Quantum Monte Carlo calculations of two neutrons in finite volume

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Nuclear Physics from Lattice QCD
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European Research Council
Established by the European Commission

- Motivation
- Lüscher formula
- Quantum Monte Carlo
- Ground and excited states in AFDMC
- Chiral effective field theory
- Extraction of scattering parameters from finite volume
- Summary and outlook

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Two neutrons in a box

Motivation

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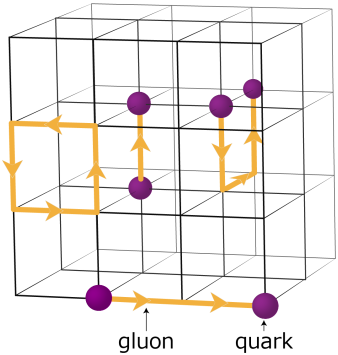
- Lattice QCD to describe nuclei from QCD



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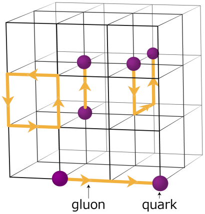
Motivation

- Lattice QCD to describe nuclei from QCD



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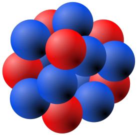
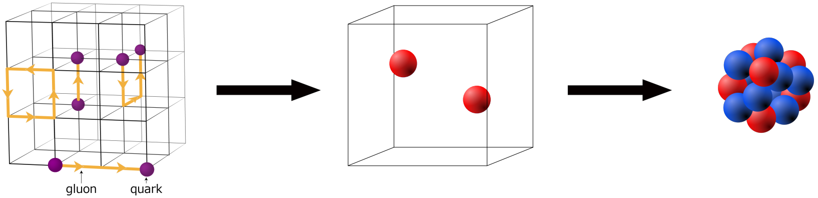


marekich/wikimedia

- However, constrained to **finite volume** and very **few particles**

Motivation

- Lattice QCD to describe nuclei from QCD



- Strategy:
  - Lattice QCD calculations for few nucleon systems
  - Matching of nuclear forces (EFT) in finite volume
  - EFT calculations of nuclear properties using advanced many-body methods

Motivation

Why two neutrons?

- Comparison to **Lüscher formula** possible $\rightarrow$ "proof of principle"
- Low-energy constants (LEC) in chiral EFT are fitted to experimental data
- Neutron-neutron scattering length cannot be measured directly

Why QMC?

- Exact method to solve Schrödinger equation
- Very successful for light nuclei
- Naturally extendable to more particles (3n, 4n, ...)

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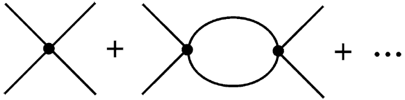
Two neutrons in finite volume
Lüscher formula

Consider interaction of nucleons *N* through contact interactions

$$\mathcal{L} = \tilde{N}^\dagger \left(i\partial_t + \frac{\nabla^2}{2M} \right) \tilde{N} + \left(\frac{\mu}{2} \right)^{4-D} [C_0 (\tilde{N}^\dagger \tilde{N})^2 + C_2^{(1)} (\tilde{N}^\dagger \nabla \tilde{N})^2 + C_2^{(2)} [i\nabla (\tilde{N}^\dagger \tilde{N})]^2 + ...]$$

$\rightarrow$ *S*-wave scattering amplitude $\mathcal{A}$



Now use

$$\mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta - ip}.$$

and periodic boundary conditions of the box to obtain energies.

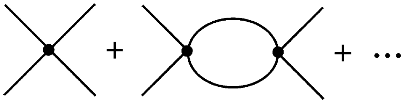
Two neutrons in finite volume
Lüscher formula

Energy $E = \frac{p^2}{m}$ of two nucleons in a box predicted by infinite volume phase shift $\delta(p)$

M. Lüscher, Commun. Math. Phys. **105**, 153 (1986).

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

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



Beane *et al.*, PLB **585**, 106 (2006).

Possible to infer scattering length, effective range, ..., from finite volume calculations ($p \cot \delta = -\frac{1}{a} + \frac{1}{2} r_e p^2 + ...$)

Finite volume energies $\rightarrow$ scattering length a, effective range r_e, ...

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Quantum Monte Carlo

QMC in three lines:

Ground state: $H|\Psi_0\rangle = E_0|\Psi_0\rangle$

Trial state: $|\Psi_T\rangle = \sum_i \alpha_i|\Psi_i\rangle$

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

QMC in more than three lines:
J. Carlson *et al.*, RMP **87**, 1067 (2015).

Quantum Monte Carlo
Trial wave function

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The trial wave function written in terms of eigenstates of H

$$\left|\Psi_T\right\rangle = \sum_i \alpha_i \left|\Psi_i\right\rangle$$

Propagate in imaginary time to project out the ground state $\left|\Psi_0\right\rangle$

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

Quantum Monte Carlo
Example

Particle in a box

$$V = \begin{cases} 0, & 0 < x < L \\ \infty, & otherwise \end{cases}$$

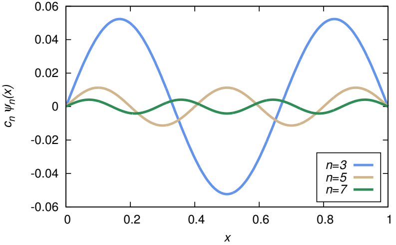
Trial wave function

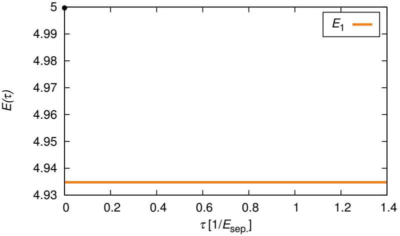
$$\Psi_T(x) = \sum_{n=1}^{\infty} c_n \Psi_n(x)$$

$$\Psi_n(x) = \sqrt{2}\sin(n\pi x)$$

Mixed estimator

$$E(\tau) = \frac{\langle \Psi_T | H e^{-(H-E_T)\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)\tau} | \Psi_T \rangle}$$





Quantum Monte Carlo
Example

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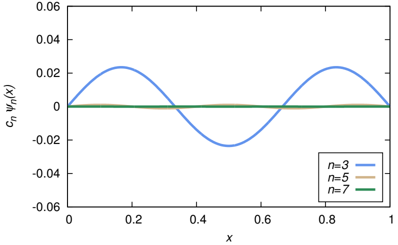

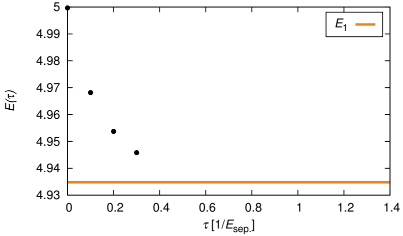

Quantum Monte Carlo
Example

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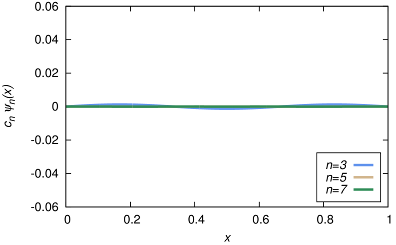

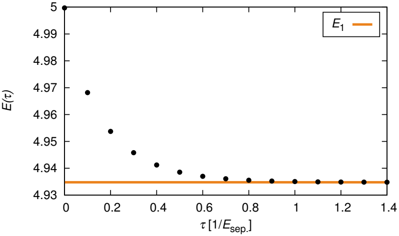

Quantum Monte Carlo
Trial wave function

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Trial wave function for N-body system:

$$\Psi_T(\mathbf{R}, S) = \prod_{i<j} f_J(r_{ij}) \Psi_{SD}(\mathbf{R}, S)$$

$$\mathbf{R} = (\mathbf{r}_1, ..., \mathbf{r_N}) \text{ and } S = (s_1, ..., s_N)$$

Jastrow function

$$f_J(r_{ij})$$

Slater determinant

$$\Psi_{SD}(\mathbf{R}, S) = \det(\{\phi_\alpha(\mathbf{r}_i, s_i)\})$$

$$\phi_\alpha(\mathbf{r}_i, s_i) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_i} \chi_{s,m_s}(s_i)$$

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Two neutrons in finite volume
Contact interaction

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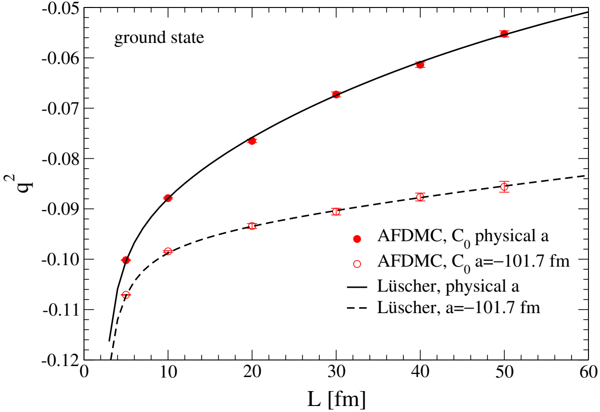
Comparison: AFDMC vs. Lüscher prediction with contact interaction

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

pionless EFT

$$E = q^2 \frac{4\pi^2}{ML^2}$$



Two neutrons in finite volume
Excited state

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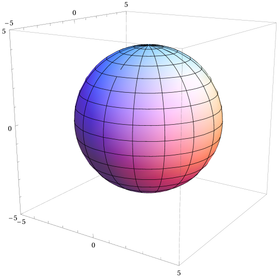
Challenging problem:

- Excited state has nodal surface $\psi(\mathbf{r}_{\text{node}}) = 0$
- QMC requires nodal surface of wave function as input (fixed node approximation, plus small release possible)



spherical nodal surface

Two neutrons in finite volume
Excited state

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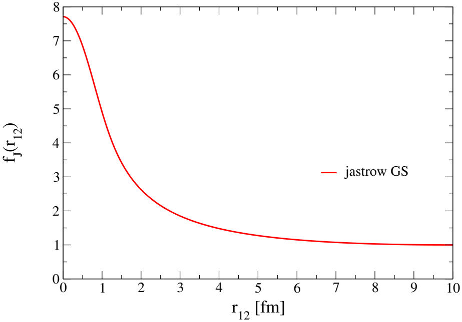
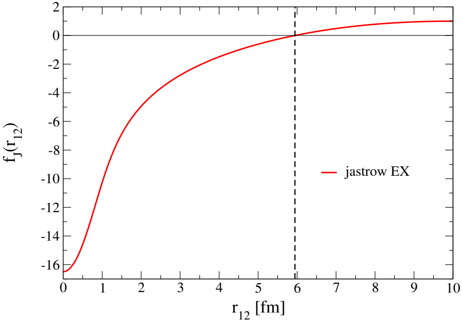
Introduce node in Jastrow function $f_J(r_{12})$ in $\Psi_T(\mathbf{R}, S) = f_J(r_{12})\Psi_{SD}(\mathbf{R}, S)$

Ground state

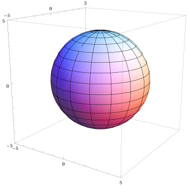


Excited state



Two neutrons in finite volume
Excited state

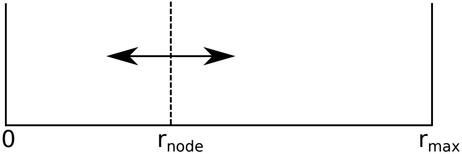
How to determine radius of the nodal surface?



For local potential Schrödinger equation

$$H\psi(\mathbf{R}) = E\psi(\mathbf{R})$$

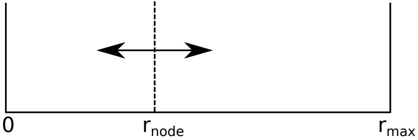
yields the same energy E independent of coordinates $\mathbf{R}$

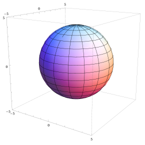


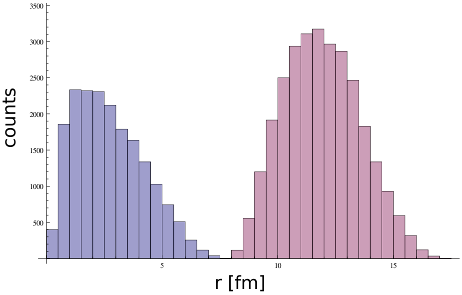
Perform separate simulations in the two pockets until $E_{\mathrm{left}} = E_{\mathrm{right}}$

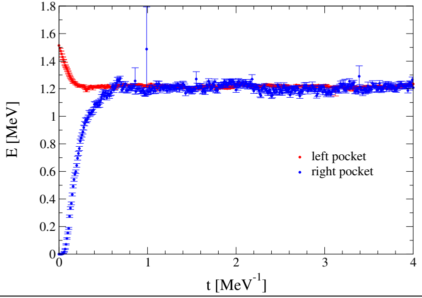
Two neutrons in finite volume
Excited state

Adjust r_{node} such that $E_{left} = E_{right}$





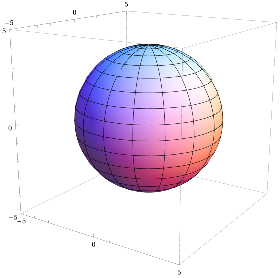


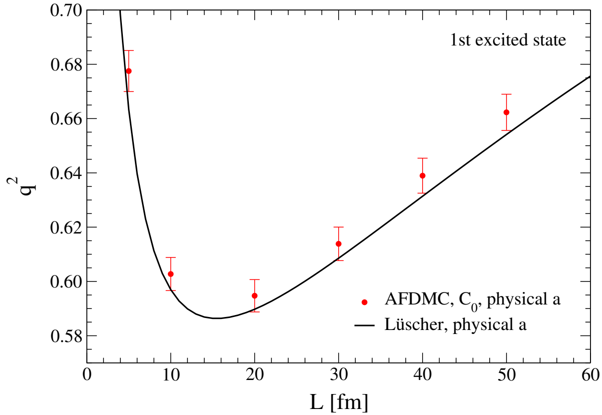


Two neutrons in finite volume
Excited state

Comparison: AFDMC vs. Lüscher prediction with contact interaction

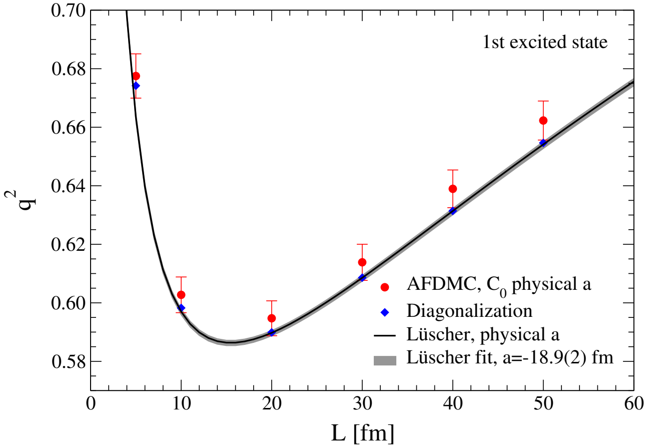
$$V(r) = C_0 \exp\left[-\left(\frac{r}{R_0}\right)^4\right]$$





Nodal surface

Determine exact nodal surface through diagonalization of $H|\psi_i\rangle = E_i|\psi_i\rangle$.



Nodal surface

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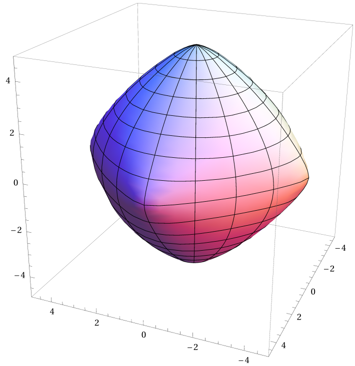
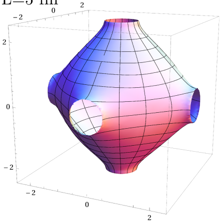
Extract nodal surface $r_{\text{node}}(\theta, \varphi)$ from first excited state $\psi_{\text{ex}}(r_{\text{node}}, \theta, \varphi) = 0$



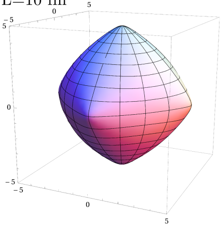
Nodal surface not spherical!

Nodal surface

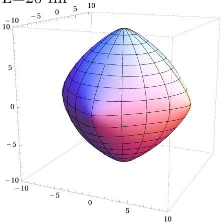
L=5 fm



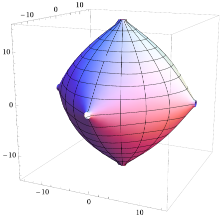
L=10 fm



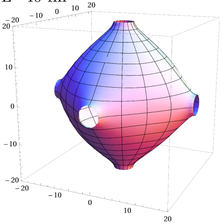
L=20 fm



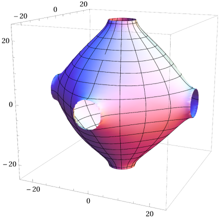
L=30 fm



L=40 fm



L=50 fm



Decomposition in cubic harmonics

Nodal surface can be decomposed in spherical harmonics

$$r_{\text{node}}(\theta, \phi) = \sum_{l} c_{lm} Y_{lm}(\theta, \phi)$$

Rotation symmetry group is broken down to the cubic symmetry group O_h

J. Muggli, Z. Angew. Math. Mech. 23, **311** (1972).

cubic harmonics

$$Y_l^c = \sum_{m=0,4,8,\ldots} c_m Y_{lm}$$

Express nodal surface in terms of cubic harmonics

$$r_{\text{node}}(\theta, \phi) = \sum_{l} c_l Y_l^c(\theta, \phi).$$

Decomposition in cubic harmonics

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Nodal surface decomposed in cubic harmonics

$$r_{\text{node}}(\theta,\phi) = \sum_l c_l Y^c_l(\theta,\phi).$$

cubic harmonics

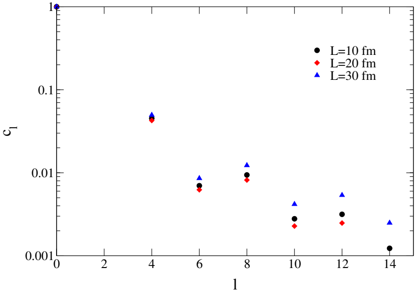
$$Y^c_l = \sum_{m=0,4,8,\ldots} c_m Y_{lm}$$

We find

$$c_l \sim \left(\frac{r_{\text{node}}}{L}\right)^l$$

Two-body scattering in infinite volume

$$R(r) \sim j_l(pr) \xrightarrow{pr \ll 1} (pr)^l$$



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cubic harmonics

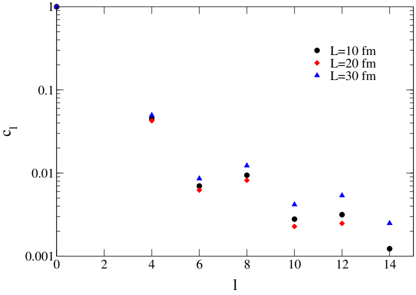
$$Y_l^c = \sum_{m=0,4,8,\ldots} c_m Y_{lm}$$

Estimate correction due to $l = 4$ contribution

$$E = \langle \psi_{l=0} | H | \psi_{l=0} \rangle + c_4^2 \langle \psi_{l=4} | H | \psi_{l=4} \rangle + \ldots$$

$$\frac{\Delta E}{E} \sim (c_4)^2 \sim 1\%$$

in agreement with results



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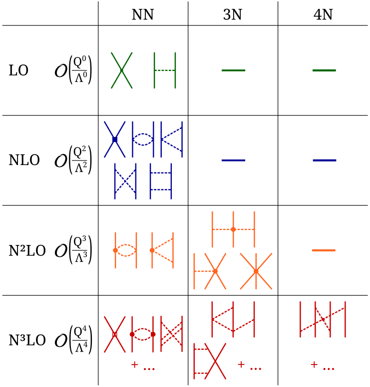
Chiral effective field theory

- Separation of scales:
  Momentum $Q \ll$ breakdown scale Λ_b
- Most general Lagrangian consistent with QCD symmetries
- Expansion in powers of $\frac{Q}{\Lambda_b}$
- Local forces up to N^{2}LO by using linearly indep. operators
  Gezerlis *et al.*, PRL **111**, 032501 (2013)



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

Limitations of Lüscher for pionful theory
Chiral leading-order (LO) potential

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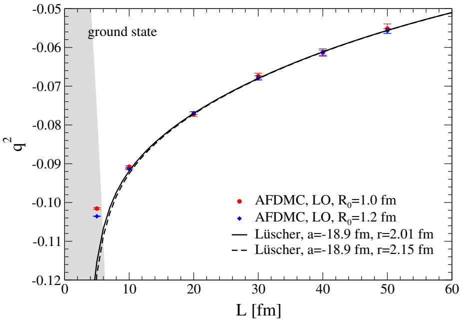
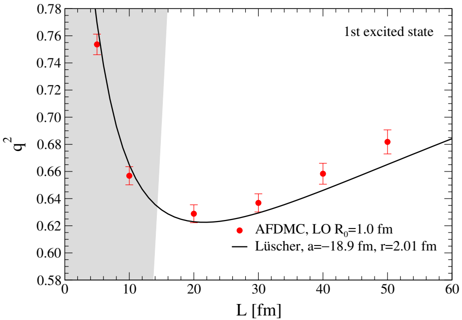
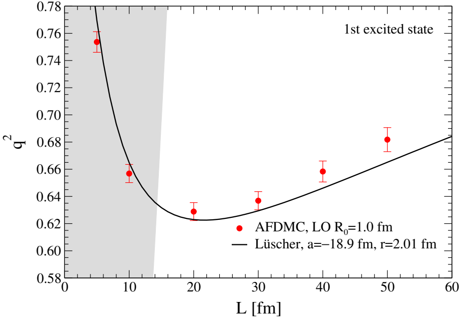
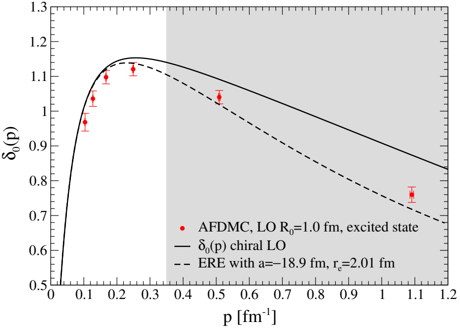




- Lüscher formula assumes zero-range interaction (pionless EFT, $|p| < m_\pi/2$)
- Not applicable for nuclear interactions at small box sizes L
- **Direct matching of lattice QCD and chiral EFT necessary for small L**

Limitations of Lüscher for pionful theory
Chiral leading-order (LO) potential





- Compare directly to phase shift
- Shows challenges for $p > m_\pi/2$

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

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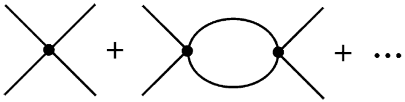
Extraction of scattering parameters from finite volume results

Energy $E = \frac{p^2}{m}$ of two nucleons in a box predicted by infinite volume phase shift $\delta(p)$
Beane *et al.*, PLB **585**, 106 (2006).

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



pionless EFT

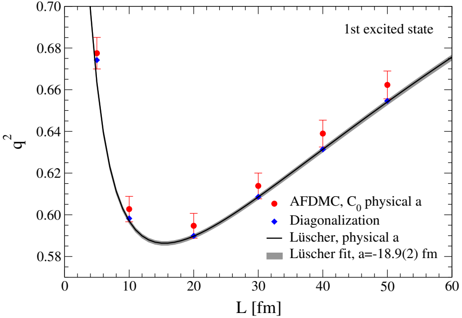
Effective range expansion:

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

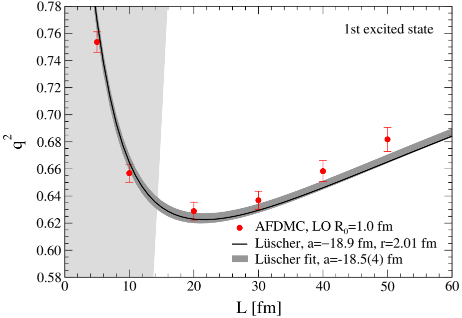
Finite volume energies $\rightarrow$ scattering length a, effective range r_e, ...

Fit to AFDMC data
Chiral NLO and N^{2}LO potentials

Fit to ground + excited state results



Contact interaction C_0



Chiral LO interaction

Fit: $a = -18.9(2)$ fm, $r_e = 1.10(1)$ fm
Exact: $a = -18.9$ fm, $r_e = 1.096$ fm

Fit: $a = -18.5(4)$ fm, $r_e = 2.00(7)$ fm
Exact: $a = -18.9$ fm, $r_e = 2.01$ fm

- Motivation
- Lüscher formula
- Quantum Monte Carlo
- Ground and excited states in AFDMC
- Chiral effective field theory
- Extraction of scattering parameters from finite volume
- Summary and outlook

Summary

- First results for two-neutron finite-volume ground and excited states in AFDMC
- Approximate construction of excited state vs. exact diagonalization
- Extraction of scattering parameters from AFDMC simulations yields accurate results
- QMC techniques can serve to match chiral EFT and lattice results beyond limitations of the Lüscher formula

Outlook

- Generalizable to more particles (3n, 4n, ...) where extensions of Lüscher's formula are only partially available
- Extraction of resonance properties through calculations of excited states

arXiv:1604.01387 **Thank you!**