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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 (N^2LO) [4, 5]. (The expansion parameter here is Q/Λ_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 N^2LO: a) the subleading contact terms in the NN sector, and b) the choice of regulator.

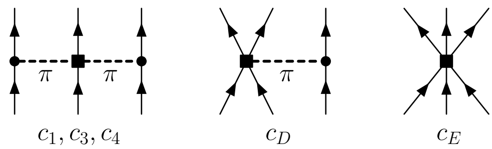

Figure 1. 3N forces at N^{2}LO.

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 $\mathbf{q}$ and the momentum transfer in the exchange channel $\mathbf{k}$. In Refs. [24, 25], instead, the choice was made to favor terms containing $\mathbf{q}$ (and isospin):

$$V_{\text{cont}}^{(2)} = C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + (C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + i\, \frac{C_5}{2}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} + C_6\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) + C_7\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\,, \tag{1}$$

which are local except for the $\mathbf{k}$-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:

$$V_{\text{long}}(r) \;\rightarrow\; V_{\text{long}}(r)\Big(1 - e^{-(r/R_0)^4}\Big)\,. \tag{2}$$

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 δ-function by introducing the same exponential factor as for the long-range regulator:

$$\delta(\mathbf{r}) \;\rightarrow\; \delta_{R_0}(\mathbf{r}) = \alpha e^{-(r/R_0)^4}\,, \tag{3}$$

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]

$$V_C = \frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \sum_{\pi(ijk)} \frac{\boldsymbol{\sigma}_i \cdot \mathbf{q}_i\, \boldsymbol{\sigma}_k \cdot \mathbf{q}_k}{(q_i^2 + m_\pi^2)(q_k^2 + m_\pi^2)}\, F_{ijk}^{\alpha\beta}\, \tau_i^\alpha\, \tau_k^\beta\,, \tag{4}$$

$$V_D = -\frac{g_A}{8f_\pi^2}\, \frac{c_D}{f_\pi^2 \Lambda_\chi} \sum_{\pi(ijk)} \frac{\boldsymbol{\sigma}_k \cdot \mathbf{q}_k}{q_k^2 + m_\pi^2}\, \boldsymbol{\sigma}_i \cdot \mathbf{q}_k\, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k\,, \tag{5}$$

$$V_E = \frac{c_E}{2f_\pi^4 \Lambda_\chi} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k\,, \tag{6}$$

Here, as in the NN sector discussed in the previous section, $\mathbf{q}_i = \mathbf{p}'_i - \mathbf{p}_i$ is the momentum transfer of particle i, while and $F^{\alpha\beta}_{ijk}$ includes the c_i contributions:

$$F^{\alpha\beta}_{ijk} = \delta^{\alpha\beta}\left[-\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2}\,\mathbf{q}_i\cdot\mathbf{q}_k\right] + \sum_\gamma \frac{c_4}{f_\pi^2}\varepsilon^{\alpha\beta\gamma}\,\tau_j^\gamma\,\boldsymbol{\sigma}_j\cdot(\mathbf{q}_i\times\mathbf{q}_k)\,.$$

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:

$$V_E^{ijk} = \frac{c_E}{2f_\pi^4\Lambda_\chi}\sum_{\pi(ijk)}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_k\,\delta(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\,. \tag{7}$$

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

$$V_D^{ijk} = \frac{c_D g_A}{24 f_\pi^4\Lambda_\chi}\sum_{\pi(ijk)}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_k\left[\frac{m_\pi^2}{4\pi}\,\delta(\mathbf{r}_{ij})X_{ik}(\mathbf{r}_{kj}) - \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_k\,\delta(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right]. \tag{8}$$

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:

$$V_{C,c_1}^{ijk} = \frac{c_1 m_\pi^4 g_A^2}{2f_\pi^4(4\pi)^2}\sum_{\pi(ijk)}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_k\,\boldsymbol{\sigma}_i\cdot\hat{\mathbf{r}}_{ij}\,\boldsymbol{\sigma}_k\cdot\hat{\mathbf{r}}_{kj}\times U(r_{ij})Y(r_{ij})U(r_{kj})Y(r_{kj})\,. \tag{9}$$

and

$$\begin{aligned} V_{C,c_3}^{ijk} &= \frac{c_3 g_A^2}{36 f_\pi^4}\sum_{\pi(ijk)}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_k \qquad (10)\\ &\times\left[\frac{m_\pi^4}{(4\pi)^2}X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj}) - \frac{m_\pi^2}{4\pi}X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj}) - \frac{m_\pi^2}{4\pi}X_{ik}(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij}) + \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_k\delta(\mathbf{r}_{ij})\,\delta(\mathbf{r}_{kj})\right]. \end{aligned}$$

and

$$\begin{aligned} V_{C,c_4}^{ijk} &= \frac{c_4 g_A^2}{72 f_\pi^4}\sum_{\pi(ijk)}\boldsymbol{\tau}_i\cdot(\boldsymbol{\tau}_k\times\boldsymbol{\tau}_j)\\ &\times\left[\frac{m_\pi^4}{2i(4\pi)^2}[X_{ij}(\mathbf{r}_{ij}),X_{kj}(\mathbf{r}_{kj})] - \frac{m_\pi^2}{4\pi}\boldsymbol{\sigma}_i\cdot(\boldsymbol{\sigma}_k\times\boldsymbol{\sigma}_j)(1-T(r_{ij}))Y(r_{ij})\delta(\mathbf{r}_{kj})\right.\\ &-\frac{m_\pi^2}{4\pi}\boldsymbol{\sigma}_i\cdot(\boldsymbol{\sigma}_k\times\boldsymbol{\sigma}_j)\left(1-T(r_{kj})\right)Y(r_{kj})\delta(\mathbf{r}_{ij}) - \frac{3m_\pi^2}{4\pi}\boldsymbol{\sigma}_i\cdot\hat{\mathbf{r}}_{ij}\,\hat{\mathbf{r}}_{ij}\cdot(\boldsymbol{\sigma}_k\times\boldsymbol{\sigma}_j)T(r_{ij})Y(r_{ij})\delta(\mathbf{r}_{kj})\\ &\left.-\frac{3m_\pi^2}{4\pi}\boldsymbol{\sigma}_k\cdot\hat{\mathbf{r}}_{kj}\,\hat{\mathbf{r}}_{kj}\cdot(\boldsymbol{\sigma}_j\times\boldsymbol{\sigma}_i)T(r_{kj})Y(r_{kj})\delta(\mathbf{r}_{ij}) + \boldsymbol{\sigma}_i\cdot(\boldsymbol{\sigma}_k\times\boldsymbol{\sigma}_j)\delta(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right]. \qquad (11) \end{aligned}$$

Note that while the Feynman diagram for V_C, in accordance with its physical intepretation, 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 replacing the δ functions by smeared-out delta functions as follows:

$$\delta(\mathbf{r}) \;\to\; \delta_{R_{3\mathrm{N}}}(\mathbf{r}) = \frac{1}{\pi\Gamma(3/4)R_{3\mathrm{N}}^3}e^{-(r/R_{3\mathrm{N}})^4}\,, \tag{12}$$

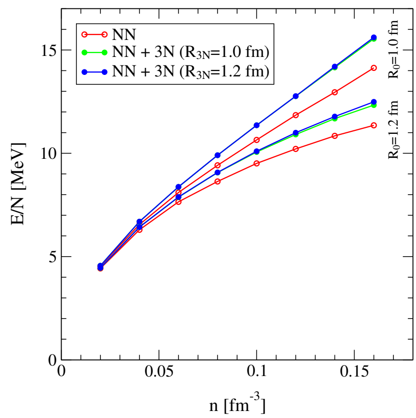

Figure 2. AFDMC energy per particle vs density for neutron matter at N^{2}LO, including both NN forces and the 3N V_C interaction. Both NN and 3N cutoffs are varied in the range 1.0 − 1.2 fm.

where $R_{3\mathrm{N}}$ 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_{long}:

$$Y(r) \;\rightarrow\; Y(r)\left(1 - e^{-(r/R_{3\mathrm{N}})^4}\right). \tag{13}$$

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 $R_{3\mathrm{N}} \rightarrow 0$ (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, $R_{3\mathrm{N}} = 1.0 - 1.2$ 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 $R_{3\mathrm{N}}$ 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].

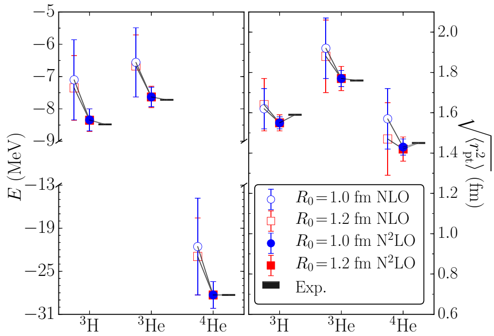

Figure 3. $A = 3, 4$ binding energies and point proton radii as compared to experiment.

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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