Quantum Monte Carlo calculations of two neutrons in a finite volume with chiral EFT interactions

Ingo Tews

(Institute for Nuclear Theory)

In collaboration with

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H.-W. Hammer, M. Hoferichter, A. Schwenk,…

Progress in Ab Initio Techniques in Nuclear Physics,

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JINA–CEE

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Outline

- Motivation
- Quantum Monte Carlo method
  - Need of local interactions (depend only on $r = r_i - r_j$)
- Local chiral interactions Gezerlis, IT *et al.*, PRL (2013) & PRC (2014), IT *et al., PRC (2016),* Lynn, IT *et al.*, PRL (2016)
- Some results for QMC with local chiral interactions
- Two neutrons in a box Klos, Lynn, IT *et al.*, PRC (2016
- Excited states
- Summary

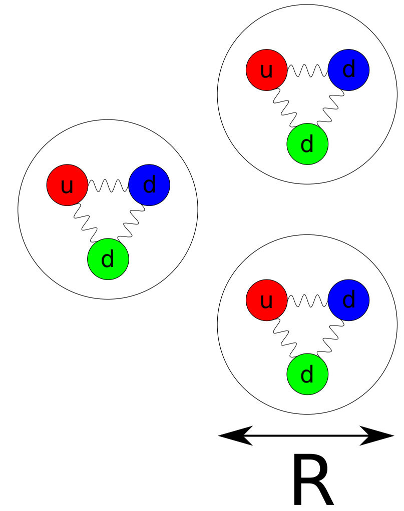
Motivation

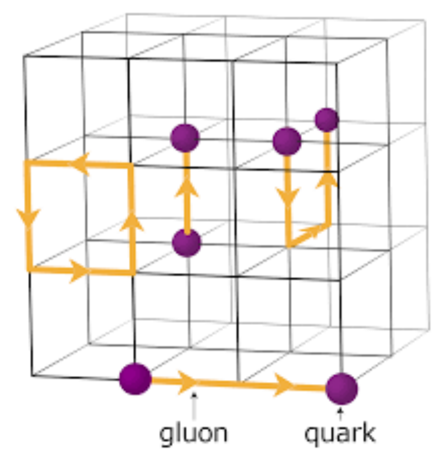
Quantum Chromodynamics (QCD)

Lattice QCD:

- Computationally very costly!
- Limited to very few particles and finite volumes.
- It could take many years for Lattice QCD calculations to describe nuclear systems (A>>2).
- At the moment not feasible for most nuclear observables.

Nuclear Physics (EOS, nuclei)





Motivation

Quantum Chromodynamics (QCD)

↓

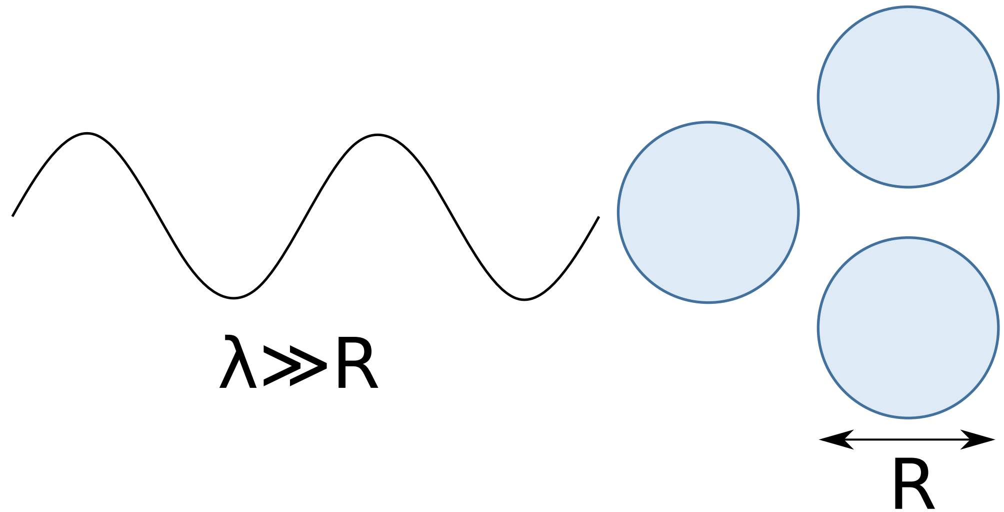
Chiral Effective field theory for nuclear forces

↓

Ab initio many-body framework

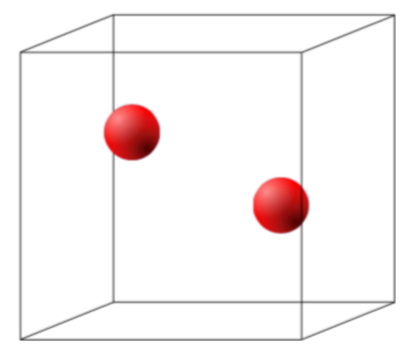
↓

Nuclear Physics (EOS, nuclei)



At low energies (long wavelength) details not resolved!

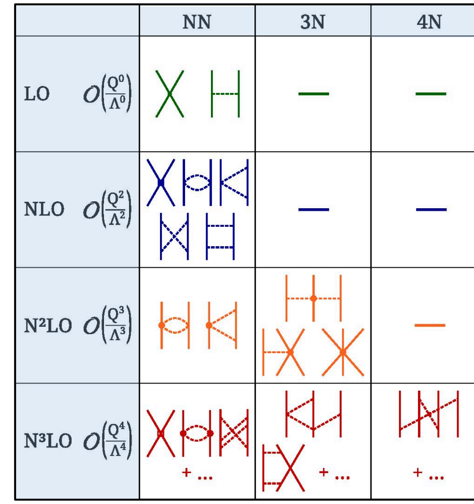
- Choose relevant degrees of freedom for low energy processes.
- Systematic expansion of interactions constrained by symmetries of QCD.



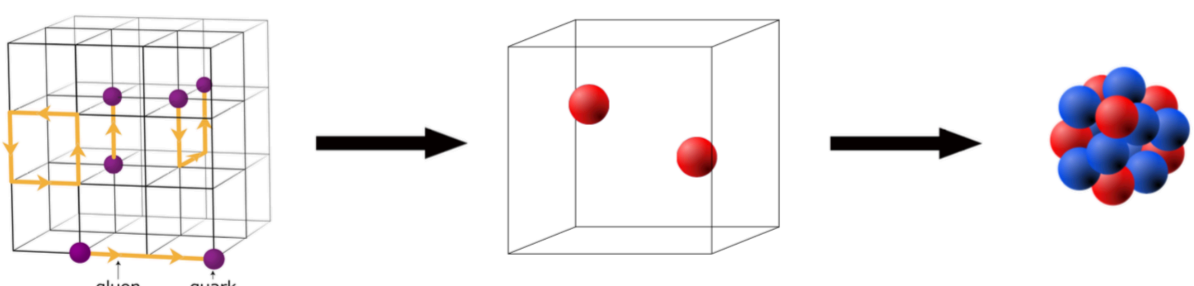
Motivation

Systematic expansion of nuclear forces in low momenta Q over breakdown scale Λ_b:

- Pions and nucleons as explicit degrees of freedom.
- Long-range physics explicit, short-range physics expanded in general operator basis.
- Couplings (LECs) fit to experimental data.
- What if data scarce or nonexistent?



- Long-term goal: Bridge the gap by matching of chiral EFT couplings to lattice QCD results to enable fully QCD-based chiral EFT predictions
- Connect ab-initio nuclear physics to the underlying theory of QCD by studying, e.g., few-nucleon (few-neutron) systems in finite volume with QMC



Credit: P. Klos

Quantum Monte Carlo method

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Solve the many-body Schrödinger equation:

$$H\left|\psi\right\rangle = -\frac{\partial}{\partial\tau}\left|\psi\right\rangle, \qquad \tau = it$$

$$\psi(R,\tau) = \int dR'^{3N} \left\langle R\right| e^{-(T+V)\tau} \left|R'\right\rangle \psi(R',0)$$

Basic steps:

- Choose trial wavefunction which overlaps with the ground state

$$\left|\psi(R,0)\right\rangle = \left|\psi_T(R,0)\right\rangle = \sum_i c_i \left|\phi_i\right\rangle \rightarrow \sum_i c_i e^{-(E_i-E_0)\tau}\left|\phi_i\right\rangle$$

- Evaluate propagator for small timestep $\Delta\tau$, feasible only for local potentials
- Make consecutive small time steps using Monte Carlo techniques to project out ground state

$$\left|\psi(R,\tau)\right\rangle \rightarrow \left|\phi_0\right\rangle \quad \text{for} \quad \tau\rightarrow\infty$$

More details:
Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt, Wiringa, RMP (2015)

Quantum Monte Carlo method

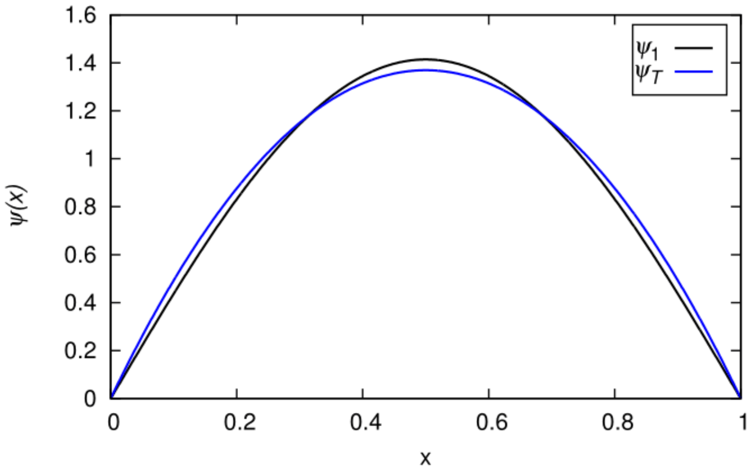
Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

Basic steps:

- Choose parabolic trial wavefunction which overlaps with the ground state

Animation by Joel Lynn, TU Darmstadt



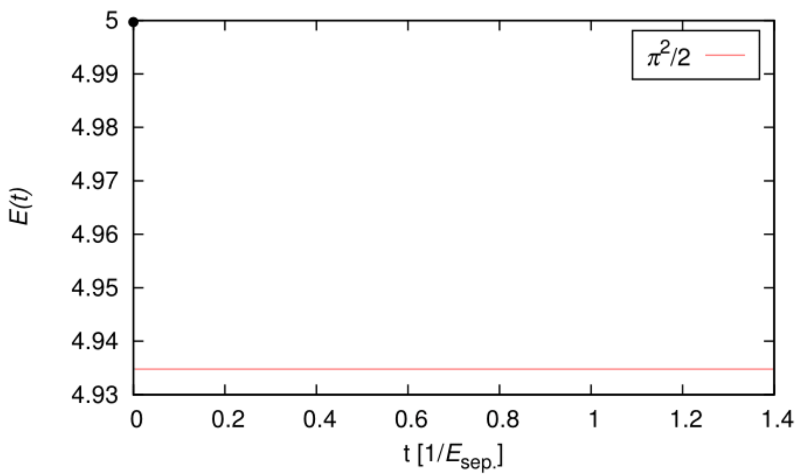
Quantum Monte Carlo method

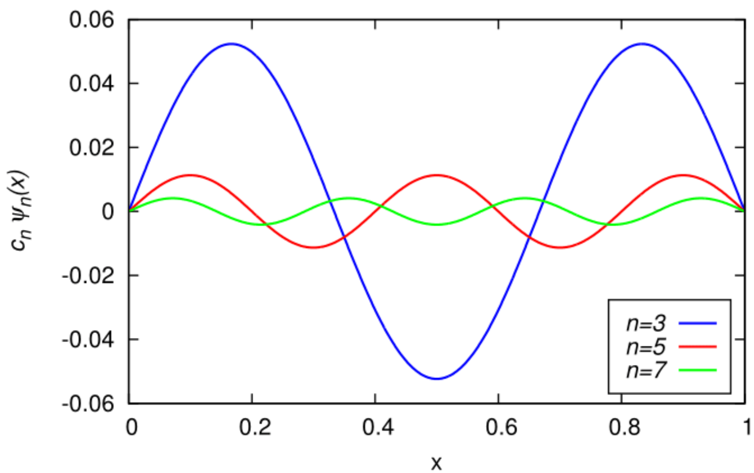
Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

- Make consecutive small timesteps, $\tau = 0.0 \left(\frac{1}{E_{\text{sep}}}\right)$

  Animation by Joel Lynn, TU Darmstadt





Quantum Monte Carlo method

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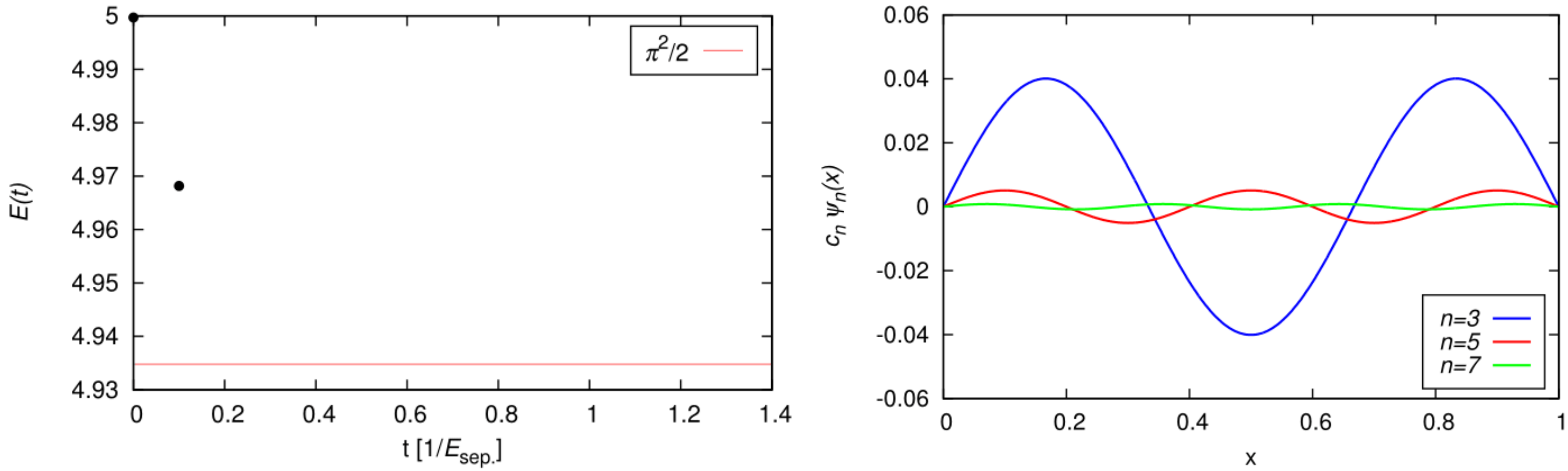
Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

- Make consecutive small timesteps, $\tau = 0.1\left(\frac{1}{E_{sep}}\right)$

Animation by Joel Lynn, TU Darmstadt



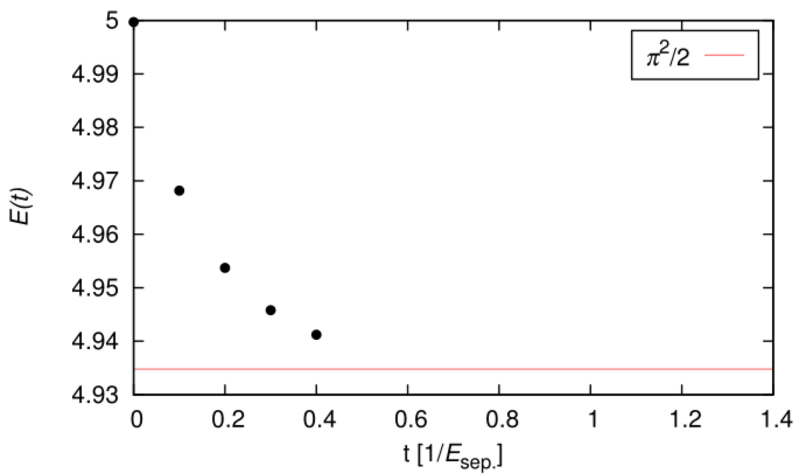
Quantum Monte Carlo method

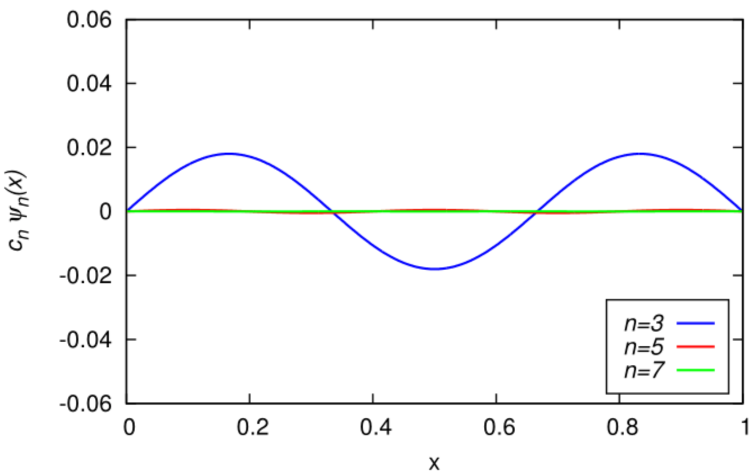
Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

- Make consecutive small timesteps, $\tau = 0.4\left(\frac{1}{E_{sep}}\right)$

Animation by Joel Lynn, TU Darmstadt





Quantum Monte Carlo method

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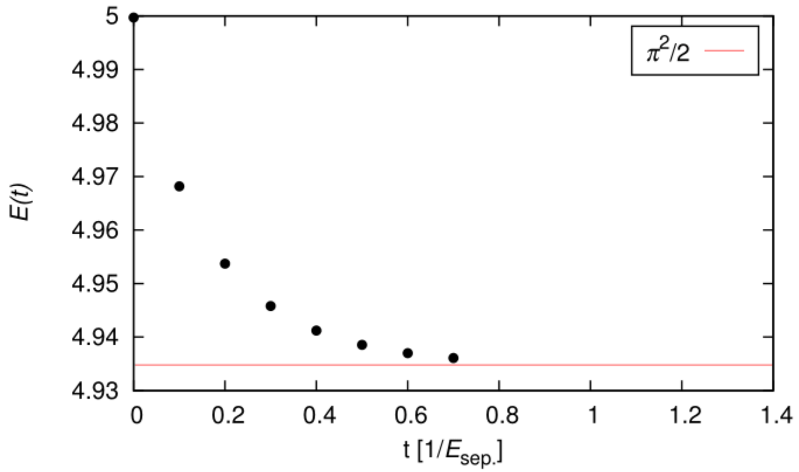
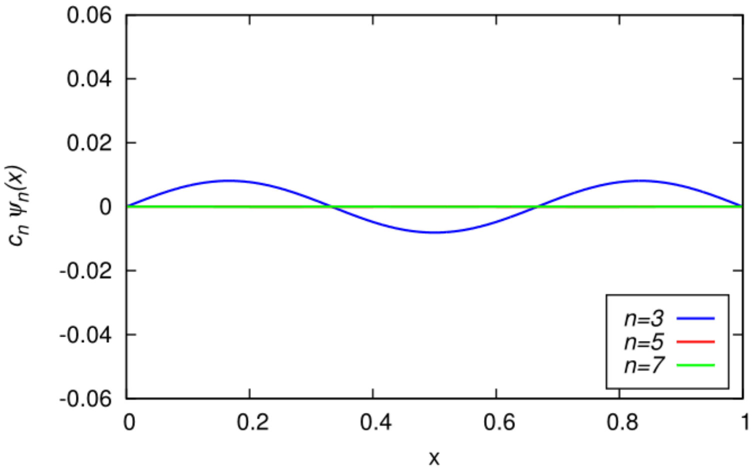
Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

- Make consecutive small timesteps, $\tau = 0.7\left(\frac{1}{E_{\mathrm{sep}}}\right)$

  Animation by Joel Lynn, TU Darmstadt





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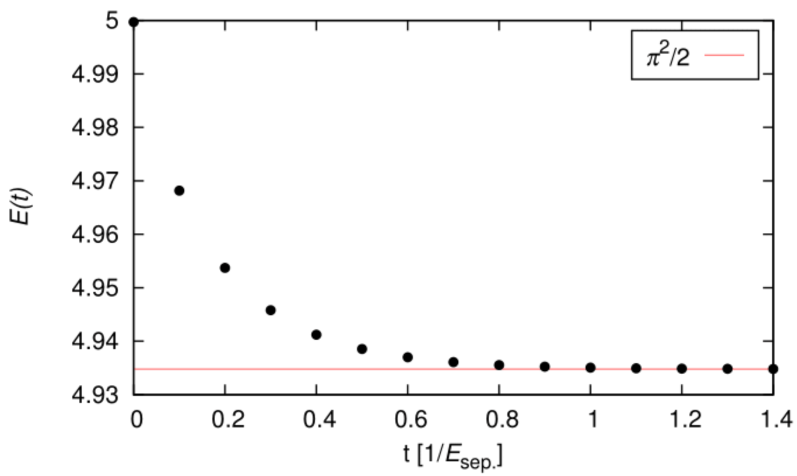
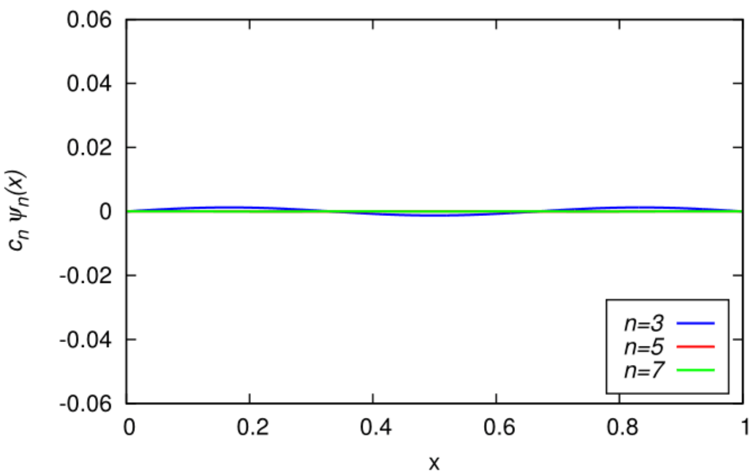
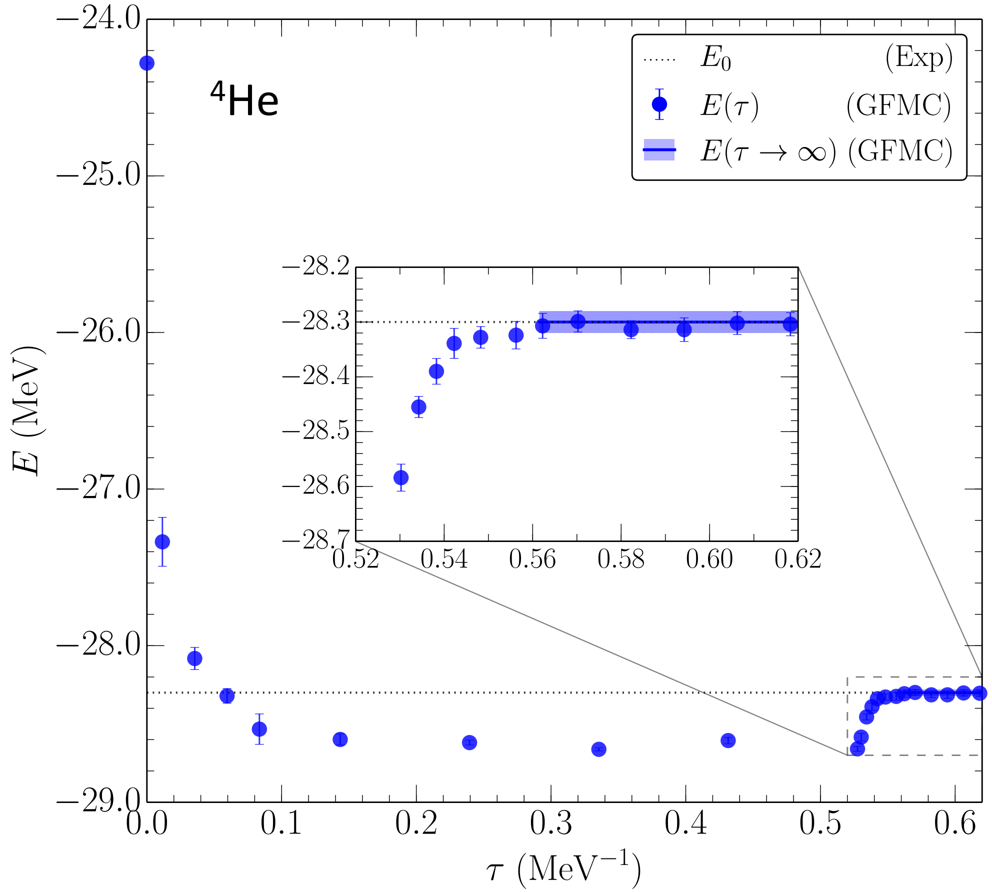


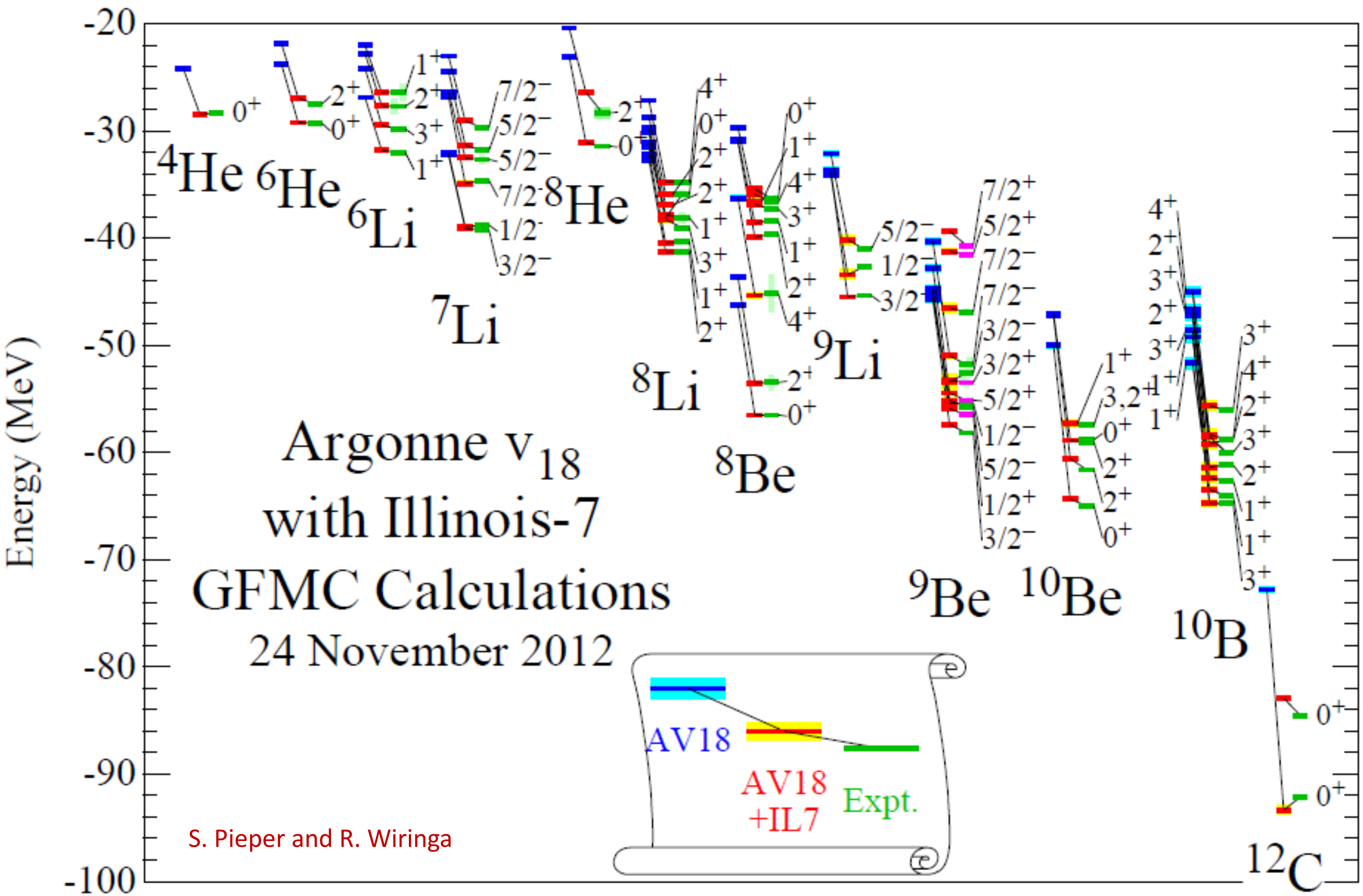


Quantum Monte Carlo method



Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, in preparation.

Quantum Monte Carlo method



Local chiral interactions

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To evaluate the propagator for small timesteps $\Delta\tau$ we need local potentials:

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

Chiral Effective Field Theory interactions generally nonlocal:

- Momentum transfer $\boldsymbol{q} \to \boldsymbol{p}' - \boldsymbol{p}$
- Momentum transfer in the exchange channel $\boldsymbol{k} = \frac{1}{2}(\boldsymbol{p} + \boldsymbol{p}')$
- Fourier transformation: $\boldsymbol{q} \to \boldsymbol{r}, \boldsymbol{k} \to$ Derivatives

Sources of nonlocalities:

- Usual regulator in relative momenta

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

- k-dependent contact operators

Solutions:

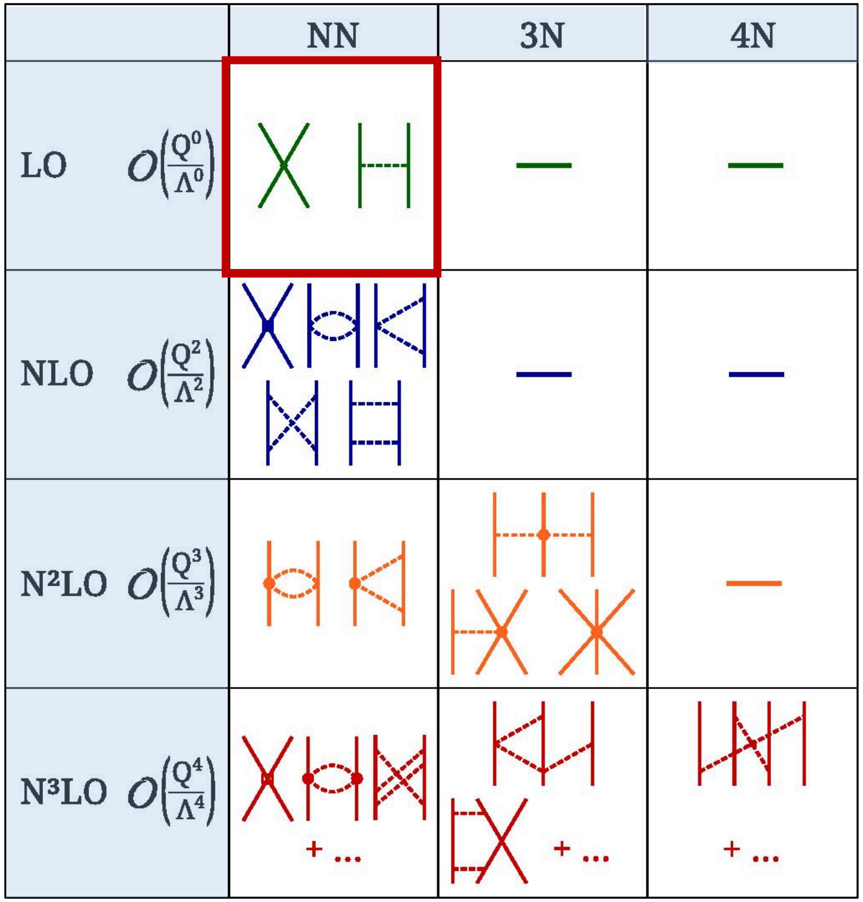
- Choose local regulators:

$$V_{\text{long}}(r) \;\to\; V_{\text{long}}(r)\left(1 - e^{-(r/R_0)^4}\right)$$

$$\delta_{R_0}(\mathbf{r}) = \alpha e^{-(r/R_0)^4}$$

- Use Fierz freedom to choose local set of contact operators

Local chiral interactions



- Leading order $V^{(0)} = V^{(0)}_{\text{cont}} + V^{\text{OPE}}$
- Pion exchange local → local regulator

$$f_{\text{long}}(r) = 1 - \exp(-r^4/R_0^4)$$

- Contact potential:

$$V^{(0)}_{\text{cont}} = \alpha_1 \mathbf{1} + \alpha_2 \sigma_1 \cdot \sigma_2 + \alpha_3 \tau_1 \cdot \tau_2 + \alpha_4 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$$

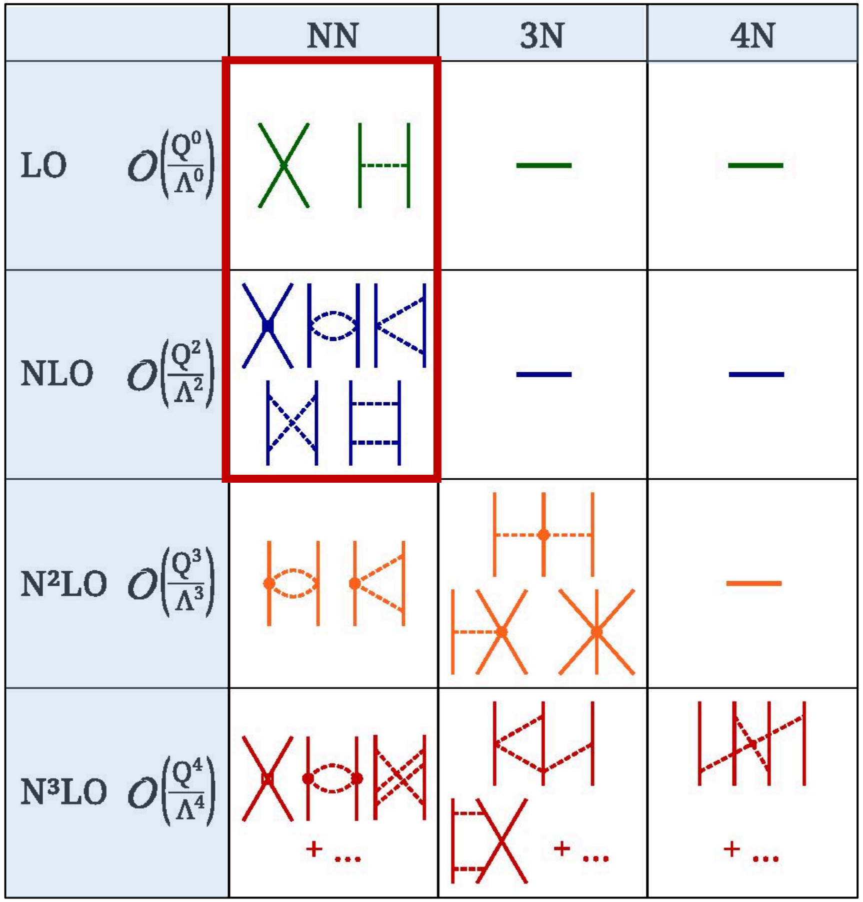
→ Only two independent (Pauli principle)

$$V^{(0)}_{\text{cont}} = C_S \mathbf{1} + C_T \sigma_1 \cdot \sigma_2$$

$$f_{\text{short}}(r) = \alpha \exp(-r^4/R_0^4)$$

Weinberg, van Kolck, Kaplan, Savage, Wise,
Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

Local chiral interactions



- Choose local set of short-range operators at NLO (7 out of 14)

$$
\begin{aligned}
V_{\mathrm{cont}}^{(2)} = {} & \gamma_1\, q^2 + \gamma_2\, q^2\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_3\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_4\, q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_5\, k^2 + \gamma_6\, k^2\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_7\, k^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_8\, k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_9\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\mathbf{q} \times \mathbf{k}) \\
& + \gamma_{10}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\mathbf{q} \times \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_{11} (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
& + \gamma_{12} (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_{13} (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \\
& + \gamma_{14} (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \,.
\end{aligned}
$$

Weinberg, van Kolck, Kaplan, Savage, Wise,
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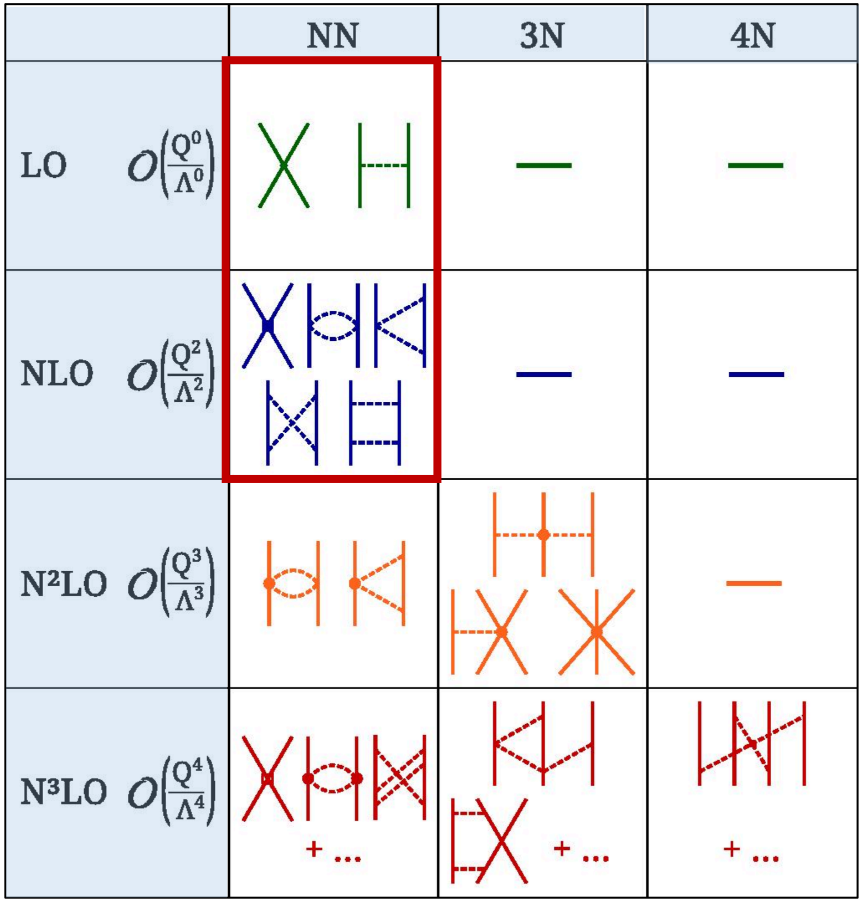
Local chiral interactions



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\begin{aligned}
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& + \gamma_4 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_5 k^2 + \gamma_6 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_7 k^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_8 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_9 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\mathbf{q} \times \mathbf{k}) \\
& + \gamma_{10} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\mathbf{q} \times \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
& + \gamma_{11} (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
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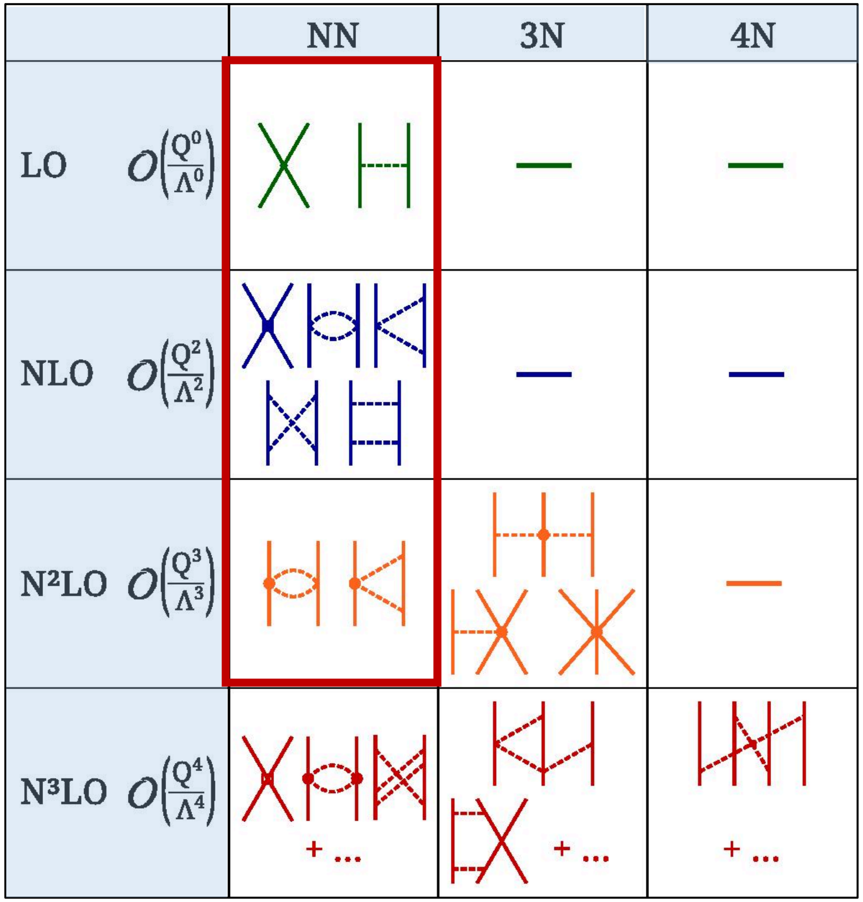
& + \gamma_{13} (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \\
& + \gamma_{14} (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \, .
\end{aligned}
$$

Local chiral interactions

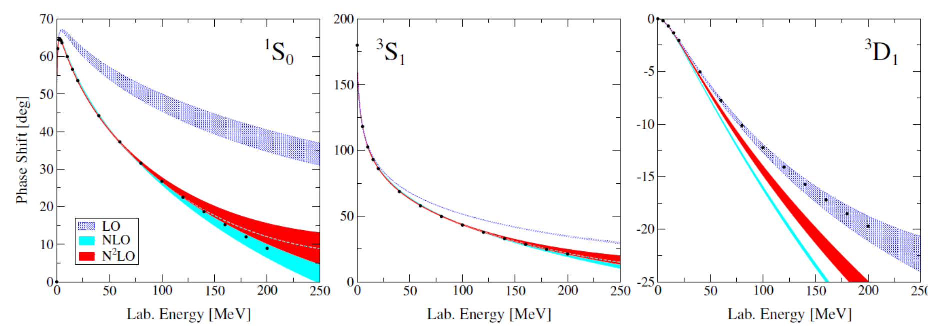


Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

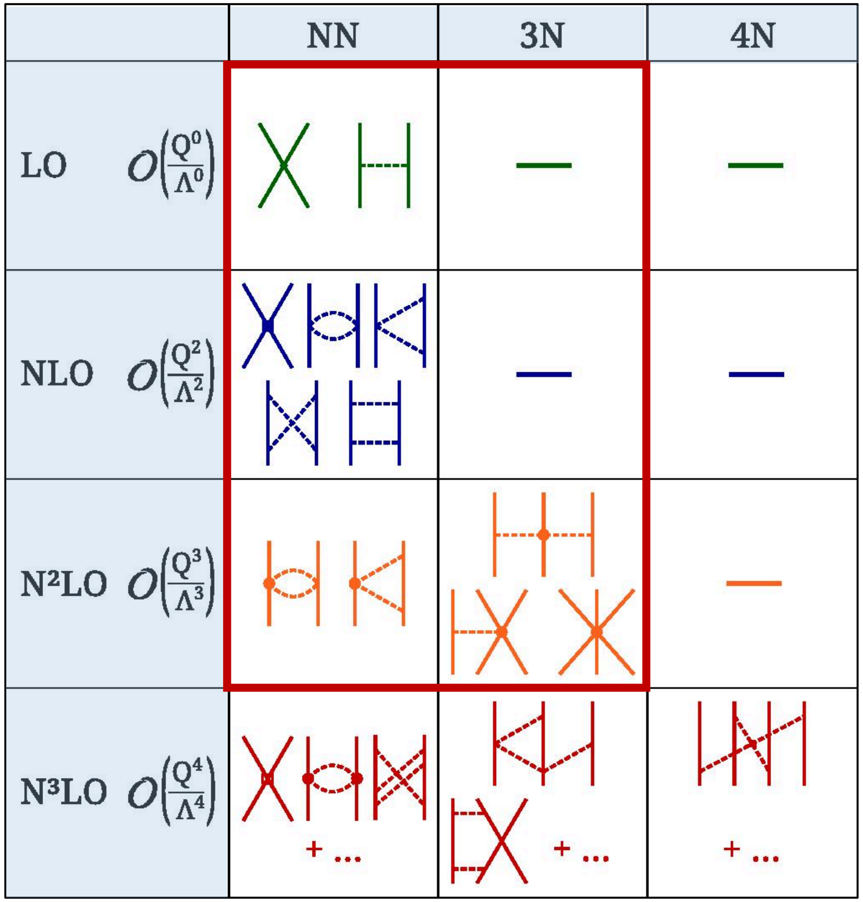
- Choose local set of short-range operators at NLO (7 out of 14)
- Pion exchanges up to N^{2}LO are local
- This freedom can be used to remove all nonlocal operators up to N^{2}LO

  Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013)
  Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

- LECs fit to phase shifts



Local chiral interactions



Weinberg, van Kolck, Kaplan, Savage, Wise,
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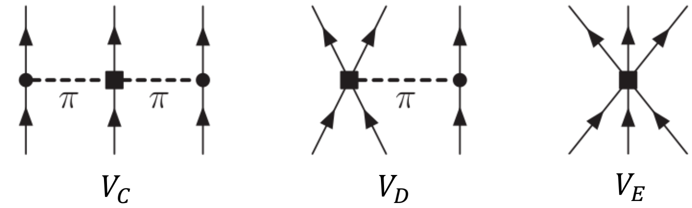
Inclusion of leading 3N forces:



Three topologies:

- Two-pion exchange V_C
- One-pion-exchange contact V_D
- Three-nucleon contact V_E

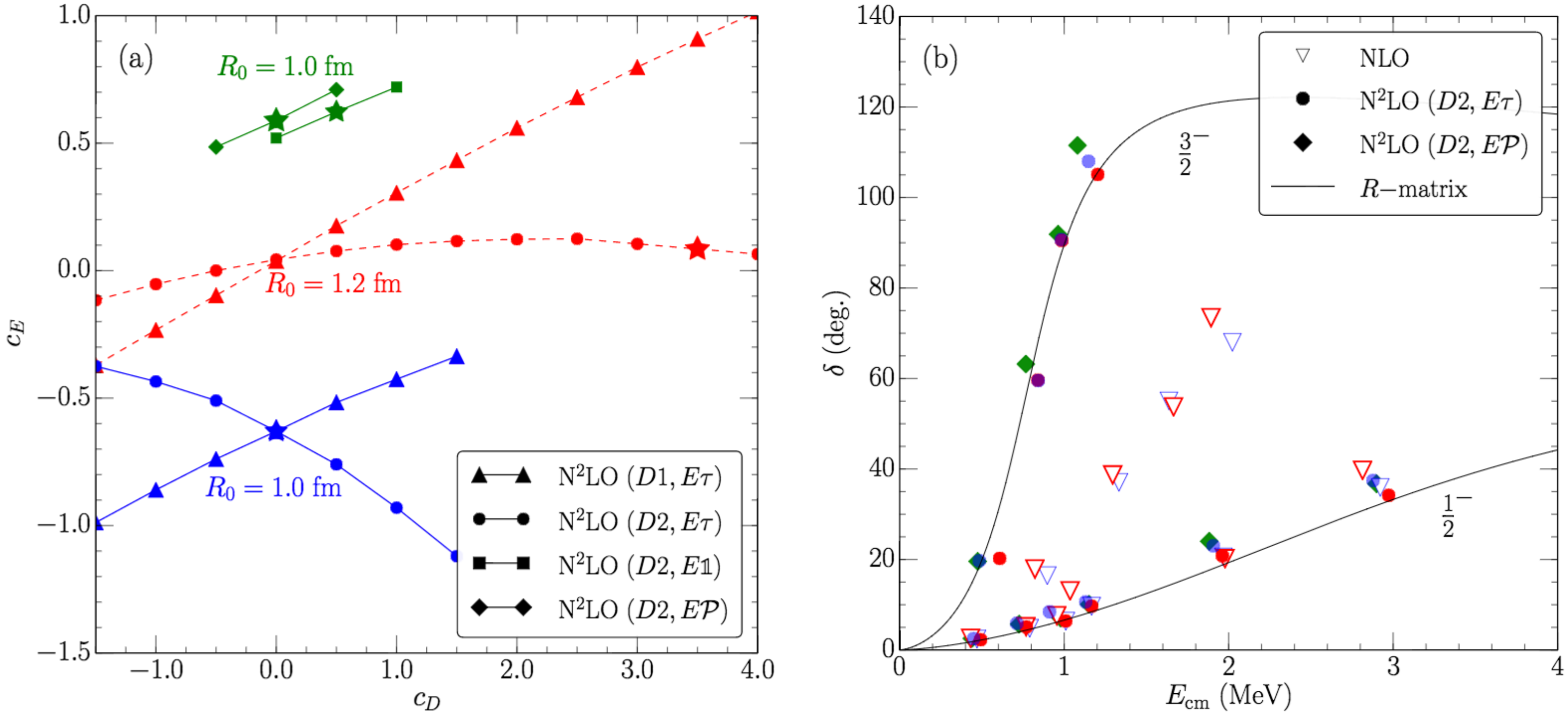
Only two new couplings: c_D and c_E.

Fit to uncorrelated observables:

- Probe properties of light nuclei: ^{4}He E_B
- Probe T=3/2 physics: n-α scattering

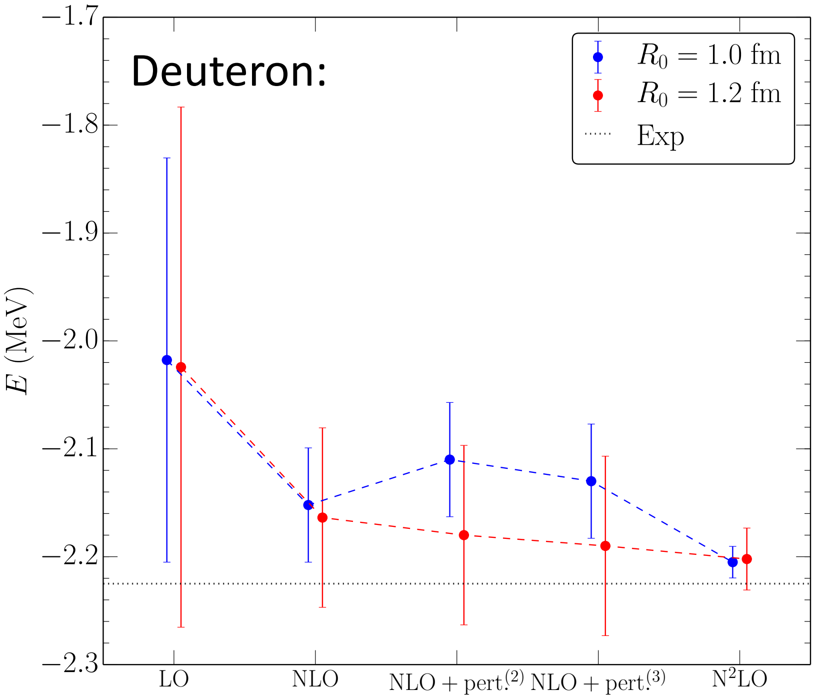
Fits of 3N LECs

- Fit c_E and c_D to ^{4}He binding energy and n-α scattering



Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

Results



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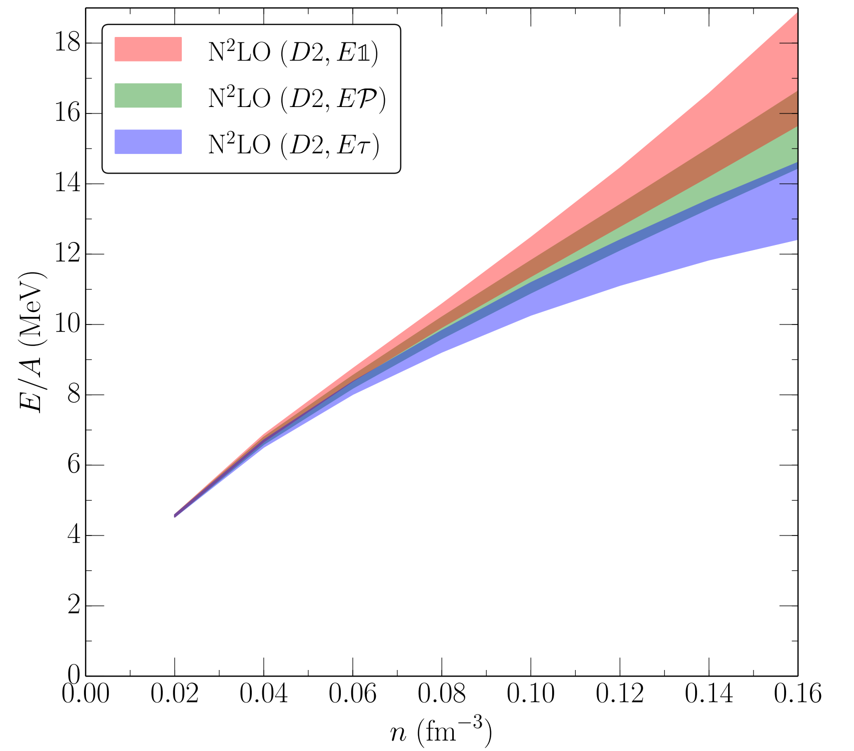
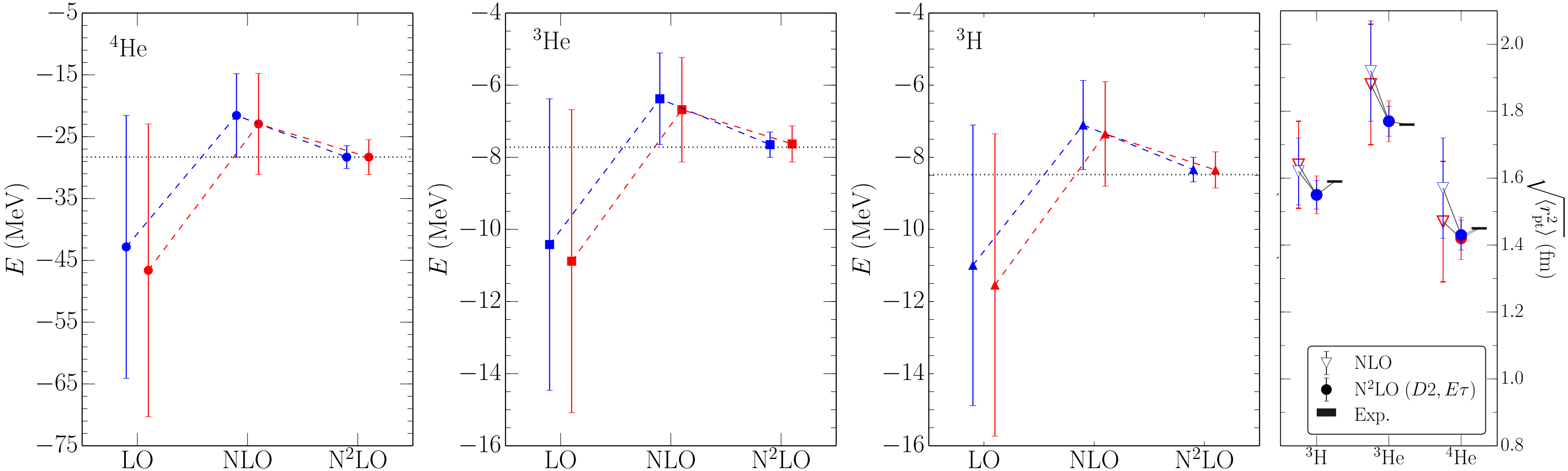


Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

- Chiral interactions at N^{2}LO simultaneously reproduce the properties of A≤5 systems and of neutron matter (uncertainty estimate as in E. Epelbaum et al, EPJ (2015))
- Commonly used phenomenological 3N interactions fail for neutron matter
  Sarsa, Fantoni, Schmidt, Pederiva, PRC (2003)

Results



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Now: two neutrons in a box

Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, PRC (2016)

Why study two neutrons in a box with QMC:

- Pure neutron systems difficult to study experimentally (e.g., nn scattering length)
- Proof of principle calculation because comparison with Luescher formula possible
- AFDMC naturally suited to calculations with periodic boundary conditions
- AFDMC naturally extendable to more particles (3n, 4n) where no Luescher formula available

Two neutrons in a box

Consider nn S-wave scattering in a cubic box with length L:

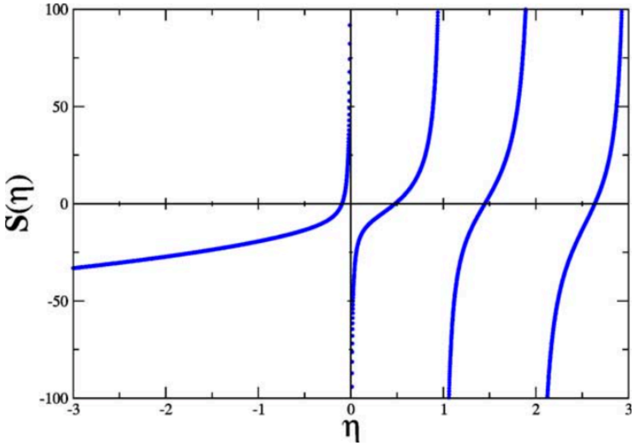
- Lüscher formula connects energy of two particles in finite volume with phase shift in the infinite volume

Lüscher, Commun. Math. Phys. (1986)

$$p \cot \delta_0(p) = \frac{1}{\pi L} S\left(\left(\frac{Lp}{2\pi}\right)^2\right)$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left(\sum_{|\mathbf{j}|<\Lambda} \frac{1}{\mathbf{j}^2 - \eta} - 4\pi\Lambda \right)$$

Beane *et al.*, PLB (2006)



- Low-energy *S*-wave scattering: use the effective-range expansion:

$$p \cot \delta_0(p) = -\frac{1}{a} + \frac{1}{2} r_e p^2 + \mathcal{O}(p^4)$$

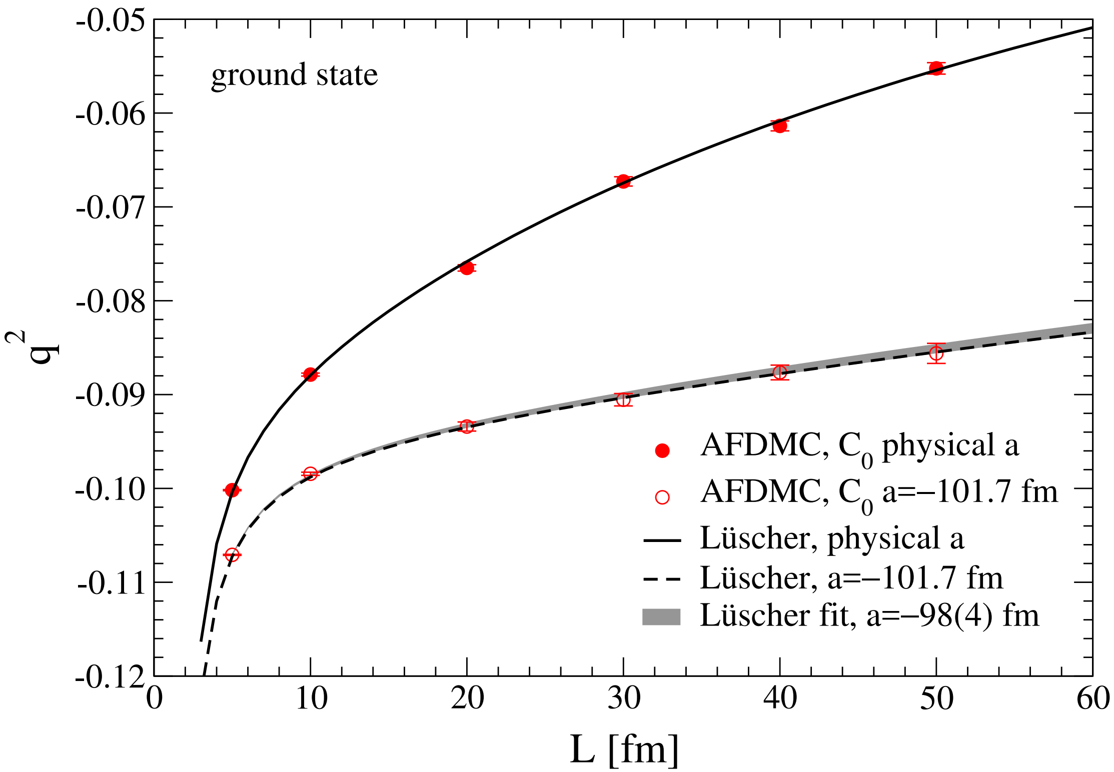
- Properties in infinite volume (scattering length, eff. range) can be determined from finite volume computations

Ground-state energies

First consider simple smeared-out contact interaction:

$$V(r) = C_0\delta(r) \to C_0\delta_{R_0}(r)$$

$$\delta_{R_0}(r) = \frac{1}{\pi\Gamma(3/4)R_0^3}\exp\left[-\left(\frac{r}{R_0}\right)^4\right]$$



Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, PRC (2016)

- Dimensionless quantity:

$$q^2 = \frac{EML^2}{4\pi^2}$$

- AFDMC precise also at extremely low densities

$$2/(50\text{ fm})^3 \sim n_0/10^4$$

TABLE I. Comparison of ground-state results for two different potentials with both the AFDMC and GFMC methods for several box sizes L.

Potential	L (fm)	q^2 AFDMC	q^2 GFMC
	5	−0.1001(3)	−0.0999(1)
C_0 physical a	10	−0.0879(7)	−0.0875(4)
	20	−0.069(2)	−0.072(2)

Ground-state energies

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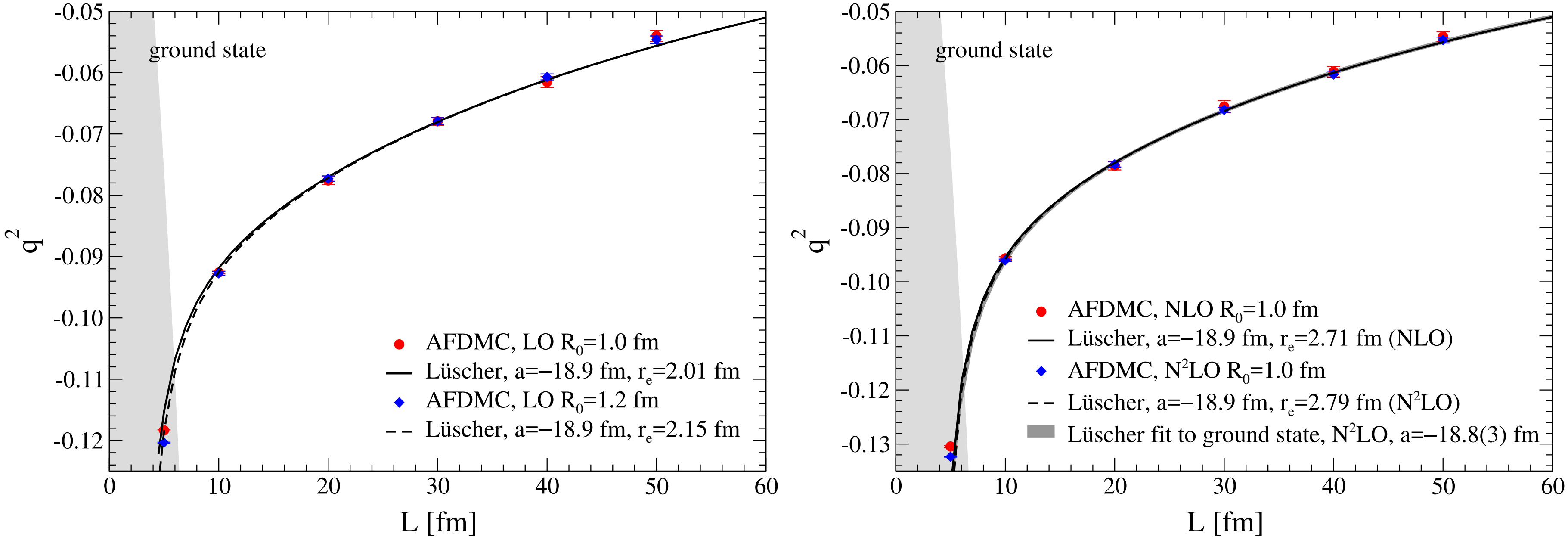
Now consider chiral EFT interactions:

- Analytic continuation of the Luescher formula (ERE) Not expected to work when pion exchanges become important, so when $p > m_\pi/2$
- Corrections go as $\exp(-m_\pi L)$, so formula valid as long as $m_\pi L$ large



Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, PRC (2016)

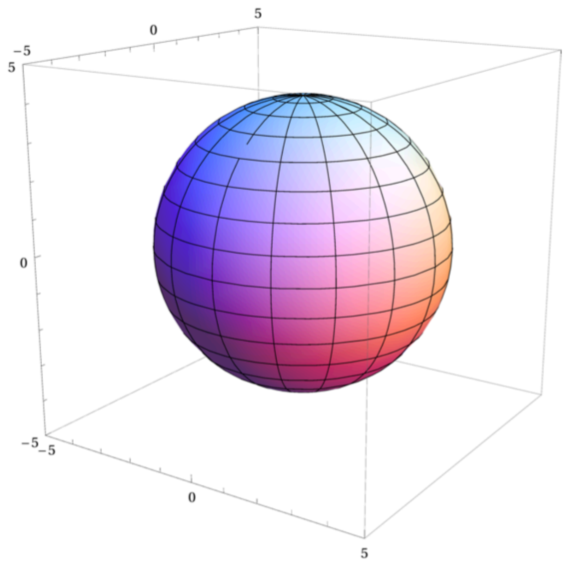
Excited states

Excited-state information desired, but challenging to obtain:

- Excited states have nodal surface in wave function.
- AFDMC uses fixed-node approximation:

  Nodal surface needed as input in trial wave function.

Insert spherical nodal surface in trial wave function (in Jastrow $f^c(r_{12})$):



$$|\psi_J\rangle = \left[\prod_{i<j} f^c(r_{ij})\right] |\Phi\rangle$$

$$\langle \mathbf{R}S|\Phi\rangle = \mathcal{A}[\langle \mathbf{r}_1 s_1|\phi_1\rangle \cdots \langle \mathbf{r}_2 s_2|\phi_2\rangle \cdots \langle \mathbf{r}_A s_A|\phi_A\rangle]$$

$$\phi_\alpha(\mathbf{r}_i, s_i) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_i} \chi_{s,m_s}(s_i) \quad \mathbf{k}_\alpha = \frac{2\pi}{L}\mathbf{n}_\alpha$$

First AFDMC calculations of excited states!

Excited states

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Jastrow functions:

$$|\psi_J\rangle = \Big[\prod_{i<j} f^c(r_{ij})\Big]|\Phi\rangle$$

$$\langle \mathbf{R}S|\Phi\rangle = \mathcal{A}[\langle \mathbf{r}_1 s_1|\phi_1\rangle \cdots \langle \mathbf{r}_2 s_2|\phi_2\rangle \cdots \langle \mathbf{r}_A s_A|\phi_A\rangle]$$

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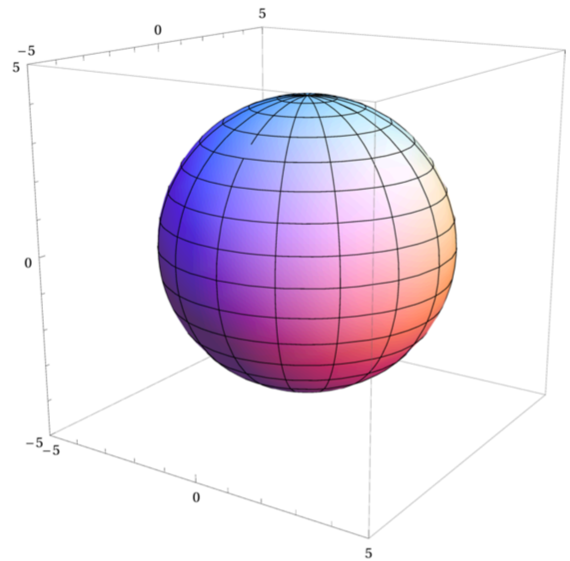
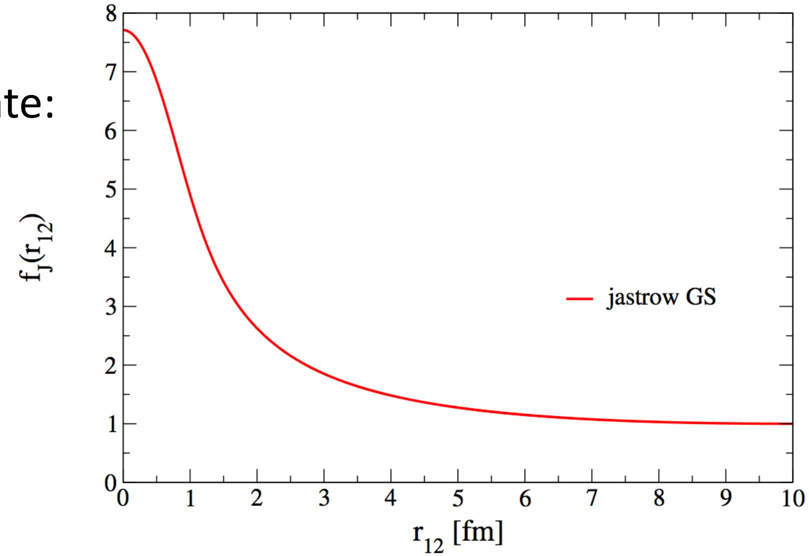
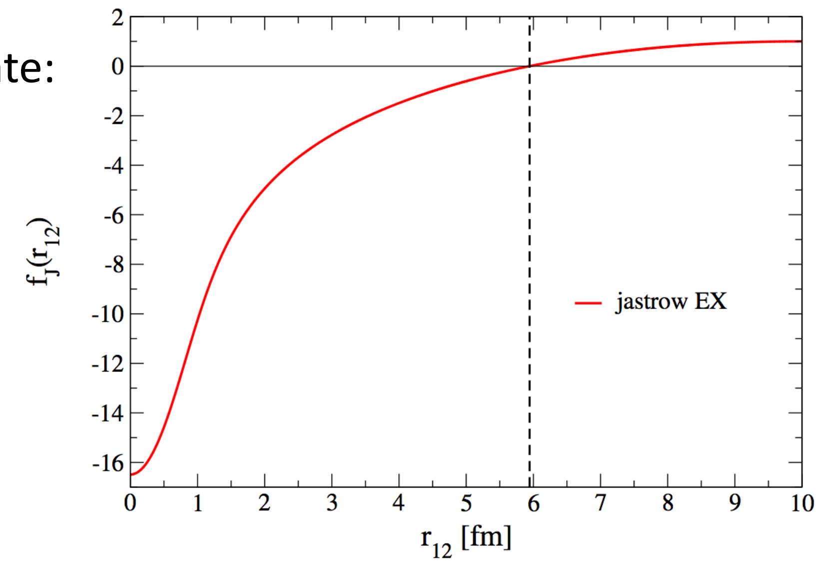


Ground state:



Excited state:

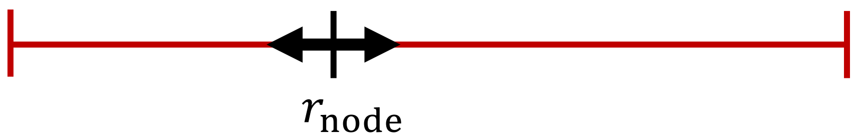


Excited states

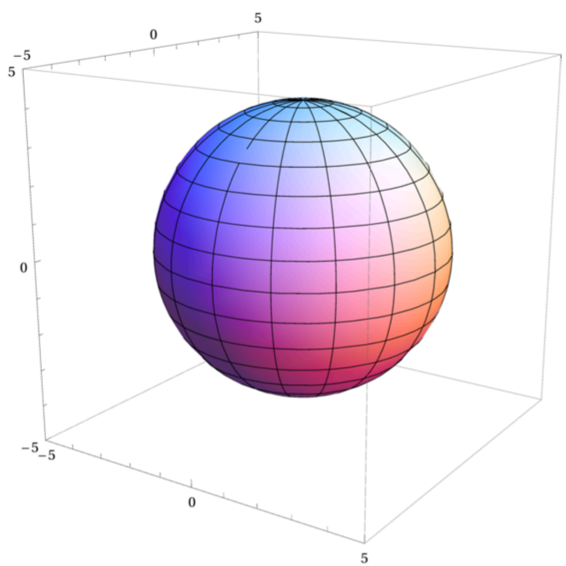
Determine nodal position: for local potential Schroedinger equation

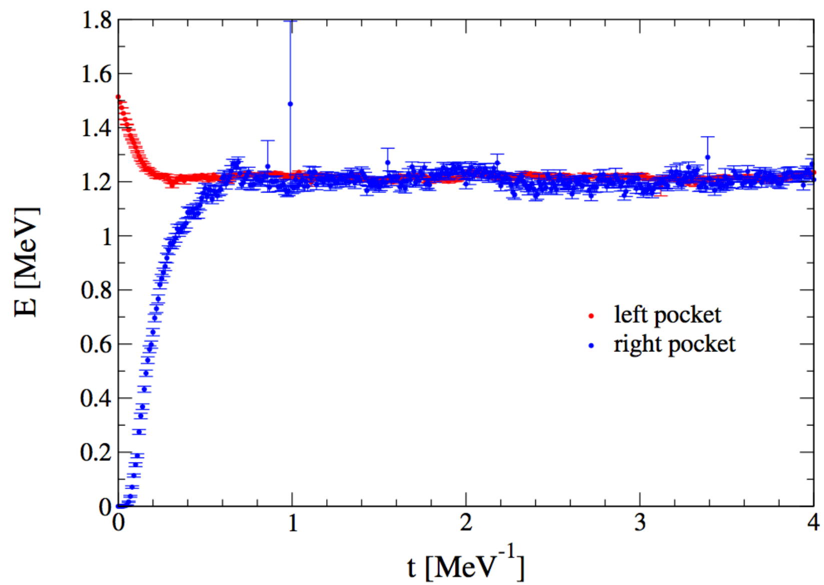
$$H\psi(\mathbf{r}_1, \mathbf{r}_2) = E\psi(\mathbf{r}_1, \mathbf{r}_2)$$

gives same energy independent of coordinates.



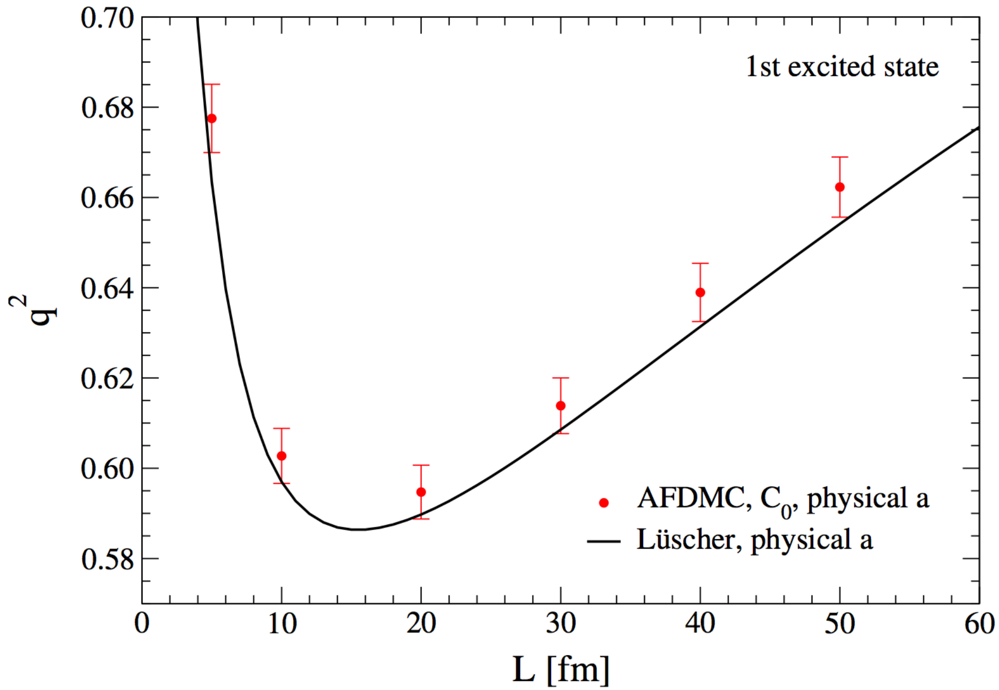
Move node until energies in both pockets are the same:





Excited states

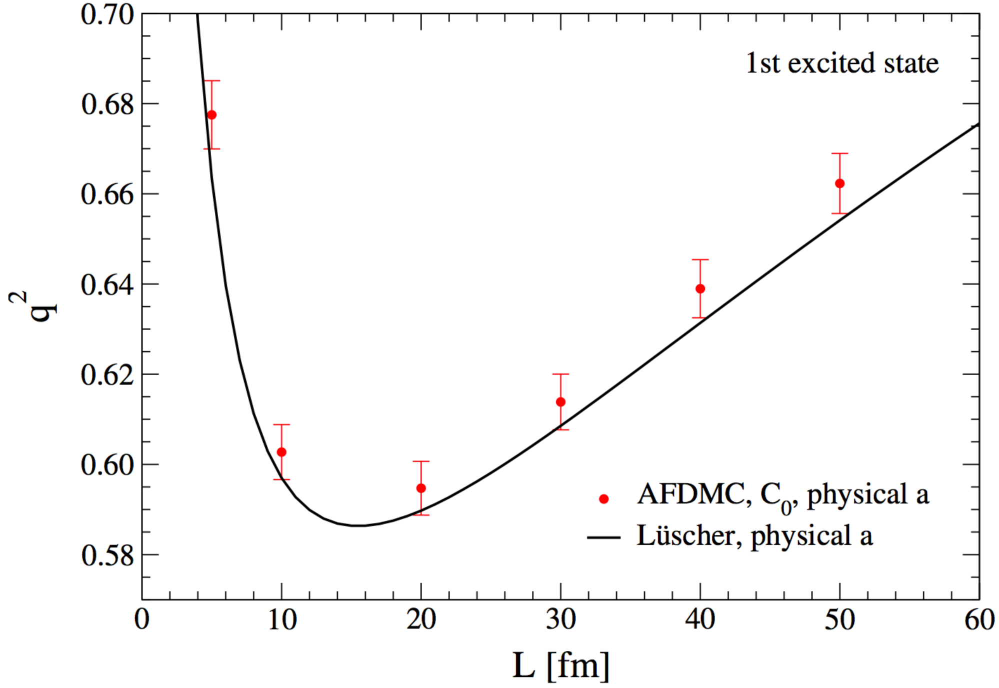
Simple smeared-out contact interaction:

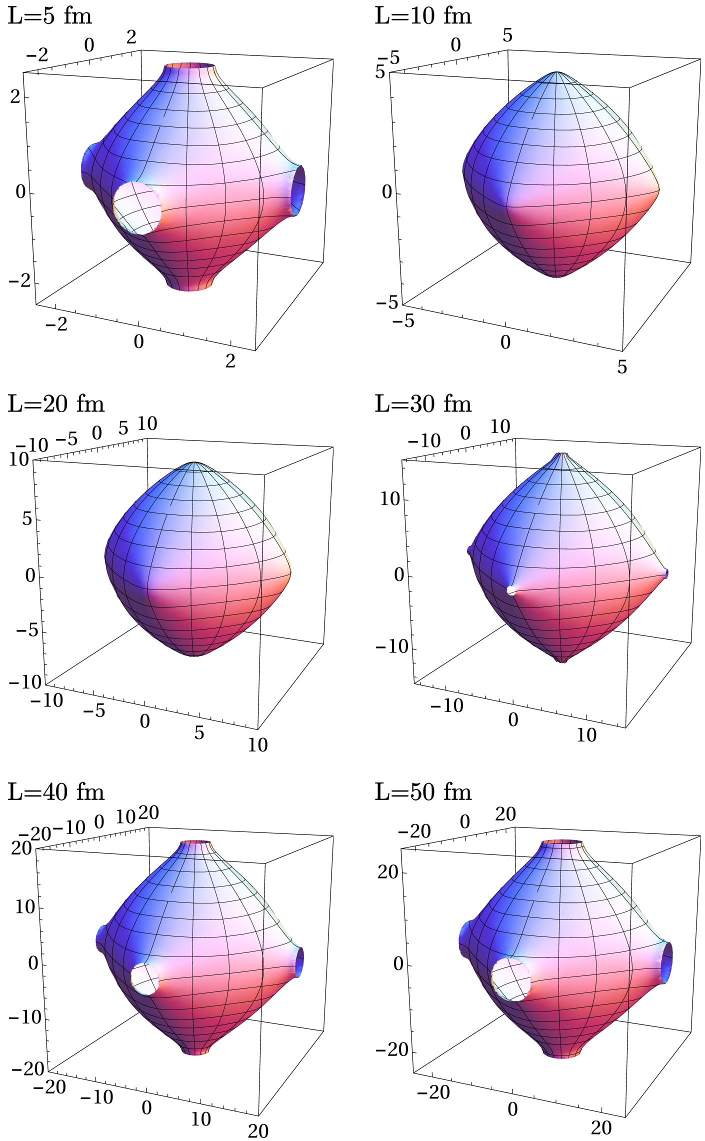


- AFDMC results systematically above the Luescher results
- Overall trend is correctly reproduced
- Nodal surface not spherical:
  - investigate exact nodal surface $r(\theta, \phi)$ using diagonalization

Excited states

Simple smeared-out contact interaction:





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Excited states

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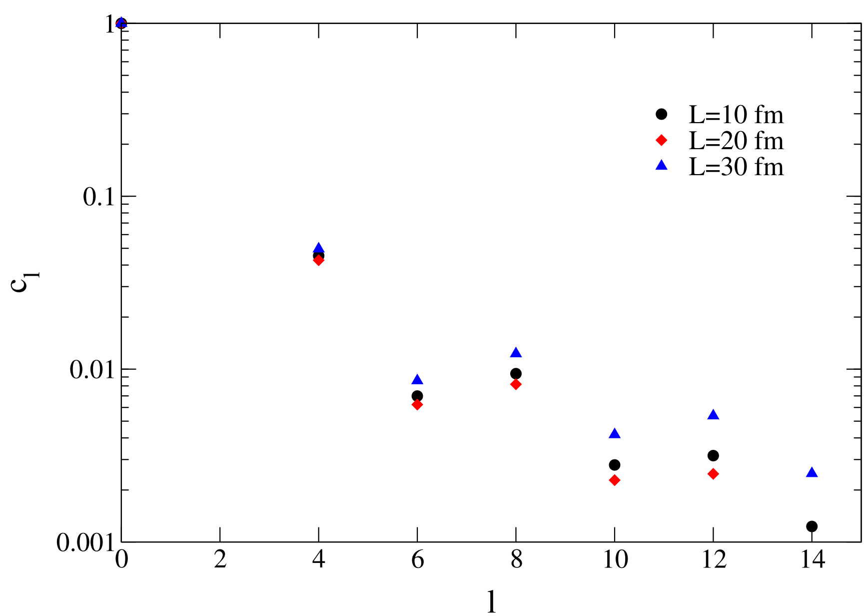
Nodal surfaces can be decomposed into cubic harmonics:

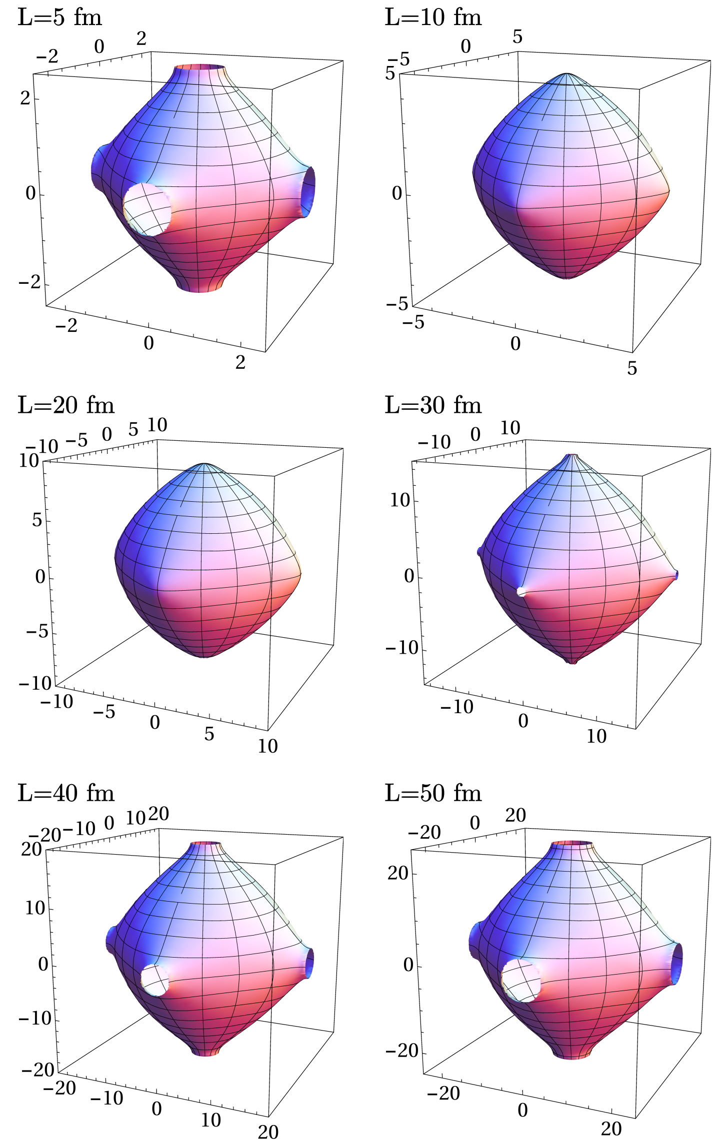
Muggli, Z. Angew. Math. Mech. (1972)

$$Y_l^c(\theta,\phi) = \sum_{m=0,4,8,\ldots} a_{lm} Y_{lm}(\theta,\phi)$$

$$r_{\mathrm{node}}(\theta,\phi) = \sum_l c_l Y_l^c(\theta,\phi)$$



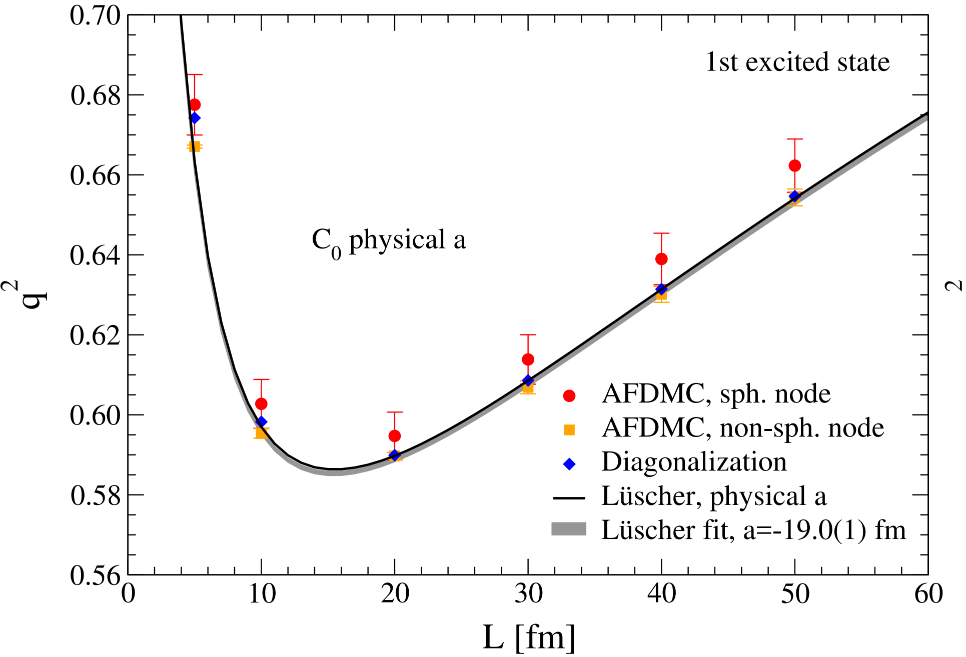
Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, PRC (2016)



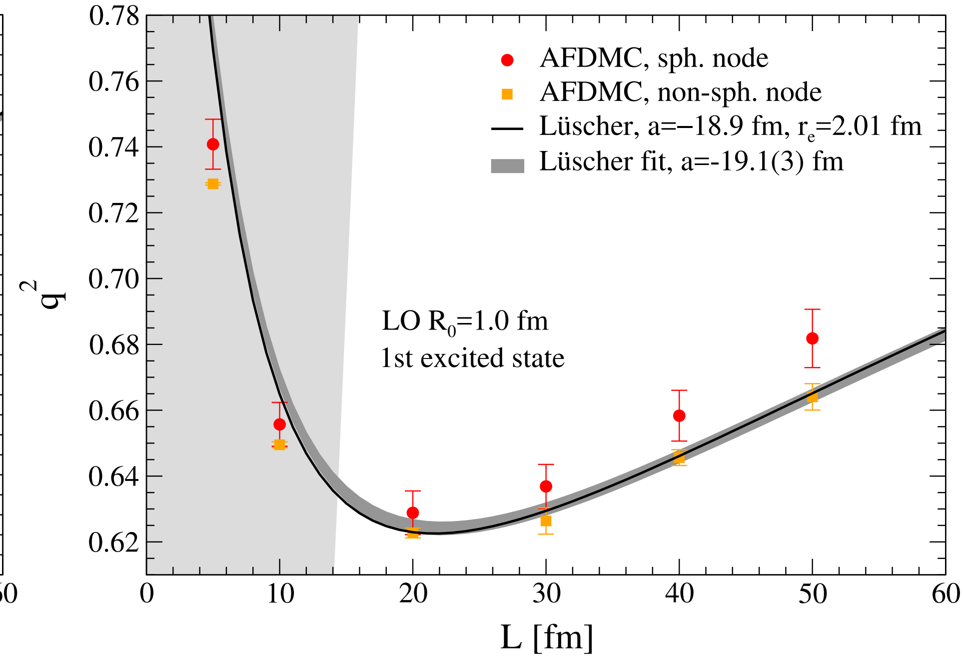
Excited states

We include first correction to spherical node:

Simple smeared-out contact interaction:



Chiral LO interaction:



Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, PRC (2016)

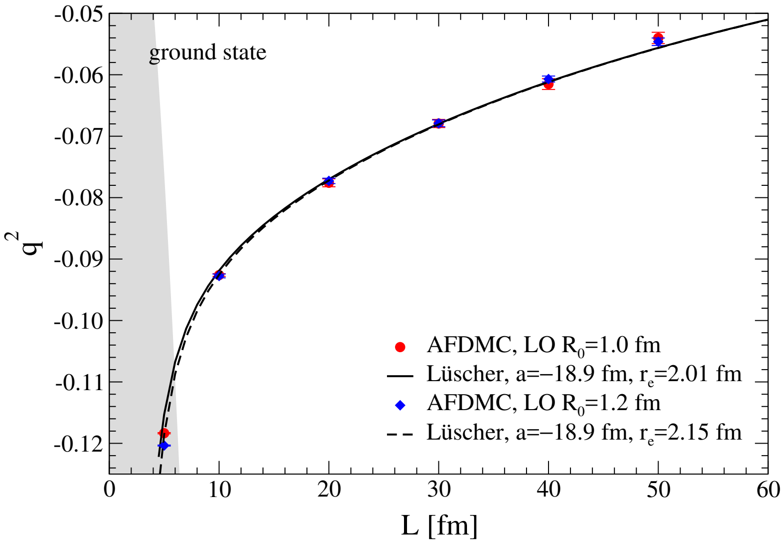
Very good agreement with Luescher results!

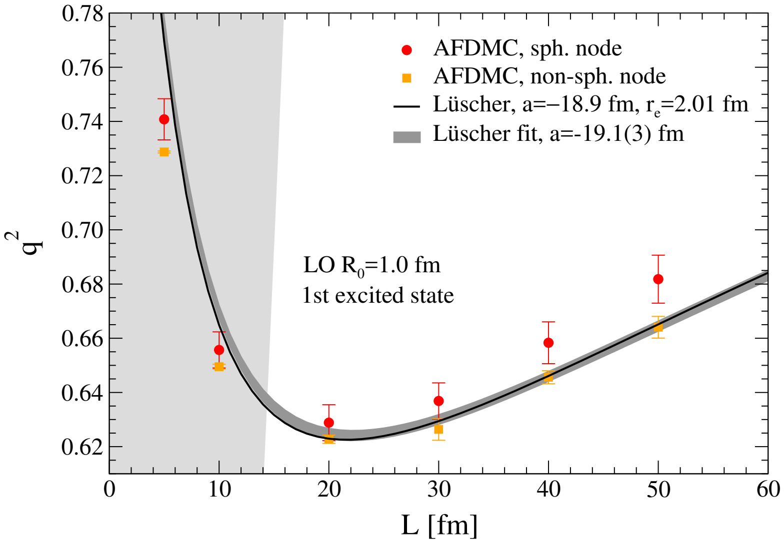
Next step: Extend to larger systems!

Summary

Quantum Monte Carlo calculations with chiral EFT interactions lead to interesting results:

- Chiral interactions at N^2LO simultaneously reproduce the properties of A=3, 4, 5 systems and of neutron matter.
- First calculations of excited states in AFDMC.
- QMC calculations provide a reliable tool to establish a bridge between lattice QCD calculations and chiral EFT.
- Possible to extend calculations to larger or different systems where no Luescher formula available.
- Finite volume calculations will eventually allow for matching LECs to Lattice QCD.





Thanks

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- Los Alamos National Laboratory:
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  A. Gezerlis
- Institute for Nuclear Theory:
  M. Hoferichter

European Research Council
Established by the European Commission

JINA–CEE

JÜLICH FORSCHUNGSZENTRUM

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Thank you!