Chiral Nucleon-Nucleon Forces in Nuclear Structure Calculations

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Nuclear physics exhibits a separation of scales

\begin{align*}
\ln Q & \quad \text{perturbative QCD} \\
\sim 1 \text{ GeV} & \quad M_{\text{QCD}} \sim m_N, m_p, 4\pi f_\pi, \ldots \\
\sim 100 \text{ MeV} & \quad M_{\text{nuc}} \sim f_\pi, 1/r_{NN}, m_\pi, \ldots \\
\sim 30 \text{ MeV} & \quad \xi \sim 1/a_{NN}
\end{align*}

To resort to \textit{EFT} could be a valuable way to describe the physics of nuclei, since the underlying theory \textit{QCD} is not solvable.
Weinberg’s “theorem”

“If one writes down the most general possible Lagrangian, including all terms consistent with assumed symmetry principles, and then calculates $S$-matrix elements with this Lagrangian to any order in perturbation theory, the result will simply be the most general possible $S$-matrix consistent with analyticity, perturbative unitarity, cluster decomposition and the assumed symmetry principles”\(^1\)

\(^1\) *S. Weinberg, Physica A* **96** 327 (1979)
Chiral EFT for nuclear theory

- Identify the relevant degrees of freedom (nucleons, pions, deltas) and symmetries of the problem (chiral symmetry).

- Build up the most general Lagrangian consistent within these constraints.

\[
\begin{align*}
\mathcal{L}_{\pi\pi} &= \frac{f_\pi^2}{4} \text{tr} \left[ \partial_\mu U \partial_\mu U^\dagger + m_\pi^2 (U + U^\dagger) \right] + \ldots \\
\mathcal{L}_{\pi N} &= \bar{\Psi} \left( i \gamma^\mu D_\mu - M_N + \frac{g_A}{2} \gamma^\mu \gamma_5 u_\mu + \ldots \right) \Psi \\
\mathcal{L}_{NN} &= -\frac{1}{2} C_S \bar{\mathbf{N}} \mathbf{N} \bar{\mathbf{N}} \mathbf{N} - \frac{1}{2} C_T (\bar{\mathbf{N}} \mathbf{\bar{\sigma}} \mathbf{N}) \cdot (\bar{\mathbf{N}} \mathbf{\bar{\sigma}} \mathbf{N}) + \ldots
\end{align*}
\]

- Perform a perturbative expansion of this Lagrangian for momenta \( q < \Lambda \), and adjust the coefficients to the physical observables (renormalization).
The chiral perturbative expansion

\begin{align*}
\text{LO} & \quad (Q/\Lambda_\chi)^0 \\
\text{NLO} & \quad (Q/\Lambda_\chi)^2 \\
\text{NNLO} & \quad (Q/\Lambda_\chi)^3 \\
\text{N^3LO} & \quad (Q/\Lambda_\chi)^4 \\
\end{align*}

2N Force \quad 3N Force \quad 4N Force
An important observation: ChPT allows the contraction of nuclear two- and many-body forces on an equal footing.

More precisely: most interaction vertices in the 3NF, as well as in the 4NF, occur in the 2NF too.

Consequently, the corresponding parameters LECs are consistently the same in the 2NF and 3NF.
A main issue: ChPT introduces a cutoff $\Lambda$ and the calculated observables depends on its choice.

Necessarily, the chiral hamiltonian has to be renormalized for each chosen cutoff via fixing the chosen LECs to fit the available experimental data ($NN$ scattering data, deuteron and triton binding energies, ...).

Cutoff invariance can be then guaranteed, at least for the two- and three-body systems.

What about the many-body systems?
Infinite nuclear matter: this is an interesting environment to study the dependence on $\Lambda$ of the results of a many-mody calculation.

We calculate infinite nuclear matter EOS starting from chiral 2NF and 3NF defined within different cutoffs.

Perturbative approach: we perform a Goldstone expansion of the binding energy per nucleon $E/A$ up to third order in the energy.

▶ ... and many, many others ...
The perturbative expansion

(a) $k_\alpha k_\beta$

(b) $k_\alpha k_\beta + k_\beta k_\alpha$

(c) $k_\alpha k_\beta + k_\beta k_\alpha$

(d) $k_\alpha k_\beta k_c k_d$

(e) $k_\alpha k_\beta k_\gamma k_\delta$
The $N^3$LO two-body potential

We consider for our study three $N^3$LO two-body potentials with different cutoffs and different regulator functions

\[
f(p', p) = \exp\left[-\left(\frac{p'}{\Lambda}ight)^2 n - \left(\frac{p}{\Lambda}\right)^2 n\right]:
\]

- $\Lambda = 500$ MeV using $n = 2$ in the regulator function\(^1\)
- $\Lambda = 450$ MeV using $n = 3$ in the regulator function
- $\Lambda = 414$ MeV using $n = 10$ in the regulator function (sharp cutoff)\(^2\)

---


Phase shifts

- Dotted black curve: $\Lambda = 500$ MeV
- Dashed blue curve: $\Lambda = 450$ MeV
- Solid red curve: $\Lambda = 414$ MeV
The $N^2$LO three-body potential

Aside the $N^3$LO two-body potentials we consider also the contribution from their corresponding three-body potentials, calculated at $N^2$LO:

They bring two more coefficients ($c_D$, $c_E$) corresponding to the contact and the $1\pi$-exchange terms, to be adjusted to the physics of the three-nucleon system.
The fit of $c_D$, $c_E$ parameters

The binding energy of the triton:
The fit of \( c_D, c_E \) parameters

The triton Gamow-Teller matrix elements of the triton via the \( \mu \) capture in \(^2\text{H}(\mu^-, \nu_\mu)\text{nn} \) and \(^3\text{He}(\mu^-, \nu_\mu)^3\text{H} \):

<table>
<thead>
<tr>
<th>( \Lambda ) cutoff (in MeV)</th>
<th>( c_D )</th>
<th>( c_E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>0.0</td>
<td>-0.17</td>
</tr>
<tr>
<td>450</td>
<td>-0.24</td>
<td>-0.11</td>
</tr>
<tr>
<td>414</td>
<td>-0.4</td>
<td>-0.07</td>
</tr>
</tbody>
</table>

The density-dependent effective $NN$ potential

The effect of the chiral $N^2$LO 3NF has been taken into account adding a density-dependent two-body potential $V_{\text{NNN}}$ to the $N^3$LO two-body one:

The perturbative expansion

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The equation of state for infinite neutron matter
The infinite neutron matter EOS

**A keypoint:** in pure neutron matter the contact interaction, \( V_E \), and the \( 1\pi \)-exchange term, \( V_D \), that appear in the \( \text{N}^2\text{LO} \) three-body force, vanish.

Therefore, the low-energy constants of \( V_E \) and \( V_D c_E, c_D \) do not play any role in the determination of the EOS of infinite neutron matter.

The EOS depends, when using with chiral 3NFs up to \( \text{N}^2\text{LO} \), only on the parameters that have been fixed in the two-nucleon system.
The infinite neutron matter EOS

$\rho$ [fm$^3$]

0.00 0.05 0.10 0.15 0.20 0.25

$E/A$ [MeV]

1st order
2nd order
3rd order
Pade’ [2|1]

$E_1$
$E_2$
$E_3$

$E_{[2|1]}$

N$^3$LO 2NF [500 MeV]
The infinite neutron matter EOS

$N^3$LO 2NF + $N^2$LO 3NF [500 MeV]

- 1st order
- 2nd order
- 3rd order
- Pade' [2|1]
The infinite neutron matter EOS

- \( \Lambda = 500 \) MeV
- \( \Lambda = 450 \) MeV
- \( \Lambda = 414 \) MeV

Two-body force only

Two-body + three-body forces

\( \rho \) [fm\(^{-3}\)]

\( E/A \) [MeV]
The equation of state for infinite symmetric nuclear matter
The infinite nuclear matter EOS

N³LO 2NF [500 MeV]

1st order
2nd order
3rd order
Pade’ [2|1]

E/A [MeV]

E₁
E₂
E₃

E_{[2|1]}

E/A [MeV]

k_F [fm⁻¹]

0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
The infinite nuclear matter EOS

N\(^3\)LO 2NF + N\(^2\)LO 3NF [500 MeV]

1st order
2nd order
3rd order
Pade’ [2|1]
The infinite nuclear matter EOS

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What has been left out ...

$3p - 3h$ 3BF diagrams:
Results for $k_F = 1.3 \text{ fm}^{-1}$

Perturbative contributions only 2NF

<table>
<thead>
<tr>
<th>Cutoff parameter $\Lambda$ (MeV)</th>
<th>414</th>
<th>450</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF contribution</td>
<td>-35.507</td>
<td>-32.786</td>
<td>-25.066</td>
</tr>
<tr>
<td>2nd order $pp$ diagram</td>
<td>-5.736</td>
<td>-8.551</td>
<td>-14.060</td>
</tr>
<tr>
<td>3rd order $pp$ diagram</td>
<td>0.017</td>
<td>-0.022</td>
<td>0.653</td>
</tr>
<tr>
<td>3rd order $hh$ diagram</td>
<td>-0.022</td>
<td>-0.021</td>
<td>-0.027</td>
</tr>
<tr>
<td>3rd order $ph$ diagram</td>
<td>1.040</td>
<td>1.200</td>
<td>-0.279</td>
</tr>
</tbody>
</table>
Results for $k_F = 1.3 \text{ fm}^{-1}$

Perturbative contributions $2\text{NF} + 3\text{NF}$

<table>
<thead>
<tr>
<th>Cutoff parameter $\Lambda$ (MeV)</th>
<th>414</th>
<th>450</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>3rd order $pp$ diagram</td>
<td>0.563</td>
<td>0.745</td>
<td>1.642</td>
</tr>
<tr>
<td>3rd order $hh$ diagram</td>
<td>-0.010</td>
<td>-0.008</td>
<td>-0.008</td>
</tr>
<tr>
<td>3rd order $ph$ diagram</td>
<td>0.581</td>
<td>0.152</td>
<td>-1.516</td>
</tr>
</tbody>
</table>
The calculated PNM and SNM EOS and the corresponding symmetry energies show in Fig. 4 and 5, respectively. The inspection of these figures shows how our results reproduce well the empirical SNM saturation point and the value of the symmetry energy at saturation density, the latter quantity being related to the isospin dependence of nuclear forces.

Two other interesting physical quantities related to PNM and SNM at saturation density are the incompressibility $K_0$ and the slope of the symmetry energy $L$.

The empirical value of the SNM incompressibility is determined from experimental data on Giant Monopole Resonance in finite nuclei, at present its accepted value is $K_0 = 230 \pm 30$ MeV [26]. From our calculations we obtain a compressibility $K_0 = 279$ MeV, a value very close to the empirical one.

The quantity $L$ determines most of the behavior of the symmetry energy in the proximity of saturation. Its empirical determination - centered at $L = 70$ MeV - is indirect and mainly based on the analysis of heavy-ion collisions at intermediate energies and nuclear structure measurements [27]. Our calculated value for $L$ is 68 MeV, in good agreement with the empirical value.

4. Concluding remarks

In this paper we have studied the properties of infinite nuclear matter employing a chiral potential. This has been done within the framework of the perturbative Goldstone expansion, using a chiral $N^3LO$ and $N^2LO$ potential with a sharp cut-off $\Lambda = 414$ MeV. The LECs involved in the potential have been chosen consistently for the two- and three-body components, and in particular the 3NF LECs $c_D$ and $c_E$ have been fixed as to reproduce the experimental $A = 3$ binding energy and Gamow-Teller matrix elements in $\beta$-decay. Our results for PNM and SNM EOS turn out to be in good agreement with the empirical properties of infinite nuclear matter. The ability to provide realistic nuclear matter predictions employing (consistent) two- and three-body interactions whose LECs are constrained by the properties of the two- and the...
Part 1: concluding remarks

- Chiral potentials with a cutoff $\Lambda \leq 500$ MeV exhibit a perturbative behavior both for infinite neutron and nuclear matter calculations.
- The EOS for infinite neutron matter shows substantial regulator independence when including 3NF contributions.
- The EOS for infinite nuclear matter shows lesser regulator independence.
Part 1: concluding remarks

- Chiral potentials with a cutoff $\Lambda \leq 500$ MeV exhibit a perturbative behavior both for infinite neutron and nuclear matter calculations.
- The EOS for infinite neutron matter shows substantial regulator independence when including 3NF contributions.
- The EOS for infinite nuclear matter shows lesser regulator independence.

Perspectives

- Improve the calculation of the perturbative expansion.
- Need of a $N^3$LO three-body force?
- Need to include four-body force effects?
Calculations for finite nuclei: the realistic shell model
▶ ... and many, many others ...
over-correcting the inadequacies of the NN interaction in these spectra that the chiral NNN interaction is clearly evident. There is an initial indication of excited states. The celebrated case of the ground state demonstrated in the odd mass nuclei for the lowest few in comparison with experiment. This is especially well-improved, and from Fig. 1, there is room for additional improvement and the NN+NNN interaction contributes significantly to improve theory.

We discuss the possibilities below. The results shown are obtained in the largest extrapolation, we can see that the best overall description of the NNN interaction, which is consistent with the NN interaction that we employed. Since this strength is some-
The realistic shell model

- The starting point is a realistic potential $V_{NN}$
- An effective shell-model hamiltonian $H_{\text{eff}}$ is then derived by way of the many-body theory of the effective hamiltonian
- The shell model calculation is performed using only quantities obtained from the effective shell-model hamiltonian, both single-particle energies and residual two-body interaction are derived from the theory
The shell-model effective hamiltonian

A very useful way to derive $H_{\text{eff}}$ is the time-dependent perturbative approach as developed by Kuo and his co-workers in the 1970s (see T. T. S. Kuo and E. Osnes, Lecture Notes in Physics vol. 364 (1990))

In this approach the effective hamiltonian $H_{\text{eff}}$ is expressed as

$$H_{\text{eff}} = \hat{Q} - \hat{Q}'\int \hat{Q} + \hat{Q}'\int \hat{Q}\int \hat{Q} - \hat{Q}'\int \hat{Q}\int \hat{Q}\int \hat{Q} \ldots ,$$

- The integral sign represents a generalized folding operation (folded diagrams are summed up at all orders using Lee-Suzuki iterative technique)
- The $\hat{Q}$-box is a collection of irreducible valence-linked Goldstone diagrams that takes into account core-polarization effects for the valence nucleons in the model space
The shell-model effective hamiltonian

\( \hat{Q} \)-box diagrams and all effective operators (electric quadrupole transitions, magnetic dipole transitions, ...) are expanded up to third order in perturbation theory.

We calculate the Padé approximant \([2|1]\) of the \( \hat{Q} \)-box, in order to obtain a better estimate of the value to which the perturbation series should converge

\[
[2|1] = V_0^{Qbox} + V_1^{Qbox} + V_2^{Qbox} (1 - (V_2^{Qbox})^{-1} V_3^{Qbox})^{-1}
\]

We include enough intermediate states so that the \( H_{\text{eff}} \) has a flat dependence on them.
\(Q\)-box perturbative expansion: 1-body diagrams
$\hat{Q}$-box perturbative expansion: 2-body diagrams
\( \hat{Q} \)-box perturbative expansion: 2-body diagrams

The shell-model effective hamiltonian

A benchmark calculation: shell-model deals with open-shell nuclei, a basic test is a nucleus that can be described as 2 nucleons outside a close-shell core.

We have chosen to test our calculations with those of NCSM for $^6\text{Li}$ with N$^3$LO potential: its structure should be made up by the $^4\text{He}$ core plus one valence proton and one valence neutron.

The comparison with NCSM needs another upgrade for our calculations, we have to start from a purely intrinsic many-body hamiltonian, so to avoid center-of-mass spurious motion:

$$H = (1 - \frac{1}{A}) \sum_i \frac{p_i^2}{2M} + \sum_{i<j} (V_{ij} - \frac{p_i \cdot p_j}{MA}) =$$

$$\sum_i \left( \frac{p_i^2}{2M} + \frac{1}{2} M \omega^2 r_i^2 \right) + \sum_{i<j} (V_{ij} - \frac{1}{2} M \omega^2 r_i^2 - \frac{p_i^2}{2MA} - \frac{p_i \cdot p_j}{MA} ) = H_0 + H_I$$
Test: $^6$Li first excited states with N$^3$LO potential
Test: $^{10}\text{B}$ first excited states with $N^3\text{LO}$ potential
The effect of three-nucleon forces: $N^3LO$ (500)
The effect of three-nucleon forces: $N^3LO$ (500)
The effect of three-nucleon forces: $N^3LO (414)$

Graphs showing the energy levels for $^6Li$ and $^8Li$ with different forces applied: 2BF, 2BF + 3BF, and Experiment (Exp) results.
The effect of three-nucleon forces: N³LO (414)

Diagram showing the energy levels of ¹⁰B and ¹²C with states labeled as 0⁺, 1⁺, 2⁺, 3⁺, and 4⁺. The diagrams compare the predictions of 2BF, 2BF + 3BF, and experimental (Exp) data.

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The effect of 3NF: oxygen isotopes with $N^3$LO (414)

Expt.
N$^3$LOW 2BF + N$^2$LOW 3BF
N$^3$LOW 2BF

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Concluding remarks

- The agreement of our results with the experimental data testifies the reliability of a microscopic shell-model calculation with chiral potentials.
- Pure three-body forces contribute positively to the improvement of theoretical results.
- Role of three-body correlations should be investigated.
- Perspectives: benchmark calculations with other many-body approaches.