Quantum Monte Carlo calculations of two neutrons in finite volume

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TALENT school on Nuclear QMC methods

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European Research Council

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Two neutrons in a box

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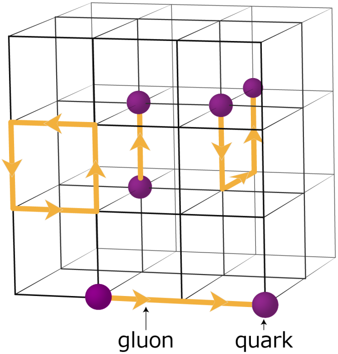
Motivation

- Lattice QCD to describe nuclei from QCD



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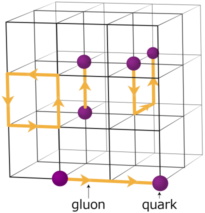
Motivation

- Lattice QCD to describe nuclei from QCD



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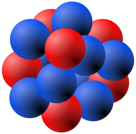
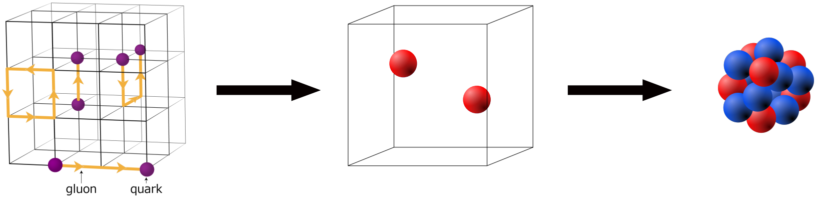


marekich/wikimedia

- 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

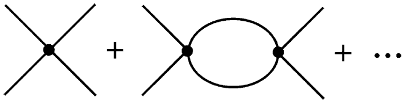
Two neutrons in finite volume
Lüscher formula

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).

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

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



pionless EFT

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, ...

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).

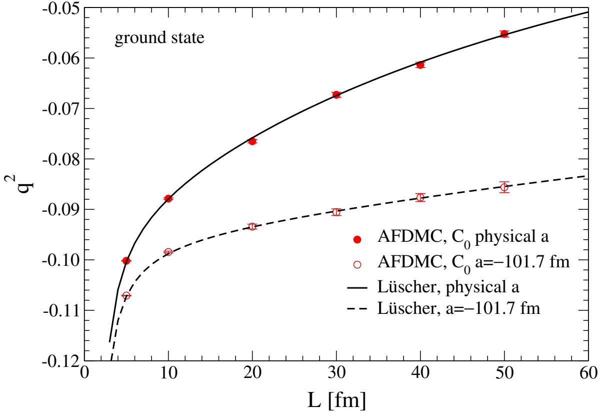
Two neutrons in finite volume
Contact interaction

Comparison: AFDMC vs. Lüscher prediction with contact interaction

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

pionless EFT

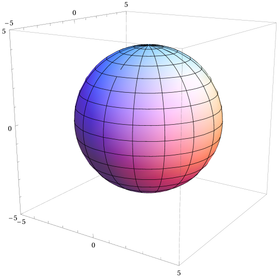
$$E = q^2 \frac{4\pi^2}{ML^2}$$



Two neutrons in finite volume
Excited state

Challenging problem:

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



spherical nodal surface

Quantum Monte Carlo
Trial wave function

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Trial wave function for N-body system:

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

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

Jastrow function

$$f_J(r_{ij})$$

Slater determinant

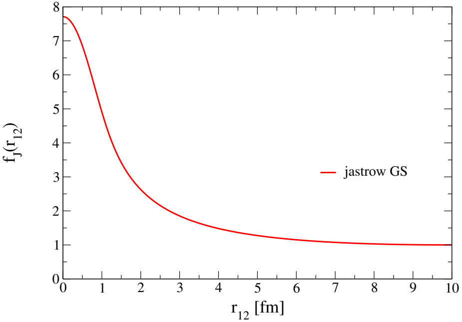
$$\Psi_{SD}(\mathbf{R}, S) = \det(\{\phi_\alpha(\mathbf{r}_i, s_i)\})$$

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

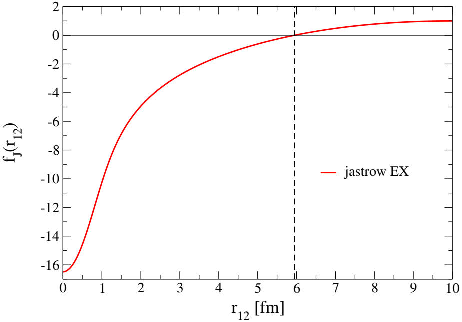
Two neutrons in finite volume
Excited state

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

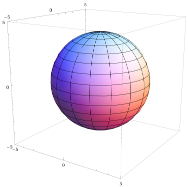
Ground state



Excited state



Two neutrons in finite volume
Excited state

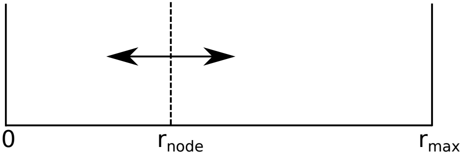


How to determine radius of the nodal surface?

For local potential Schrödinger equation

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

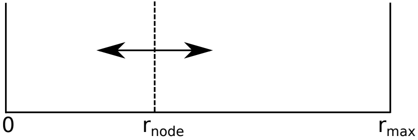
yields the same energy E independent of coordinates $\mathbf{R}$

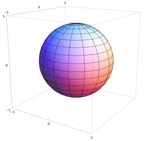


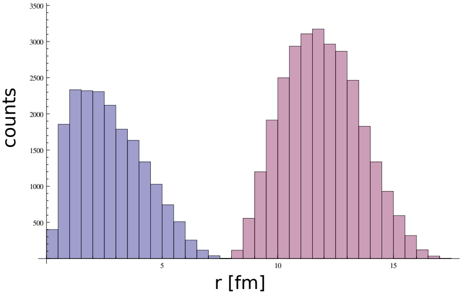
Perform separate simulations in the two pockets until $E_{left} = E_{right}$

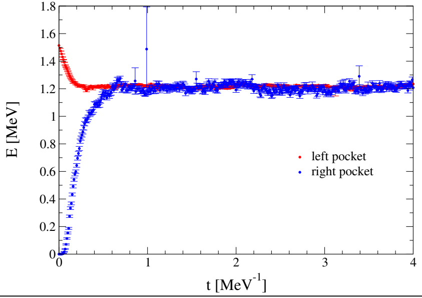
Two neutrons in finite volume
Excited state

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





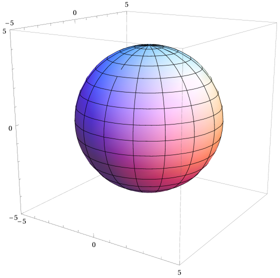


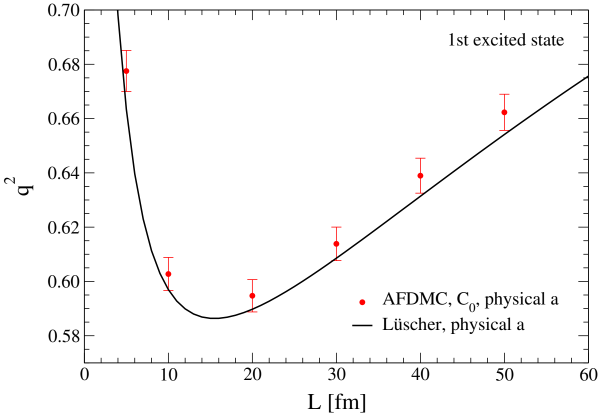


Two neutrons in finite volume
Excited state

Comparison: AFDMC vs. Lüscher prediction with contact interaction

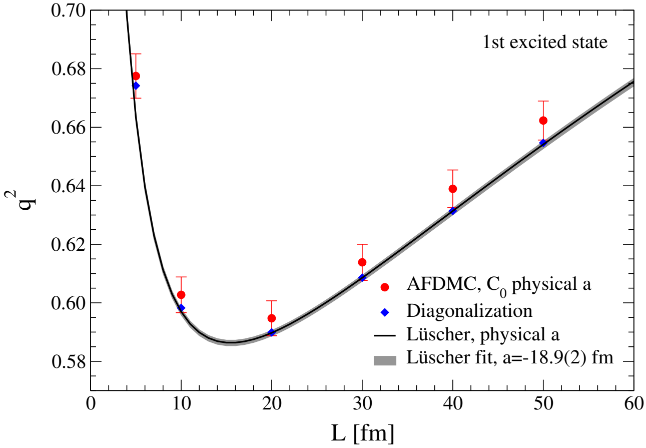
$$V(r) = C_0 \exp\left[-\left(\frac{r}{R_0}\right)^4\right]$$





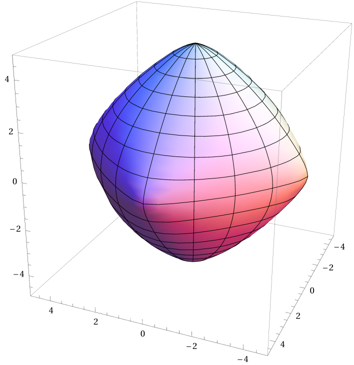
Nodal surface

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



Nodal surface

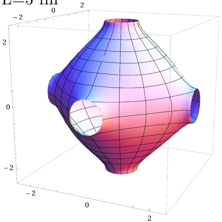
Extract nodal surface $r_{\text{node}}(\theta, \varphi)$ from first excited state $\psi_{\text{ex}}(r_{\text{node}}, \theta, \varphi) = 0$



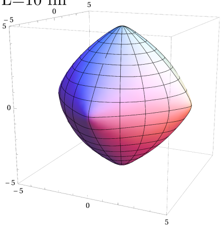
Nodal surface not spherical!

Nodal surface

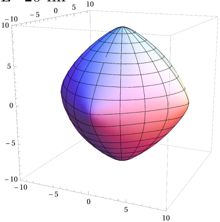
L=5 fm



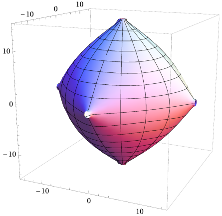
L=10 fm



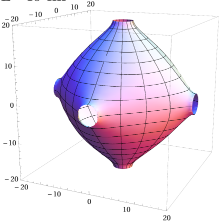
L=20 fm



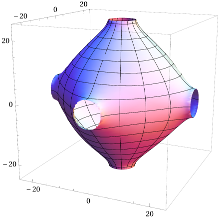
L=30 fm



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

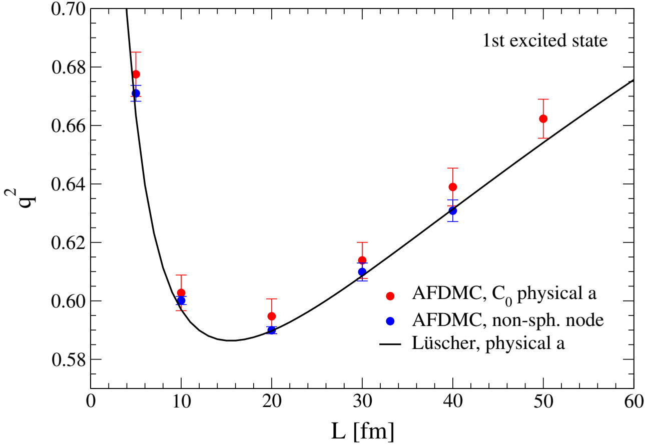
$$Y_l^c = \sum_{m=0,4,8,\ldots} c_m Y_{lm}$$

Express nodal surface in terms of cubic harmonics

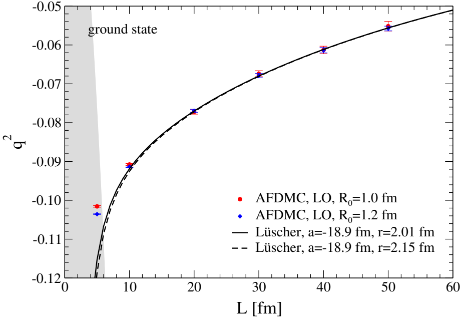
$$r_{\text{node}}(\theta,\phi) = \sum_l c_l Y_l^c(\theta,\phi).$$

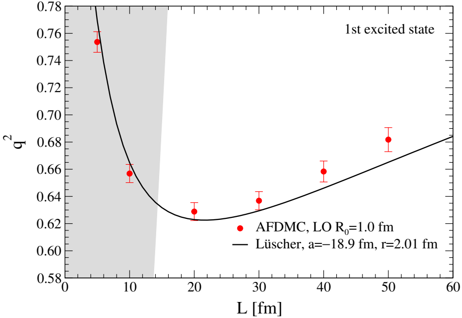
Two neutrons in finite volume
Improved nodal surface

Add non-spherical contribution: $r_{\mathrm{node}}(\theta, \phi) = c_0\, Y_0^c(\theta, \phi) + c_4\, Y_4^c(\theta, \phi)$



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





- 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**

Summary

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- 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!