Lattice simulations of nuclear structure

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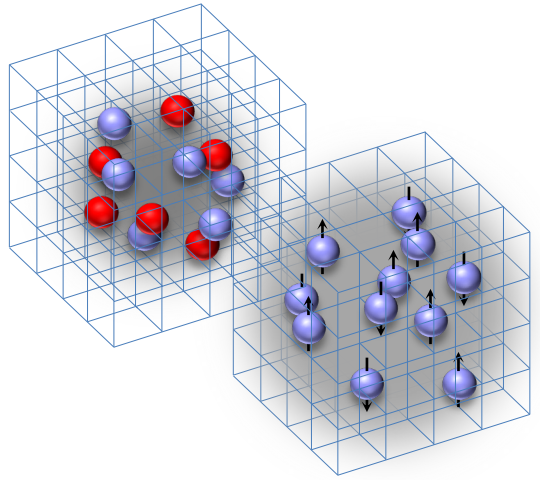
Nuclear physics at the edge of stability
ECT* Trento
July 4, 2022



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MICHIGAN STATE UNIVERSITY

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project

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Outline

Lattice effective field theory

Nuclear physics near a quantum phase transition

Spin-isospin exchange symmetry

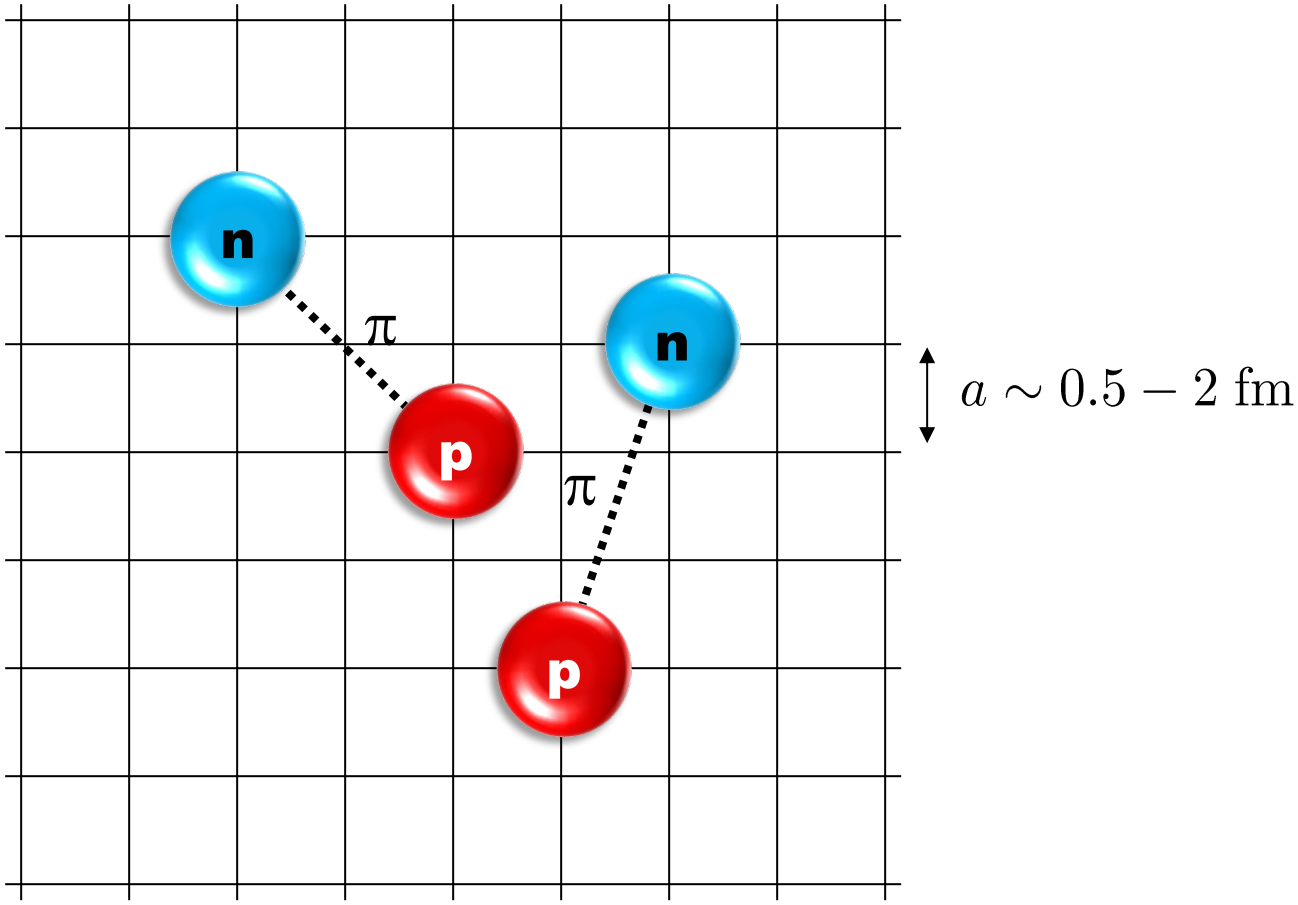
Essential elements for nuclear binding

Structure of the carbon-12 states

Wave function matching

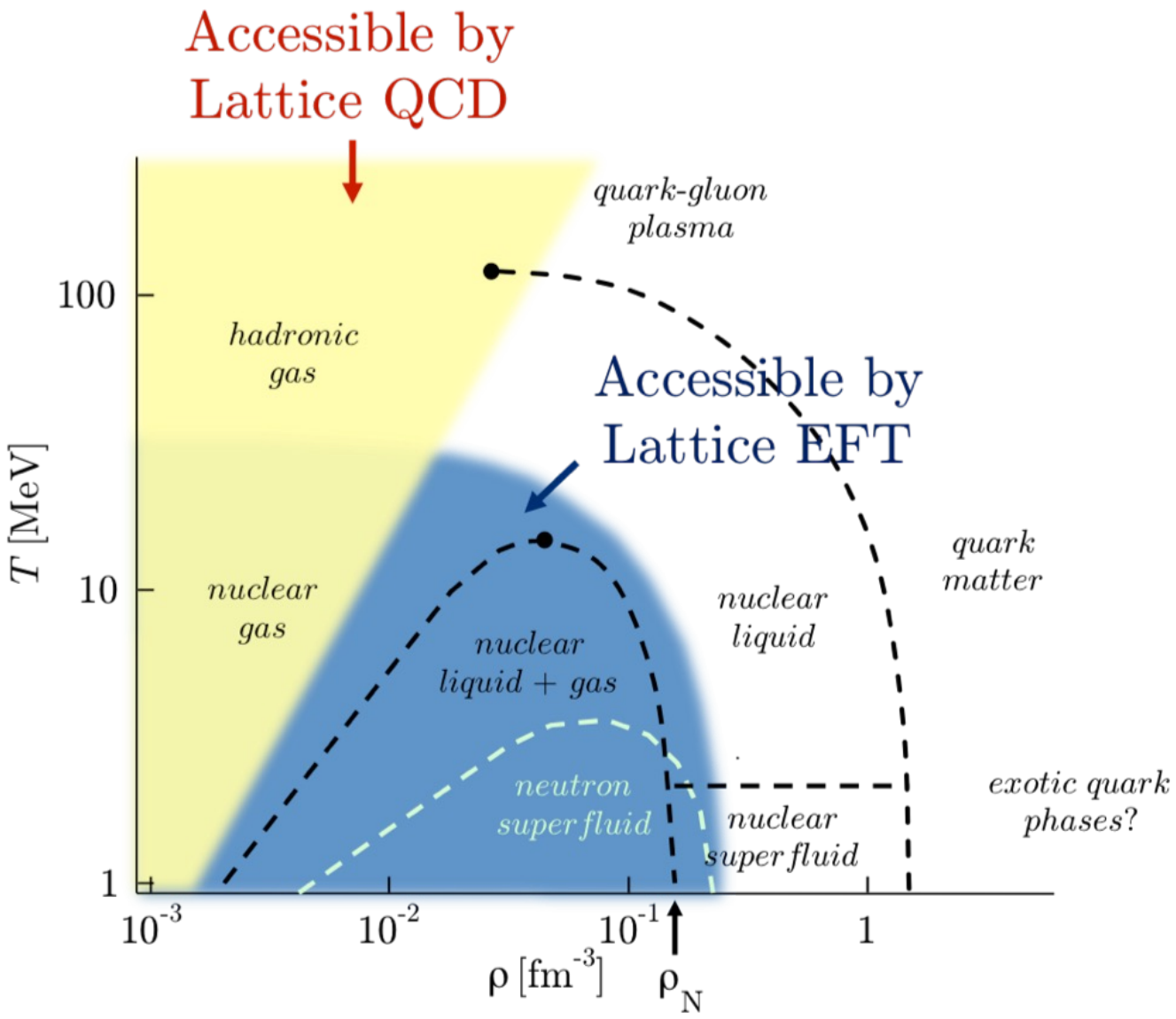
Summary

Lattice effective field theory



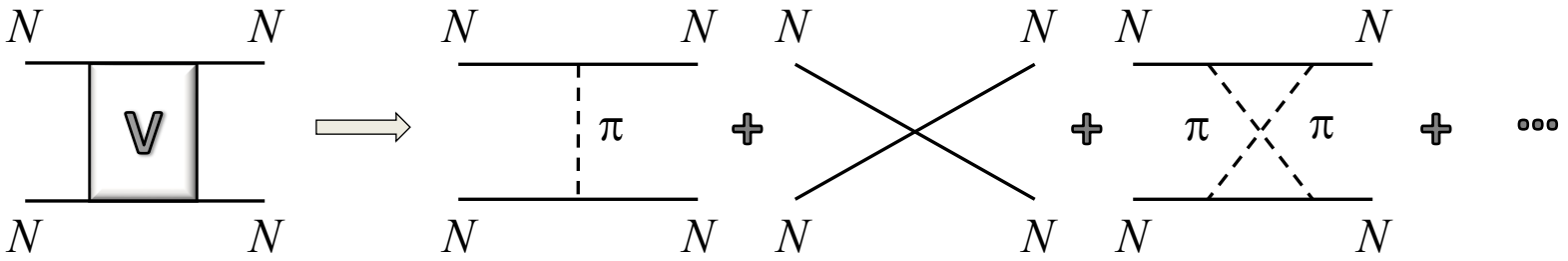
D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer


Accessible by
Lattice QCD
quark-gluon
plasma
hadronic
gas
Accessible by
Lattice EFT
quark
matter
nuclear
gas
nuclear
liquid
nuclear
liquid + gas
neutron
superfluid
nuclear
superfluid
exotic quark
phases?
100
10
1
T [MeV]
10^-3
10^-2
10^-1
1
ρ [fm^-3]
ρ_N

Chiral effective field theory

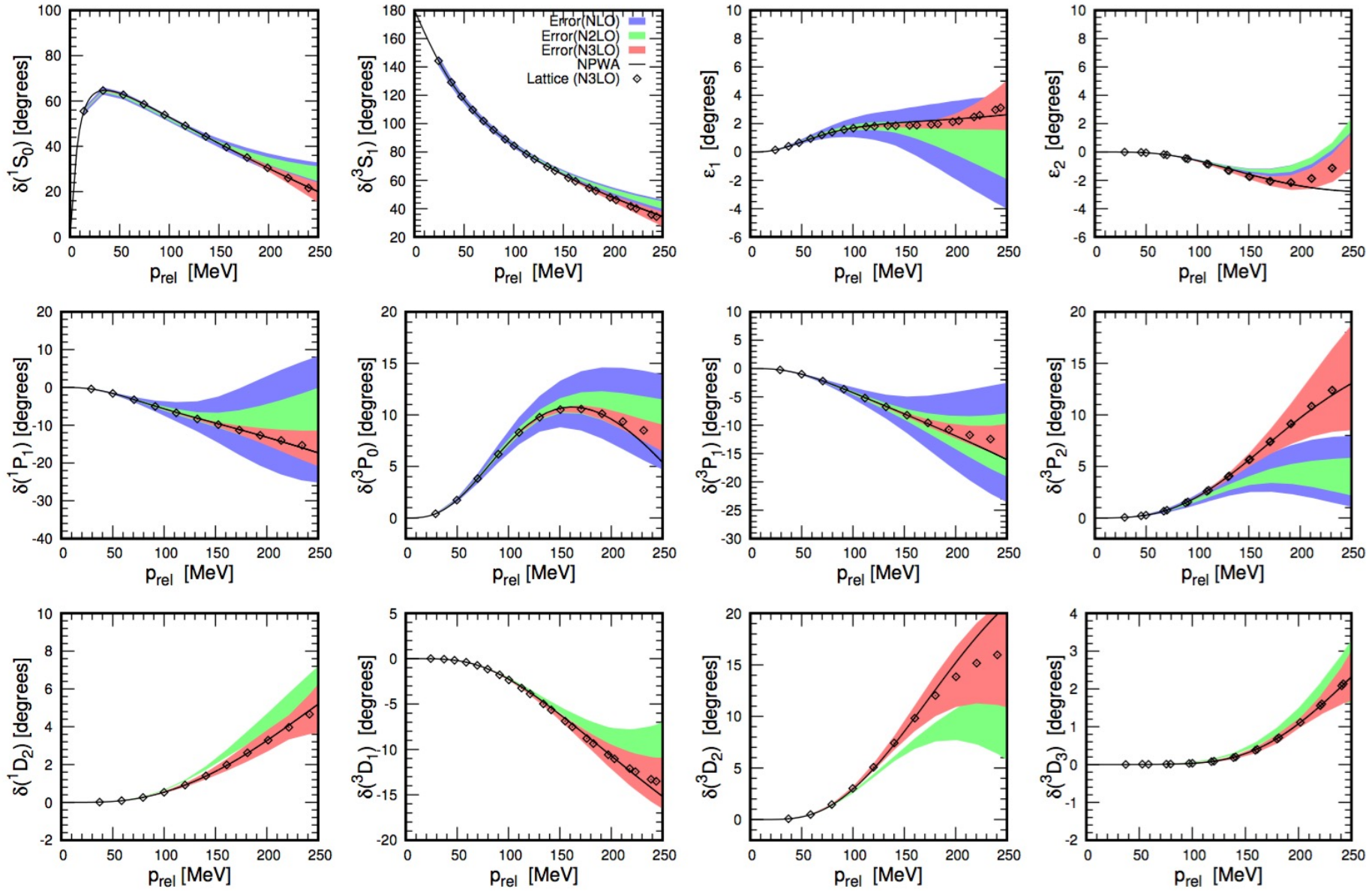
Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

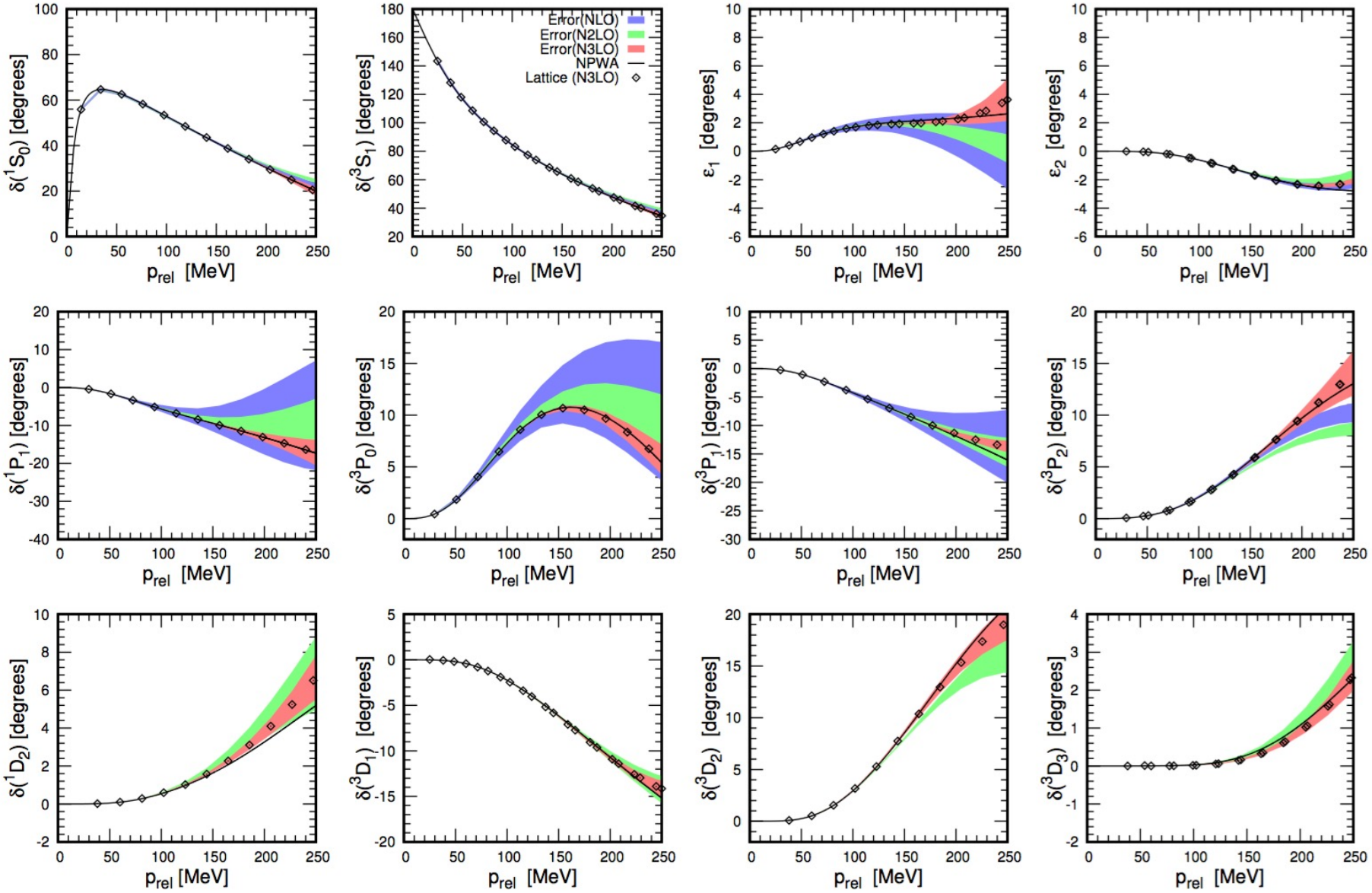
Leading order (LO) Next-to-leading order (NLO)

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



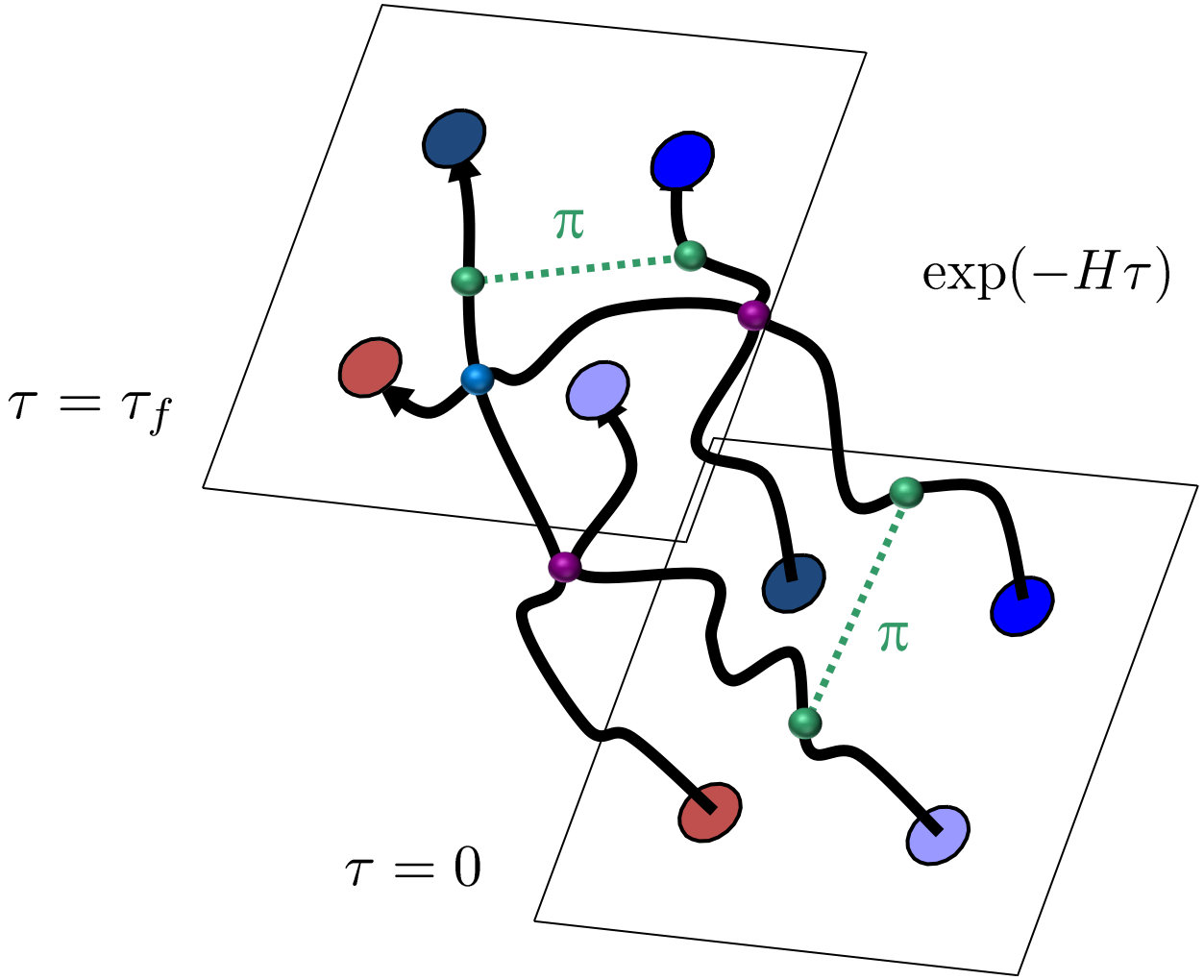
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

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



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

Euclidean time projection



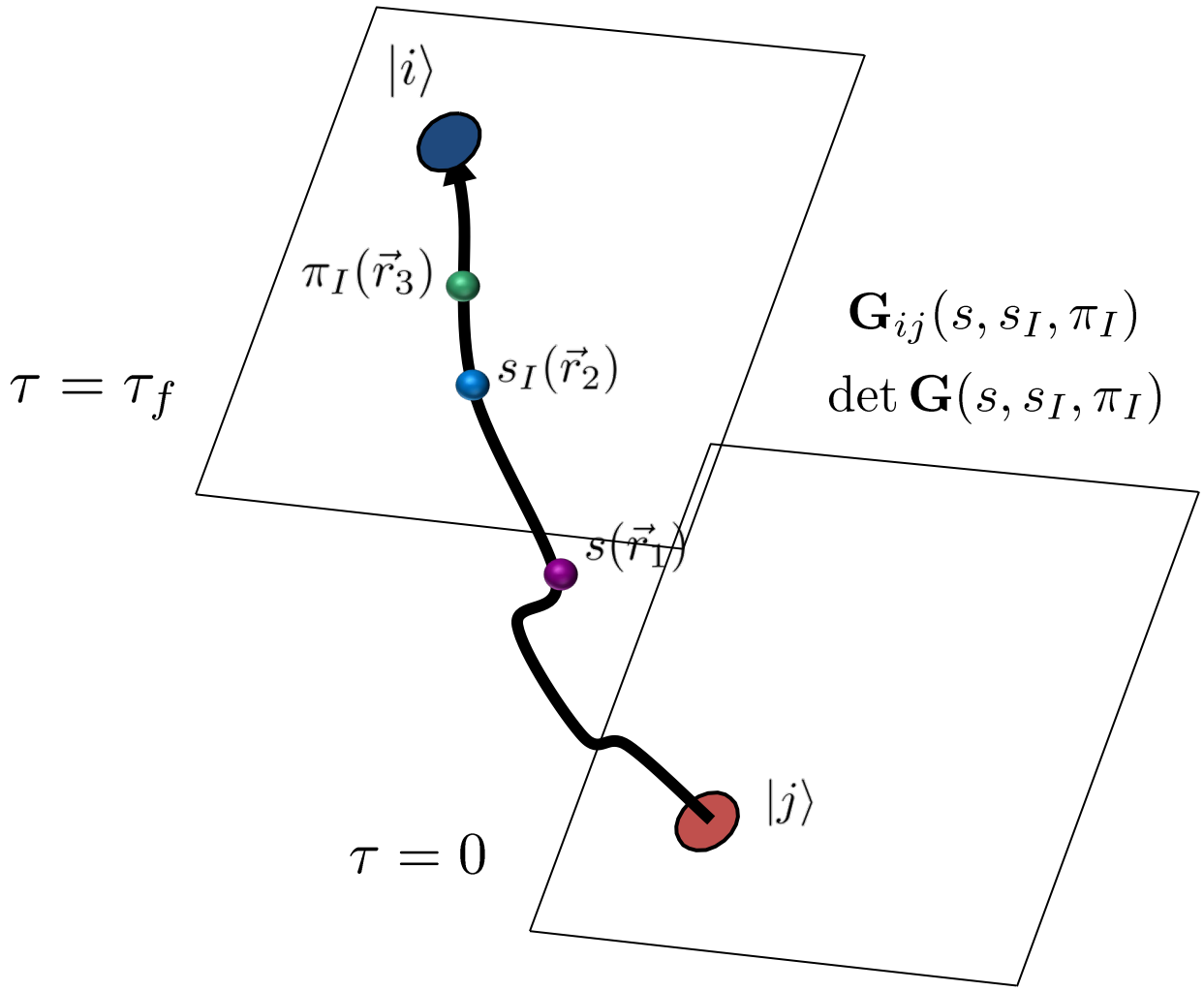
Auxiliary field method

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

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

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

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


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = \tau_f$
$\tau = 0$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{G}(s, s_I, \pi_I)$

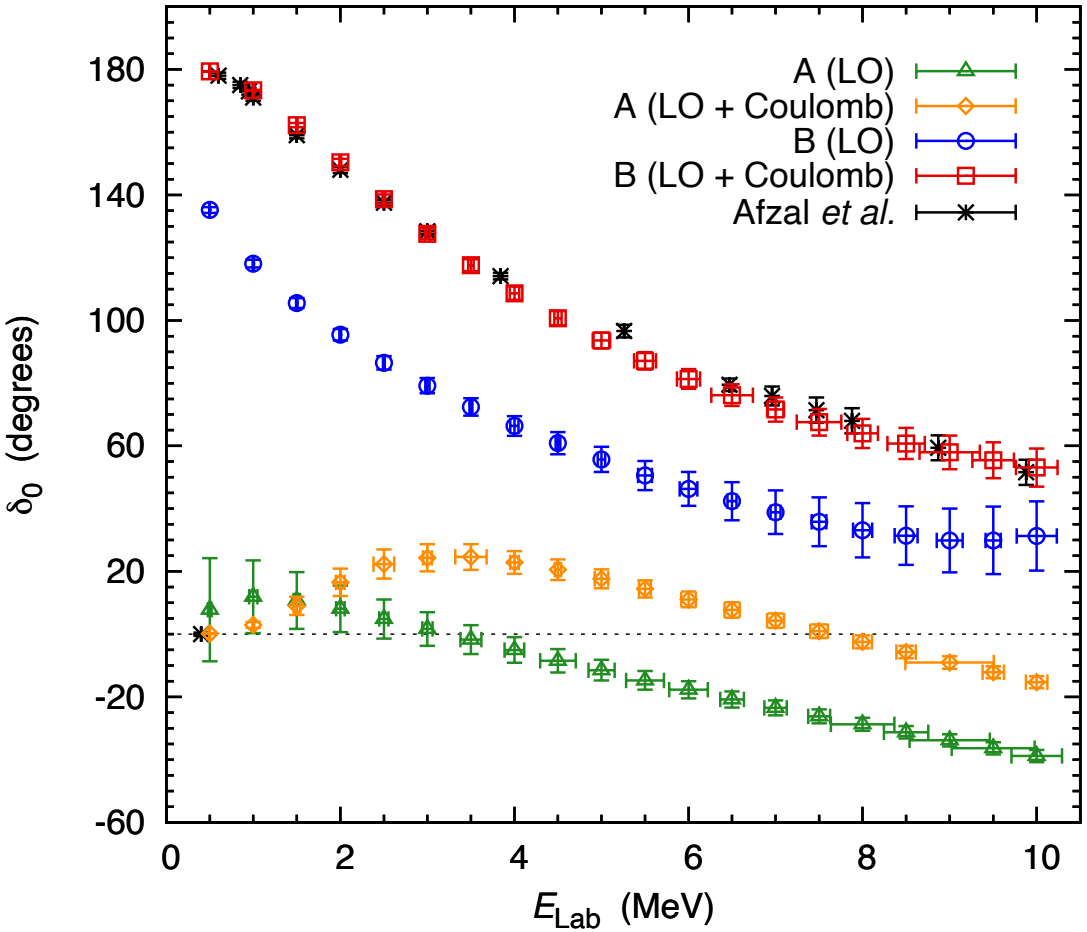
Nuclear physics near a quantum phase transition

We consider two different interactions, A and B, at leading order (LO) in chiral effective field theory. They both have the same one-pion exchange potential and Coulomb potential. The difference between A and B resides with their short-range interactions.

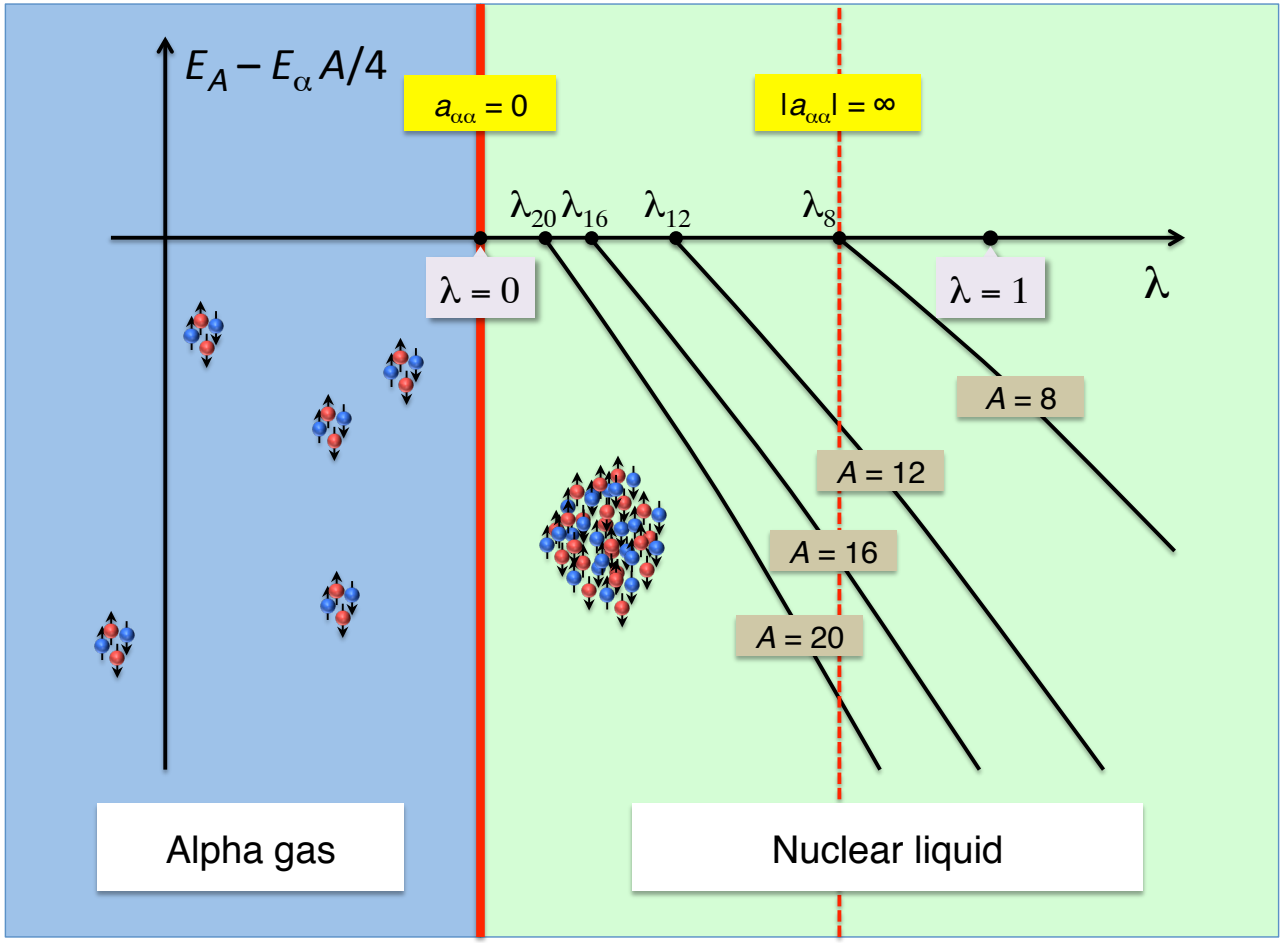
Interaction A	Interaction B
Nonlocal short-range interaction	Nonlocal short-range interaction + Local short-range interaction

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

alpha-alpha S-wave 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)

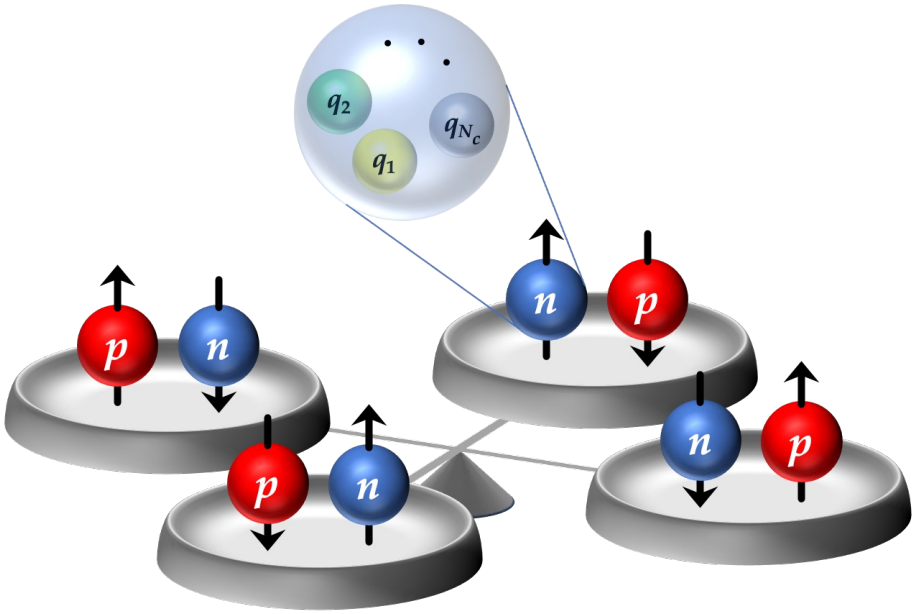
Spin-isospin exchange symmetry

Kaplan, Savage, PLB 365, 244 (1996)

Kaplan, Manohar, PRC 56, 76 (1997)

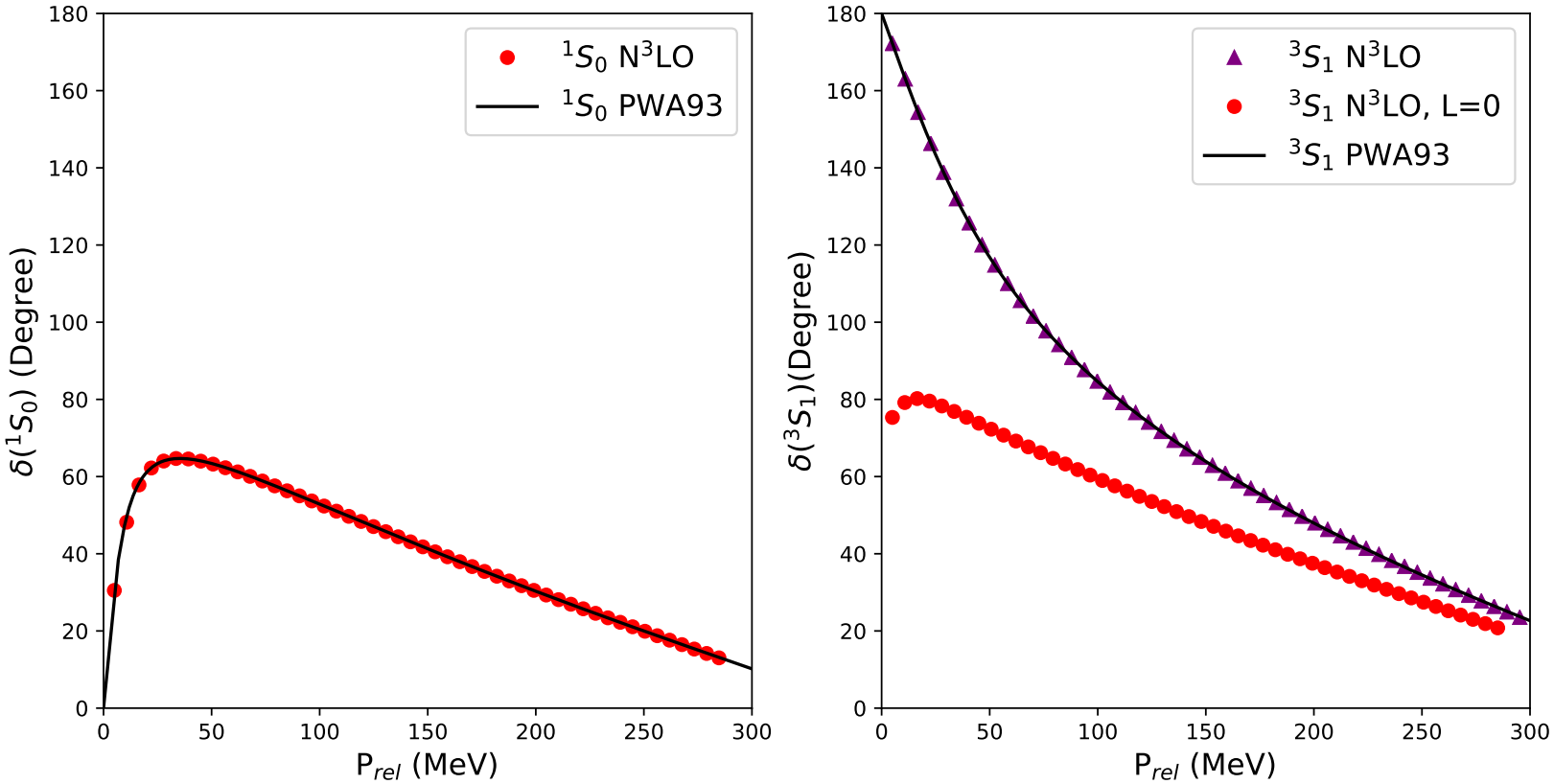
Calle Gordon, Arriola, PRC 80, 014002 (2009)

$$V^{2N}_{\text{large}-N_c} = V_C + \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 W_S + (3\hat{r} \cdot \vec{\sigma}_1 \hat{r} \cdot \vec{\sigma}_2 - \vec{\sigma}_1 \cdot \vec{\sigma}_2)\vec{\tau}_1 \cdot \vec{\tau}_2 W_T$$



D.L., Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, Meißner, PRL 127, 062501 (2021)

$$\Lambda_{\mathrm{large}-N_c} \sim 500 \text{ MeV}$$



D.L., Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, Meißner, PRL 127, 062501 (2021)

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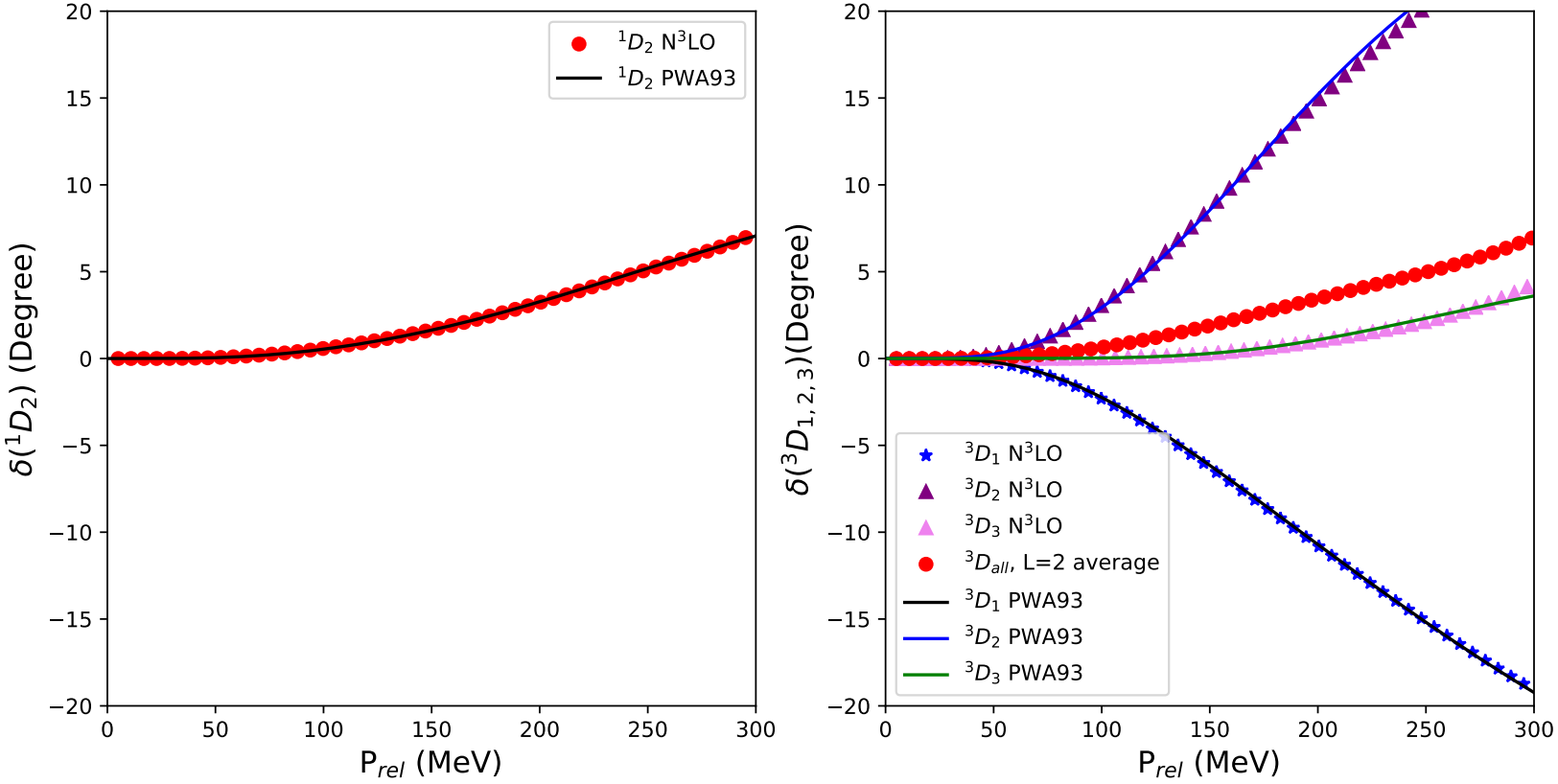


D.L., Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, Meißner, PRL 127, 062501 (2021)

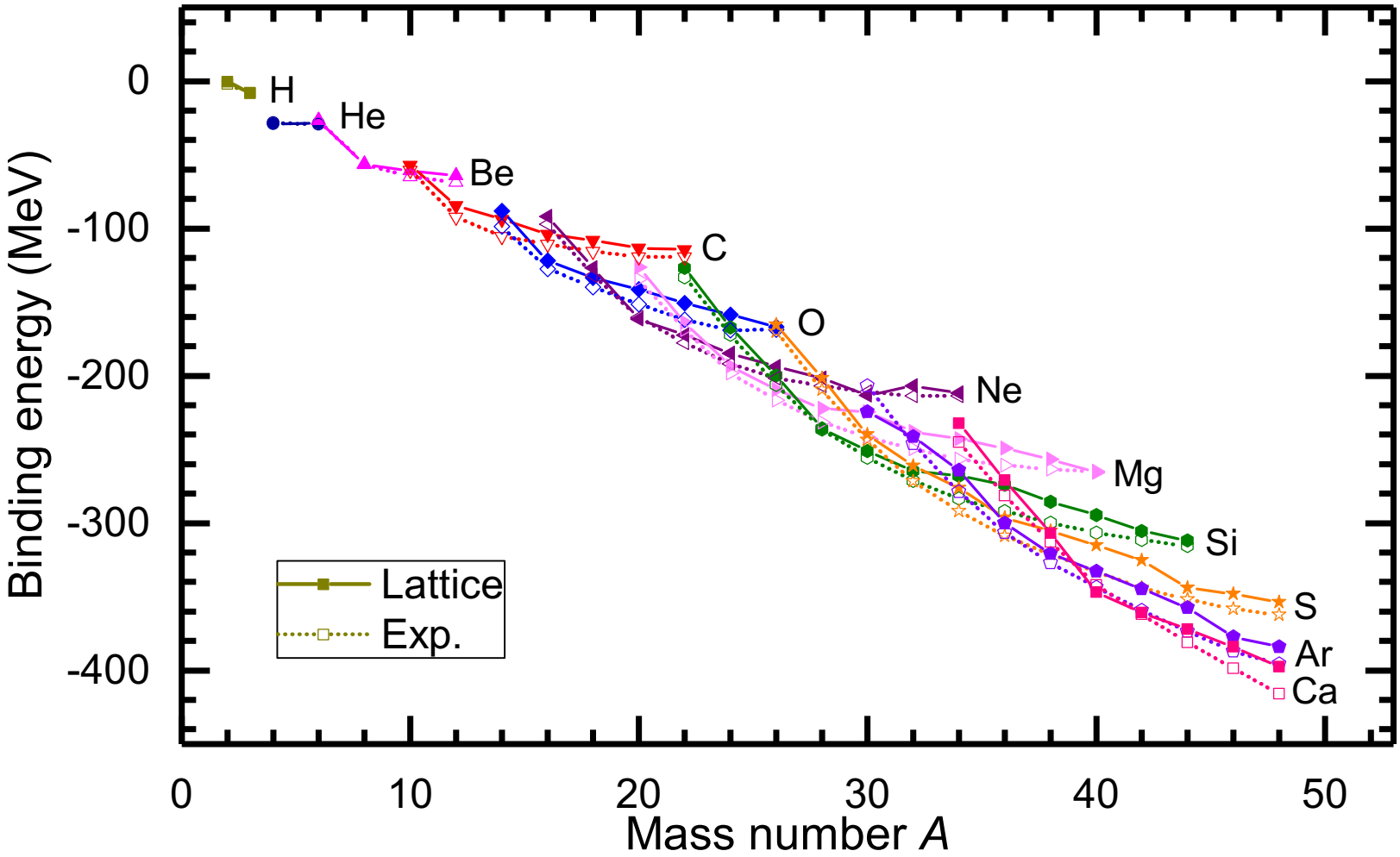
Essential elements for nuclear binding

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

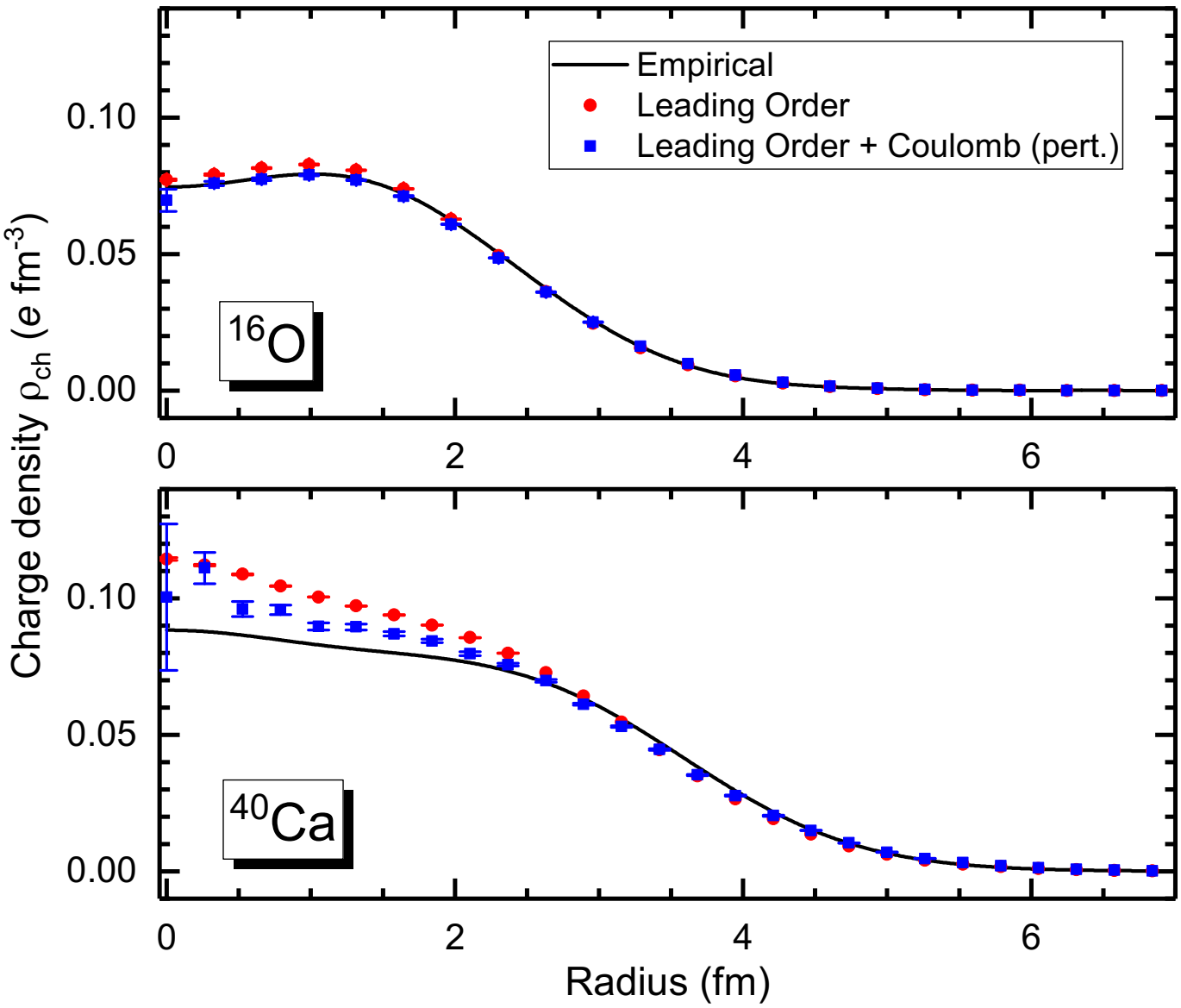
Except for the Coulomb potential, the interaction is invariant under Wigner's SU(4) symmetry.



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

	B	Exp.	$R_{\rm ch}$	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

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

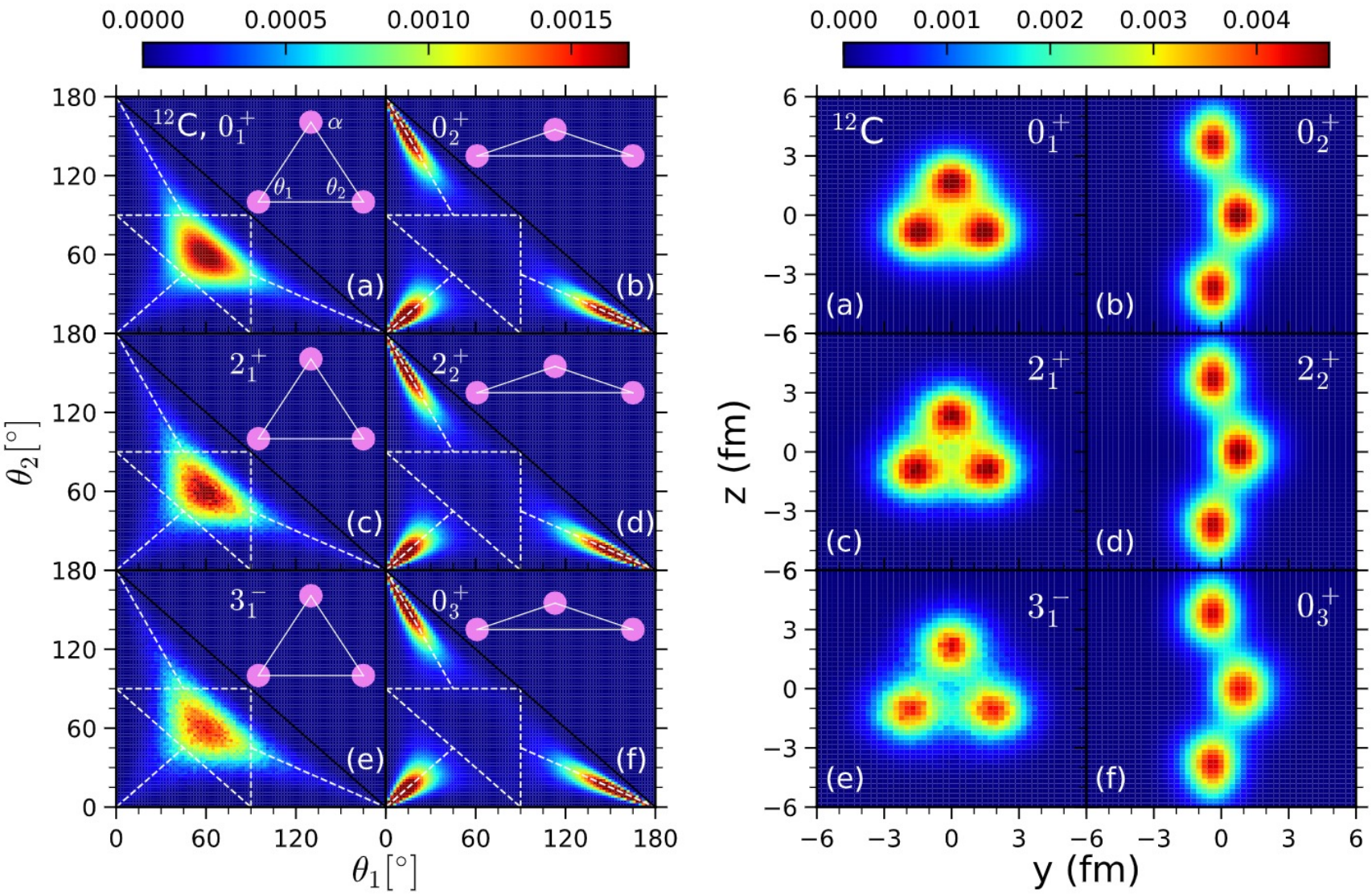


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

Structure and spectrum of ^{12}C

Shen, Lähde, D.L. Meißner, EPJA 57, 276 (2021)

State	$a = 1.97$ fm	$a = 1.64$ fm	Experiment
0_1^+	$-92.15(3)$	$-92.12(4)$	-92.162
2_1^+	$-88.87(4)$	$-88.19(17)$	-87.722
0_2^+	$-85.20(15)$	$-85.23(22)$	-84.508
3_1^-	$-84.9(2)$	$-83.3(5)$	$-82.521(5)$
2_2^+	$-83.5(2)$	$-83.1(5)$	$-82.29(6)$
0_3^+	$-80.0(3)$	$-79.2(6)$	$-81.9(3)$
1_1^-	$-81.5(4)$	$-79.7(4)$	$-81.315(4)$
2_1^-	$-78.6(2)$	$-76.1(2)$	$-80.326(4)$
1_1^+	$-79.67(11)$	$-78.14(24)$	$-79.452(6)$
4_1^-	$-78.1(2)$	$-75.5(5)$	$-78.846(20)$
4_1^+	$-80.99(11)$	$-79.1(6)$	$-78.083(5)$
2_3^+	$-79.9(4)$	$-77.9(2)$	-76.056
0_4^+	$-79.25(11)$	$-76.94(18)$	-74.402



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

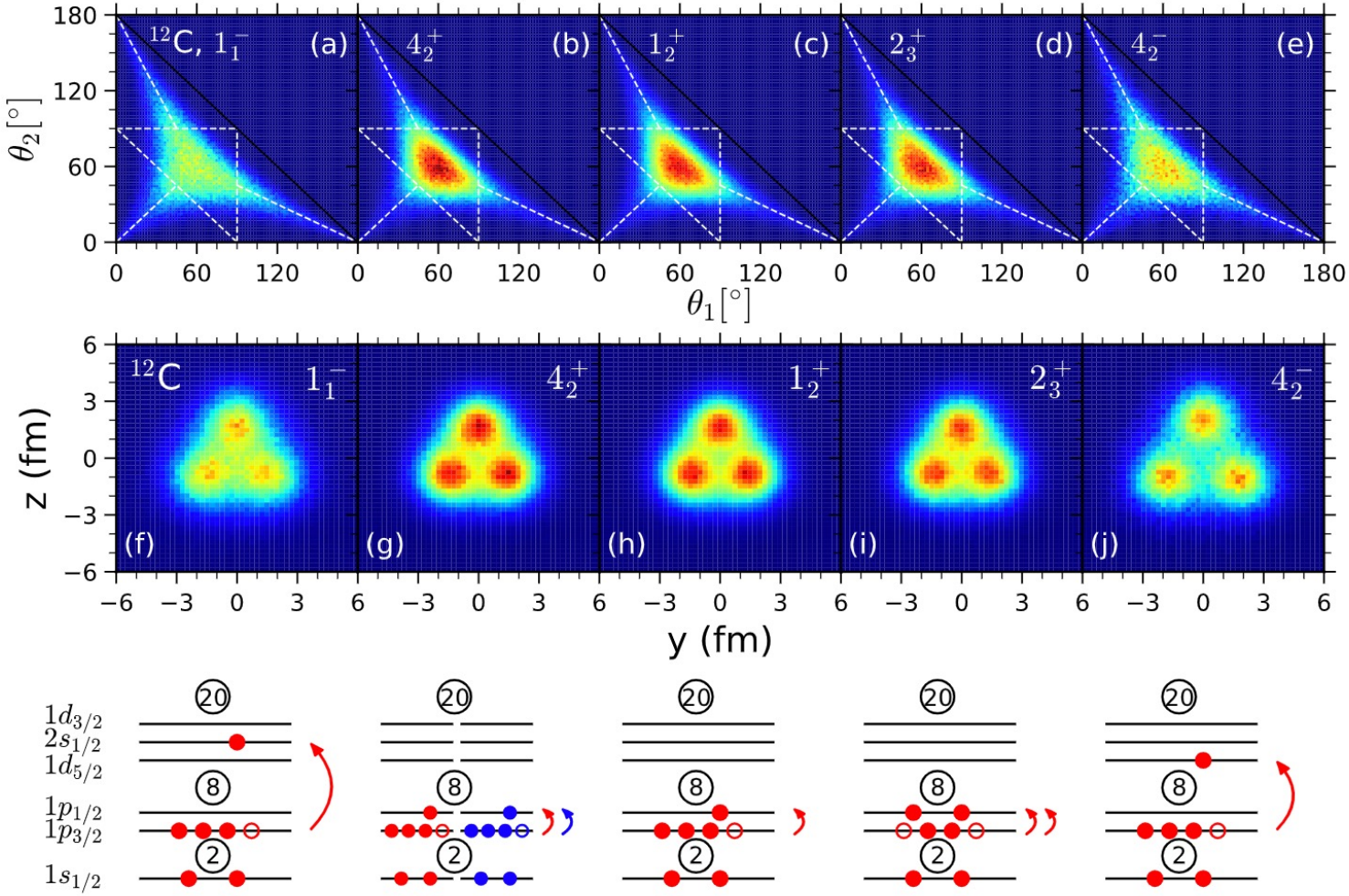


Figure S3: **Top Panel:** Density distribution for the two inner angles of the triangle formed by the three alpha clusters. **Middle Panel:** Tomographic projection of the nuclear density. **Lower Panel:** Sketch of the orbitals for the shell model initial states used in each of these calculations.

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

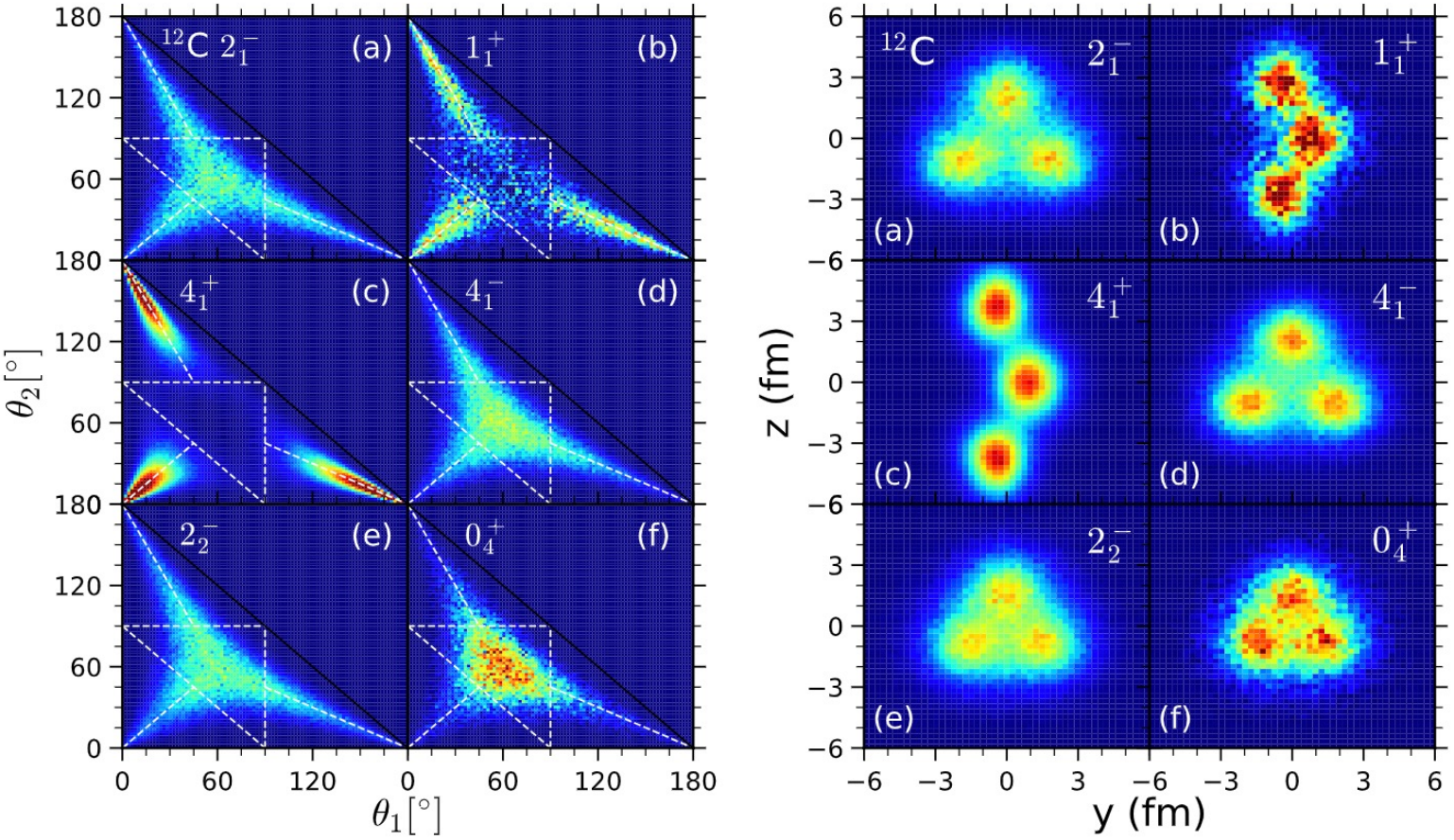
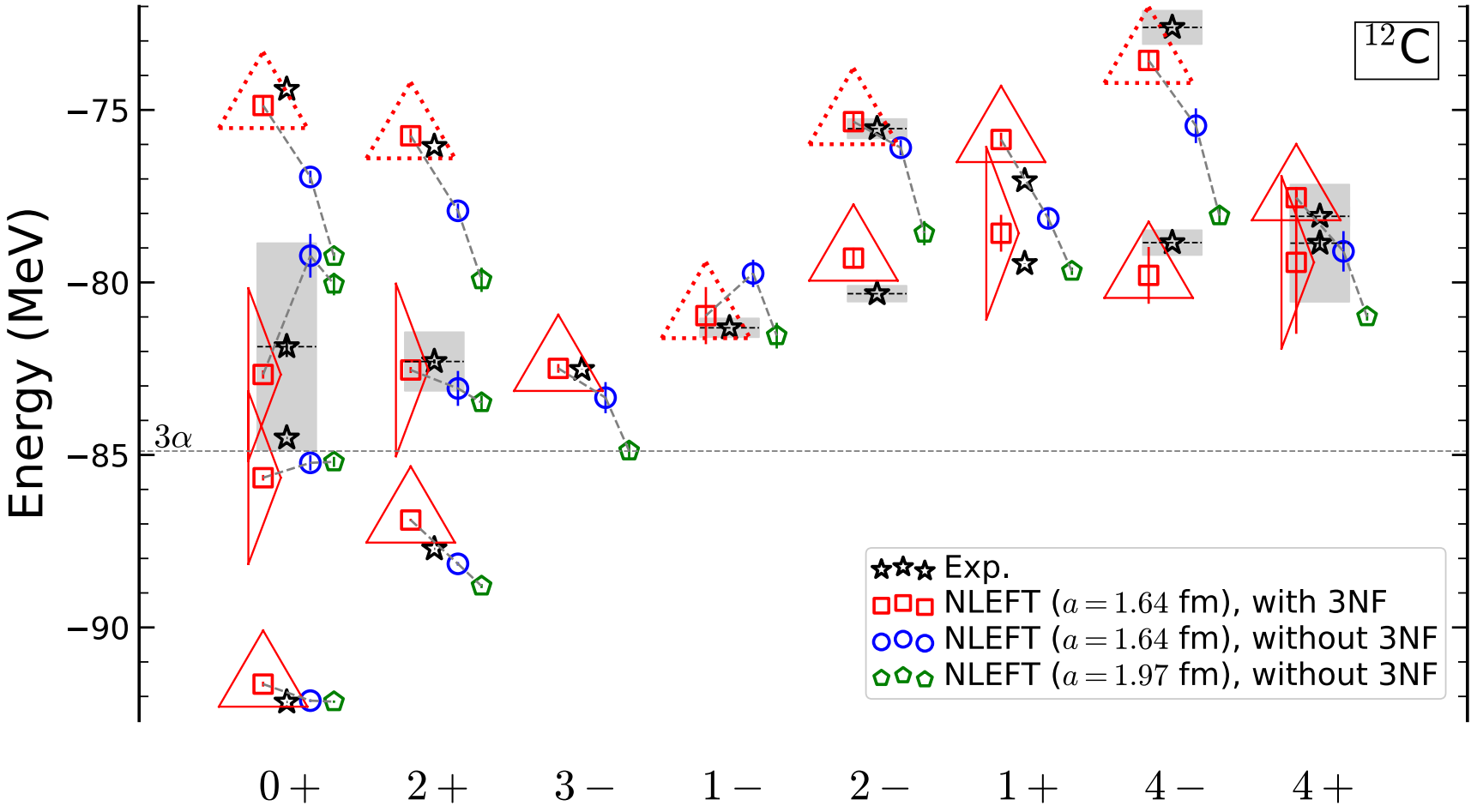


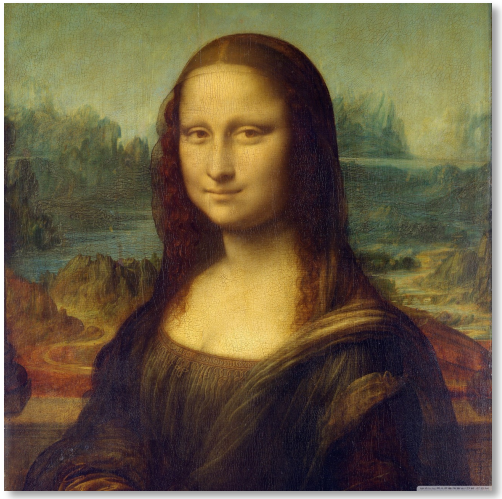
Figure S4: **Left Panel:** Density distribution for the two inner angles of the triangle formed by the three alpha clusters. **Right Panel:** Tomographic projection of the nuclear density. From (a) to (f), the selected states are ordered by their energies from low to high.

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



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

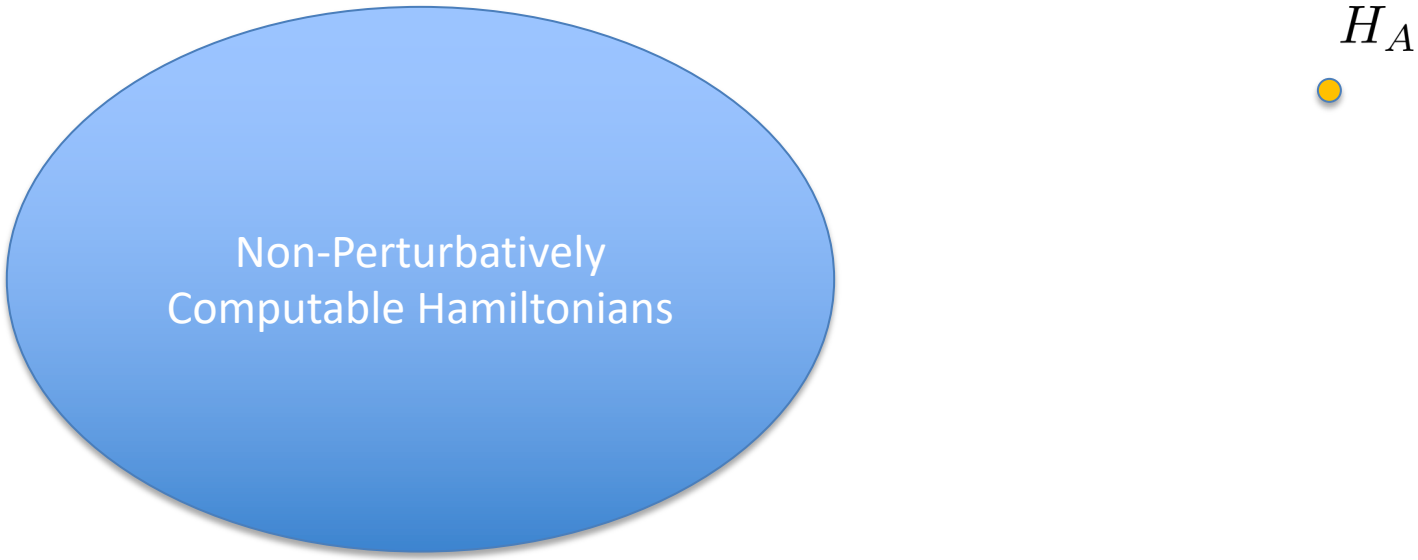
Wave function matching

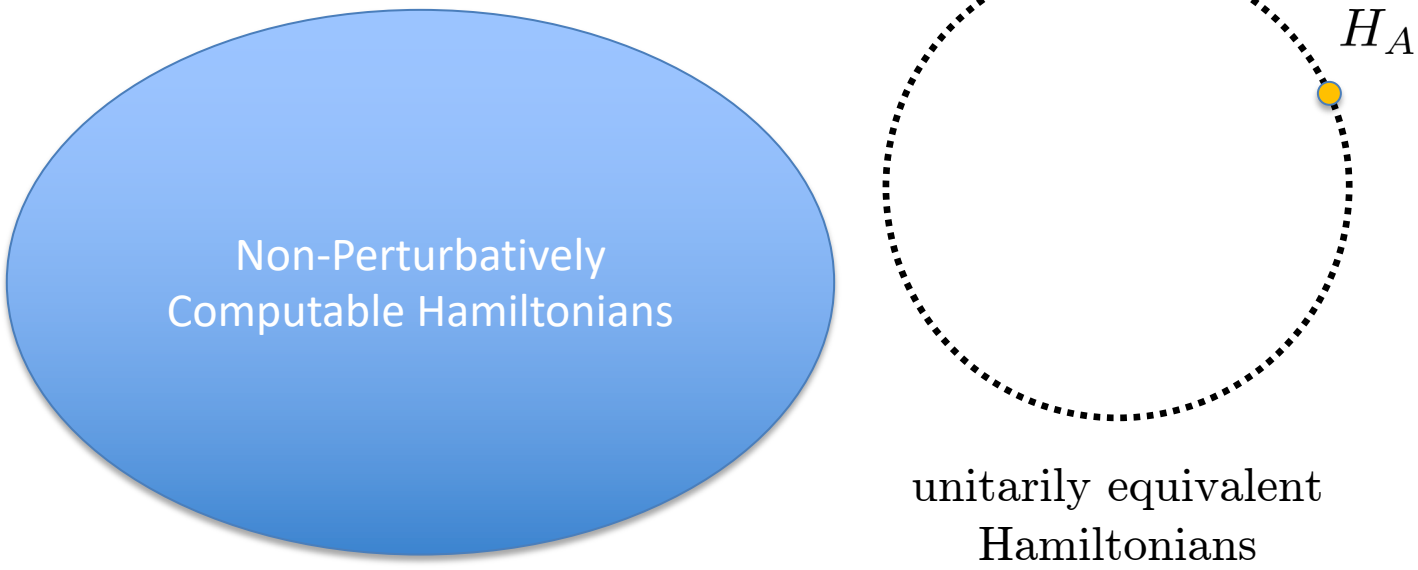


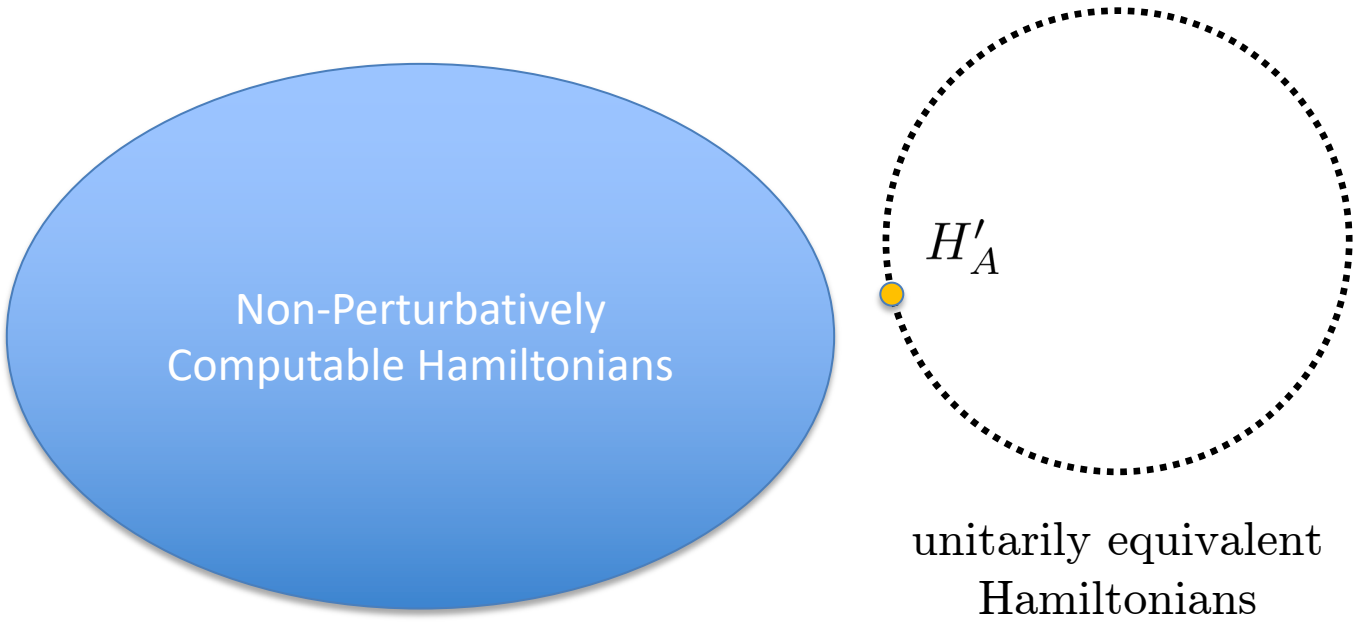
Work in progress: Elhatisari, Bovermann, et al.

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.

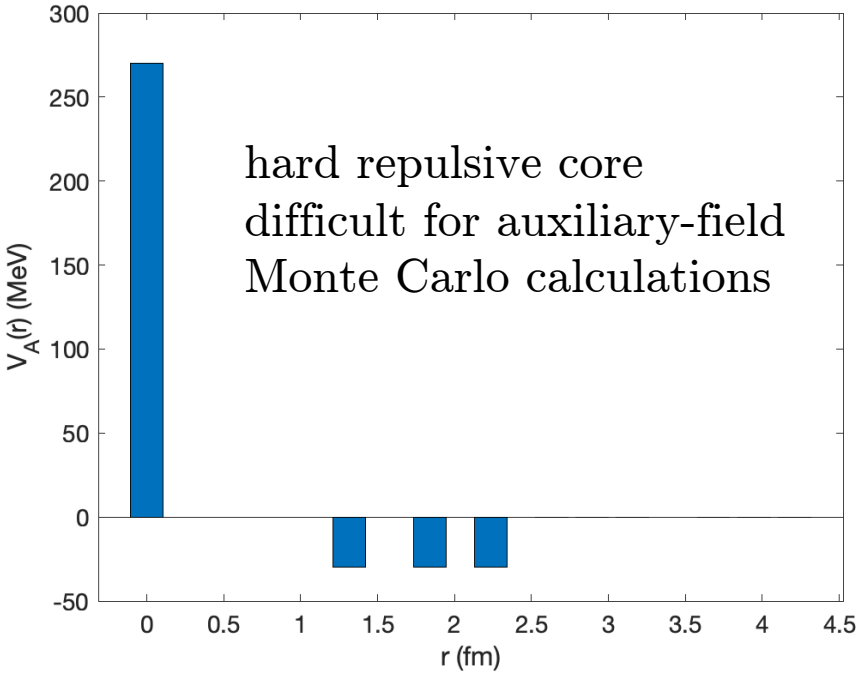

Non-Perturbatively
Computable Hamiltonians
H_A


Non-Perturbatively
Computable Hamiltonians
H_A
unitarily equivalent
Hamiltonians

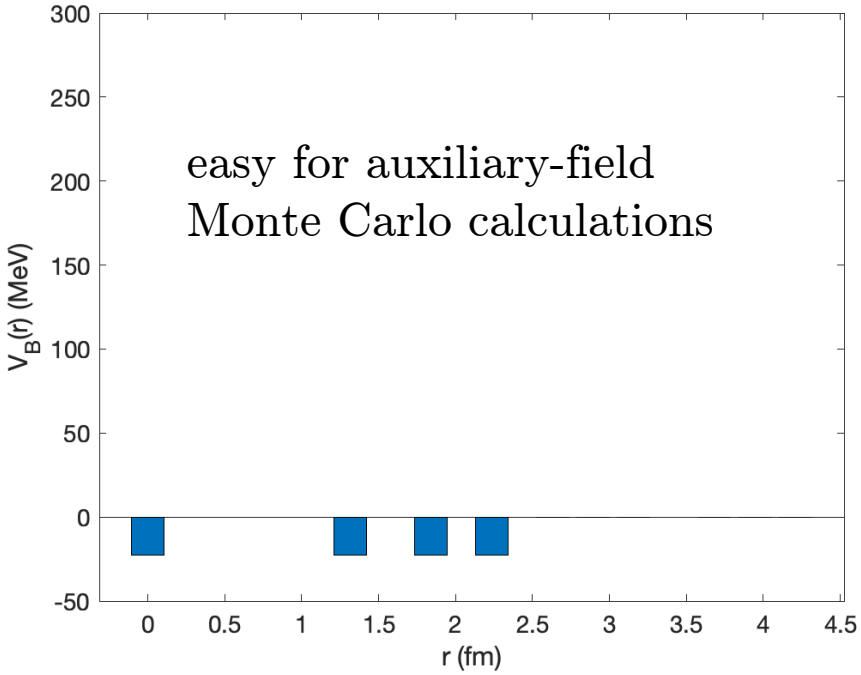

Non-Perturbatively
Computable Hamiltonians
H'_A
unitarily equivalent
Hamiltonians

Wave function matching

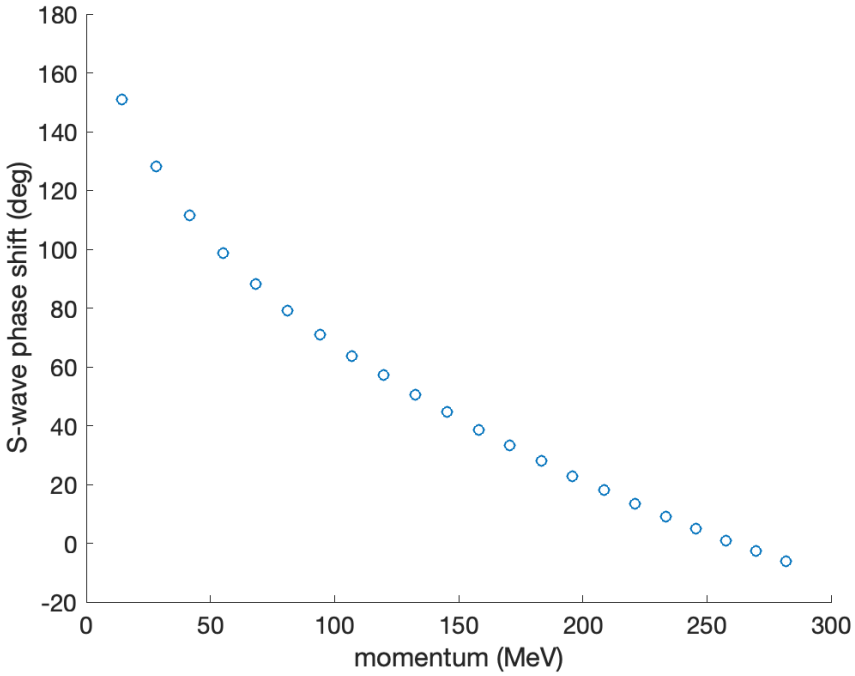
$V_A(r)$



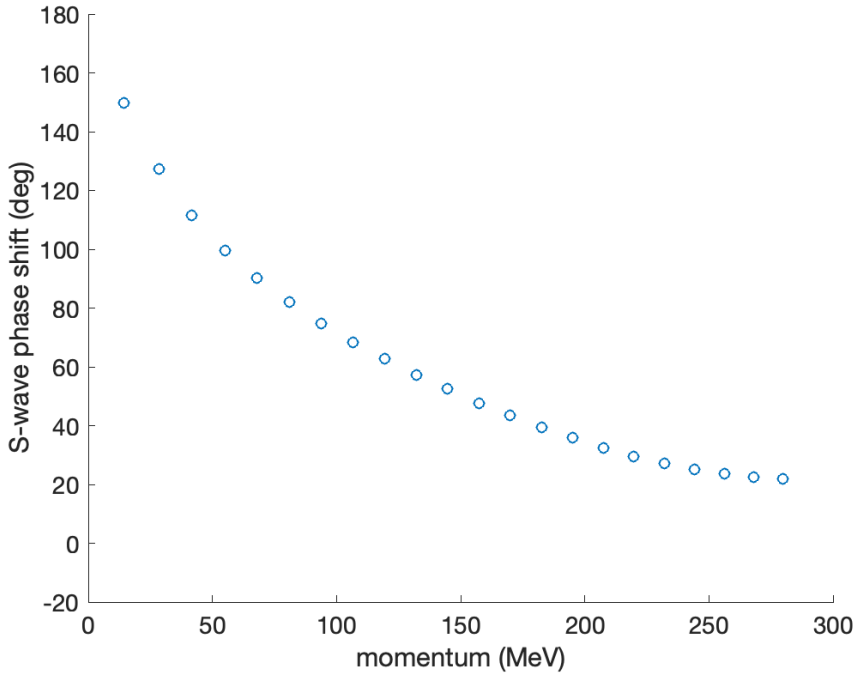
$V_B(r)$



$V_A(r)$


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

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

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

$$U : P\,|\psi_A^0\rangle\,/\|P\,|\psi_A^0\rangle\,\| \rightarrow P\,|\psi_B^0\rangle\,/\|P\,|\psi_B^0\rangle\,\|$$

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

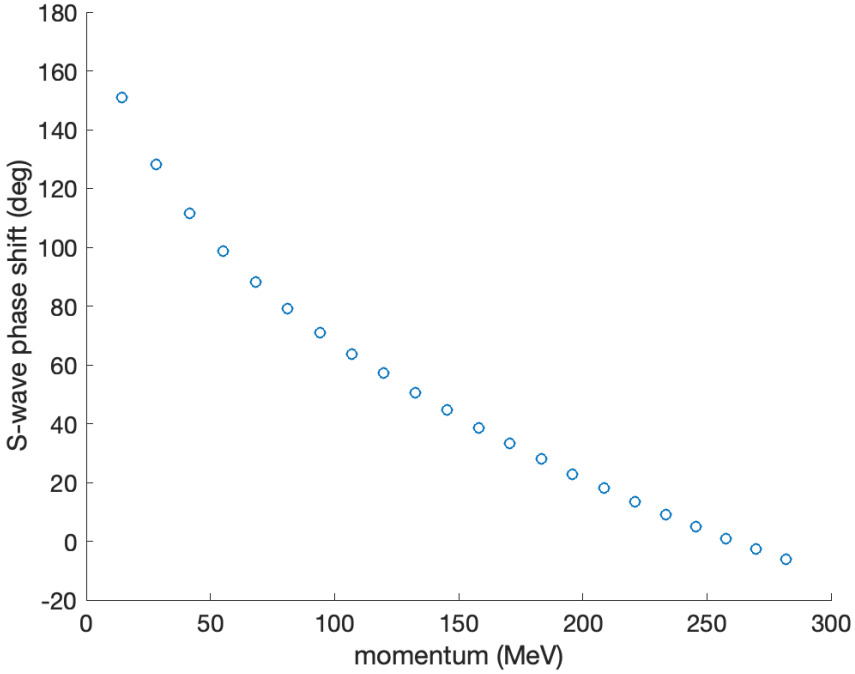
$$U : H_A \rightarrow H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

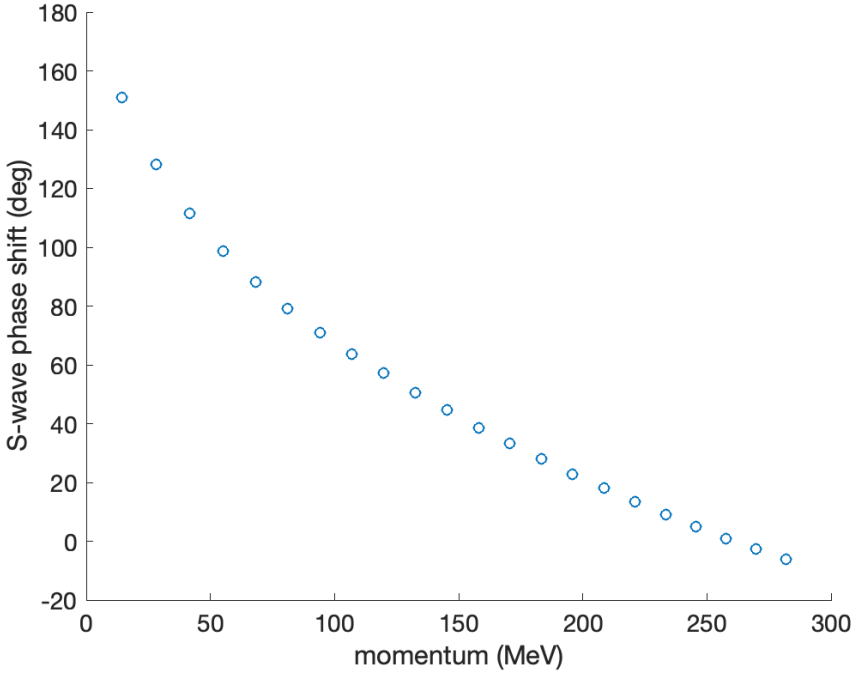
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

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

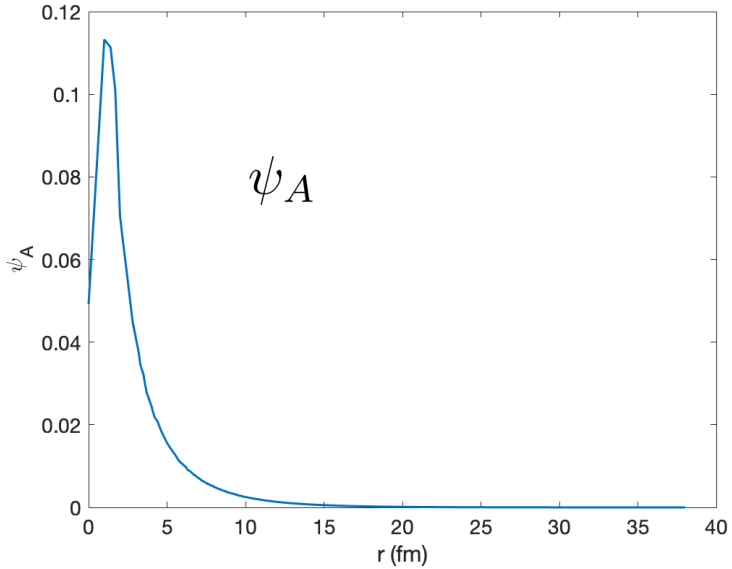
$V_A(r)$

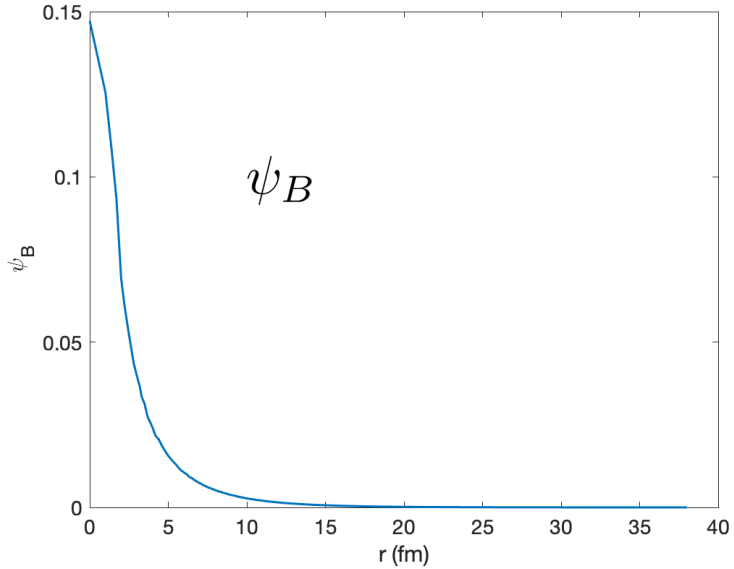


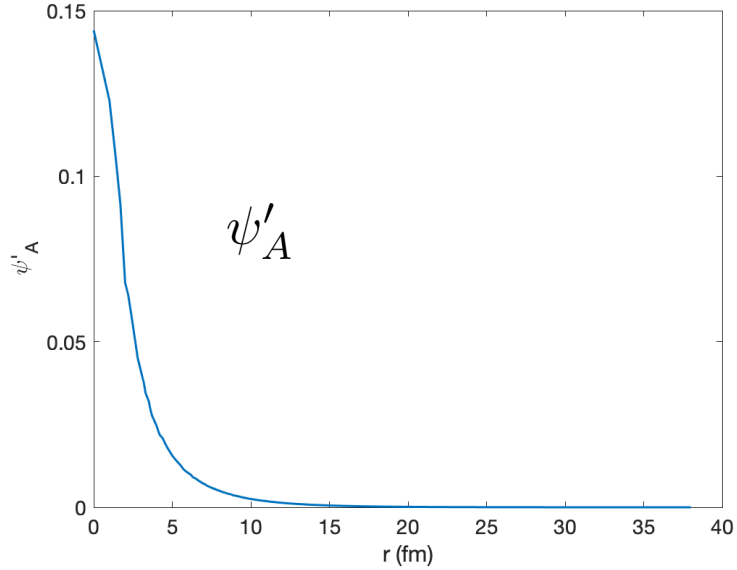
$V'_A(r, r')$



Ground state wave functions





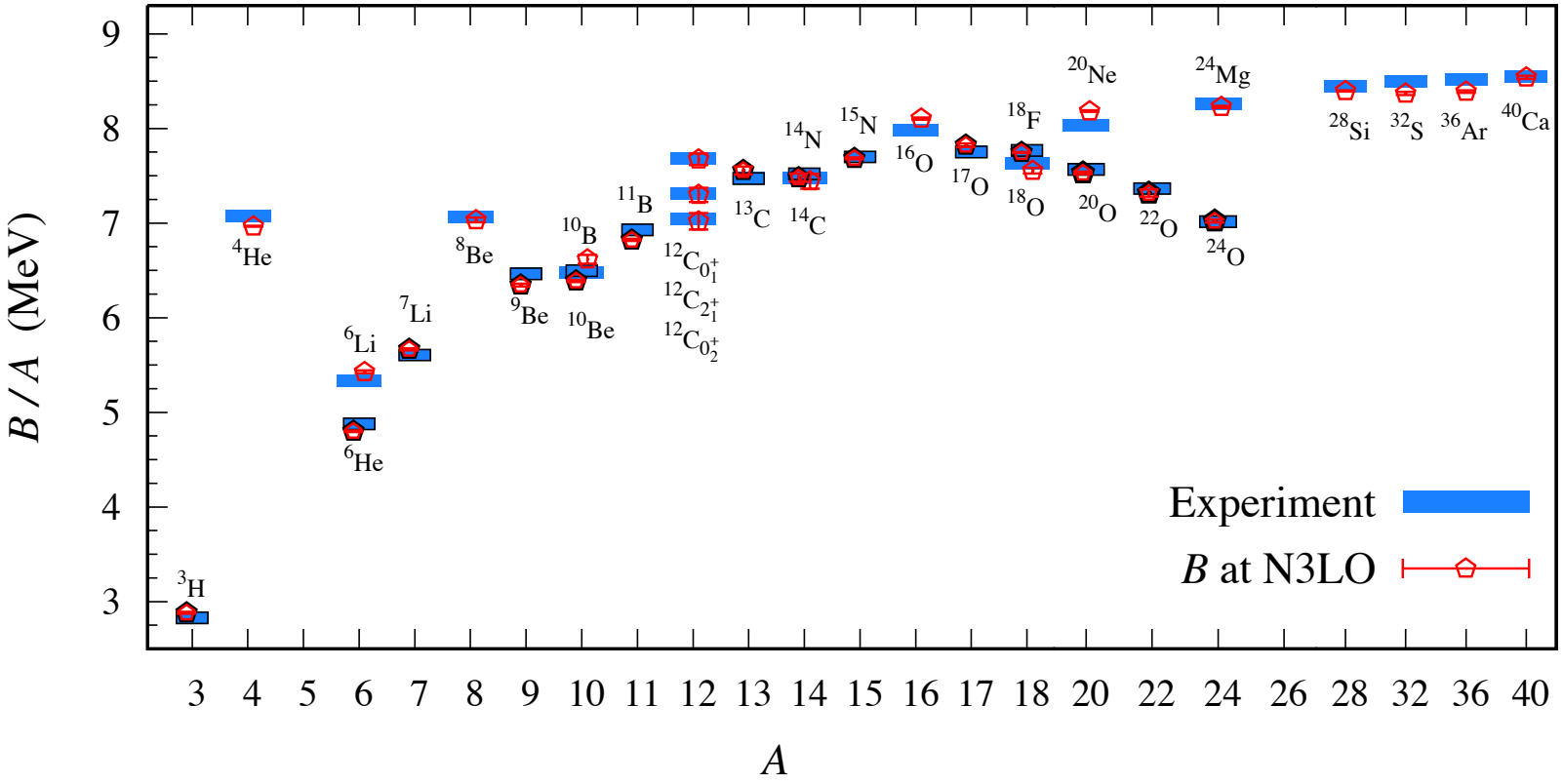


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

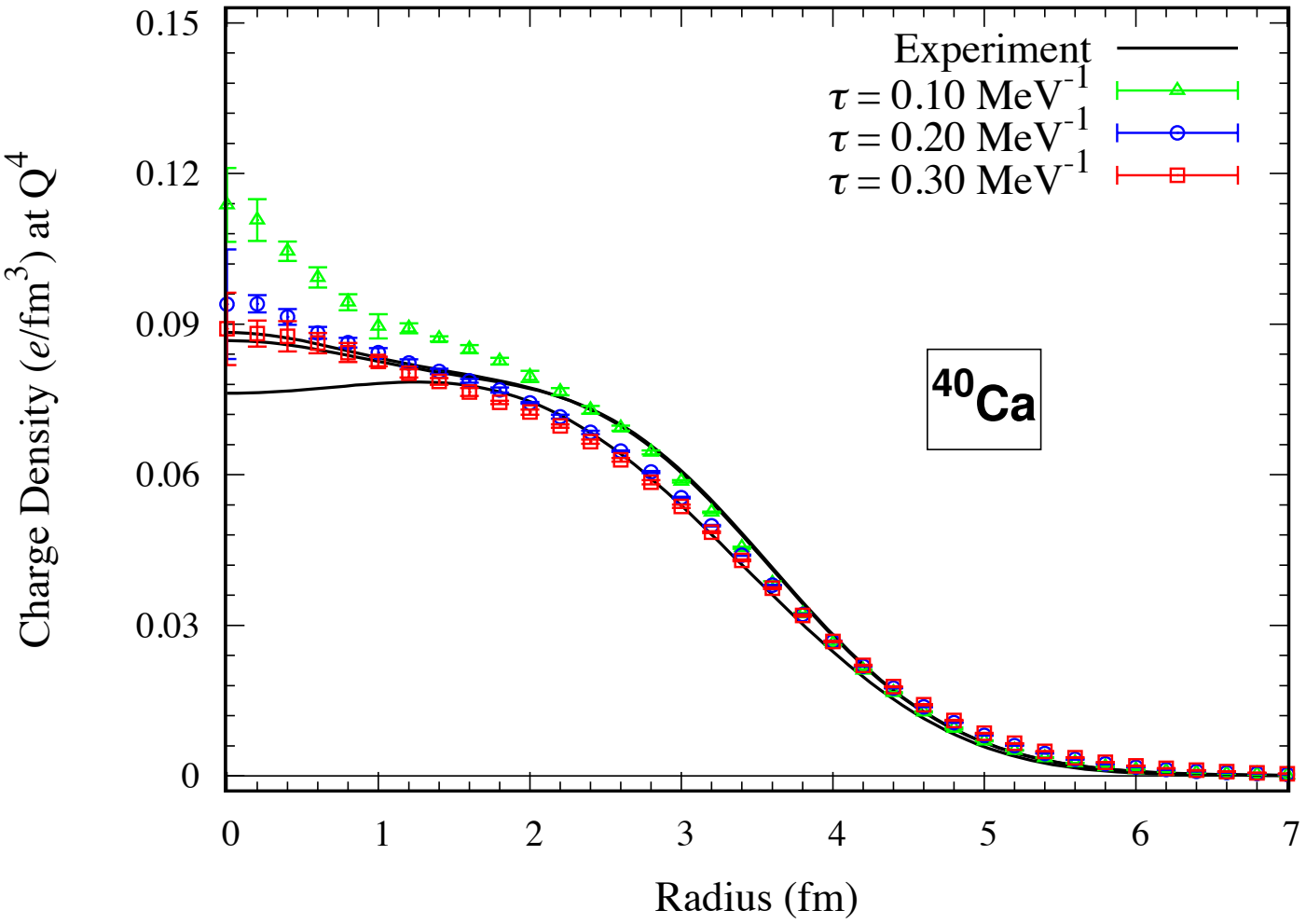
$R = 2.6$ fm

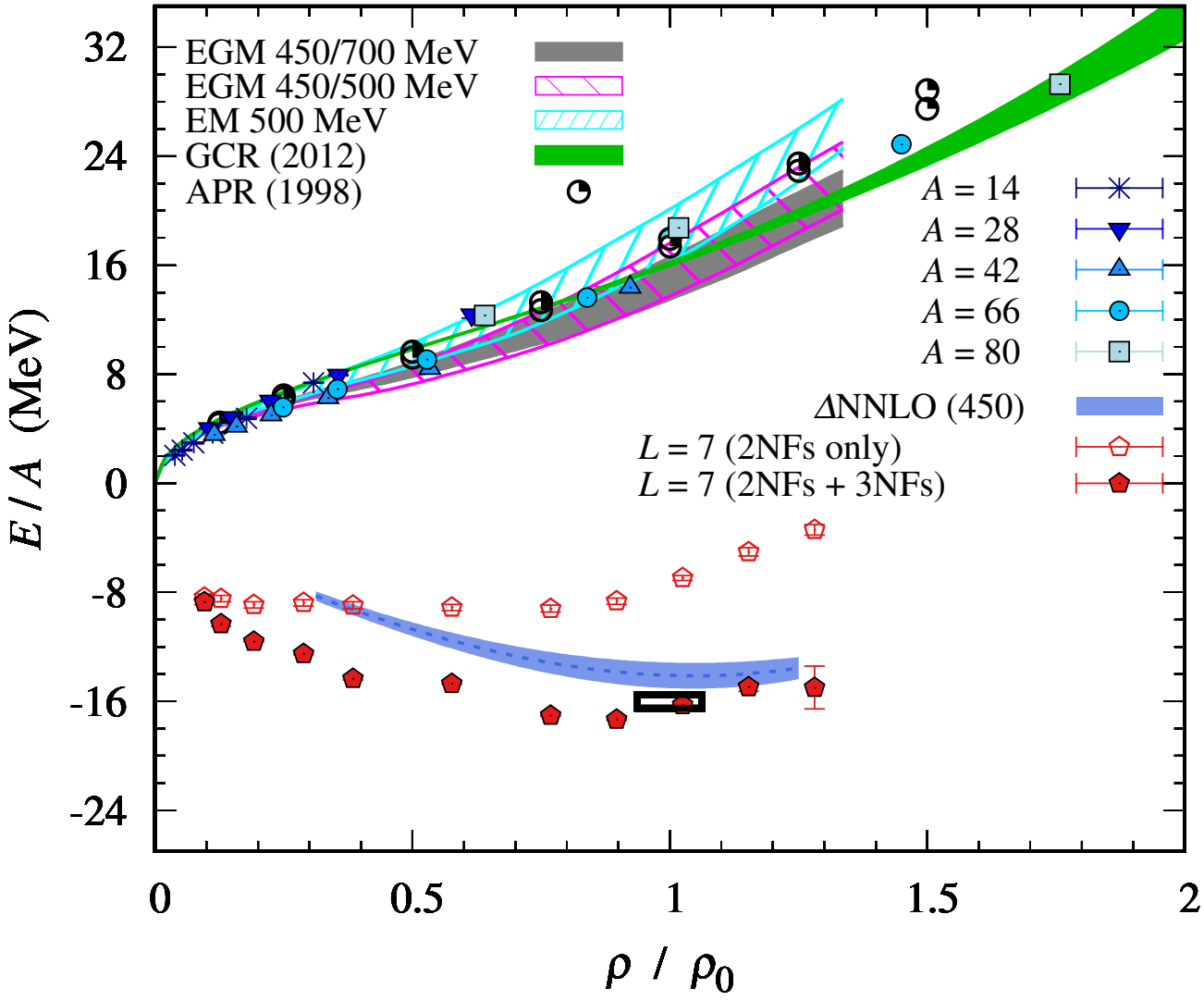
$E_{A,n} = E'_{A,n}$ (MeV)	$\langle\psi_{B,n}\|H_A\|\psi_{B,n}\rangle$ (MeV)	$\langle\psi_{B,n}\|H'_A\|\psi_{B,n}\rangle$ (MeV)
-1.2186	3.0088	-1.1597
0.2196	0.3289	0.2212
0.8523	1.1275	0.8577
1.8610	2.2528	1.8719
3.2279	3.6991	3.2477
4.9454	5.4786	4.9798
7.0104	7.5996	7.0680
9.4208	10.0674	9.5137
12.1721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

Chiral lattice results at N3LO using wave function matching



Work in progress: Elhatisari, Bovermann, et al.


Experiment
τ = 0.10 MeV-1
τ = 0.20 MeV-1
τ = 0.30 MeV-1
40Ca
Charge Density (e/fm3) at Q4
Radius (fm)
0.15
0.12
0.09
0.06
0.03
0
0
1
2
3
4
5
6
7


EGM 450/700 MeV
EGM 450/500 MeV
EM 500 MeV
GCR (2012)
APR (1998)
A = 14
A = 28
A = 42
A = 66
A = 80
ΔNNLO (450)
L = 7 (2NFs only)
L = 7 (2NFs + 3NFs)
E / A (MeV)
ρ / ρ0
32
24
16
8
0
-8
-16
-24
0
0.5
1
1.5
2

Summary

We started with an introduction to lattice effective field theory. We showed that symmetric nuclear matter is near a quantum phase transition. We presented large-N_c arguments and numerical evidence that nuclear physics is close to Wigner's SU(4) symmetric limit. We then studied the nuclear states of carbon-12 and found that alpha cluster structures with two different geometries. We concluded with a discussion of a new method called wave function matching. This enables high-fidelity calculations of nuclear structure from *ab initio* lattice Monte Carlo simulations.