

Wave function matching and the quantum many-body problem

Dean Lee
Facility for Rare Isotope Beams
Michigan State University
NLEFT Collaboration

Hirschegg 2023 – Effective field theories for nuclei and nuclear matter
*EMMI Workshop and International Workshop XLIX on
Gross Properties of Nuclei and Nuclear Excitations*
January 19, 2023



Outline

Tale of two interactions

Essential elements for nuclear binding

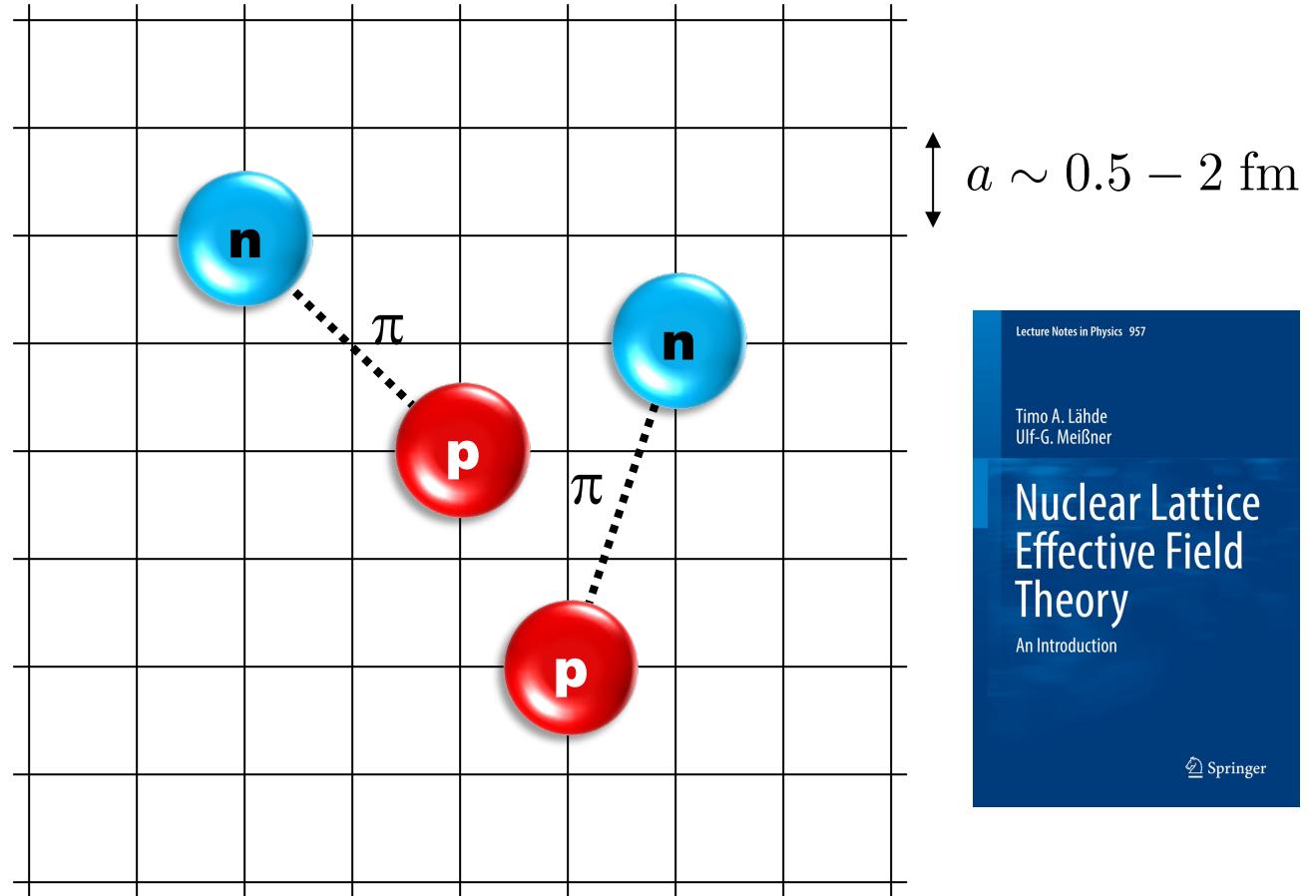
Wave function matching

Chiral effective field theory results at N3LO

Summary

Lattice effective field theory

See Ulf's talk from Wednesday



Lähde, Meißner, Nuclear Lattice Effective Field Theory, Springer (2019)
D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

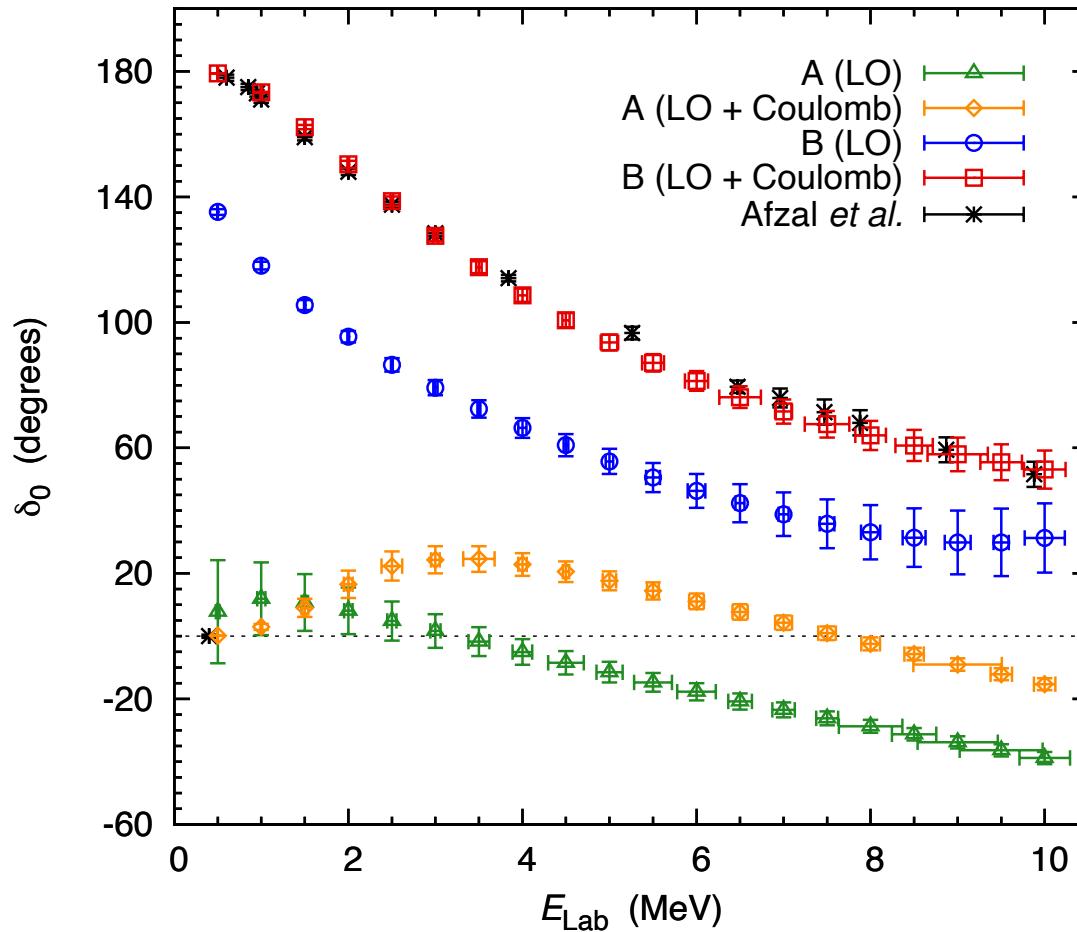
A tale of two interactions

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.

<u>Interaction A</u>	<u>Interaction B</u>
Nonlocal short-range interaction	Nonlocal short-range interaction + Local short-range interaction

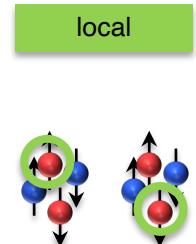
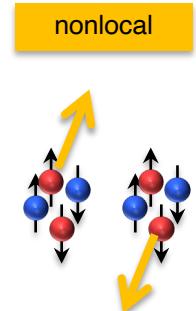
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak,
PRL 117, 132501 (2016)

alpha-alpha S-wave scattering



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

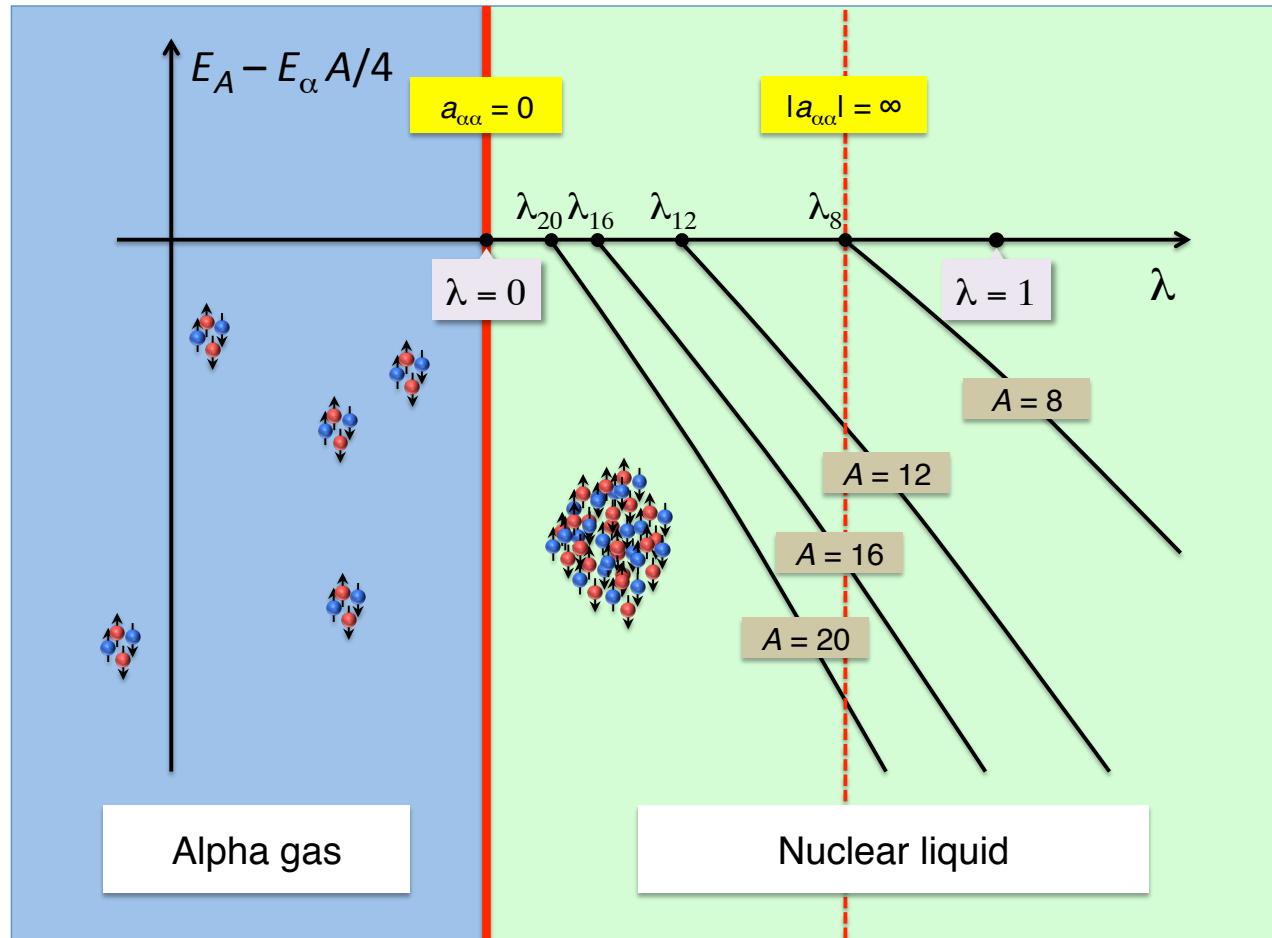
Sensitivity to short-distance physics



Rokash, Epelbaum, Krebs, D.L., PRL 118, 232502 (2017)

Kanada-En'yo, D.L., PRC 103, 024318 (2021)

Nuclear physics near a quantum phase transition



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

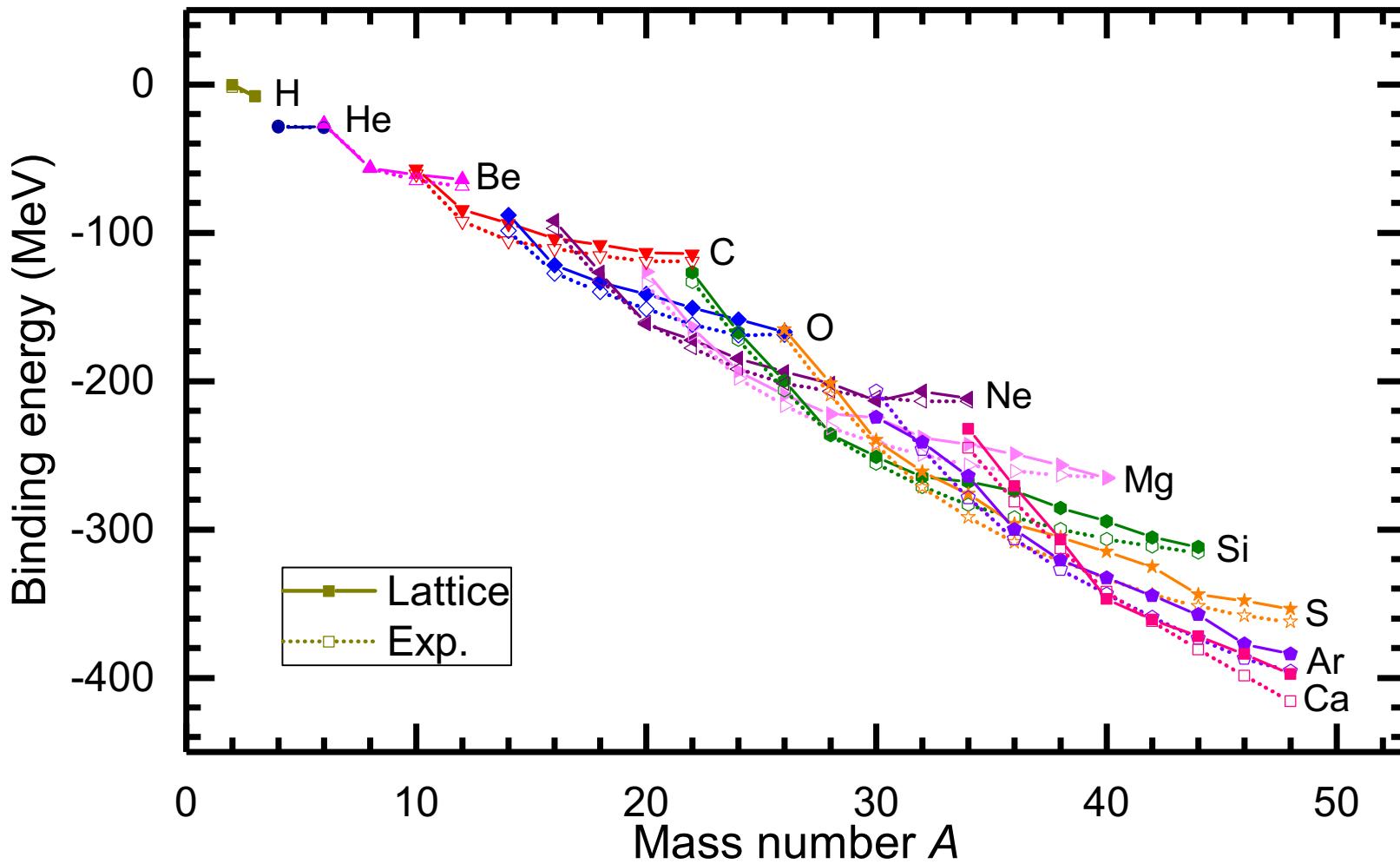
fit to $A > 3$

The lattice Hamiltonian has the form of a smeared four-component Hubbard model with two-body and three-body interactions

$$H_{\text{SU}(4)} = H_{\text{free}} + \frac{1}{2!} C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{1}{3!} C_3 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3$$

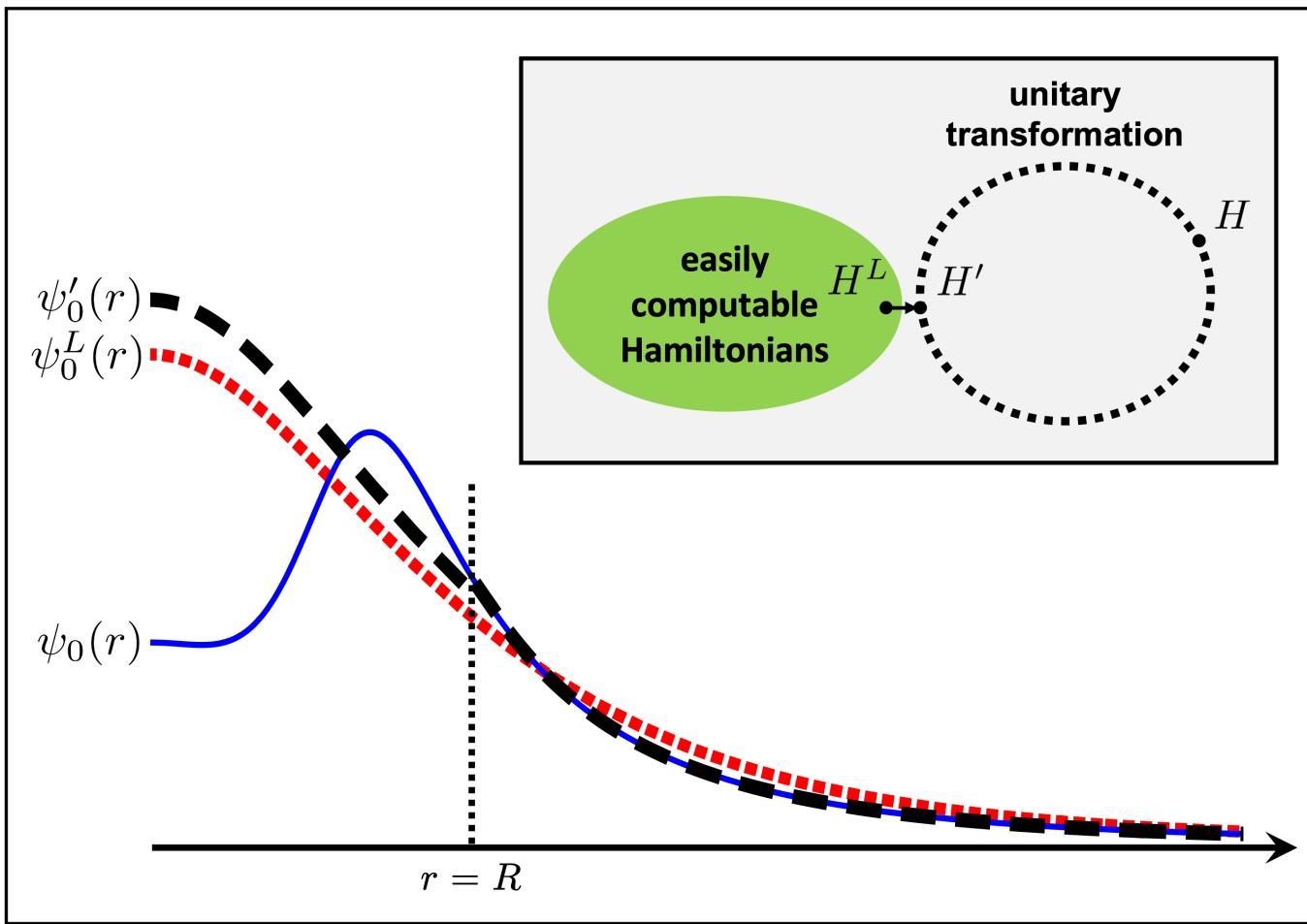
$$\tilde{\rho}(\mathbf{n}) = \sum_i \tilde{a}_i^\dagger(\mathbf{n}) \tilde{a}_i(\mathbf{n}) + s_L \sum_{|\mathbf{n}' - \mathbf{n}|=1} \sum_i \tilde{a}_i^\dagger(\mathbf{n}') \tilde{a}_i(\mathbf{n}')$$

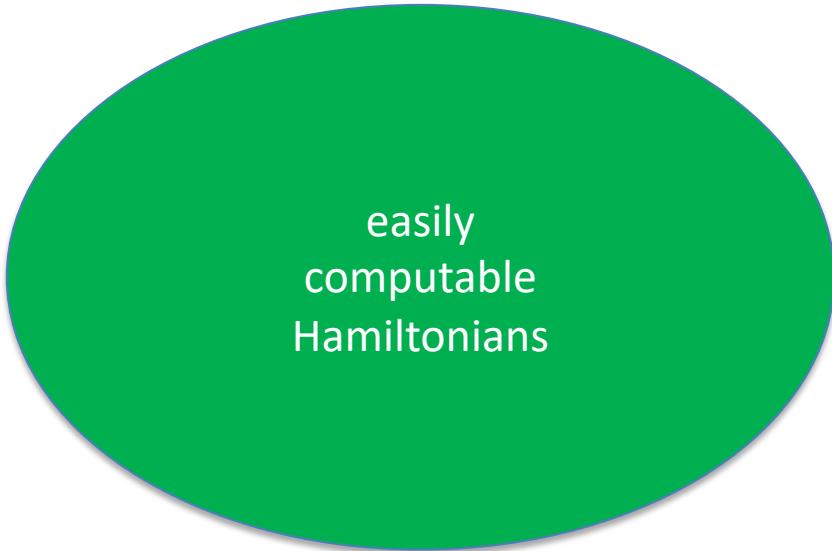
$$\tilde{a}_i(\mathbf{n}) = a_i(\mathbf{n}) + s_{NL} \sum_{|\mathbf{n}' - \mathbf{n}|=1} a_i(\mathbf{n}')$$



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.

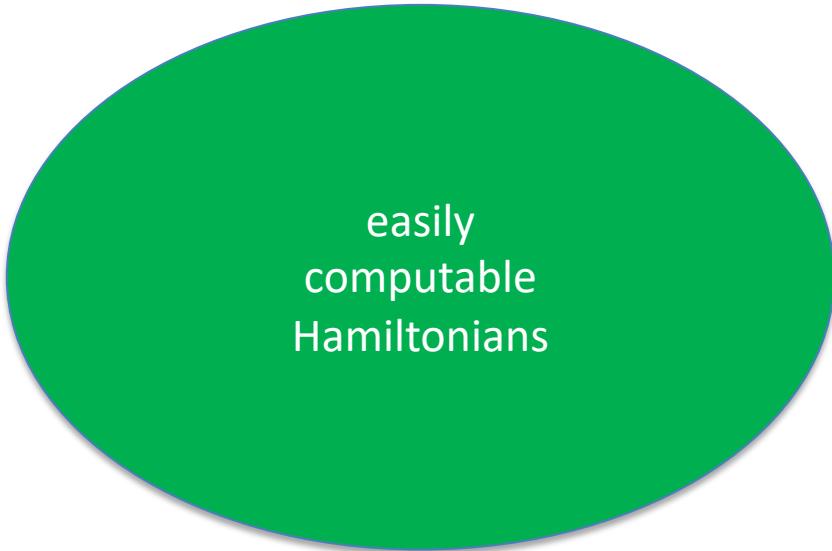
Wave function matching



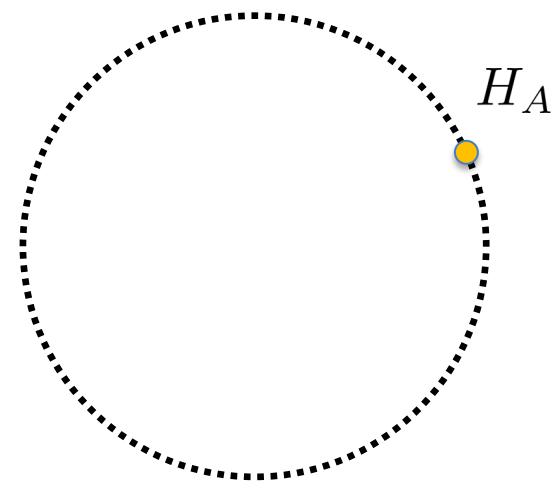


easily
computable
Hamiltonians

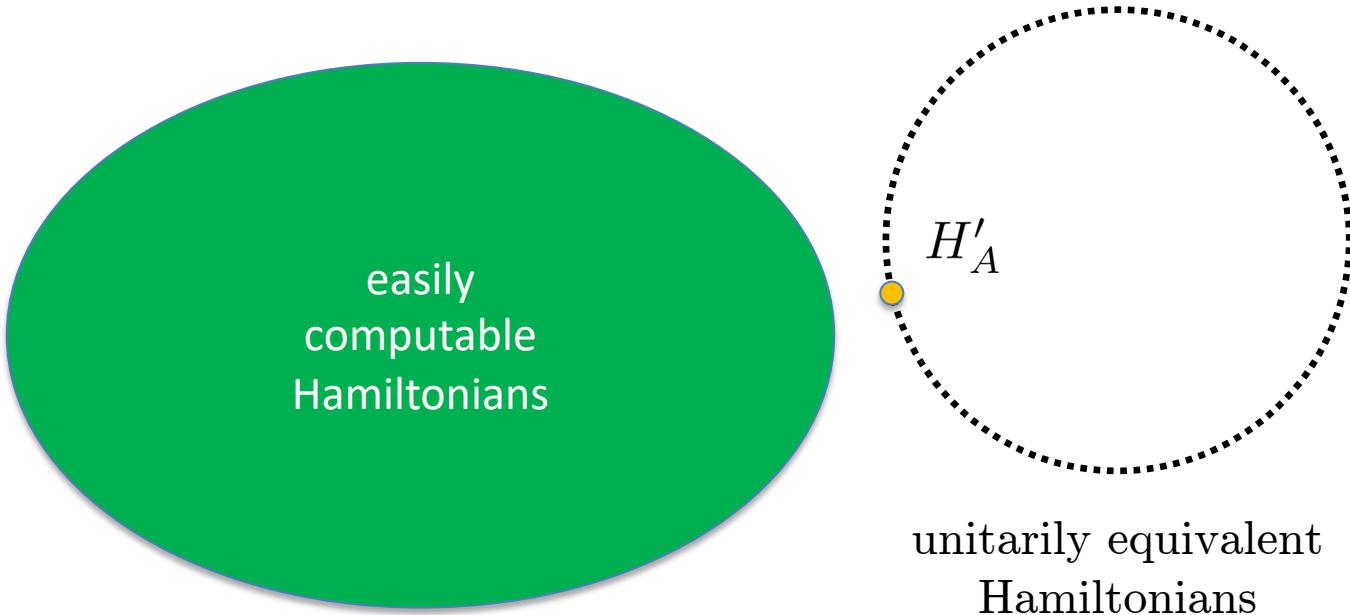
H_A

easily
computable
Hamiltonians



unitarily equivalent
Hamiltonians



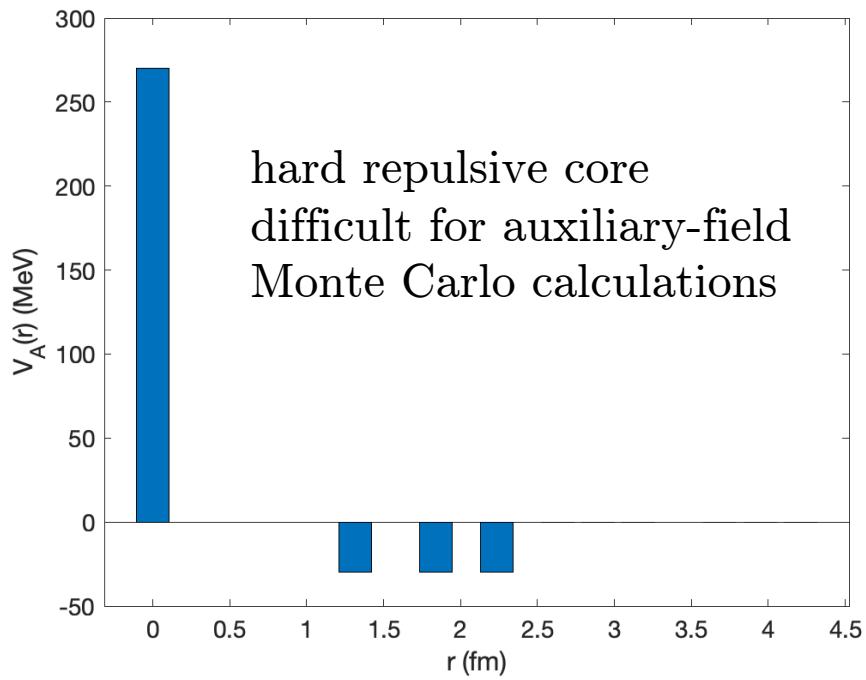
easily
computable
Hamiltonians

H'_A

unitarily equivalent
Hamiltonians

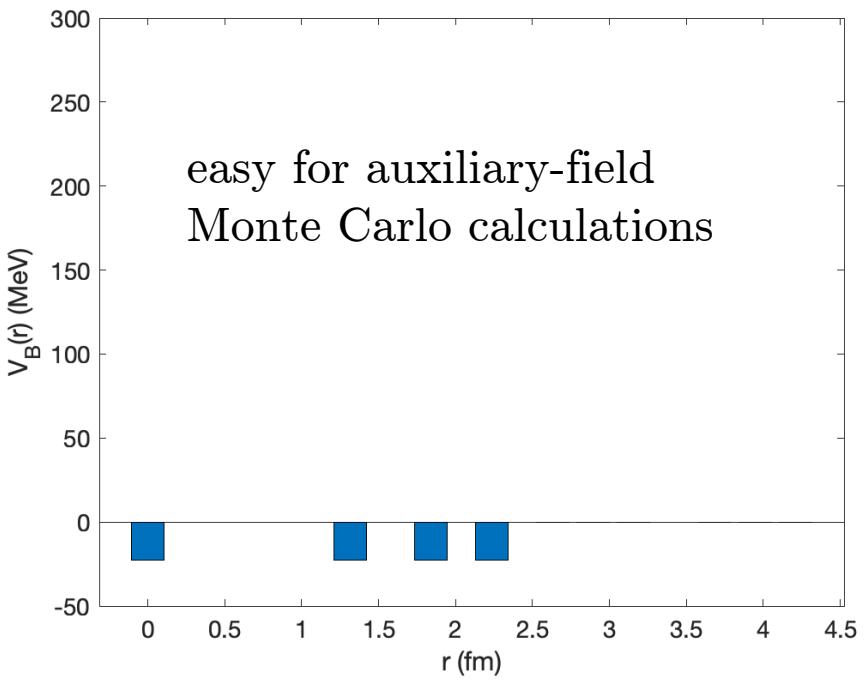
Wave function matching

$$V_A(r)$$

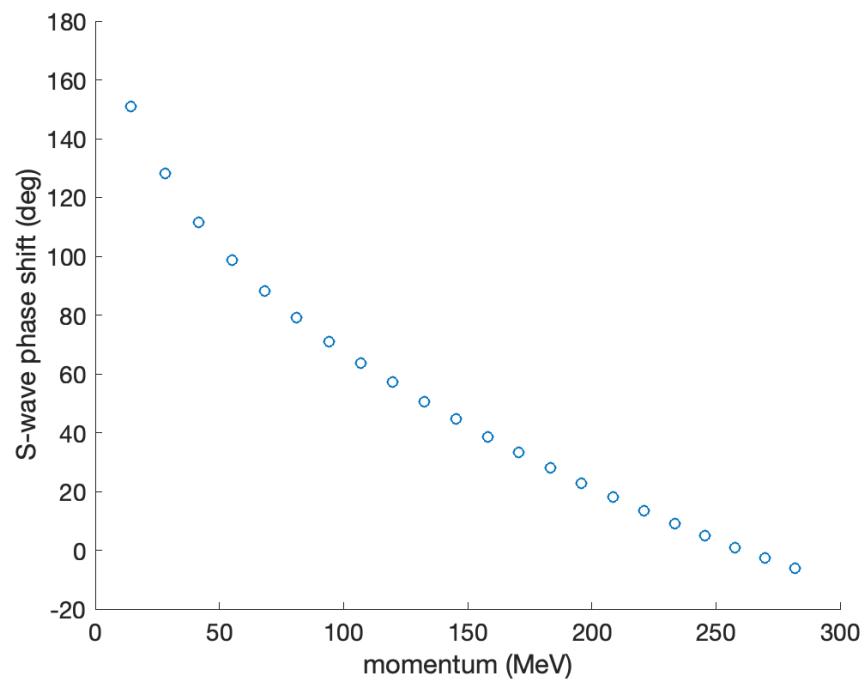
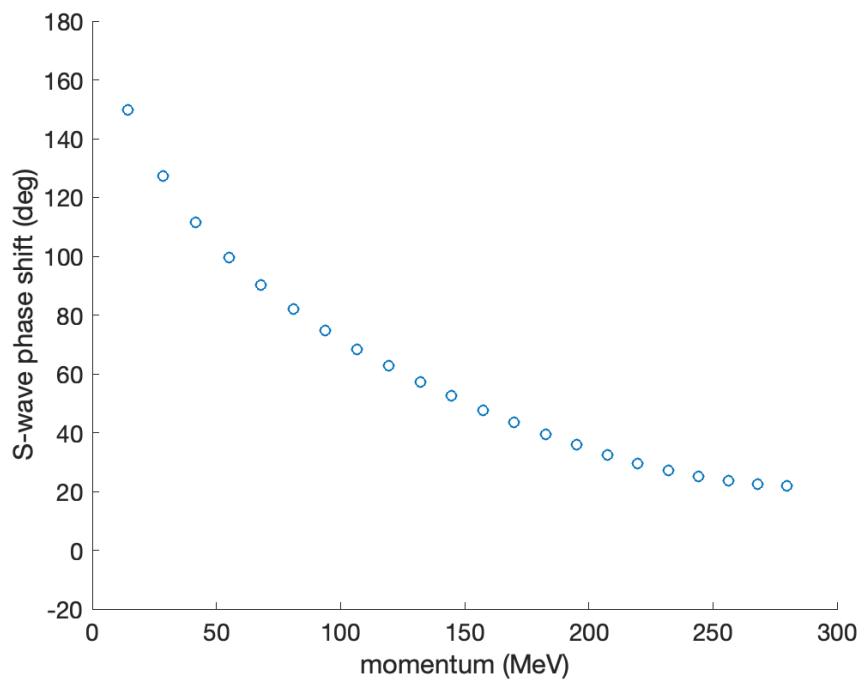


hard repulsive core
difficult for auxiliary-field
Monte Carlo calculations

$$V_B(r)$$



easy for auxiliary-field
Monte Carlo calculations

$V_A(r)$  $V_B(r)$ 

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

$$H_A |\psi_{A,n}\rangle = (K + V_A) |\psi_{A,n}\rangle = E_{A,n} |\psi_{A,n}\rangle$$

$$H_B |\psi_{B,n}\rangle = (K + V_B) |\psi_{B,n}\rangle = E_{B,n} |\psi_{B,n}\rangle$$

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

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

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

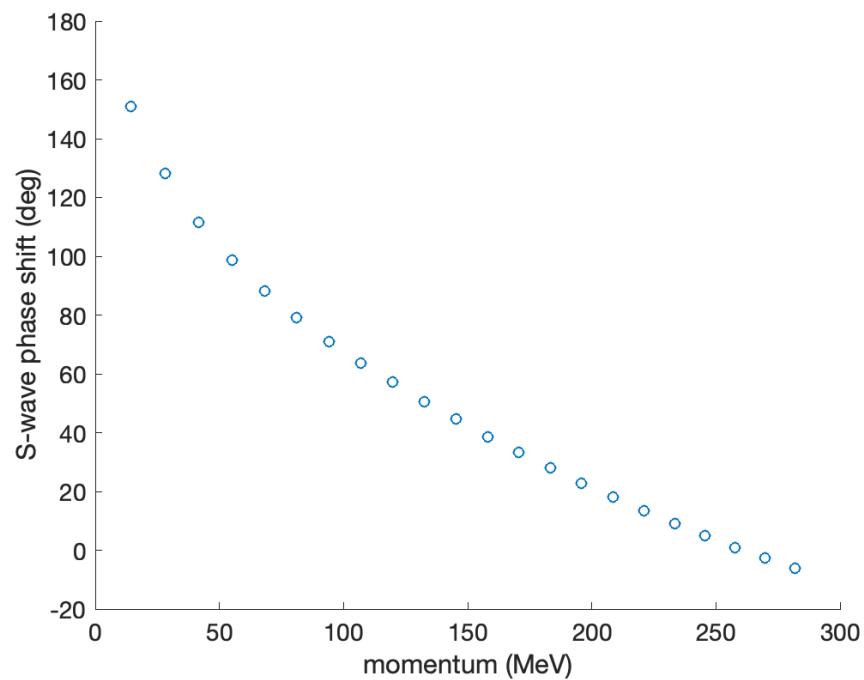
$$U : H_A \rightarrow H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

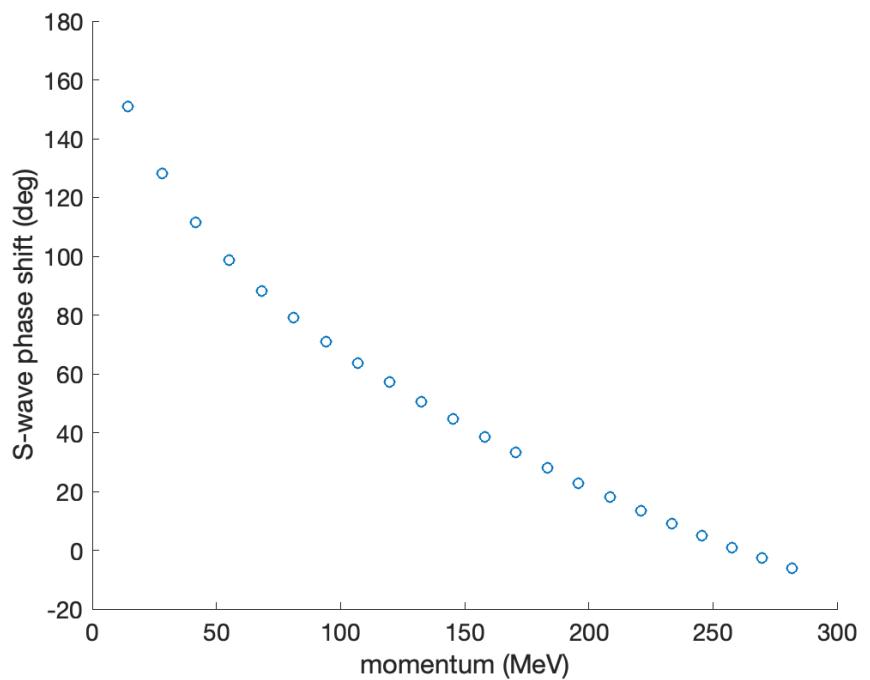
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

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

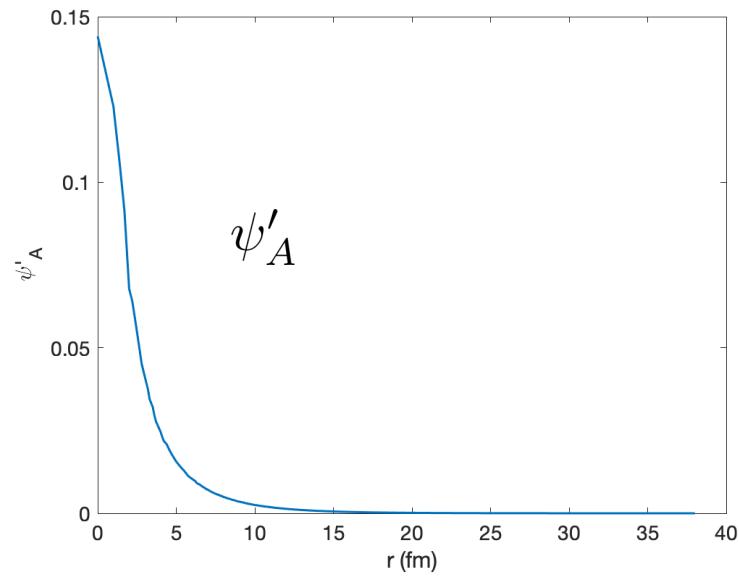
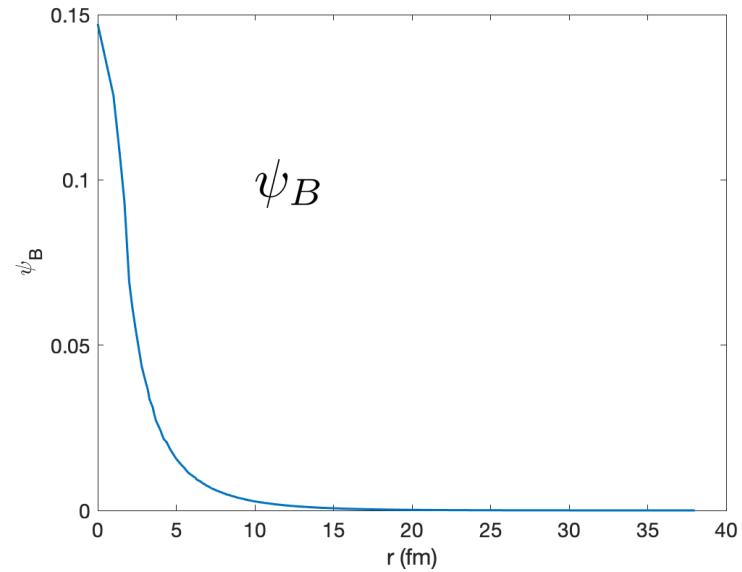
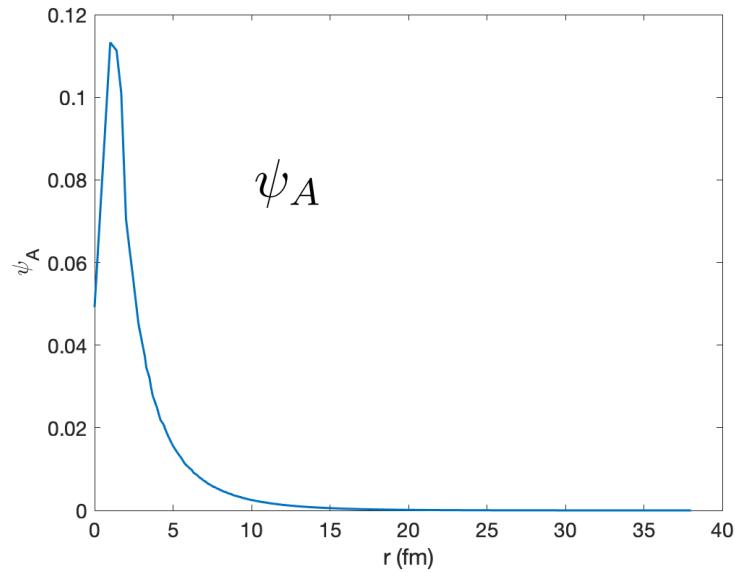
$$V_A(r)$$



$$V'_A(r, r')$$



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.

$$R = 2.6 \text{ fm}$$

$E_{A,n} = E'_{A,n}$ (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

Hamiltonian translators

Suppose U_{AB} is a unitary transformation mapping all the eigenvectors of H_B to all the eigenvectors of H_A . Let U_{BA} be the inverse of U_{AB} . We note the curious fact that

$$H'_A = U_{BA} H_A U_{AB}$$

has the eigenvectors of H_B but has the eigenvalues of H_A . We call U_{AB} and U_{BA} Hamiltonian translators.

We can construct a Hamiltonian translator using quantum adiabatic evolution

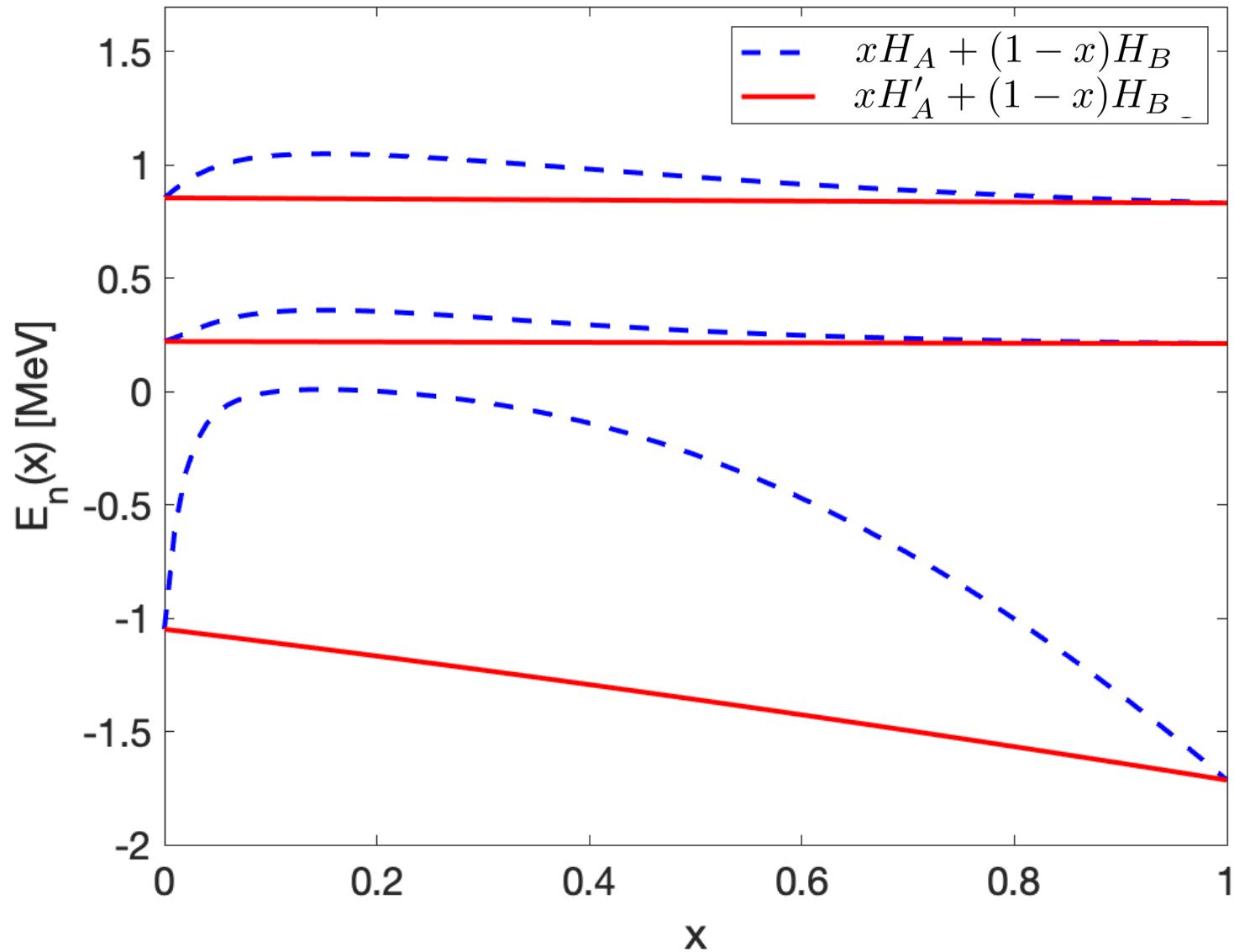
$$U_T = \lim_{T \rightarrow \infty} \overleftarrow{\mathcal{T}} \exp \left[-i \int_0^T H_T(t) dt \right]$$

where $H_T(t)$ smoothly interpolates between H_B and H_A as t goes from 0 to T .

Wave function matching is an approximate Hamiltonian translator at the two-body level.

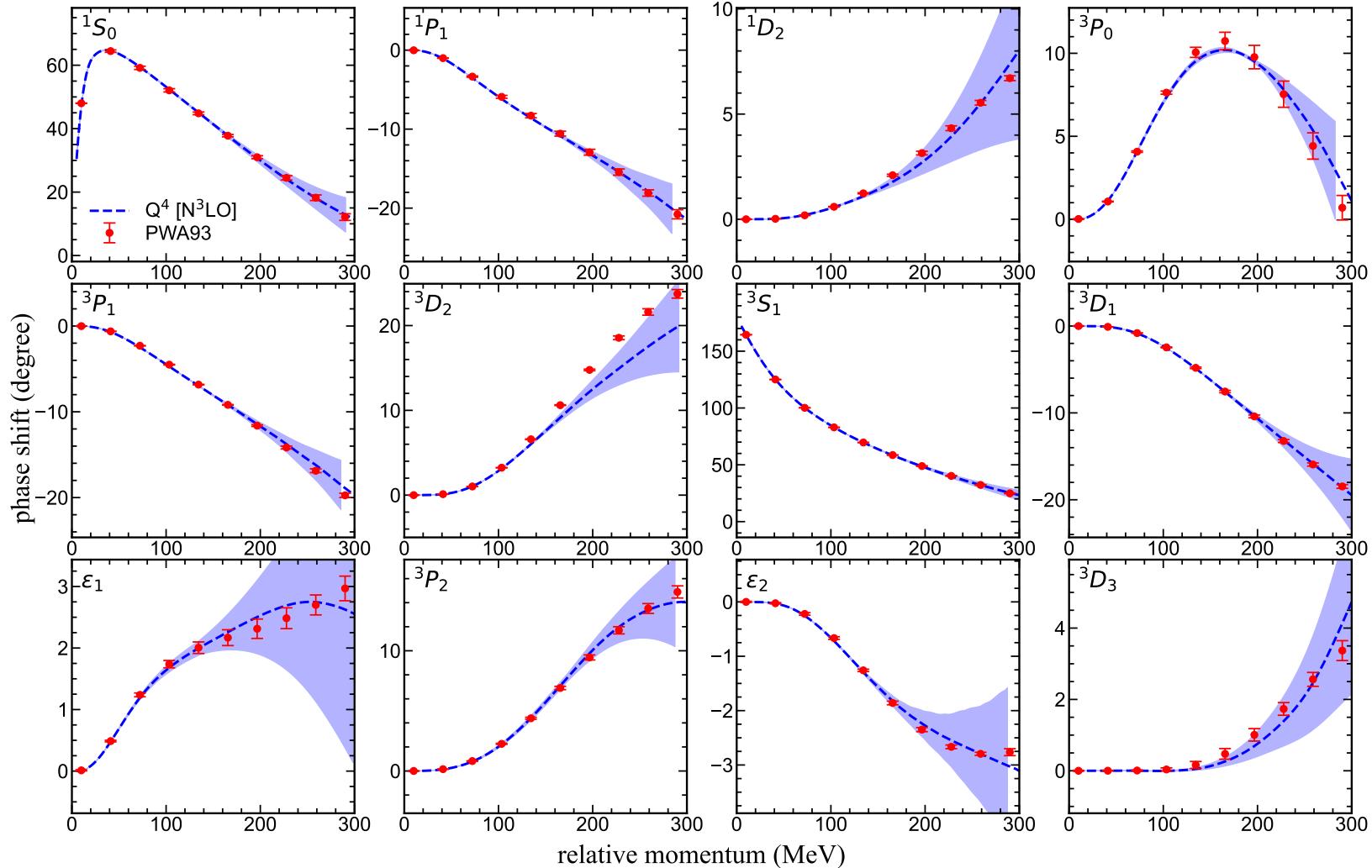
B

A

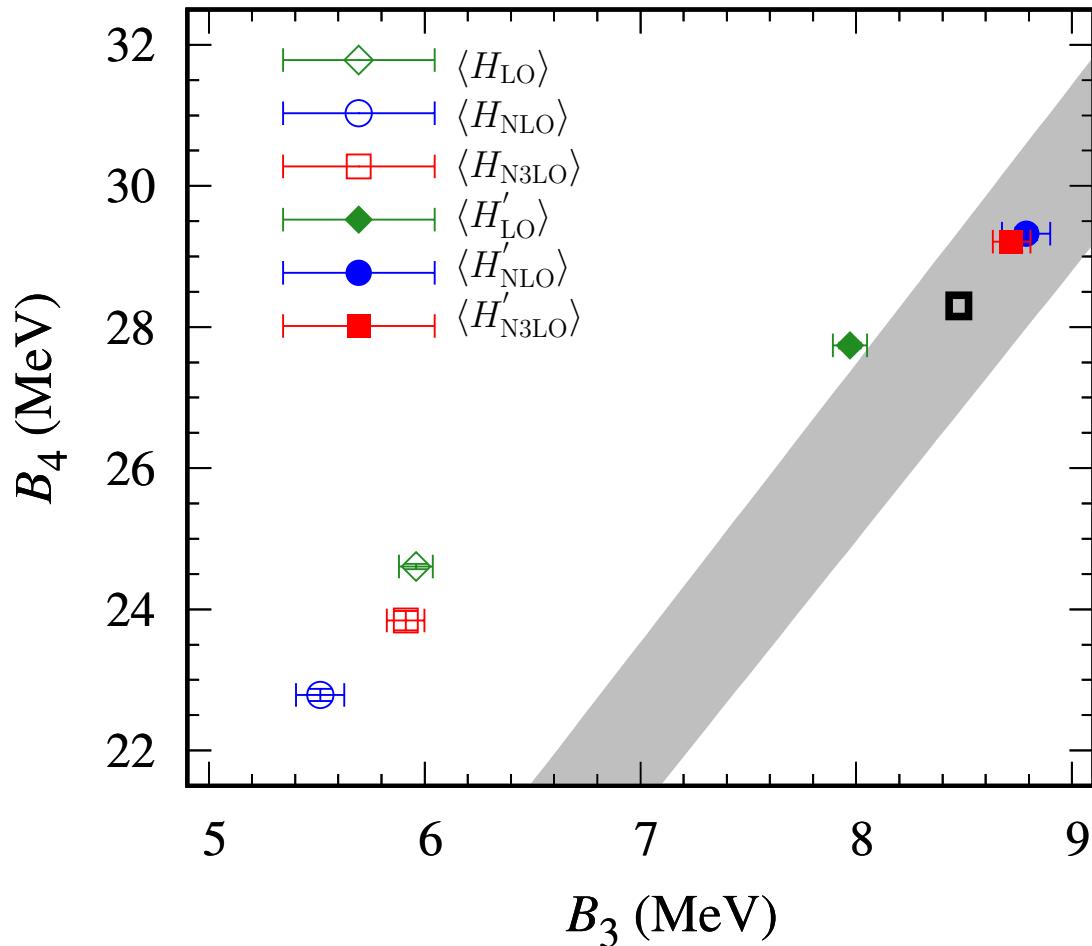


straight lines mean the eigenvectors don't change with x

N3LO chiral effective field theory interaction

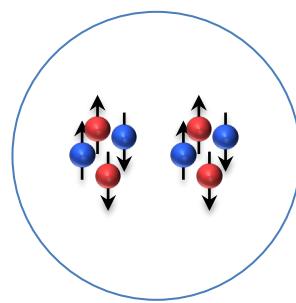


Tjon line

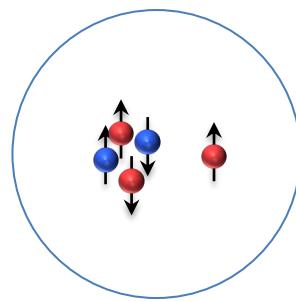
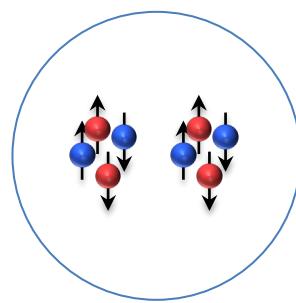


Tjon, Phys. Lett. B 56, 217 (1975); Nogga, Kamada, Glöckle, Phys. Rev. Lett. 85, 944 (2000);
Platter, Hammer, Meißner, Phys. Lett. B607, 254 (2005)

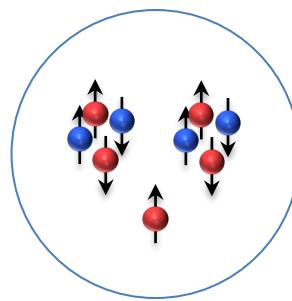
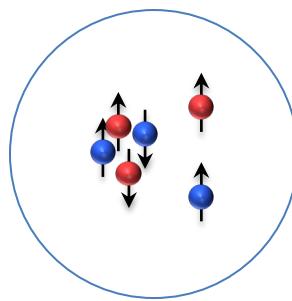
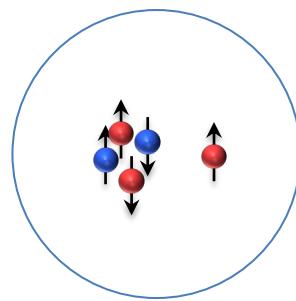
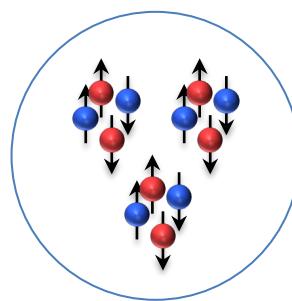
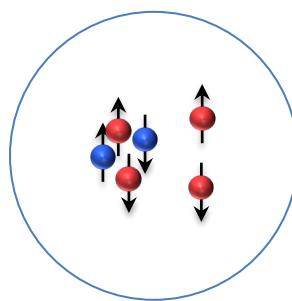
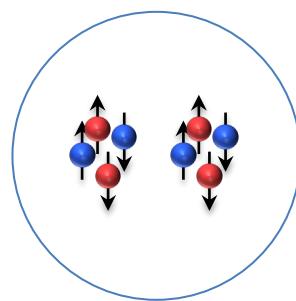
Sensitivity to short-distance physics



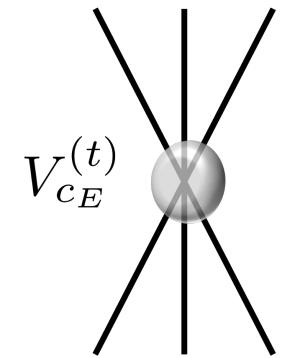
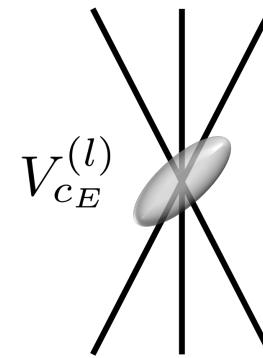
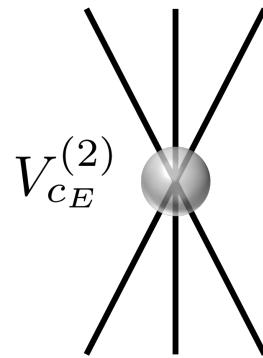
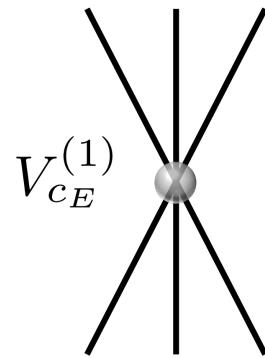
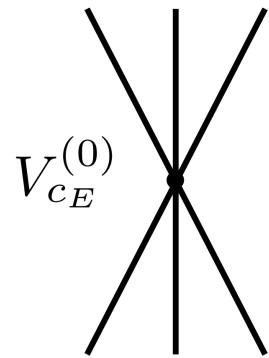
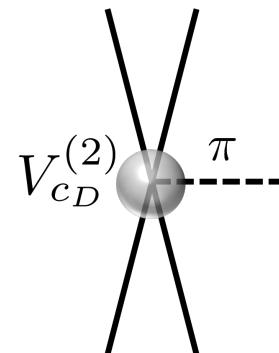
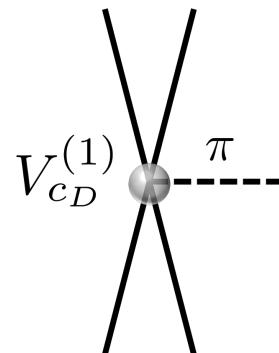
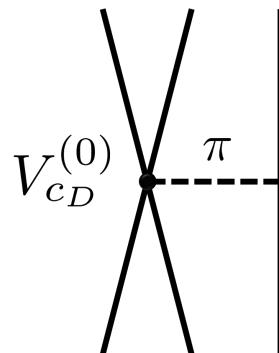
Sensitivity to short-distance physics



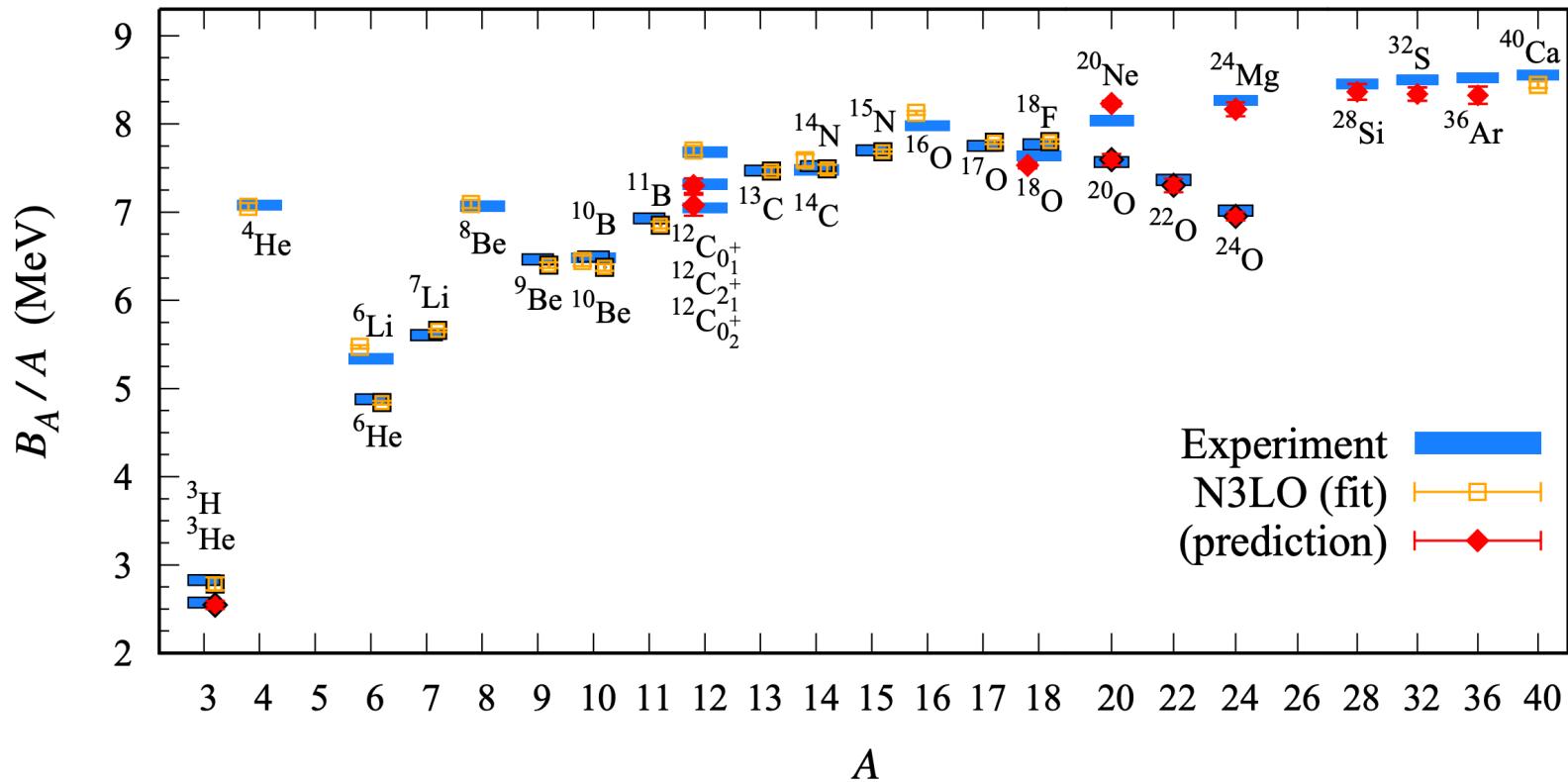
Sensitivity to short-distance physics



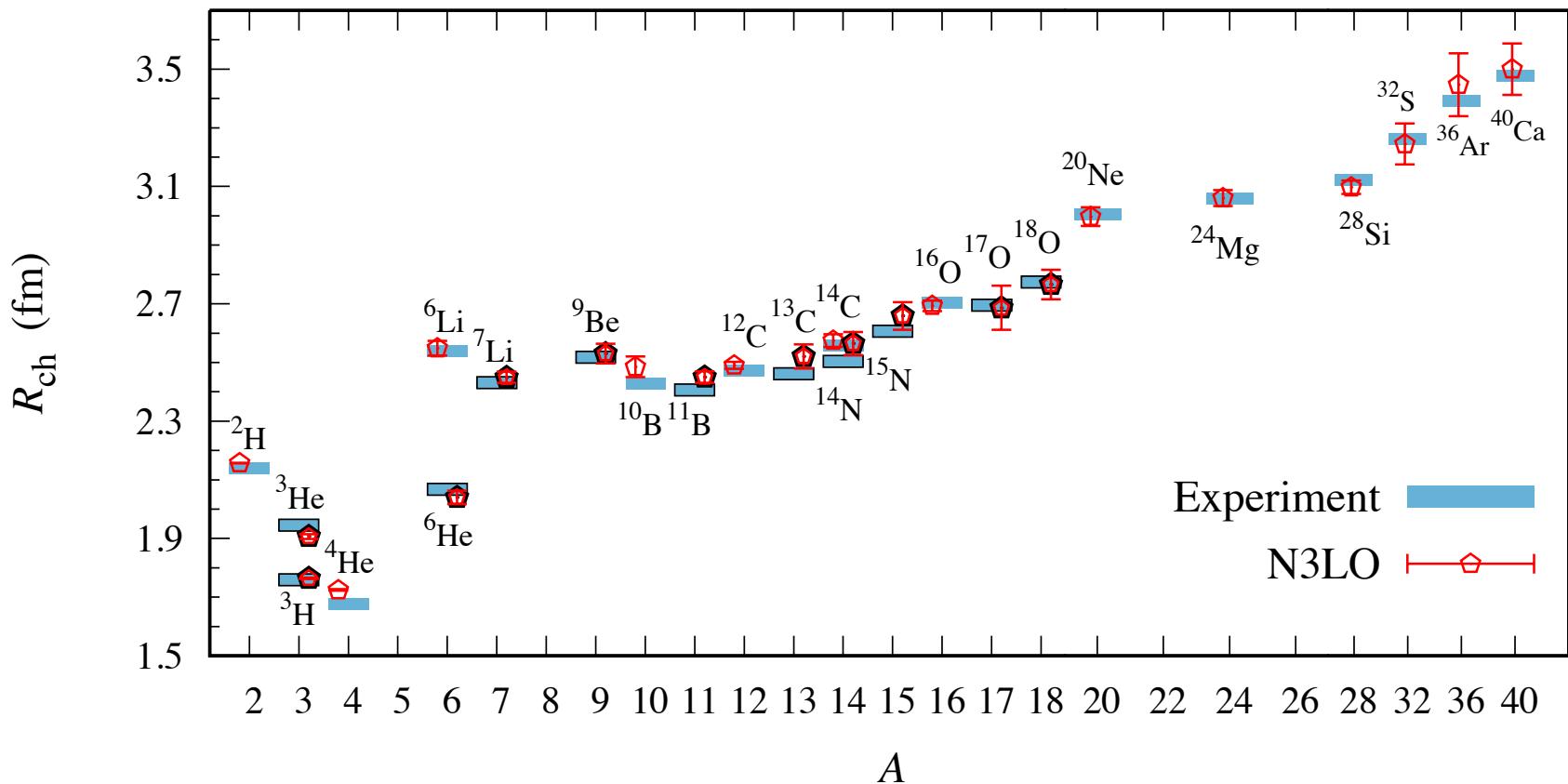
Short-distance three-nucleon interactions



Binding energy per nucleon



Charge radius



Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim,
Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin, arXiv: 2210.17488

Neutron and nuclear matter

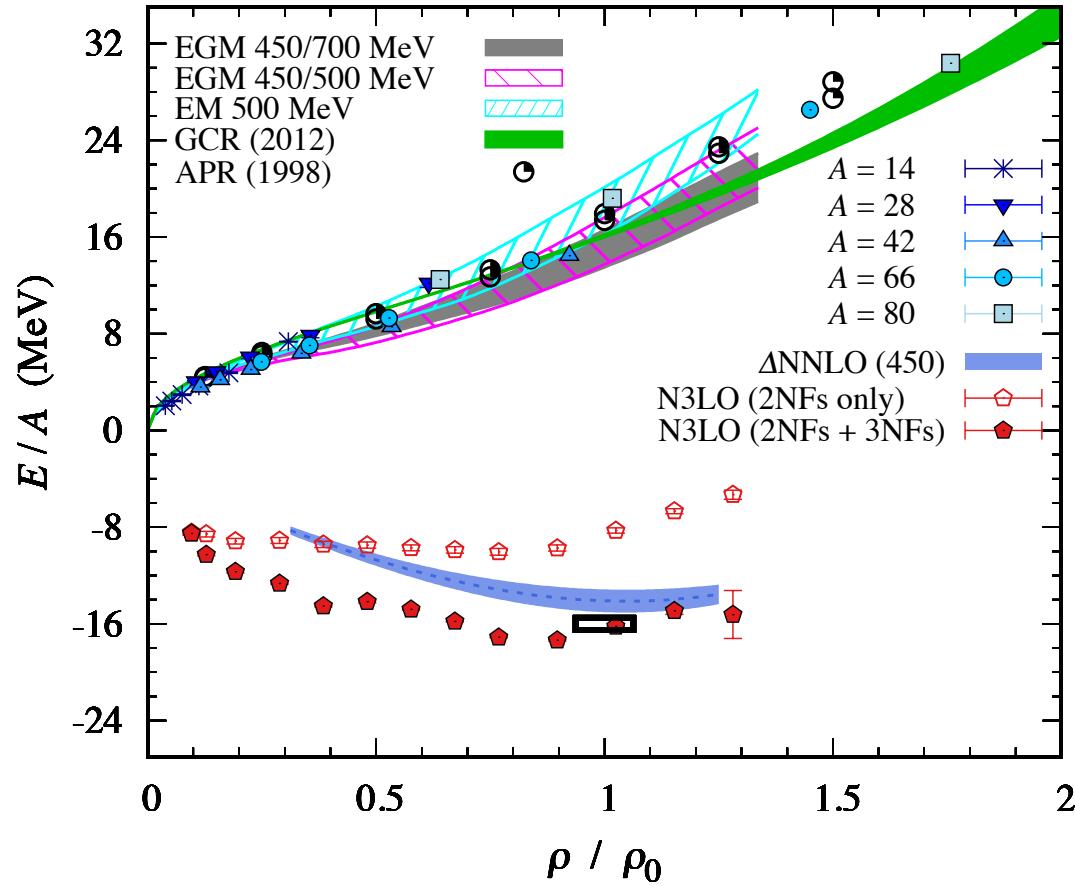
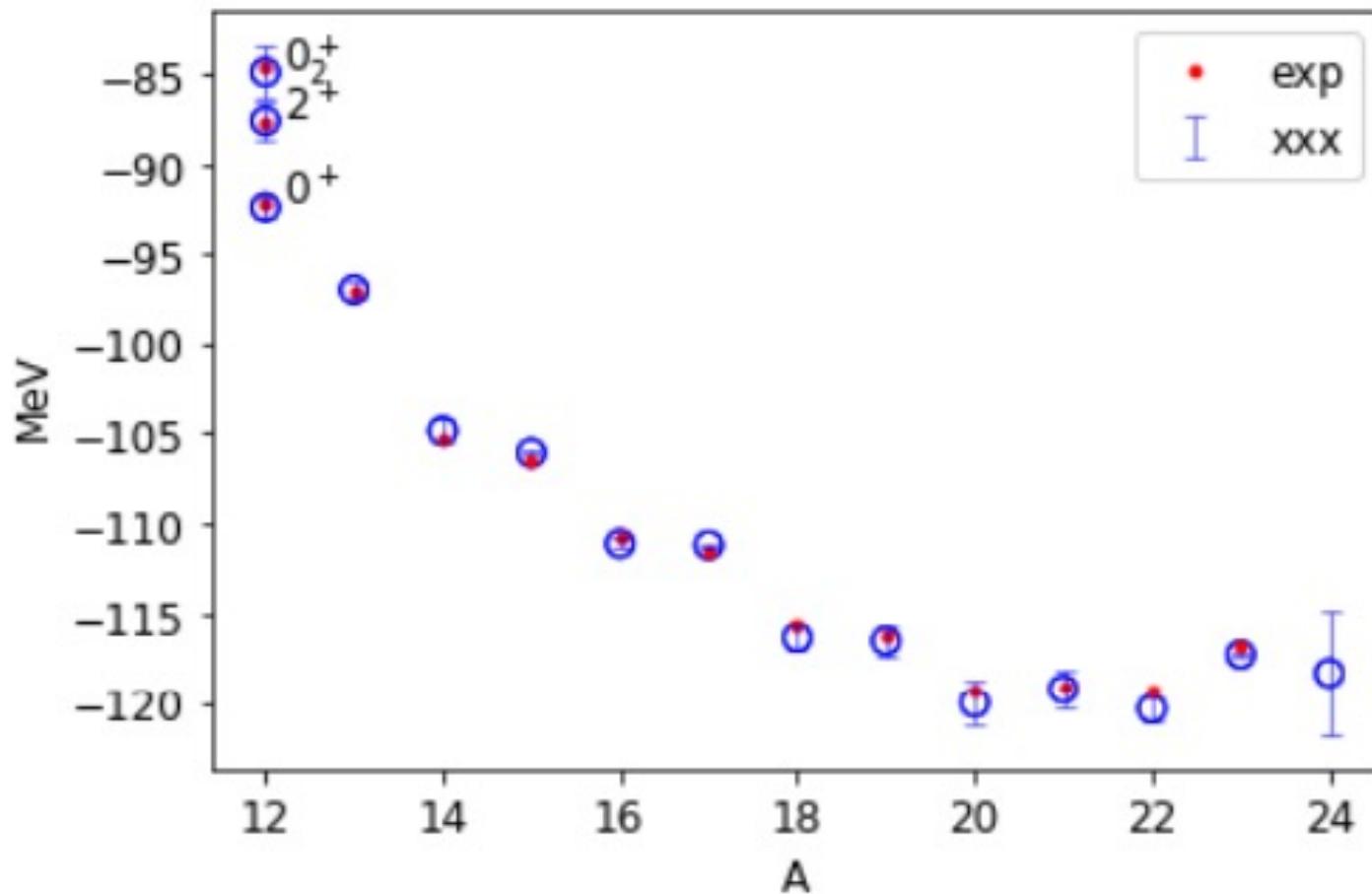


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim,
Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin, arXiv: 2210.17488

Carbon isotopes



Some things to do:

Calculate the binding energies, radii, and structure of the isotopic chains of carbon, oxygen, silicon, and calcium.

Search for clustering in medium mass nuclei.

Adapt and optimize GPU codes for Frontier and the new supercomputer at Forschungszentrum Jülich and extend calculations to heavy nuclei.

Extract ANC s from finite-volume energy corrections. See Sebastian's talk from Wednesday.

Extend calculations to light and medium mass hypernuclei.

Calculate resonance widths.

Compute thermodynamic properties of neutron matter and symmetric and asymmetric nuclear matter.

Summary

We started with a discussion of the differences between local and nonlocal interactions and the fact that the interaction between two alpha particles is sensitive to short-distance physics. We used this information to produce a simple interaction that gave a decent description of light and medium mass nuclei.

We then introduced the technique of wave function. We demonstrated the basic concepts using simple examples and then applied wave function matching to calculations at N3LO in chiral effective field theory. We are able to control sensitivity to short-distance physics using several three-nucleon interactions beyond N3LO.