Quantum Monte Carlo with Chiral Effective Field Theory Interactions: An Update

Alexandros Gezerlis

UNIVERSITY of GUELPH

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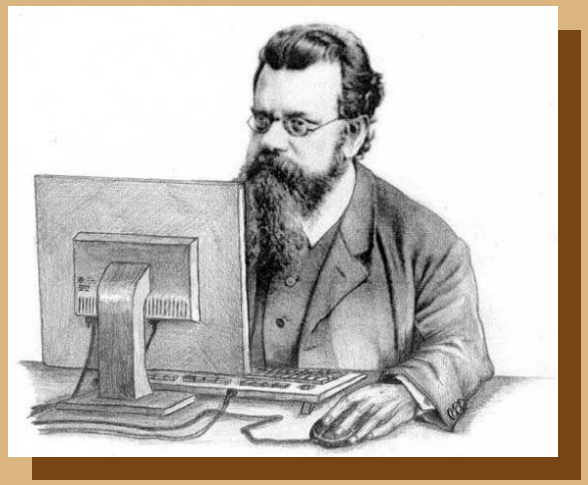
Thanks to my collaborators

- Joe Carlson (LANL)
- Evgeny Epelbaum (Bochum)
- Stefano Gandolfi (LANL)
- Kai Hebeler (OSU)
- **Joel Lynn (LANL)**
- Andreas Nogga (Juelich)
- Achim Schwenk (Darmstadt)
- **Ingo Tews (Darmstadt)**

Outline



Credit: Bernhard Reischl

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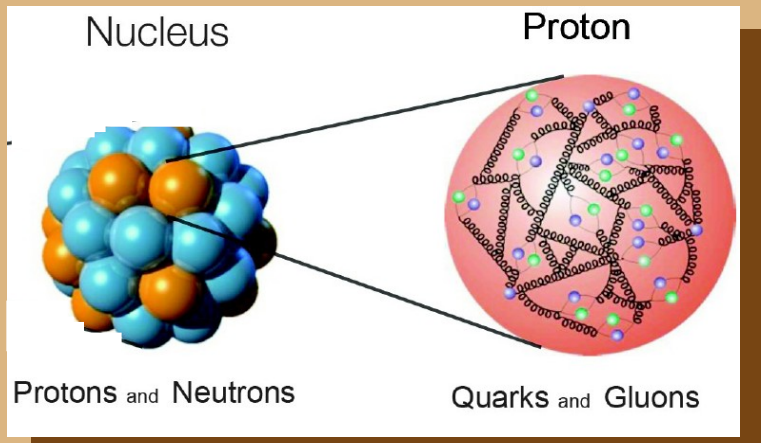

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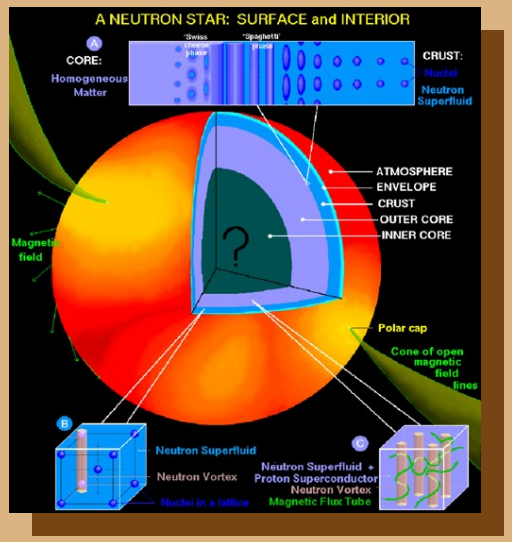

Credit: Dany Page

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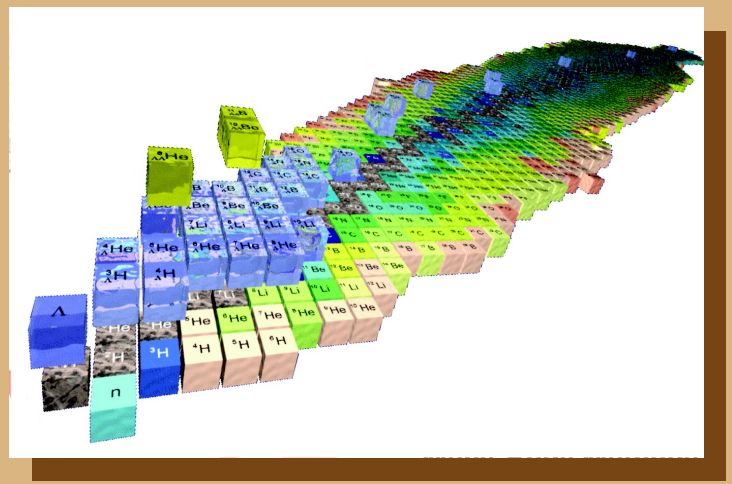


Let's start with Quantum Monte Carlo

Quantum Monte Carlo

A family of microscopic simulation methods,
very successful in other areas of physics (and chemistry)

Ground State of the Electron Gas by a Stochastic Method

Abstract | References | Citing Articles (6,935) | Page Images

Download: PDF (234 kB) Export: BibTeX or EndNote (RIS)

D. M. Ceperley
National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, California 94720

B. J. Alder
Lawrence Livermore Laboratory, University of California, Livermore, California 94550

Received 16 April 1980; published in the issue dated 18 August 1980

An exact stochastic simulation of the Schroedinger equation for charged bosons and fermions has been used to calculate the correlation energies, to locate the transitions to their respective crystal phases at zero temperature within 10%, and to establish the stability at intermediate densities of a ferromagnetic fluid of electrons.

URL: http://link.aps.org.subzero.lib.uoguelph.ca/doi/10.1103/PhysRevLett.45.566
DOI: 10.1103/PhysRevLett.45.566
PACS: 67.90.+i, 71.45.Gm

Continuum Quantum Monte Carlo

Rudiments of Diffusion Monte Carlo:

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau}\Psi_V$$
$$\to \alpha_0 e^{-(E_0-E_T)\tau}\Psi_0$$

How to do? Start somewhere and evolve

$$\psi(\mathbf{R},\tau) = \int G(\mathbf{R},\mathbf{R}',\tau)\psi(\mathbf{R}',0)d\mathbf{R}'$$

With a standard propagator

$$G(\mathbf{R},\mathbf{R}',\tau) = \langle \mathbf{R}|e^{-(H-E_0)\tau}|\mathbf{R}'\rangle$$

Cut up into many time slices

$$G(\mathbf{R},\mathbf{R}',\Delta\tau) \approx e^{-\frac{V(\mathbf{R})+V(\mathbf{R}')}{2}\Delta\tau}\left(\frac{m}{2\pi\hbar^2\tau}\right)^{\frac{3A}{2}} e^{-\frac{m|\mathbf{R}-\mathbf{R}'|^2}{2\hbar^2\tau}}$$

Quantum Monte Carlo

What about more general Hamiltonians?

$$H = -\frac{\hbar^2}{2m}\sum_{j=1,N}\nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl}$$

Focus on the two-body interactions for now

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k}\sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

Eight channels often enough (e.g. Argonne v8')

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$

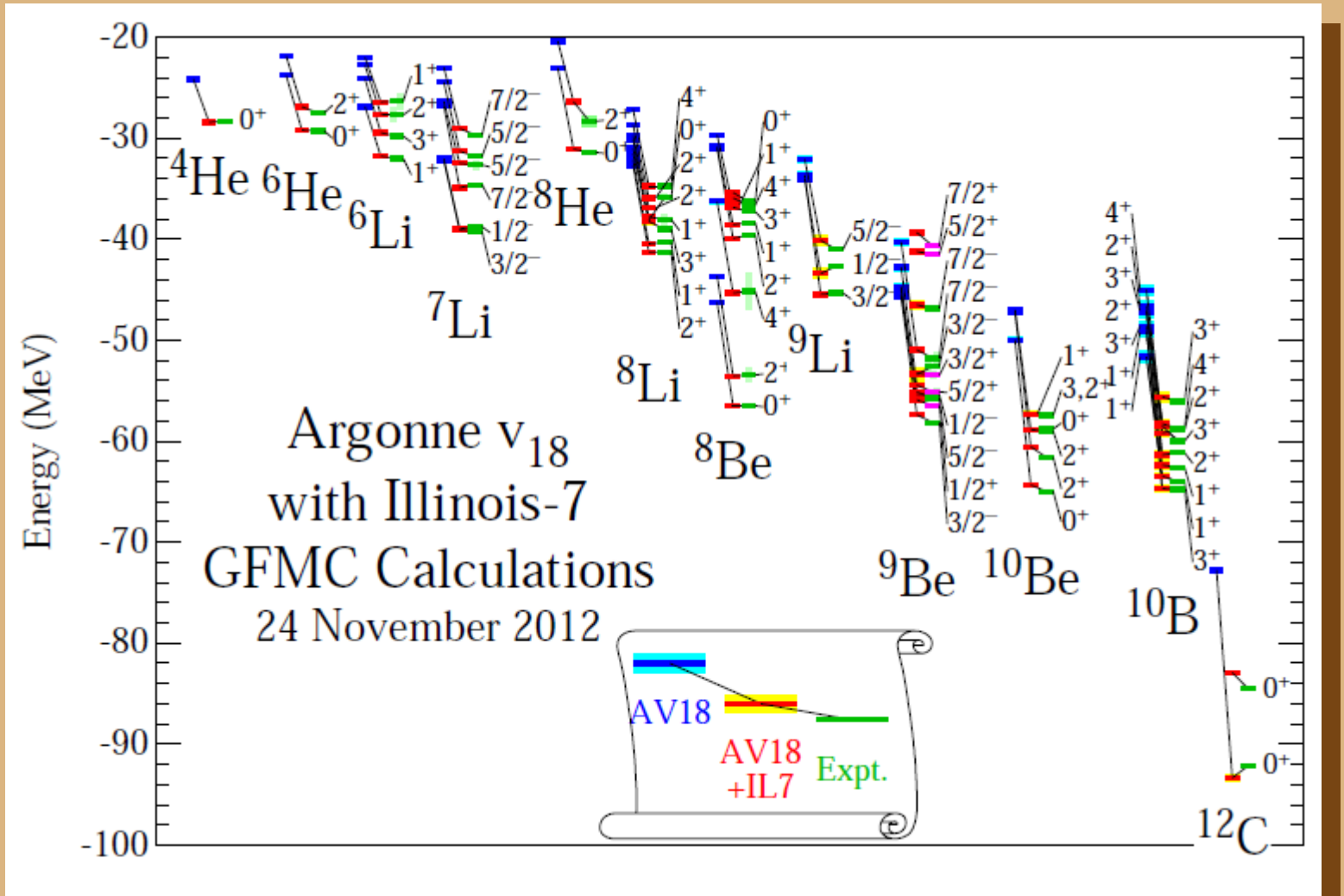
With tensor: $S_{jk} = 3(\hat{r}_{jk} \cdot \sigma_j)(\hat{r}_{jk} \cdot \sigma_k) - \sigma_j \cdot \sigma_k$

And spin, orbit: $\mathbf{S}_{jk} = \frac{\hbar}{2}(\sigma_j + \sigma_k)$

$$\mathbf{L}_{jk} = \frac{\hbar}{2\imath}(\mathbf{r}_j - \mathbf{r}_k) \times (\nabla_j - \nabla_k)$$

Nuclear GFMC

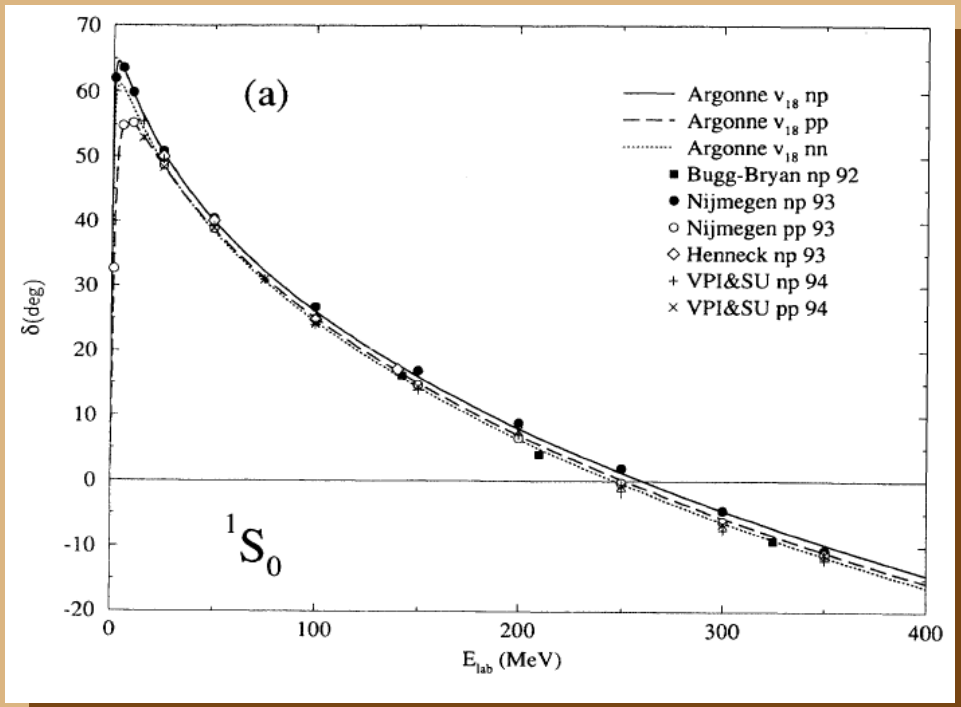
Green's Function Monte Carlo is very accurate and very expensive

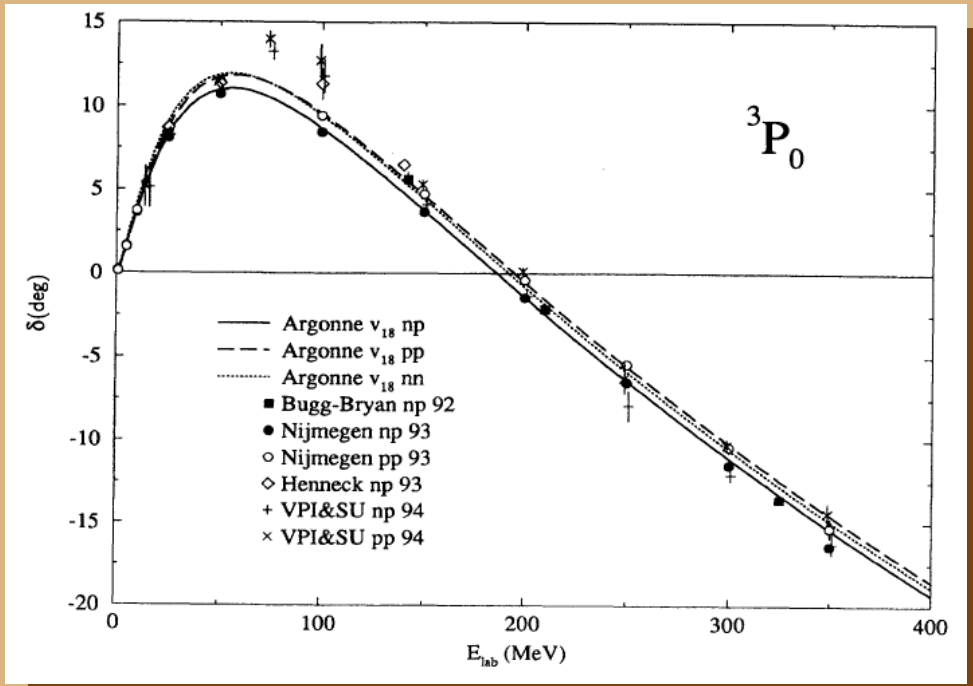


Credit: Steve Pieper

Uses phenomenological forces

Historically, nuclear QMC has utilized local, high-quality, phenomenological interactions of the Argonne/Urbana/Illinois family

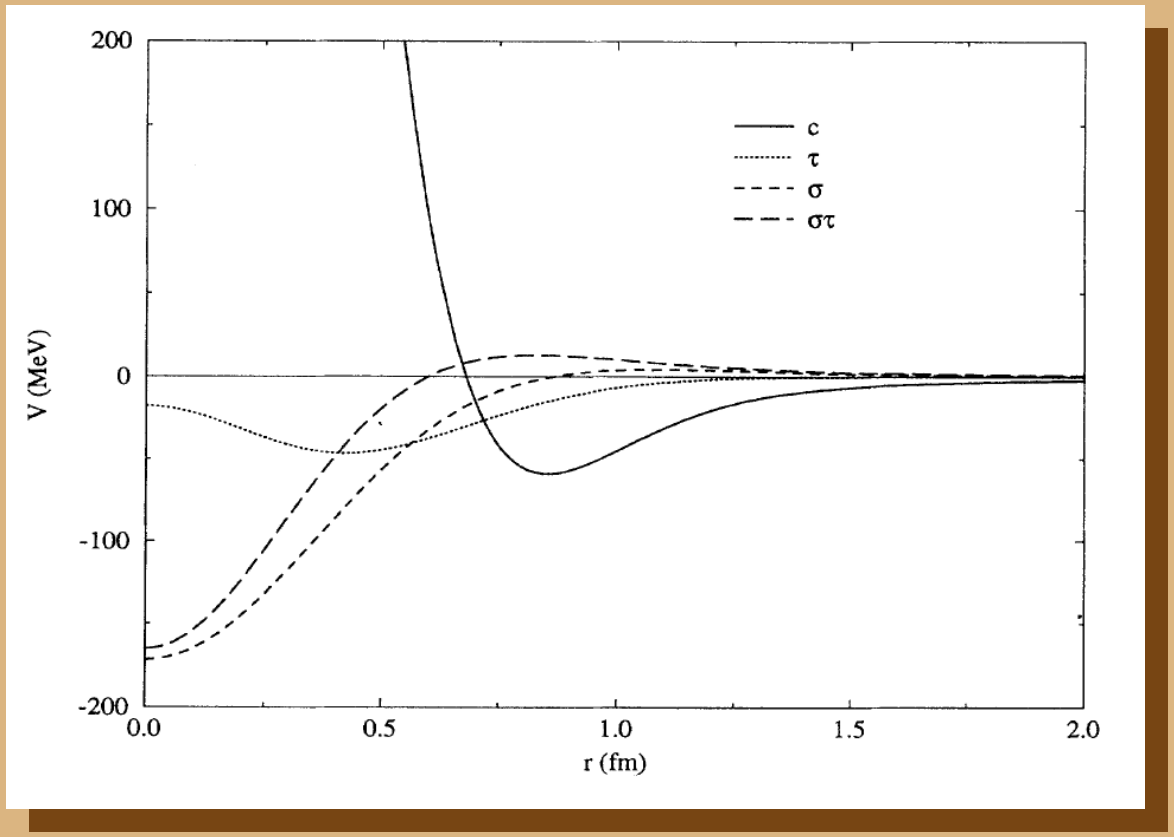




Credit: Bob Wiringa

Historically, phenomenological = hard

The nucleon-nucleon part of these interactions (Argonne v18) turns out (due to its locality) to be very hard/repulsive at short distances



Credit: Bob Wiringa

This also makes it non-perturbative at the many-body level

In summary

Local high-quality phenomenology is hard

Consubstantial with the successes of nuclear QMC,
difficult to use in most other many-body methods

Chiral EFT
a) is connected to symmetries of QCD
b) has consistent many-body forces, and
c) allows us to produce systematic uncertainty bands
also happens to be non-local (such are the *sumbebekota*)

Heavily used in other methods, but not used in nuclear QMC

How to go beyond?

Eliminate the reason chiral EFT was unused by powerful nuclear QMC methods (non-locality): this talk

Other approaches also being pursued:

Nuclear Theory

Real-Space Imaginary-Time Propagators for Non-Local Nucleon-Nucleon Potentials

J. E. Lynn, K. E. Schmidt

(Submitted on 31 May 2012 (v1), last revised 26 Jul 2012 (this version, v2))

Nuclear structure quantum Monte Carlo methods such as Green's function or auxiliary field diffusion Monte Carlo have used phenomenological local real-space potentials containing as few derivatives as possible, such as the Argonne-Urbana family of interactions, to make sampling simple and efficient. Basis set methods such as no-core shell model and coupled-cluster techniques typically use softer non-local potentials because of their more rapid convergence with basis set size. These non-local potentials are usually defined in momentum space and are often based on effective field theory. Comparisons of the results of the two types of methods can be difficult when different potentials are used. We show methods for evaluating the real-space imaginary-time propagators needed to perform quantum Monte Carlo calculations using such non-local potentials. We explore the universality of the large imaginary time propagators for different potentials and discuss how non-local potentials can be used in quantum Monte Carlo calculations.

Nuclear Theory

Effective Field Theory for Lattice Nuclei

N.Barnea, L.Contessi, D. Gazit, F. Pederiva, U. van Kolck

(Submitted on 20 Nov 2013)

We show how nuclear effective field theory (EFT) and ab initio nuclear-structure methods can turn input from lattice quantum chromodynamics (LQCD) into predictions for the properties of nuclei. We argue that pionless EFT is the appropriate theory to describe the light nuclei obtained in recent LQCD simulations carried out at pion masses much heavier than the physical pion mass. We solve the EFT using the effective-interaction hyperspherical harmonics and auxiliary-field diffusion Monte Carlo methods. Fitting the three leading-order EFT parameters to the deuteron, dineutron and triton LQCD energies at $m_\pi \approx 800$ MeV, we reproduce the corresponding alpha-particle binding and predict the binding energies of mass-5 and 6 ground states.

Nuclear Theory

Quantum Monte Carlo calculations of neutron matter with non-local chiral interactions

Alessandro Roggero, Abhishek Mukherjee, Francesco Pederiva

(Submitted on 7 Feb 2014)

We present fully non-perturbative quantum Monte Carlo calculations with non-local chiral effective field theory (EFT) interactions for the ground state properties of neutron matter. The equation of state, the nucleon chemical potentials and the momentum distribution in pure neutron matter up to one and a half times the nuclear saturation density are computed with a newly optimized chiral EFT interaction at next-to-next-to-leading order. This work opens the way to systematic order by order benchmarking of chiral EFT interactions, and \emph{ab initio} prediction of nuclear properties while respecting the symmetries of quantum chromodynamics.

Turning to chiral EFT

Nuclear Hamiltonian: chiral EFT

Attempt to build on QCD in a systematic manner

Exploit separation of scales: $a_{^1S_0} = (11 \text{ MeV})^{-1}$

$$m_\pi = 140 \text{ MeV}$$

$$\Lambda = 4\pi f_\pi \approx 1 \text{ GeV}$$

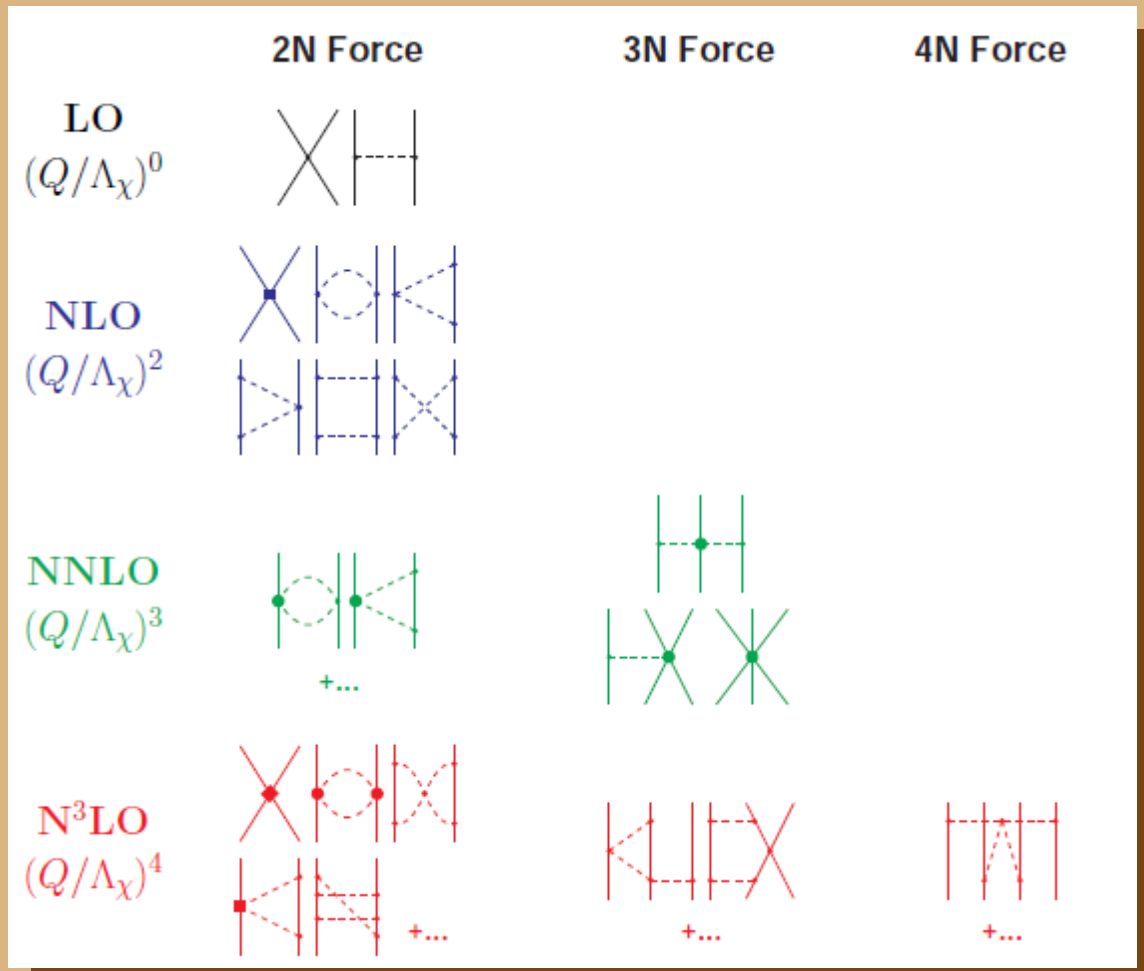
Chiral Effective Field Theory approach:

Use nucleons and pions as degrees of freedom

Systematically expand in $\frac{Q}{\Lambda_\chi}$

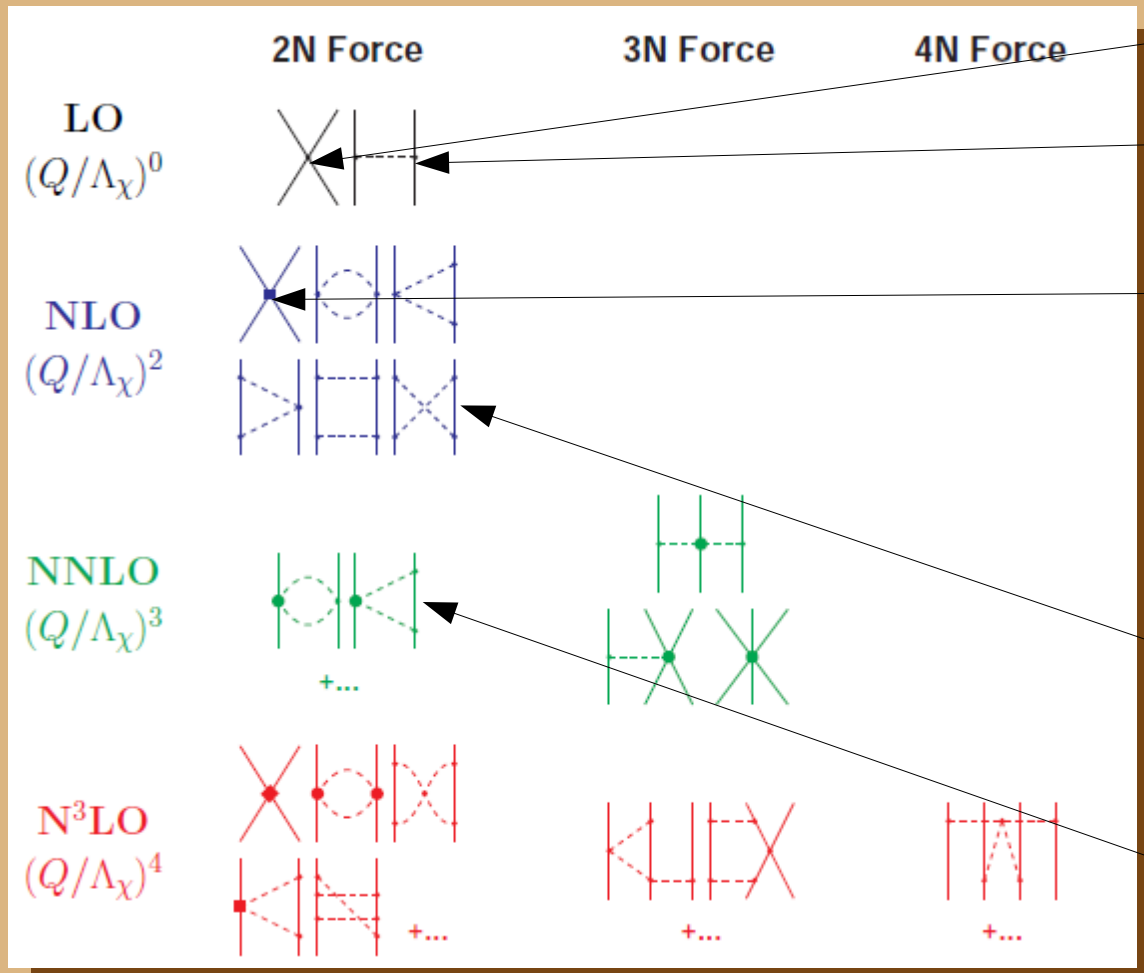
Program introduced by S. Weinberg, now taken over by the nuclear community

Nuclear Hamiltonian: chiral EFT



- Attempts to connect with underlying theory (QCD)
- Systematic low-momentum expansion
- Consistent many-body forces
- Low-energy constants from experiment or lattice QCD
- Until now non-local in coordinate space, so unused in continuum QMC
- Power counting's relation to renormalization still an open question

Nuclear Hamiltonian: chiral EFT



$$V_{\rm ct}^{(0)} = C_S + C_T\ \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$$

$$V_{1\pi}^{(0)} = -\left(\frac{g_A}{2f_\pi}\right)^2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \frac{(\boldsymbol{\sigma}_1\cdot\mathbf{q})(\boldsymbol{\sigma}_2\cdot\mathbf{q})}{q^2+m_\pi^2}$$

$$\begin{aligned} V_{\rm ct}^{(2)} &= C_1\ q^2 + C_2\ k^2 \\ &+ \left(C_3\ q^2 + C_4\ k^2\right)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \\ &+ i\frac{C_5}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\mathbf{q}\times\mathbf{k}) \\ &+ C_6(\boldsymbol{\sigma}_1\cdot\mathbf{q})(\boldsymbol{\sigma}_2\cdot\mathbf{q}) \\ &+ C_7(\boldsymbol{\sigma}_1\cdot\mathbf{k})(\boldsymbol{\sigma}_2\cdot\mathbf{k}) \end{aligned}$$

Long-studied two-pion exchange

Contains couplings from πN scattering

Regulator and dictionary:

$$f(p,p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$$

$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

$$\mathbf{p}' = (\mathbf{p}'_1 - \mathbf{p}'_2)/2 \qquad \mathbf{q} = \mathbf{p}' - \mathbf{p}$$

What is local

Successful nuclear QMC program constrained to use local potentials as input.

What does "local" mean?

In particle physics: potential is defined at one point in space-time (contact)

In nuclear physics:

$$\langle \mathbf{r}'|\hat{V}|\mathbf{r}\rangle = \begin{cases} V(\mathbf{r})\ \delta^3(\mathbf{r}'-\mathbf{r}) & \text{if local.} \\ V(\mathbf{r}',\mathbf{r}) & \text{if nonlocal.} \end{cases}$$

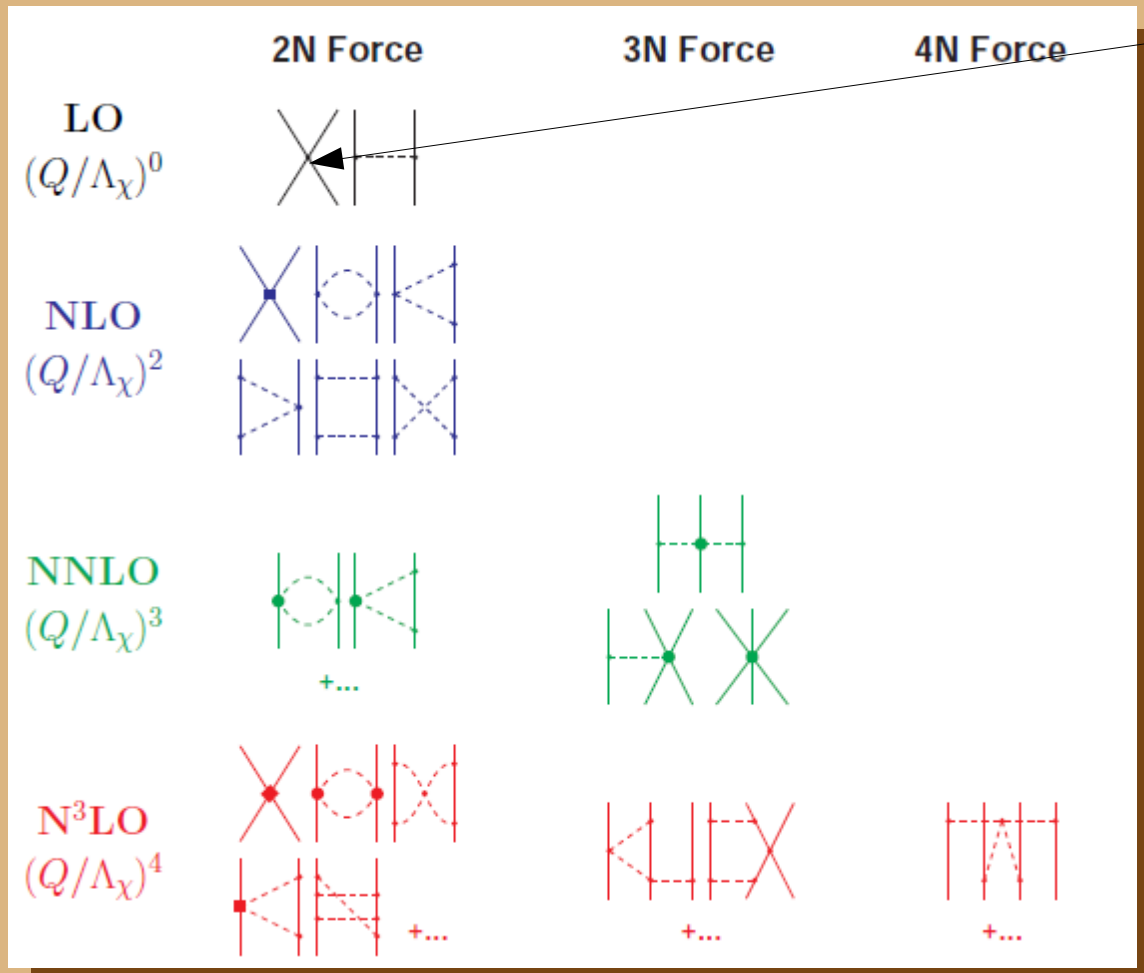
which is equivalent to

$$\langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle = \begin{cases} V(\mathbf{p}'-\mathbf{p}) & \text{if local.} \\ V(\mathbf{p}',\mathbf{p}) & \text{if nonlocal.} \end{cases}$$

Reminder: in our terminology local is function of $\mathbf{q}$ only

Turning to the resolution

Nuclear Hamiltonian: chiral EFT



$$V_{\rm ct}^{(0)} = C_S + C_T\ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Merely the standard choice.

Actually 4 terms in full set
"consistent with the symmetries of QCD"

$$V_{\rm ct}^{(0)} = C_1 + C_2\ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_3\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + C_4\ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

Pick 2 and antisymmetrize

In the general case

Eliminate both sources of non-locality

Write down a local energy-independent NN potential

- Use local pion-exchange regulator $f_{\rm long}(r) = 1 - e^{-(r/R_0)^4}$

cf. $f(p,p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$

In the general case

Eliminate both sources of non-locality

Write down a local energy-independent NN potential

- Use local pion-exchange regulator $f_{\rm long}(r) = 1 - e^{-(r/R_0)^4}$
- Pick 7 different contacts at NLO, just make sure that when antisymmetrized they lead to a set obeying the required symmetry principles (as above)

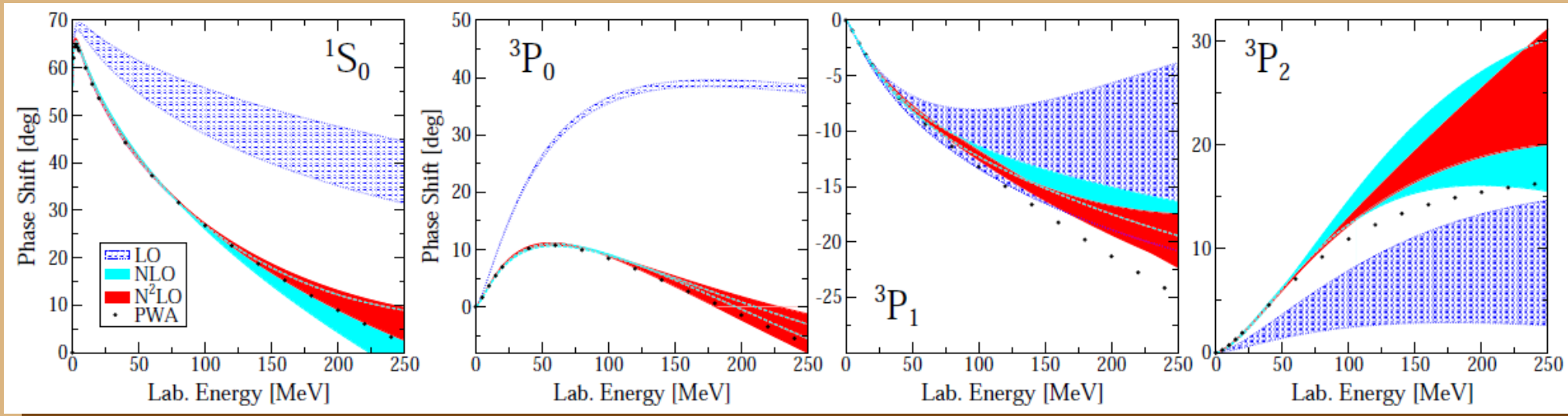
$$
\begin{aligned}
V_{\rm ct}^{(2)} &= C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
&+ \left(C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i\,\frac{C_5}{2}\,(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\
&+ C_6\,(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7\,(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2
\end{aligned}
$$

cf.

$$
\begin{aligned}
V_{\rm ct}^{(2)} &= C_1\, q^2 + C_2\, k^2 \\
&+ \left(C_3\, q^2 + C_4\, k^2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i\,\frac{C_5}{2}\,(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{q} \times \mathbf{k}) \\
&+ C_6\,(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k})
\end{aligned}
$$

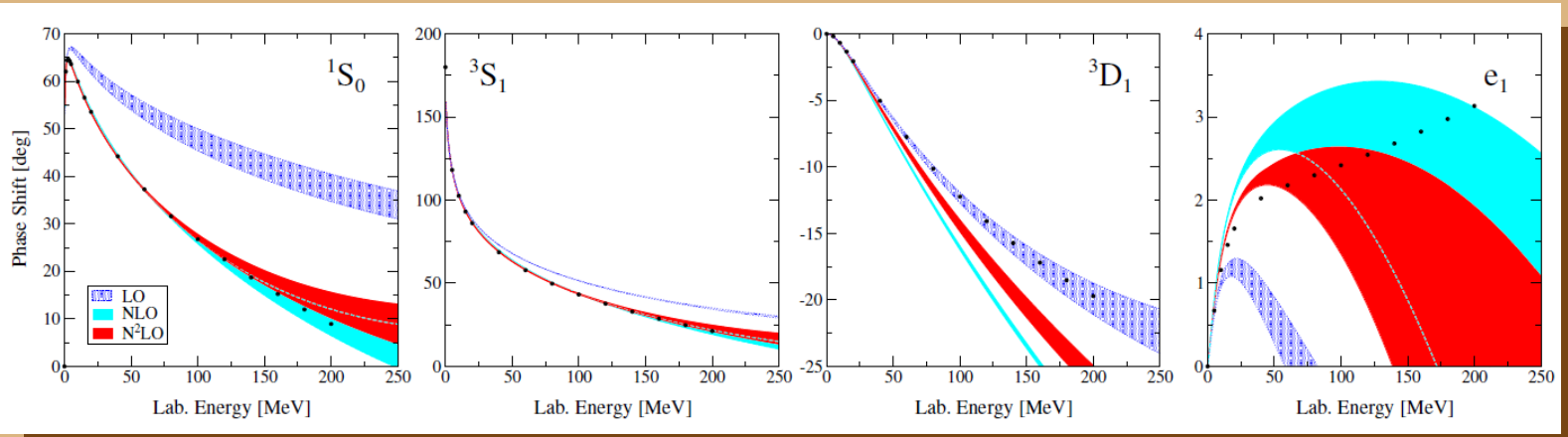
Phase shifts

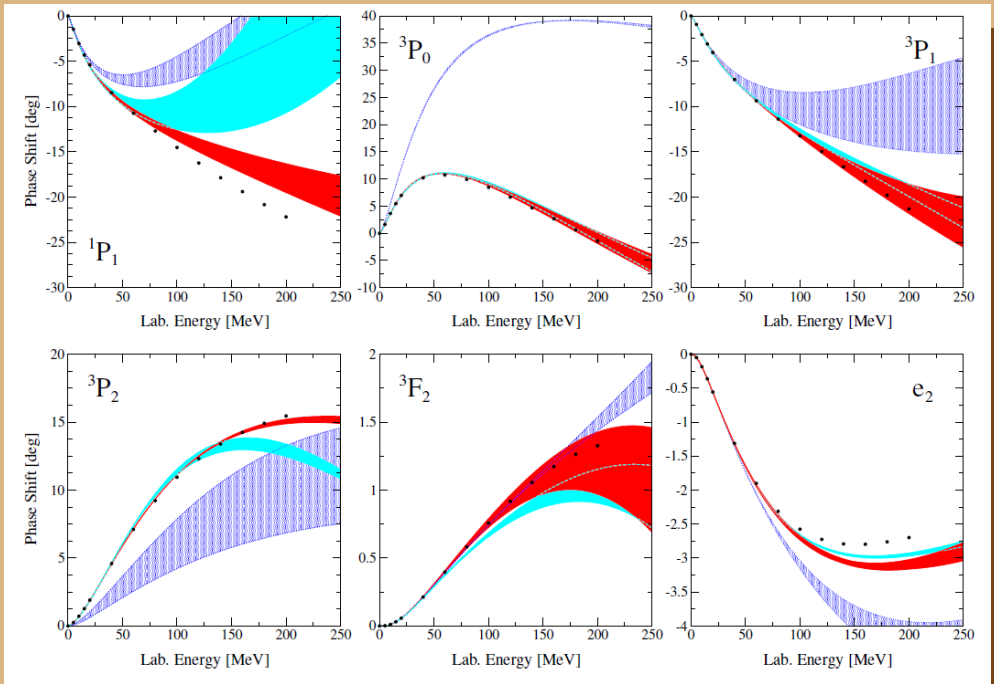
Order-by-order systematic trend evident



A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

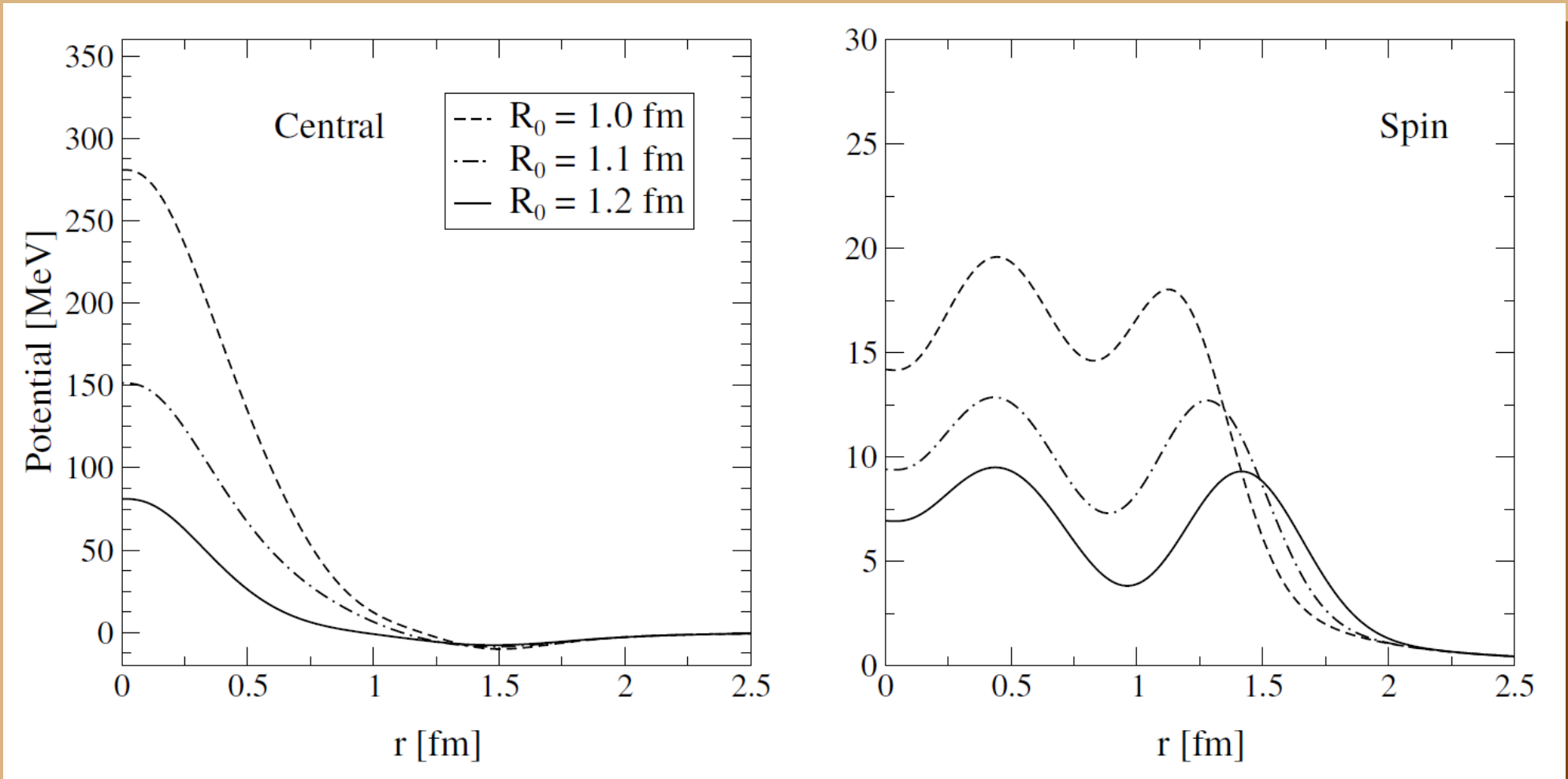
Updated phase shifts





A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, in preparation

Since it's local, let's plot it (N^2LO)



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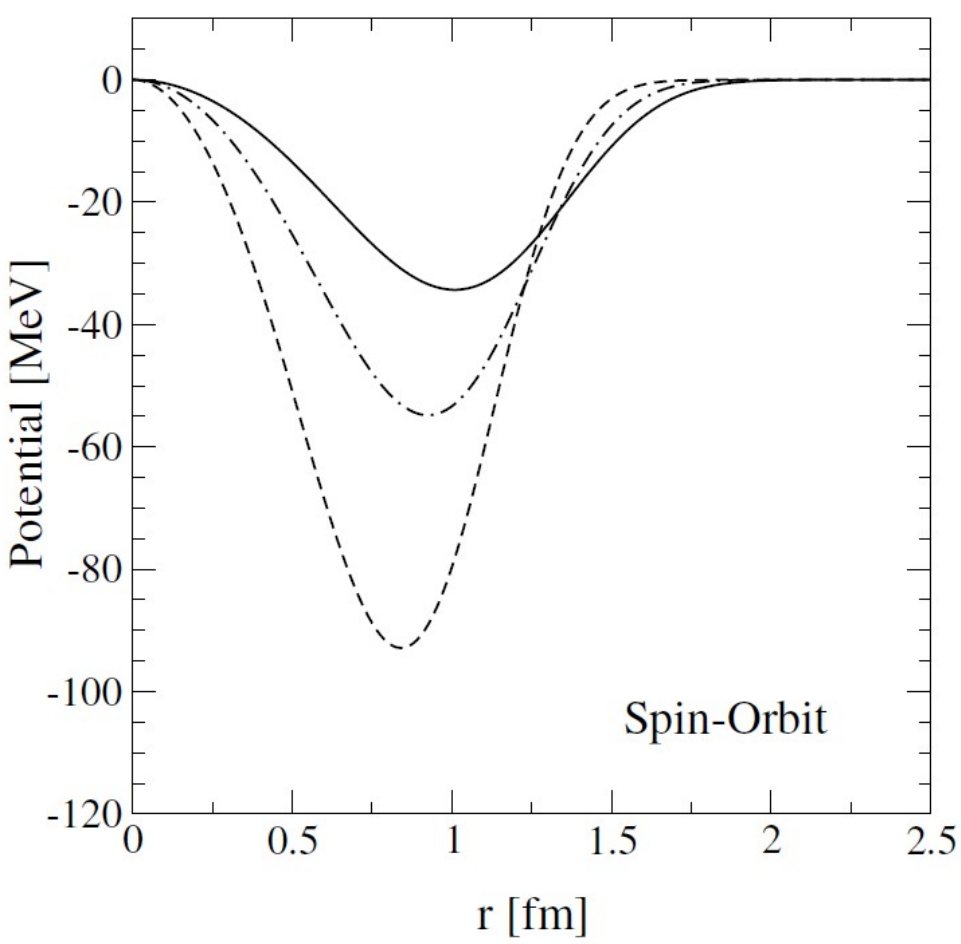
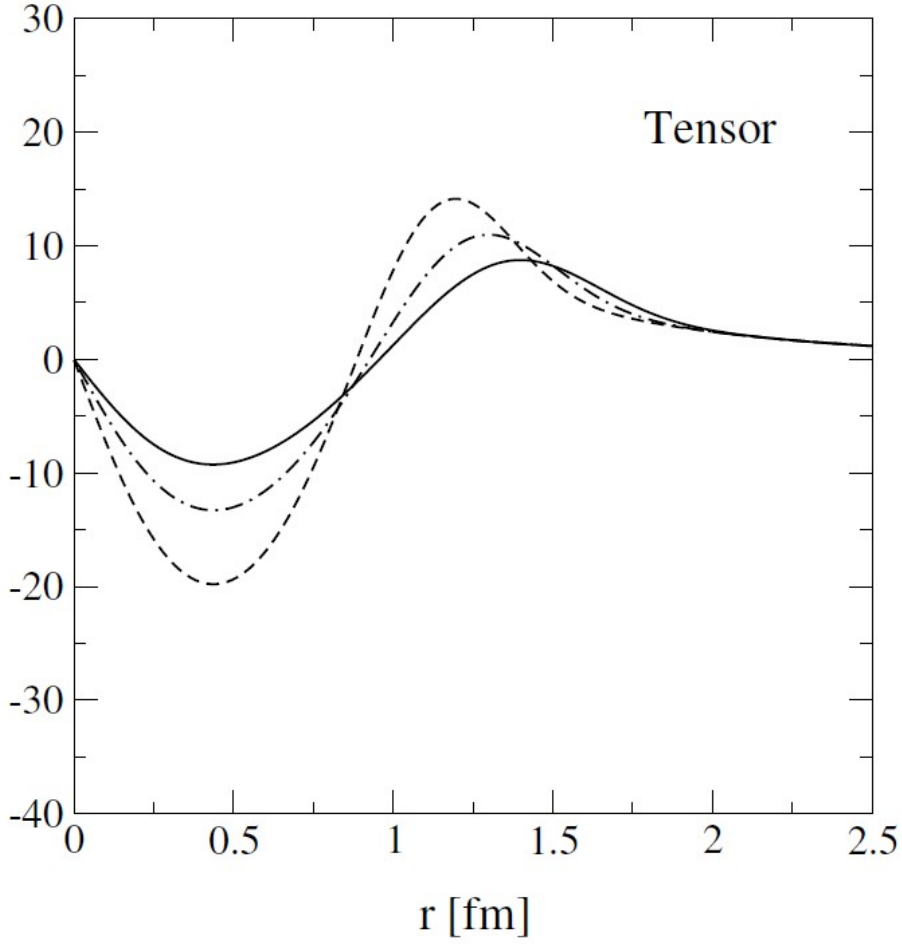
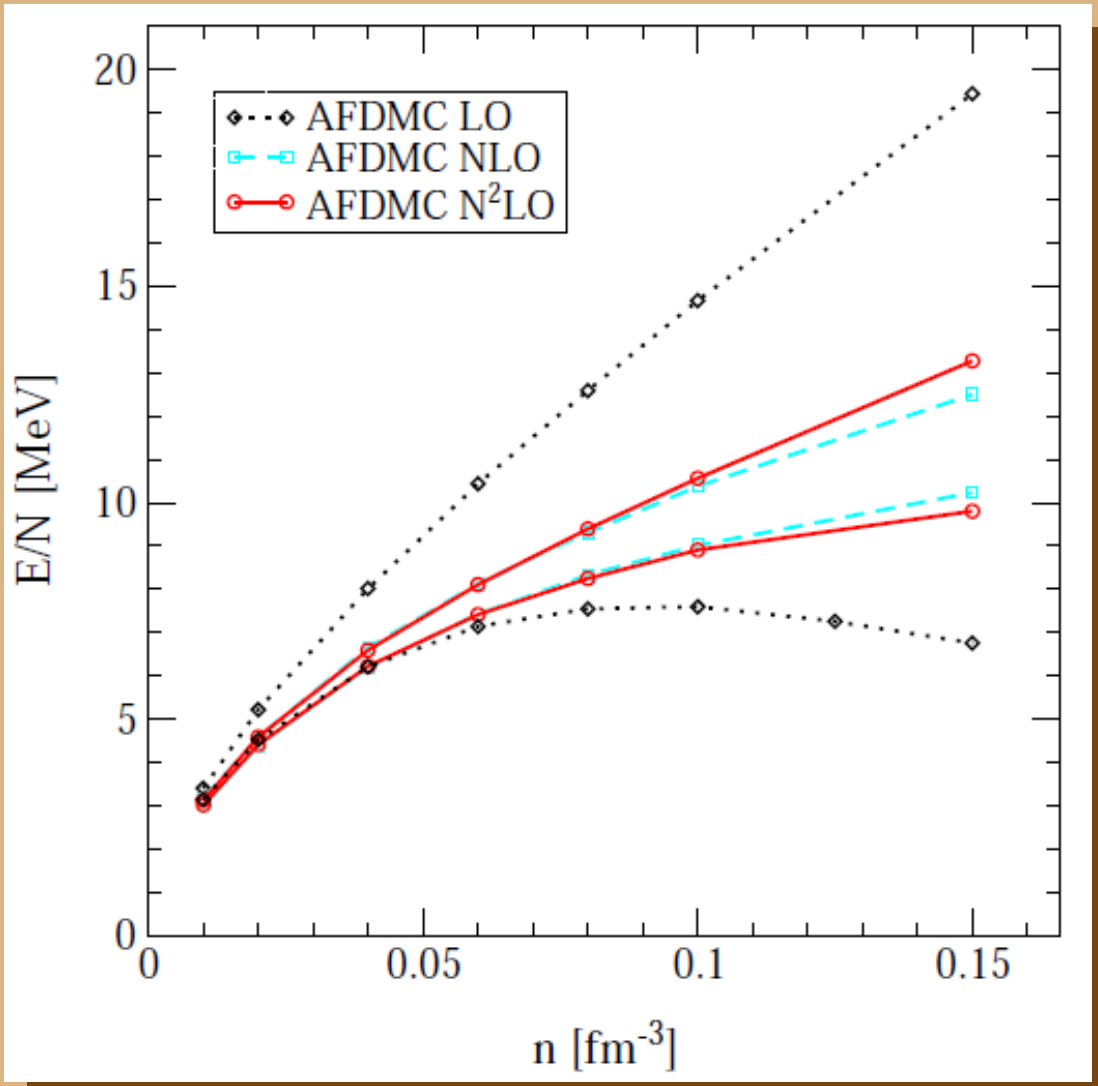




A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, in preparation

Chiral EFT in QMC

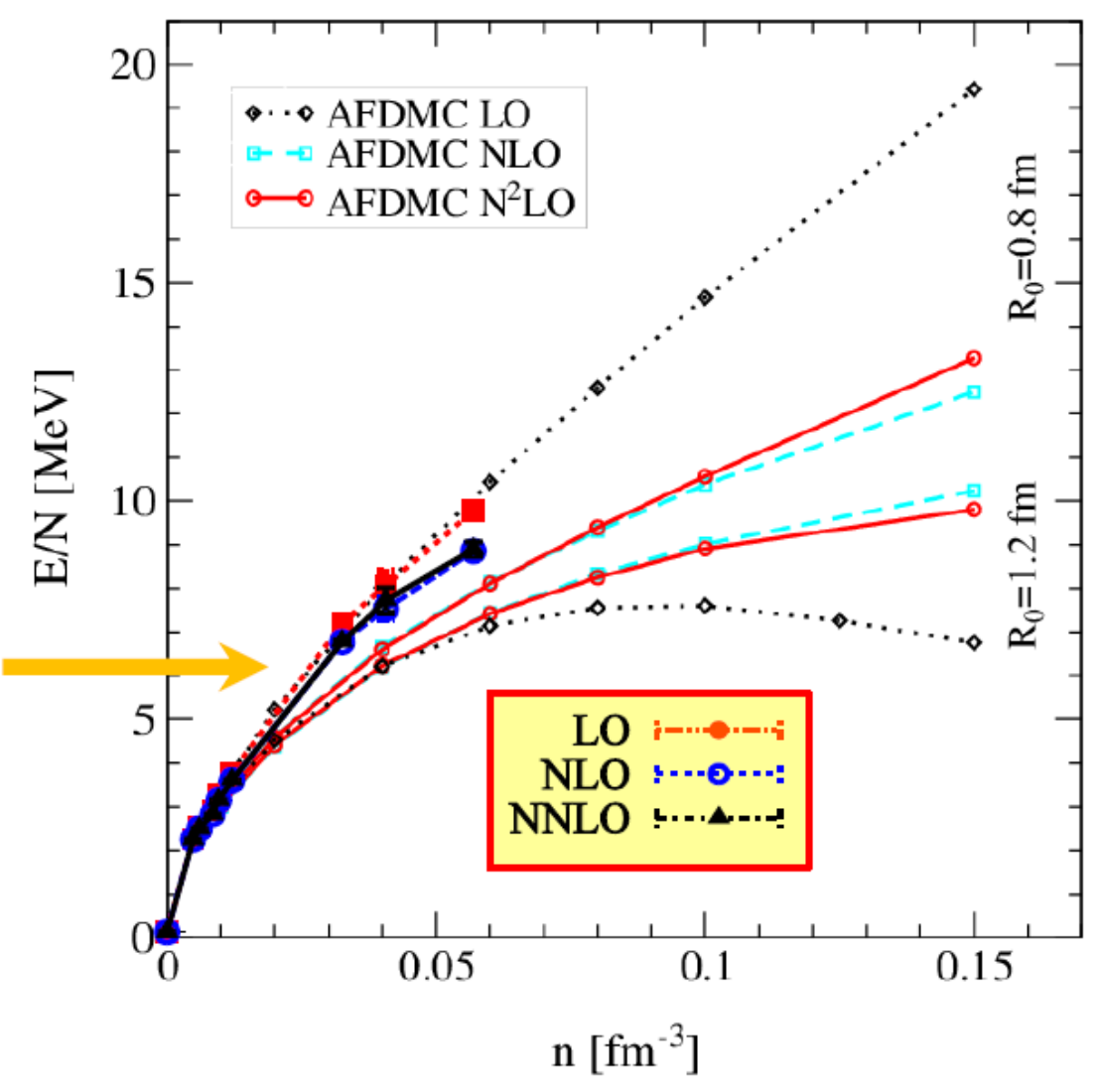


- Use Auxiliary-Field Diffusion Monte Carlo to handle the full interaction
- First ever non-perturbative systematic error bands
- Band sizes to be expected
- Many-body forces will emerge systematically

NEUTRONS

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

Chiral EFT in lattice QMC



- Complementary Quantum Monte Carlo approach that has already been using chiral EFT forces
- Preliminary results

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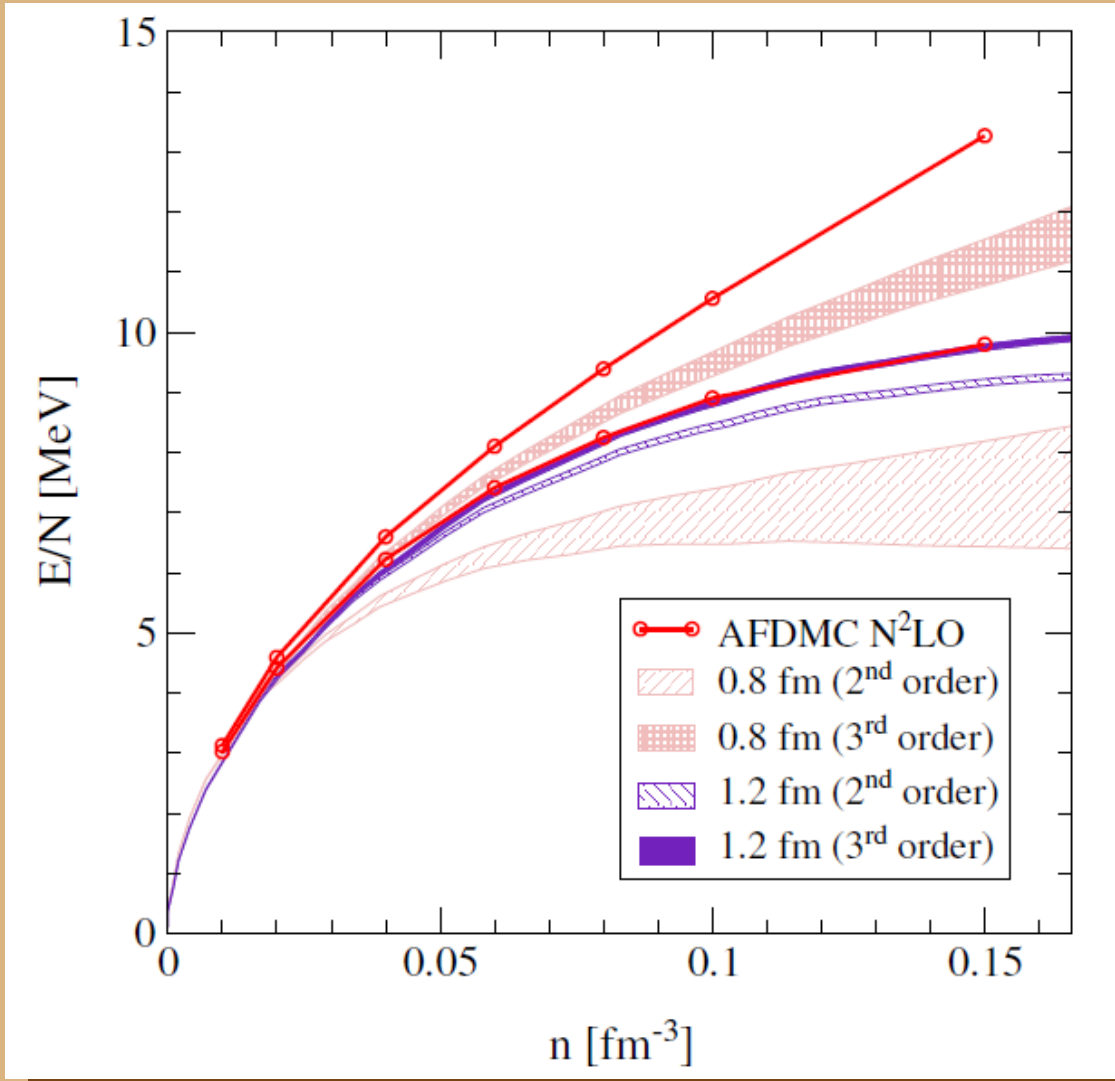
Dean Lee/nuclear lattice EFT collaboration

QMC vs MBPT



- Comparison with many-body perturbation approach
- MBPT bands come from diff. single-particle spectra
- Soft potential in excellent agreement with AFDMC
- Hard potential slower to converge

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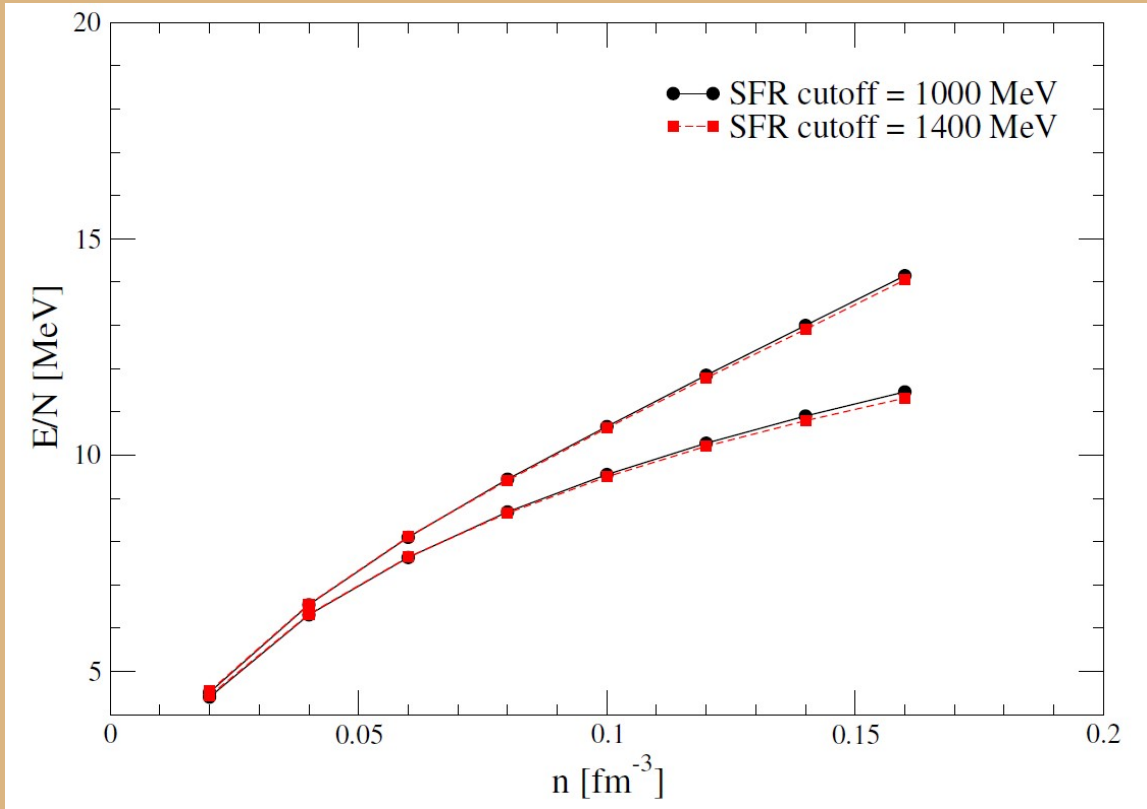
A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

Newer results: SFR cutoff



- New, better fits to higher energies
- Spectral-function regularization cutoff (kept fixed before) now varied
- Clearly shows lack of dependence

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A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, in preparation

Newer results: perturbativeness

First-ever opportunity to non-perturbatively test pertubativeness

- Use one chiral order in the propagator (many-body evolution), another chiral order when evaluating observables

- As for all observables that do not commute with the Hamiltonian, we need to explicitly extrapolate:

$$\langle H \rangle_{NLO+N^2LO} = \langle T+V \rangle_{NLO} - \langle V \rangle^{\rm ex}_{NLO} + \langle V \rangle^{\rm ex}_{N^2LO}$$

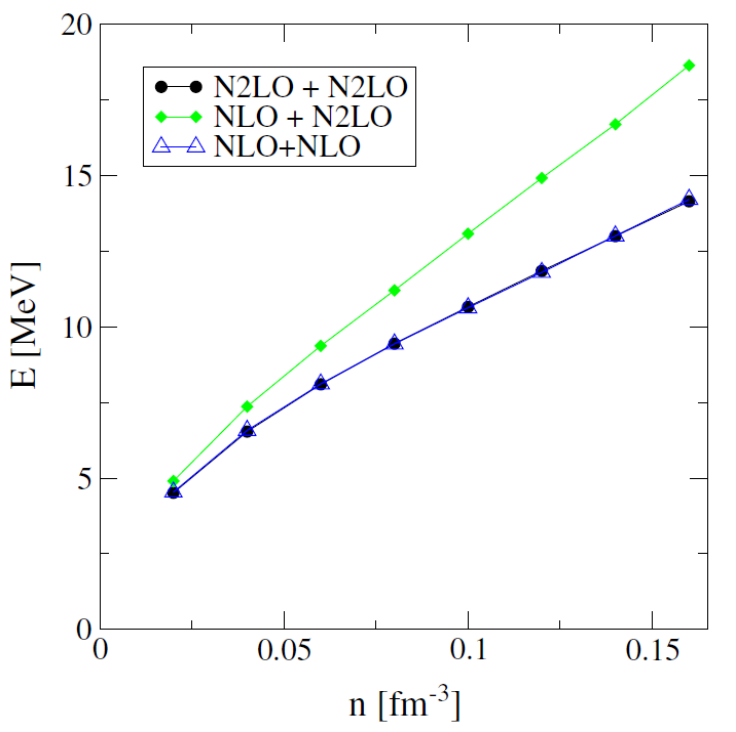
where

$$\langle \Phi | \hat{V} | \Phi \rangle^{\rm ex} = 2\langle \Phi | \hat{V} | \Psi_V \rangle - \langle \Psi_V | \hat{V} | \Psi_V \rangle$$

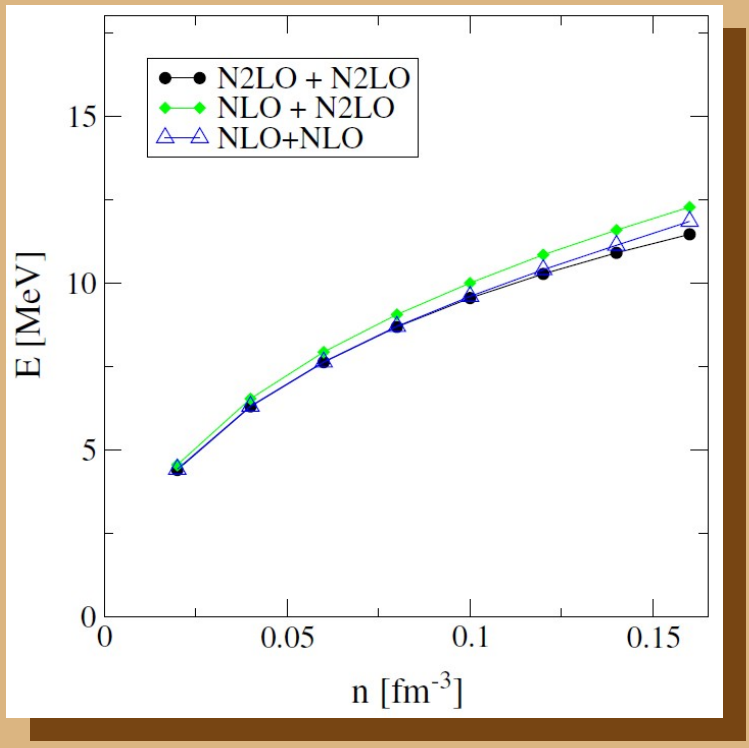
- If VMC is poor, extrapolation will be poor.

Newer results: perturbativeness

Hard(ish)
R_0 = 1.0 fm
Λ = 500 MeV



Soft
R_0 = 1.2 fm
Λ = 400 MeV



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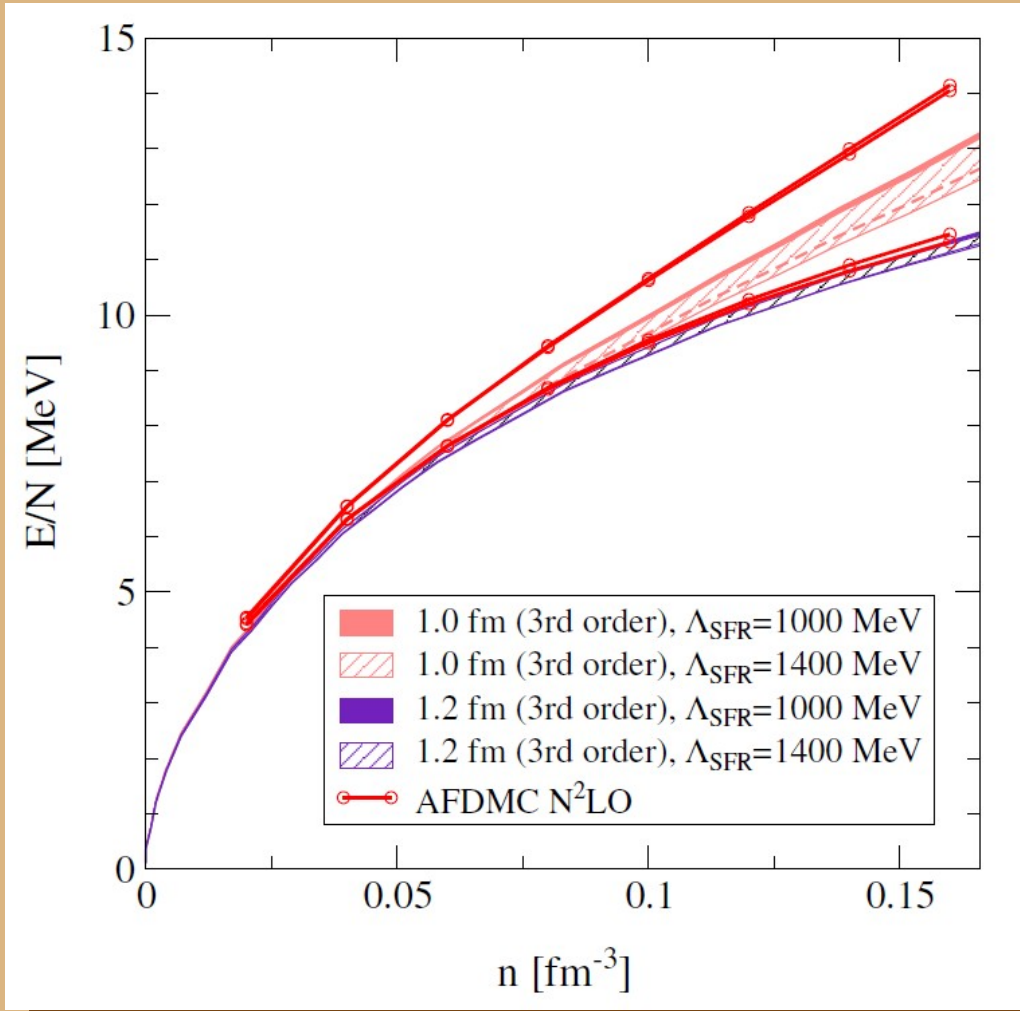
Newer results



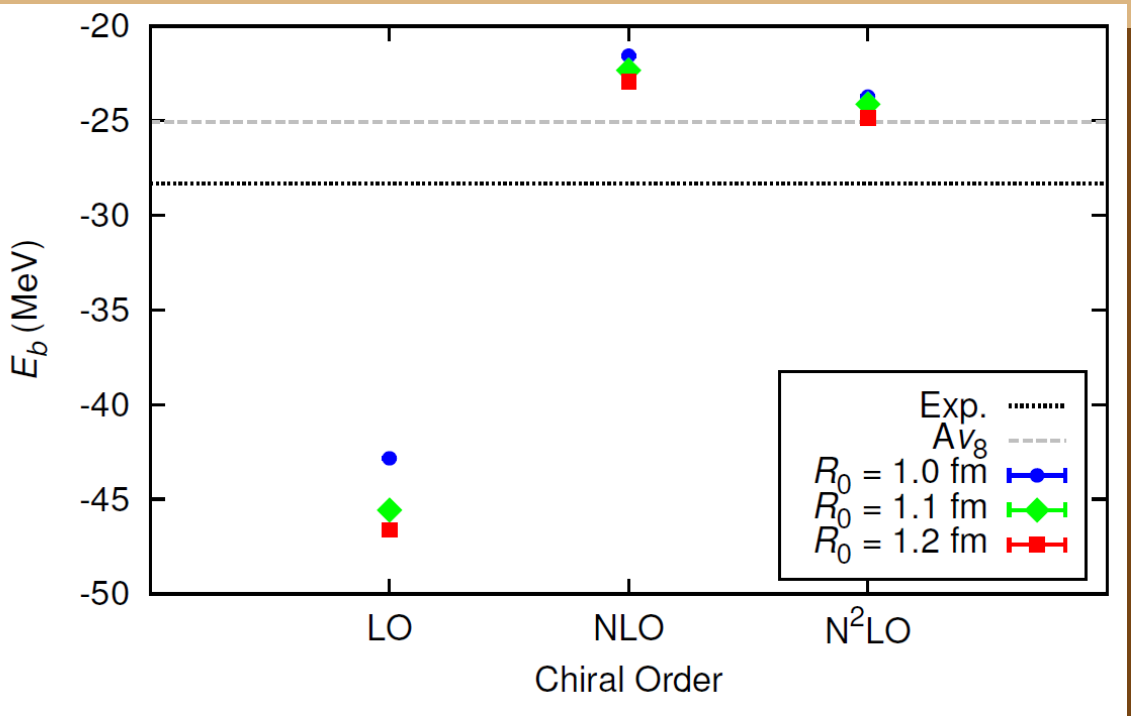
- Comparison with many-body perturbation approach
- Once again, soft potential is nearly identical to AFDMC
- Once again, SFR cutoff does not matter

NEUTRONS

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, in preparation

Now turn to finite nuclei

New results with chiral forces

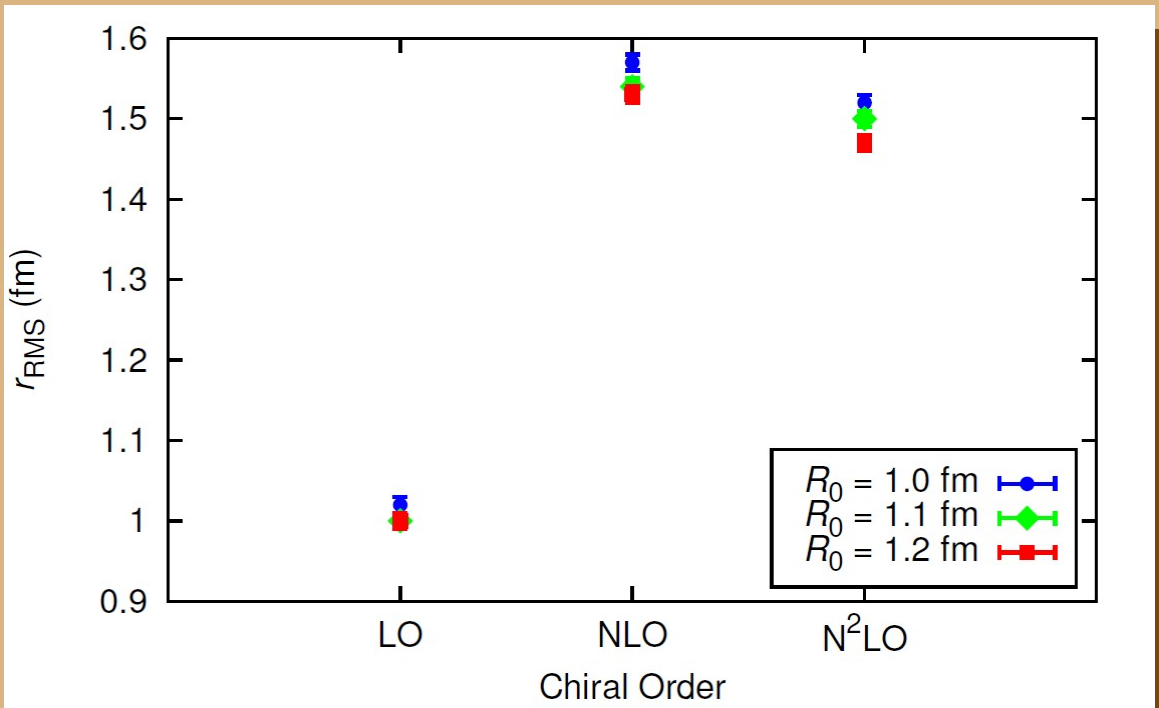


- Binding energy of ^{4}He
- Non-perturbative systematic error bands
- All results are strong force + Coulomb, no NNN

NUCLEONS

J. E. Lynn, A. Gezerlis, J. Carlson, E. Epelbaum, S. Gandolfi, A. Schwenk, in preparation

New results with chiral forces

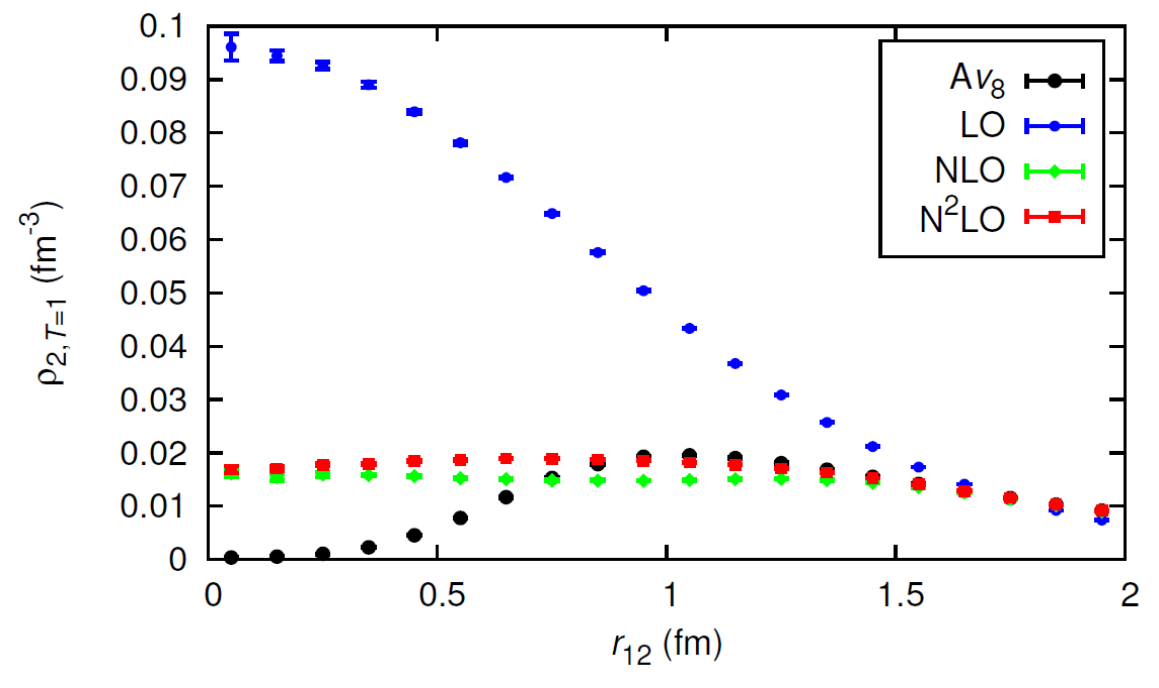


- rms radii for ^{4}He
- Systematic error bands
- All results are strong force + Coulomb, no NNN

NUCLEONS

J. E. Lynn, A. Gezerlis, J. Carlson, E. Epelbaum, S. Gandolfi, A. Schwenk, in preparation

New results with chiral forces



- Two-nucleon densities in ^{4}He (for R_0 = 1.2 fm)
- Appropriately normalized:

$$g_{2n,k}(r) = A \sum_{i<j} \langle \Psi | \delta(r - r_{ij}) O_{ij}^k | \Psi \rangle$$

- Quantifies softness of potential

NUCLEONS

J. E. Lynn, A. Gezerlis, J. Carlson, E. Epelbaum, S. Gandolfi, A. Schwenk, in preparation

Conclusions

- Chiral EFT (whether hard or soft) can now be used in continuum Quantum Monte Carlo methods
- Non-perturbative systematic error bands can be produced (for both light nuclei and infinite matter)
- The perturbativeness of different orders can be directly tested