Wave function matching and the quantum many-body problem

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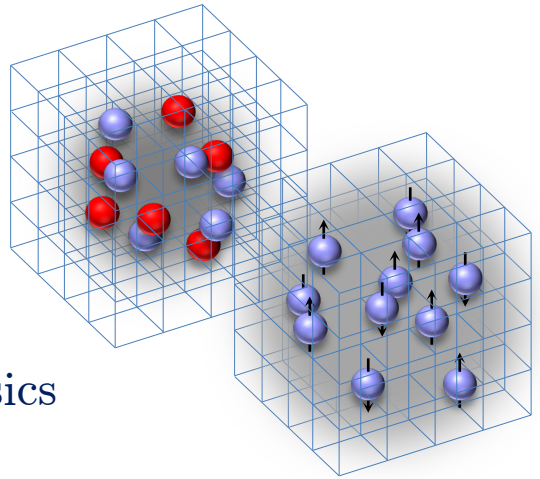
Michigan State University
NLEFT Collaboration



Progress in *Ab Initio* Techniques in Nuclear Physics
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FRIB MICHIGAN STATE UNIVERSITY NUCLEI Nuclear Computational Low-Energy Initiative A SciDAC-4 Project JÜLICH FORSCHUNGSZENTRUM OAK RIDGE National Laboratory LEADERSHIP COMPUTING FACILITY

Outline

Tale of two interactions

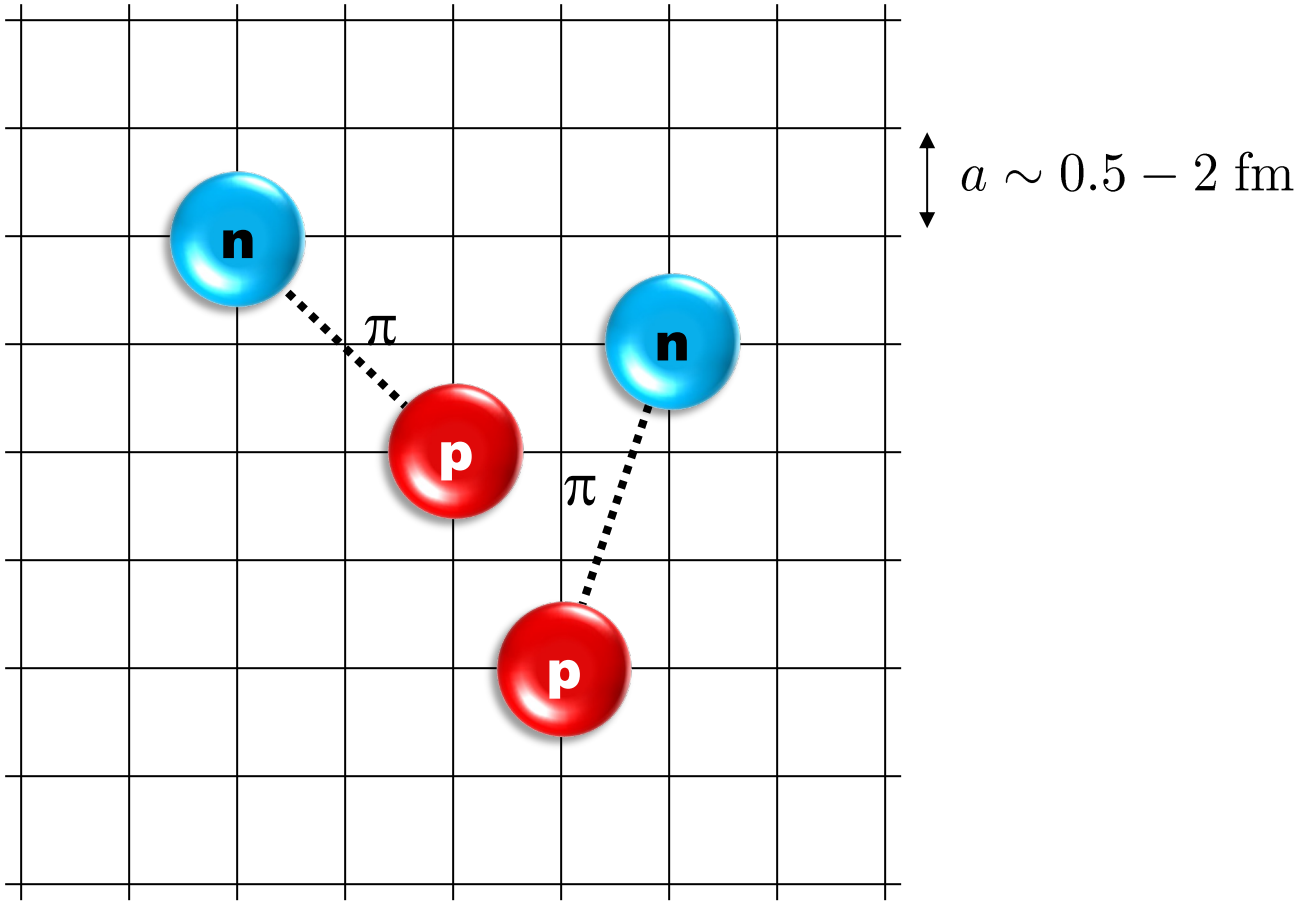
Essential elements for nuclear binding

Wave function matching

Chiral effective field theory results at N3LO

Summary

Lattice effective field theory



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

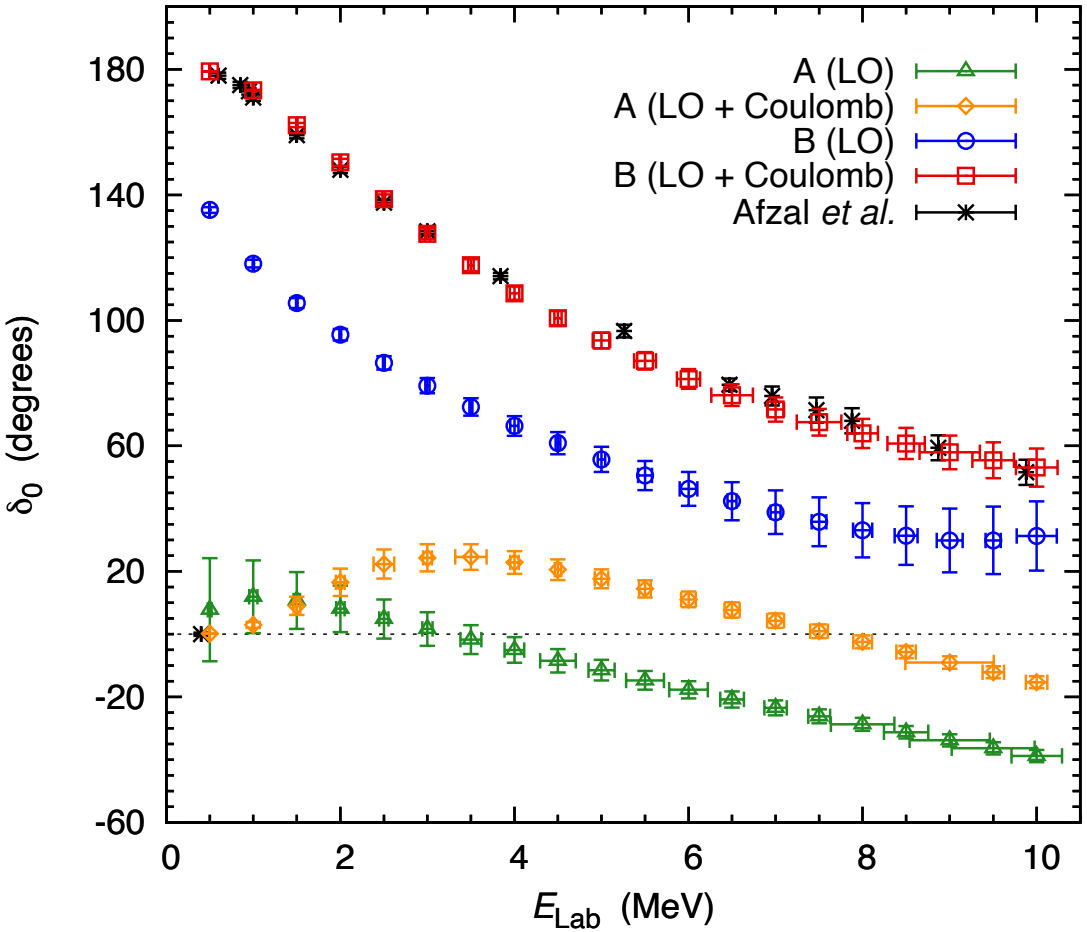
A tale of two interactions

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.

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

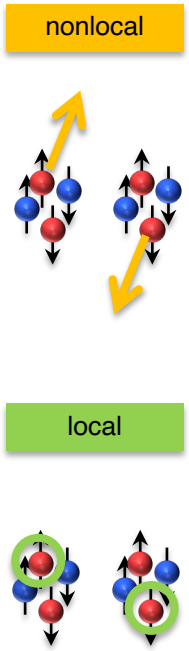
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Alpha-alpha S-wave scattering



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

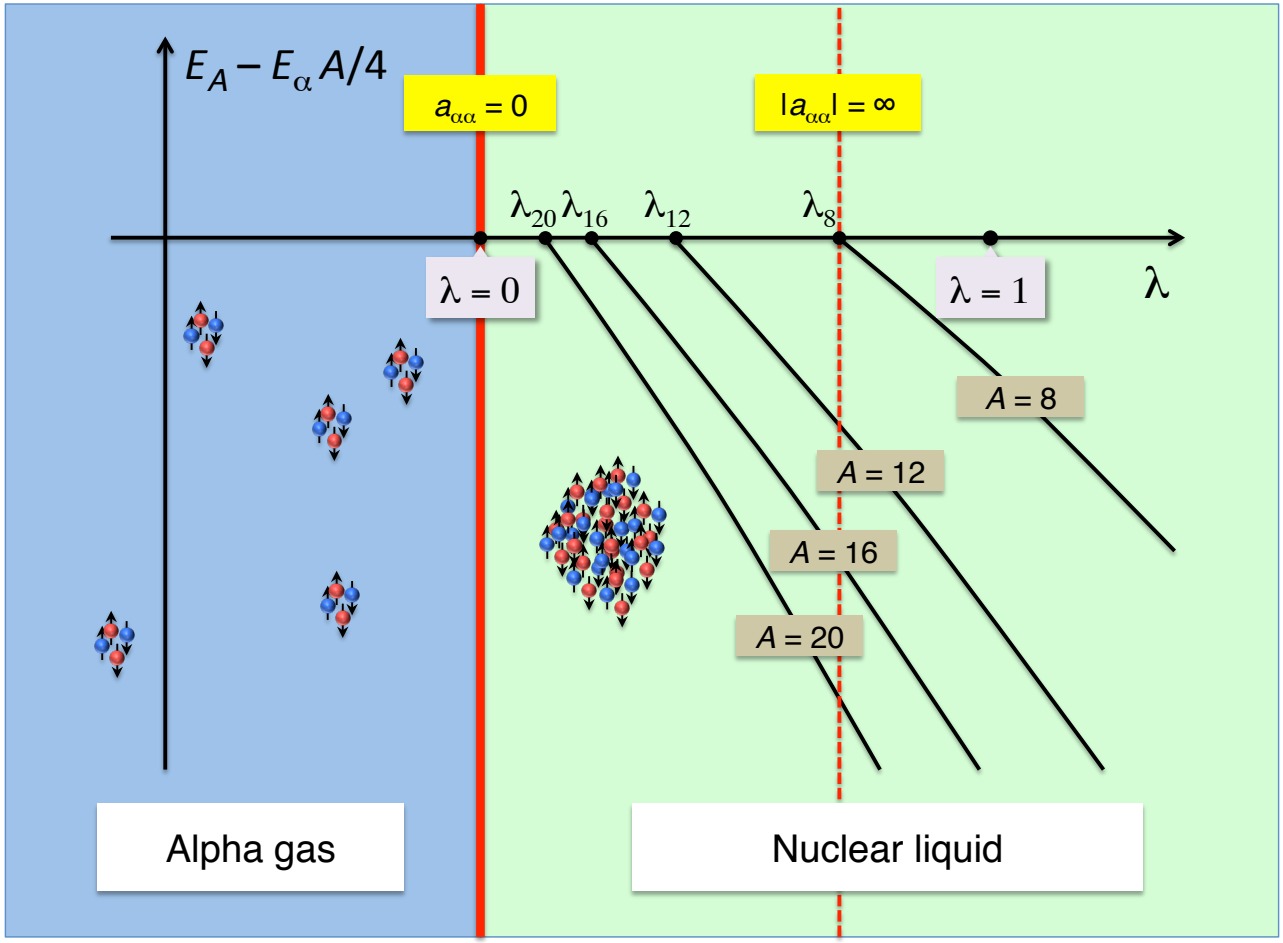
Sensitivity to short-distance physics



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

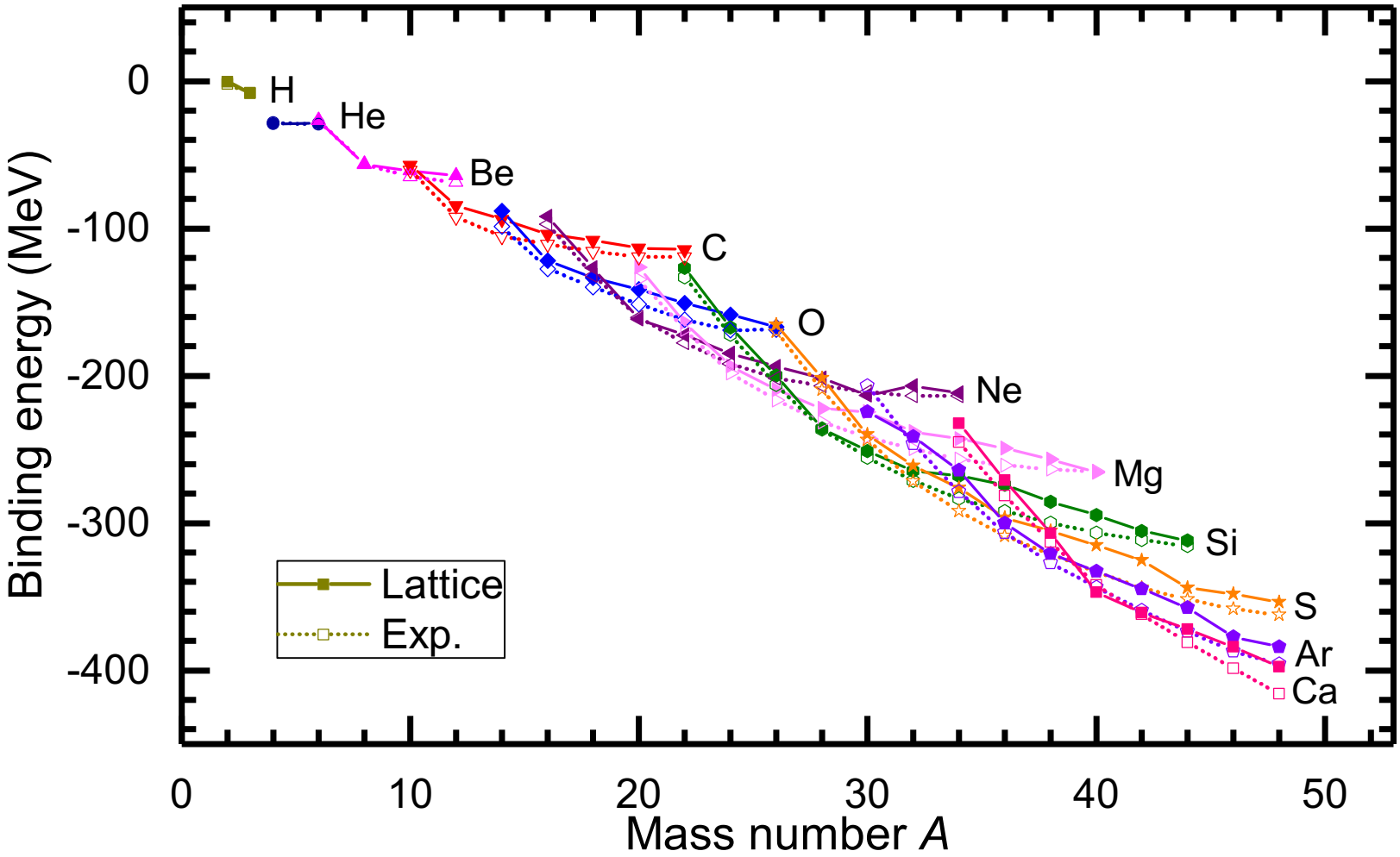
fit to A > 3

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

$$H_{\mathrm{SU}(4)} = H_{\mathrm{free}} + \tfrac{1}{2!} C_2 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^2 + \tfrac{1}{3!} C_3 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^3$$

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

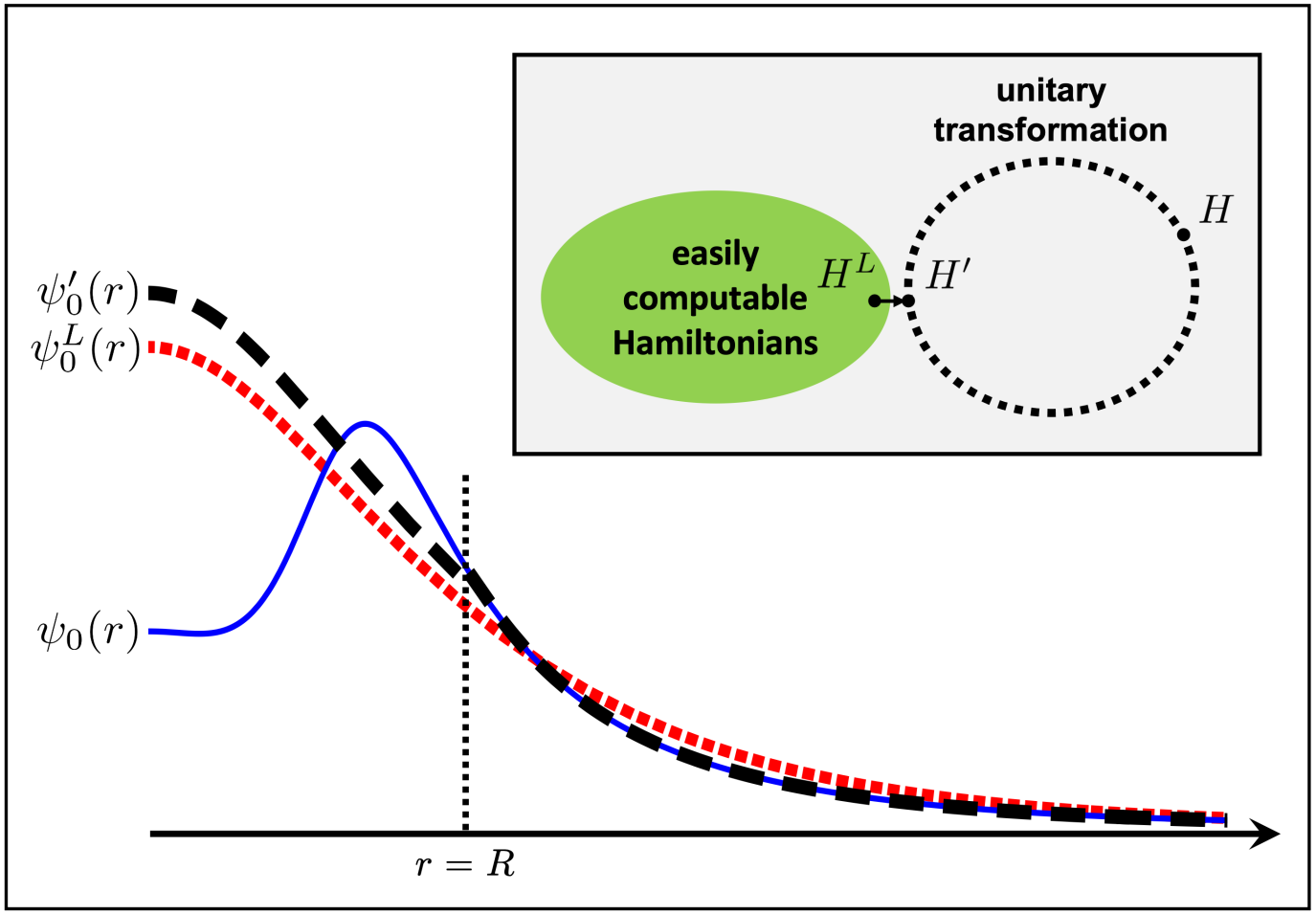
$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}')$$



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

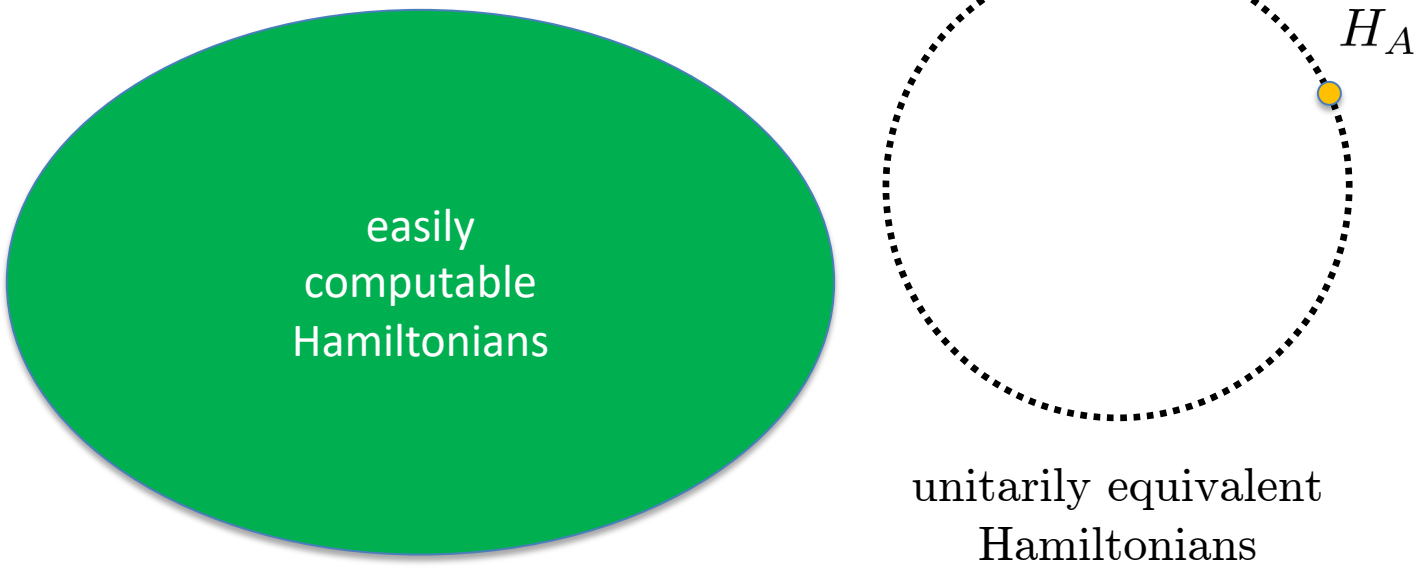
Lattice Monte Carlo simulations can compute highly nontrivial correlations in nuclear many-body systems. Unfortunately, sign oscillations prevent direct simulations using a high-fidelity Hamiltonian based on chiral effective field theory due to short-range repulsion.

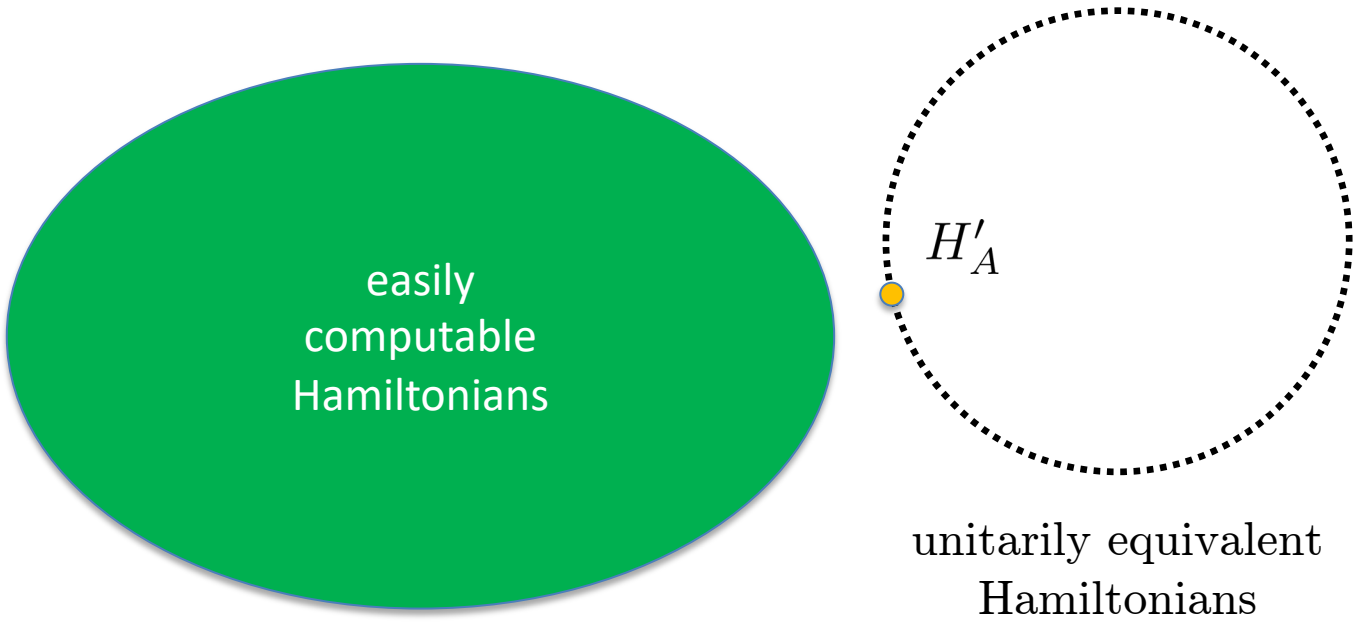
Wave function matching



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

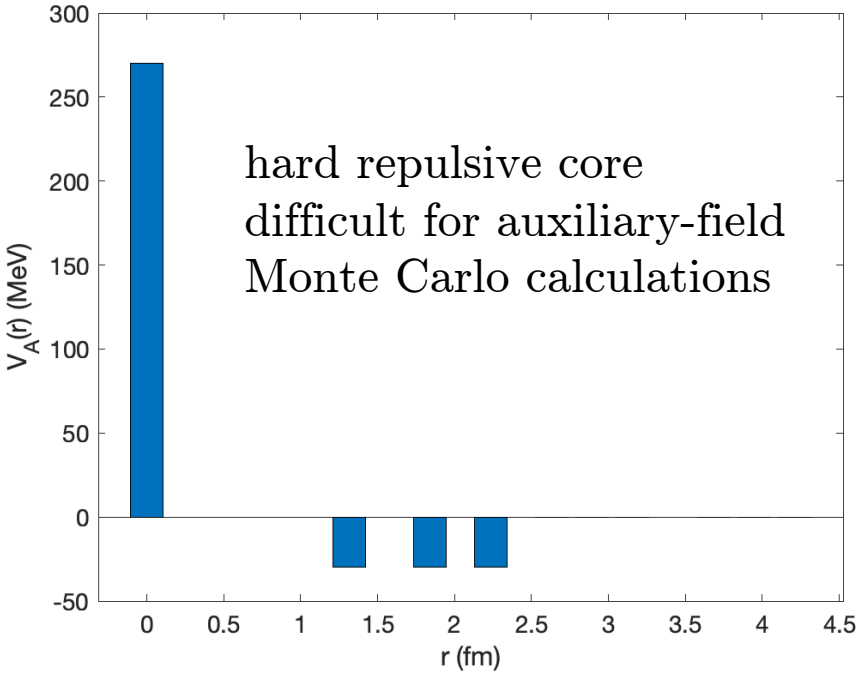

easily
computable
Hamiltonians
H_A


easily
computable
Hamiltonians
H_A
unitarily equivalent
Hamiltonians


easily
computable
Hamiltonians
H'_A
unitarily equivalent
Hamiltonians

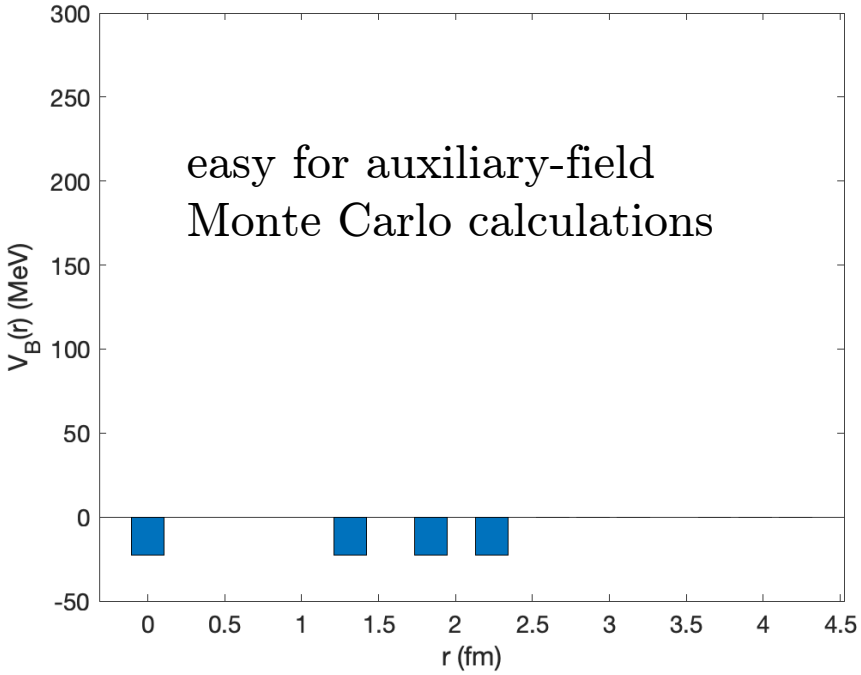
Wave function matching

$V_A(r)$



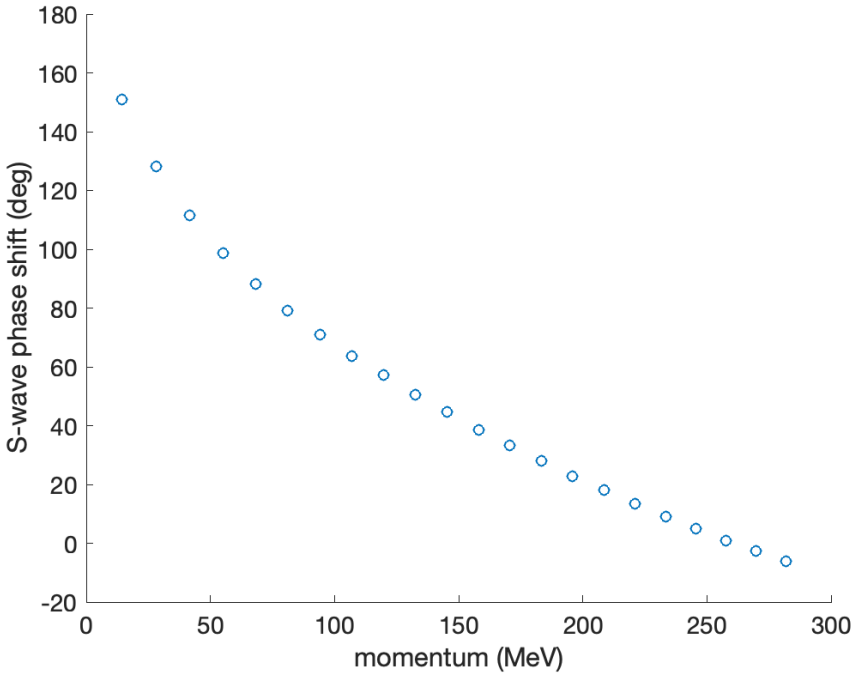
hard repulsive core
difficult for auxiliary-field
Monte Carlo calculations

$V_B(r)$

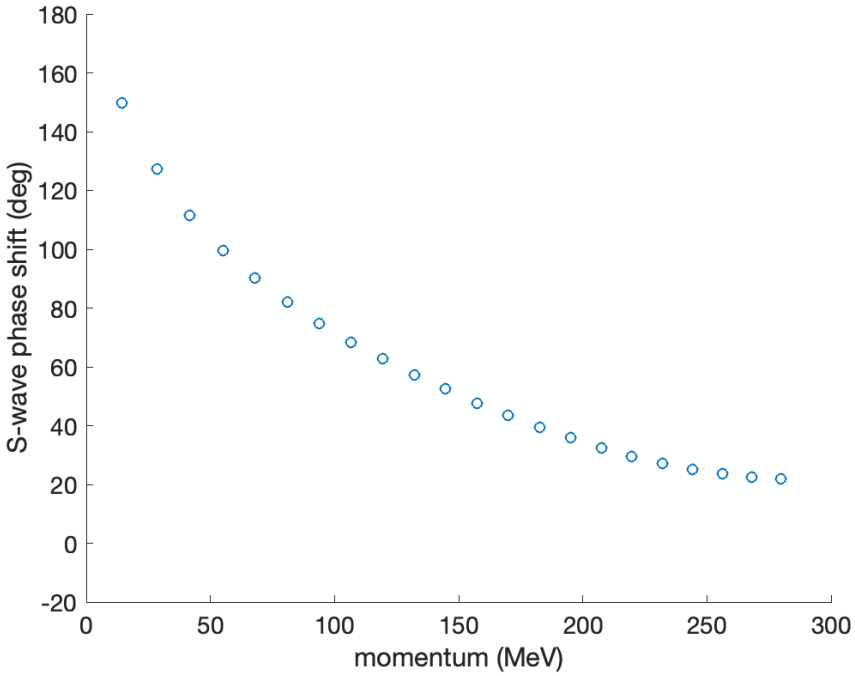


easy for auxiliary-field
Monte Carlo calculations

$V_A(r)$


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
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80
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40
20
0
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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

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

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

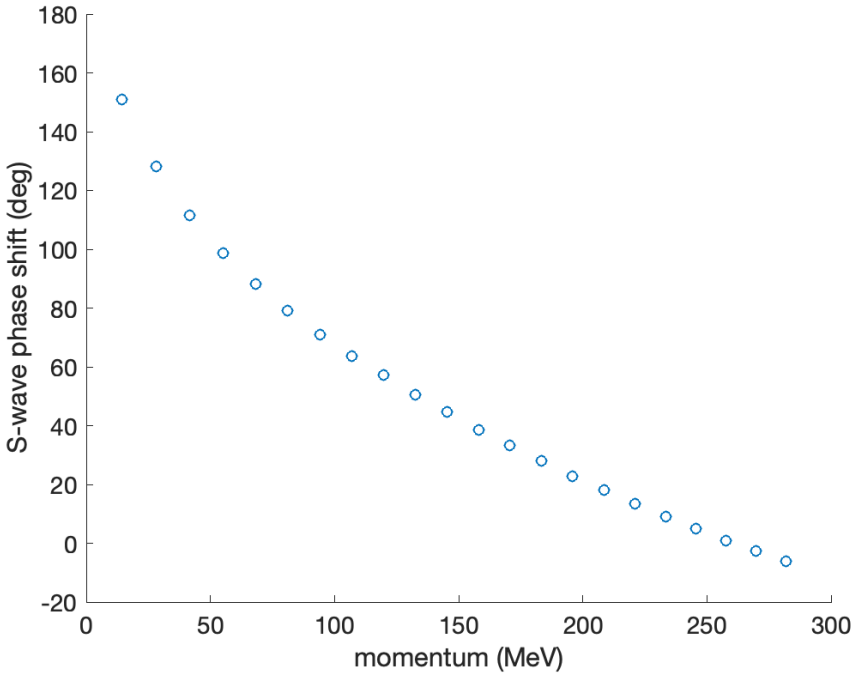
$$U : H_A \rightarrow H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

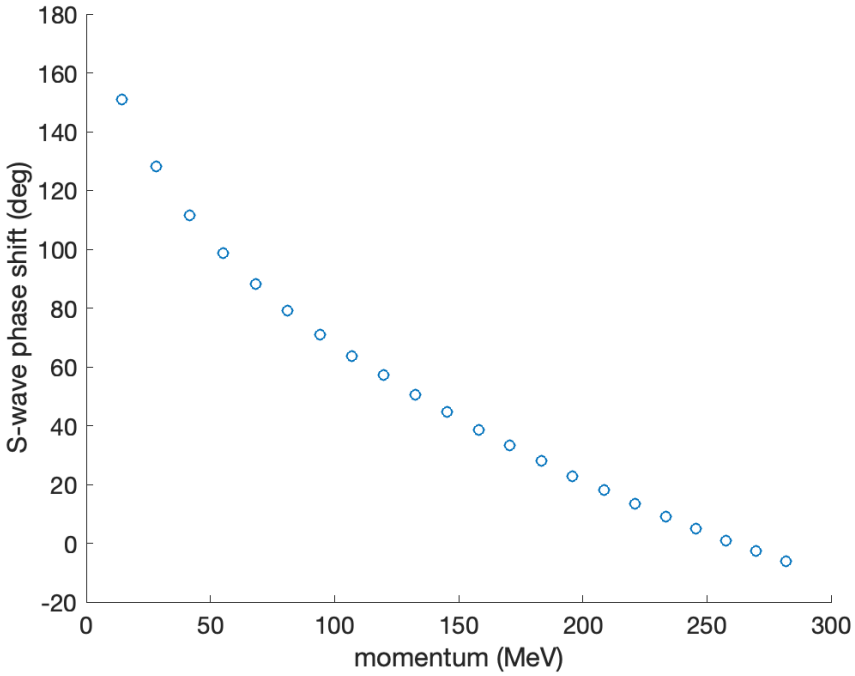
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

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

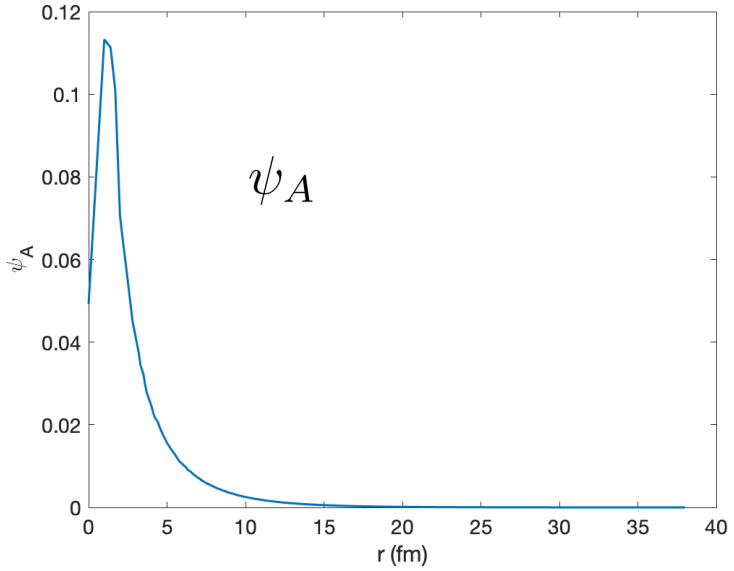
$V_A(r)$

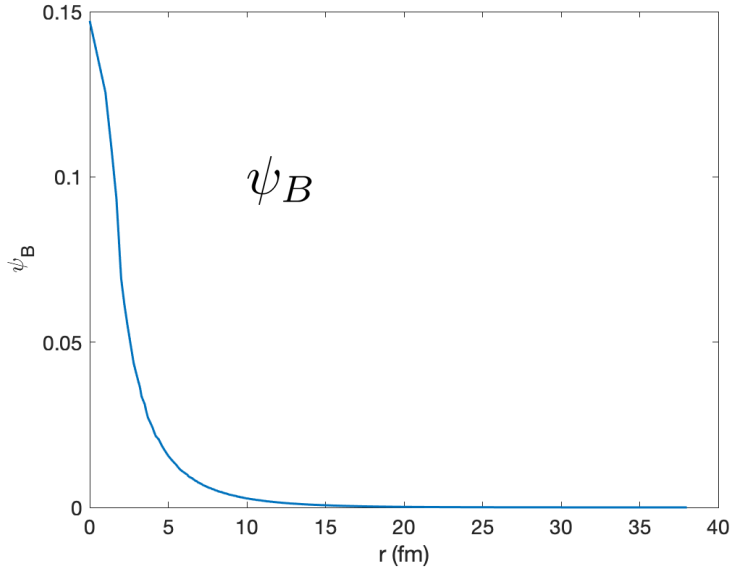


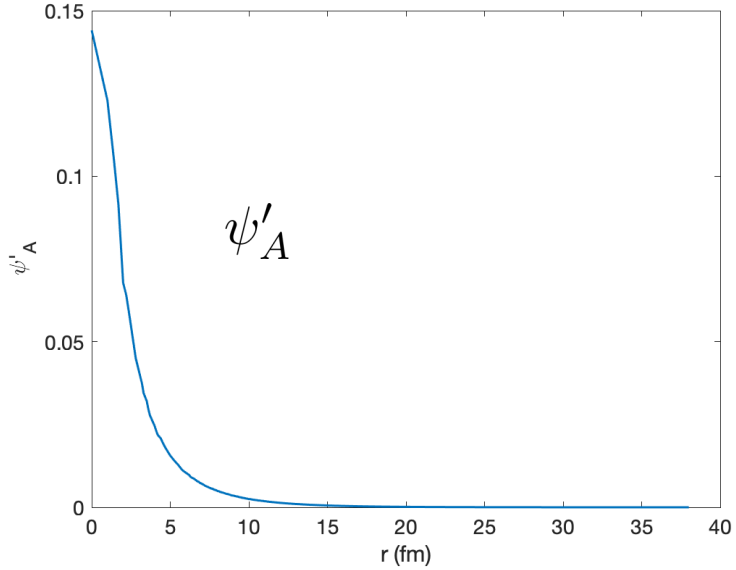
$V'_A(r, r')$



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.

$R = 2.6$ 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

Analyticity

The unitary transformation used in wave function matching is locally integrable and differs from the identity only within a compact domain. The nontrivial part of the transformation is

$$f(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}') \equiv U(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}') - \delta_{\mathbf{S},\mathbf{S}'}\delta_{\mathbf{I},\mathbf{I}'}\delta^3(\mathbf{r}-\mathbf{r}')$$

$$f(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}') = 0 \qquad \text{if} \;\; |\mathbf{r}| > R \;\; \text{or} \;\; |\mathbf{r}'| > R$$

In momentum space, the nontrivial part is

$$\tilde{f}(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{p},\mathbf{p}') = \int d^3\mathbf{r} d^3\mathbf{r}' e^{i\mathbf{p}\cdot\mathbf{r}} e^{i\mathbf{p}'\cdot\mathbf{r}'} f(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}')$$

The momentum space nontrivial part is differentiable for all values of momenta.

$$\nabla_{\mathbf{p}} \tilde{f}(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{p},\mathbf{p}') = \int d^3\mathbf{r} d^3\mathbf{r}' \; i\mathbf{r} \; e^{i\mathbf{p}\cdot\mathbf{r}} e^{i\mathbf{p}'\cdot\mathbf{r}'} \, f(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}')$$

$$\nabla_{\mathbf{p}'} \tilde{f}(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{p},\mathbf{p}') = \int d^3\mathbf{r} d^3\mathbf{r}' \; i\mathbf{r}' \; e^{i\mathbf{p}\cdot\mathbf{r}} e^{i\mathbf{p}'\cdot\mathbf{r}'} \, f(\mathbf{S},\mathbf{S}';\mathbf{I},\mathbf{I}';\mathbf{r},\mathbf{r}')$$

The wave function matching transformation is analytic everywhere in momentum space. It does not produce any new non-analytic behavior. It defines a new low-energy effective field theory with the same breakdown scale as the original low-energy effective field theory.

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

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

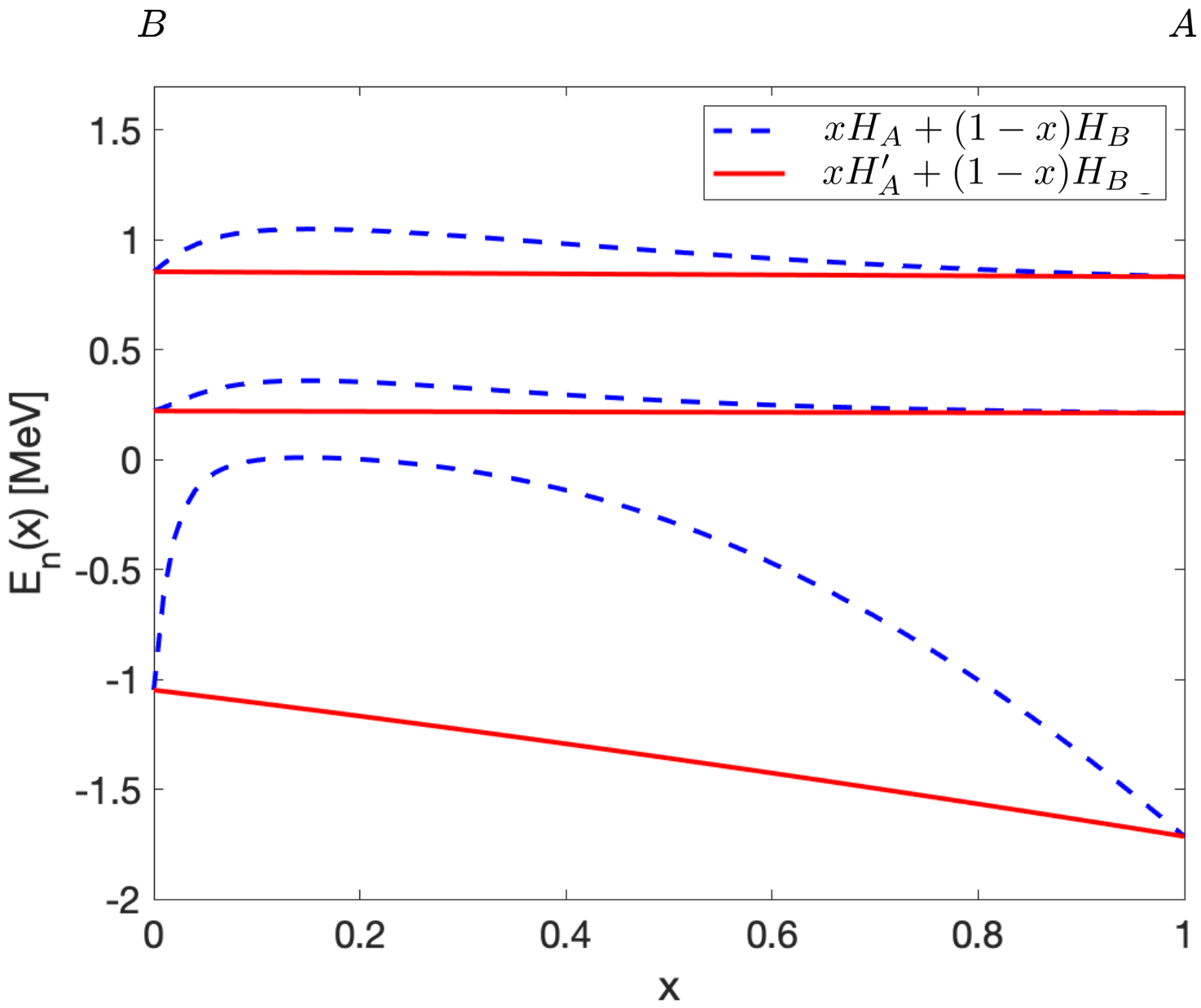
has the eigenvectors of H_B but has the eigenvalues of H_A. We call U_{AB} and U_{BA} Hamiltonian translators.

We can construct a Hamiltonian translator using quantum adiabatic evolution

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

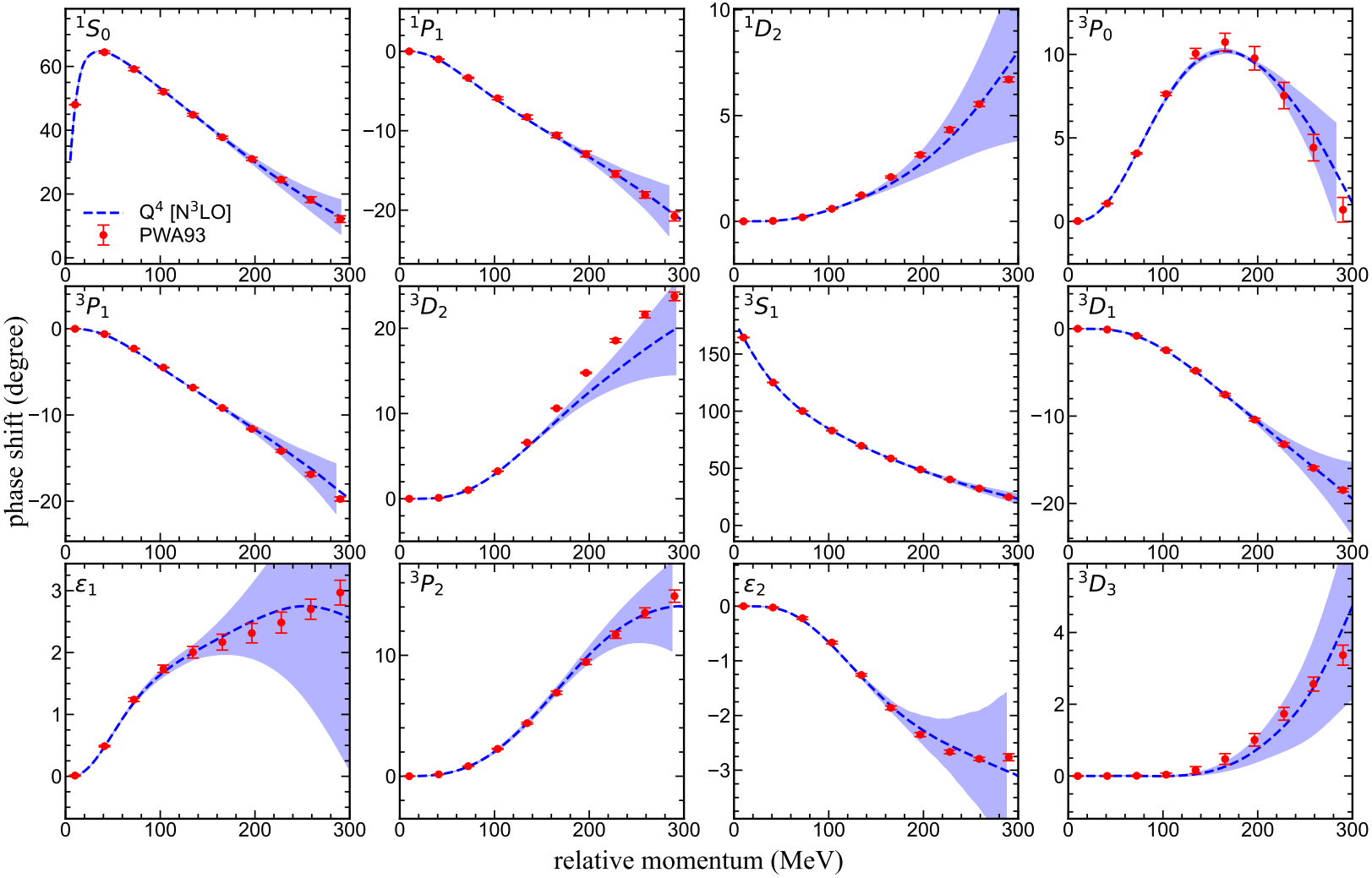
where $H_T(t)$ smoothly interpolates between H_B and H_A as t goes from 0 to T.

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

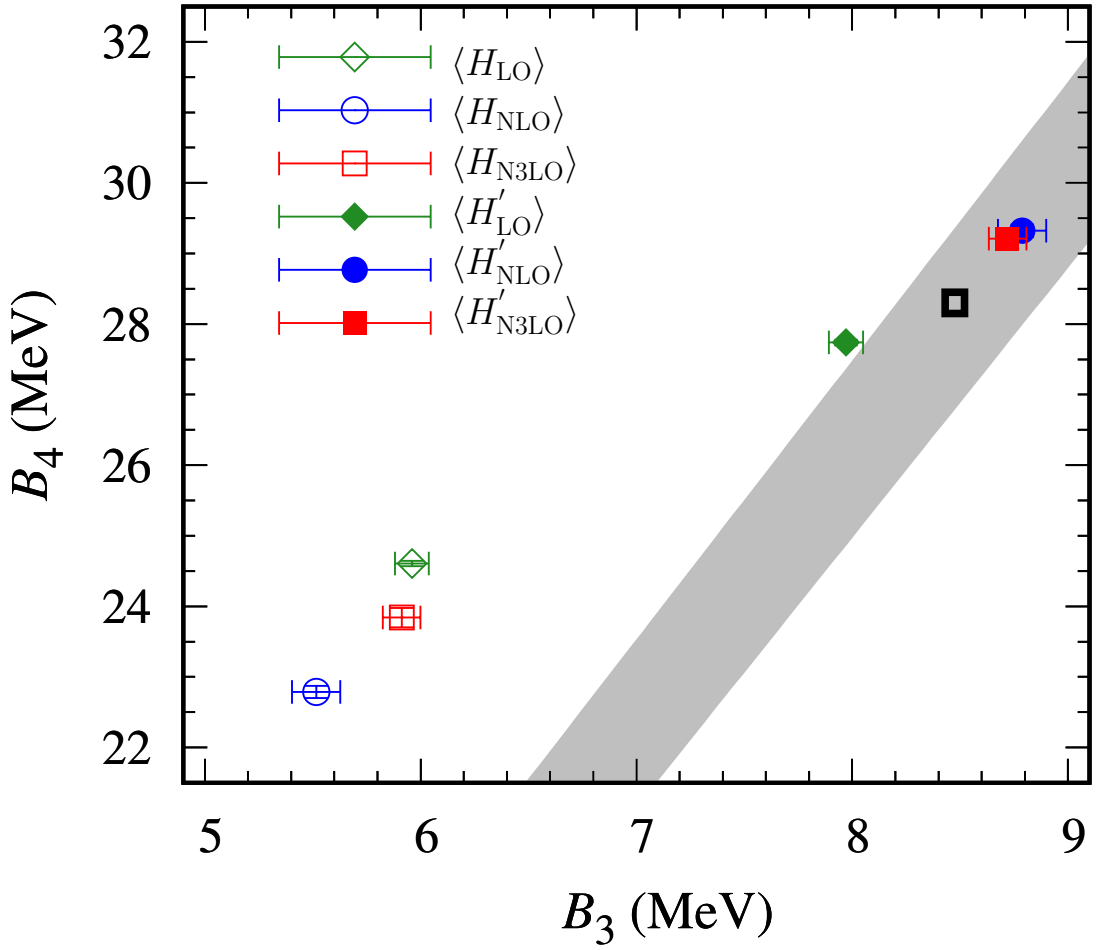


straight lines mean the eigenvectors don't change with x

N3LO chiral effective field theory interaction

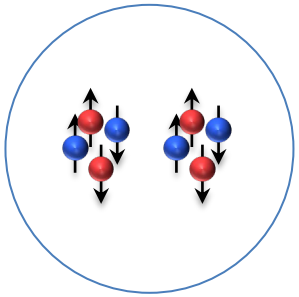


Tjon line

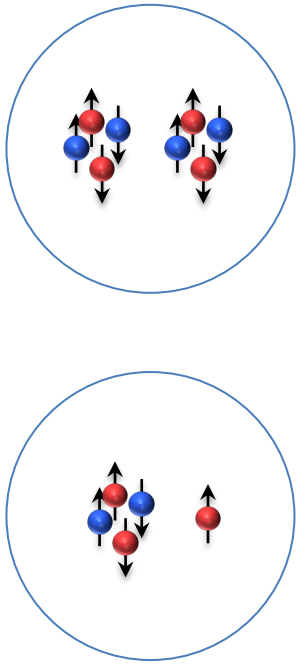


Tjon, Phys. Lett. B 56, 217 (1975); Nogga, Kamada, Glöckle, Phys. Rev. Lett. 85, 944 (2000); Platter, Hammer, Meißner, Phys. Lett. B607, 254 (2005)

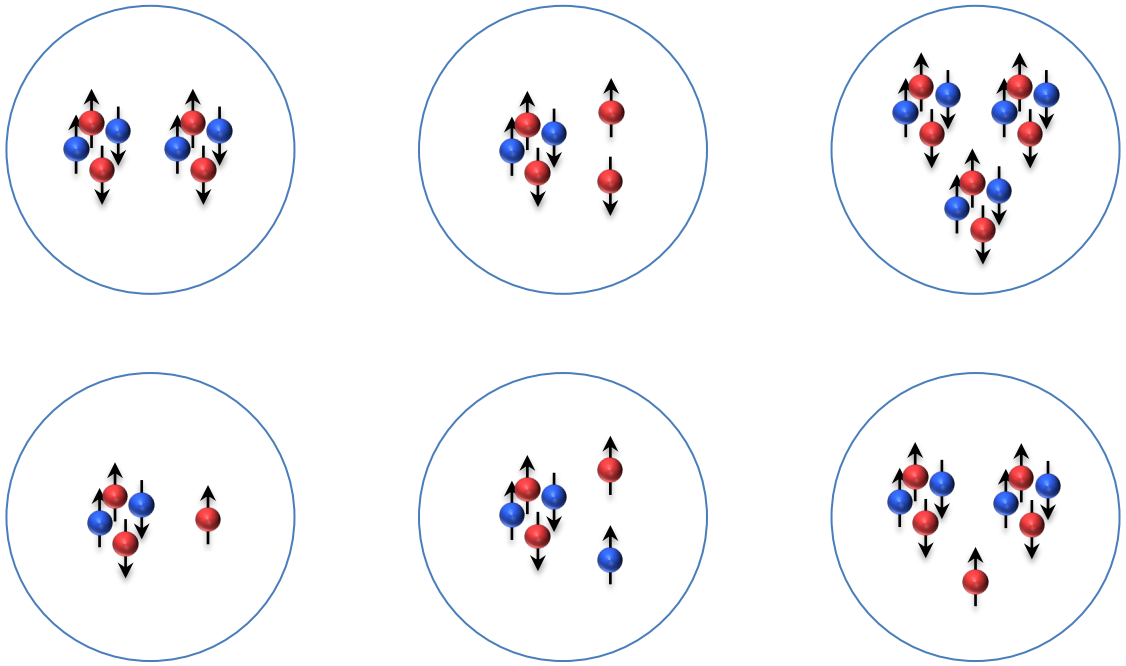
Sensitivity to short-distance physics



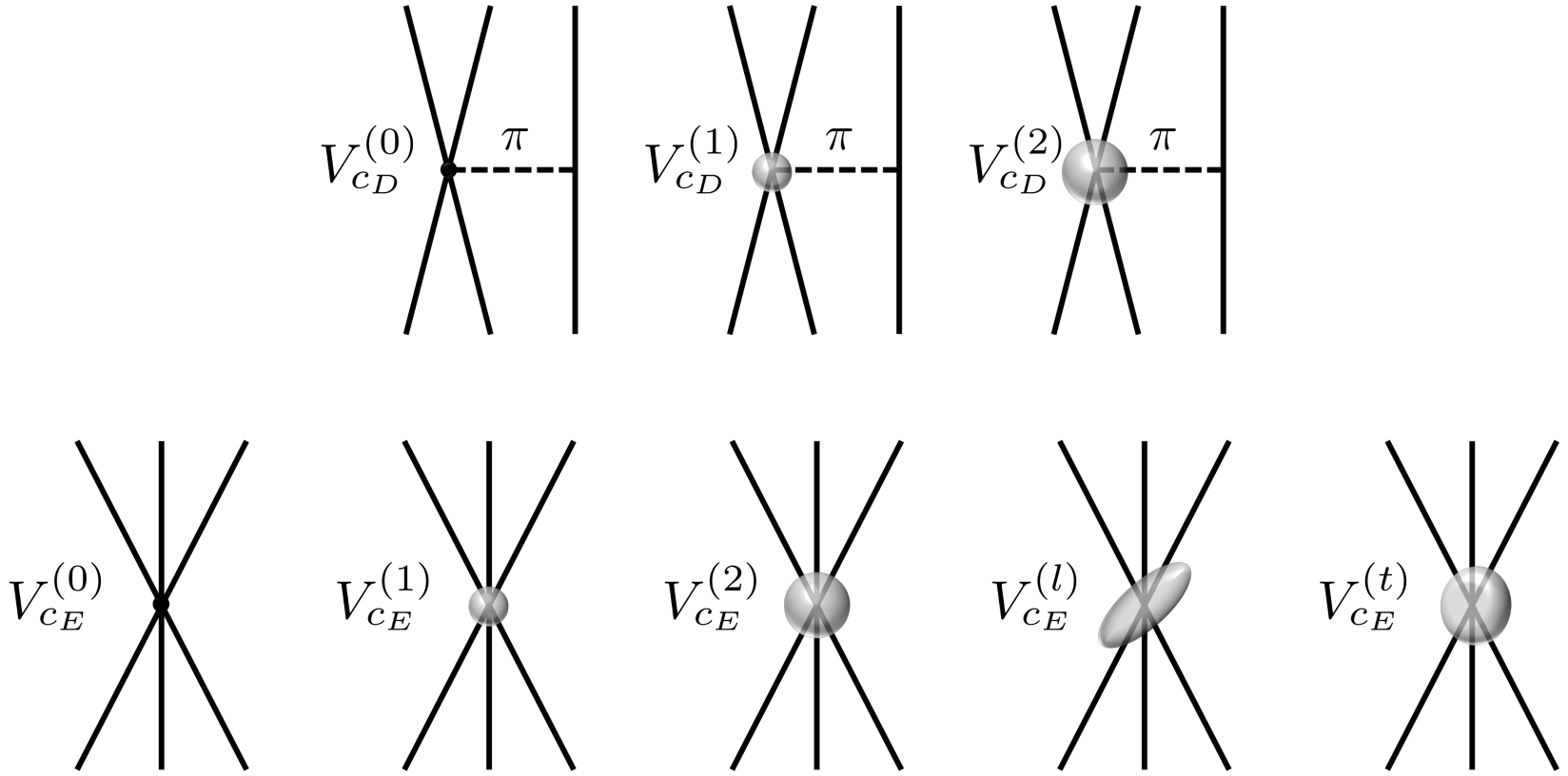
Sensitivity to short-distance physics



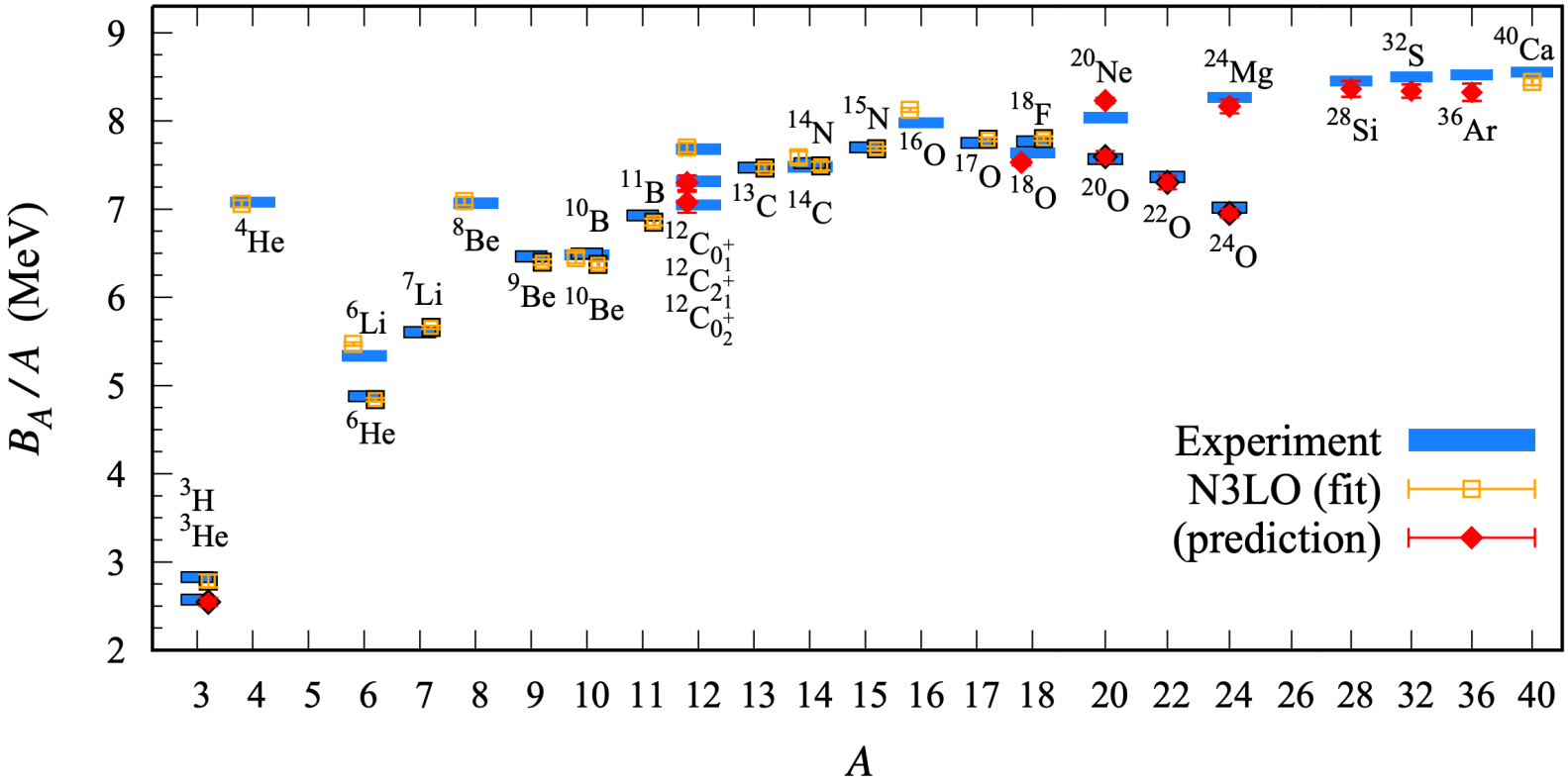
Sensitivity to short-distance physics



Short-distance three-nucleon interactions

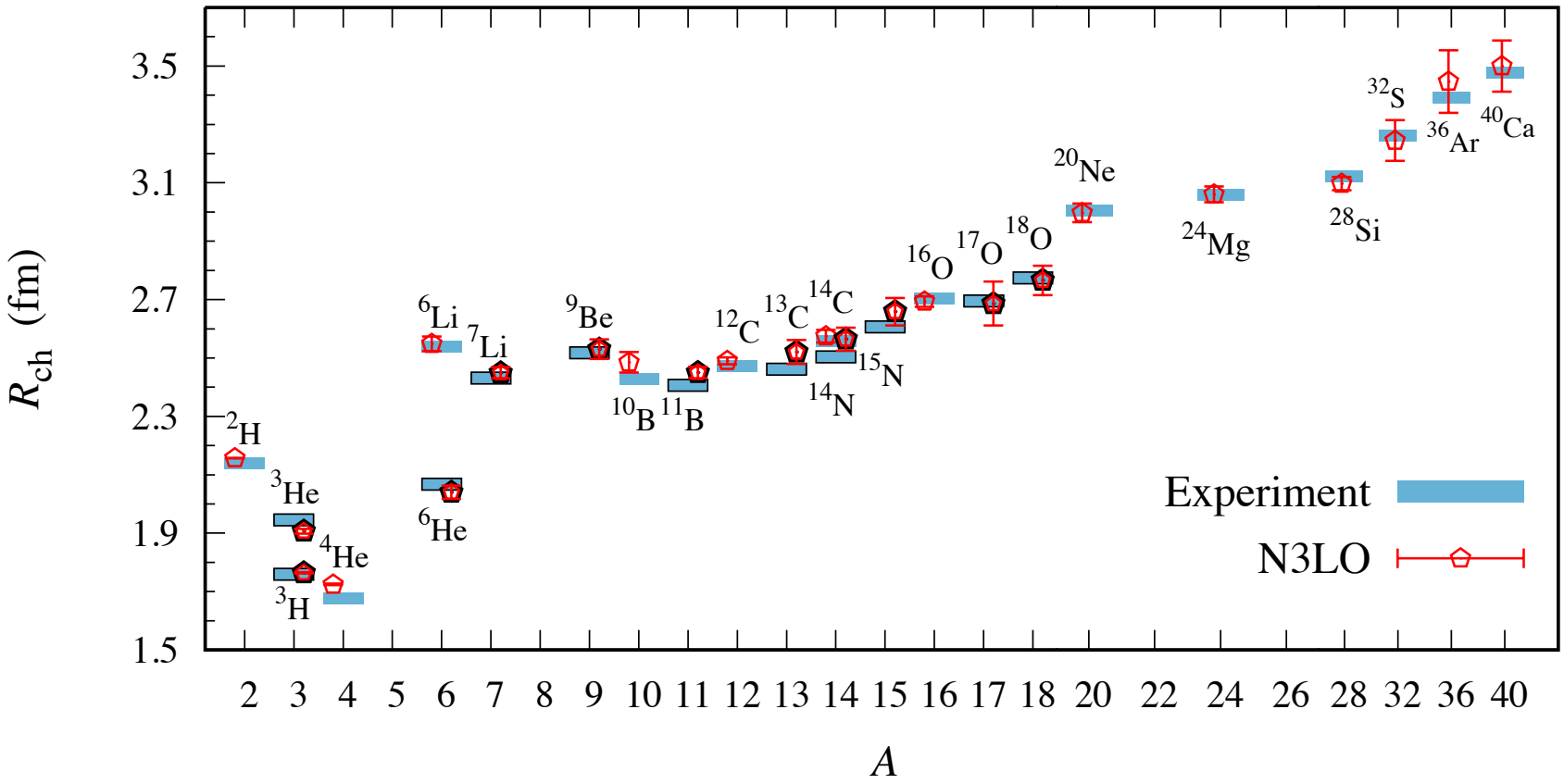


Binding energy per nucleon



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

Charge radius



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Neutron and nuclear matter

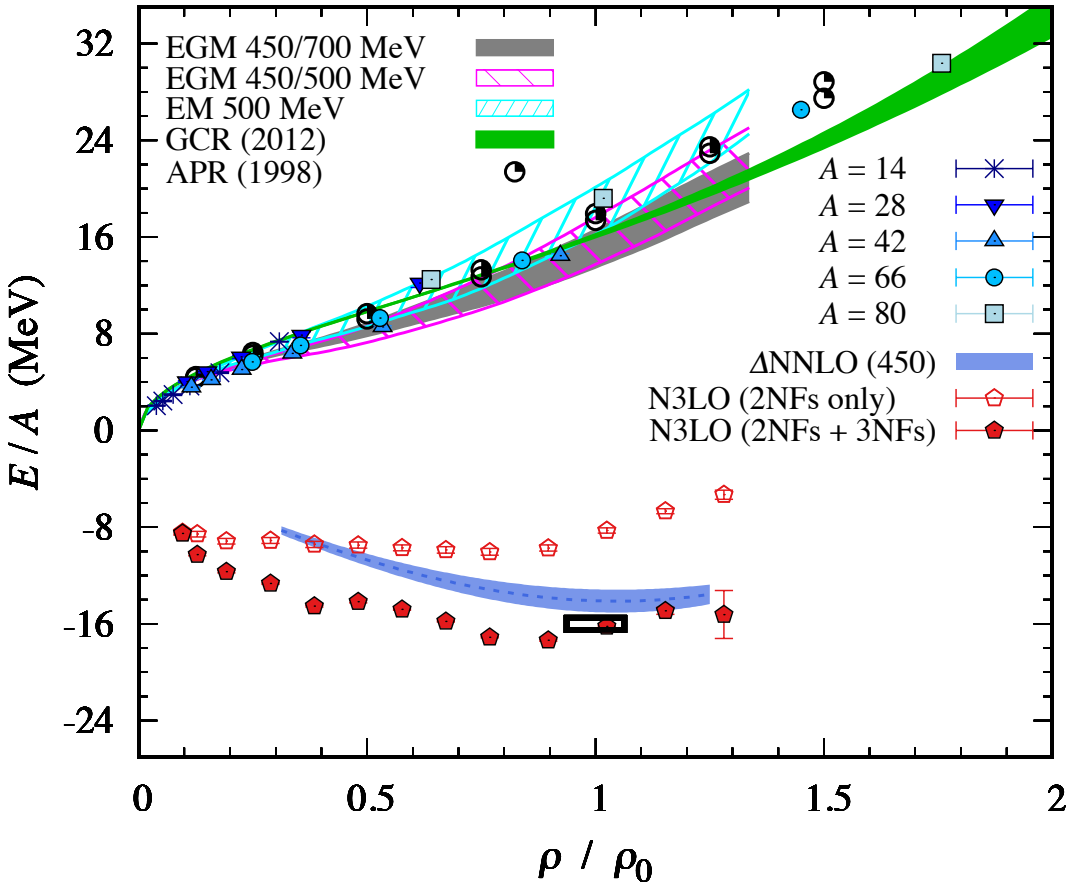
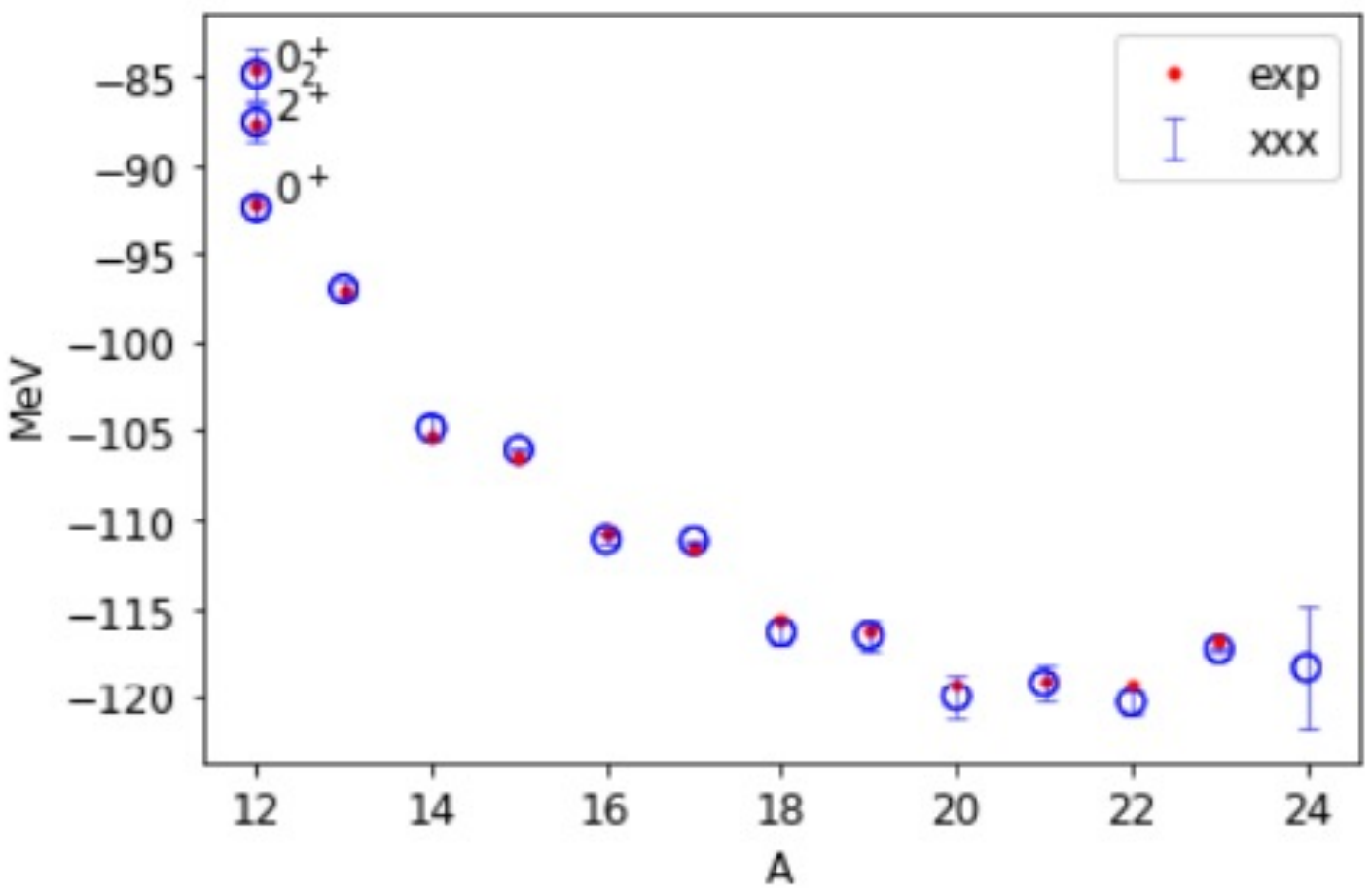


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

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



M. Kim, Song, Y. Kim, et al., work in progress

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.