New Developments in Nuclear Lattice Effective Field Theory Simulations

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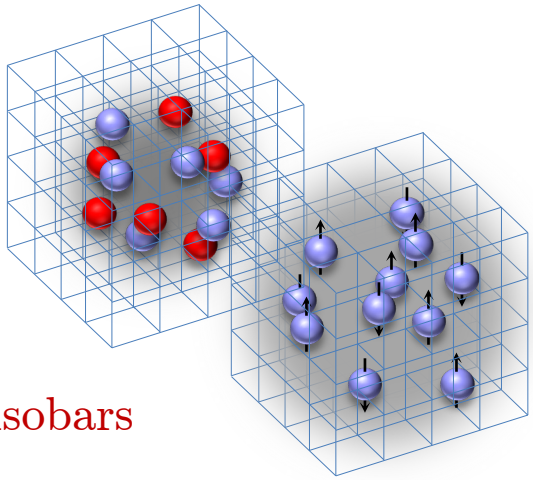


EMMI Rapid Reaction Task Force
Nuclear physics confronts relativistic collisions of isobars
Part 2: October 12-14, 2022
University of Heidelberg

Outline

Lattice effective field theory

Adiabatic projection method

A tale of two interactions

Essential elements for nuclear binding

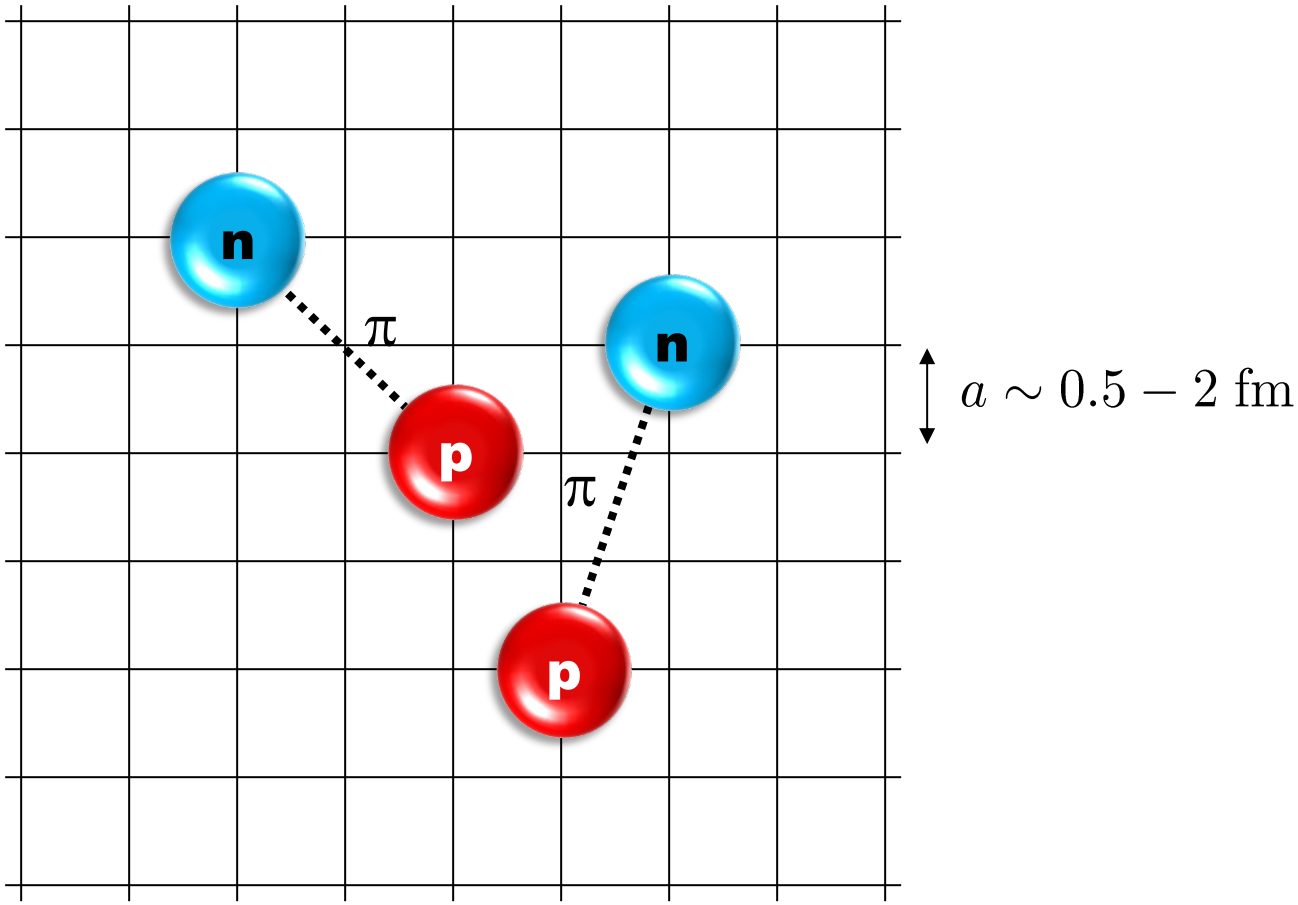
Pinhole algorithm

Structure and spectrum of ^{12}C

Wave function matching

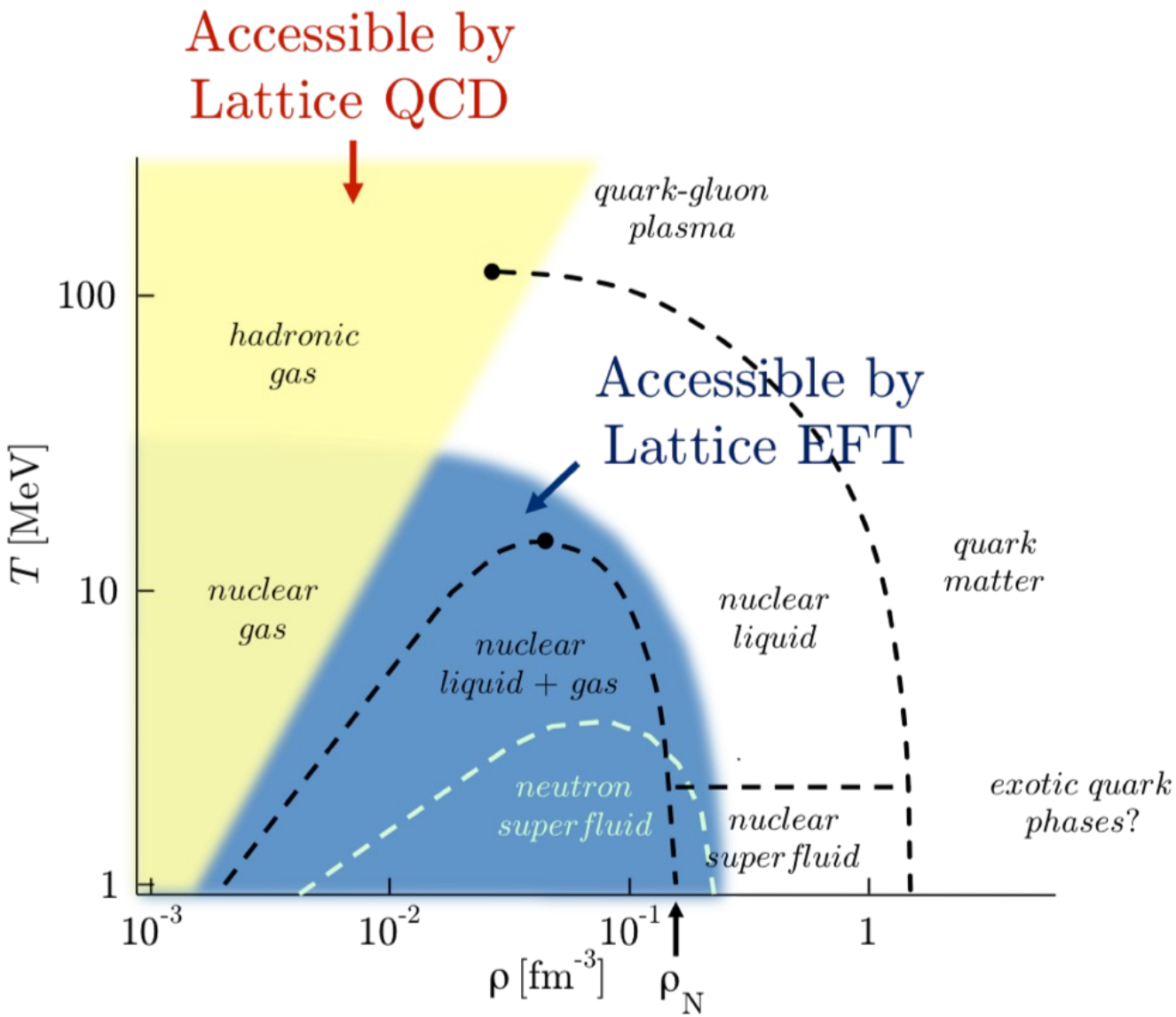
Summary

Lattice effective field theory



[D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)]

[Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer]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10
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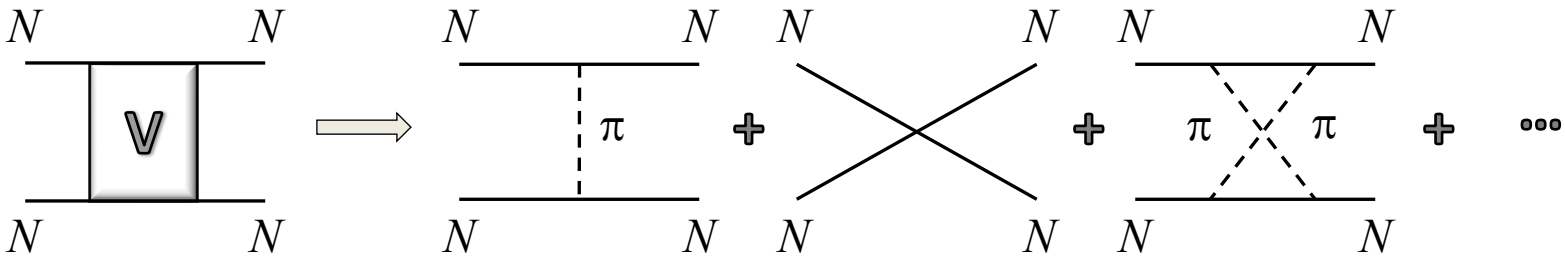
ρ [fm^-3]
ρ_N

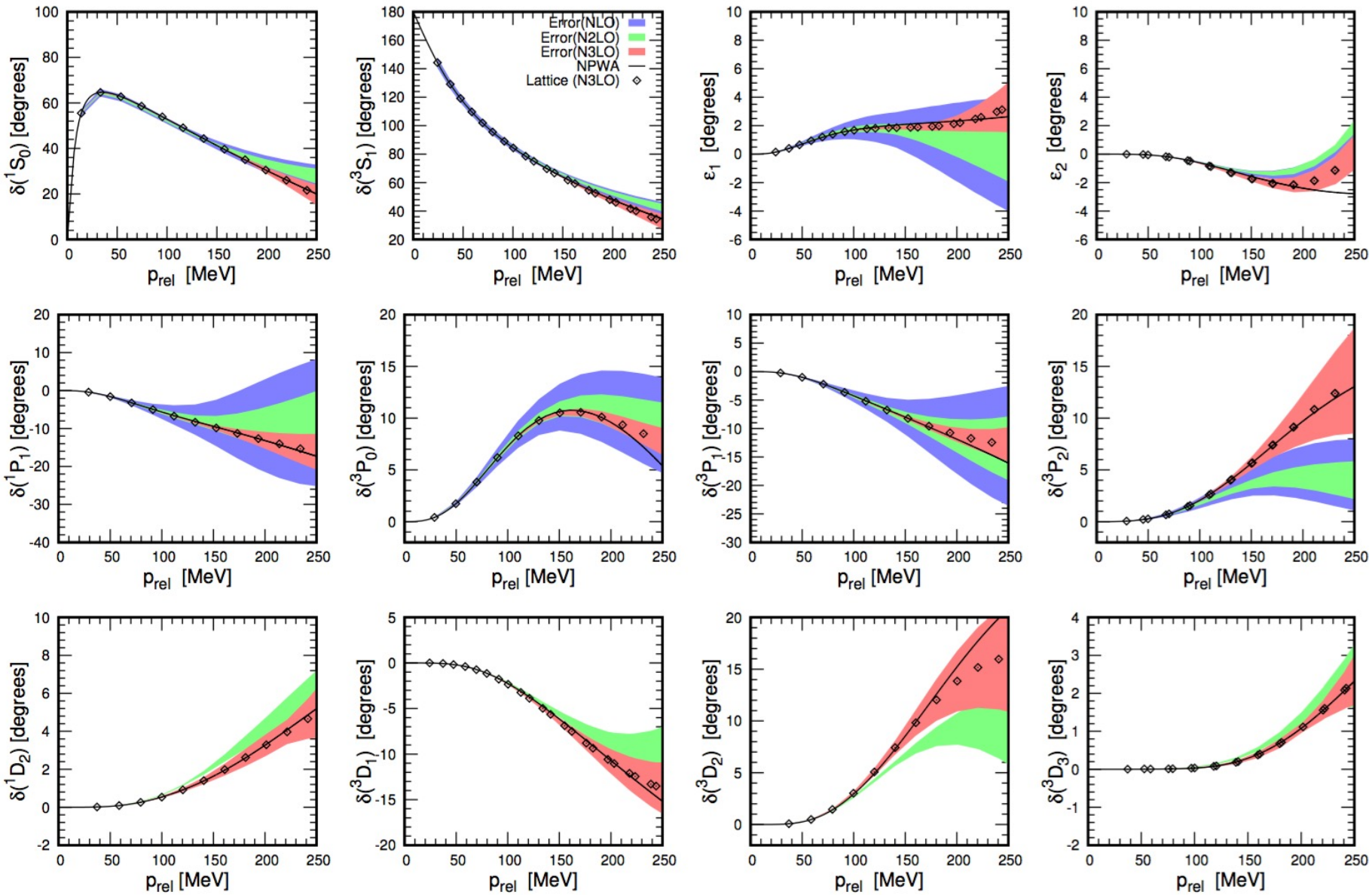
Chiral effective field theory

Construct the effective potential order by order



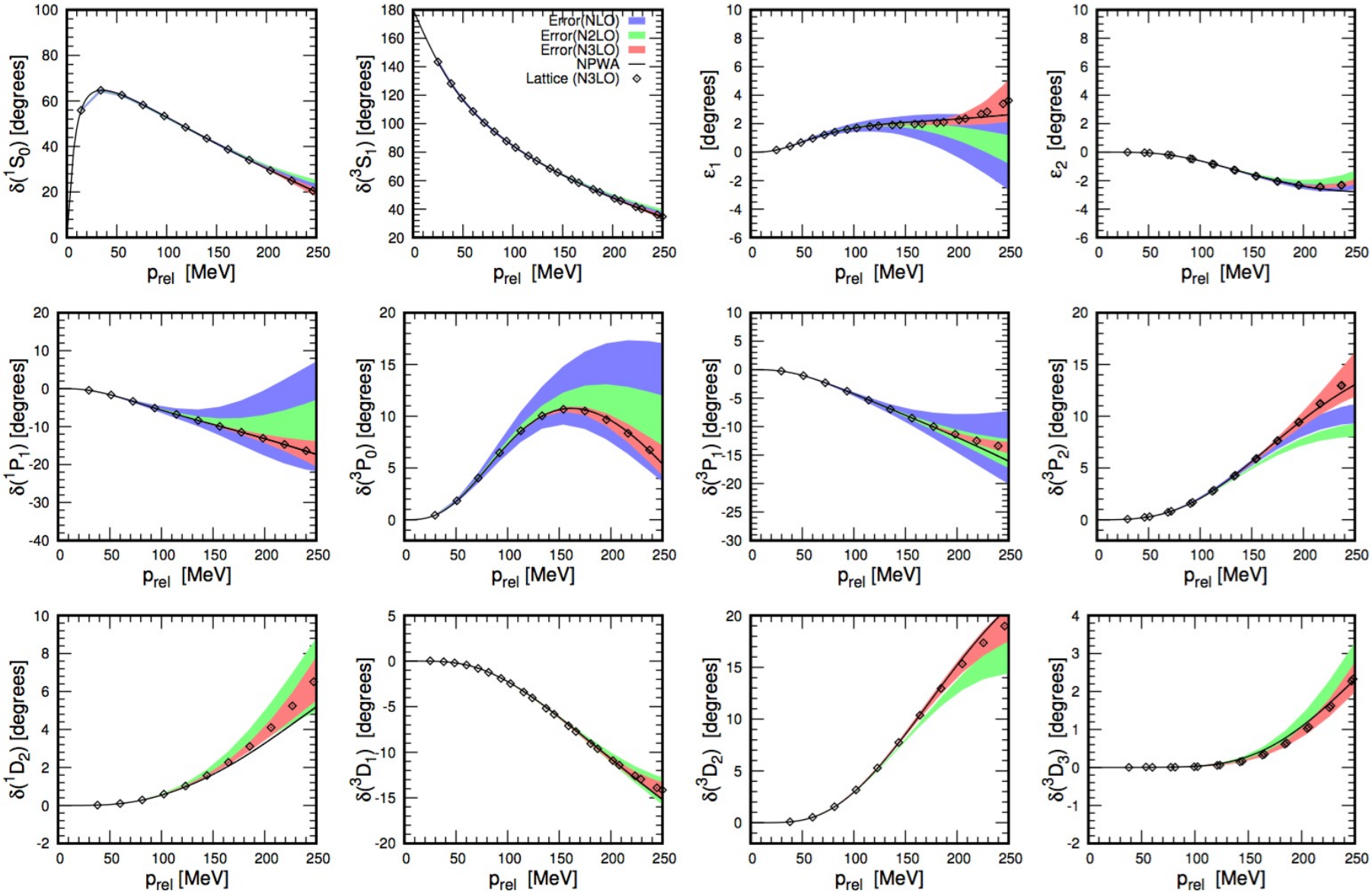
$$\underbrace{V^{\mathrm{OPEP}}\ \text{Contact interactions}}_{\text{Leading order (LO)}}\quad \underbrace{V^{\mathrm{TPEP}}\qquad\qquad}_{\text{Next-to-leading order (NLO)}}$$

$a = 1.315\,\mathrm{fm}$

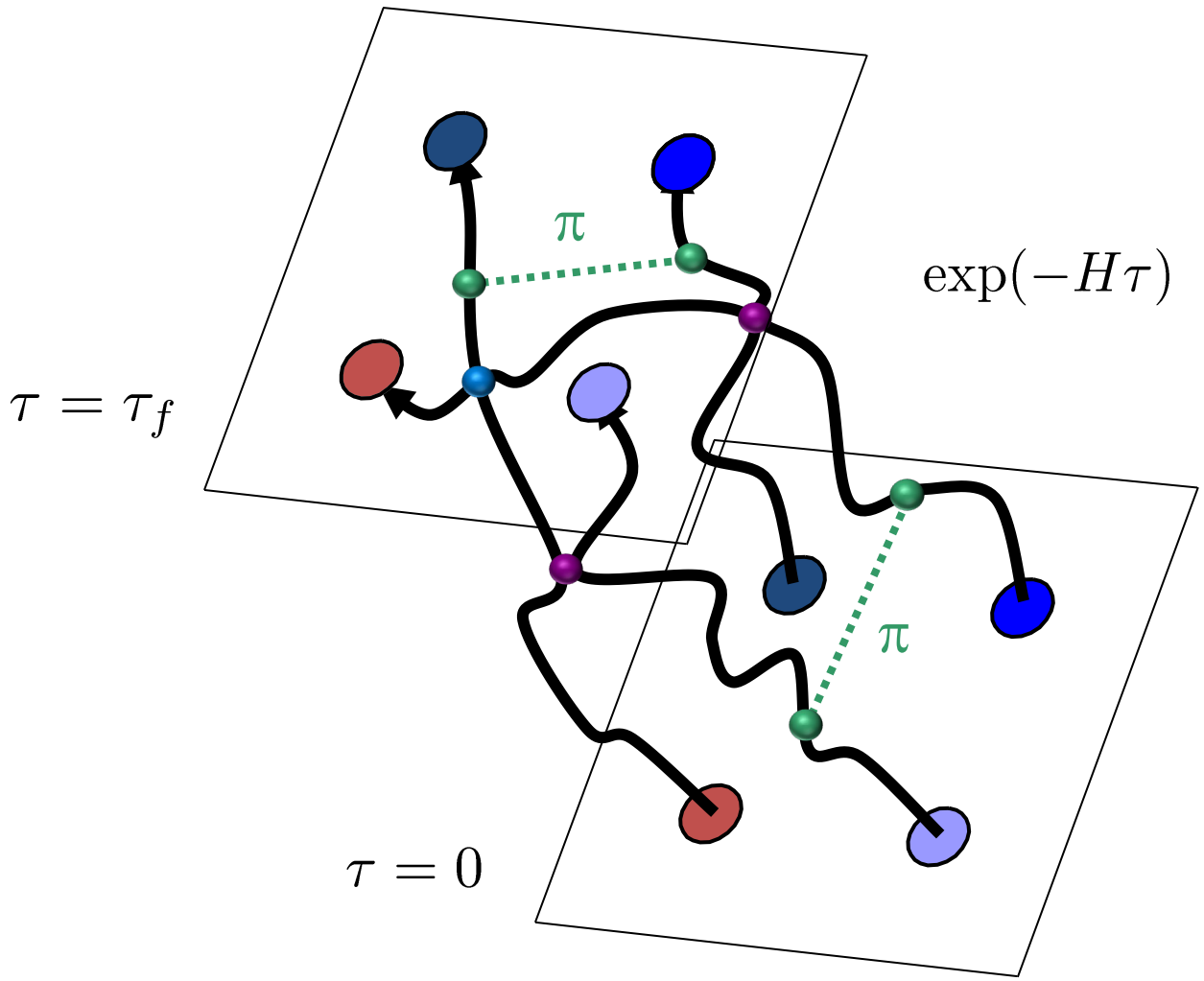


[Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)]

$a = 0.987\,\mathrm{fm}$



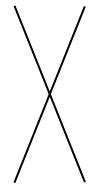
Euclidean time projection



Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right]$$

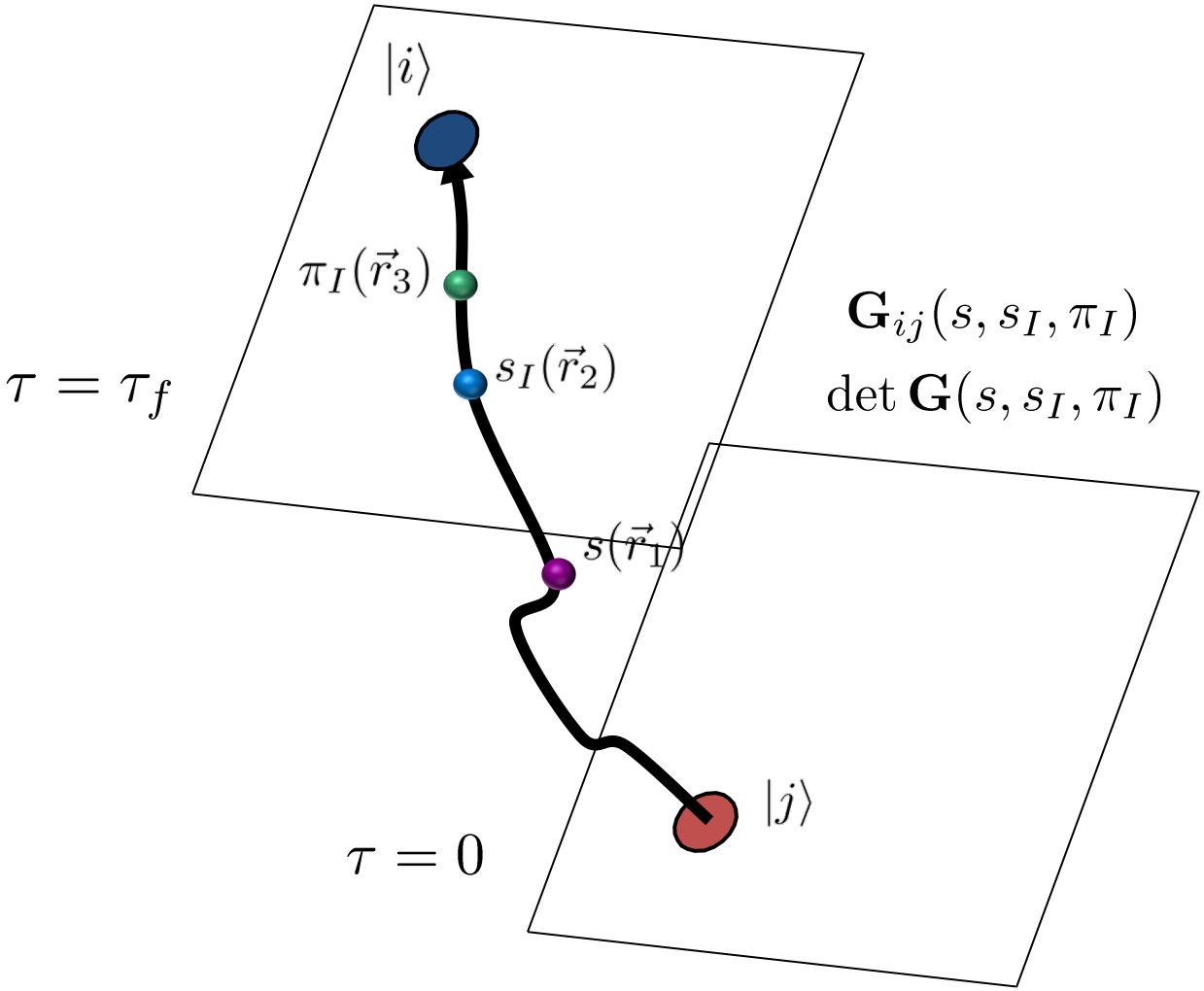


$$(N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right]$$

$$sN^\dagger N$$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.



$$\mathbf{G}_{ij}(s, s_I, \pi_I)$$

$$\det \mathbf{G}(s, s_I, \pi_I)$$

Adiabatic projection method

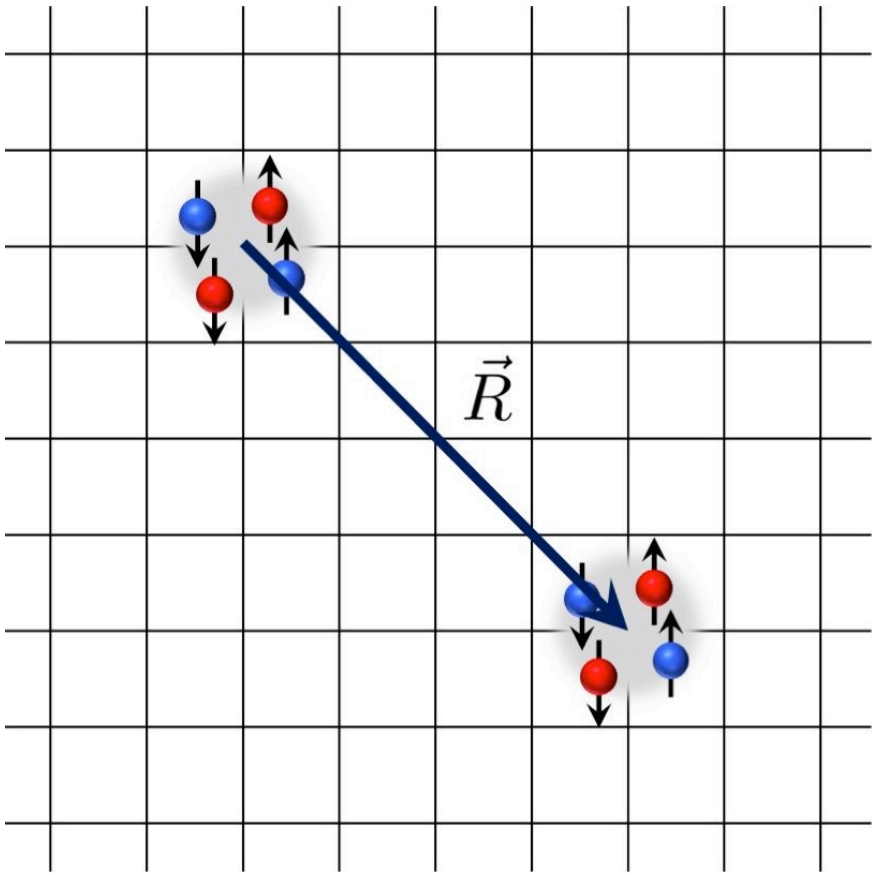
The adiabatic projection method is a first principles method for scattering and reactions. Strategy is to divide the problem into two parts.

In the first part, use Euclidean time projection and lattice Monte Carlo to derive an *abinitio*low-energy cluster Hamiltonian, called the adiabatic Hamiltonian.

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

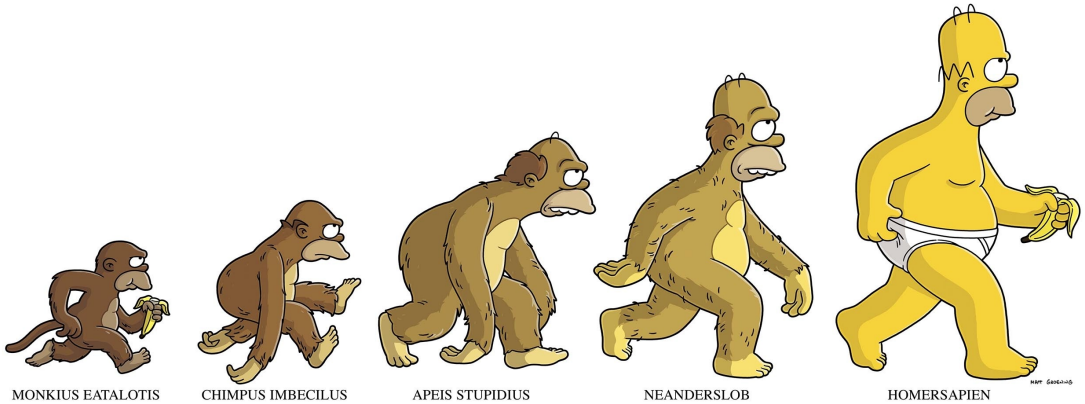
Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



We then evolve the clusters with Euclidean time

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



HOMERSAPIEN M. Groening

Effective cluster-cluster Hamiltonian is constructed from these states

We evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we also construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian. We can read off the scattering phase shifts for the asymptotic long-distance properties of the scattering wave functions.

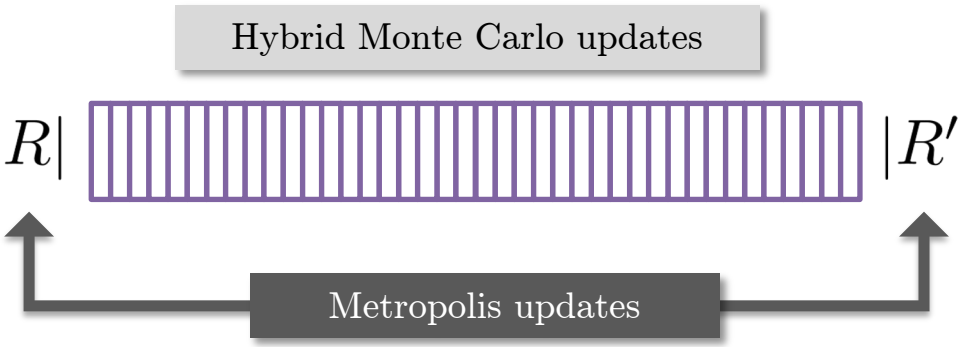
Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 106, 054612, 2015
Elhatisari, D.L., PRC 90, 064001, 2014

We use projections onto spherical harmonics defined on sets of lattice points with the same distance from the origin.

$$|R\rangle^{L,L_z} = \sum_{\vec{R}'} Y_{L,L_z}(\hat{R}')\delta_{R,|\vec{R}'|}|\vec{R}'\rangle$$

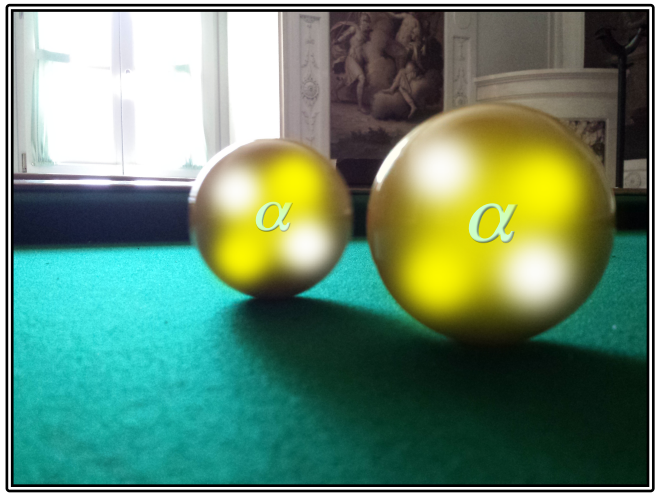
New algorithm developed for auxiliary field updates and initial/final state updates

$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R|$$



$$|R'\rangle^{L,L_z}$$

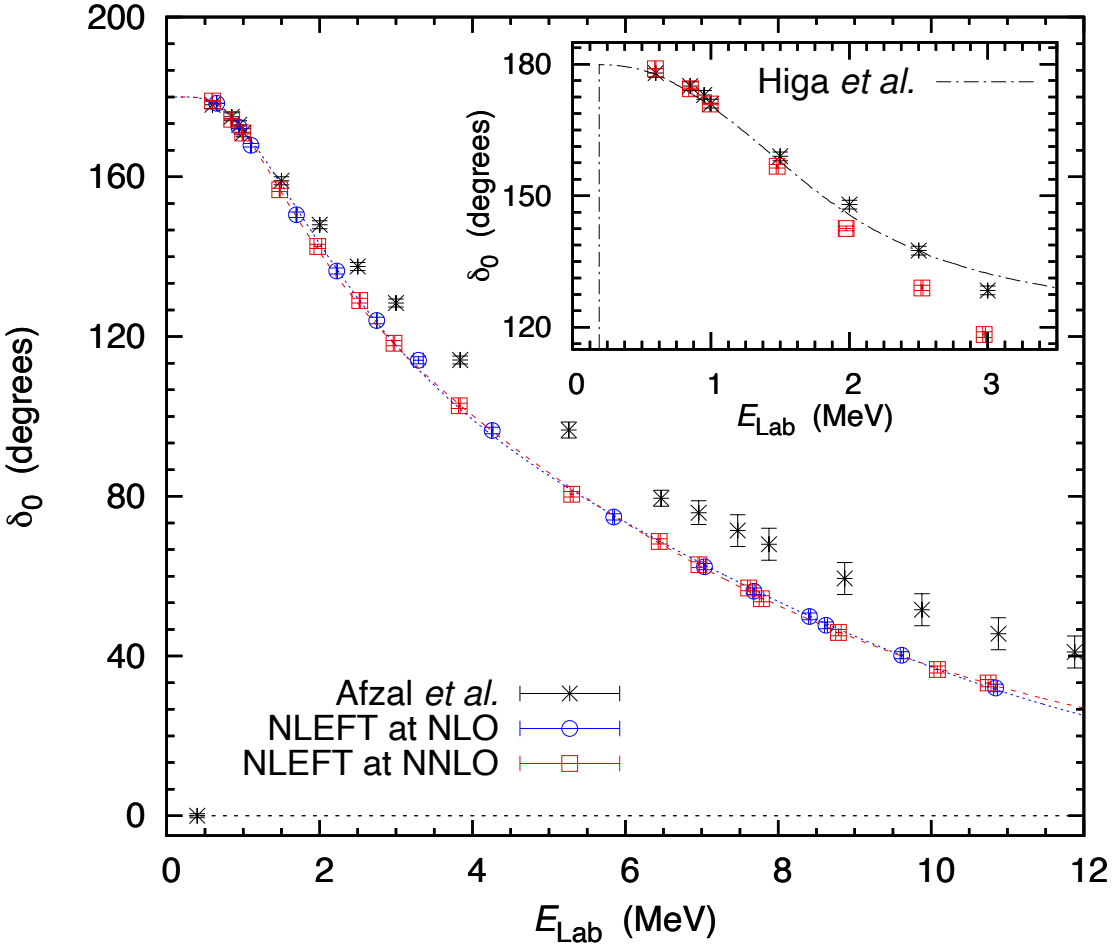
$$\underline{{}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}}$$



Lattice simulations for alpha-alpha scattering using adiabatic projection method. The computational scaling of the method is roughly quadratic in the number of nucleons.

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

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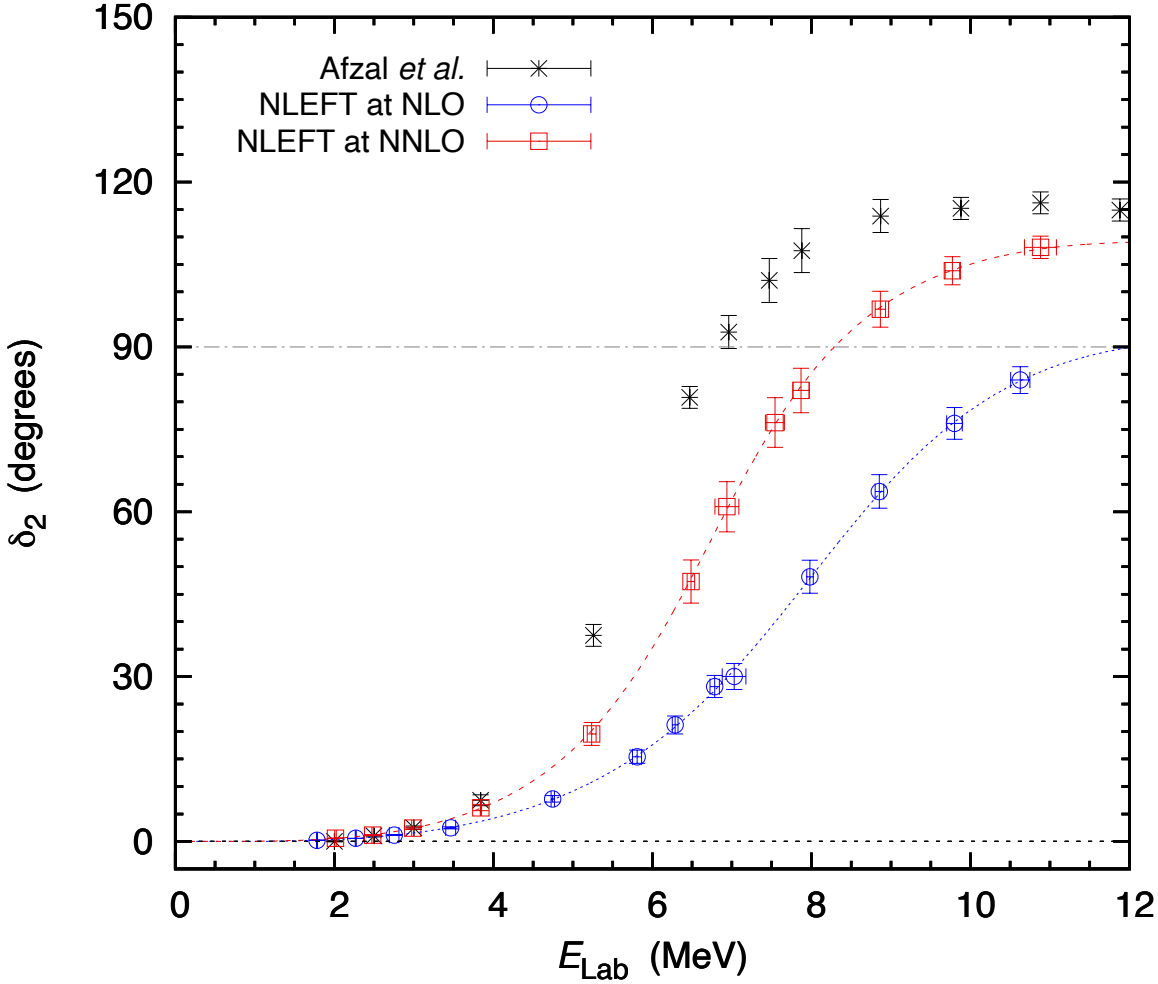

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

A tale of two interactions

Two different chiral LO interactions, A and B, that are nearly the same for up to four nucleon systems. However, they disagree strongly for systems with more nucleons.

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{8}Be	−58.61(14)	−59.73(6)	−56.51(14)	−57.29(7)	−56.591
^{12}C	−88.2(3)	−95.0(5)	−84.0(3)	−89.9(5)	−92.162
^{16}O	−117.5(6)	−135.4(7)	−110.5(6)	−126.0(7)	−127.619
^{20}Ne	−148(1)	−178(1)	−137(1)	−164(1)	−160.645

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

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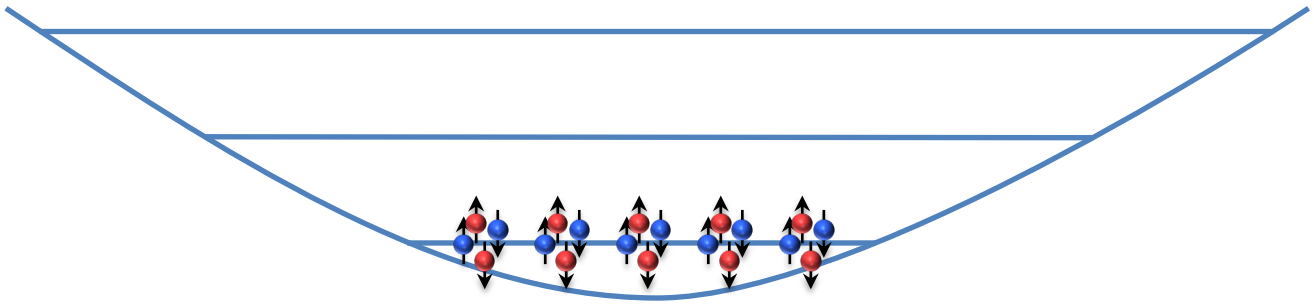
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

$$\frac{E_{^{12}\mathrm{C}}}{E_{^{4}\mathrm{He}}} = 3.00(1)$$

$$\frac{E_{^{16}\mathrm{O}}}{E_{^{4}\mathrm{He}}} = 4.00(2)$$

$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^{4}\mathrm{He}}} = 5.03(3)$$

Bose condensate of alpha particles!



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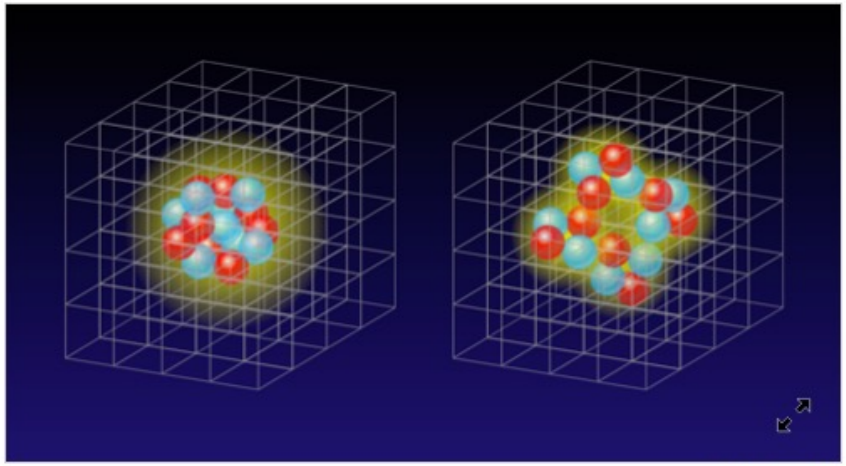
Viewpoint: Uncovering a Quantum Phase Transition in Nuclei

David J. Dean, Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

September 19, 2016 • *Physics* 9, 106

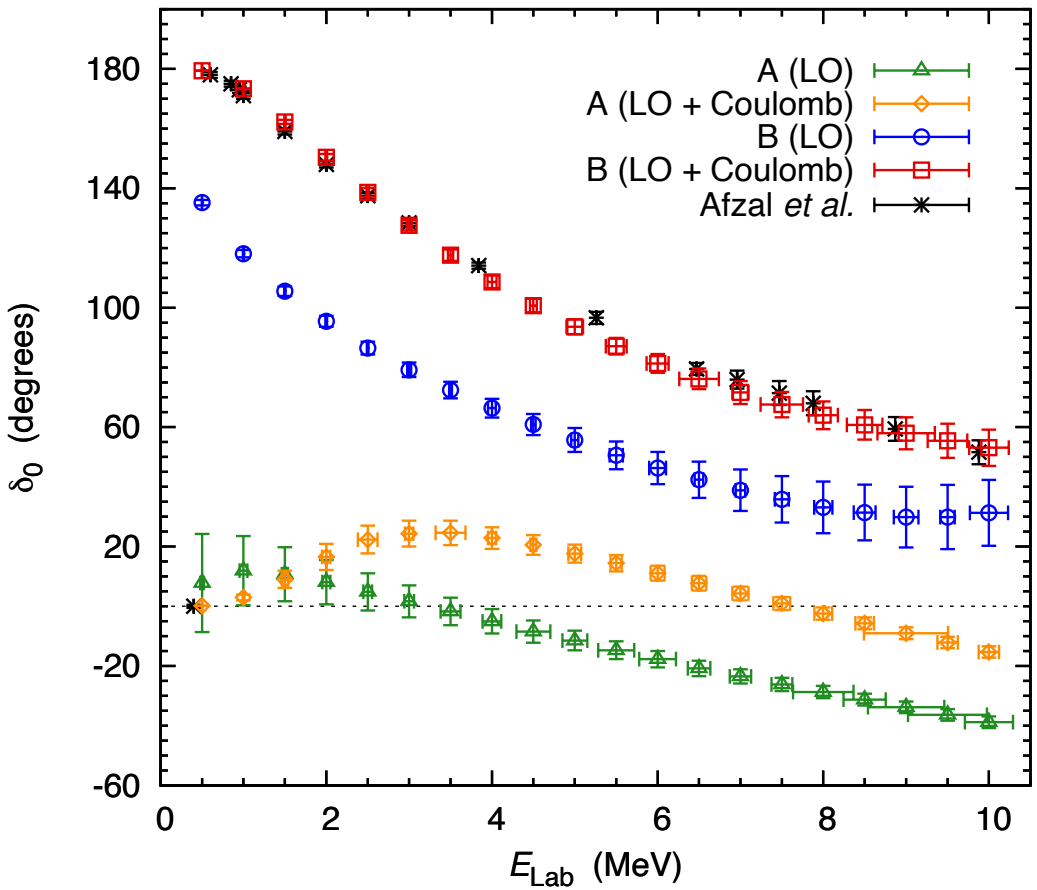
Simulations predict that the ground states of certain light nuclei lie near a quantum phase transition between a liquid-like phase and a phase involving clusters of alpha particles.



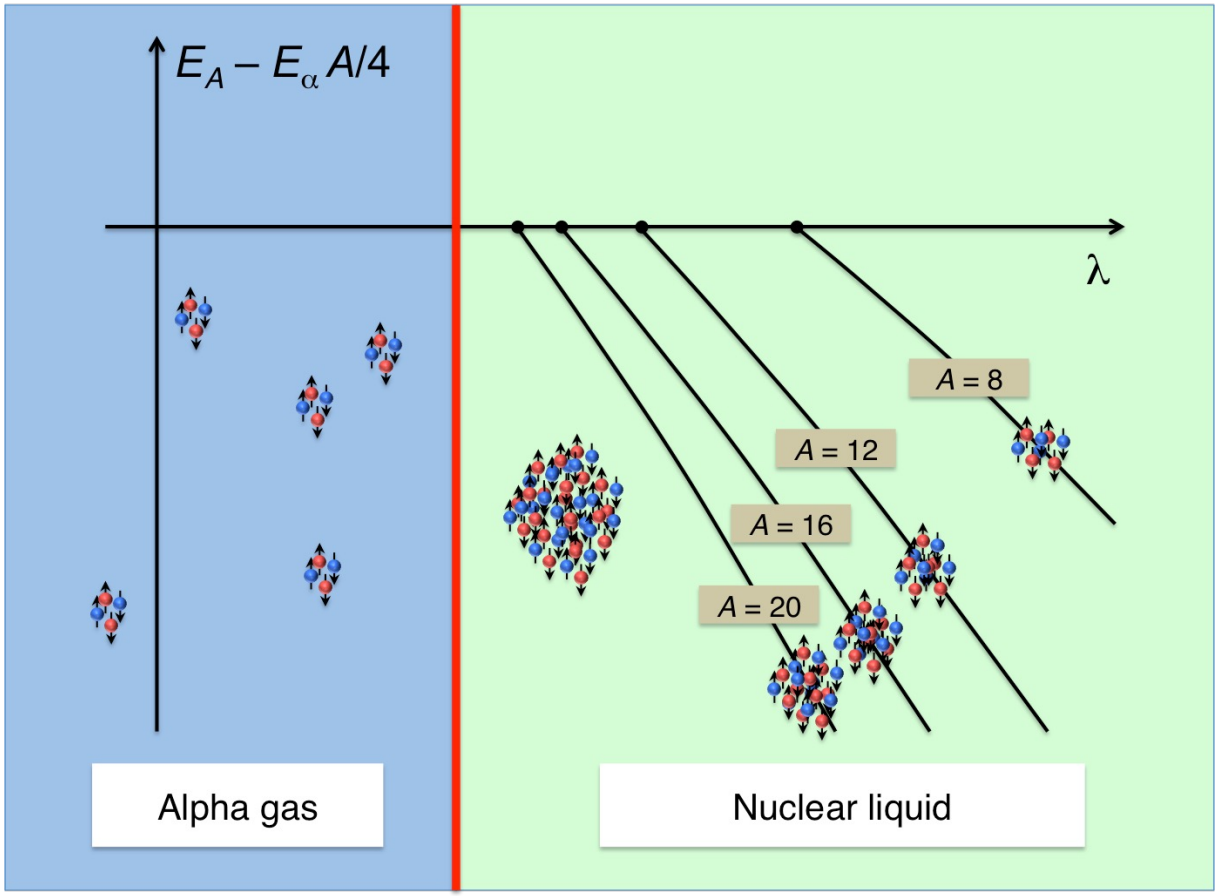
APS/Alan Stonebraker

Figure 1: Lee and colleagues performed simulations of a nucleus in which they tweaked the interaction between nucleons (protons and neutrons) [1]. They found that, depending on the form of the interaction, the nucleus lay on either side of a quantum phase transition. The transition is between (left) a phase in which protons and neutrons are evenly distributed (a Fermi liquid) to (right) a phase in which the protons and neutrons cluster into alpha particles. **Show less**

alpha-alpha scattering



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Essential elements for nuclear binding

What is the minimal nuclear interaction that can reproduce the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii?

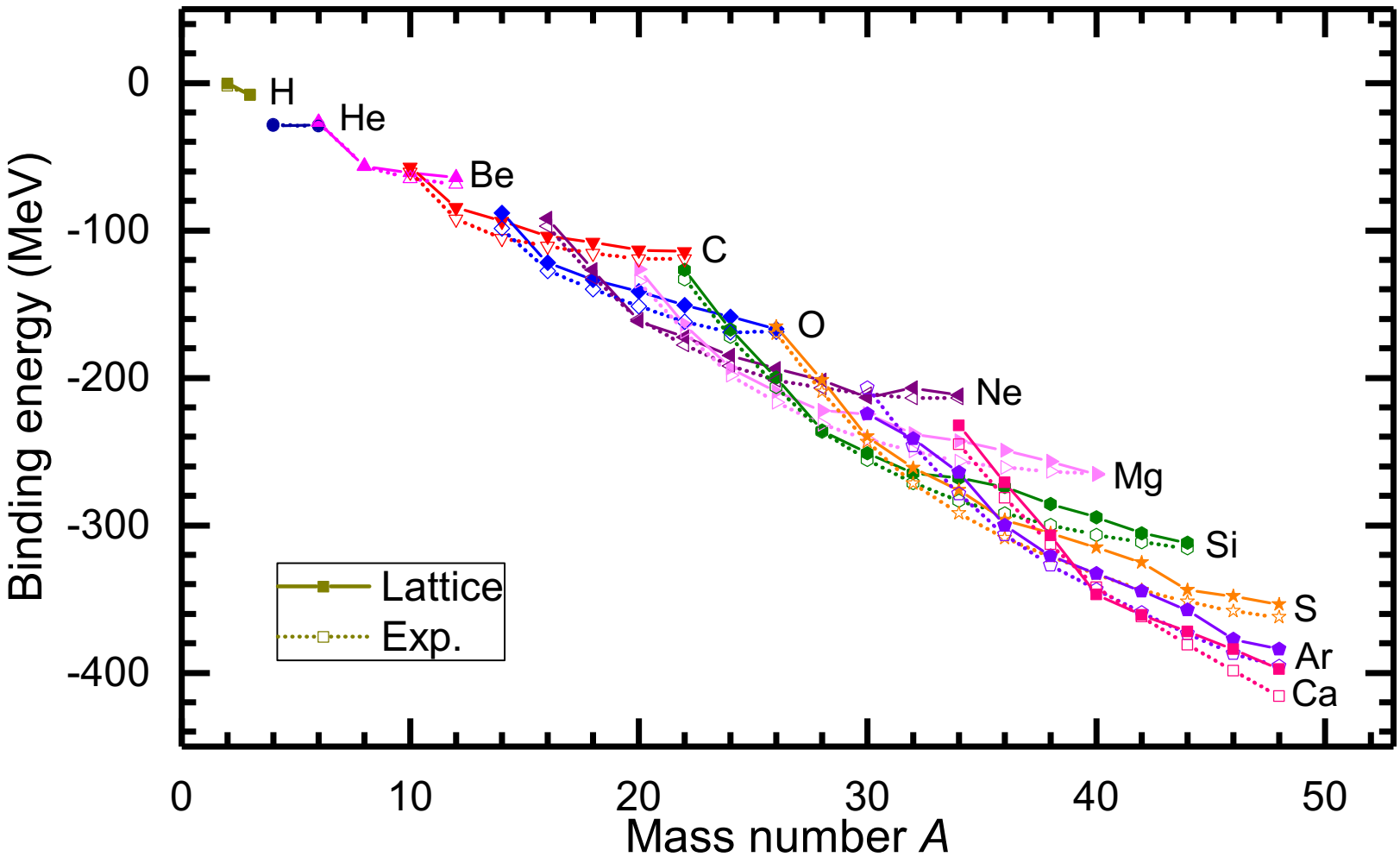
We construct an interaction with only four parameters.

1. Strength of the two-nucleon S-wave interaction
2. Range of the two-nucleon S-wave interaction
3. Strength of three-nucleon contact interaction

fit to $A = 2, 3$ systems

4. Range of the local part of the two-nucleon interaction

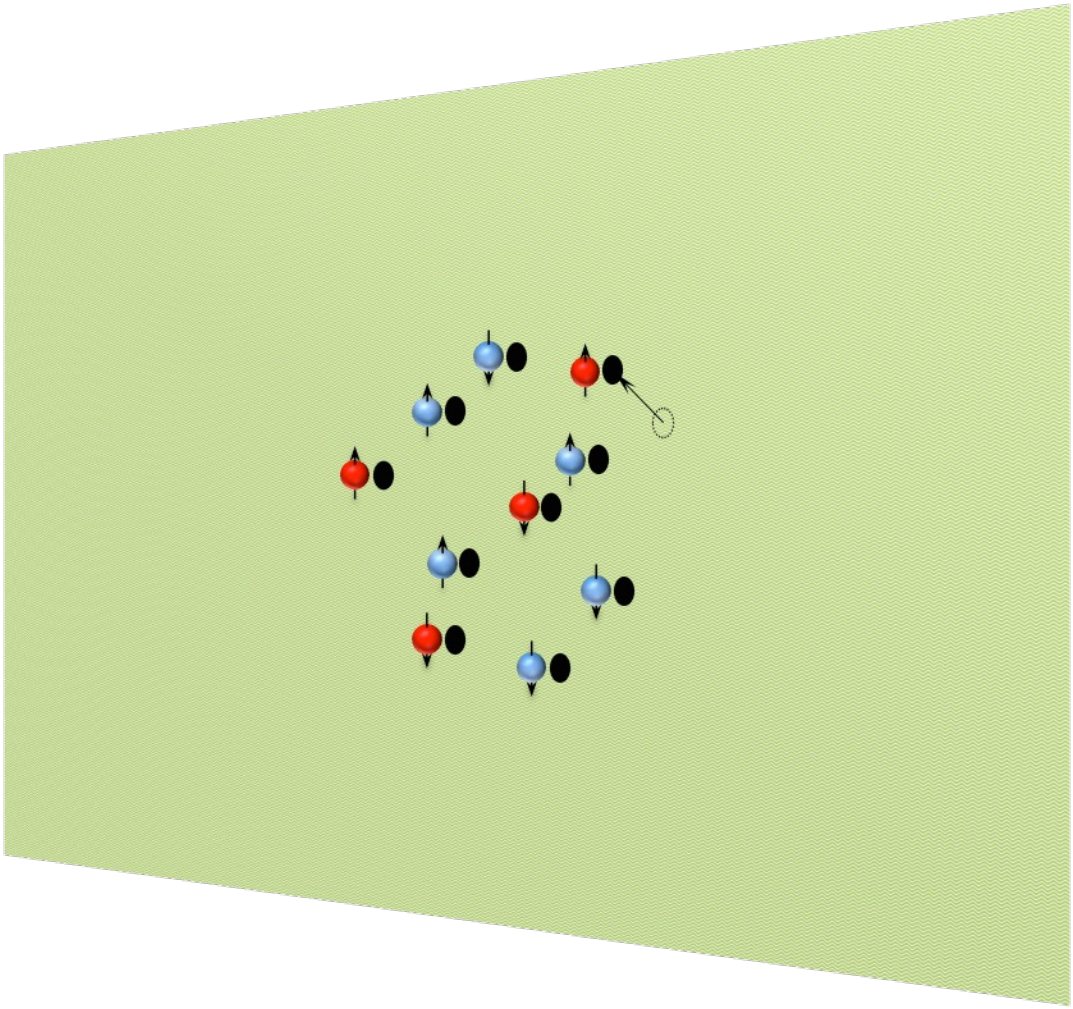
fit to A > 3



Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

	B	Exp.	R_{ch}	Exp.
^{3}H	8.48(2)(0)	8.48	1.90(1)(1)	1.76
^{3}He	7.75(2)(0)	7.72	1.99(1)(1)	1.97
^{4}He	28.89(1)(1)	28.3	1.72(1)(3)	1.68
^{16}O	121.9(1)(3)	127.6	2.74(1)(1)	2.70
^{20}Ne	161.6(1)(1)	160.6	2.95(1)(1)	3.01
^{24}Mg	193.5(02)(17)	198.3	3.13(1)(2)	3.06
^{28}Si	235.8(04)(17)	236.5	3.26(1)(1)	3.12
^{40}Ca	346.8(6)(5)	342.1	3.42(1)(3)	3.48

Pinhole algorithm



Seeing Structure with Pinholes

Consider the density operator for nucleon with spin i and isospin j

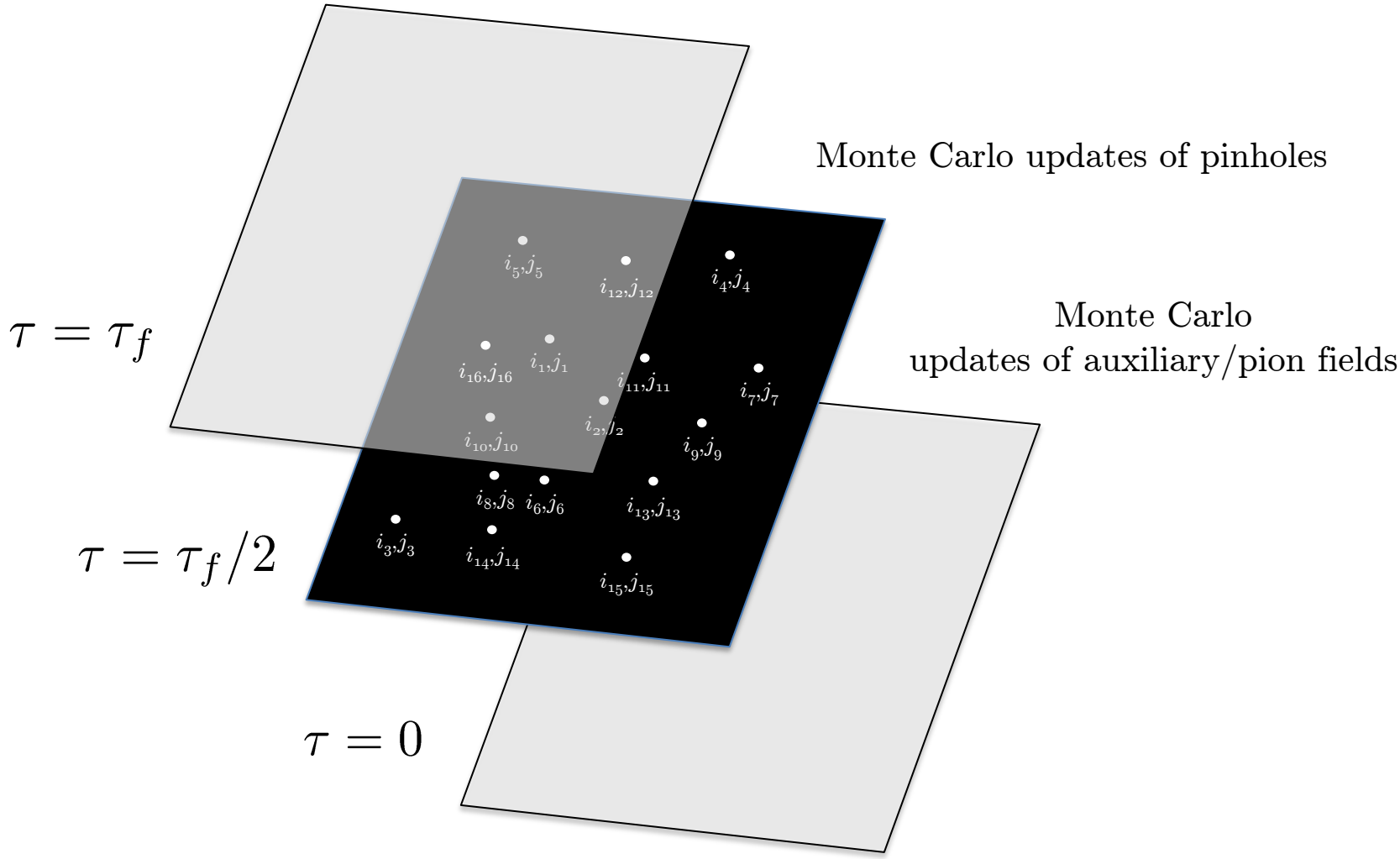
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

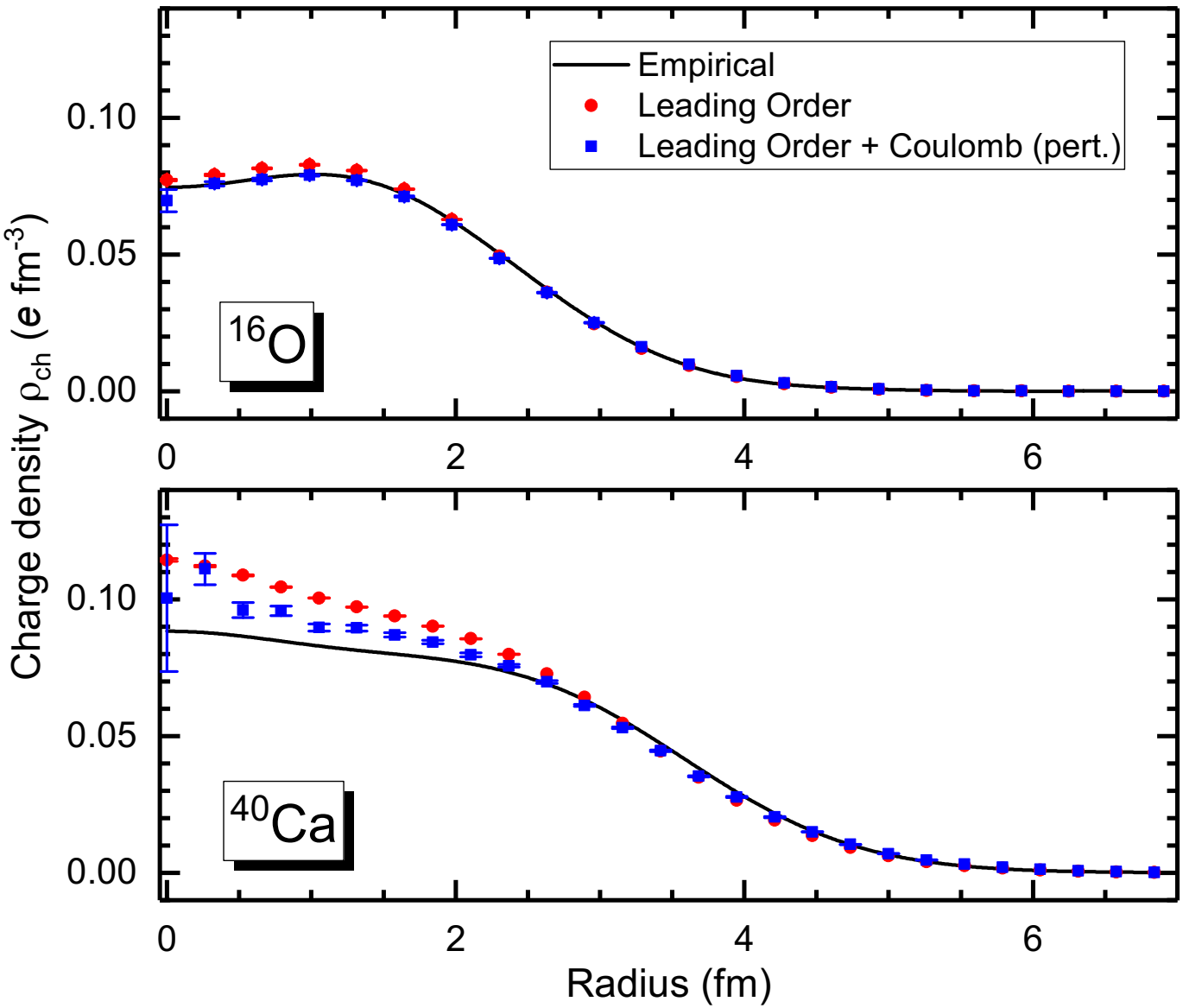
$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$

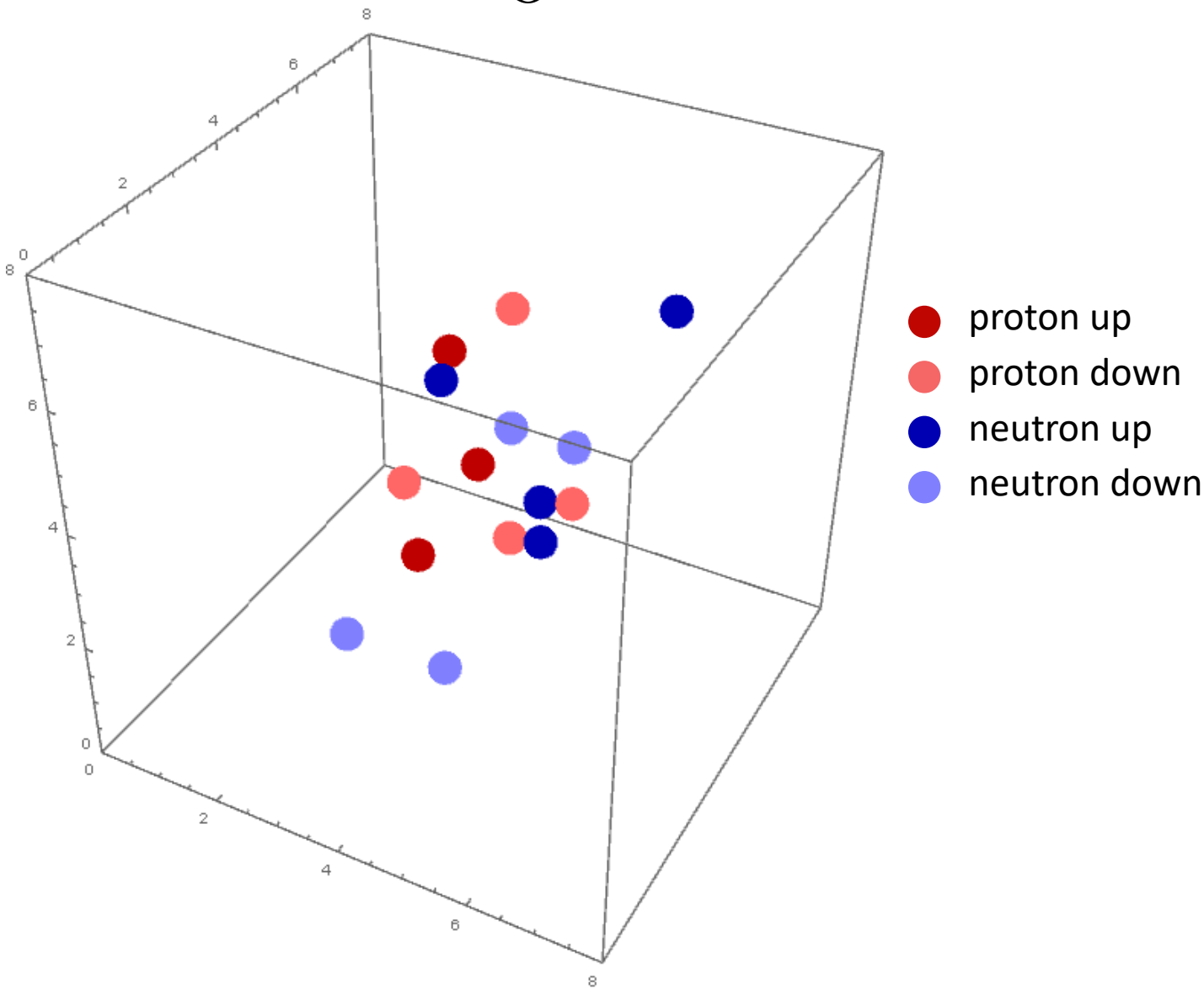


Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



[Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)]

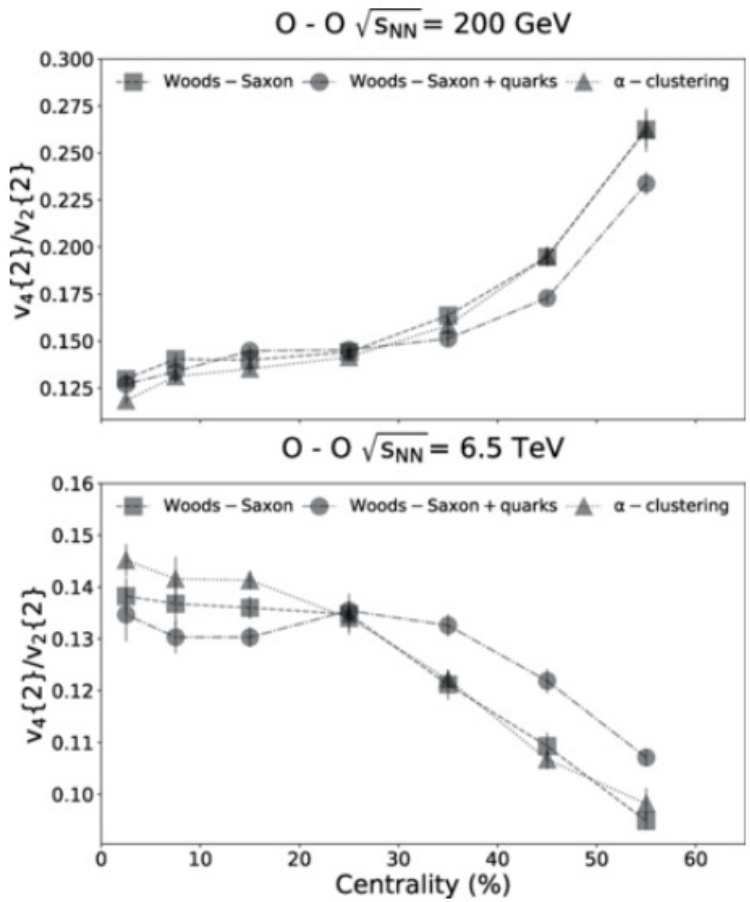
^{16}O



$^{16}O^{16}O$ collisions at energies available at the BNL Relativistic Heavy Ion Collider and at the CERN Large Hadron Collider comparing α clustering versus substructure

Nicholas Summerfield, Bing-Nan Lu, Christopher Plumberg, Dean Lee, Jacquelyn Noronha-Hostler, and Anthony Timmins

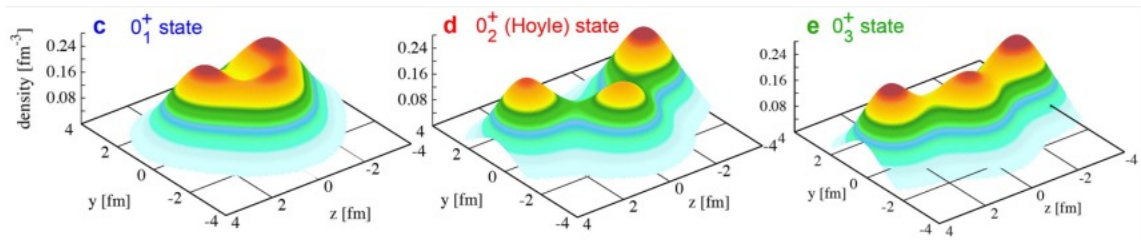
Phys. Rev. C **104**, L041901 – Published 4 October 2021

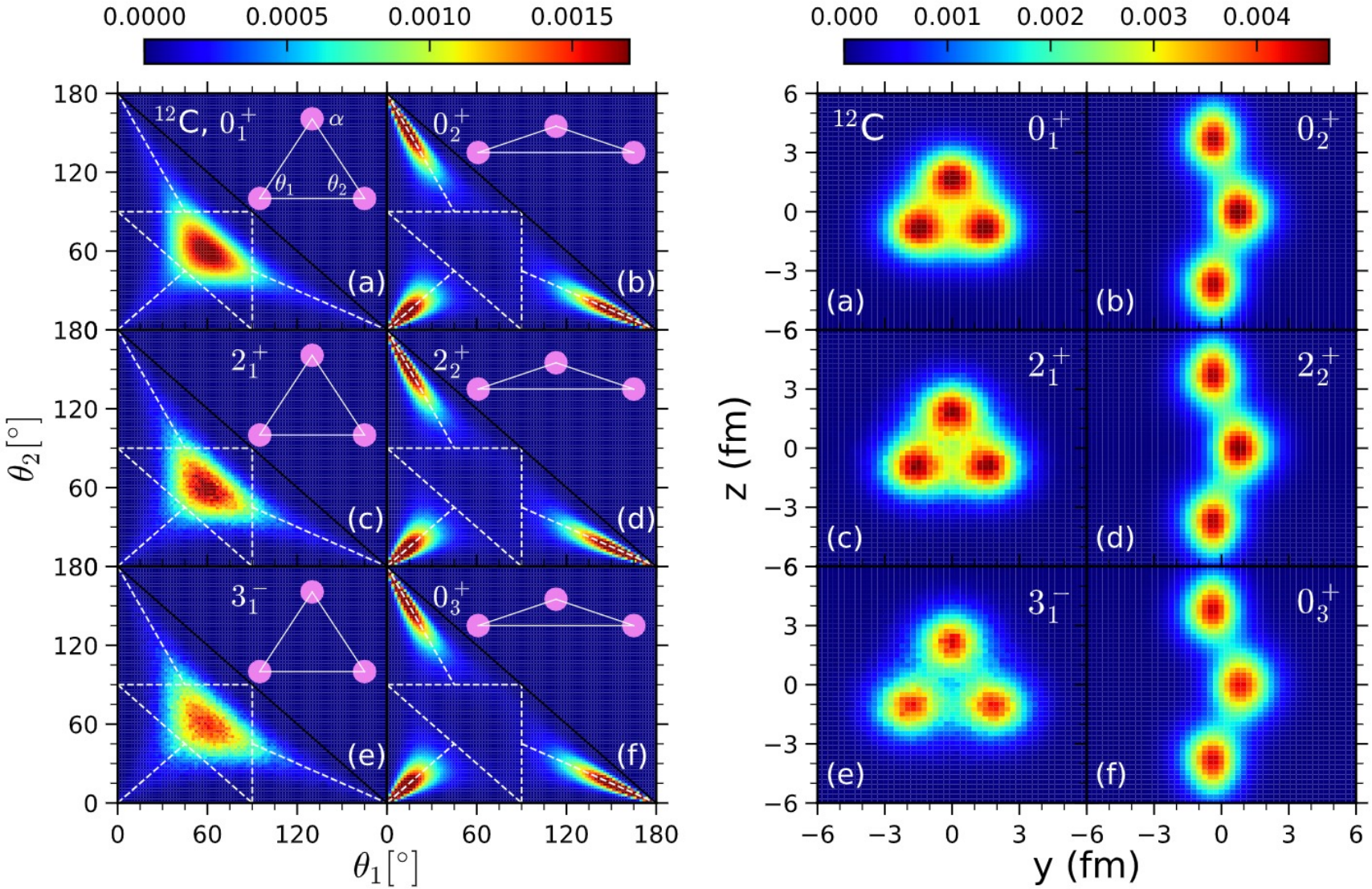


Structure and spectrum of ^{12}C

Ab initio No-Core Monte Carlo Shell Model calculations of ^{12}C

Otsuka et al., Nat. Comm. 13:2234 (2022)





Shen, Elhatisari, Lähde, D.L., Lu, Meißner, arXiv:2202.13596

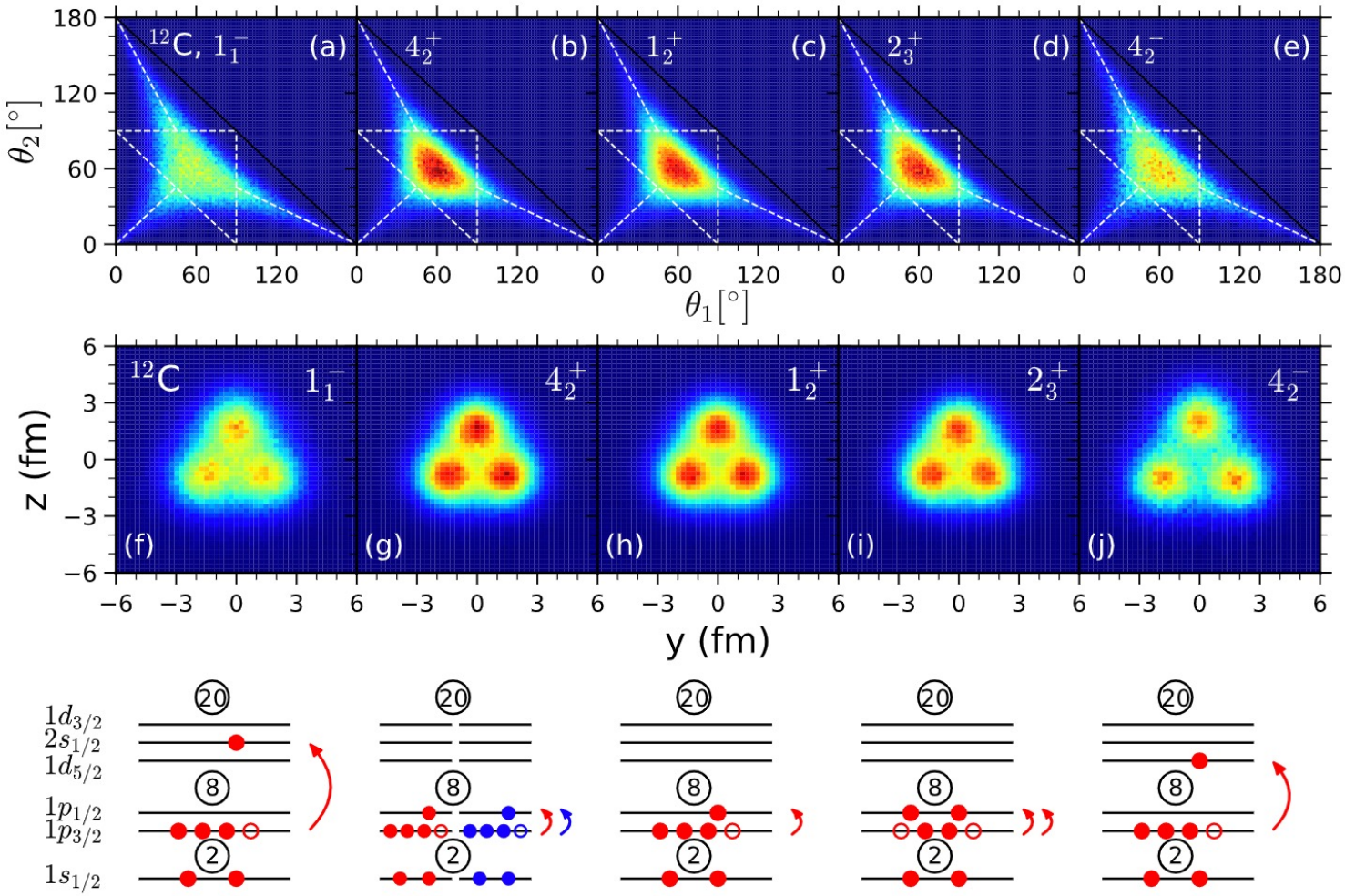


Figure S3: **Top Panel:** Density distribution for the two inner angles of the triangle formed by the three alpha clusters. **Middle Panel:** Tomographic projection of the nuclear density. **Lower Panel:** Sketch of the orbitals for the shell model initial states used in each of these calculations.

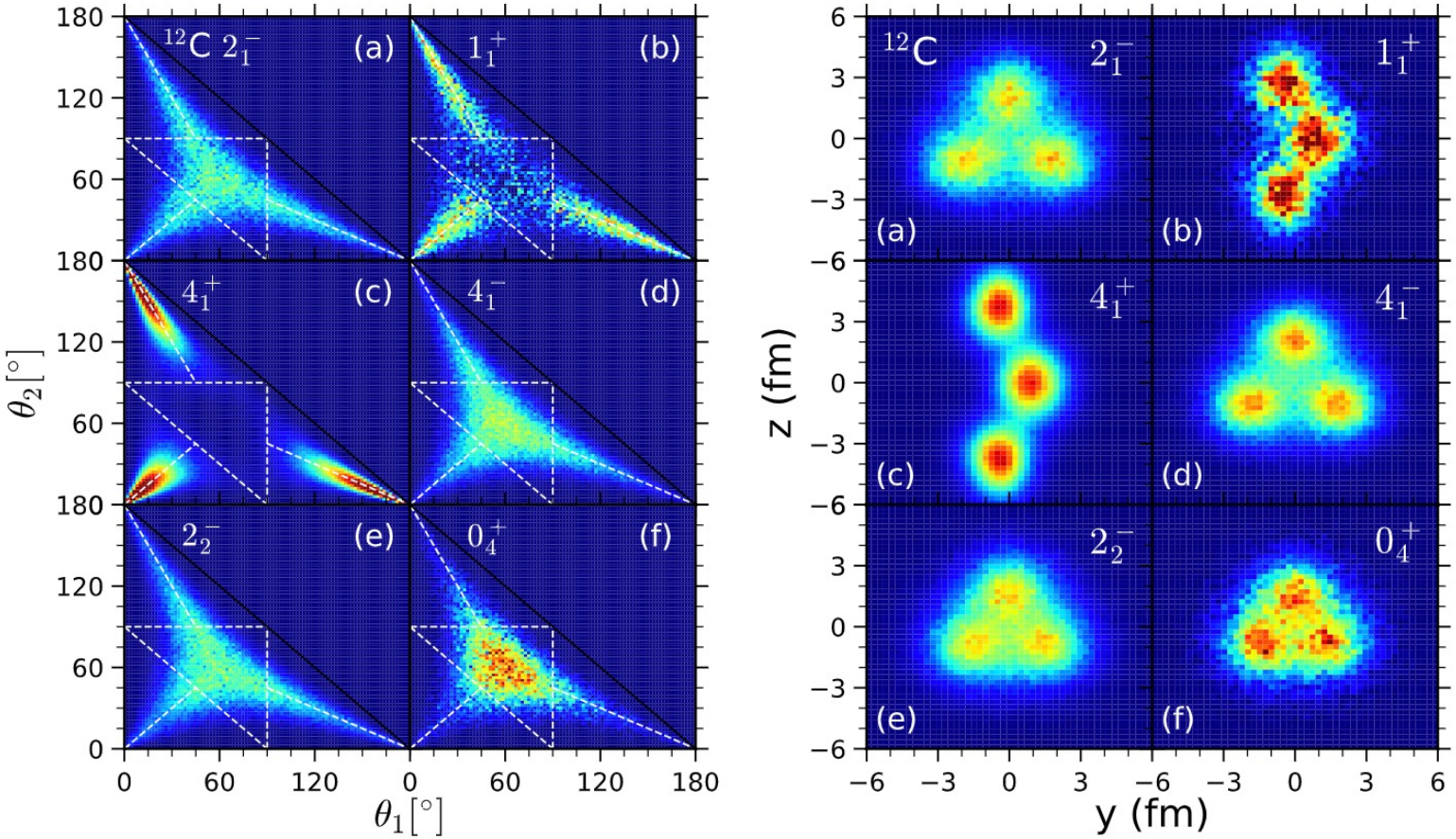
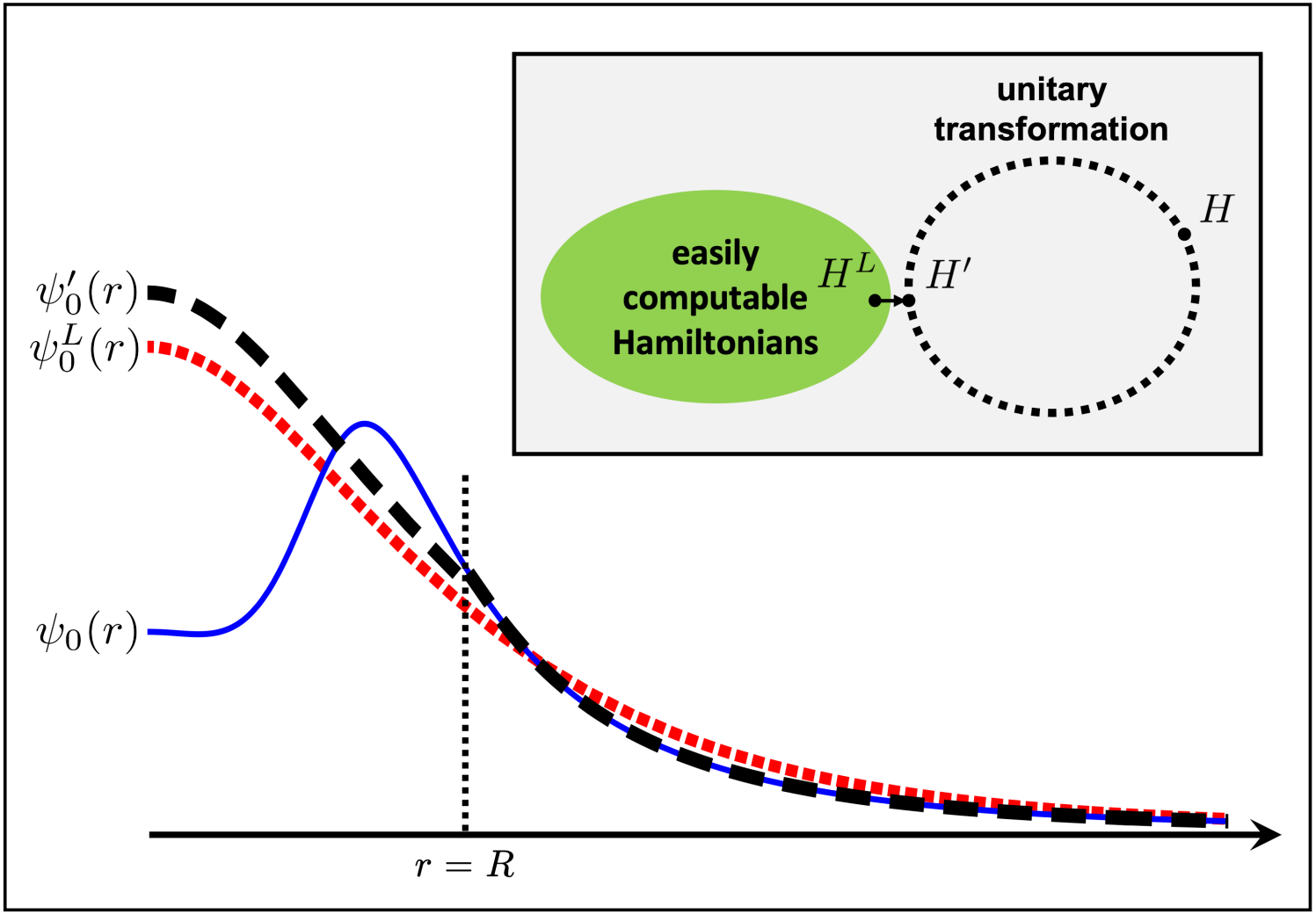


Figure S4: **Left Panel:** Density distribution for the two inner angles of the triangle formed by the three alpha clusters. **Right Panel:** Tomographic projection of the nuclear density. From (a) to (f), the selected states are ordered by their energies from low to high.

Wave function matching

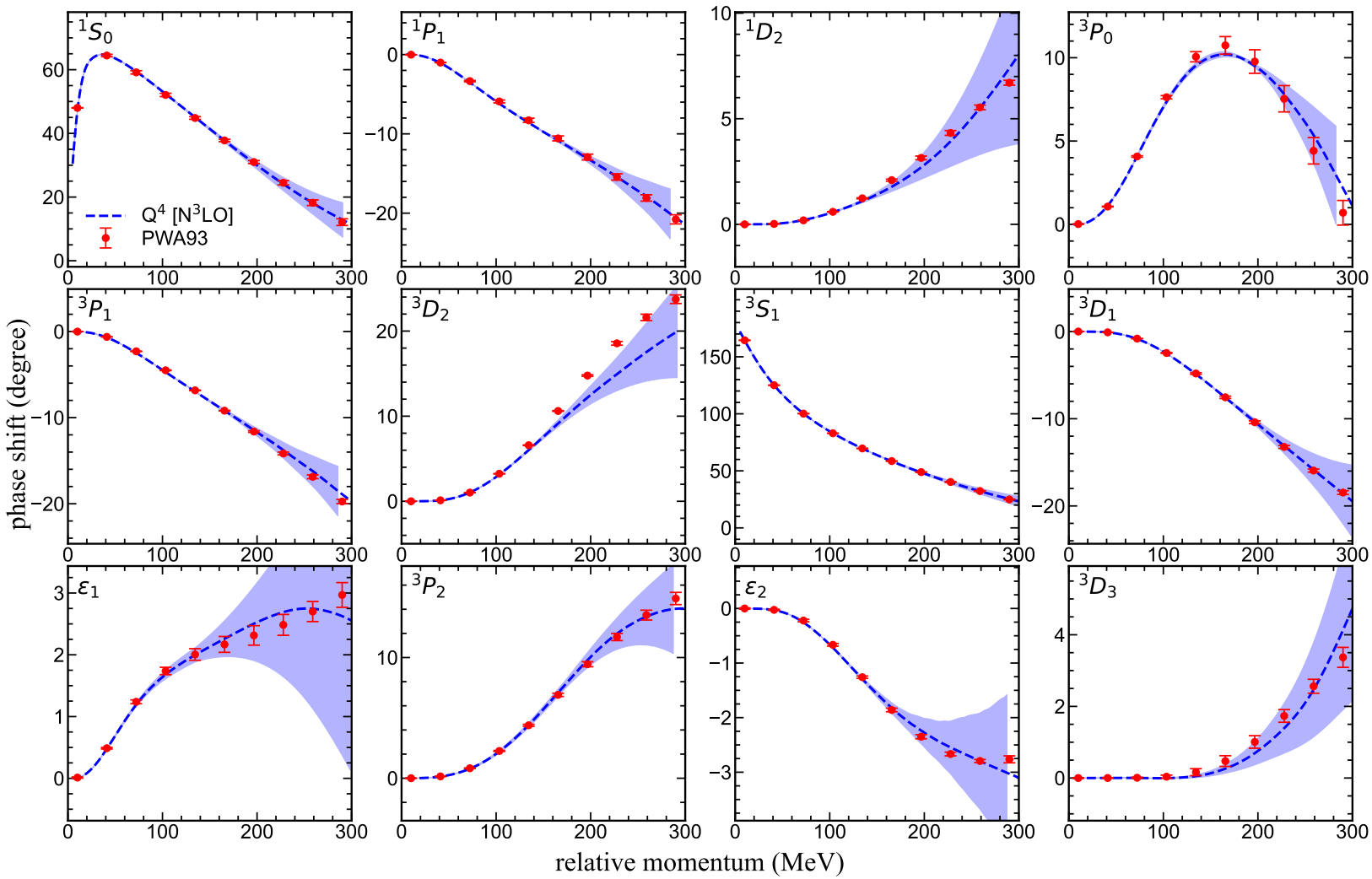


Work in progress: Elhatisari, Bovermann, et al.

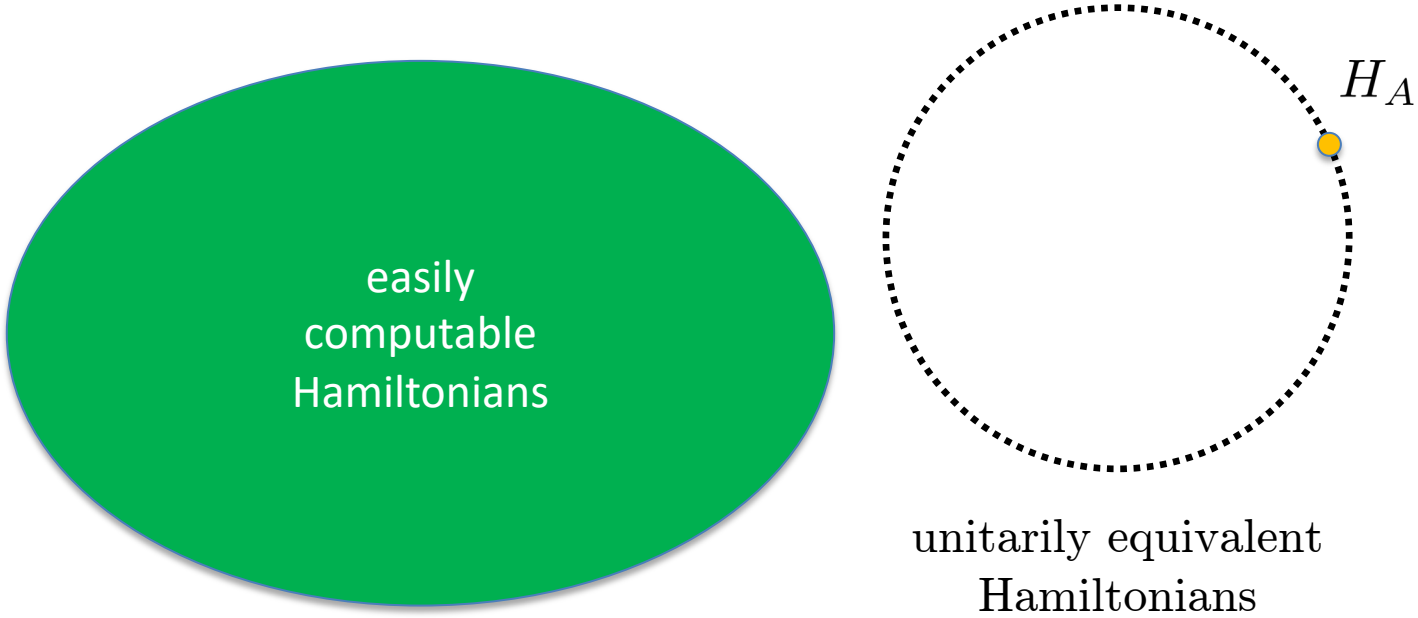
Lattice Monte Carlo simulations can compute highly nontrivial correlations in nuclear many-body systems. Unfortunately, sign oscillations prevent direct simulations using a high-fidelity Hamiltonian based on chiral effective field theory due to short-range repulsion.

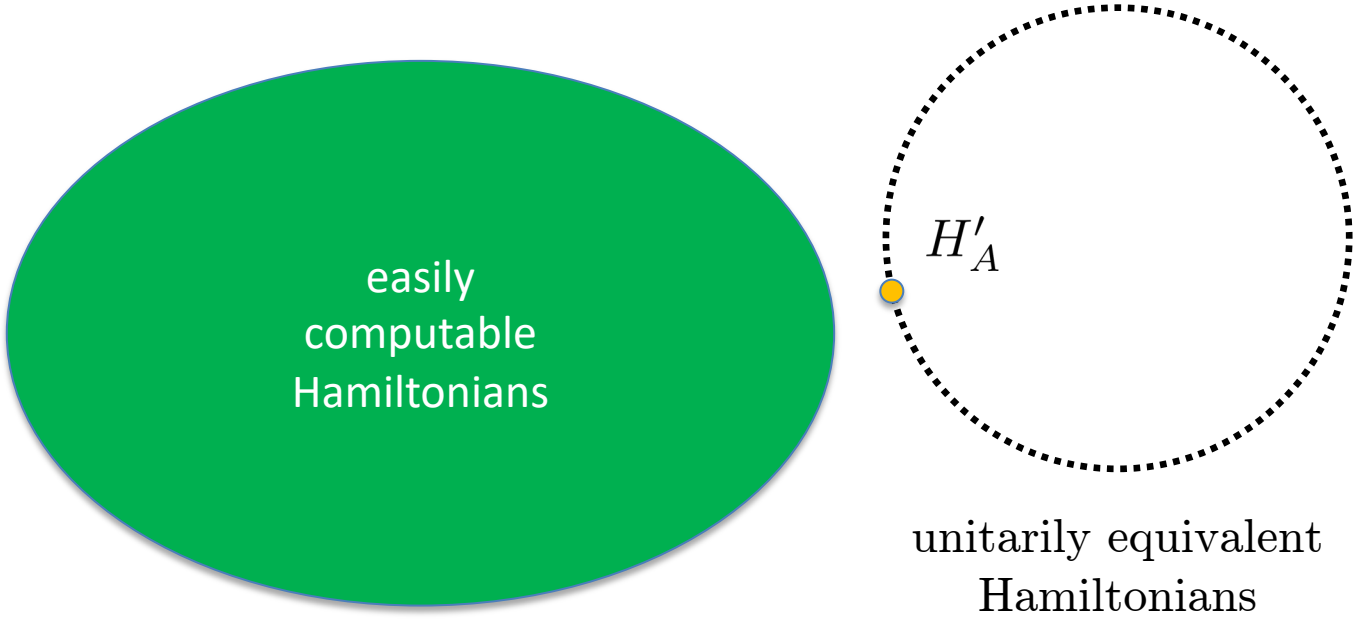
Wave function matching solves this problem by means of unitary transformations and perturbation theory. By using unitary transformations, we construct a high-fidelity Hamiltonian that can be reached by perturbation theory, starting from a Hamiltonian without a sign problem.

N3LO chiral interaction



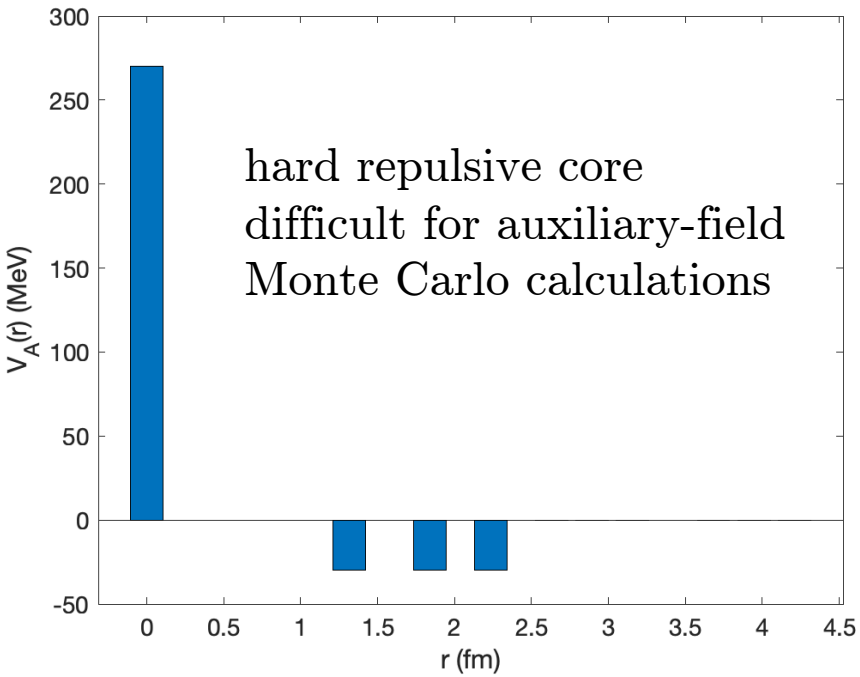

easily
computable
Hamiltonians
H_A


easily
computable
Hamiltonians
H_A
unitarily equivalent
Hamiltonians

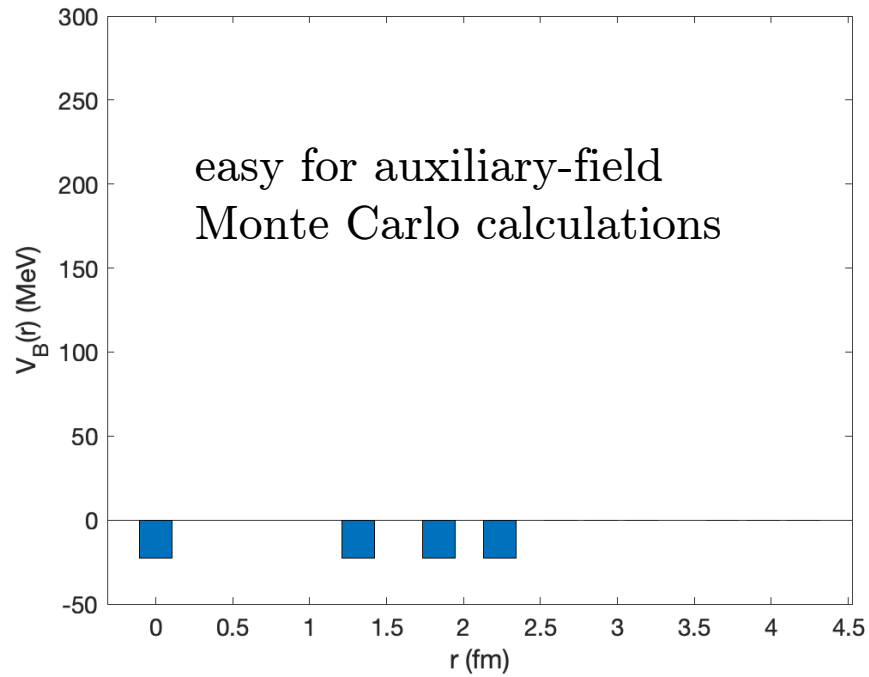

easily
computable
Hamiltonians
H'_A
unitarily equivalent
Hamiltonians

Wave function matching

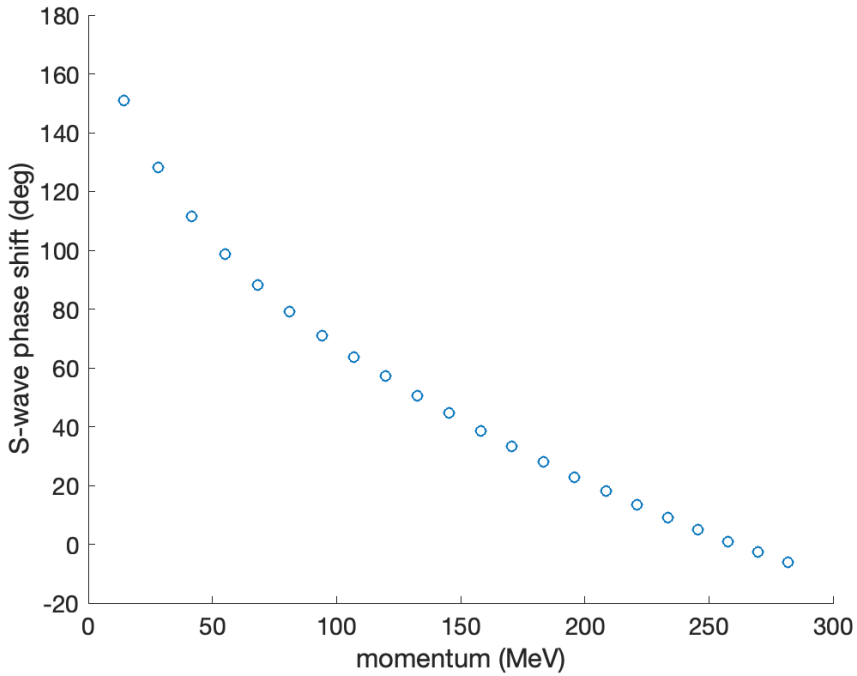
$V_A(r)$



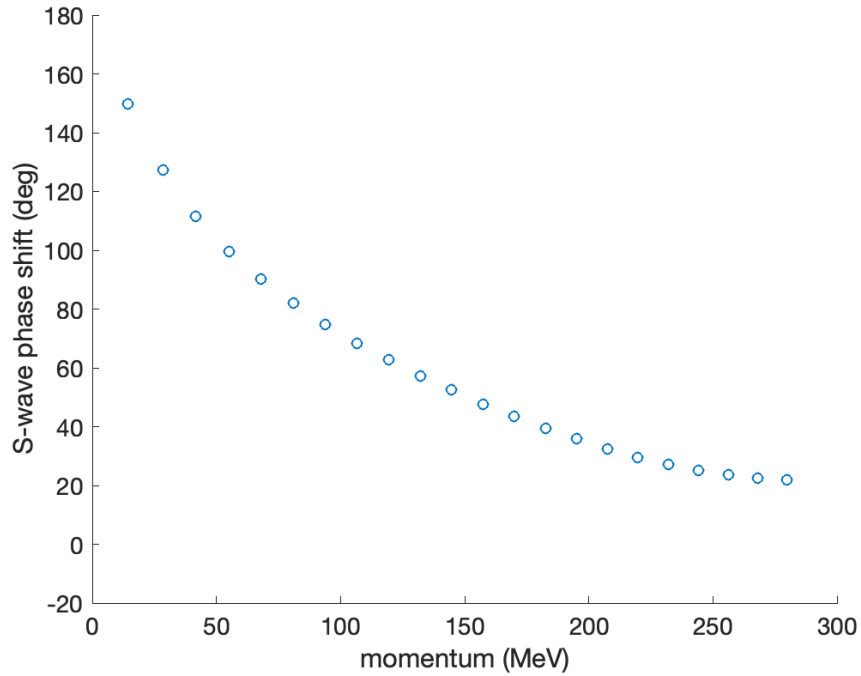
$V_B(r)$



$V_A(r)$


S-wave phase shift (deg)
momentum (MeV)
180
160
140
120
100
80
60
40
20
0
-20
0
50
100
150
200
250
300

$V_B(r)$


S-wave phase shift (deg)
momentum (MeV)
180
160
140
120
100
80
60
40
20
0
-20
0
50
100
150
200
250
300

Let us write the eigenenergies and eigenfunctions for the two interactions as

$$H_A \left|\psi_{A,n}\right\rangle = \left(K + V_A\right) \left|\psi_{A,n}\right\rangle = E_{A,n} \left|\psi_{A,n}\right\rangle$$
$$H_B \left|\psi_{B,n}\right\rangle = \left(K + V_B\right) \left|\psi_{B,n}\right\rangle = E_{B,n} \left|\psi_{B,n}\right\rangle$$

We would like to compute the eigenenergies of H_A starting from the eigenfunctions of H_B and using first-order perturbation theory.

Not surprisingly, this does not work very well. The interactions V_A and V_B are quite different.

$E_{A,n}$ (MeV)	$\langle\psi_{B,n}\|H_A\|\psi_{B,n}\rangle$ (MeV)
-1.2186	3.0088
0.2196	0.3289
0.8523	1.1275
1.8610	2.2528
3.2279	3.6991
4.9454	5.4786
7.0104	7.5996
9.4208	10.0674
12.1721	12.8799
15.2669	16.0458

Let P be a projection operator that is nonzero only for separation distances r less than R. We define a short-distance unitary operator U such that

$$U : P\left|\psi_A^0\right\rangle / \left\| P\left|\psi_A^0\right\rangle \right\| \to P\left|\psi_B^0\right\rangle / \left\| P\left|\psi_B^0\right\rangle \right\|$$

There are many possible choices for U. The corresponding action of U on the Hamiltonian is

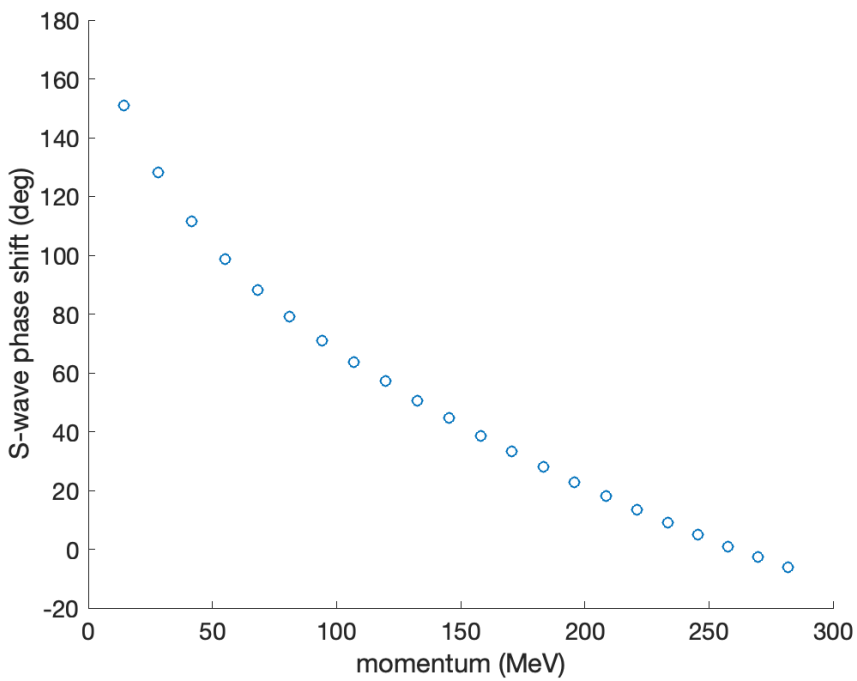
$$U : H_A \to H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

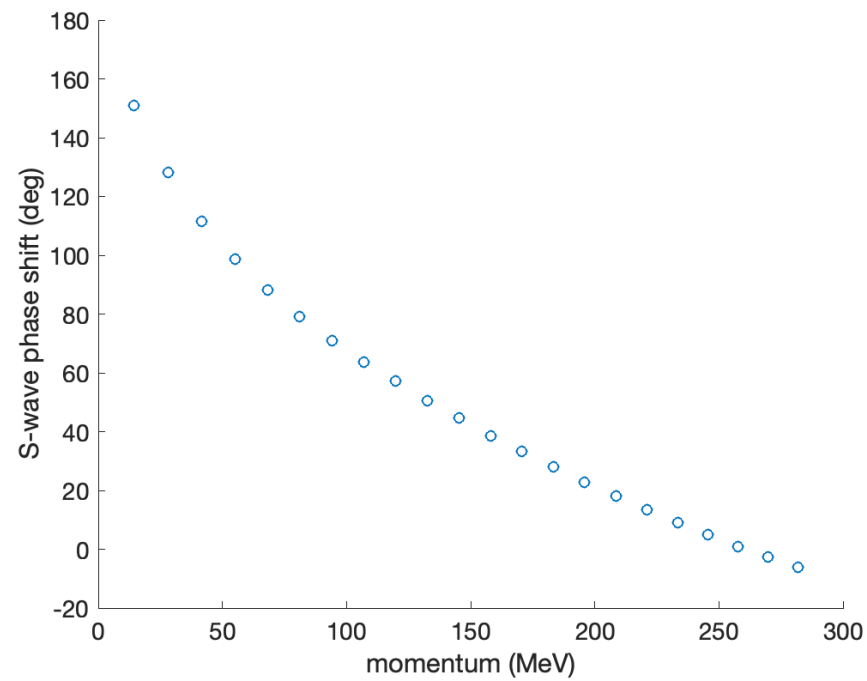
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

Since they are unitarily equivalent, the phase shifts are exactly the same

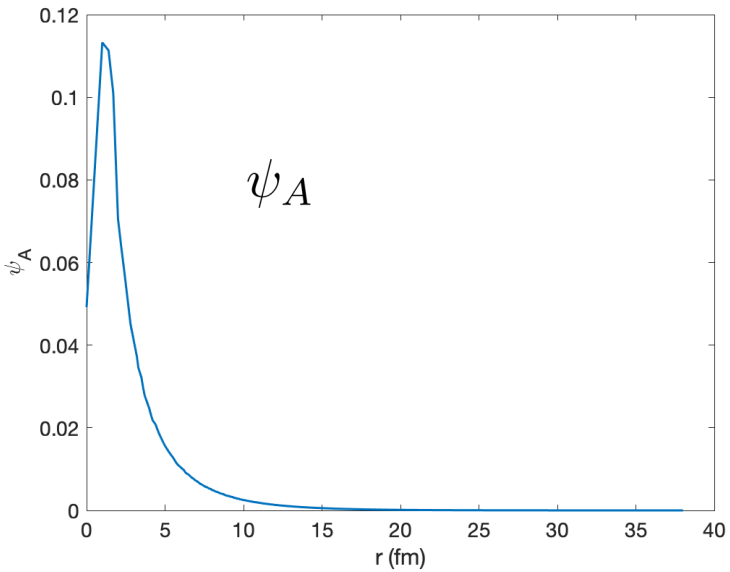
$V_A(r)$

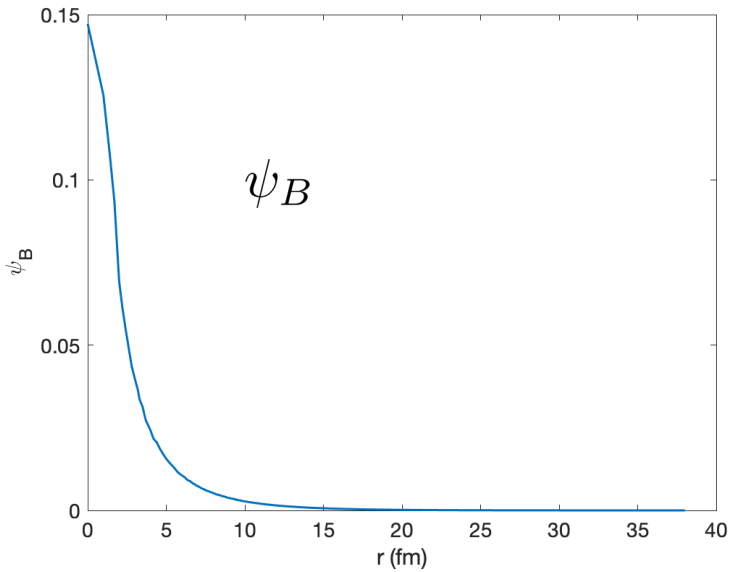


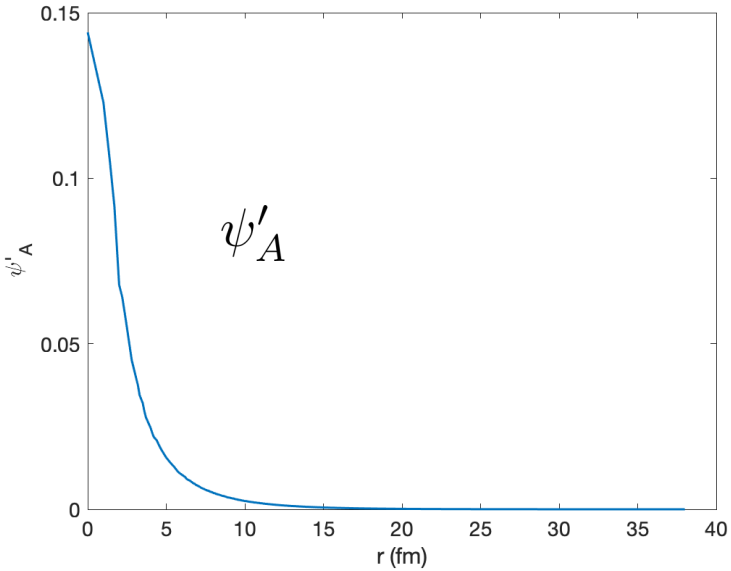
$V'_A(r, r')$



Ground state wave functions





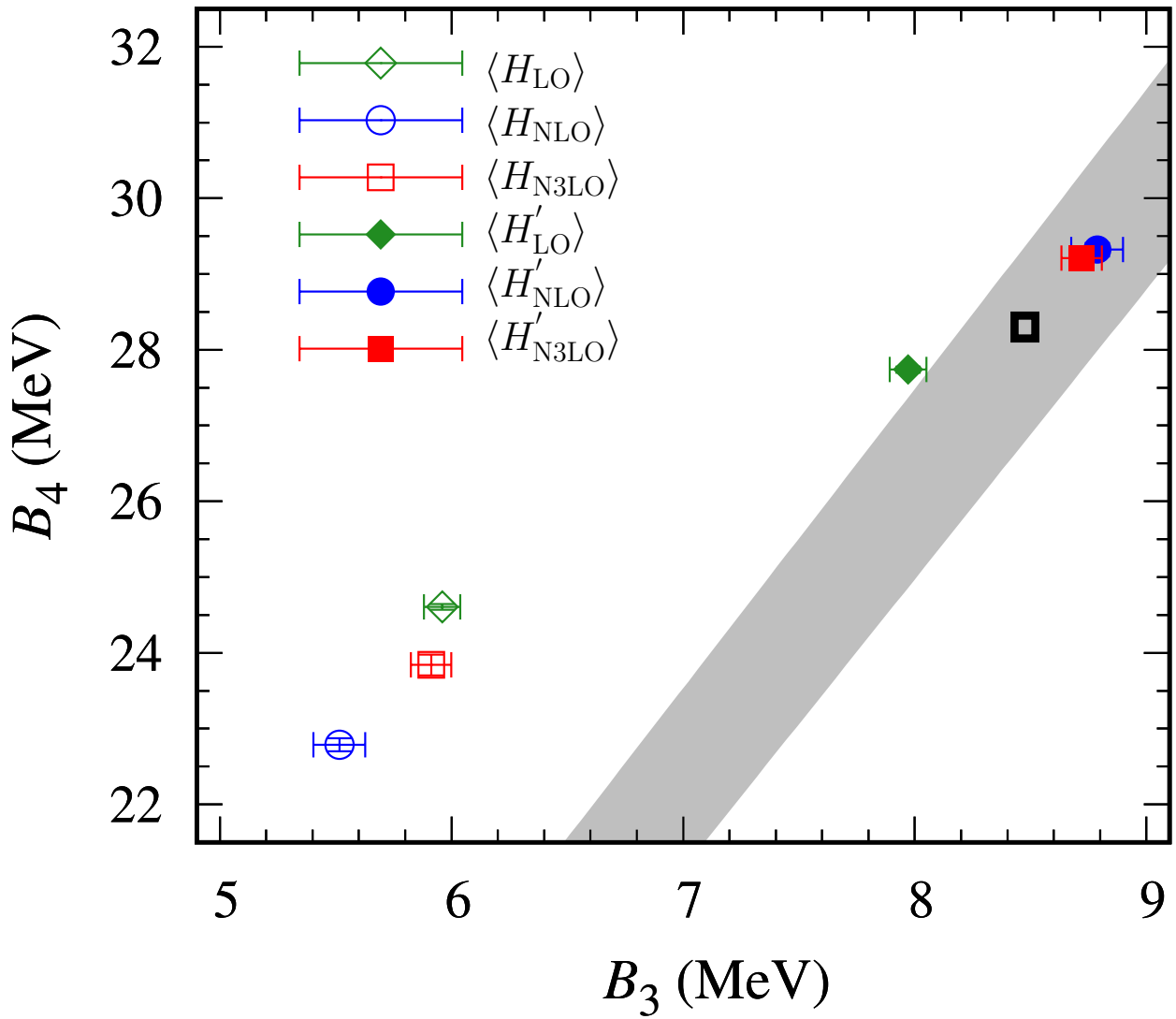


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

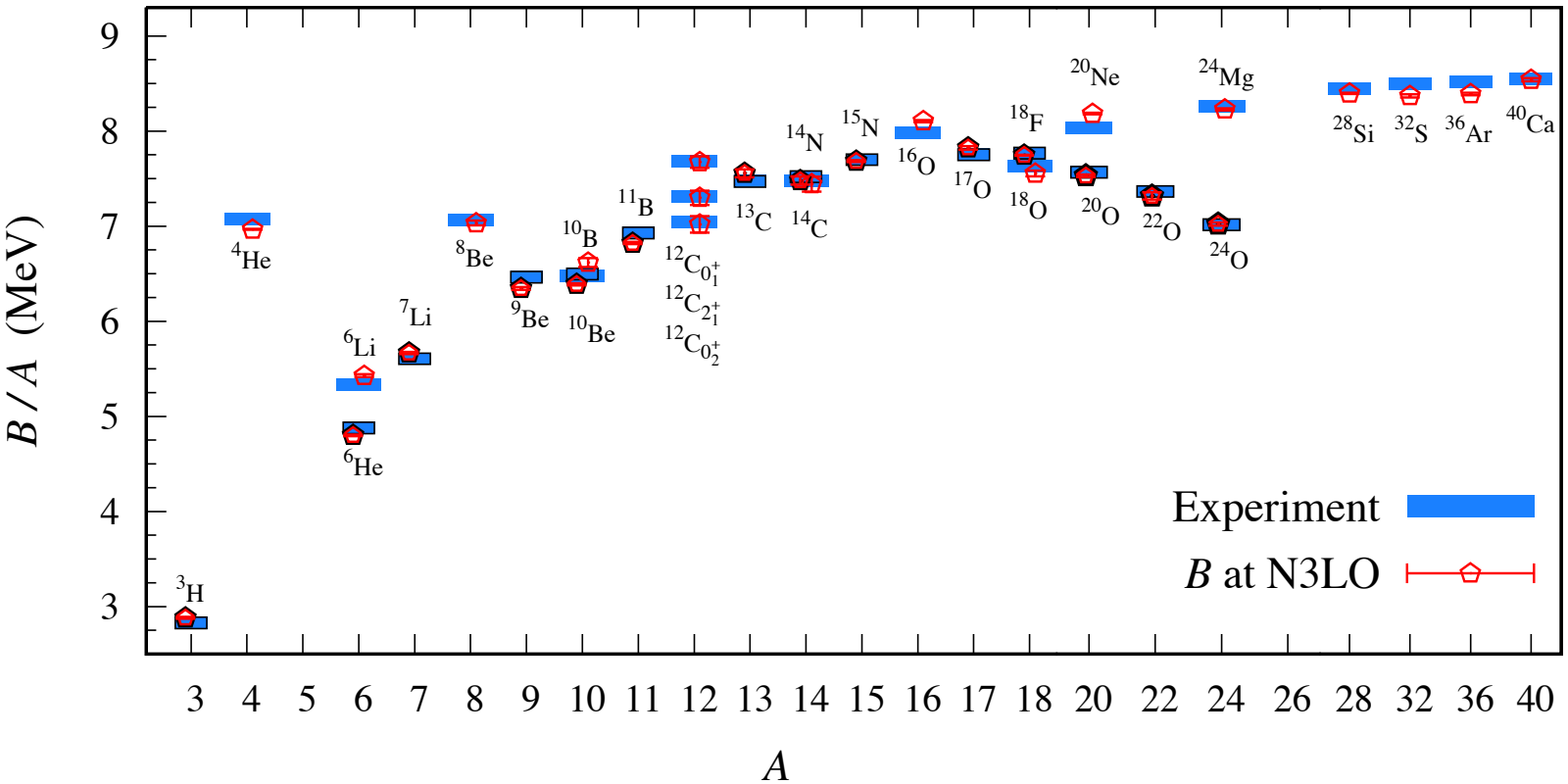
$R = 2.6$ fm

$E_{A,n} = E'_{A,n}$ (MeV)	$\langle\psi_{B,n}\|H_A\|\psi_{B,n}\rangle$ (MeV)	$\langle\psi_{B,n}\|H'_A\|\psi_{B,n}\rangle$ (MeV)
-1.2186	3.0088	-1.1597
0.2196	0.3289	0.2212
0.8523	1.1275	0.8577
1.8610	2.2528	1.8719
3.2279	3.6991	3.2477
4.9454	5.4786	4.9798
7.0104	7.5996	7.0680
9.4208	10.0674	9.5137
12.1721	12.8799	12.3163
15.2669	16.0458	15.4840

Tjon line

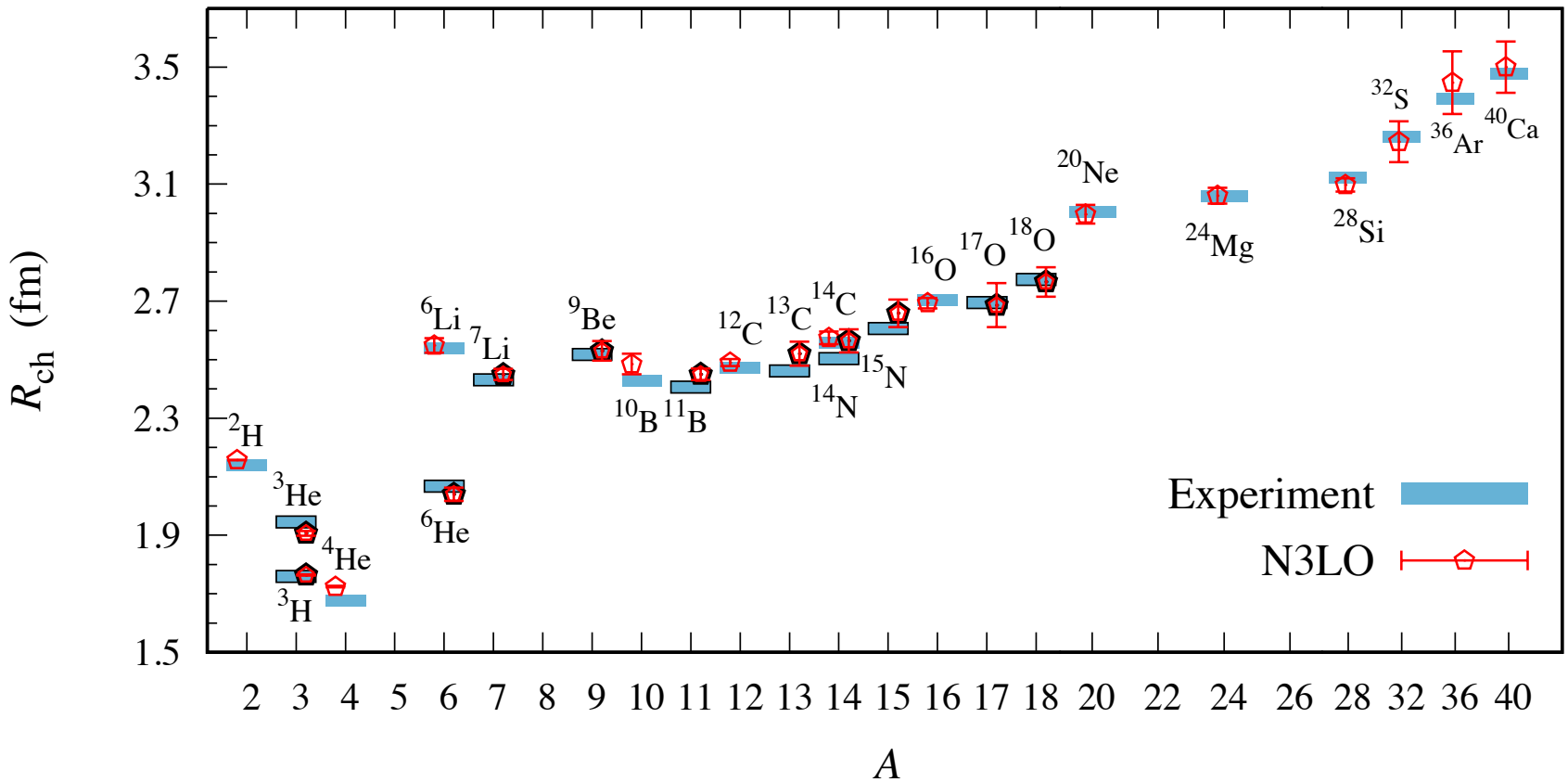

$\langle H_{\rm LO} \rangle$
$\langle H_{\rm NLO} \rangle$
$\langle H_{\rm N3LO} \rangle$
$\langle H'_{\rm LO} \rangle$
$\langle H'_{\rm NLO} \rangle$
$\langle H'_{\rm N3LO} \rangle$
32
30
28
26
24
22
B_4 (MeV)
5
6
7
8
9
B_3 (MeV)

Binding energy per nucleon

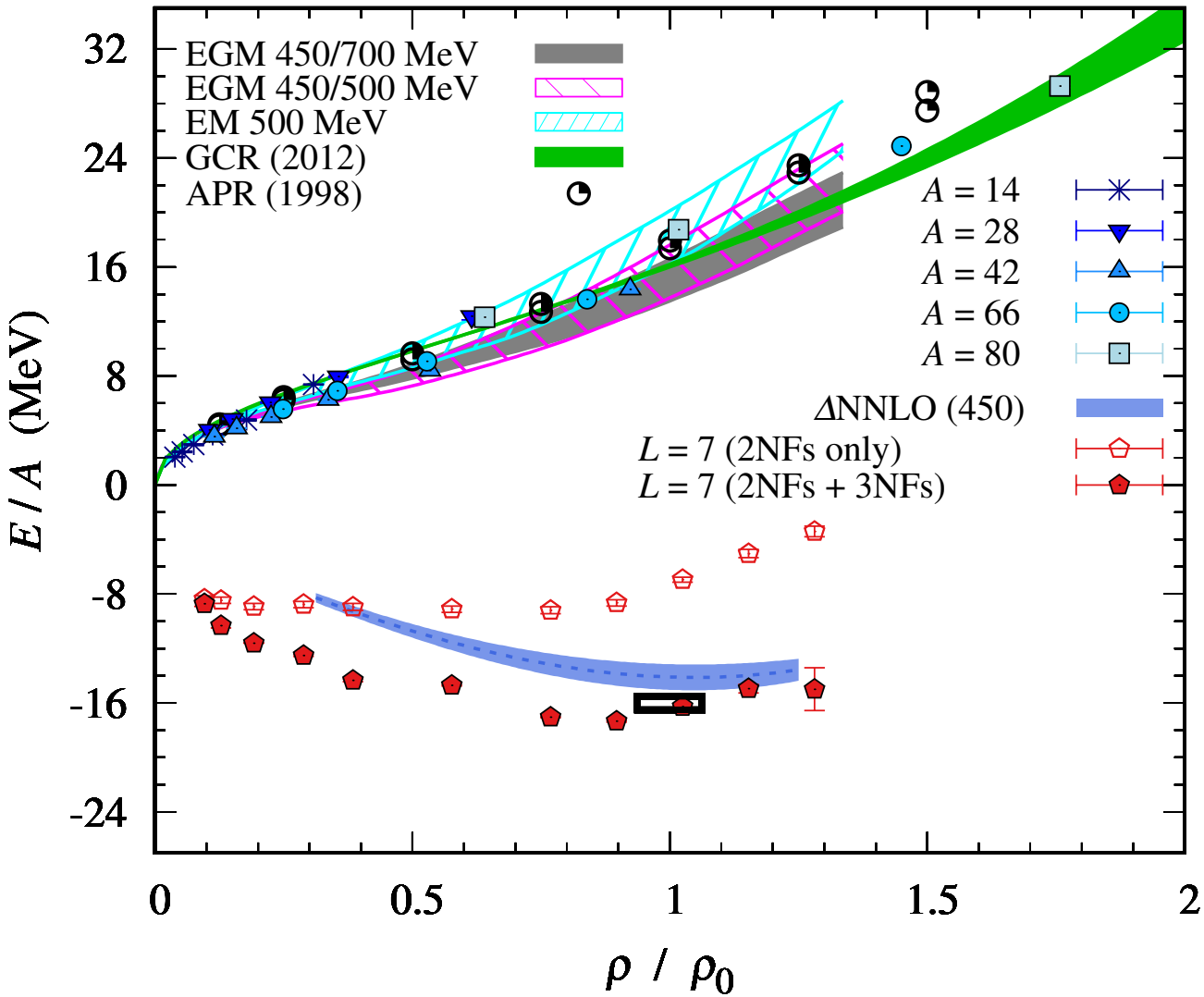


Work in progress: Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin

Charge radius



Work in progress: Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin



Work in progress: Elhatisari, Bovermann, et al.

Summary

We started with an introduction to lattice effective field theory. We then discussed alpha-alpha scattering using the adiabatic projection method and showed that nuclear physics is close to a quantum phase transition. We then introduced the pinhole algorithm for determining probability distributions of nucleons in position space with full correlations and discussed nuclear structure, alpha clustering, and the intrinsic structure of the low-lying ^{12}C states. We concluded with a discussion of wave function matching for high-fidelity calculations at N3LO order.