NLO and N$^2$LO for two different values of the NN cutoff, $R_0 = 1.0$ fm (equal to $R_{3N}$) and $R_0 = 1.2$ fm (equal to $R_{3N}$). The N$^2$LO potential does a reasonable job of reproducing both the energies and the radii. Note that this figure displays error bars at each order of the chiral expansion and each value of the NN cutoff. These are produced using the approach discussed in Refs. [29–31].

6 Summary & Conclusions

In this contribution I have briefly gone over the main features of local chiral NN and 3N forces at N$^2$LO. In addition to showing the general expressions appearing in these potentials, I have discussed the main results for the ground-state energy of pure infinite neutron matter when varying the 3N cutoff from $R_{3N} = 1.0$ fm to $R_{3N} = 1.2$ fm. The dependence on this cutoff was much smaller than the dependence on the NN cutoff, $R_0$. This finding is part of a larger study showing that there is still much to be learned concerning local versus nonlocal regulators. I also touched upon the significance of the two 3N couplings, $c_D$ and $c_E$, novel ways to constrain these, as well as their effects in light nuclei.

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