Wave function matching

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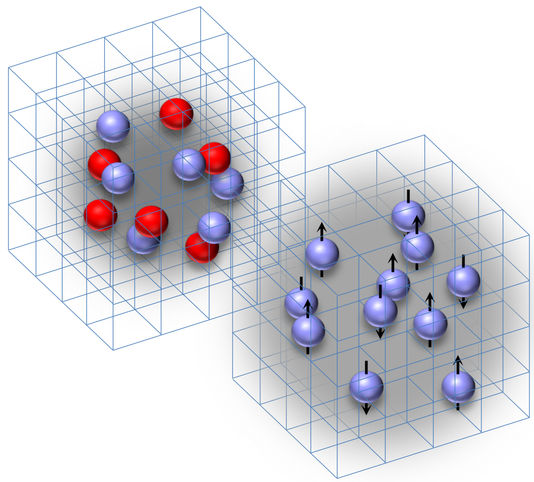


ERC EXOTIC Workshop
Frontiers in Nuclear Physics
Bethe Center for Theoretical Physics
University of Bonn
November 22, 2023

Outline

Essential elements for nuclear binding

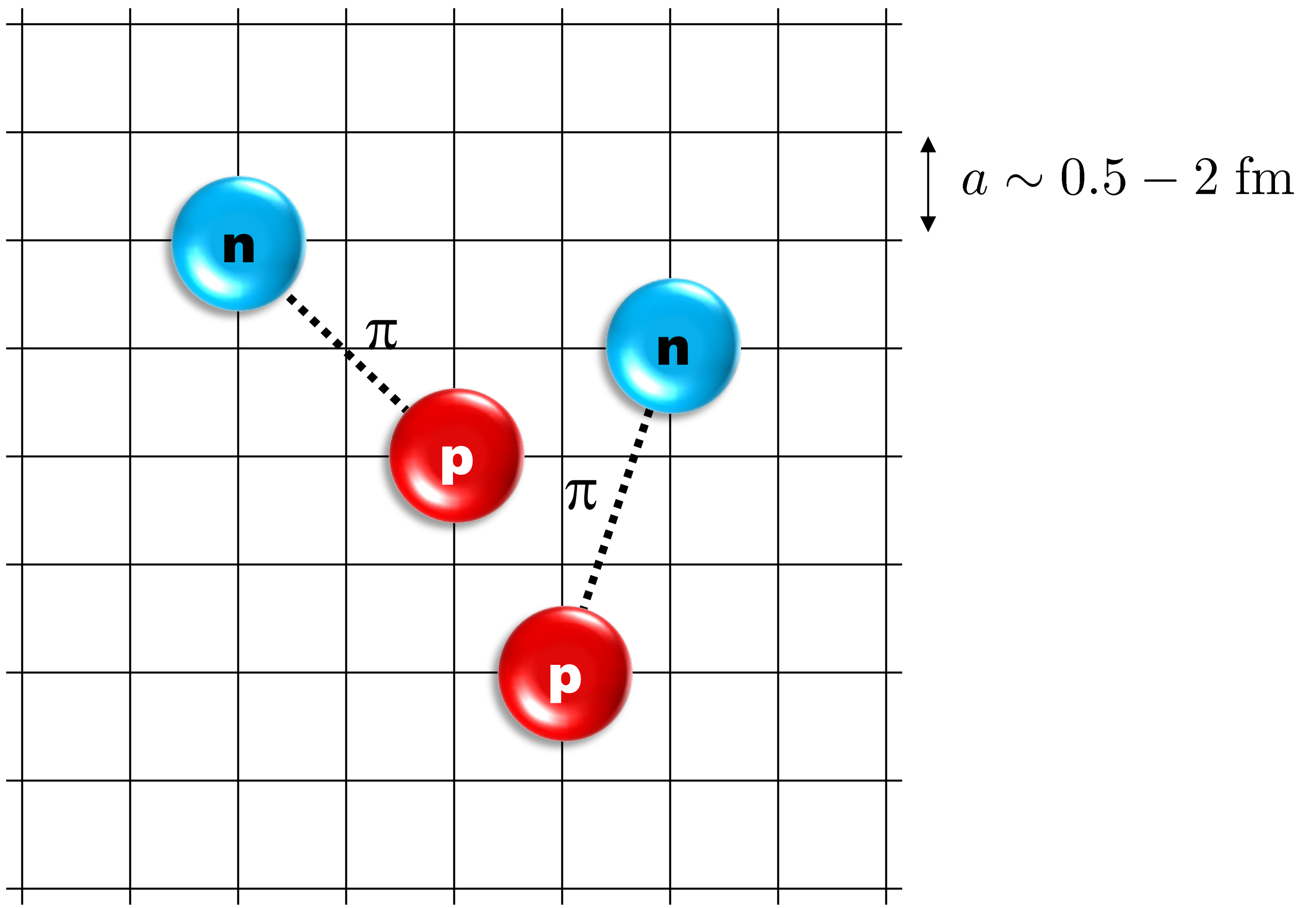
Wave function matching

Applications to nuclear structure

Theory of wave function matching

Summary

Lattice effective field theory



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

Essential elements for nuclear binding

See Shihang's talk from Tuesday

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)

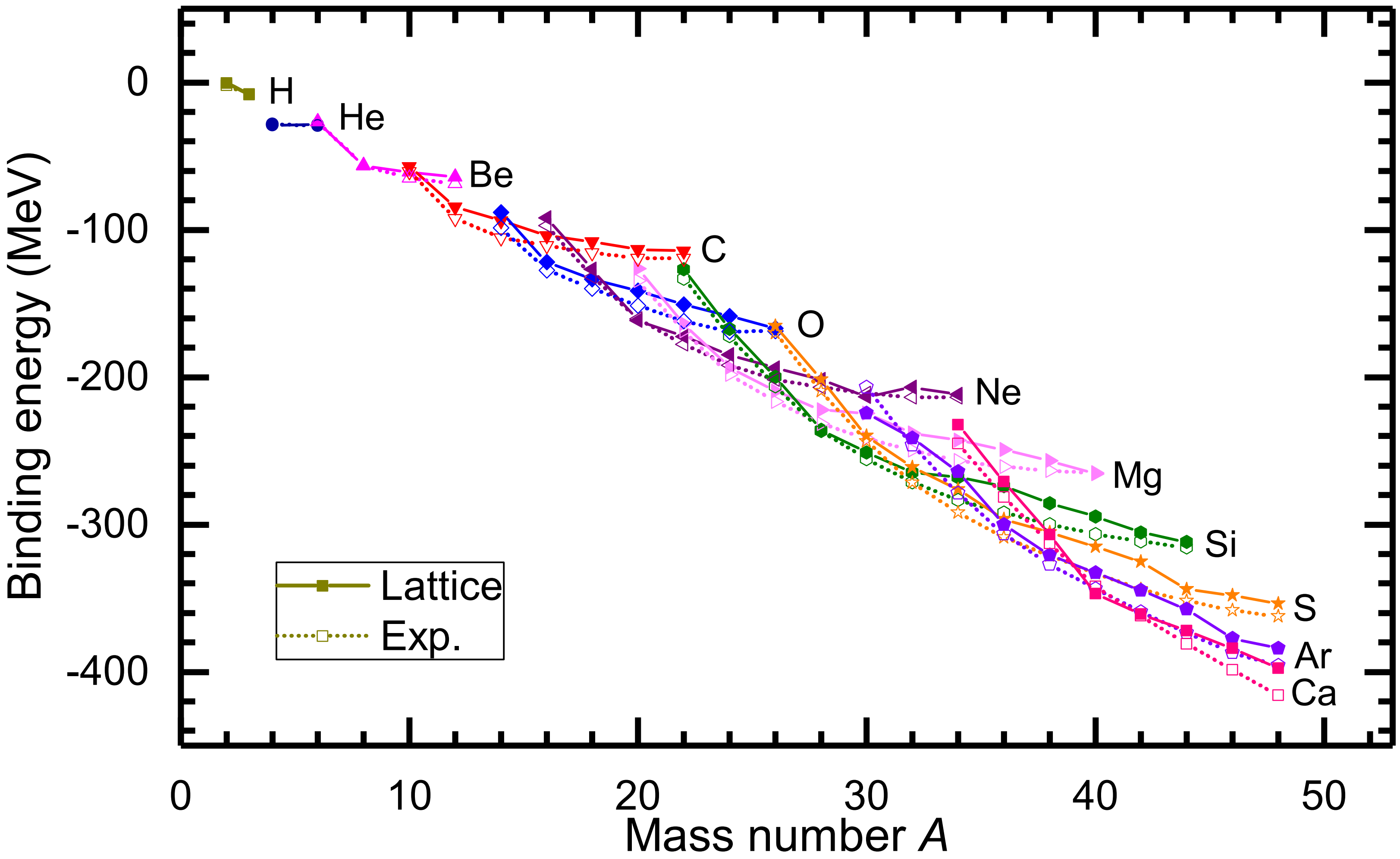
The lattice Hamiltonian has the form of a smeared four-component Hubbard model with two-body and three-body interactions

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

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

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

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

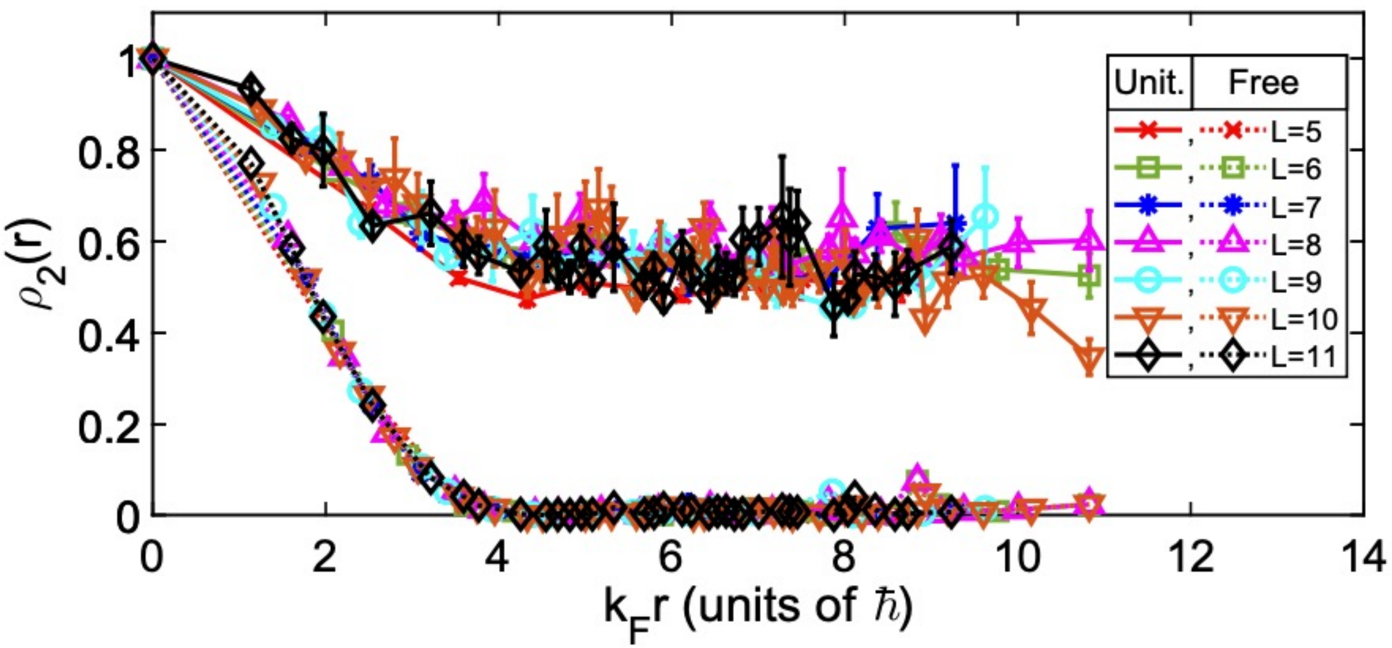


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

Lattice Monte Carlo simulations can compute highly nontrivial correlations in quantum many-body systems …

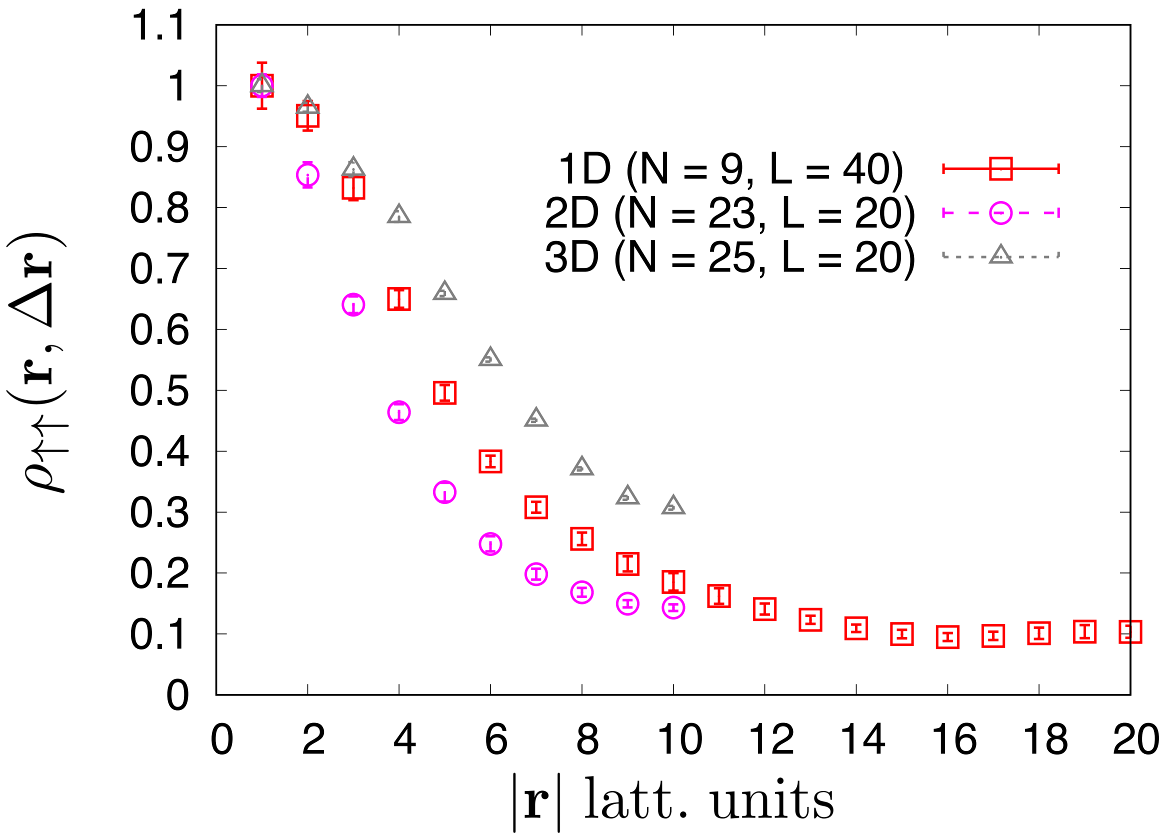
Superfluidity

Ground state S-wave superfluid long-range order in the unitary limit



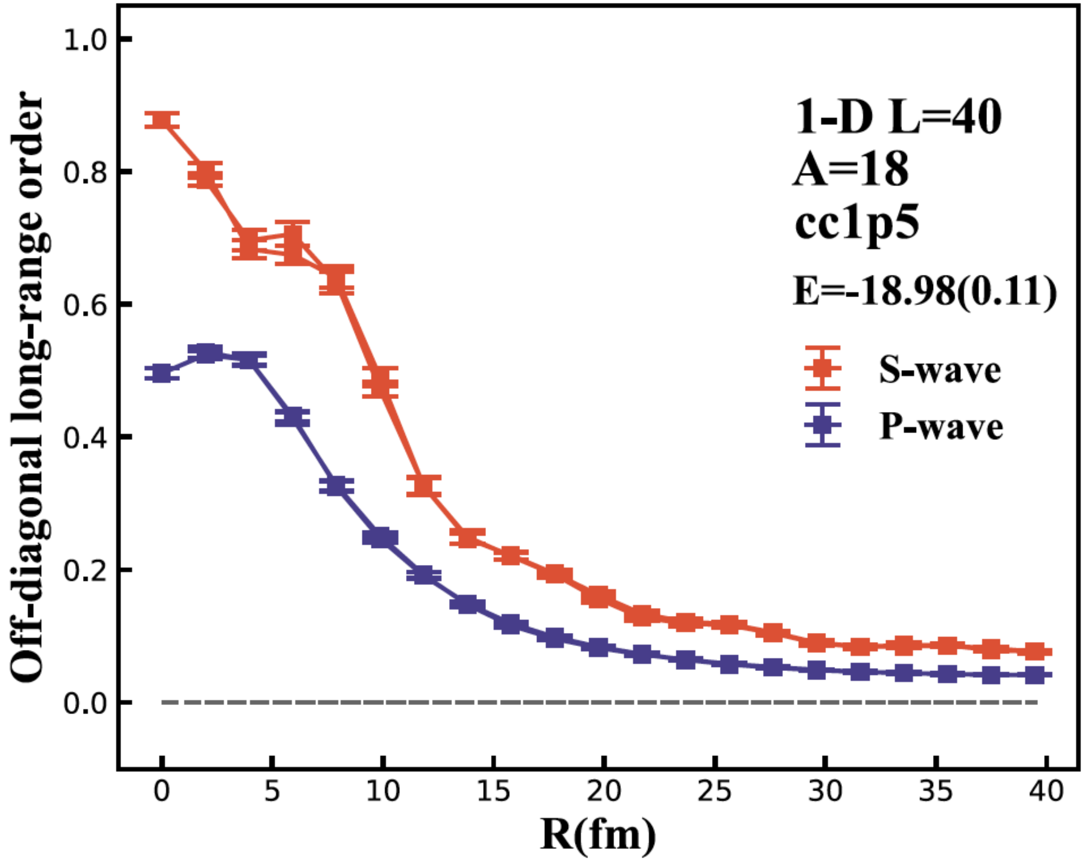
He, Li, Lu, D.L., Phys. Rev. A 101, 063615 (2020)

Ground state P-wave superfluid long-range order for polarized fermions



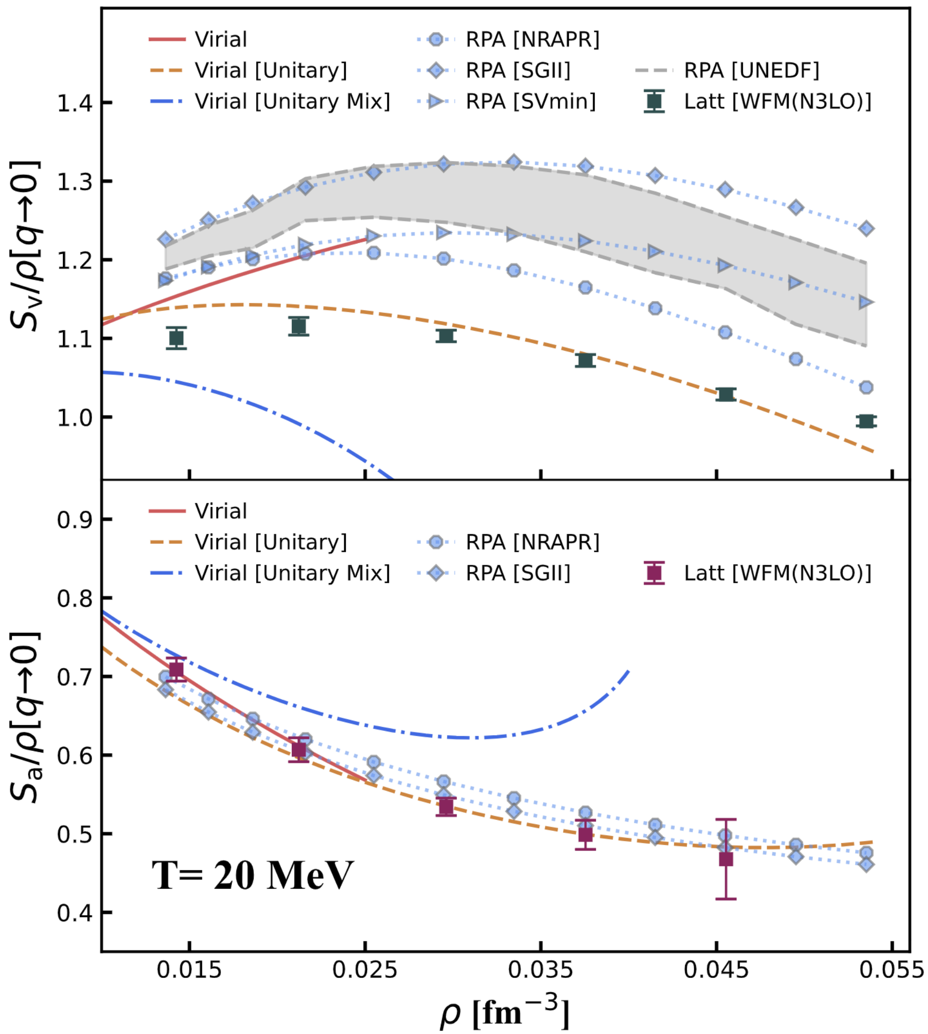
Work in progress: Ma, Given, Hicks, Carlson, Gandolfi, Gezerlis, Palkanoglou, Schmidt, D.L.

Spin-balanced fermions: Simultaneous S-wave and P-wave superfluidity



Work in progress: Ma, Given, Hicks, Carlson, Gandolfi, Gezerlis, Palkanoglou, Schmidt, D.L.

Static structure factors for hot dilute neutron matter

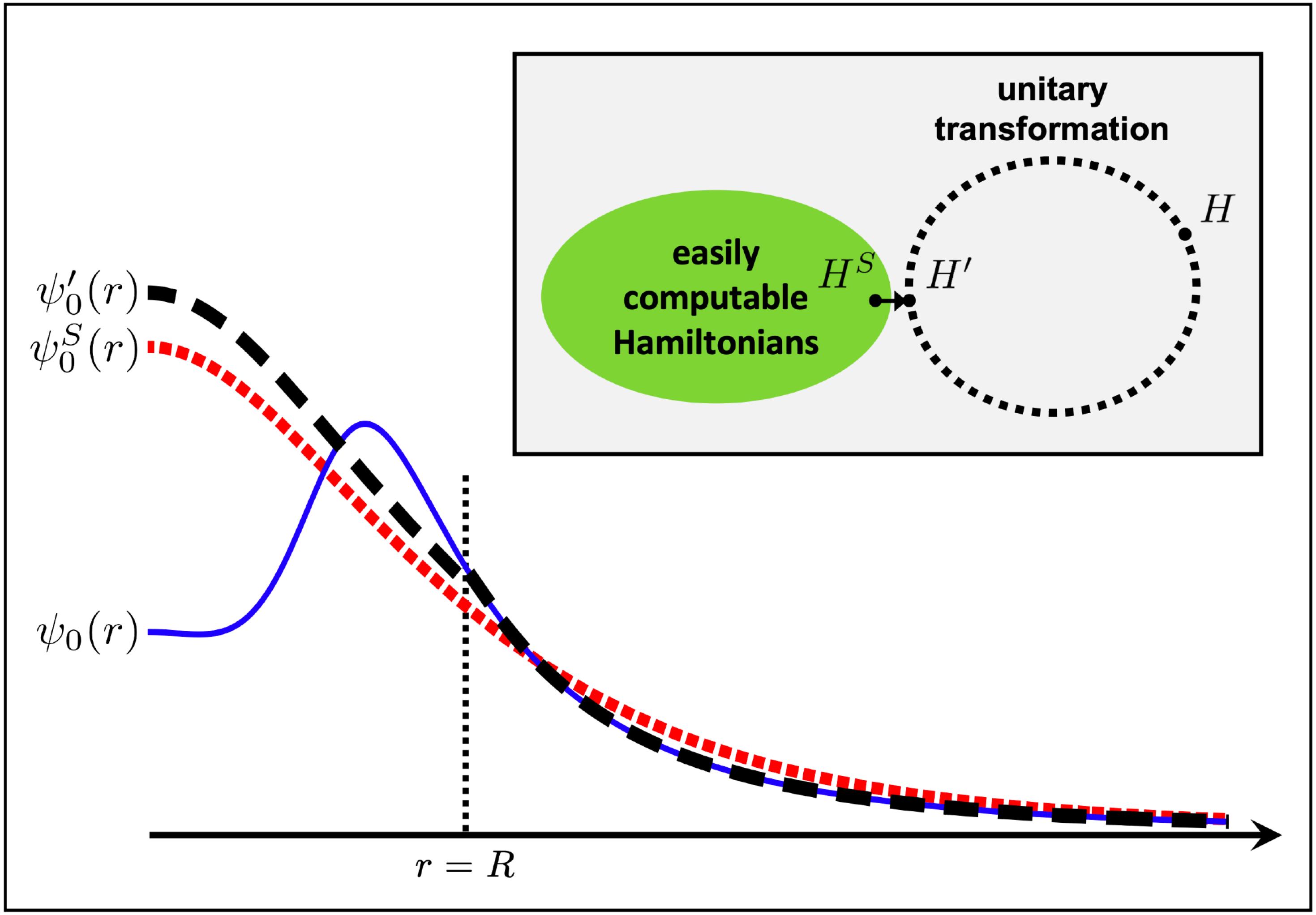


Ma, Lin, Lu, Elhatisari, D.L., Li, Meißner, Steiner, Wang, arXiv:2306.04500

Lattice Monte Carlo simulations can compute highly nontrivial correlations in quantum 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.

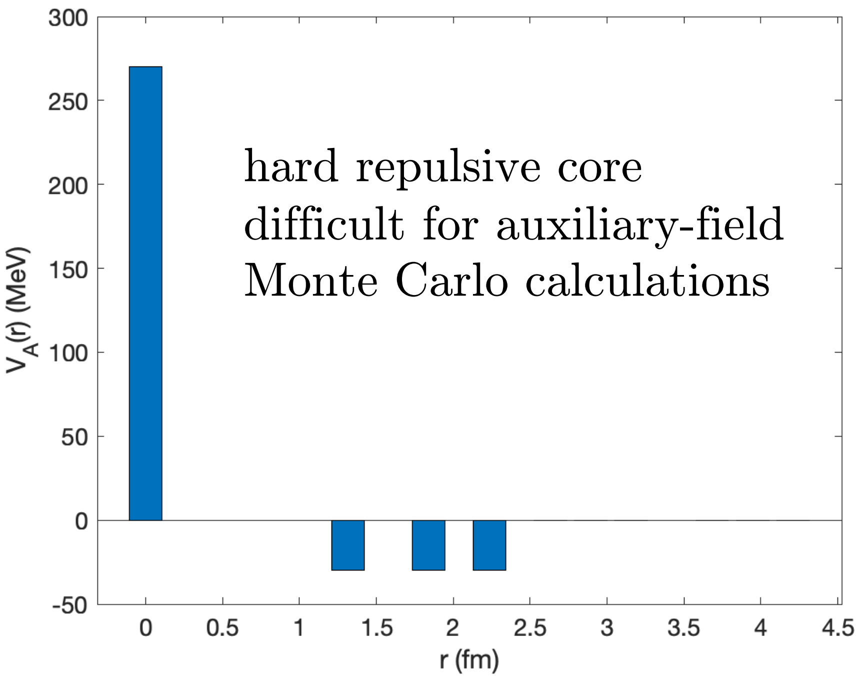
Wave function matching



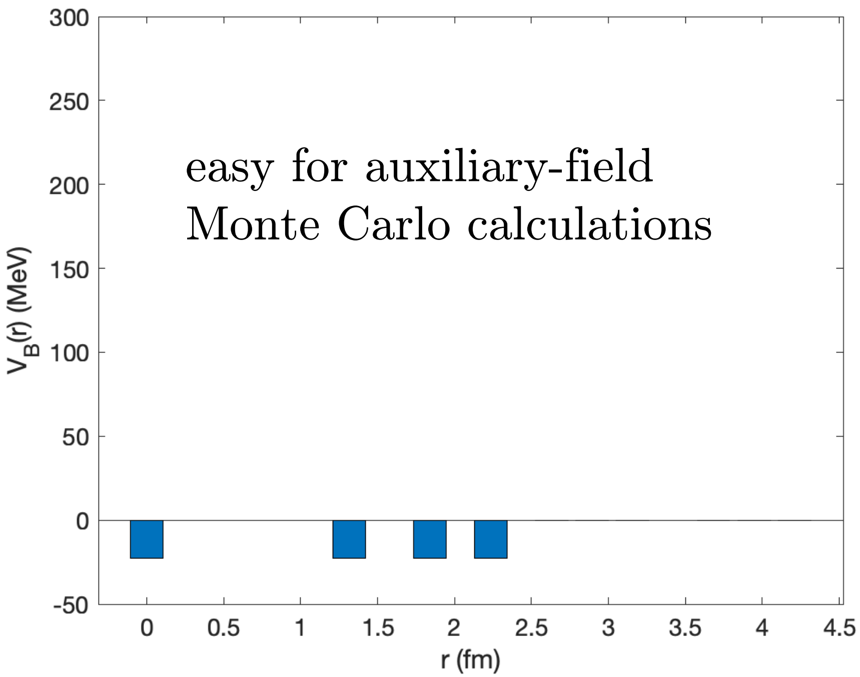
Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin, arXiv: 2210.17488

Wave function matching

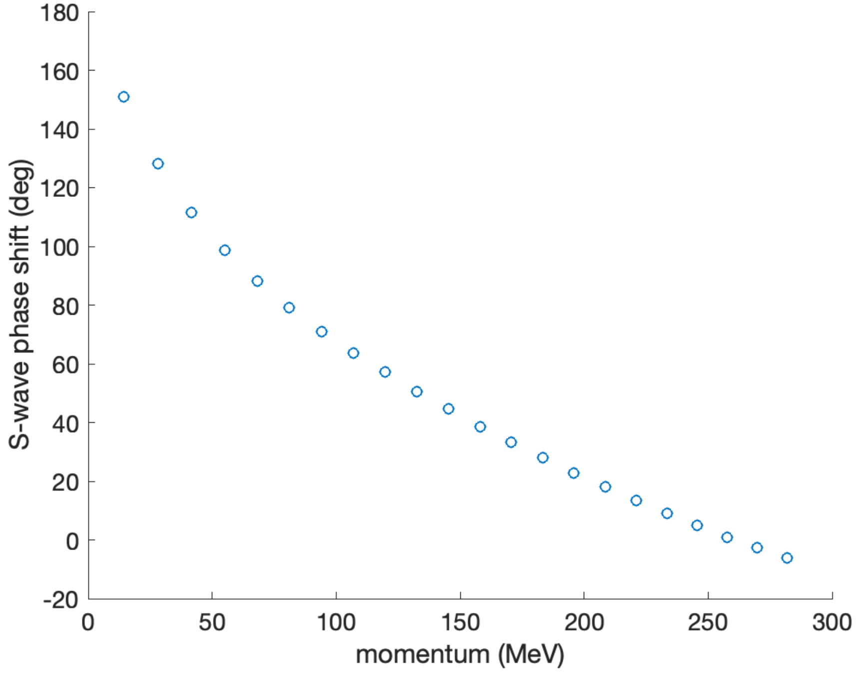
$V_A(r)$



$V_B(r)$

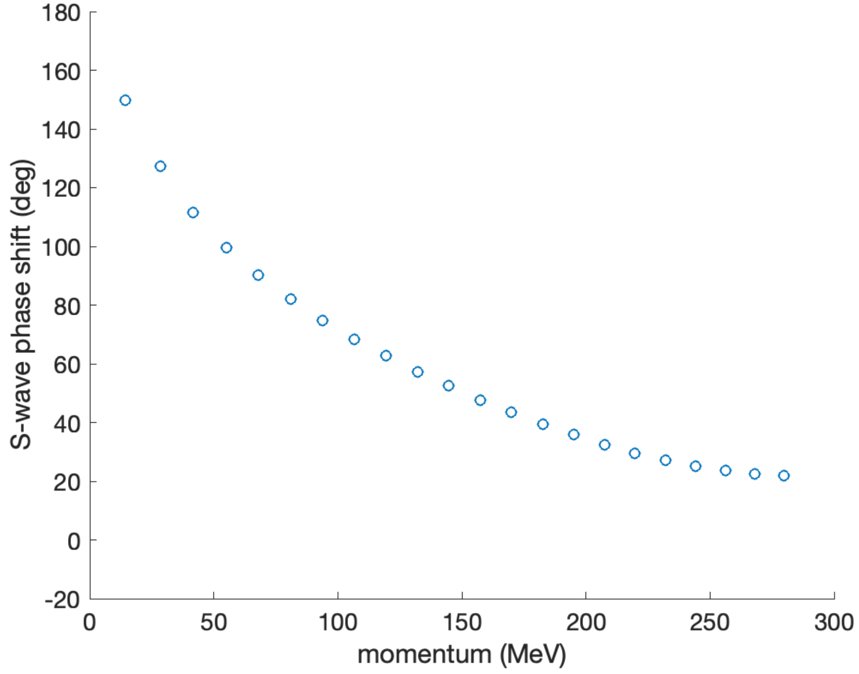


$V_A(r)$



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

$V_B(r)$



S-wave phase shift (deg)
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150
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250
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momentum (MeV)

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)	$\langle \psi_{B,n} \vert H_A \vert \psi_{B,n} \rangle$ (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_R be a projection operator that is nonzero only for separation distances r less than R.

We define a finite-range unitary operator U that vanishes beyond distance R. We require that

$$U : \frac{P_R|\psi_B^0\rangle}{\|P_R|\psi_B^0\rangle\|} \to \frac{P_R|\psi_A^0\rangle}{\|P_R|\psi_A^0\rangle\|}$$

There are many possible choices to complete the unitary transformation.

$$U : |\phi_j\rangle \to U\,|\phi_j\rangle$$

$$|\phi_j\rangle \perp P_R\,|\psi_B^0\rangle \qquad j = 1, 2, \cdots$$

Bovermann, Epelbaum, Krebs, Lähde, D.L., PoS, LATTICE2021

The corresponding action of U on the Hamiltonian is

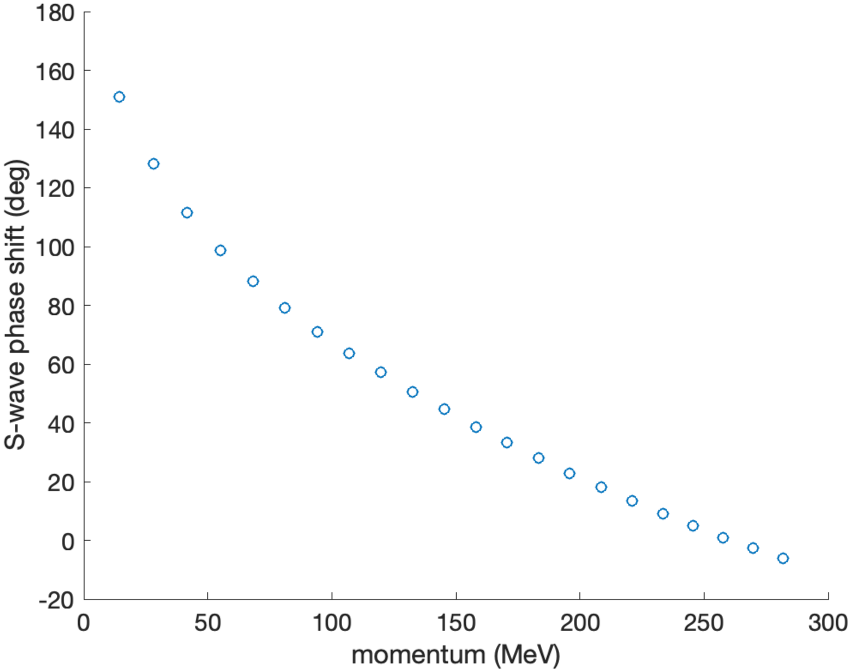
$$U : H_A \to H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

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

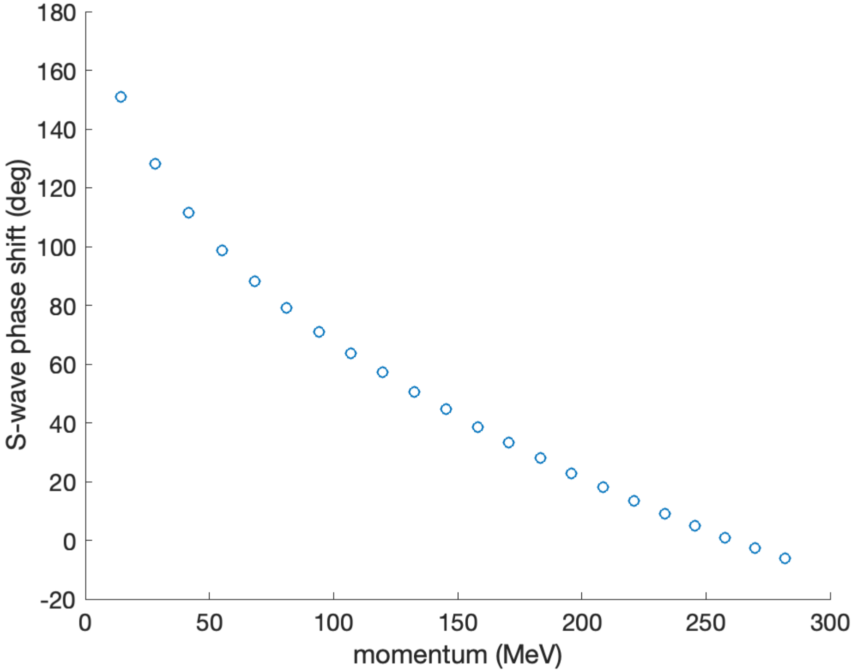
Since they are unitarily equivalent, the phase shifts for the original and transformed Hamiltonians are exactly the same

$$V_A(r)$$



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

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



S-wave phase shift (deg)
180
160
140
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250
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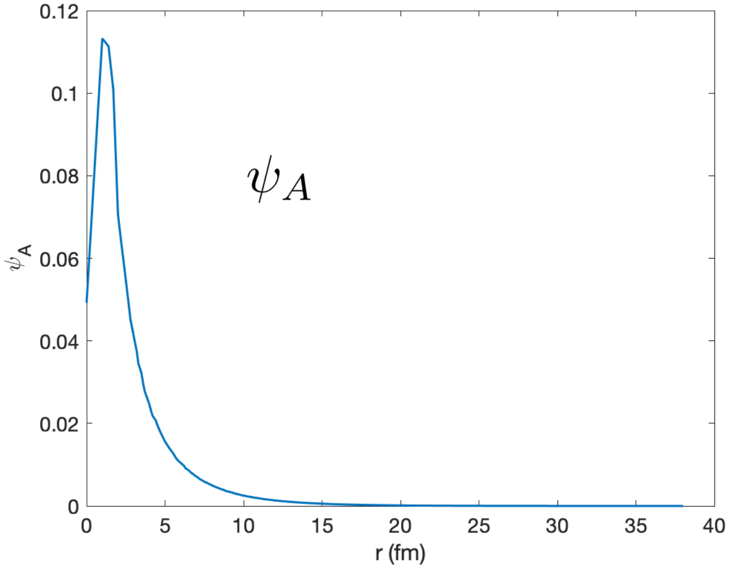
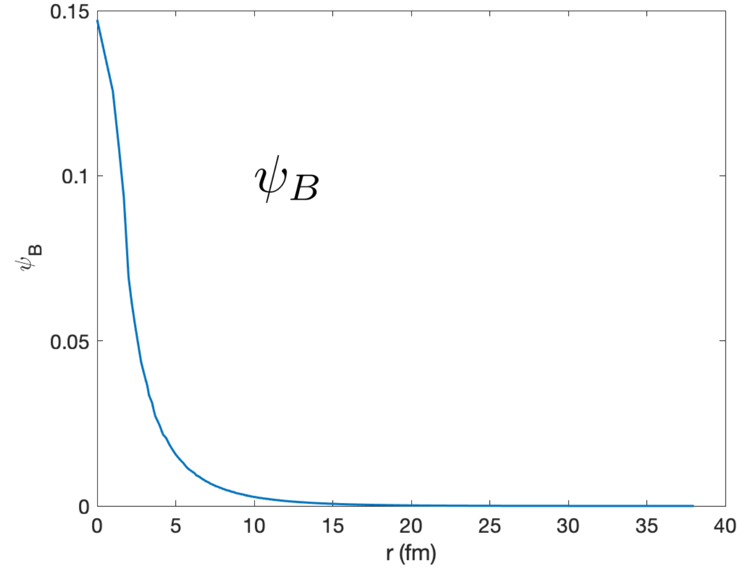
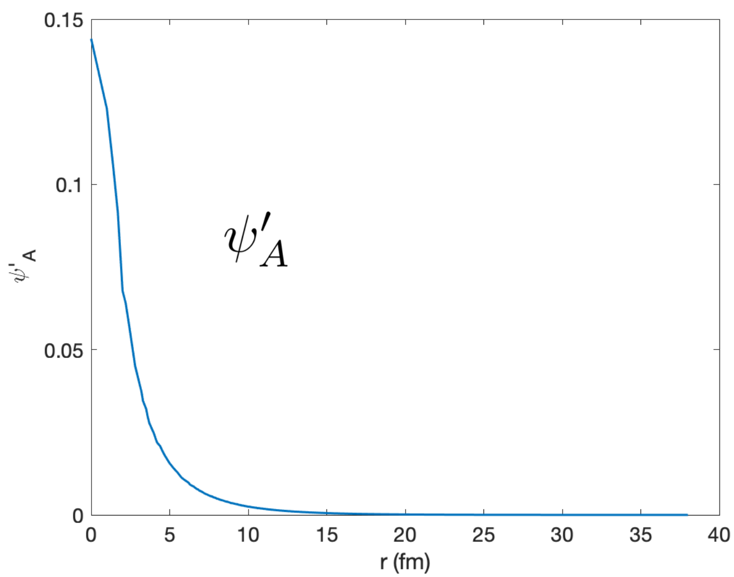
momentum (MeV)

Ground state wave functions





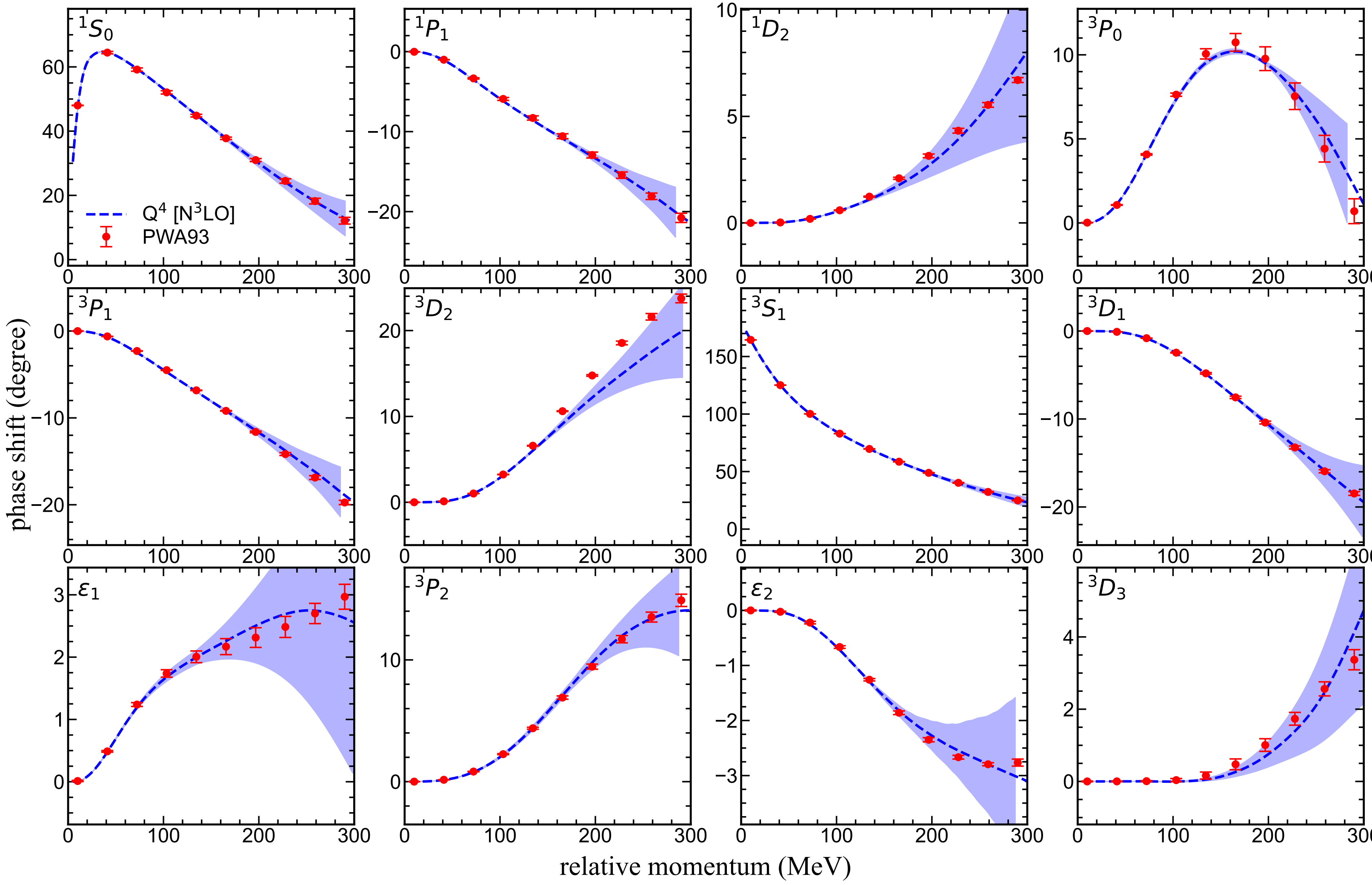


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

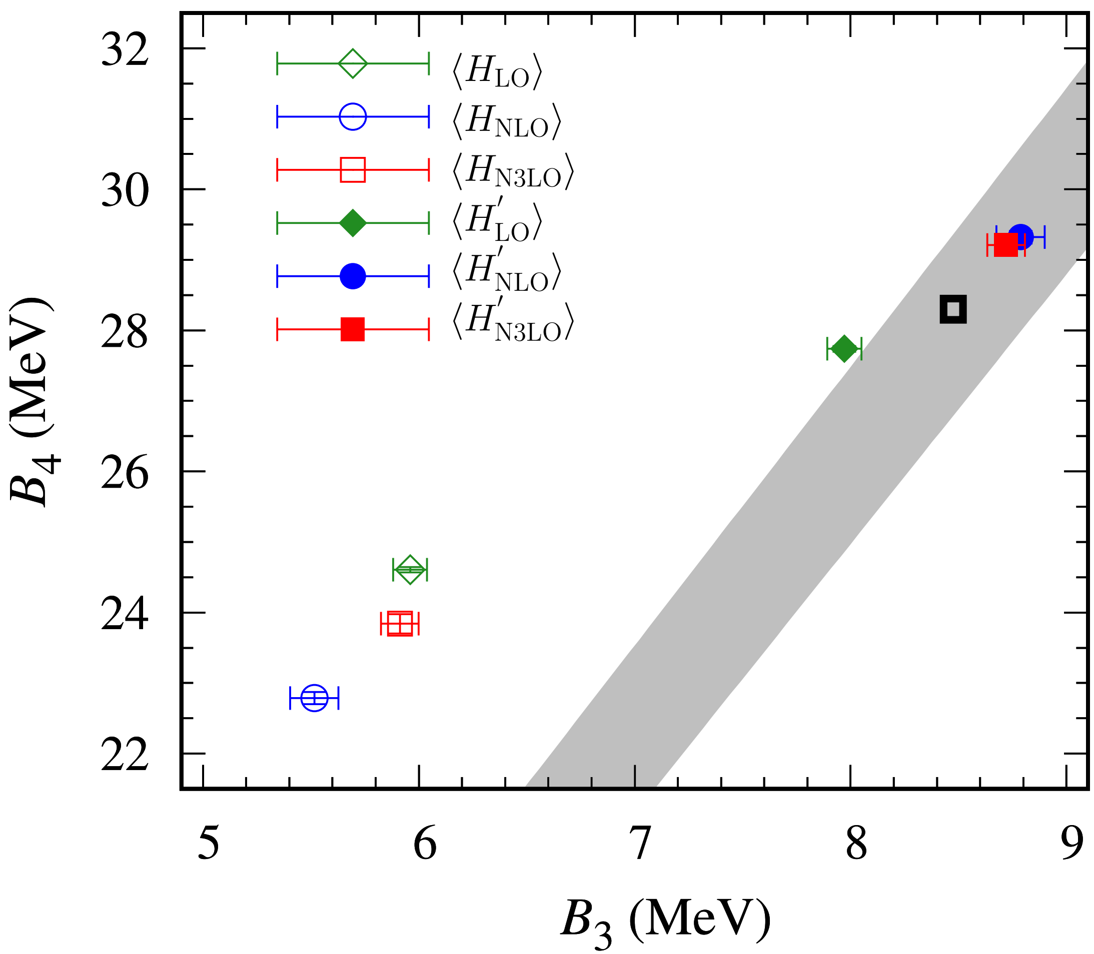
$R = 2.6$ fm

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

N3LO chiral effective field theory interaction

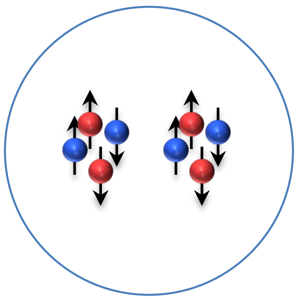


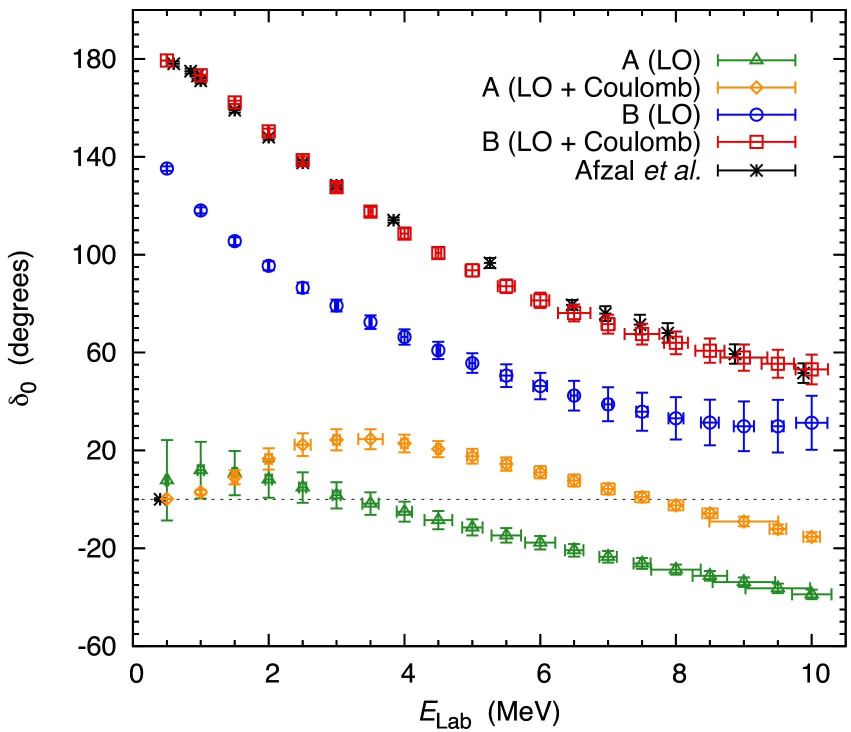
Tjon line



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

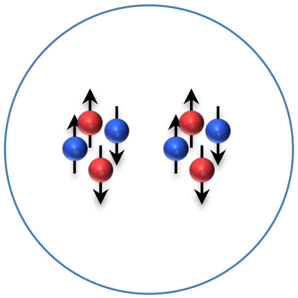
Sensitivity to short-distance physics

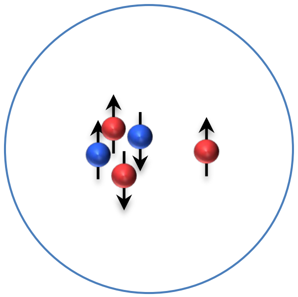




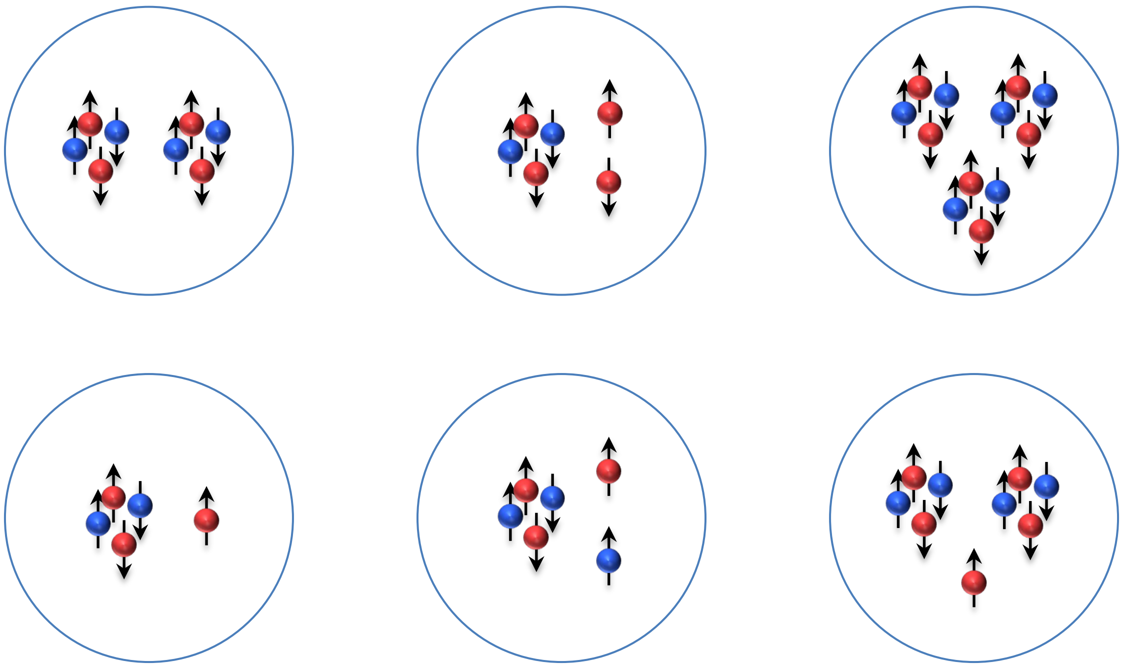
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Sensitivity to short-distance physics

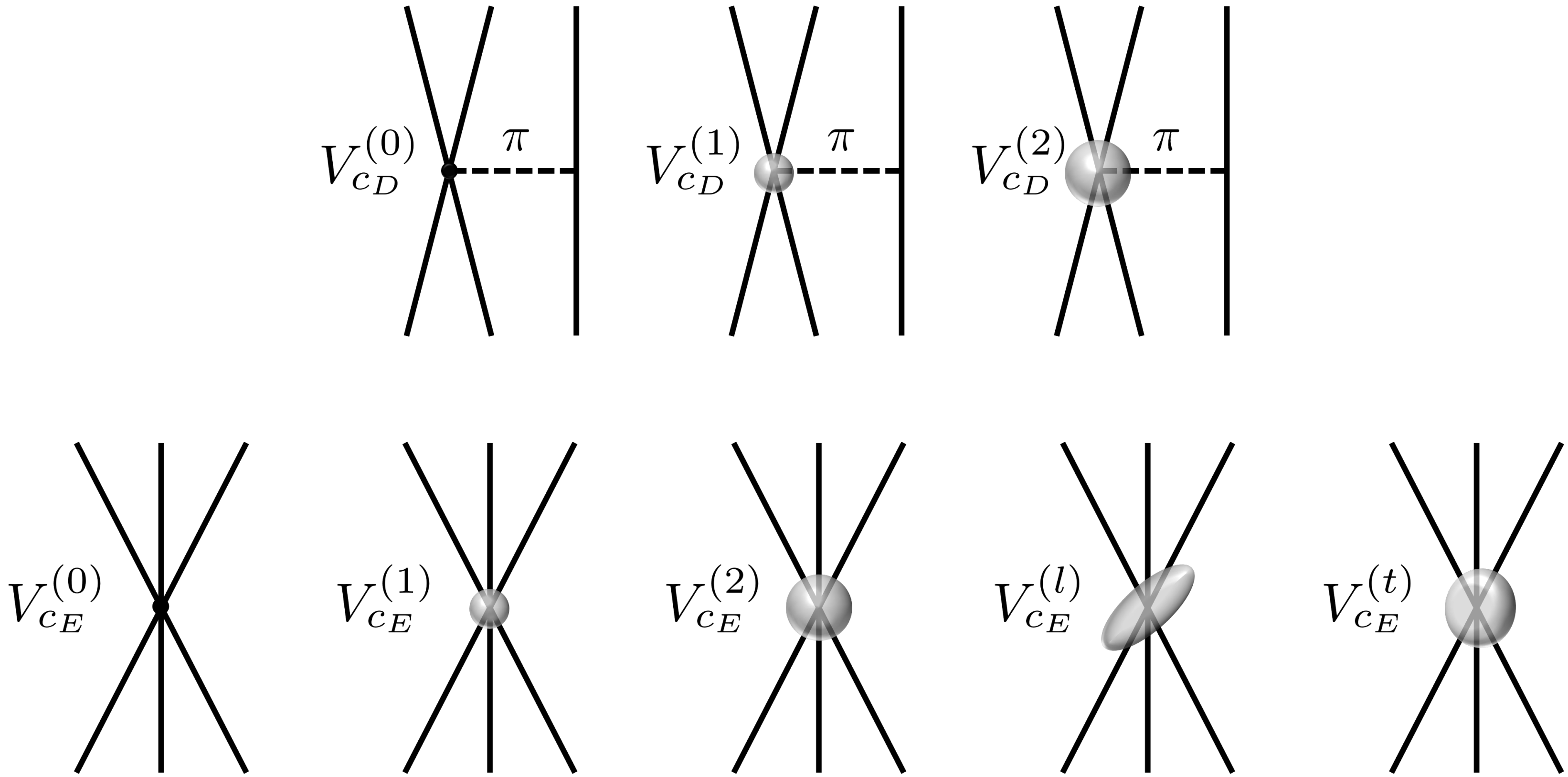




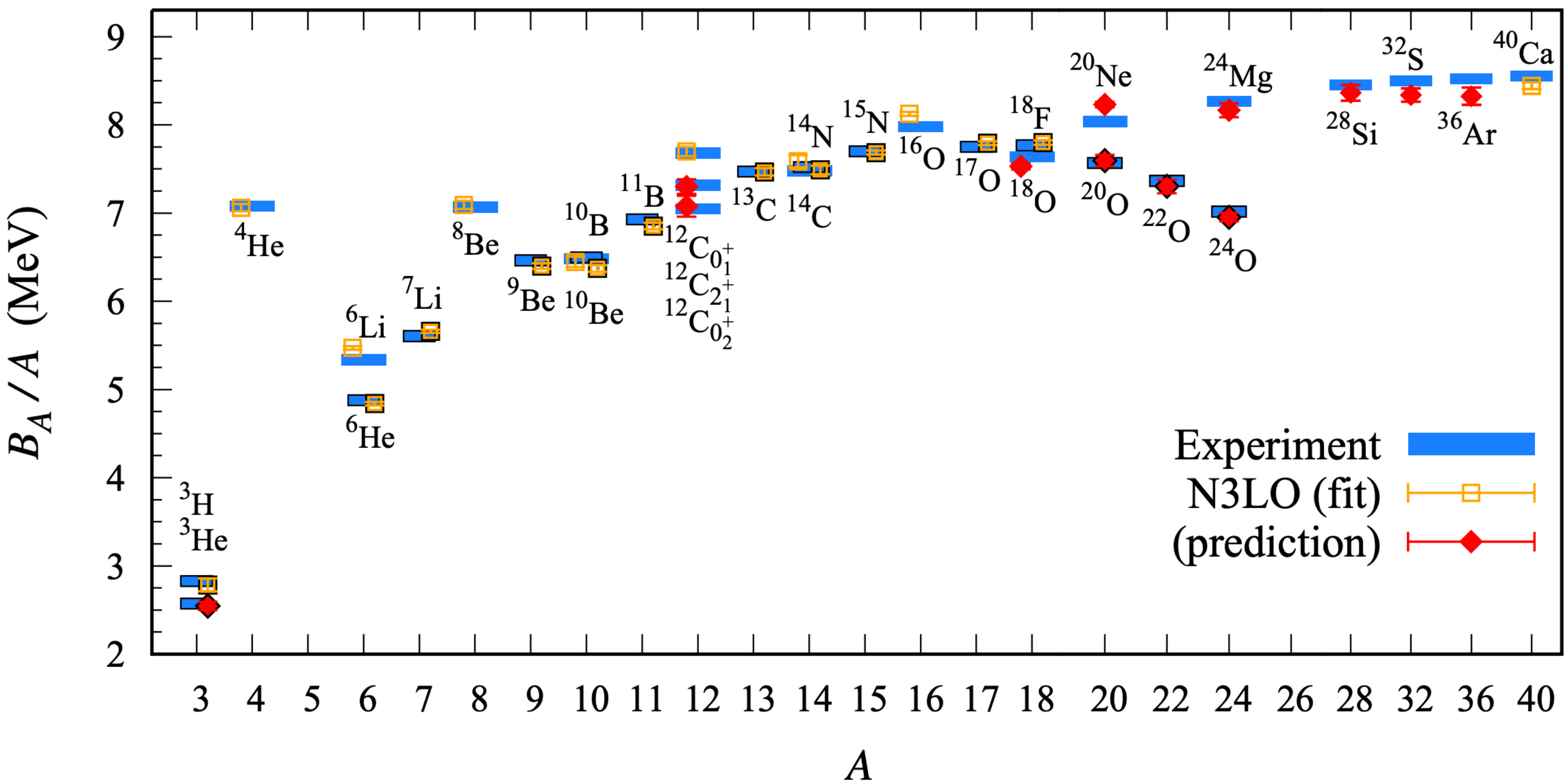
Sensitivity to short-distance physics



Short-distance three-nucleon interactions

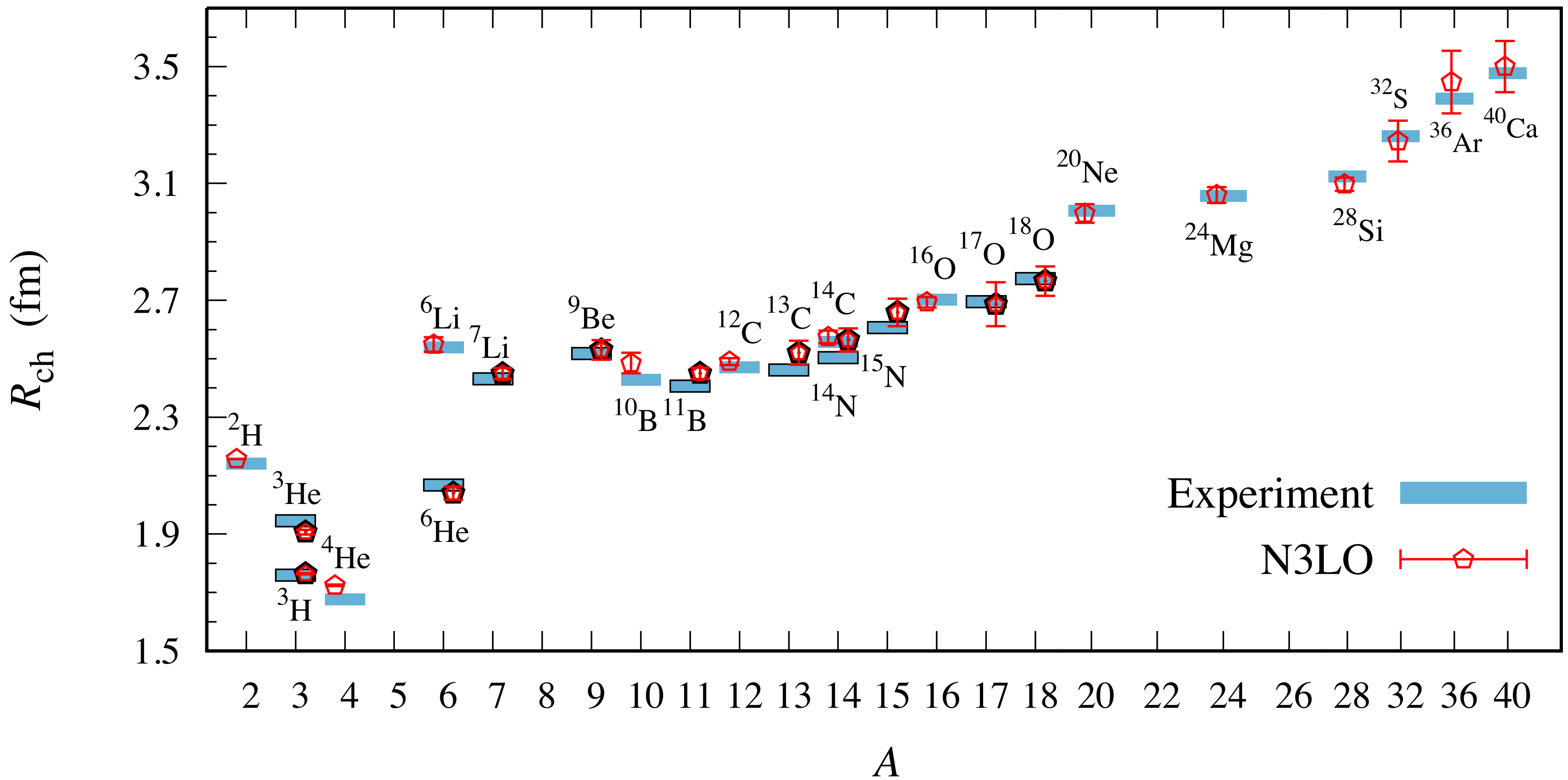


<u>Binding energy per nucleon</u>



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



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

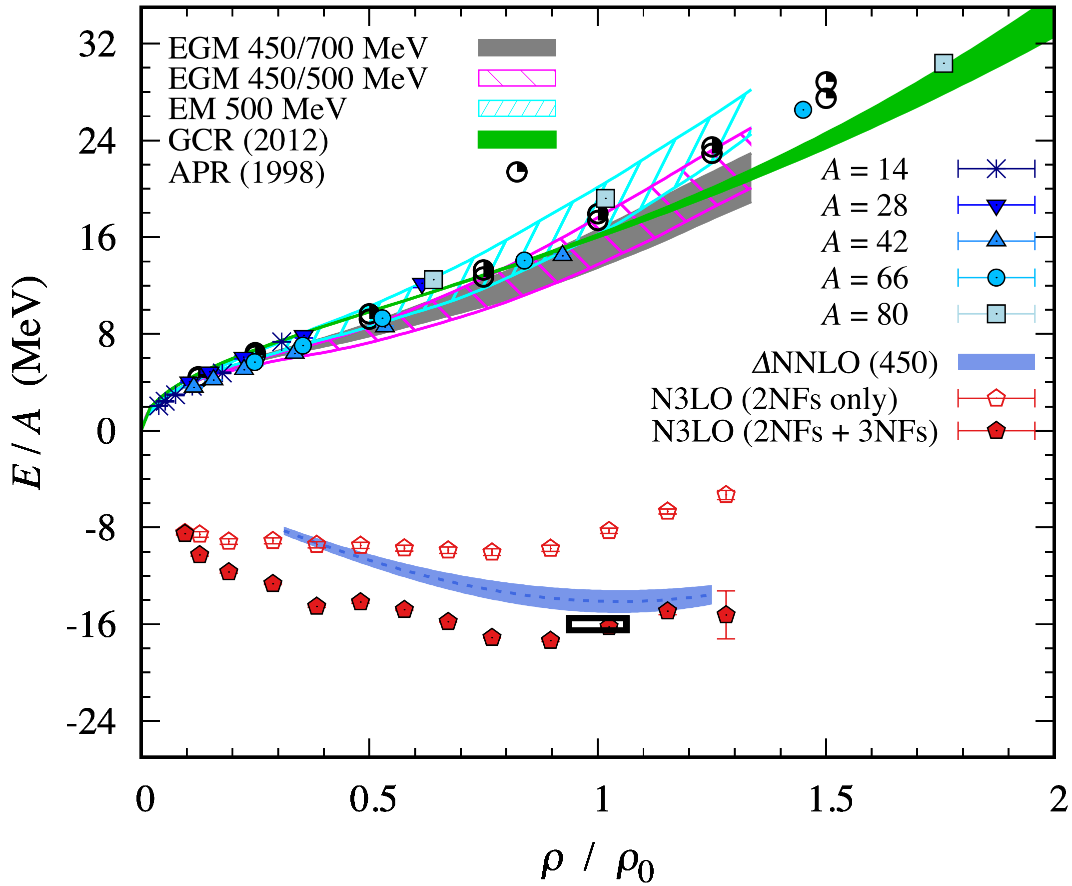


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

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

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

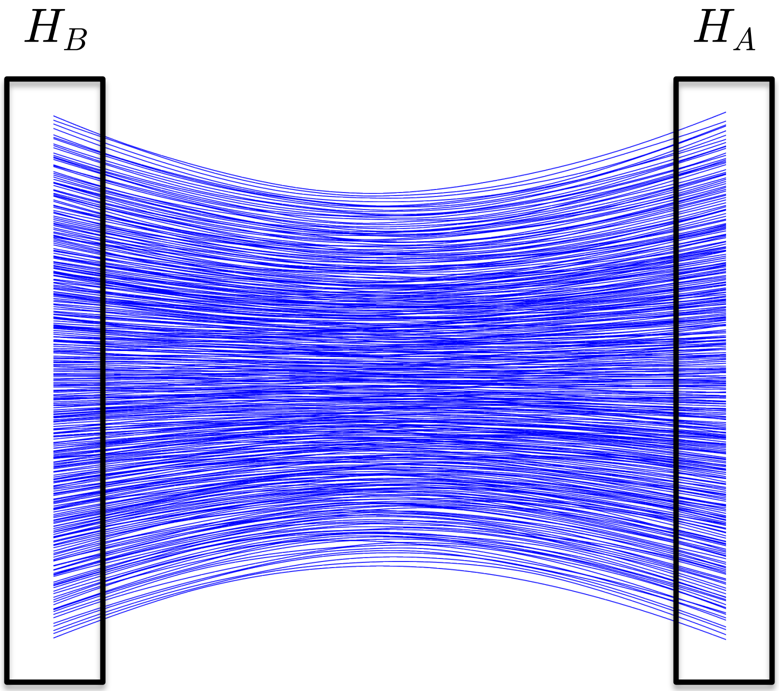
$$H'_A = U_{BA} H_A U_{AB}$$

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.

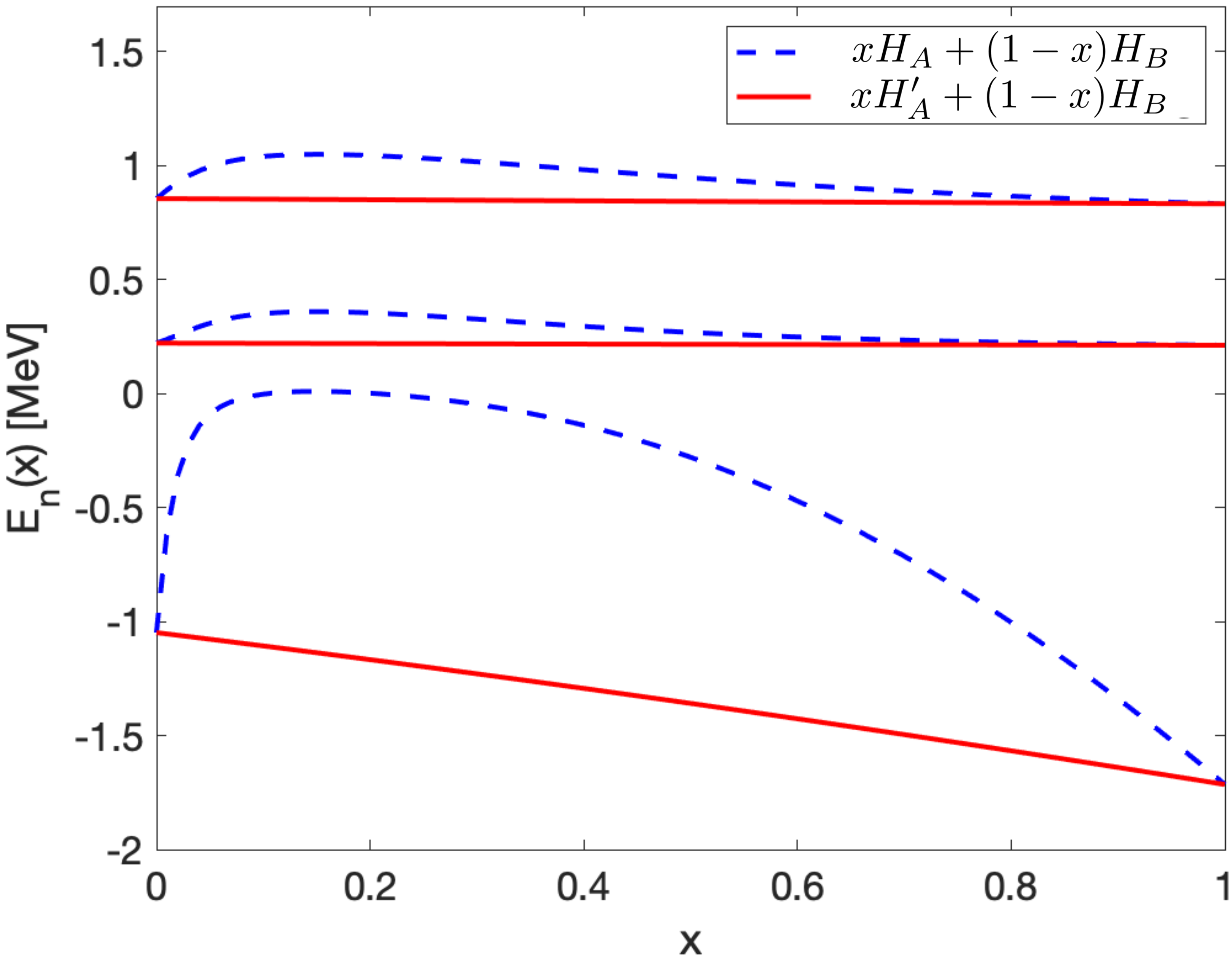


Wave function matching is an approximate Hamiltonian translator for low-energy two-body states.

$$U : \frac{P_R|\psi_B^0\rangle}{\|P_R|\psi_B^0\rangle\|} \to \frac{P_R|\psi_A^0\rangle}{\|P_R|\psi_A^0\rangle\|}$$

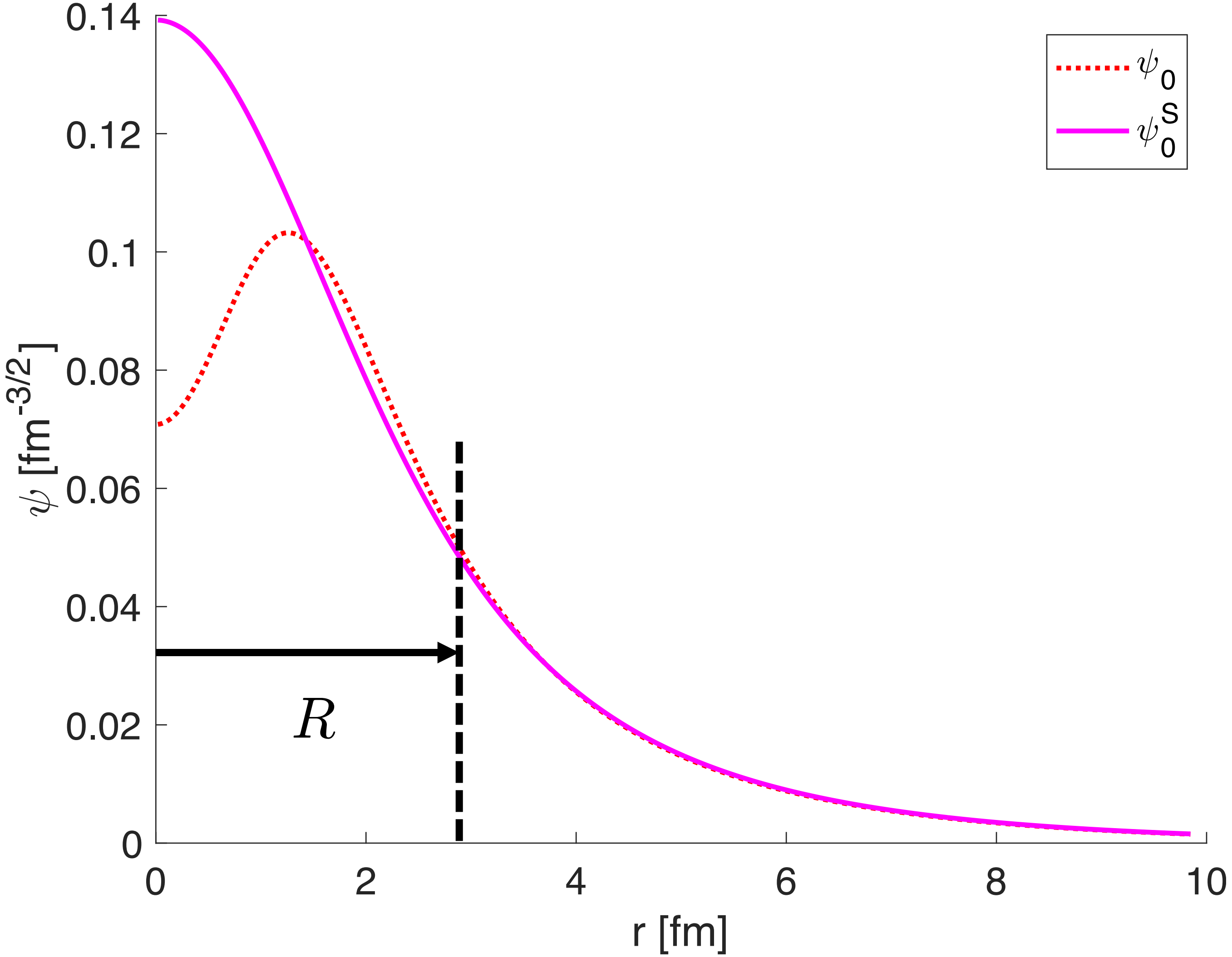
$$U : H_A \to H_A' = U^\dagger H_A U$$

H_B H_A, H'_A

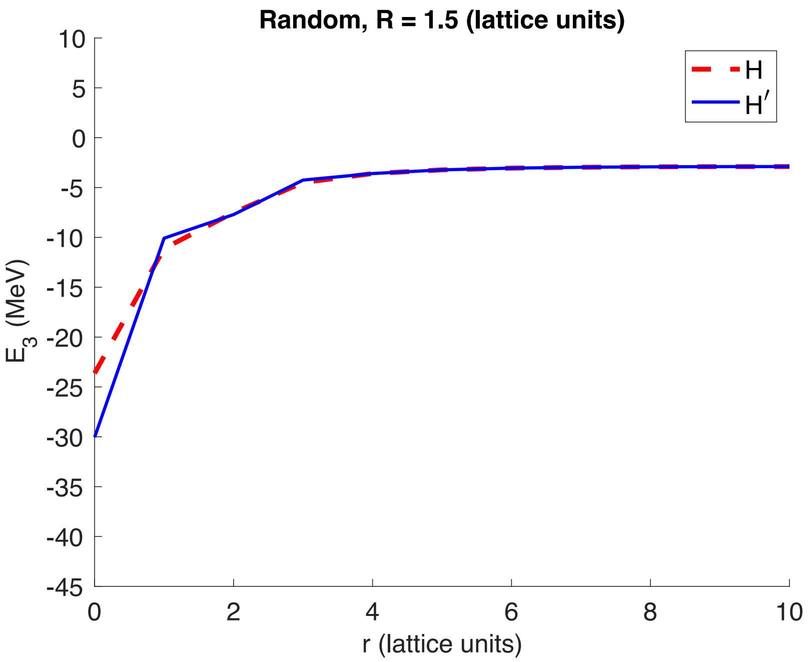


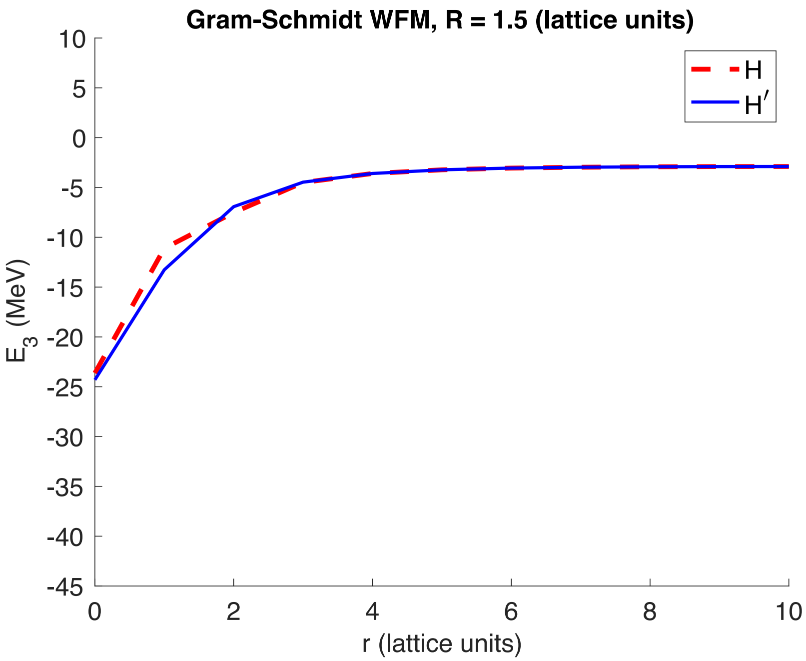
straight lines mean the eigenvectors don't change with x

Dependence on wave function matching radius

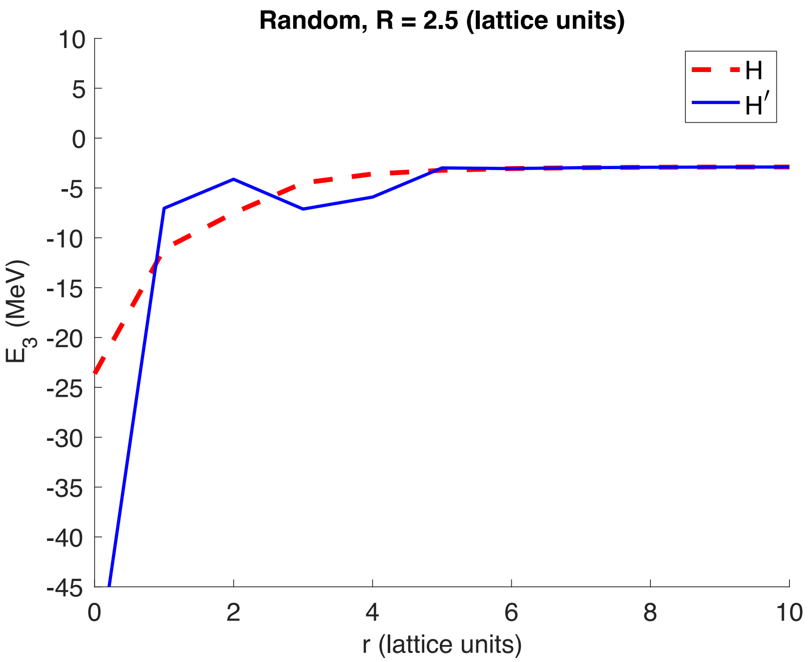


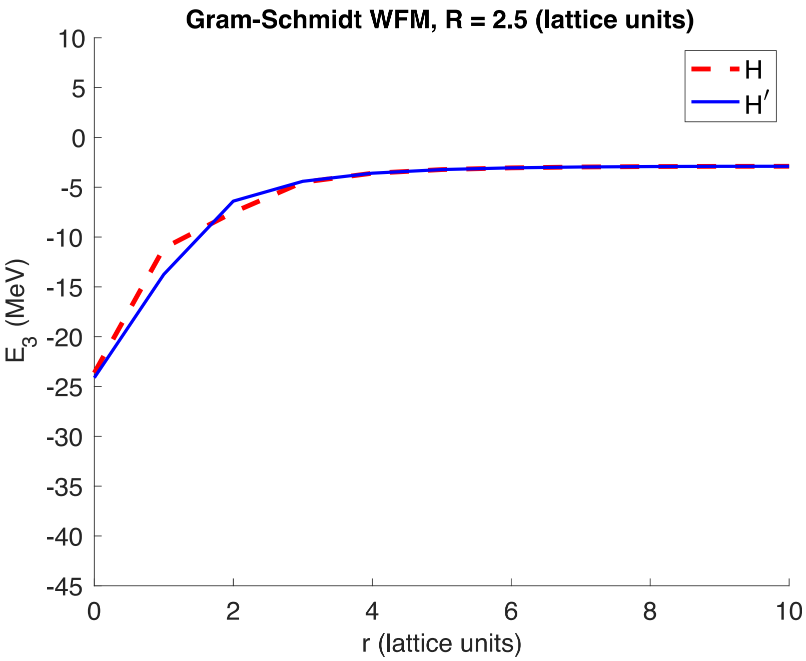
1D system with two infinitely heavy particles and one light particle



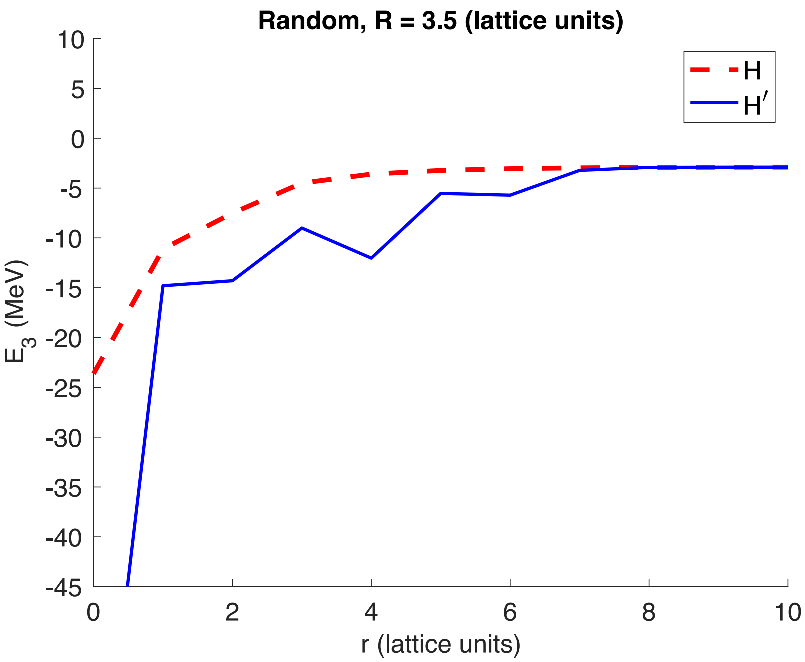


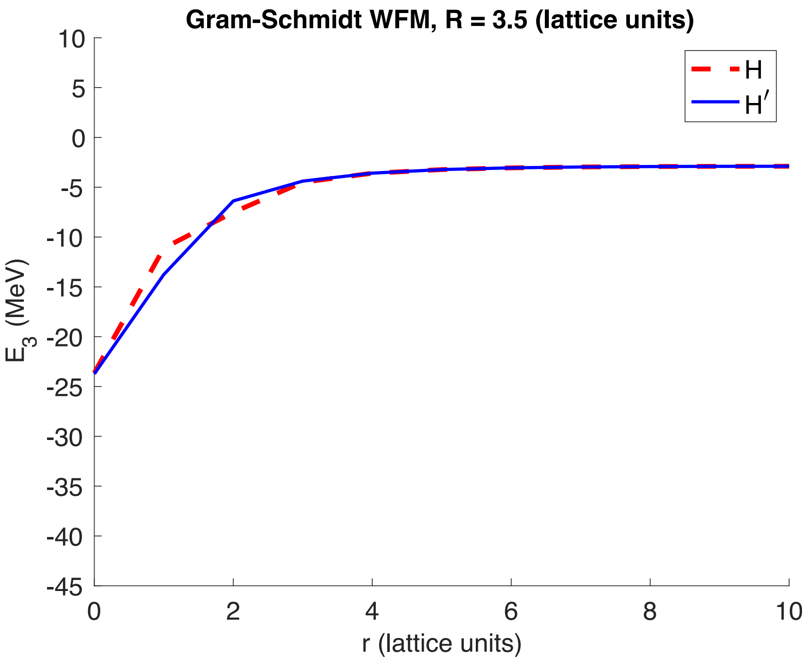
1D system with two infinitely heavy particles and one light particle





1D system with two infinitely heavy particles and one light particle





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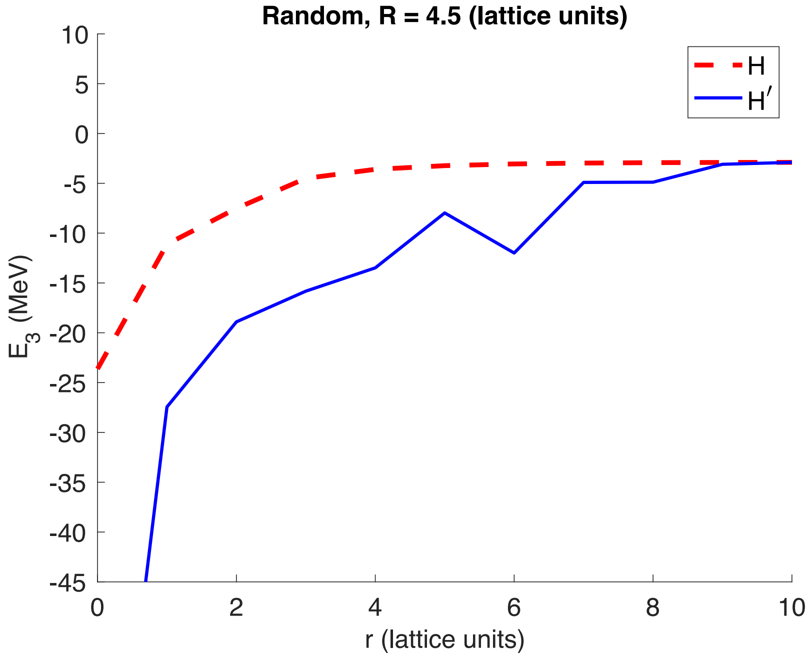
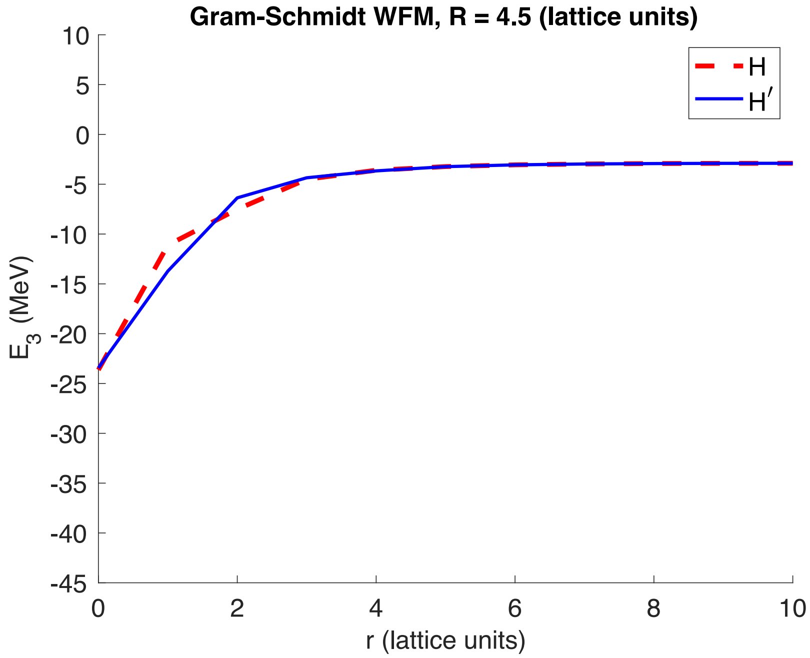
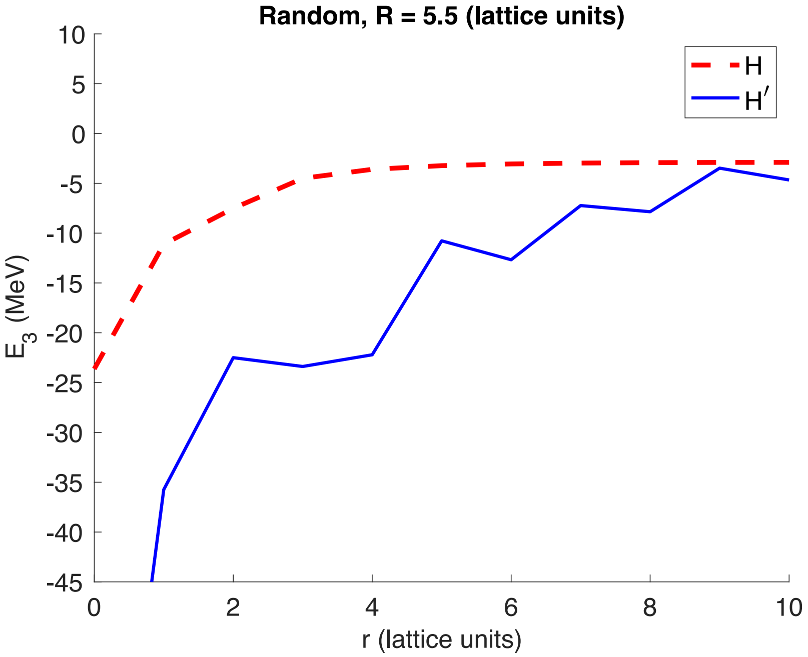
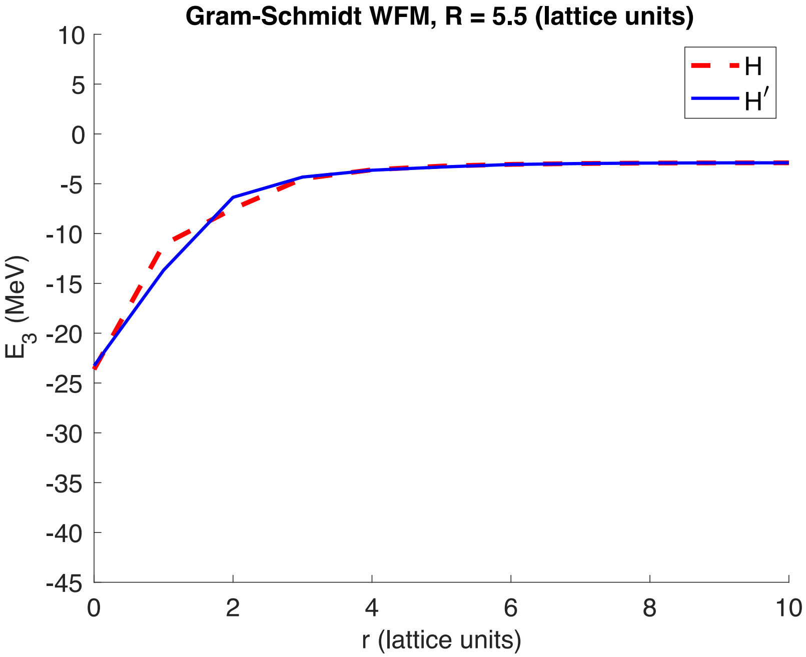
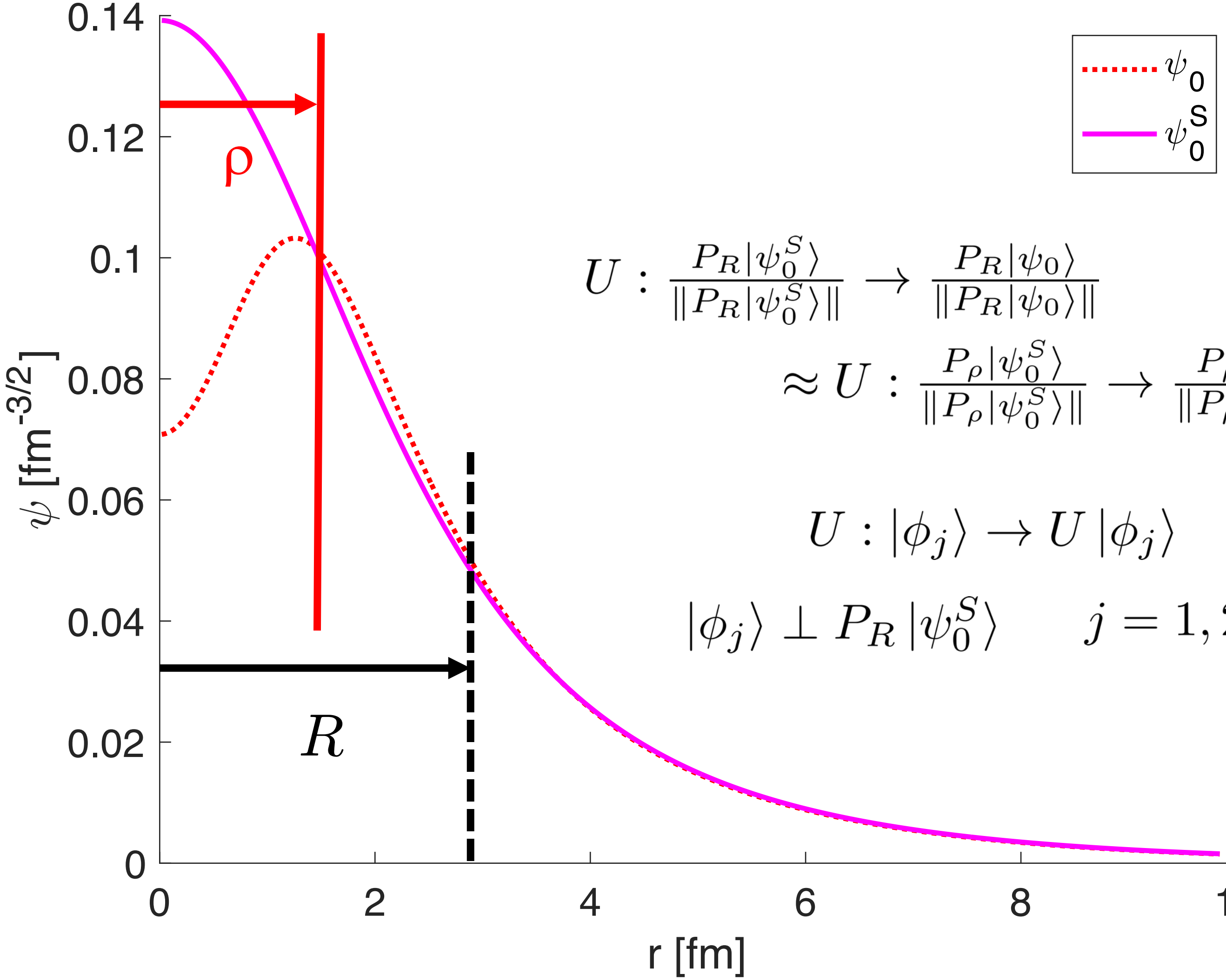




1D system with two infinitely heavy particles and one light particle







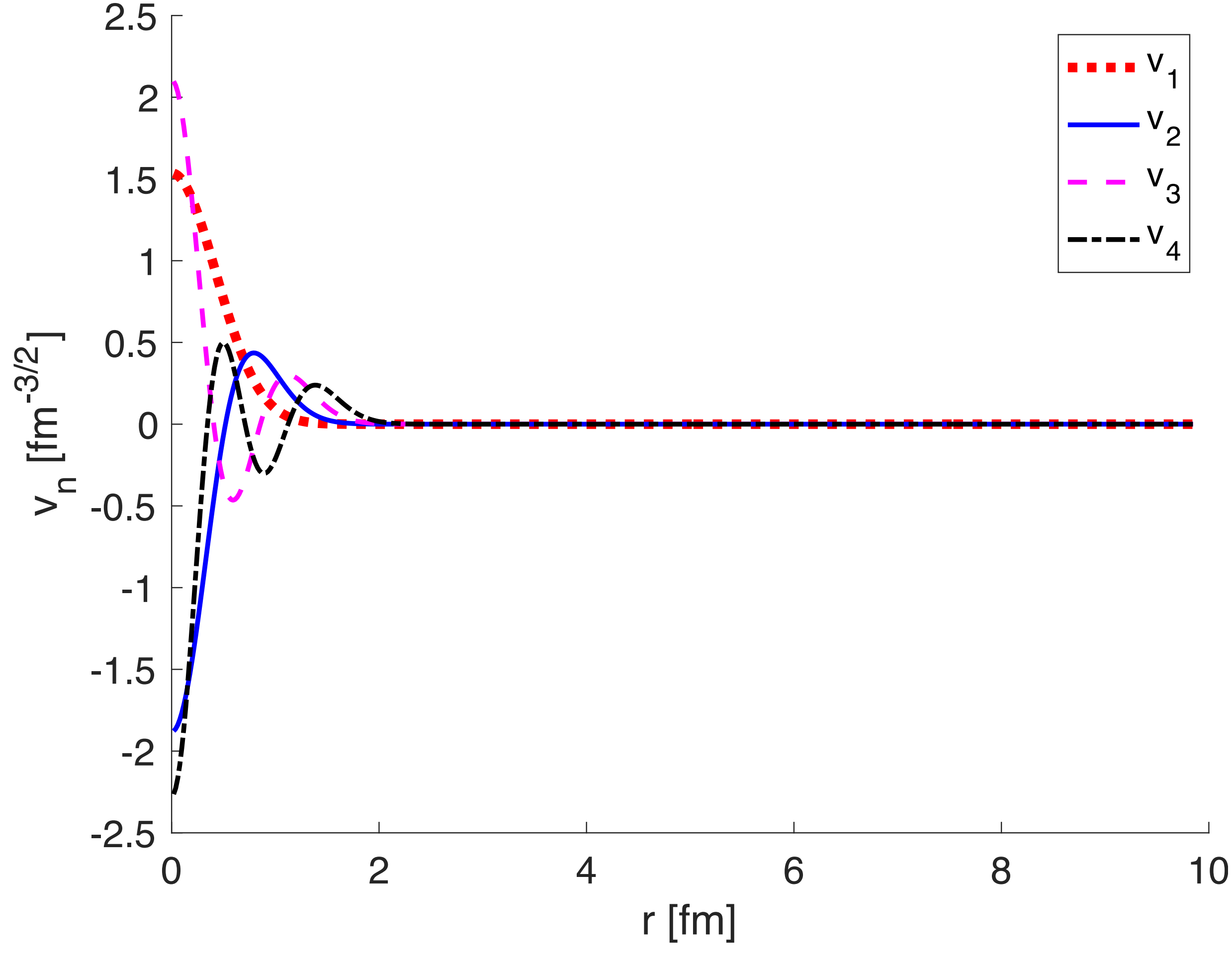
$$U : \frac{P_R|\psi_0^S\rangle}{\|P_R|\psi_0^S\rangle\|} \to \frac{P_R|\psi_0\rangle}{\|P_R|\psi_0\rangle\|}$$

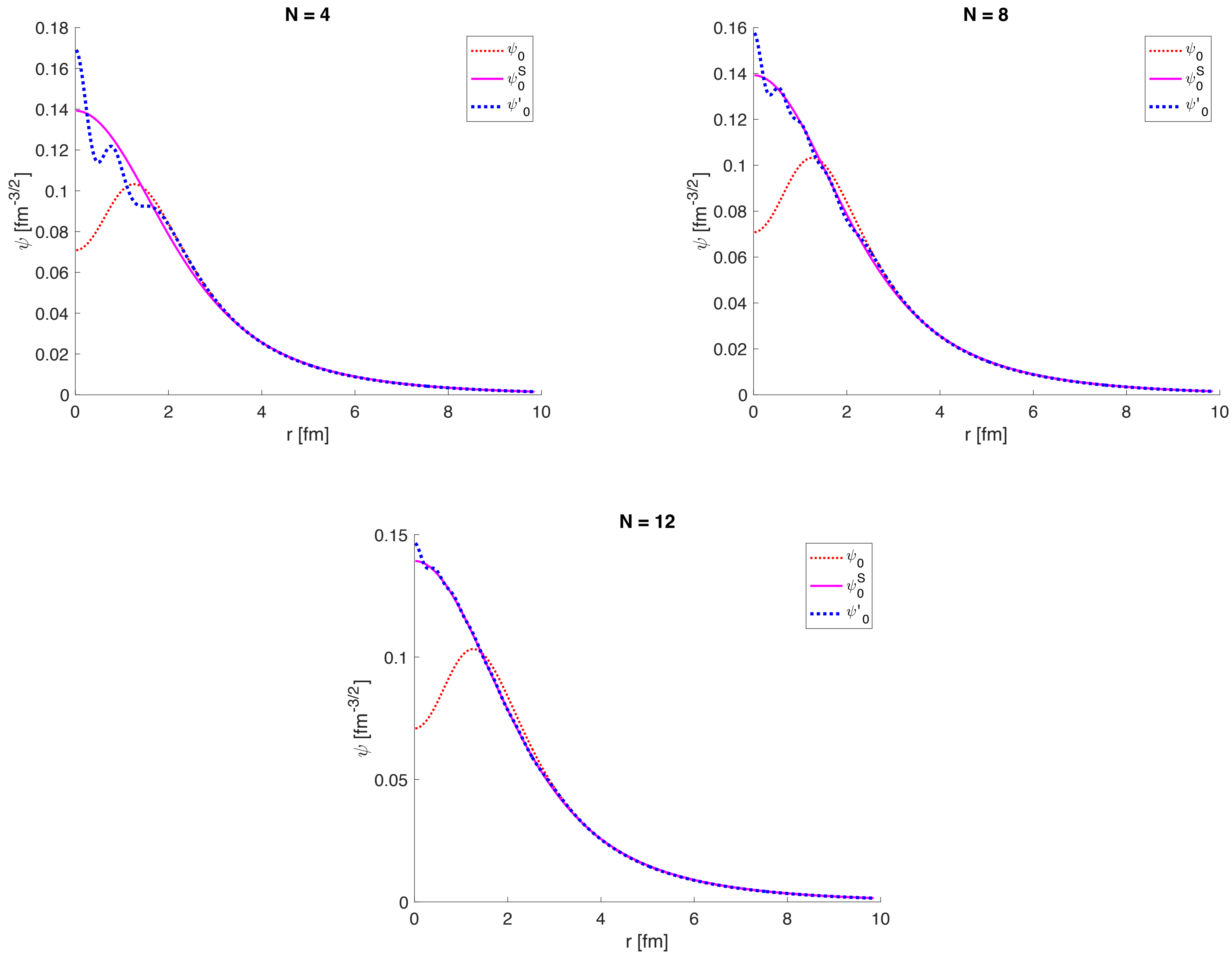
$$\approx U : \frac{P_\rho|\psi_0^S\rangle}{\|P_\rho|\psi_0^S\rangle\|} \to \frac{P_\rho|\psi_0\rangle}{\|P_\rho|\psi_0\rangle\|}$$

$$U : |\phi_j\rangle \to U\,|\phi_j\rangle$$

$$|\phi_j\rangle \perp P_R\,|\psi_0^S\rangle \qquad j = 1, 2, \cdots$$

Wave function matching in continuous space





N = 4
N = 8
N = 12
ψ [fm^-3/2]
r [fm]
ψ_0
ψ^S_0
ψ'_0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.05
0.15
2
4
6
8
10

Summary

We started with a simplified interaction that reproduced the essential elements of nuclear interactions. We then introduced the main topic, wave function matching. We demonstrated the basic concepts using simple examples and applied wave function matching to calculations of nuclear structure at N3LO in chiral effective field theory. We then discussed some theoretical concepts associated with wave function matching.