Quantum Monte Carlo Calculations Of Light Nuclei With Chiral Interactions

Nuclear Physics from Lattice QCD

TECHNISCHE UNIVERSITÄT DARMSTADT

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NERSC

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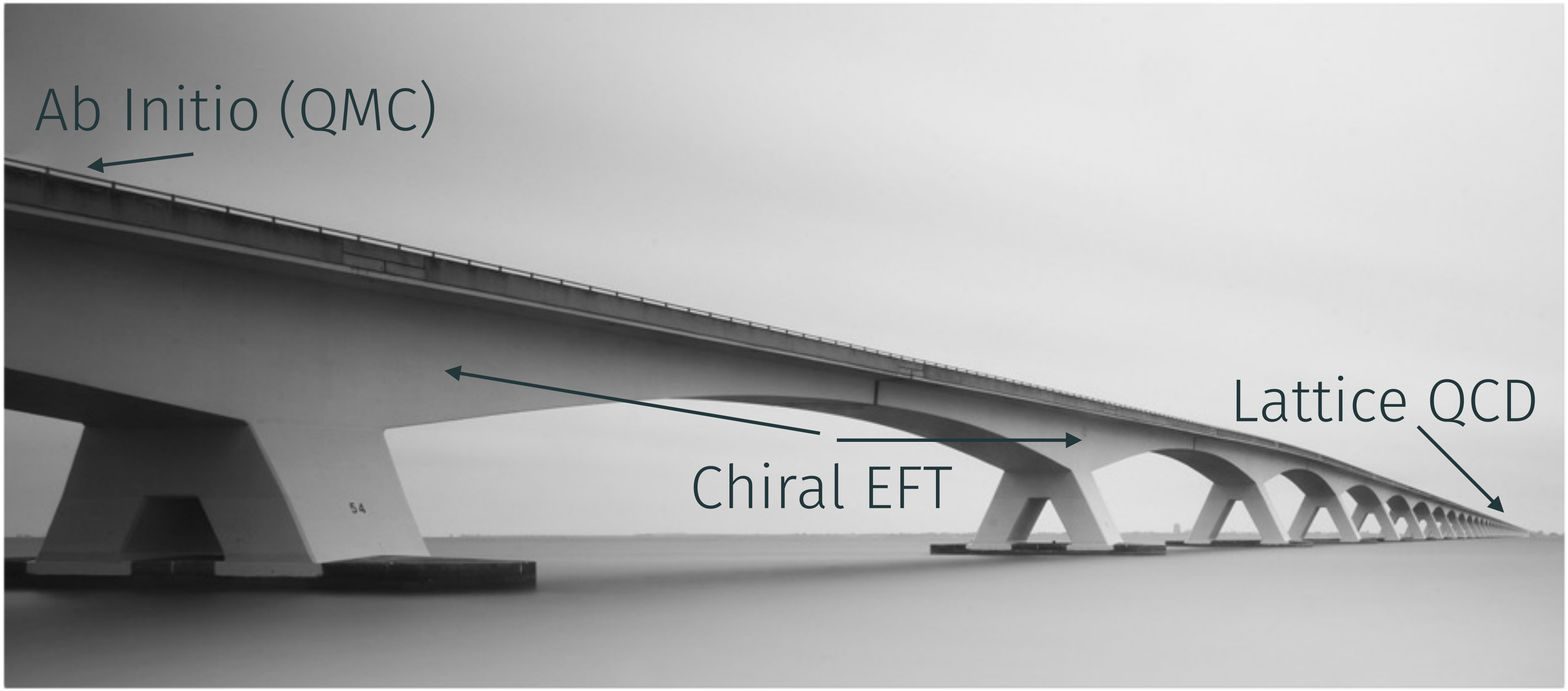
April 13, 2016

Building A Bridge



Outline

- Quantum Monte Carlo
- Chiral EFT
- Three-Nucleon Interaction
- Fits and Results
- Finite Volume Calculations
- Summary

Quantum Monte Carlo (QMC)

QMC

QMC in two lines:

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

$$\lim_{\tau\to\infty} e^{-H\tau}\left|\Psi_T\right\rangle \to \left|\Psi_0\right\rangle$$

QMC in more than two lines:

J. Carlson et al, RMP **87**, 1067 (2015).

QMC - Variational Monte Carlo (VMC)

1. Guess a trial wave function Ψ_T and generate a random position: $\mathrm{R} = \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_A$.

2. Use the Metropolis algorithm to generate new positions R' based on the probability $P = \frac{|\Psi_T(\mathrm{R}')|^2}{|\Psi_T(\mathrm{R})|^2}$. (Yields a set of “walkers” distributed according to $|\Psi_T|^2$).

3. Invoke the variational principle: $E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} > E_0$.

QMC - Diffusion Monte Carlo

- The wave function is imperfect: $|\Psi_T\rangle = \sum_{i=0}^{\infty} \alpha_i |\Psi_i\rangle$.
- Propagate in imaginary time to project out the ground state $|\Psi_0\rangle$.

$$
\begin{aligned}
|\Psi(\tau)\rangle &= e^{-(H-E_T)\tau} |\Psi_T\rangle \\
&= e^{-(E_0-E_T)\tau}[\alpha_0 |\Psi_0\rangle + \sum_{i\neq 0} \alpha_i e^{-(E_i-E_0)\tau} |\Psi_i\rangle].
\end{aligned}
$$

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\end{aligned}
$$

$$
|\Psi(\tau)\rangle \xrightarrow{\tau\to\infty} |\Psi_0\rangle .
$$

QMC - An Example

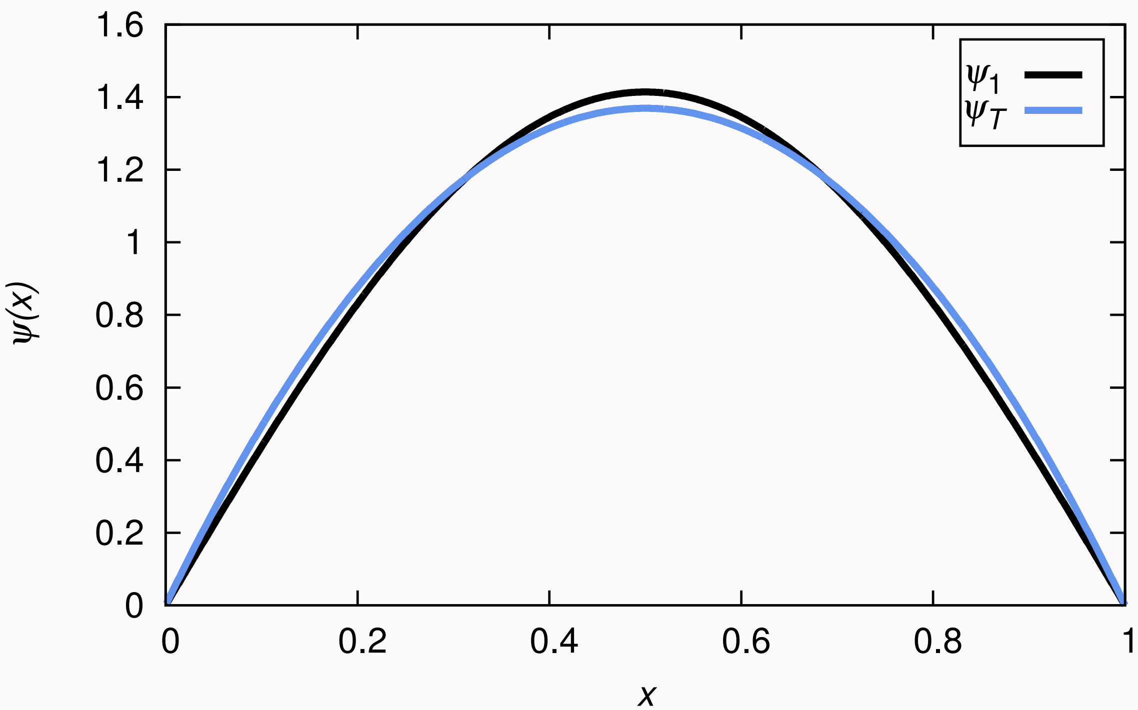
$$H = \frac{p_x^2}{2m} + V(x), \;\; V = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

$$\hbar = m = L = 1$$

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

Trial wave function; e.g.

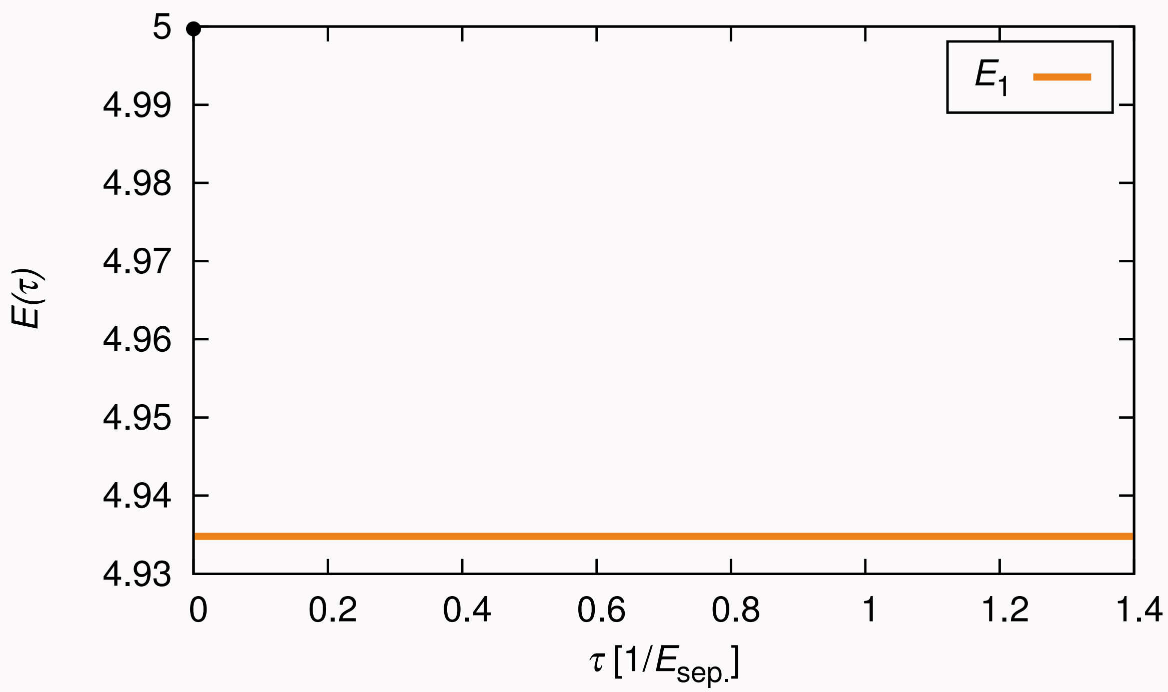
$$\Psi_T(x) = \sqrt{30}x(1-x).$$

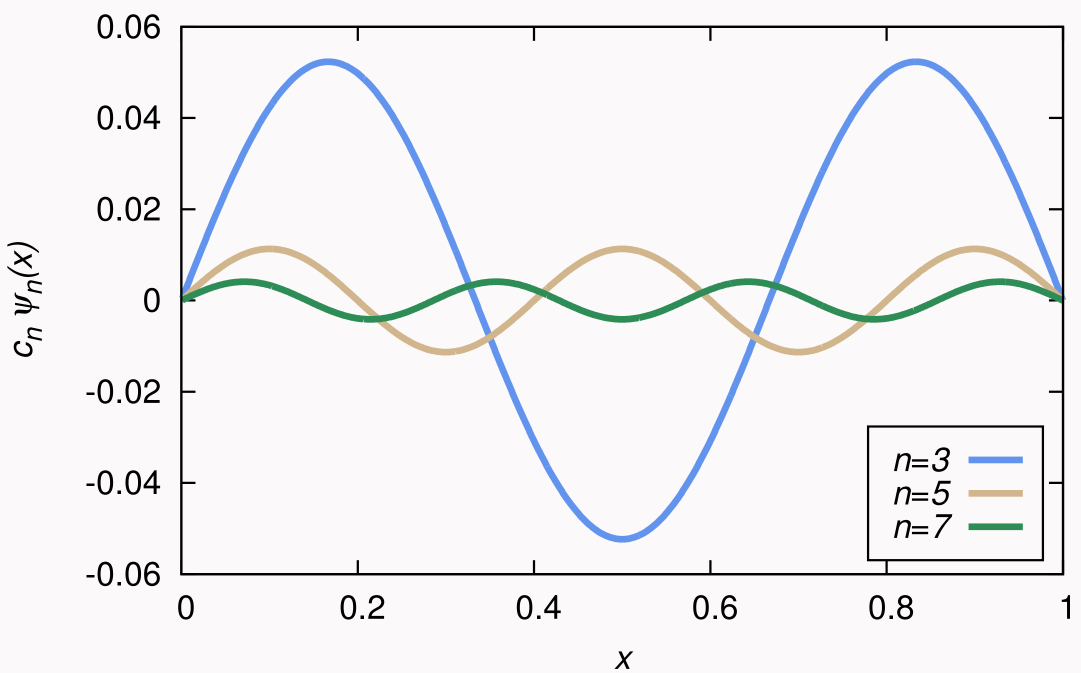


QMC - An Example

$$E(\tau) = \frac{\langle \Psi_T | H e^{-(H-E_T)\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)\tau} | \Psi_T \rangle}, \quad \Psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\tau = 0.0(1/E_{\text{sep}})$$

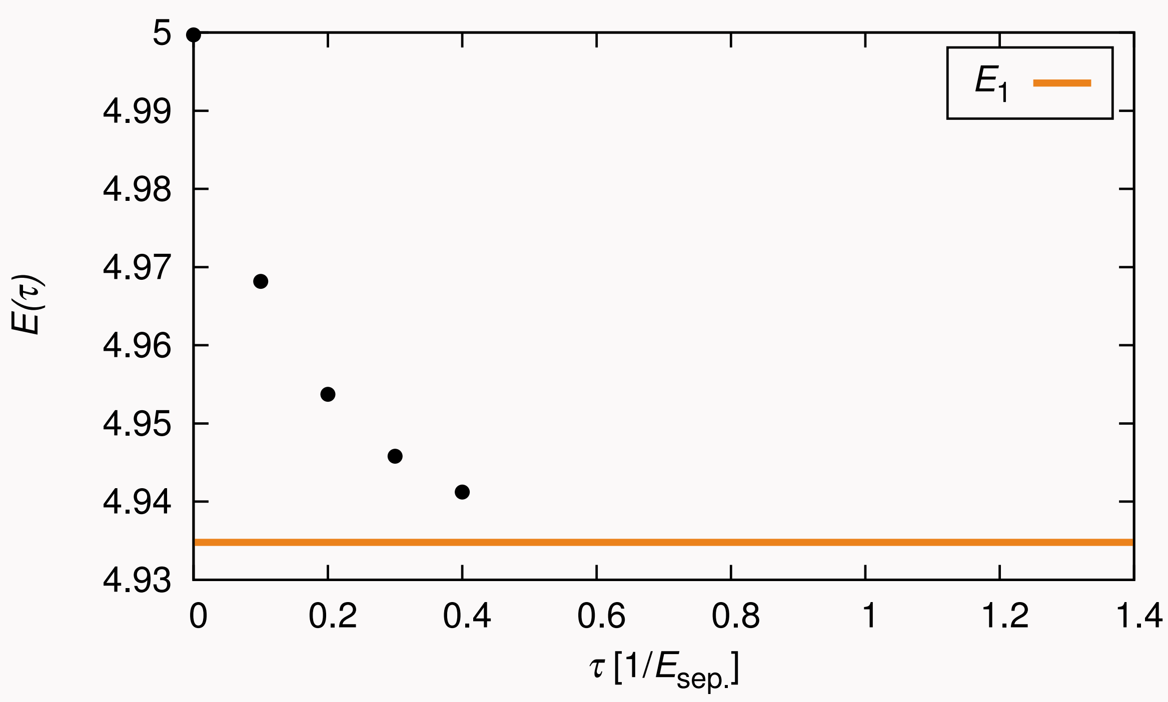


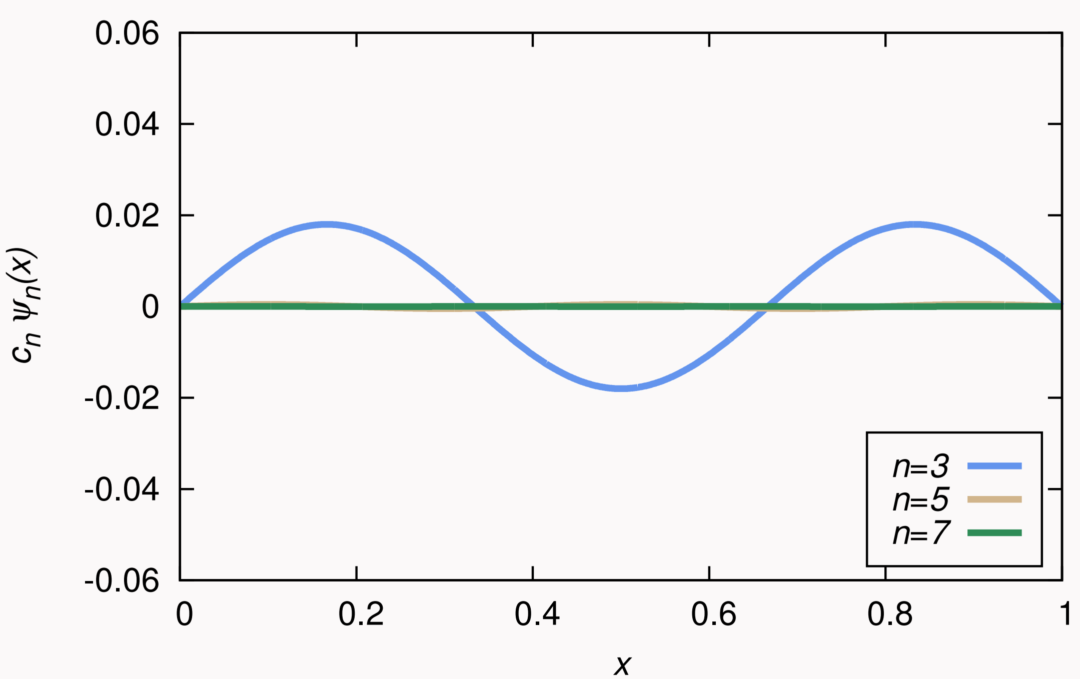


QMC - An Example

$$E(\tau) = \frac{\langle \Psi_T | H e^{-(H-E_T)\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)\tau} | \Psi_T \rangle}, \quad \Psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\tau = 0.4(1/E_{\text{sep}})$$

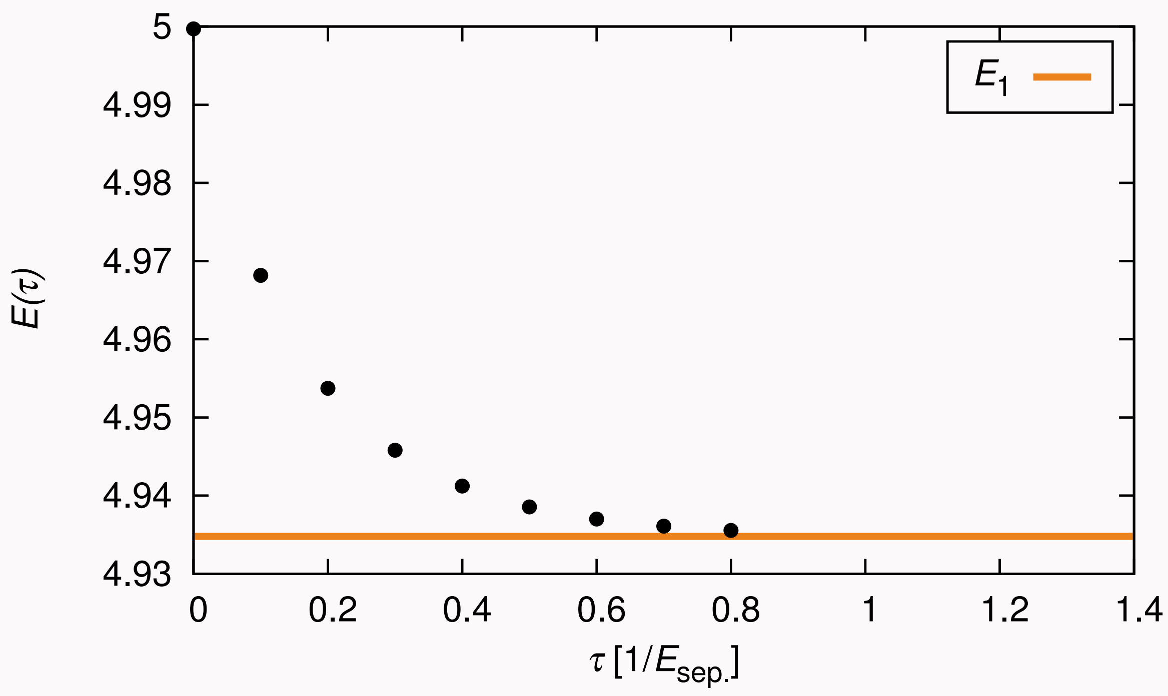


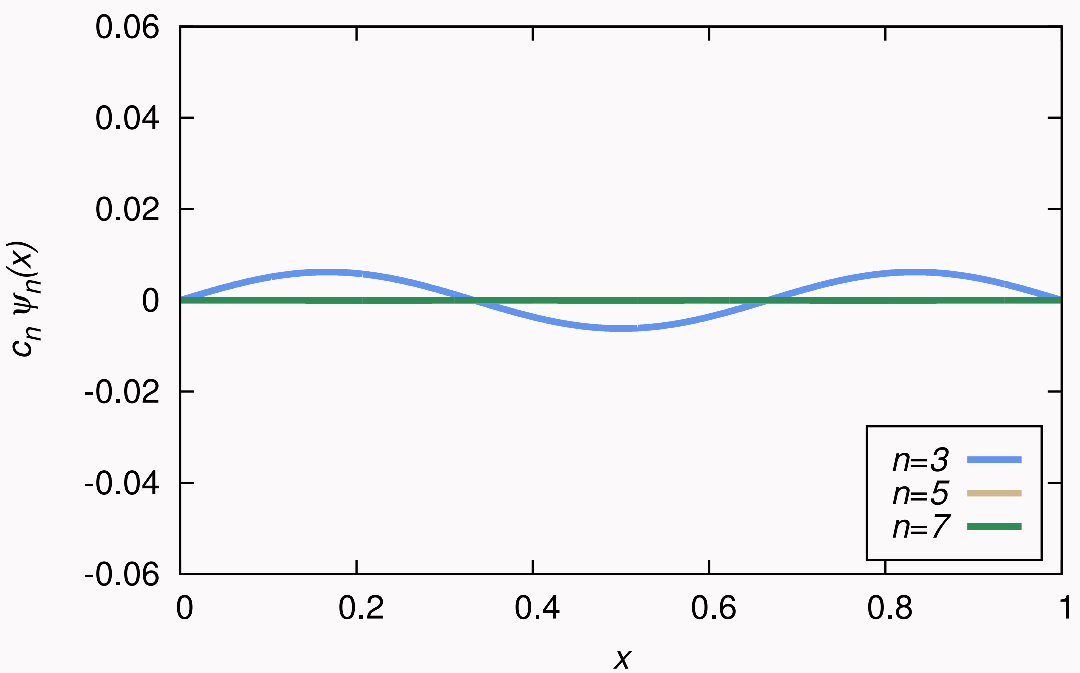


QMC - An Example

$$E(\tau) = \frac{\langle \Psi_T | H e^{-(H-E_T)\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)\tau} | \Psi_T \rangle}, \quad \Psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\tau = 0.8(1/E_{\mathrm{sep}})$$

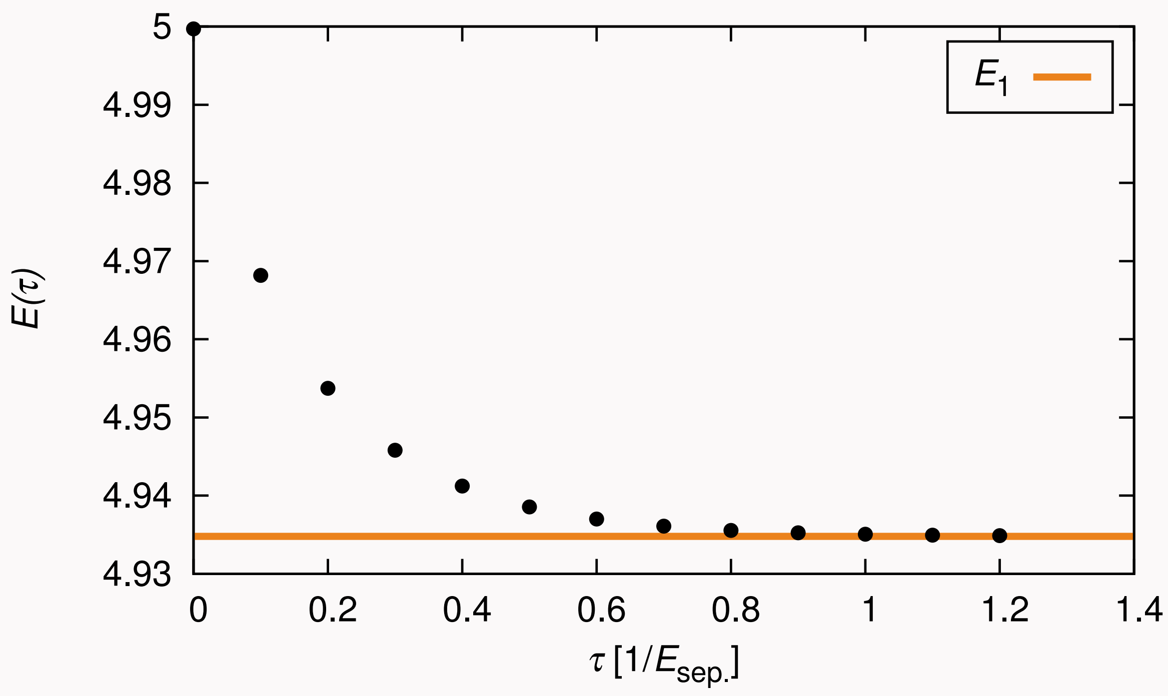


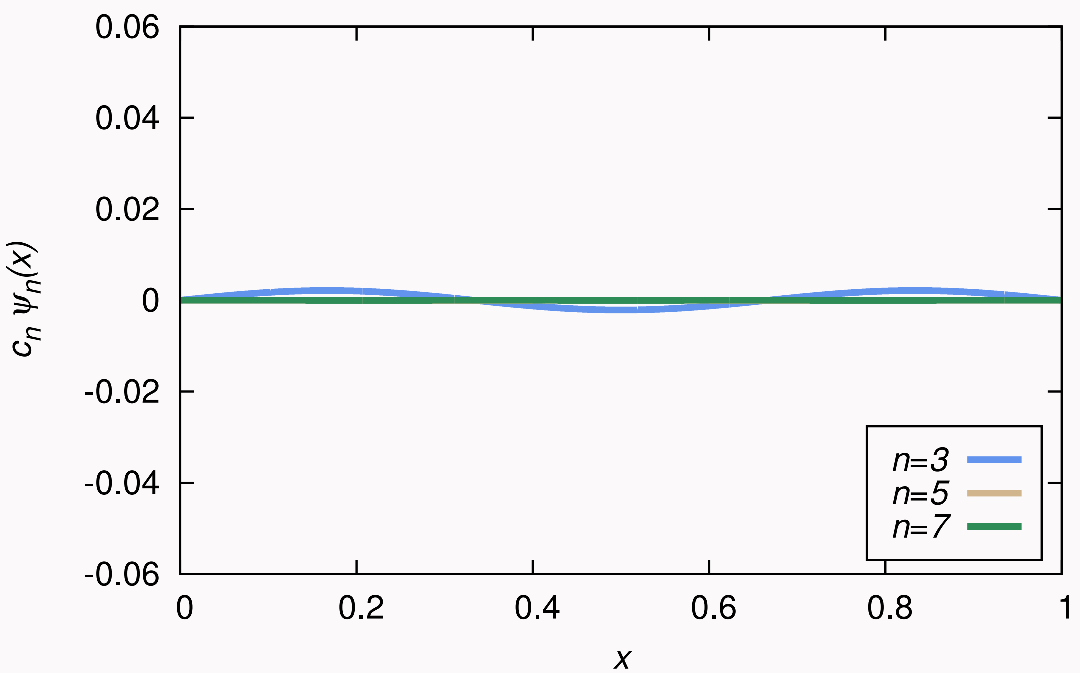


QMC - An Example

$$E(\tau) = \frac{\langle \Psi_T | H e^{-(H-E_T)\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)\tau} | \Psi_T \rangle}, \quad \Psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

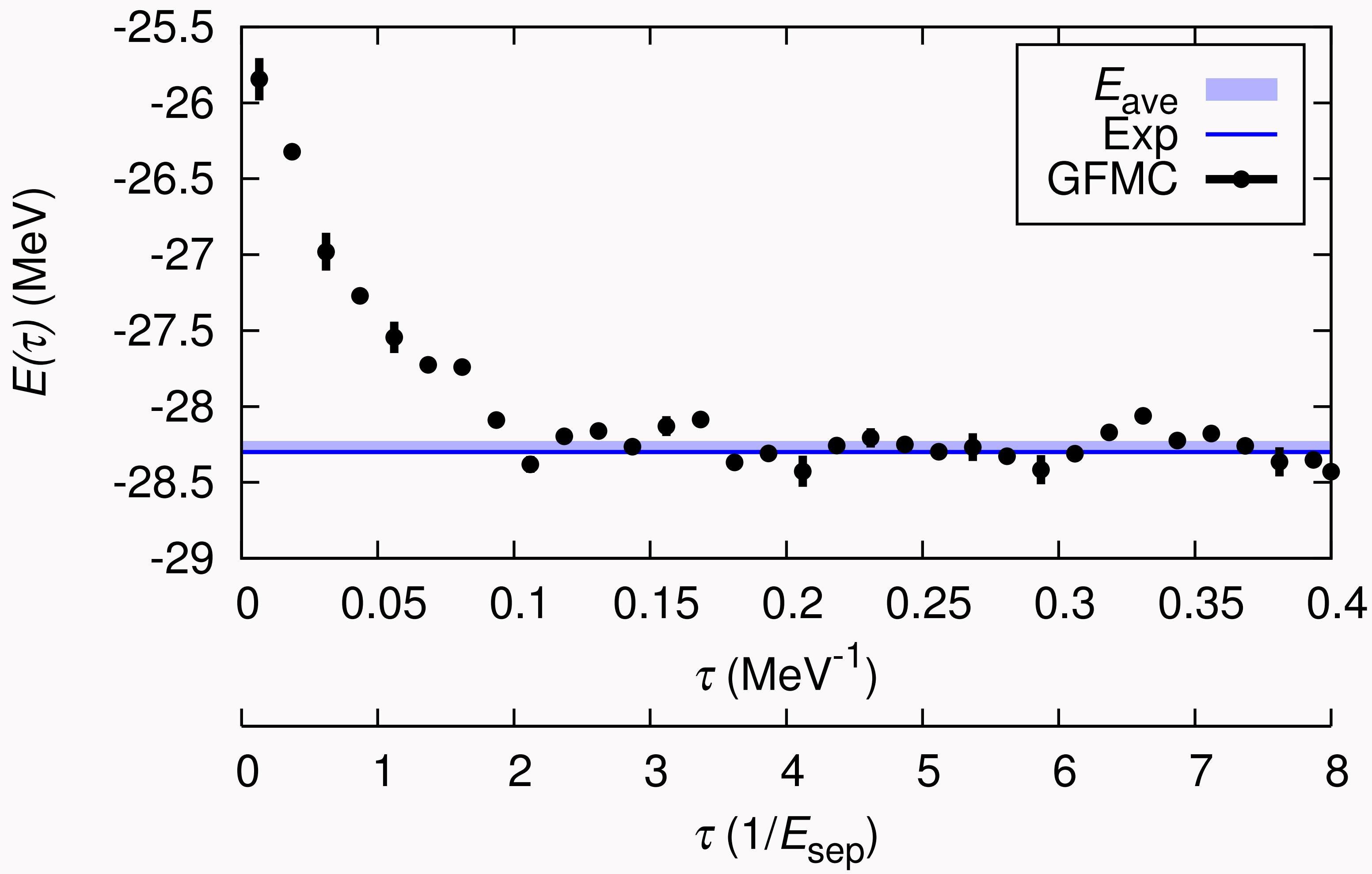
$$\tau = 1.2 \ (1/E_{\text{sep}})$$





QMC - An Example

For ^{4}He, $1/E_{sep} = 1/|E_\alpha - E_t| \approx 0.05\ \text{MeV}^{-1}$.



The Hamiltonian

Of course, the Hamiltonian is much more complicated in nuclear physics.

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \cdots$$

Chiral Effective Field Theory (EFT)

Chiral EFT

Chiral EFT in two lines:

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{2g^2}\text{Tr}(G_{\mu\nu}G^{\mu\nu}) + \bar{q}i\gamma^{\nu}D_{\nu}q - \bar{q}\mathcal{M}q \rightarrow \text{Chiral symmetry}$$

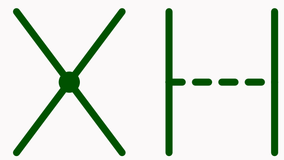
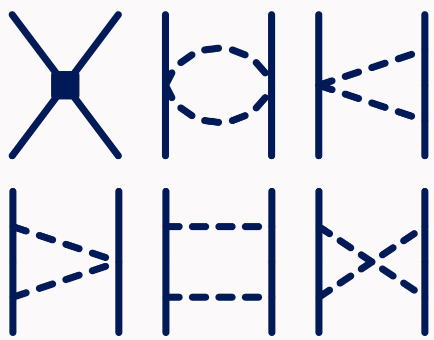
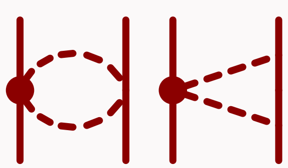
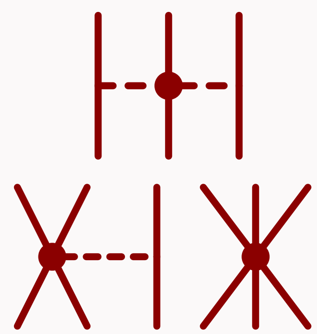
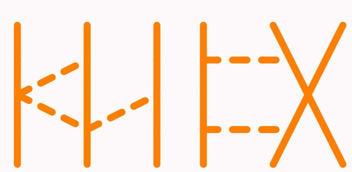
$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \cdots$$

More Details:

E. Epelbaum et al, RMP **81**, 1773 (2009);

R. Machleidt et al, Phys. Rep. **503**, (2011).

Chiral EFT

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		–
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		–
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

- Chiral EFT: Expand in powers of Q/Λ_b.
  $Q \sim m_\pi \sim 100$ MeV
  $\Lambda_b \sim 500$ MeV
- Long-range physics: π exchanges.
- Short-range physics: Contacts × LECs.
- Many-body forces & currents enter systematically.

Chiral EFT - Open Questions

- Power counting - Weinberg scheme ill defined but appears to give converging results, KSW scheme well defined but doesn't appear to give converging results. What's the right counting?

- Regulator choices - Since we take cutoff finite, these now matter. How much?

- Cutoff effects - Can we reduce cutoff effects?

- Delta degrees of freedom - Are these important for convergence of the expansion?

- Is there a better way forward?

Chiral EFT

Local construction possible[1] up to N^2LO.

Definitions.

$$\mathbf{q} = \mathbf{p} - \mathbf{p}', \ \mathbf{k} = \mathbf{p} + \mathbf{p}'$$

Regulator:

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

Contacts:

$\propto \mathbf{q}$ and $\mathbf{k}$

[1] A. Gezerlis et al, PRL **111** 032501 (2013); JEL et al, PRL **113** 192501 (2014); A. Gezerlis et al, PRC **90** 054323 (2014)

Chiral EFT

Local construction possible[1] up to N^2LO.

Definitions.

$$\mathbf{q} = \mathbf{p} - \mathbf{p}', \ \mathbf{k} = \mathbf{p} + \mathbf{p}'$$

Regulator:

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

$$\rightarrow f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4} \ : \ R_0 = 1.0, 1.1, 1.2 \text{ fm.}$$

Contacts:

~~$\propto$ **q** and **k**~~

→ Choose contacts $\propto$ **q** (As much as possible!)

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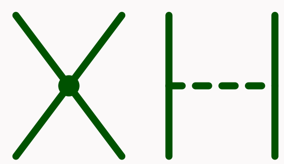
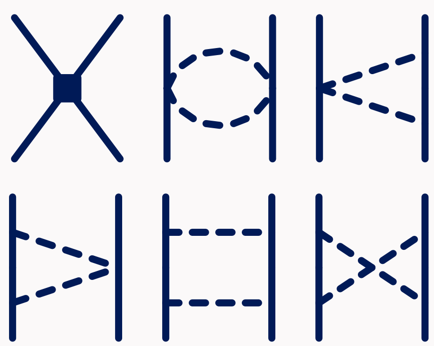
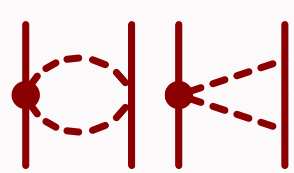
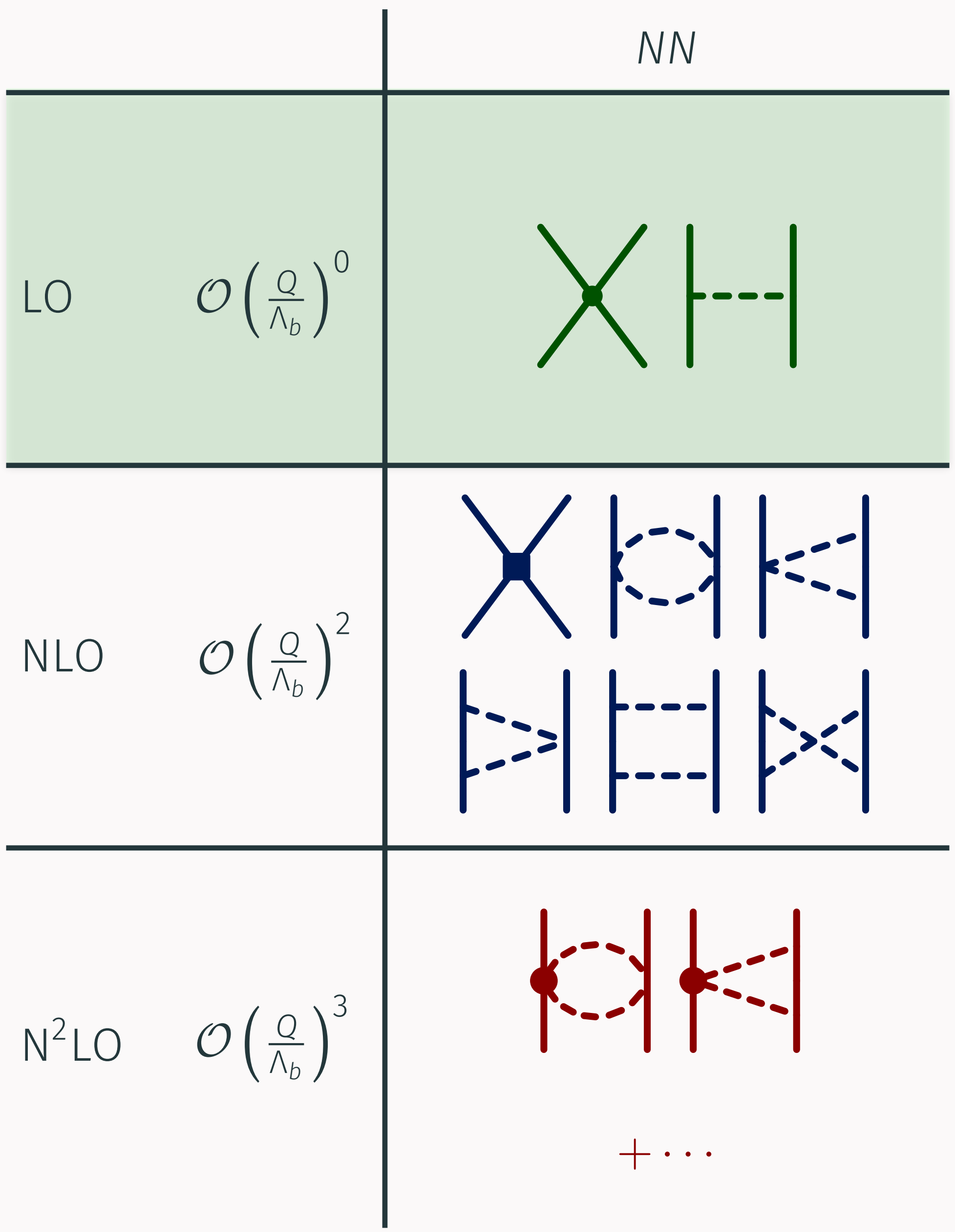
Chiral EFT

		NN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$

Chiral EFT



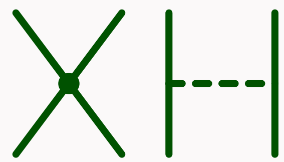
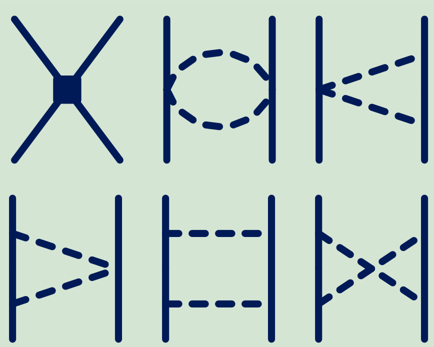
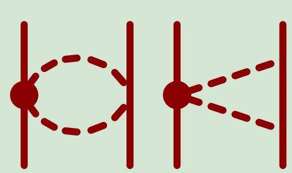
$$V^{(0)}_{\text{cont}} = \alpha_1 + \alpha_2(\sigma_1 \cdot \sigma_2) + \alpha_3(\tau_1 \cdot \tau_2) + \alpha_4(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$$

Pauli Exclusion Principle

$\rightarrow$ Only two independent contacts!

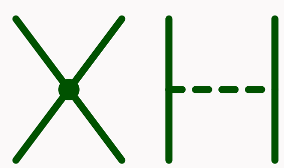
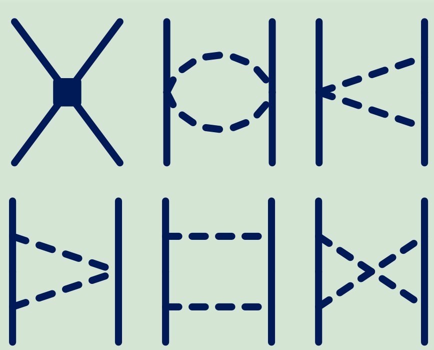
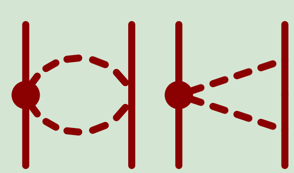
$$V^{(0)}_{\text{cont}} = C_S + C_T(\sigma_1 \cdot \sigma_2)$$

Chiral EFT

		NN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$

$$
\begin{aligned}
V^{(2)}_{\text{cont}} = {} & \gamma_1 q^2 + \gamma_2 q^2 (\sigma_1 \cdot \sigma_2) \\
& + \gamma_3 q^2 (\tau_1 \cdot \tau_2) + \gamma_4 q^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
& + \gamma_5 k^2 + \gamma_6 k^2 (\sigma_1 \cdot \sigma_2) + \gamma_7 k^2 (\tau_1 \cdot \tau_2) \\
& + \gamma_8 k^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
& + (\sigma_1 + \sigma_2)(\mathbf{q} \times \mathbf{k})(\gamma_9 + \gamma_{10}(\tau_1 \cdot \tau_2)) \\
& + (\sigma_1 \cdot \mathbf{q})(\sigma_2 \cdot \mathbf{q})(\gamma_{11} + \gamma_{12}(\tau_1 \cdot \tau_2)) \\
& + (\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k})(\gamma_{13} + \gamma_{14}(\tau_1 \cdot \tau_2))
\end{aligned}
$$

Chiral EFT

		NN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$

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V^{(2)}_{\text{cont}} = {} & \gamma_1 q^2 + \gamma_2 q^2(\sigma_1\cdot\sigma_2) \\
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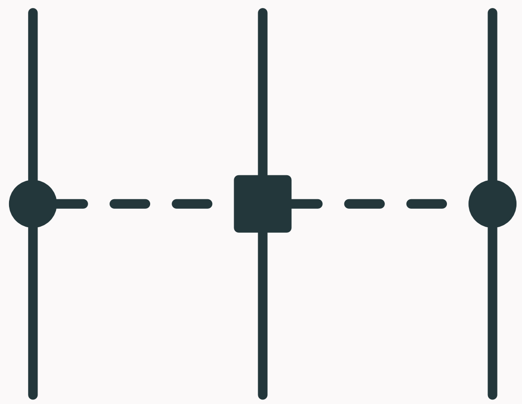
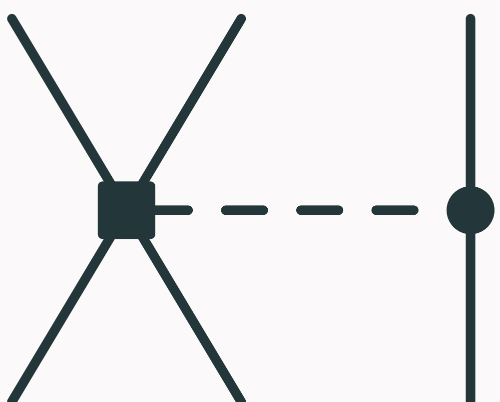
& + \gamma_5 k^2 + \gamma_6 k^2(\sigma_1\cdot\sigma_2) + \gamma_7 k^2(\tau_1\cdot\tau_2) \\
& + \gamma_8 k^2(\sigma_1\cdot\sigma_2)(\tau_1\cdot\tau_2) \\
& + (\sigma_1+\sigma_2)(\mathbf{q}\times\mathbf{k})(\gamma_9 + \gamma_{10}(\tau_1\cdot\tau_2)) \\
& + (\sigma_1\cdot\mathbf{q})(\sigma_2\cdot\mathbf{q})(\gamma_{11} + \gamma_{12}(\tau_1\cdot\tau_2)) \\
& + (\sigma_1\cdot\mathbf{k})(\sigma_2\cdot\mathbf{k})(\gamma_{13} + \gamma_{14}(\tau_1\cdot\tau_2))
\end{aligned}
$$

Three-Nucleon Interaction

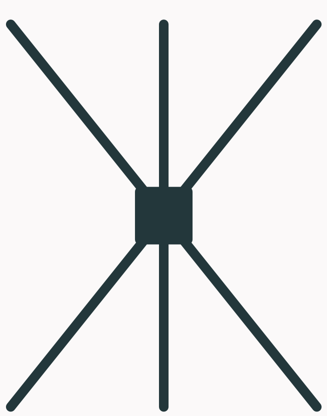
Three-Nucleon Interaction



c_1, c_3, c_4

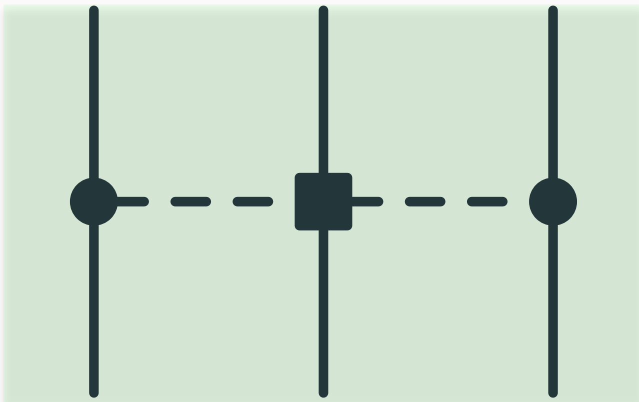


c_D

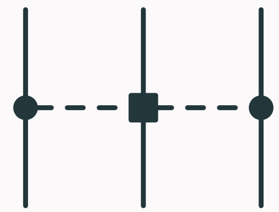


c_E

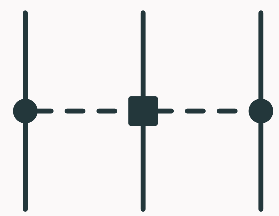
Three-Nucleon Interaction



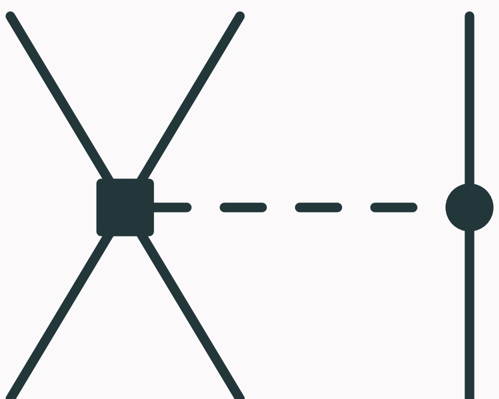
$c_1,\ c_3,\ c_4$

$\mathcal{F}\Big\{$  $\Big\}$ $\rightarrow\sim$ Tucson-Melbourne a' Term

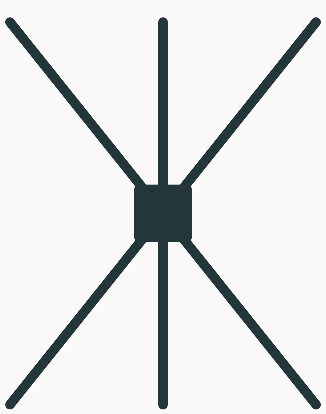
c_1

$\mathcal{F}\Big\{$  $\Big\}$ $\rightarrow\sim$ Fujita-Miyazawa

$c_3,\ c_4$

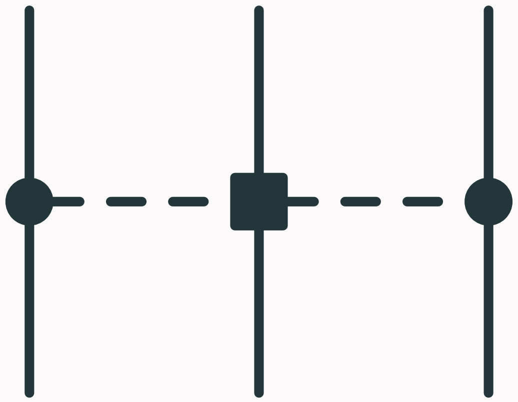


c_D

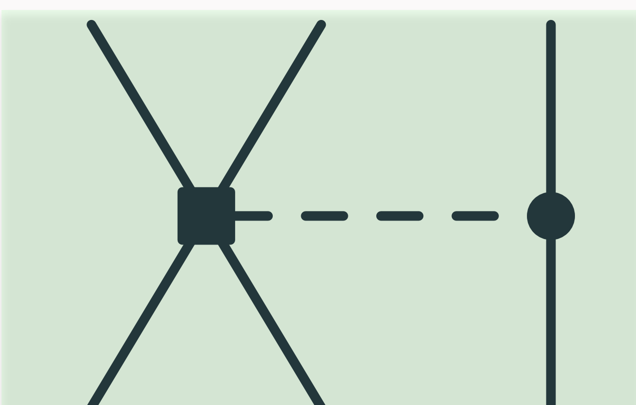


c_E

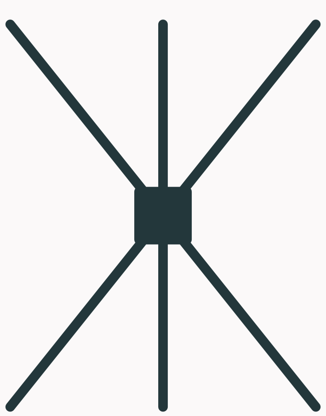
Three-Nucleon Interaction



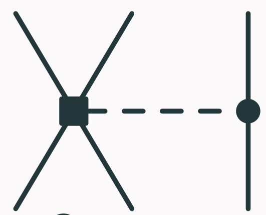
$c_1,\ c_3,\ c_4$



c_D



c_E

$\mathcal{F}\Big\{$  $\Big\} \rightarrow 1\pi\text{-Exchange} + \text{Contact}$

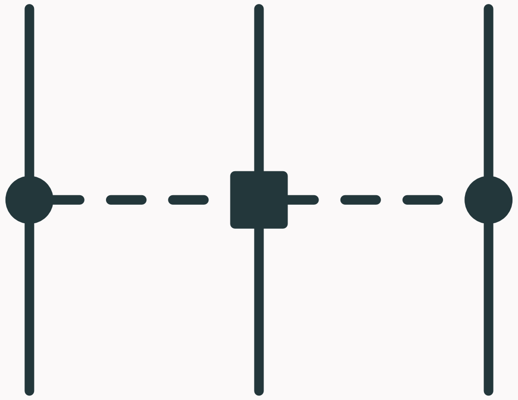
$$V_{D1} \propto \sum_{i<j<k} \sum_{\text{cyc.}} (\tau_i \cdot \tau_k) \times$$

$$\left[X_{ik}(\mathbf{r}_{kj})\Delta_{ij} + X_{ik}(\mathbf{r}_{ij})\Delta_{kj} - \frac{2^3\pi}{m_\pi^3}(\sigma_i \cdot \sigma_k)\Delta_{ij}\Delta_{kj} \right]$$

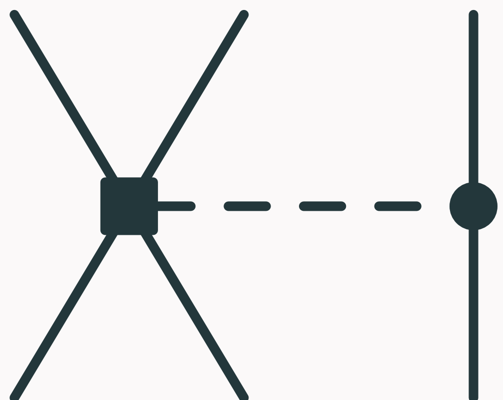
$$V_{D2} \propto \sum_{i<j<k} \sum_{\text{cyc.}} (\tau_i \cdot \tau_k) \times$$

$$\left[X_{ik} - \frac{2^2\pi}{m_\pi^3}(\sigma_i \cdot \sigma_k)\Delta_{ik} \right](\Delta_{ij} + \Delta_{kj})$$

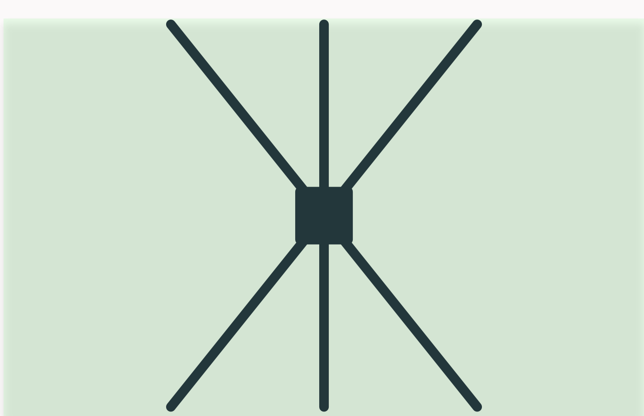
Three-Nucleon Interaction



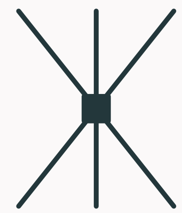
$c_1,\ c_3,\ c_4$



c_D



c_E

$\mathcal{F}\Big\{$  $\Big\} \rightarrow$ Contact

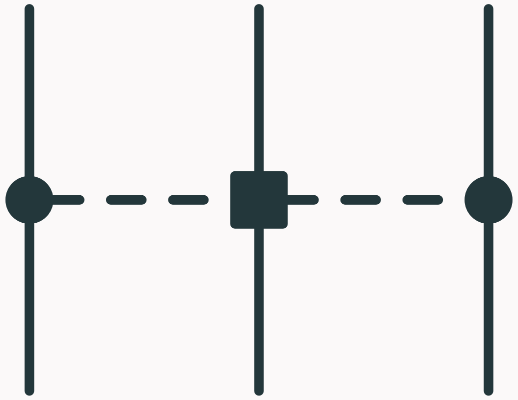
c_E

$$V_E \propto \sum_{i<j<k} \sum_{\text{cyc.}} O_{ijk} \Delta_{ij} \Delta_{kj}$$

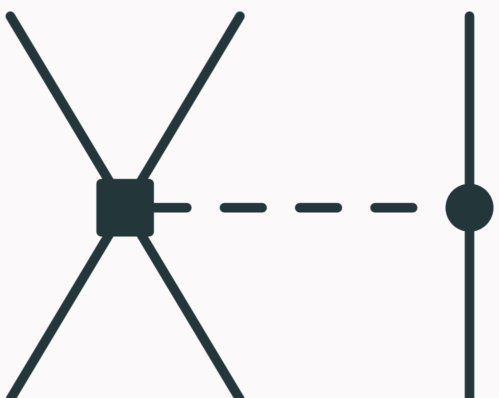
Fierz rearrangement freedom

$$O_{ijk} = \{\mathbb{1}, \sigma_i \cdot \sigma_j, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j,$$
$$\sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]\}$$

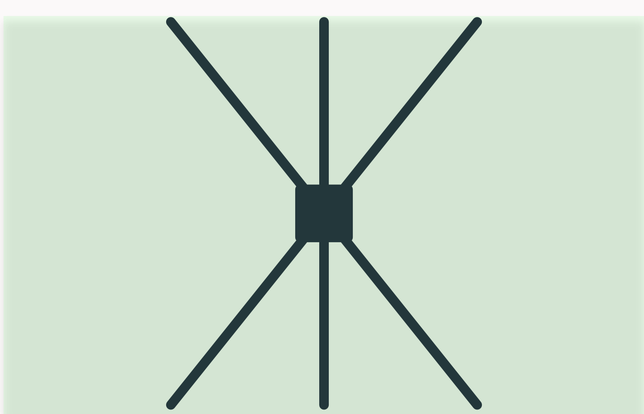
Three-Nucleon Interaction



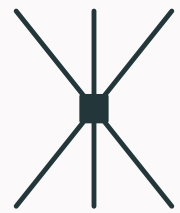
$c_1,\ c_3,\ c_4$



c_D



c_E

$\mathcal{F}\Big\{$  $\Big\}$ → Contact

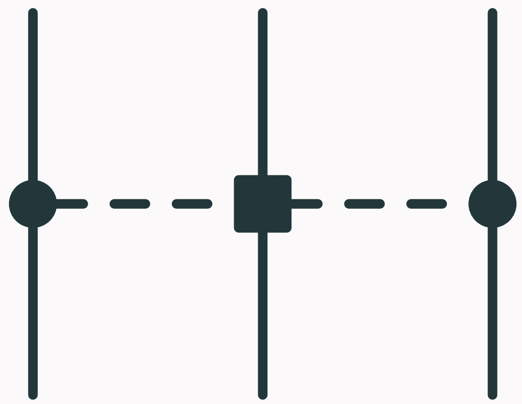
c_E

$$V_E \propto \sum_{i<j<k} \sum_{\text{cyc.}} O_{ijk} \Delta_{ij} \Delta_{kj},\ \Delta_{ij} \propto e^{-(r_{ij}/R_0)^4}$$

~~Fierz rearrangement freedom~~

$$O_{ijk} = \{\mathbb{1}, \sigma_i \cdot \sigma_j, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j,$$
$$\sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]\}$$

Three-Nucleon Interaction



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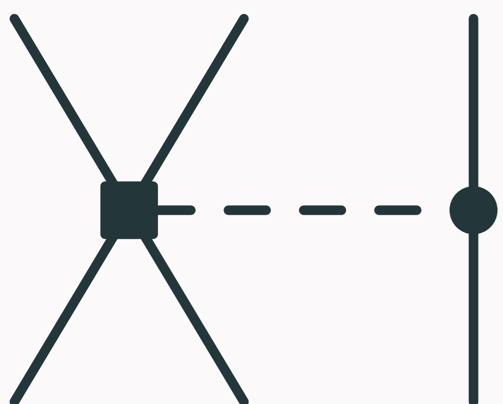
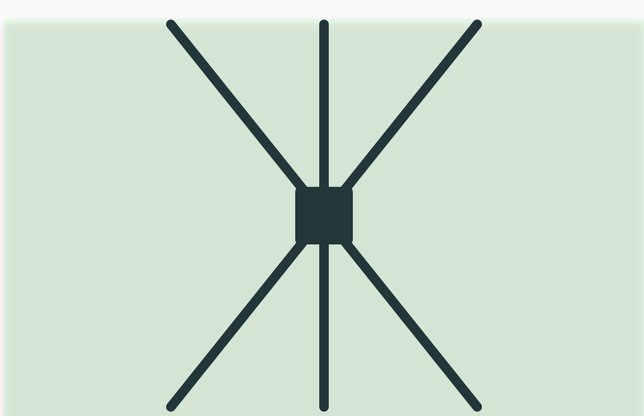
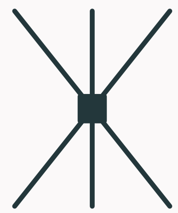


c_D



c_E

$\mathcal{F}\Big\{$  $\Big\} \rightarrow$ Contact

c_E

$$V_{E\tau} \propto \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \Delta_{ij} \Delta_{kj}$$

$$V_{E\mathbb{1}} \propto \sum_{i<j<k} \sum_{\text{cyc}} \Delta_{ij} \Delta_{kj}$$

$$V_{E\mathcal{P}} \propto \sum_{i<j<k} \sum_{\text{cyc}} \mathcal{P} \Delta_{ij} \Delta_{kj},$$

$$\mathcal{P} = \frac{1}{36}\Big(3 - \sum_{i<j} \sigma_i \cdot \sigma_j\Big)\Big(3 - \sum_{k<\ell} \tau_k \cdot \tau_\ell\Big)$$

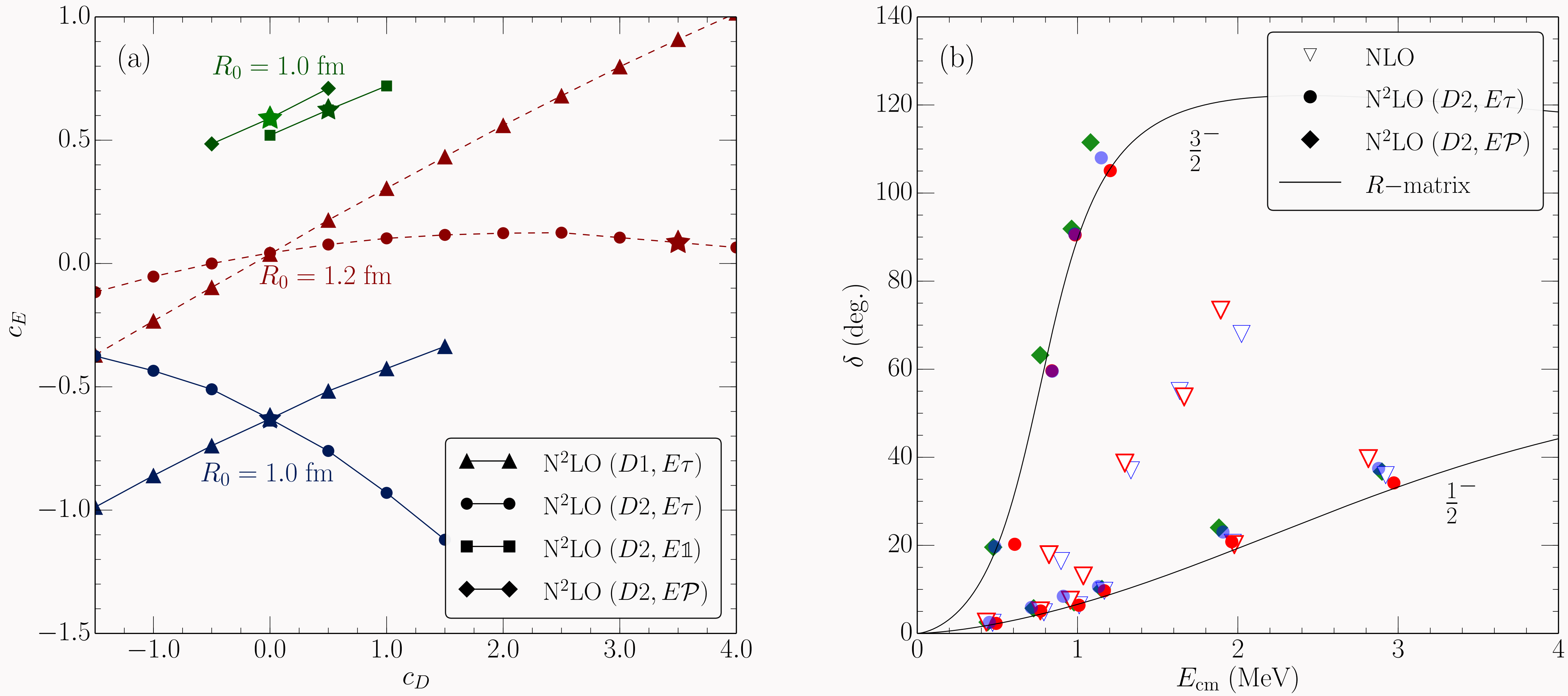
Fits

Choosing Observables

What to fit c_D and c_E to?

- Uncorrelated observables.
- Probe properties of light nuclei: ^{4}He E_B.
- Probe $T = 3/2$ physics: n-α scattering phase shifts.

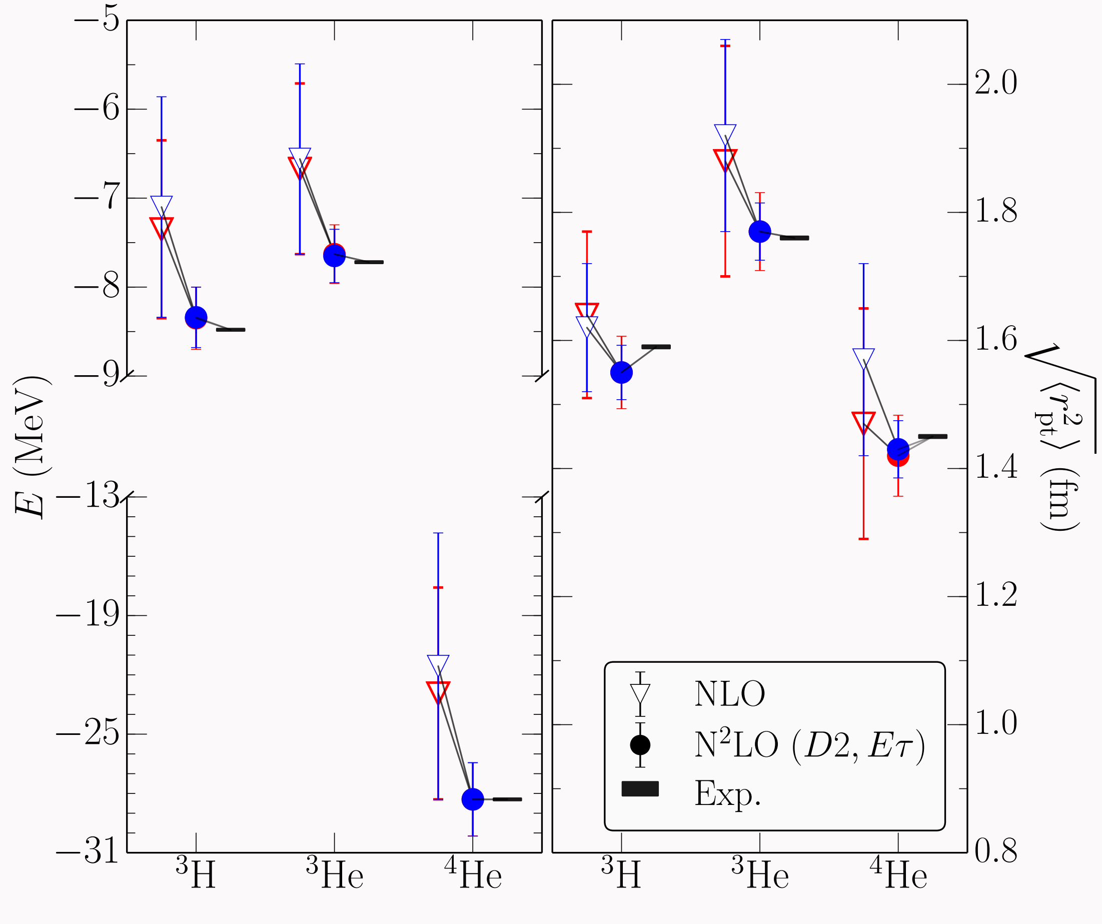
Fits

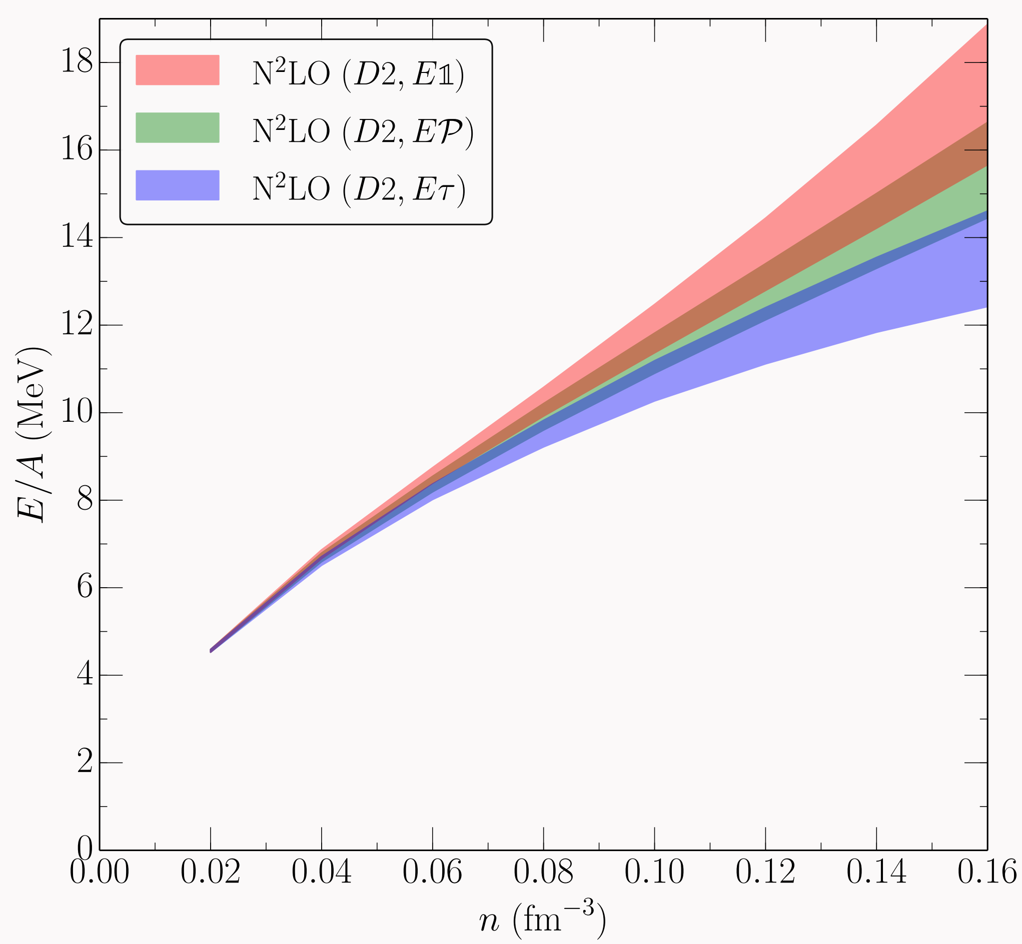


JEL et al, PRL **116**, 062501 (2016)

Results

A simultaneous description of properties of light nuclei, n-α scattering and neutron matter is possible. Uncertainty analysis as in E. Epelbaum et al, EPJ **A51**, 53 (2015).





JEL et al, PRL **116**, 062501 (2016)

Finite Volume Calculations

Motivation - Nuclei In Finite Volume

- Lattice QCD is the only *ab initio* method available to solve QCD directly at low energies.
- Computational costs mean in our lifetimes, Lattice QCD will not likely simulate, e.g., ^{12}C.
- Need some connection between Lattice QCD and *ab initio* low-energy nuclear theory;
  e.g. obtaining LECs in chiral EFT from Lattice simulations.

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  e.g. obtaining LECs in chiral EFT from Lattice simulations. Now add filler text! Yeah. I like this
  Use Lattice ideas to extract resonant properties from finite volume calculations.

Motivation - Lüscher Formula

- Take a simple scattering problem $np \to d\gamma$.
  Near threshold radiative capture in the $^1S_0$ channel.

- Might expect $L \gg |a^{^1S_0}|, |a^{^3S_1}|$, with, e.g.
  $a^{^1S_0} = -23.71$ fm.

- Not so! Lüscher $\to p \cot \delta_0(p) = \frac{1}{\pi L} S\left[\left(\frac{Lp}{2\pi}\right)^2\right]$,

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

More On The Lüscher Formula

For low-energy S-wave scattering, can use the effective-range expansion:

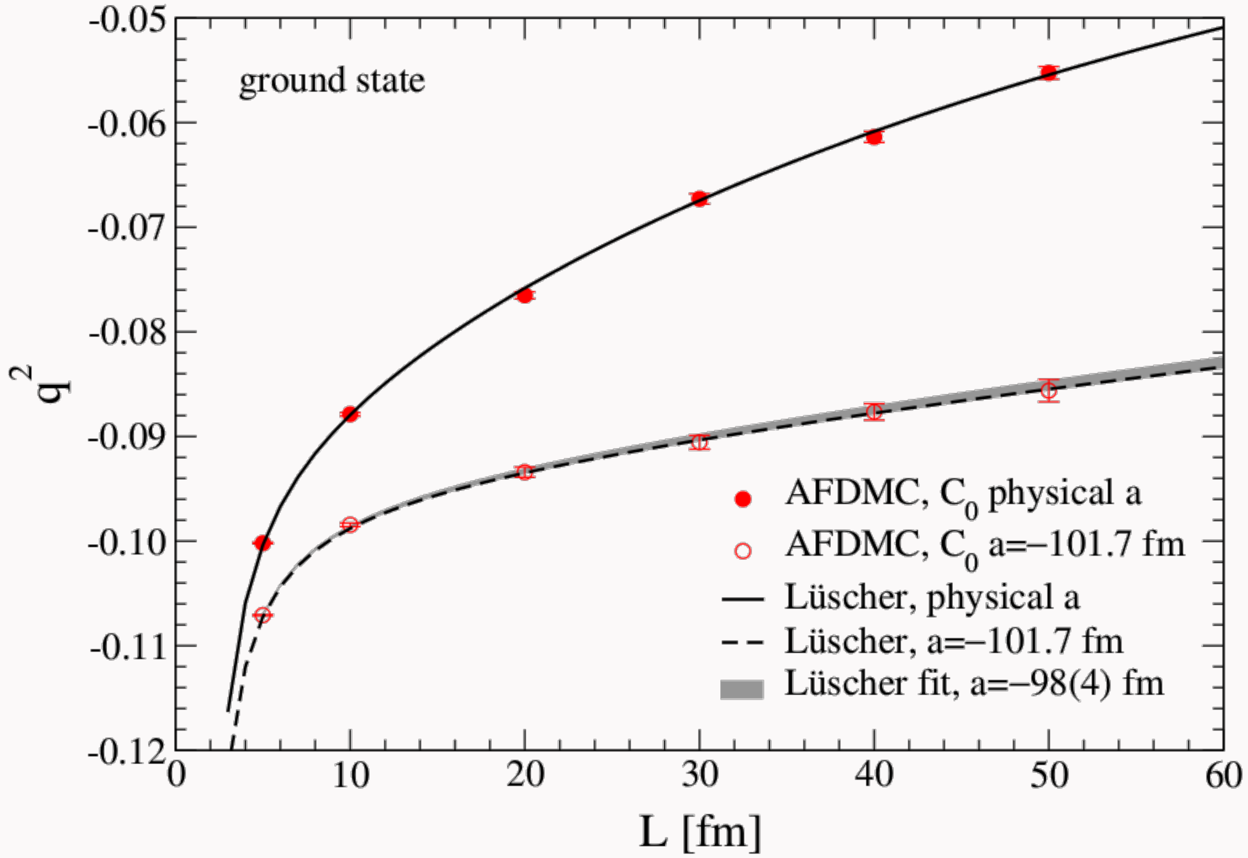
$$-\frac{1}{a^{(^1S_0)}} + \frac{1}{2} r_e^{(^1S_0)} p^2 = \frac{1}{\pi L} S\left[\left(\frac{Lp}{2\pi}\right)^2\right].$$

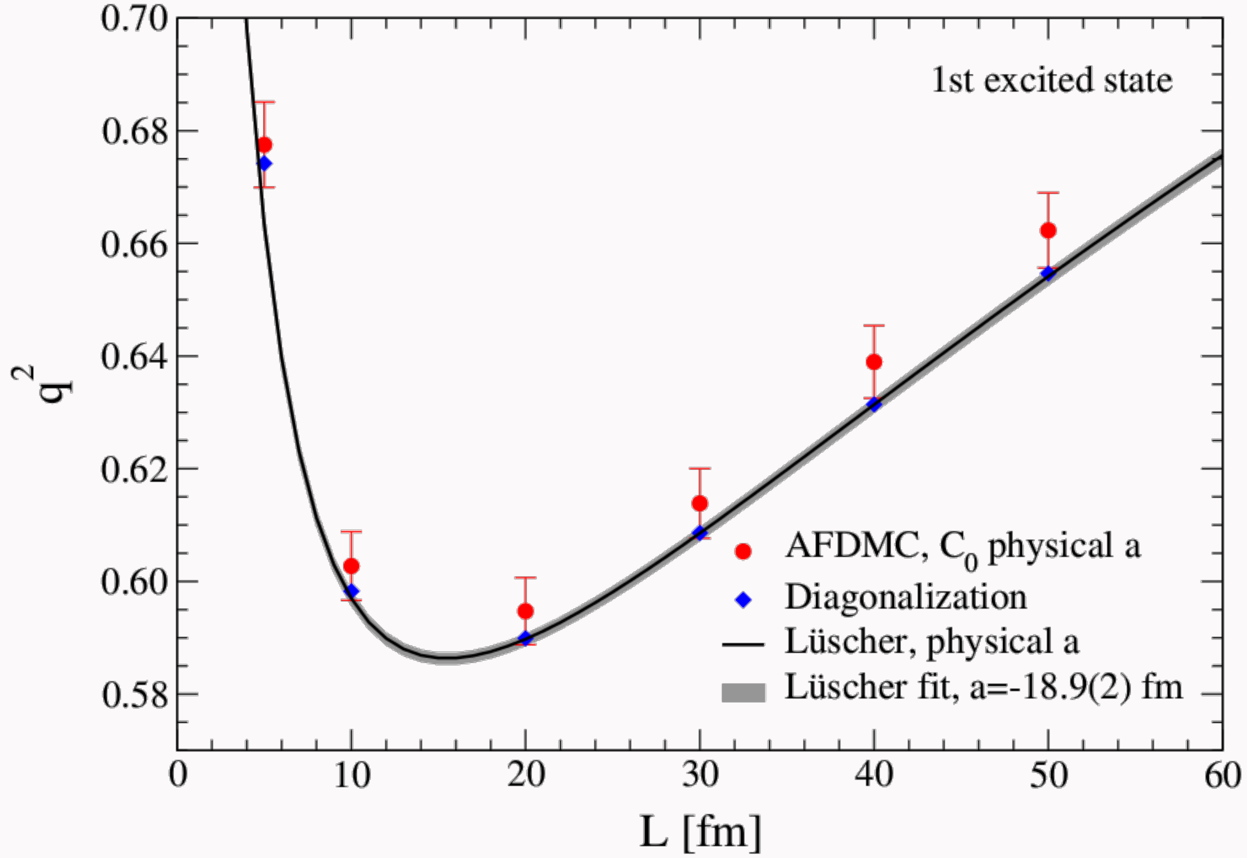
Consider first two neutrons only and a contact interaction (smeared out)

$$V(r) = C_0 \exp\left[-\left(\frac{r}{R_0}\right)^4\right].$$

Introduce $q = pL/2\pi$.

Results - Contact





First AFDMC calculations of excited states.

P. Klos et al, arXiv:1604.01387 [nucl-th]

$2n$ In Finite Volume With Chiral Interactions

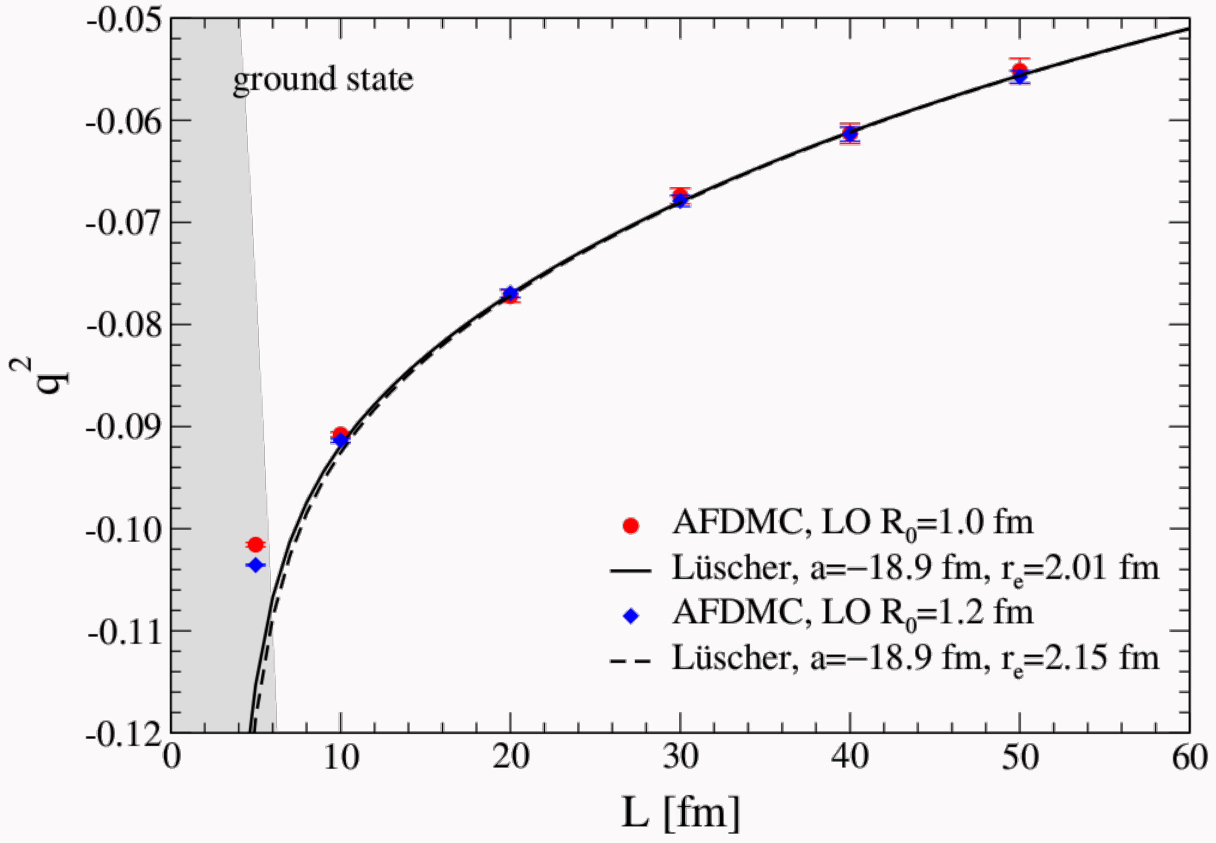
Now consider chiral EFT interactions.

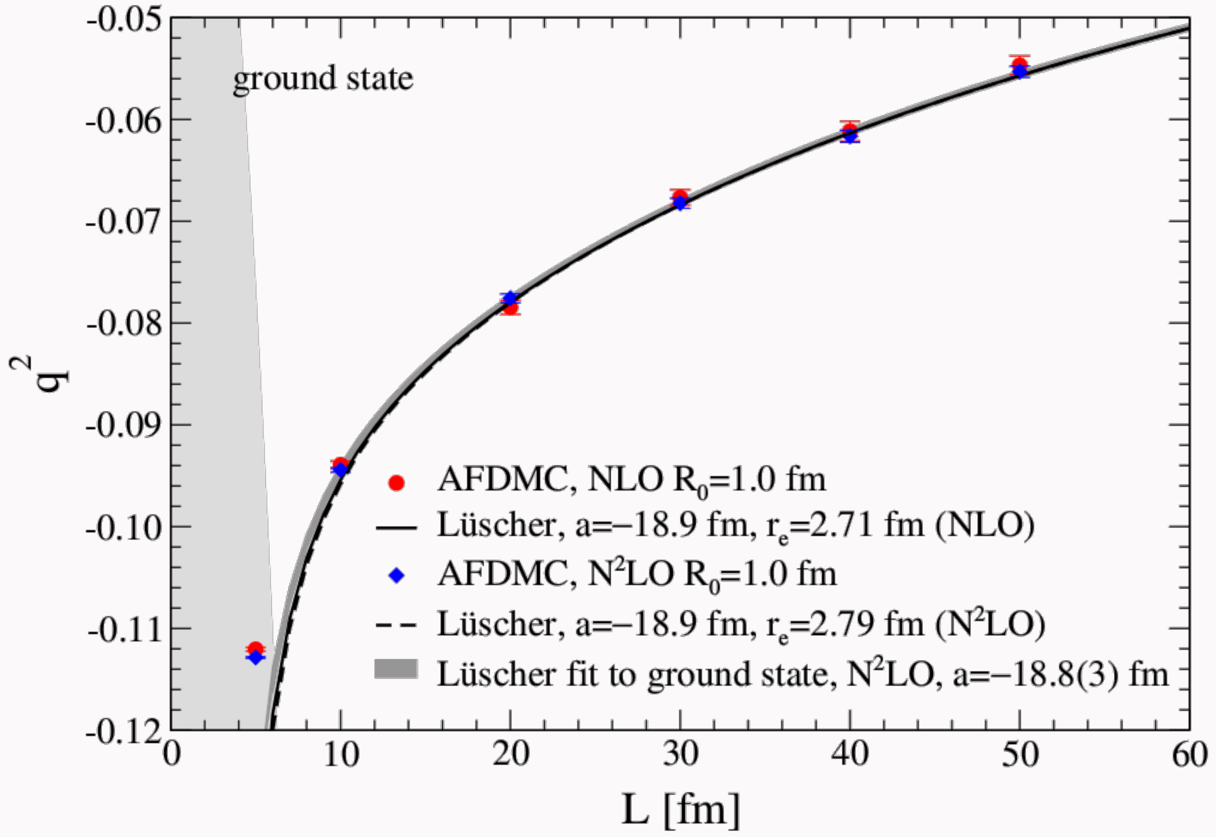
Standard Lüscher formula assumes $\not{\pi}$ EFT.

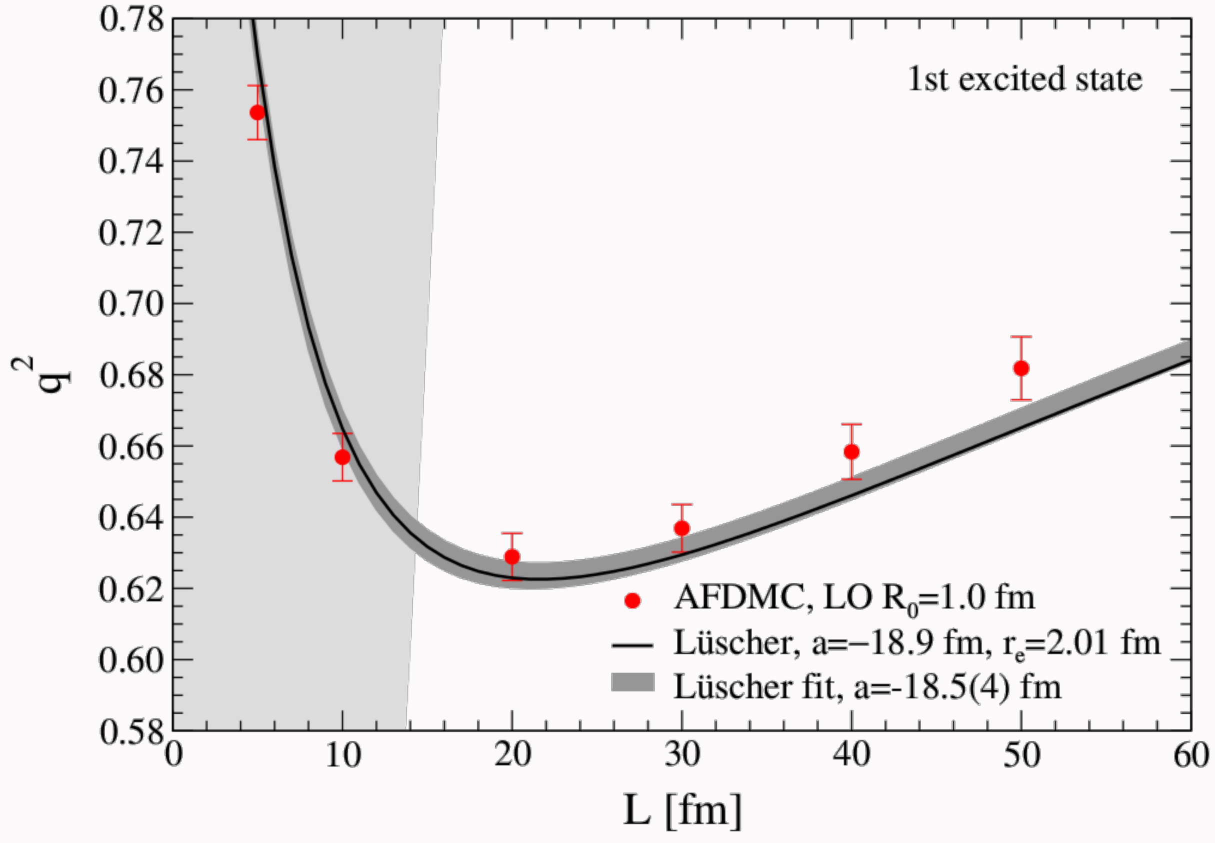
$$|p| \lesssim m_\pi/2$$

Corrections ~ $e^{-m_\pi L}$

Results - Chiral EFT







P. Klos et al, arXiv:1604.01387 [nucl-th]

Summary

- QMC + Chiral EFT is possible and yields new insights.
- More studies of power counting, regulator choices and effects, and cutoff dependencies are necessary.
- Chiral two- and three-nucleon interactions at N^2LO have sufficient freedom to give a good description of light nuclei, n-α scattering, and neutron matter.
- Calculations of nuclei in finite volume could eventually allow for comparison to Lattice QCD calculations.

Thank You!