Properties of nuclei from chiral EFT interactions

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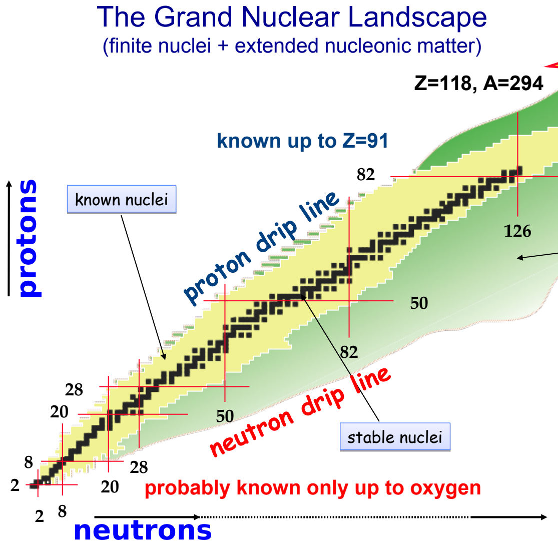
NUCLEI Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY

www.computingnuclei.org

NERSC National Energy Research Scientific Computing Center



neutron stars

Outline

- The nuclear Hamiltonian and the method
- Nuclear energies and charge radii
- Nuclear and neutron matter EOS
- Electro-magnetic currents and nuclear magnetic moments
- Conclusions

Nuclear Hamiltonian

Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

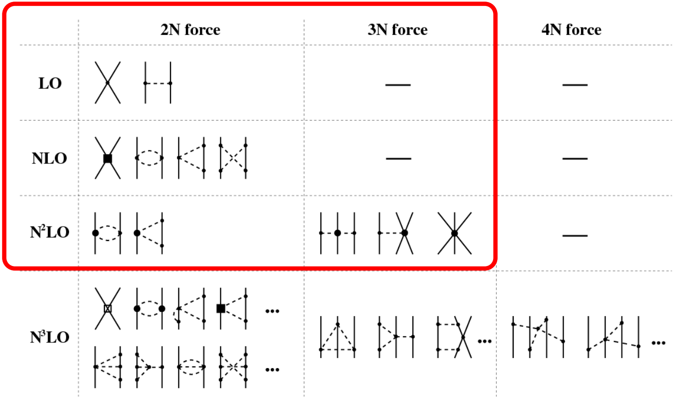
$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

v_{ij} NN fitted on scattering data.

V_{ijk} typically constrained to reproduce light systems (A=3,4).

- "Phenomenological/traditional" interactions (Argonne/Illinois)
- Local chiral forces up to N^{2}LO (Gezerlis, et al. PRL 111, 032501 (2013), PRC 90, 054323 (2014), Lynn, et al. PRL 116, 062501 (2016)).

Nuclear Hamiltonian



Expansion in powers of Q/Λ, Q$\sim$100 MeV, Λ $\sim$1 GeV.

Long-range physics given by pion-exchanges (no free parameters).

Short-range physics: contact interactions (LECs) to fit.

Operators need to be regulated $\rightarrow$ cutoff dependency!

Order's expansion provides a way to quantify uncertainties!

Truncation error estimate

Error quantification (one possible scheme). Define

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right),$$

where p is a typical nucleon's momentum or k_F for matter, Λ_b is the cutoff, and calculate:

$$\Delta(N2LO) = \max\left(Q^4|\hat{O}_{LO}|,\ Q^2|\hat{O}_{LO} - \hat{O}_{NLO}|,\ Q|\hat{O}_{NLO} - \hat{O}_{N2LO}\right)$$

Epelbaum, Krebs, Meissner (2014).

Quantum Monte Carlo

Propagation in imaginary time:

$$H\,\psi(\vec{r}_1 \ldots \vec{r}_N) = E\,\psi(\vec{r}_1 \ldots \vec{r}_N) \qquad \psi(t) = e^{-(H-E_T)t}\psi(0)$$

Ground-state extracted in the limit of $t \to \infty$.

Propagation performed by

$$\psi(R,t) = \langle R|\psi(t)\rangle = \int dR'\,G(R,R',t)\psi(R',0)$$

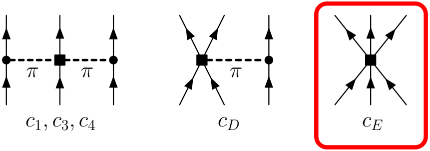
- Importance sampling: $G(R,R',t) \to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, bigger systems, less accurate than GFMC

Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 2-3 %.

See Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Chiral three-body forces, some issue



Equivalent forms of operators entering in V_E (Fierz-rearrangement):

$$1, \quad \sigma_i\cdot\sigma_j, \quad \tau_i\cdot\tau_j, \quad \sigma_i\cdot\sigma_j\tau_i\cdot\tau_j, \quad \sigma_i\cdot\sigma_j\tau_i\cdot\tau_k, \quad [(\sigma_i\times\sigma_j)\cdot\sigma_k][(\tau_i\times\tau_j)\cdot\tau_k]$$

Epelbaum et al (2002). We investigated the following choices:

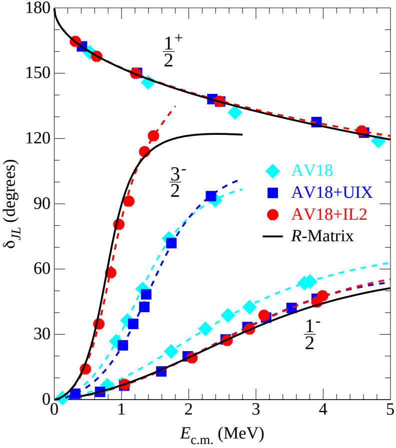
$$V_{E\tau} = \frac{c_E}{\Lambda_\chi F_\pi^4}\sum_{i<j<k}\sum_{\text{cyc}}\tau_i\cdot\tau_k\delta(r_{kj})\delta(r_{ij})$$

$$V_{E1} = \frac{c_E}{\Lambda_\chi F_\pi^4}\sum_{i<j<k}\sum_{\text{cyc}}\delta(r_{kj})\delta(r_{ij})$$

Qualitative differences expected, i.e. consider ^{4}He vs neutron matter!

Chiral three-body forces

Coefficients c_D and c_E fit to reproduce the binding energy of ^{4}He and neutron-^{4}He scattering. $\rightarrow$ more information on T=3/2 part of three-body interaction. (vs A=3, 4)



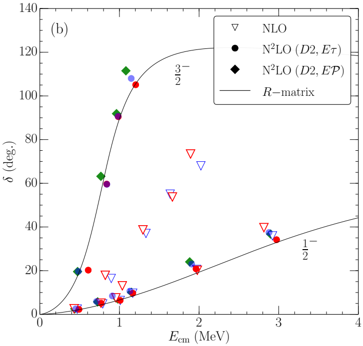
GFMC neutron-^{4}He results using Argonne Hamiltonians.

Nollett, Pieper, Wiringa, Carlson, Hale, PRL (2007).

^{4}He binding energy and p-wave n-^{4}He scattering

Regulator: $\delta(r) = \frac{1}{\pi\Gamma(3/4)R_0^3}\exp(-(r/R_0)^4)$

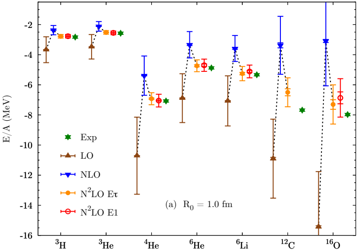
Cutoff R_0 taken consistently with the two-body interaction.

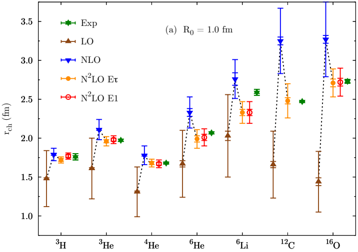


Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

AFDMC calculations

Energies and charge radii, cutoff 1.0 fm:





Lonardoni, et al., PRL (2018), PRC (2018).

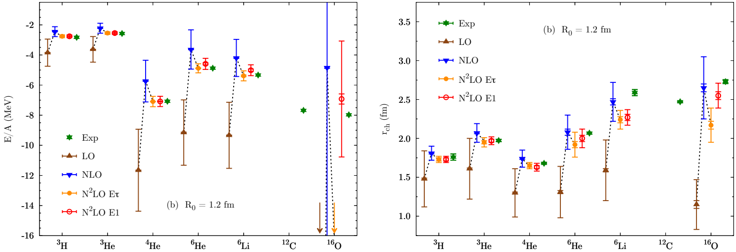
Qualitative good description of both energies and radii.

Good convergence (although uncertainties still large if LO included).

Different V_E operators give similar results.

AFDMC calculations

Energies and charge radii, cutoff 1.2 fm:

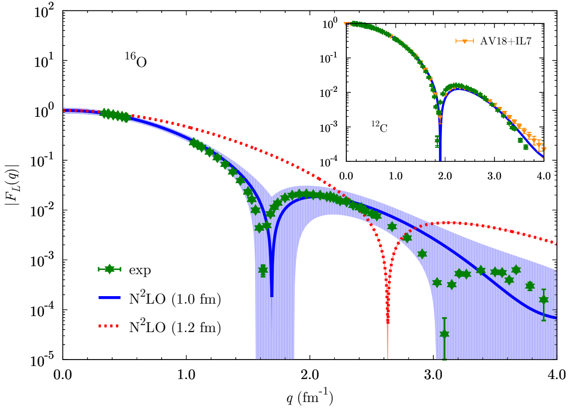


Lonardoni, et al., PRL (2018), PRC (2018).

Qualitative good description up to A=6.

Different V_E operators give very different results for ^{16}O.

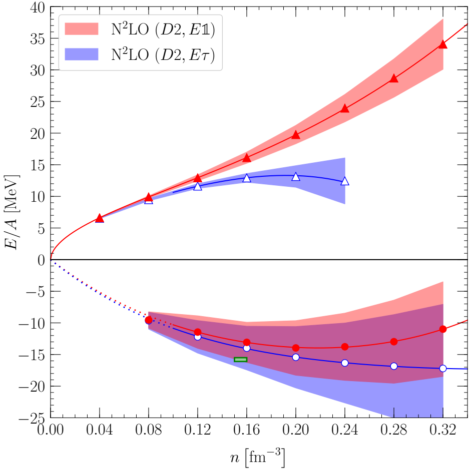
Charge form factor



Lonardoni, et al., PRL (2018), PRC (2018).

Hard interaction reproduces exp. Similar good results for other nuclei.

Nuclear and neutron matter EOS

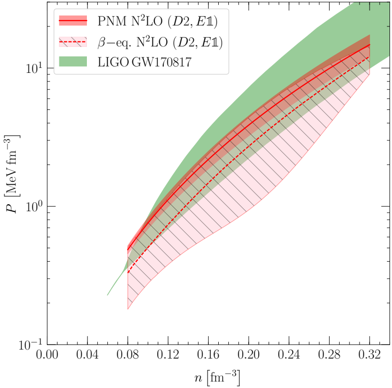


Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Symmetric nuclear matter less dependent upon the choice of V_E (cf. nuclei). E_τ is very bad for neutron matter.

Nuclear and neutron matter EOS

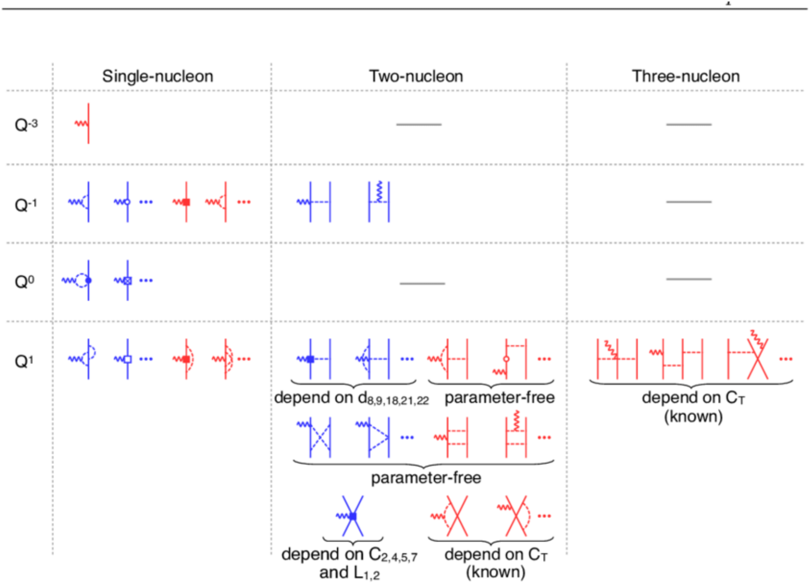
Pressure of pure neutron matter and $\beta-$equilibrated matter.



Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Very good agreement with LIGO posterior from GW.

Electro-magnetic currents



Electro-magnetic currents

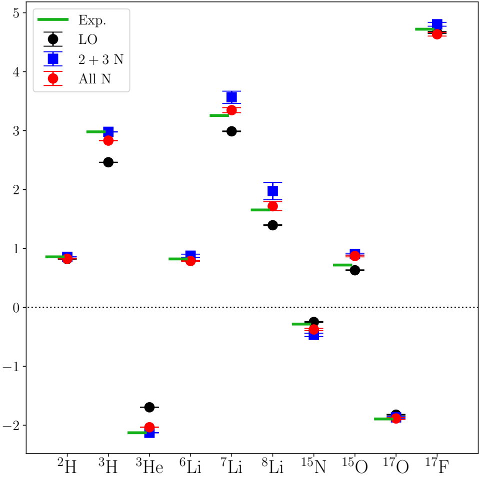
But, within chiral EFT, there are different ways to construct the currents.

Hamiltonian	Pisa/Norfolk/WUSTL	Bochum
Q^0 LO	Q^{-2} LO	Q^{-3} LO
Q^1 –	Q^{-1} NLO	Q^{-2} –
Q^2 NLO	Q^0 N2LO	Q^{-1} NLO
Q^3 N2LO	Q^1 N3LO	Q^0 N2LO
		Q^1 N3LO
	2 LECS (contact)	2 LECS (contact)
	1 LEC (OPE)	

Understanding which currents to use, chiral order, regulators, continuity equation, etc., is still work in progress.

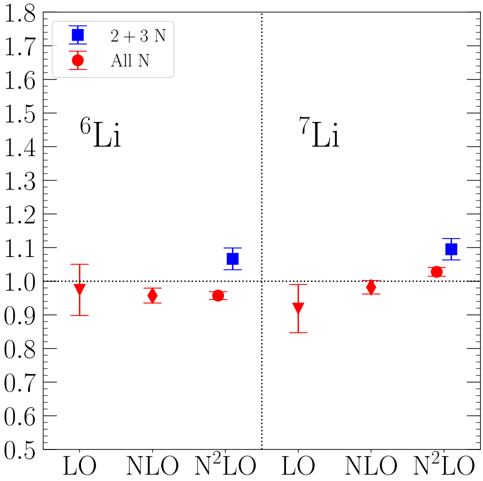
The Pisa/etc currents will be used in the next few slides (with some adjustment...).

Fit: up to A=3 or including all nuclei.



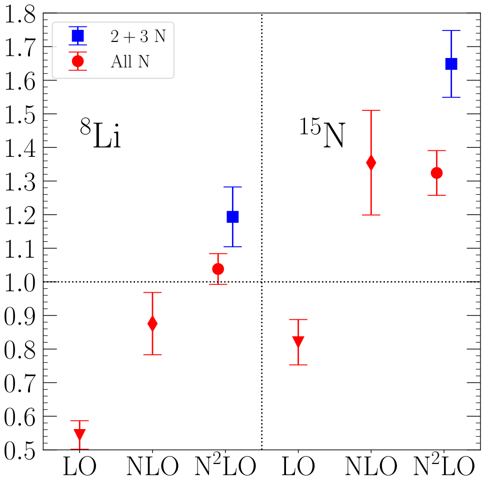
Nuclear magnetic moments

Order by order calculation. Same order in the Hamiltonian and currents.



Pretty good convergence.

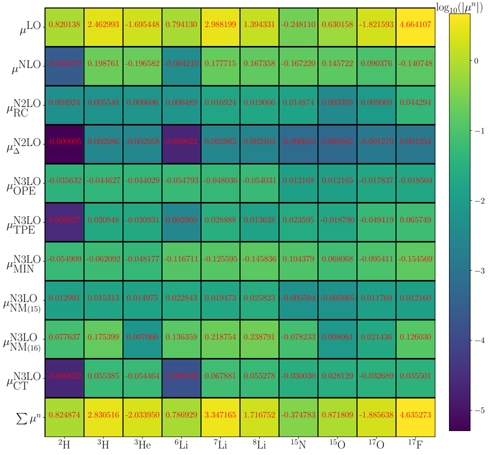
Nuclear magnetic moments



In these cases the convergence is not clear (LO errors are smaller than NLO).

Nuclear magnetic moments

Magnetic moments, single contributions.



In several cases, the contribution of N3LO terms is larger than N2LO and NLO.

Conclusions

- Chiral EFT provides a way to constrain nuclear interactions and estimate systematic uncertainties
- Nuclear energies and radii well reproduced by the hard interaction. But several issues with the softer one.
- Role of V_E critical for neutron matter, but symmetric nuclear matter is qualitatively ok.
- EOS compatible with GW observations.
- Still a lot of work to do to derive EM currents in a consistent way (work in progress).
- Overall good description of nuclear magnetic moments. Best fitting strategy not clear yet.
- Convergence with the chiral expansion not clear.

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