New Algorithms for the Nuclear Many-Body Problem

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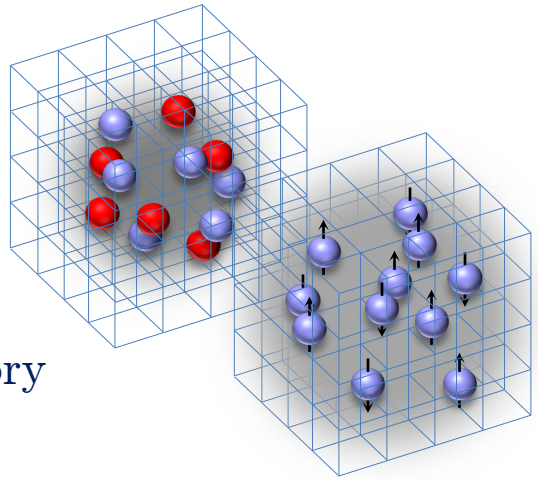
NLEFT Collaboration



Workshop on Progress in Ab Initio Nuclear Theory
TRIUMF, Vancouver
February 27, 2024

NUCLEI Nuclear Computational Low-Energy Initiative
A SciDAC-5 Project

JÜLICH FORSCHUNGSZENTRUM

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

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MICHIGAN STATE UNIVERSITY

In memory of our dear friend and colleague, Rup.
He is greatly missed.

Outline

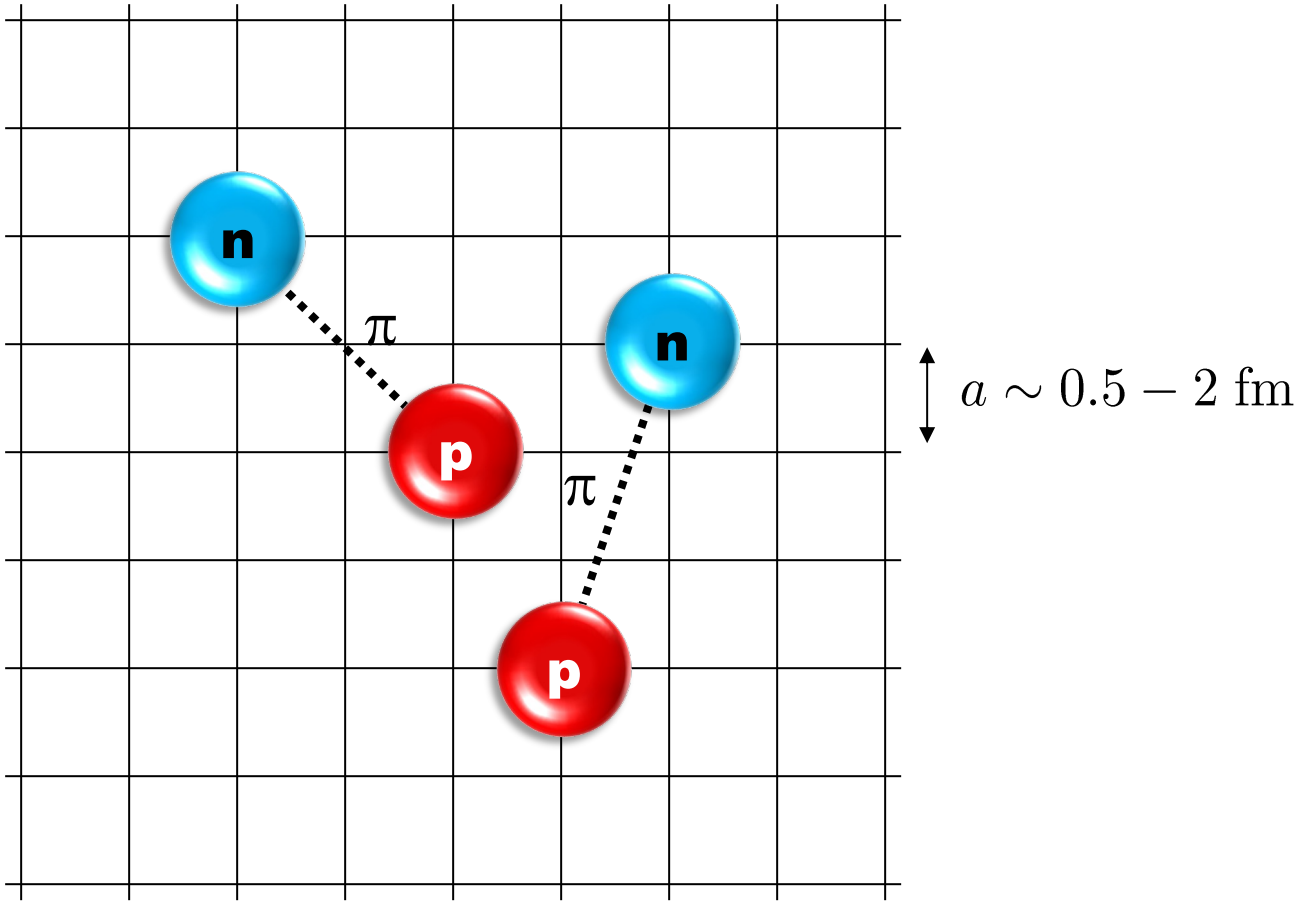
Lattice effective field theory

Floating block method

Wave function matching

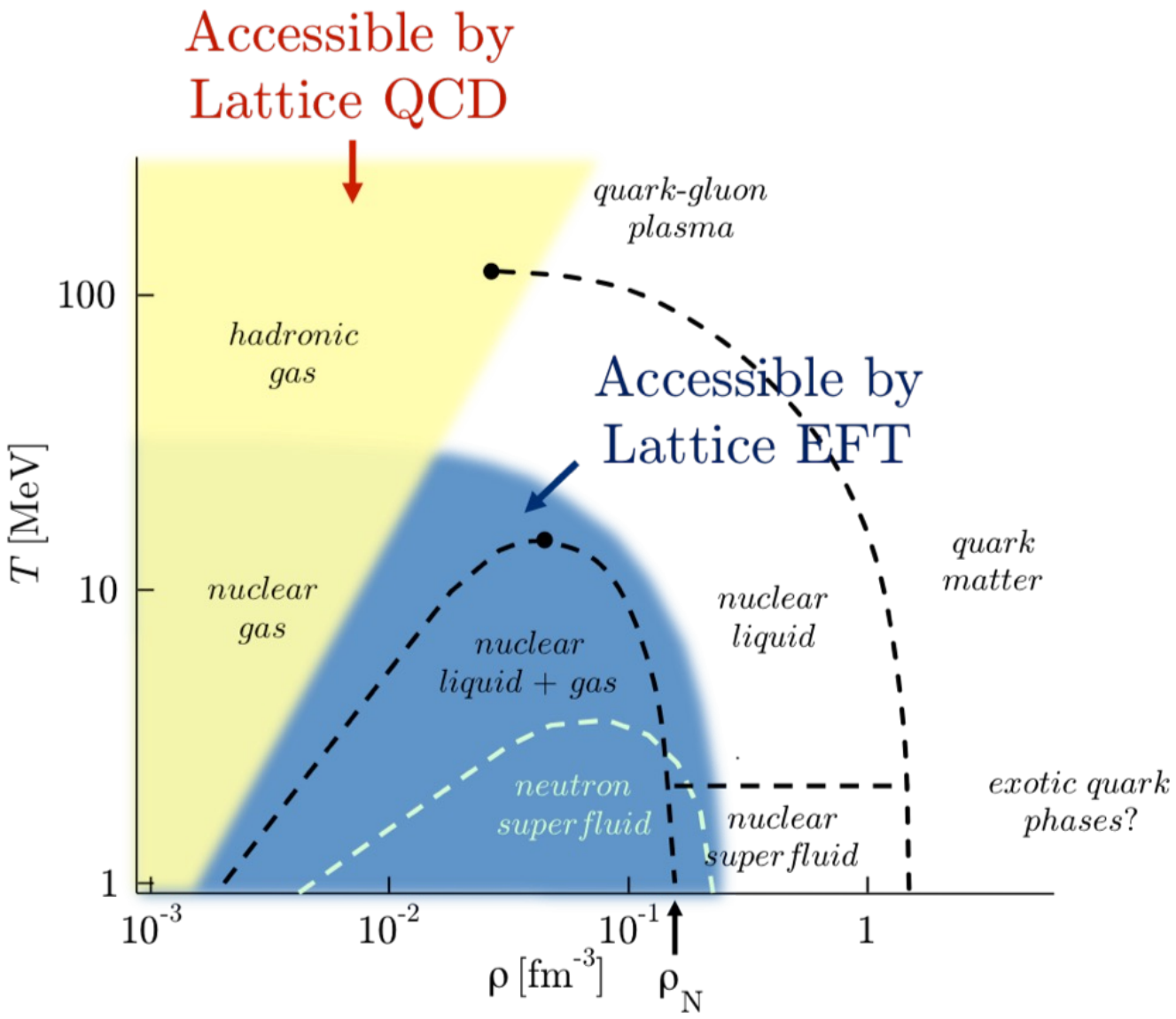
Summary

Lattice effective field theory



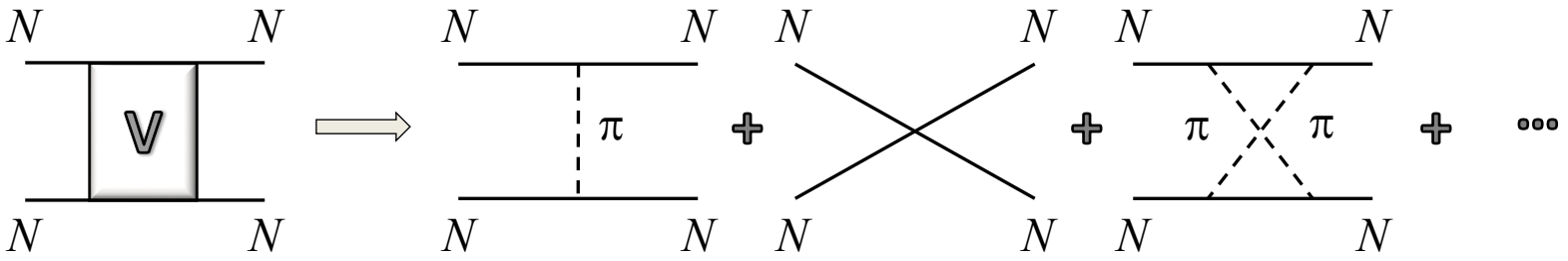
D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

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

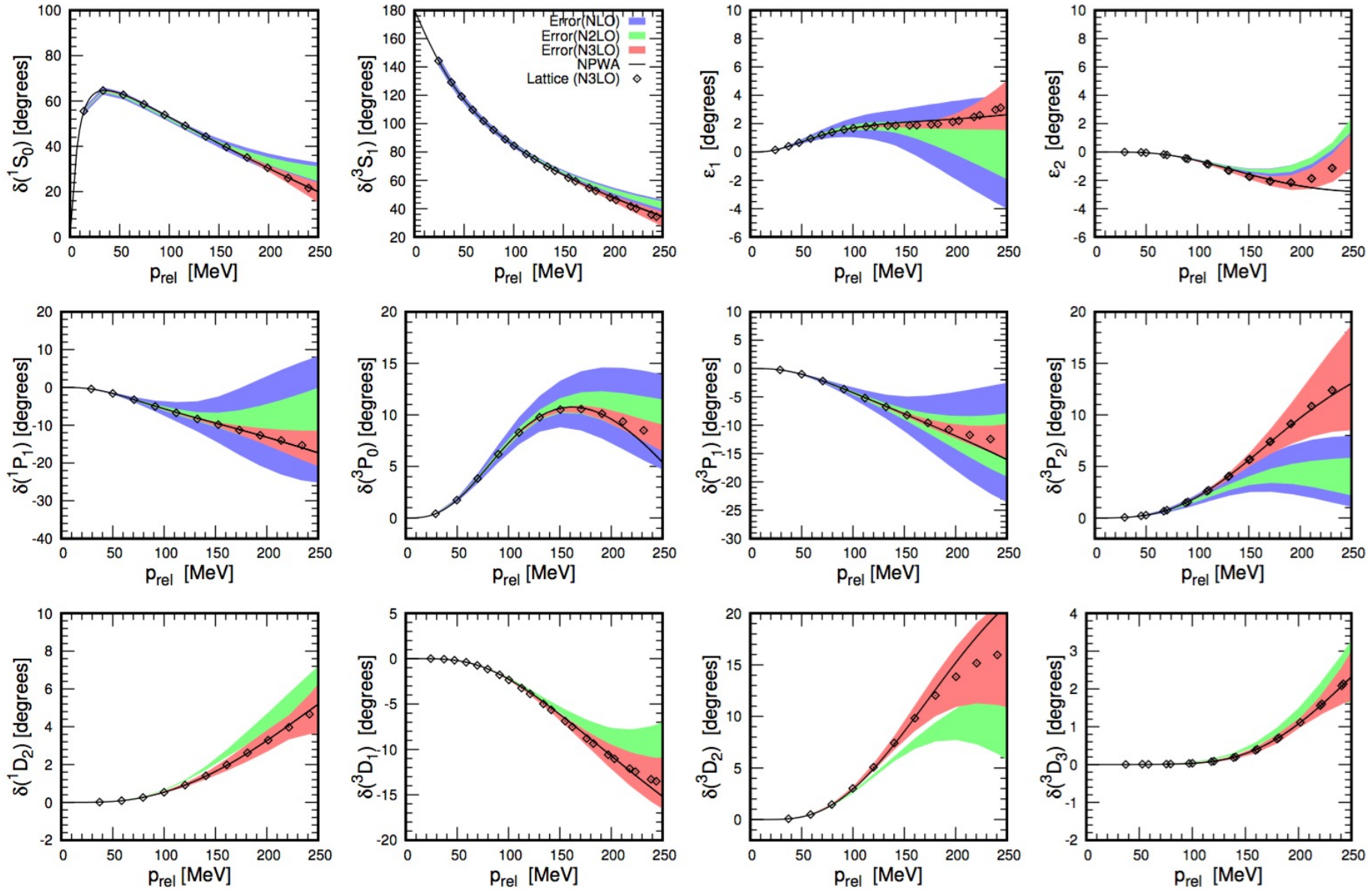
Construct the effective potential order by order



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

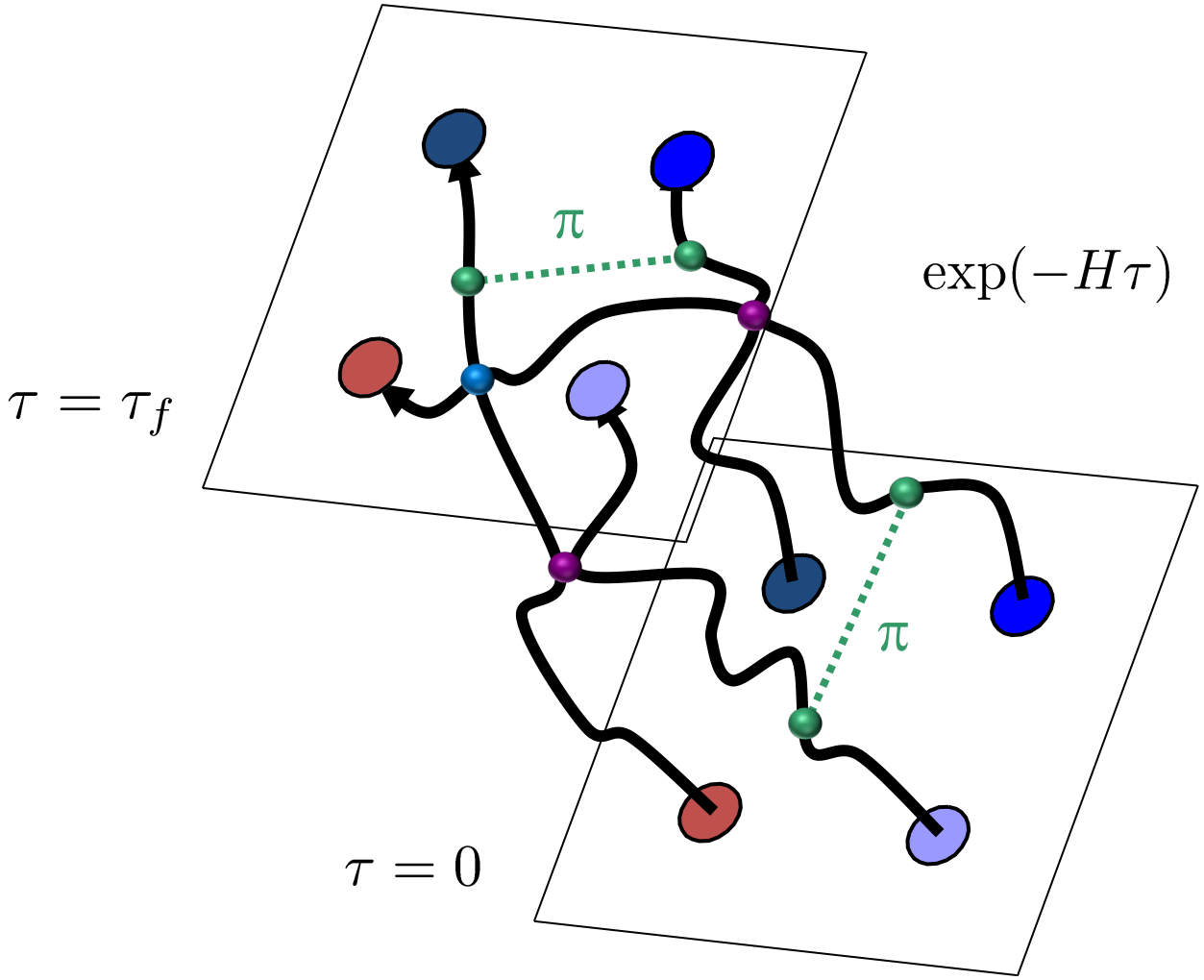
Leading order (LO) Next-to-leading order (NLO)

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

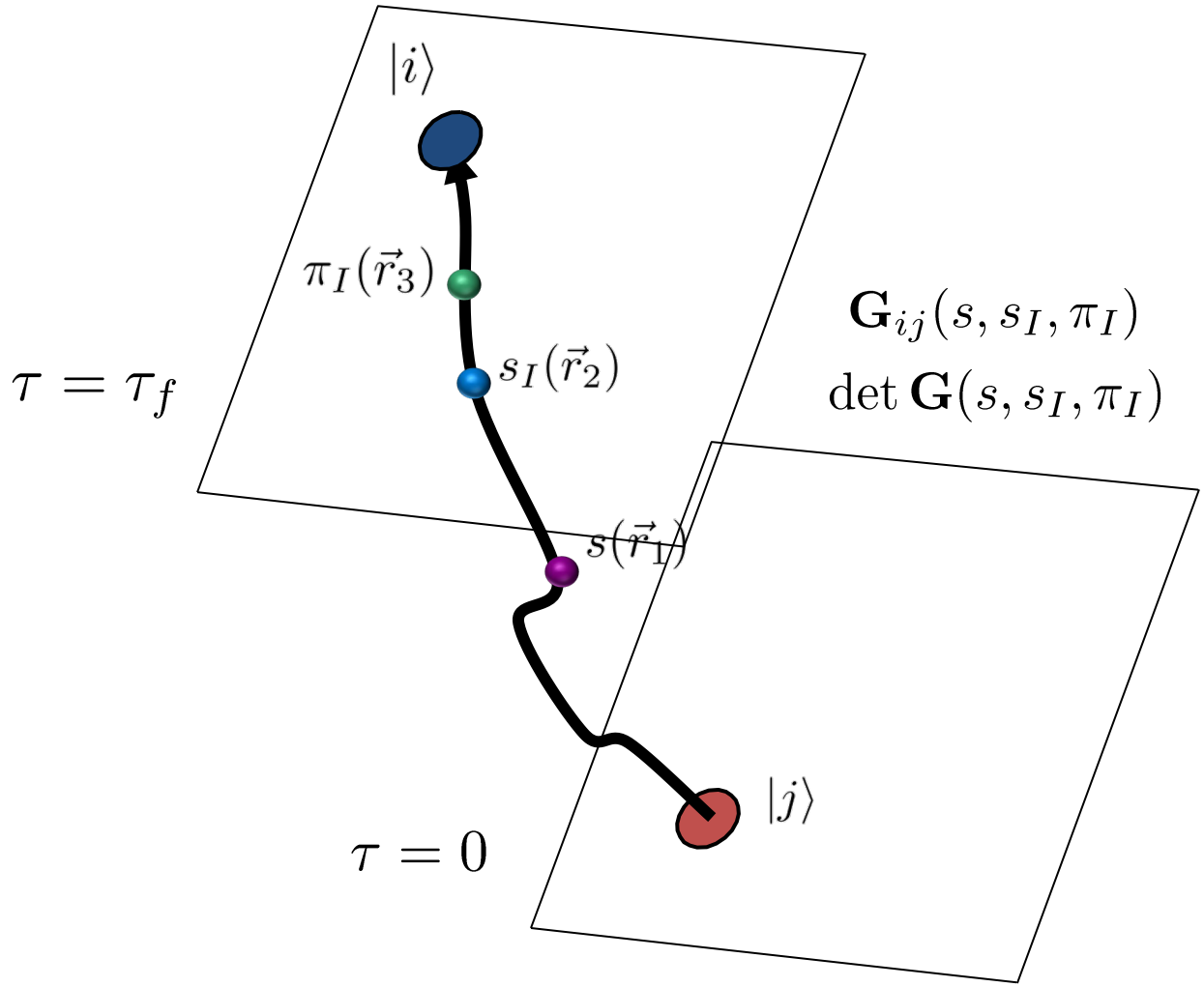


Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, Phys. Rev. C 98, 044002 (2018)

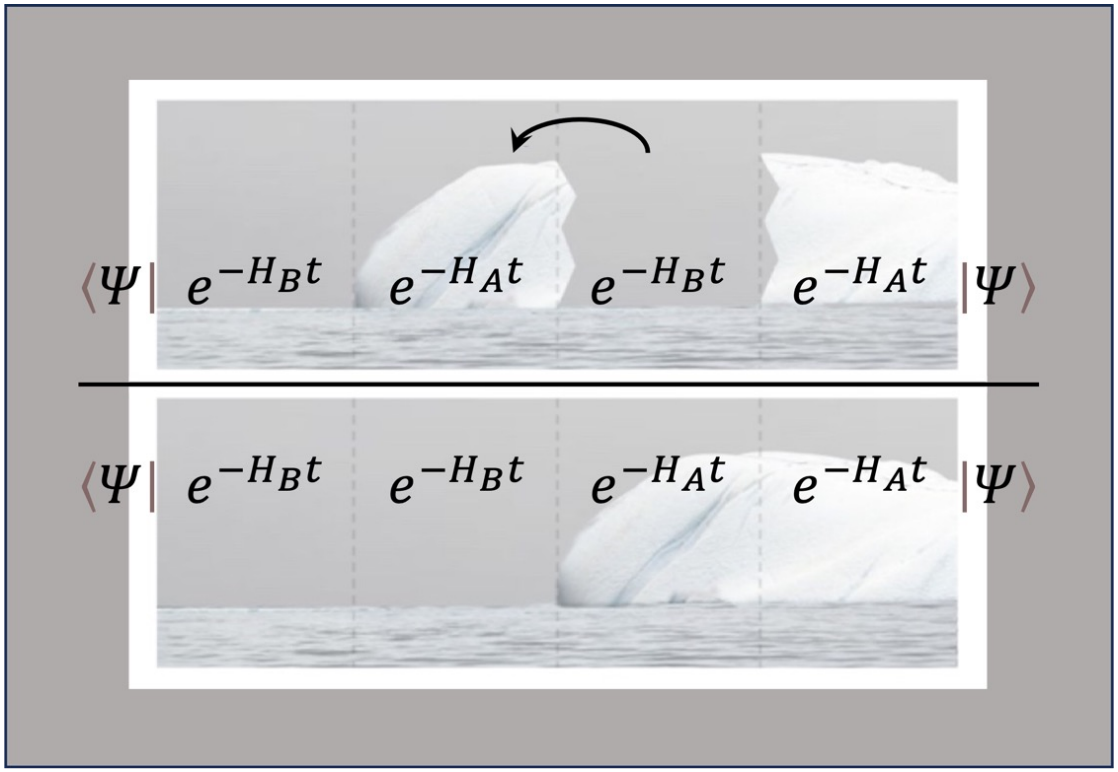
Euclidean time projection



Auxiliary field method



Floating block method



Sarkar, D.L., Meißner, Phys. Rev. Lett. 131, 242503 (2023)

In the limit of large Euclidean time, we can use quantum Monte Carlo calculations to produce the ground state wave function

$$\exp(-H\tau)\,|\psi_{\rm init}\rangle \approx |\psi_0\rangle \exp(-E_0\tau)\,\langle\psi_0|\psi_{\rm init}\rangle$$

Suppose that the Hamiltonian depends smoothly on some parameter c. We would like to perform eigenvector continuation of the ground state

$$H(c)\,|\psi_0(c)\rangle = E_0(c)\,|\psi_0(c)\rangle$$

We then need to compute norm matrix elements and Hamiltonian matrix elements

$$N_{j,k} = \langle\psi_0(c_j)|\psi_0(c_k)\rangle$$
$$H_{j,k}(c) = \langle\psi_0(c_j)|H(c)|\psi_0(c_k)\rangle$$

and solve the generalized eigenvalue problem

$$\sum_k H_{j,k}(c) v_k = E_0^{EC}(c) \sum_k N_{j,k} v_k$$

There is no problem to calculate ratios of Hamiltonian and norm matrix elements

$$\frac{H_{j,k}(c)}{N_{j,k}} \approx \frac{\langle \psi_{\text{init}} | \exp[-H(c_j)\tau] H(c) \exp[-H(c_k)\tau] | \psi_{\text{init}} \rangle}{\langle \psi_{\text{init}} | \exp[-H(c_j)\tau] \exp[-H(c_k)\tau] | \psi_{\text{init}} \rangle}$$

But it is difficult to compute the norm matrix elements. The standard approach is to compute the ratio of the norm matrix elements to some reference amplitude

$$\frac{N_{j,k}}{N_{\text{ref}}} \approx \frac{\langle \psi_{\text{init}} | \exp[-H(c_j)\tau] \exp[-H(c_k)\tau] | \psi_{\text{init}} \rangle}{\langle \psi_{\text{init}} | \exp[-H(c_{\text{ref}})\tau] \exp[-H(c_{\text{ref}})\tau] | \psi_{\text{init}} \rangle}$$

But the large exponential factors due to differences in the ground energies make the Monte Carlo sampling very difficult.

Floating block method

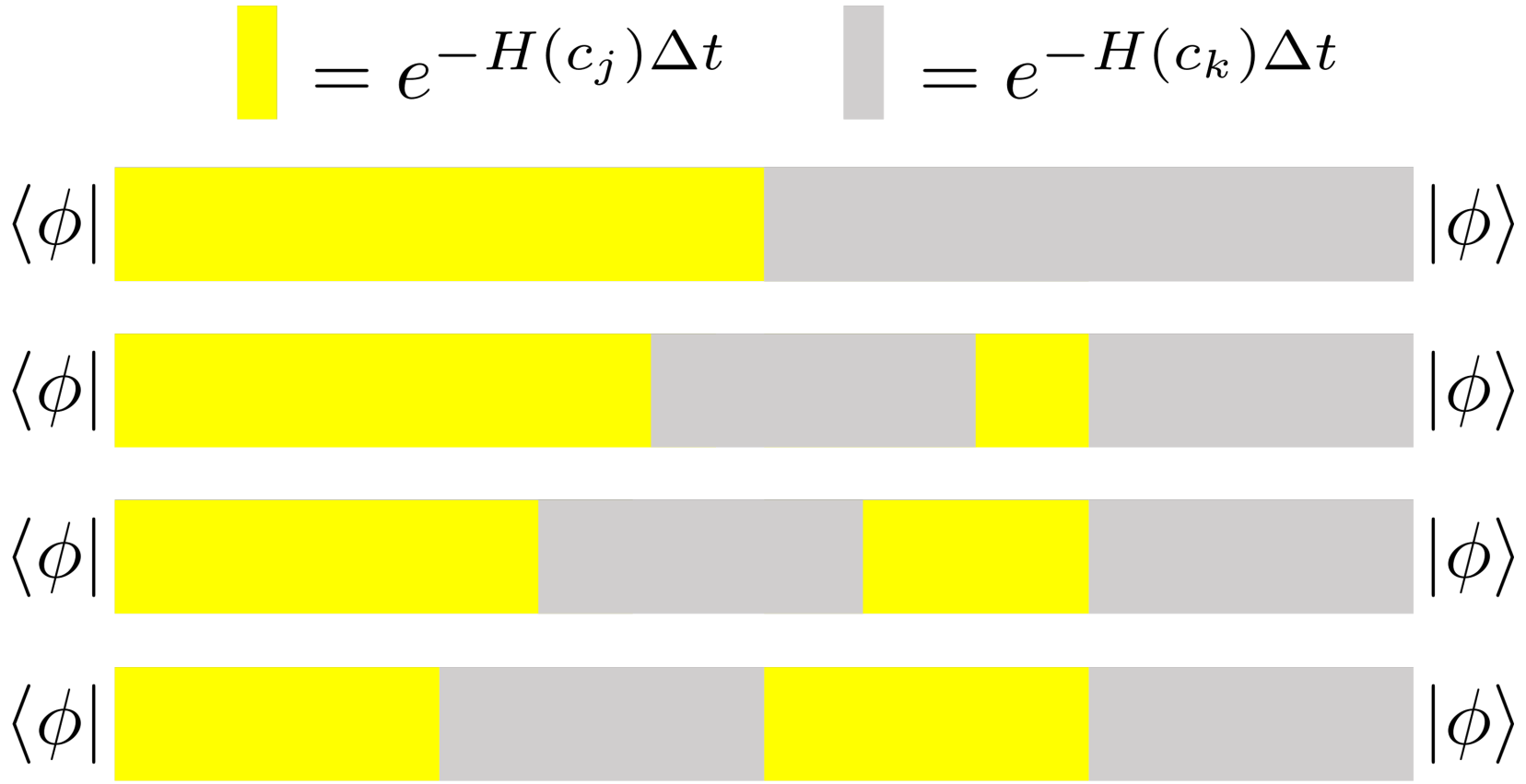
The floating block method solves this problem by computing ratios where the exponential factors of the ground state energies cancel.

$$|N_{j,k}|^2 = |\,\langle\psi_0(c_j)|\psi_0(c_k)\rangle\,|^2 \approx$$

$$\frac{\langle\psi_{\text{init}}|\exp[-H(c_j)\tau]\exp[-H(c_k)\tau]\exp[-H(c_j)\tau]\exp[-H(c_k)\tau]|\psi_{\text{init}}\rangle}{\langle\psi_{\text{init}}|\exp[-2H(c_j)\tau]\exp[-2H(c_k)\tau]|\psi_{\text{init}}\rangle}$$

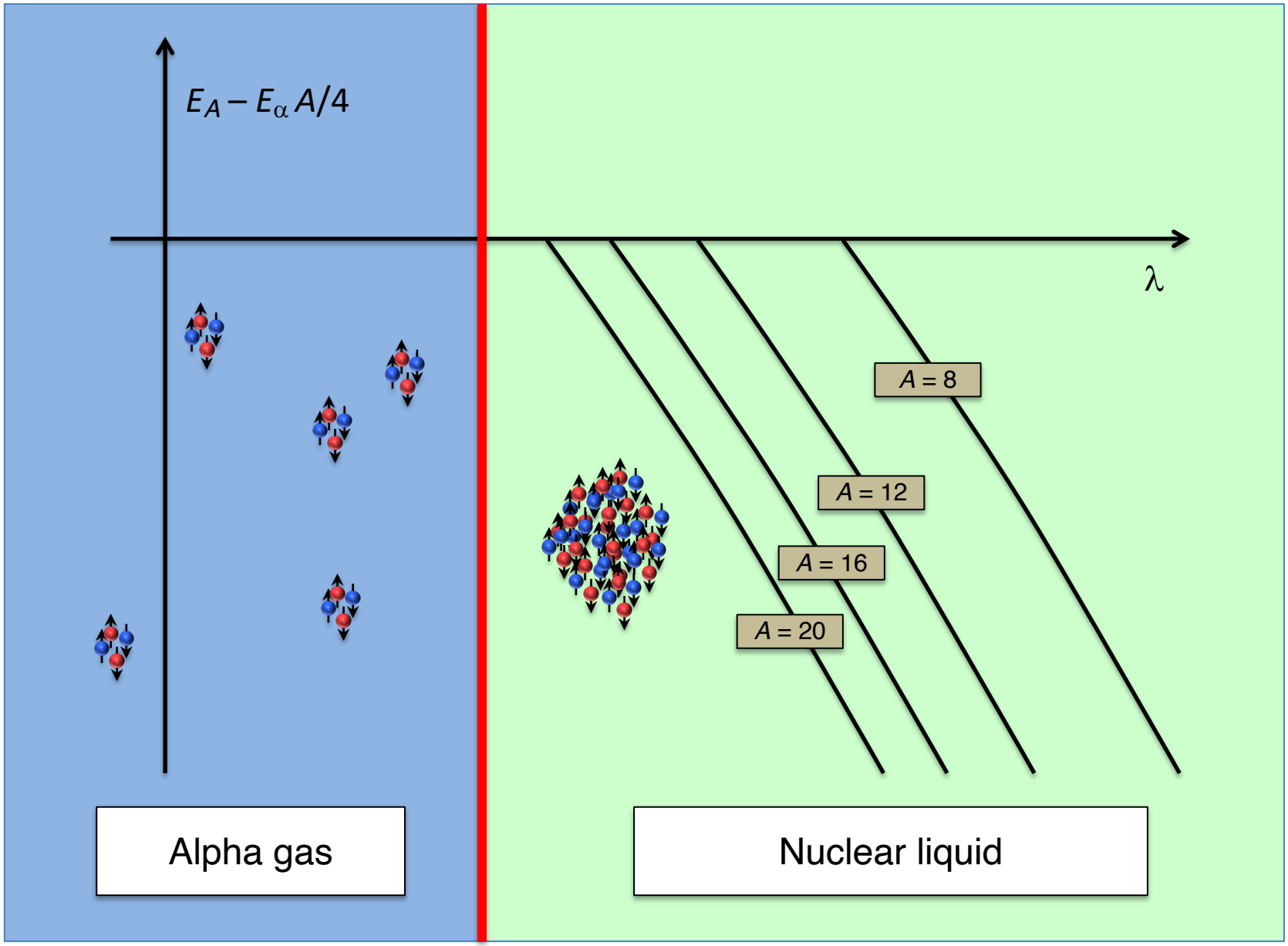
Sarkar, D.L., Meißner, Phys. Rev. Lett. 131, 242503 (2023)

$$\frac{\langle\psi_{\text{init}}|\exp[-H(c_j)\tau]\exp[-H(c_k)\tau]\exp[-H(c_j)\tau]\exp[-H(c_k)\tau]|\psi_{\text{init}}\rangle}{\langle\psi_{\text{init}}|\exp[-2H(c_j)\tau]\exp[-2H(c_k)\tau]|\psi_{\text{init}}\rangle}$$



In order to compute the phase, we calculate the ratio

$$\frac{N_{j,k}}{|N_{j,k}|} \approx \frac{\langle\psi_{\text{init}}|\exp[-2H(c_j)\tau]\exp[-2H(c_k)\tau]|\psi_{\text{init}}\rangle}{|\langle\psi_{\text{init}}|\exp[-2H(c_j)\tau]\exp[-2H(c_k)\tau]|\psi_{\text{init}}\rangle|}$$



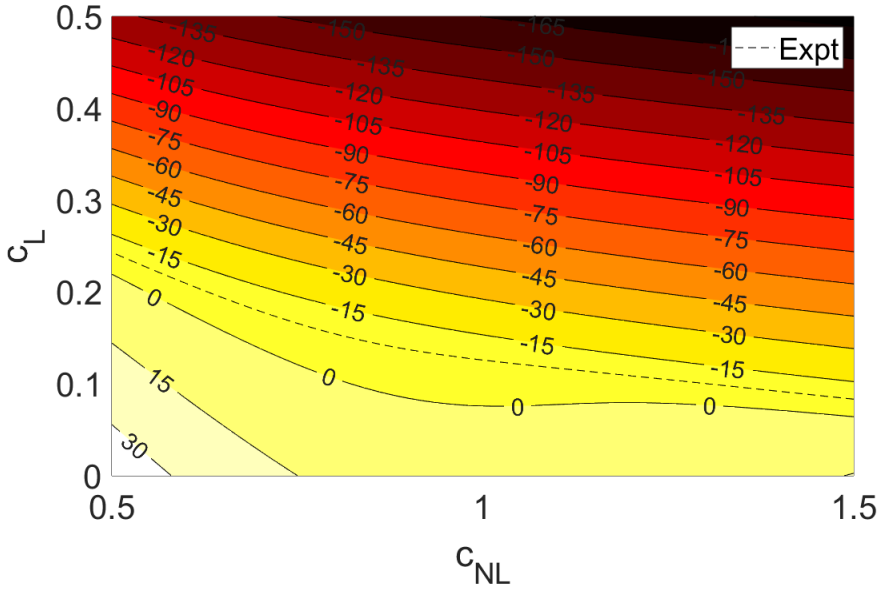
Elhatisari, et al., Phys. Rev. Lett. 117, 132501 (2016)

(c_L, c_{NL})	Full Simulation	2nd order EC	3rd order EC	4th order EC
(0.8,0.2)	-338.57 ± 0.03	-330.63 ± 0.26	-333.15 ± 1.85	-333.24 ± 1.14
(0.8,0.1)	-295.33 ± 0.02	-290.04 ± 0.24	-292.08 ± 1.51	-292.17 ± 1.03
(0.9,0.1)	-381.81 ± 0.02	-369.12 ± 0.28	-372.63 ± 2.24	-372.77 ± 1.83
(0.8,0.3)	-382.41 ± 0.03	-371.22 ± 0.27	-374.24 ± 2.25	-374.34 ± 1.42
(0.4,0.6)	-177.15 ± 0.05	-177.25 ± 0.19	-177.32 ± 0.46	-177.33 ± 0.24
(0.4,0.7)	-217.73 ± 0.04	-217.70 ± 0.19	-217.71 ± 0.38	-217.72 ± 0.21
(0.3,0.7)	-141.11 ± 0.05	-139.63 ± 0.19	-141.09 ± 0.71	-141.10 ± 0.35
(0.4,0.8)	-259.35 ± 0.06	-258.19 ± 0.20	-258.31 ± 0.30	-258.32 ± 0.28
(0.2,0.6)	-41.54 ± 0.05	-31.91 ± 0.15	-37.75 ± 0.50	-41.64 ± 0.14
(0.2,0.2)	31.26 ± 0.02	101.48 ± 0.17	99.18 ± 1.86	69.72 ± 1.77
(0.8,0.8)	-606.63 ± 0.05	-574.23 ± 0.37	-579.97 ± 4.02	-580.12 ± 2.70

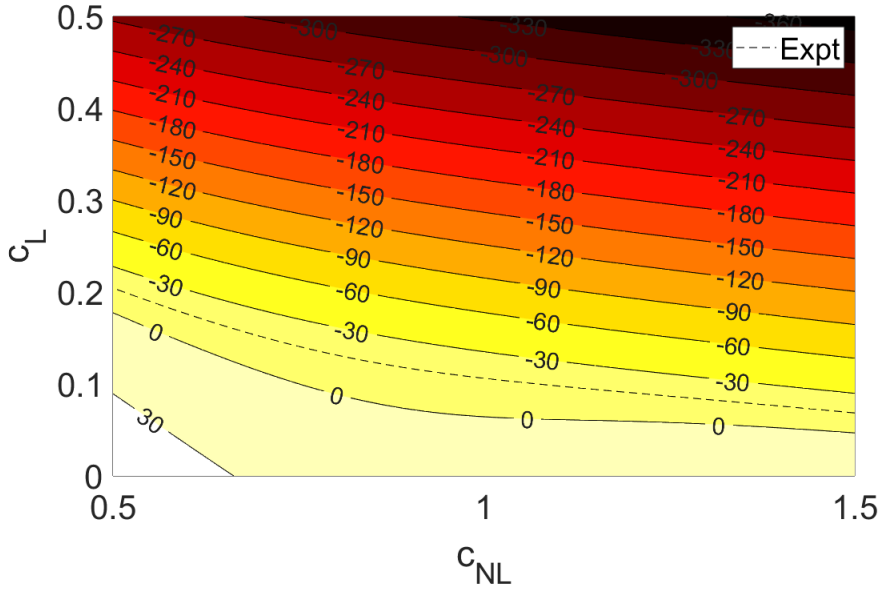
TABLE I: Comparison of the EC emulator prediction and full simulations results for ^{12}C. The training points added to the EC subspace progressively are: $(c_L, c_{NL}) = (0.5, 0.5)$, $(0.2, 0.8)$, $(0, 1)$, and $(0.2, 0.6)$.

Sarkar, D.L., Meißner, Phys. Rev. Lett. 131, 242503 (2023)

$E(^{12}\mathrm{C}) - 3E(^{4}\mathrm{He})$

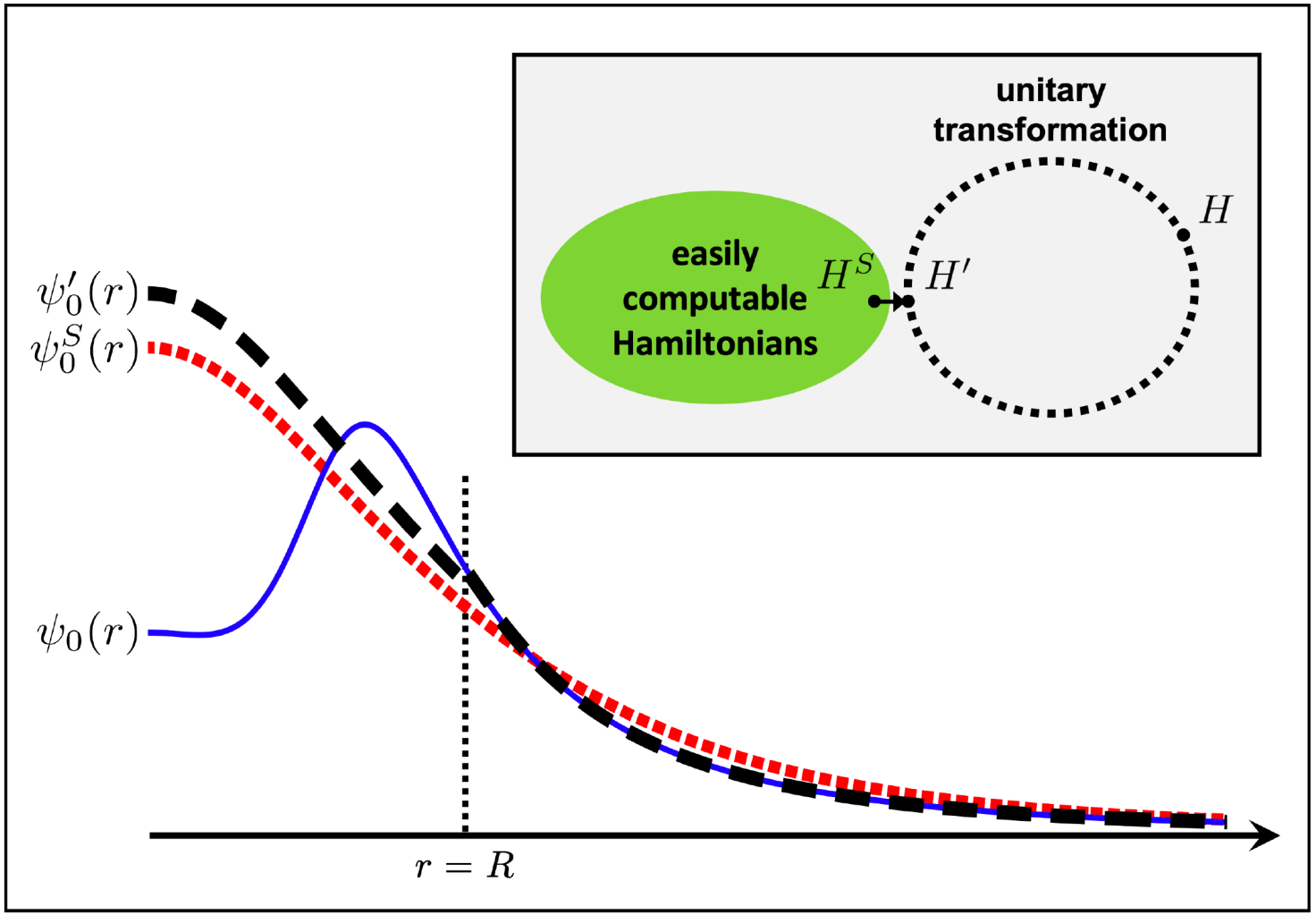


$E(^{16}\mathrm{O}) - 4E(^{4}\mathrm{He})$



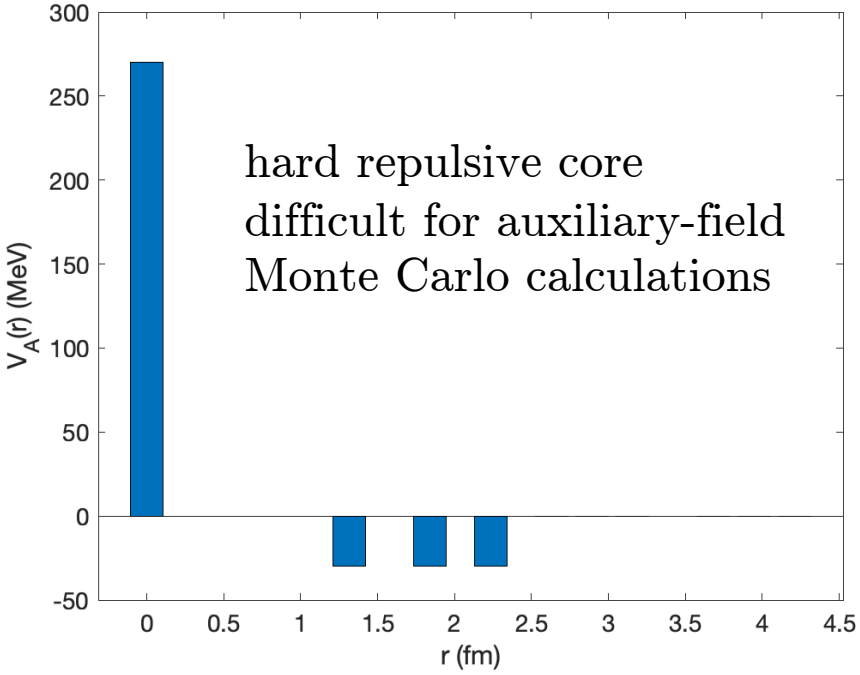
Sarkar, D.L., Meißner, Phys. Rev. Lett. 131, 242503 (2023)

Wave function matching

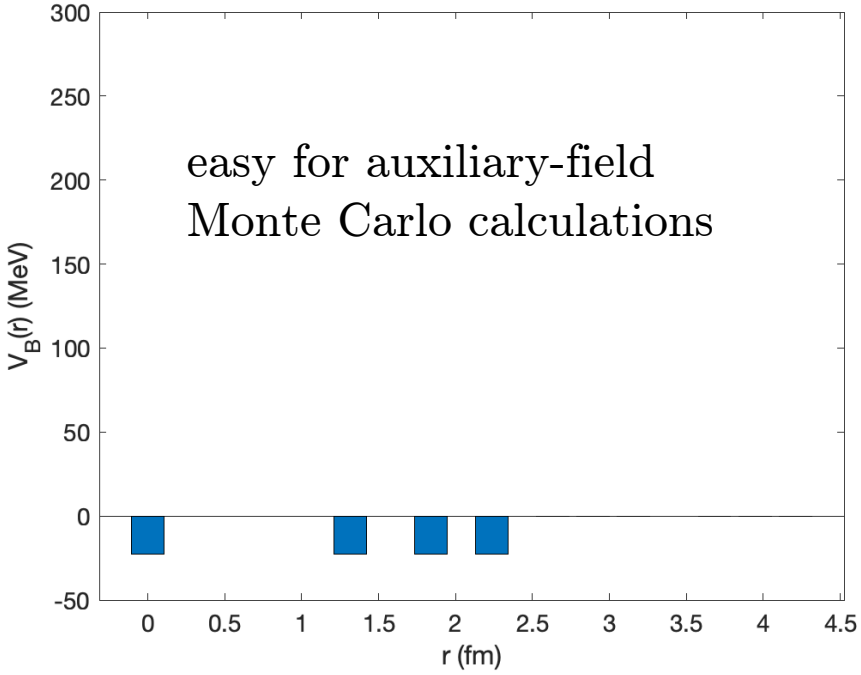


Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, arXiv: 2210.17488

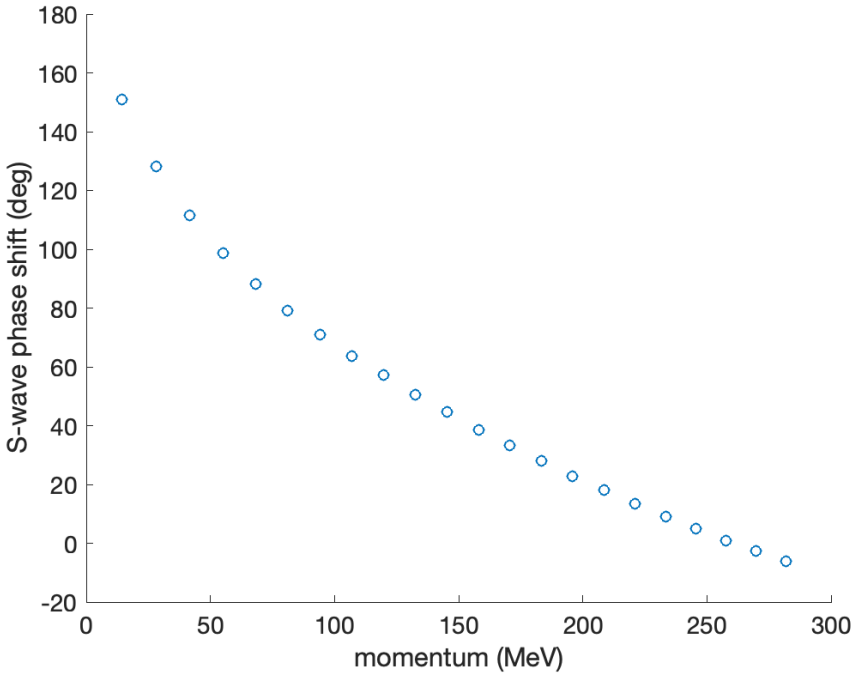
$V_A(r)$


hard repulsive core
difficult for auxiliary-field
Monte Carlo calculations
300
250
200
150
100
50
0
-50
$V_A(r)$ (MeV)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
r (fm)

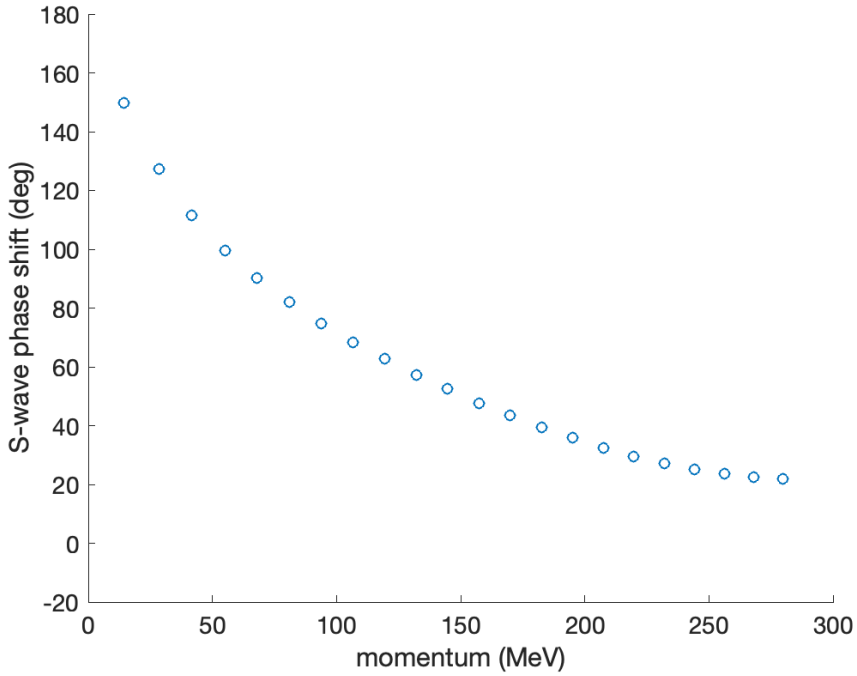
$V_B(r)$


easy for auxiliary-field
Monte Carlo calculations
300
250
200
150
100
50
0
-50
$V_B(r)$ (MeV)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
r (fm)

$V_A(r)$


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_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

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

There are many possible choices to complete the unitary transformation.

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

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

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

The corresponding action of U on the Hamiltonian is

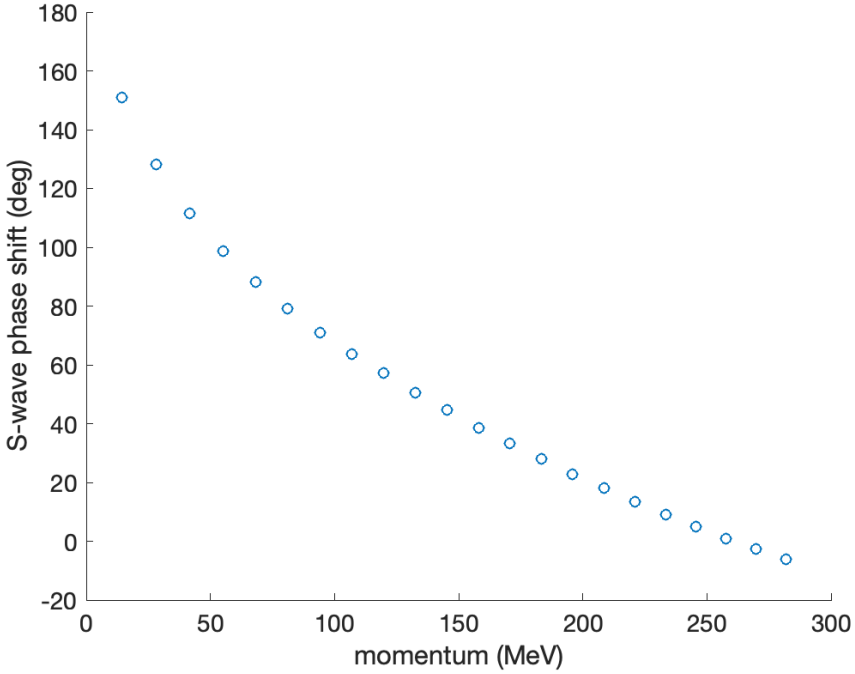
$$U : H_A \to H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

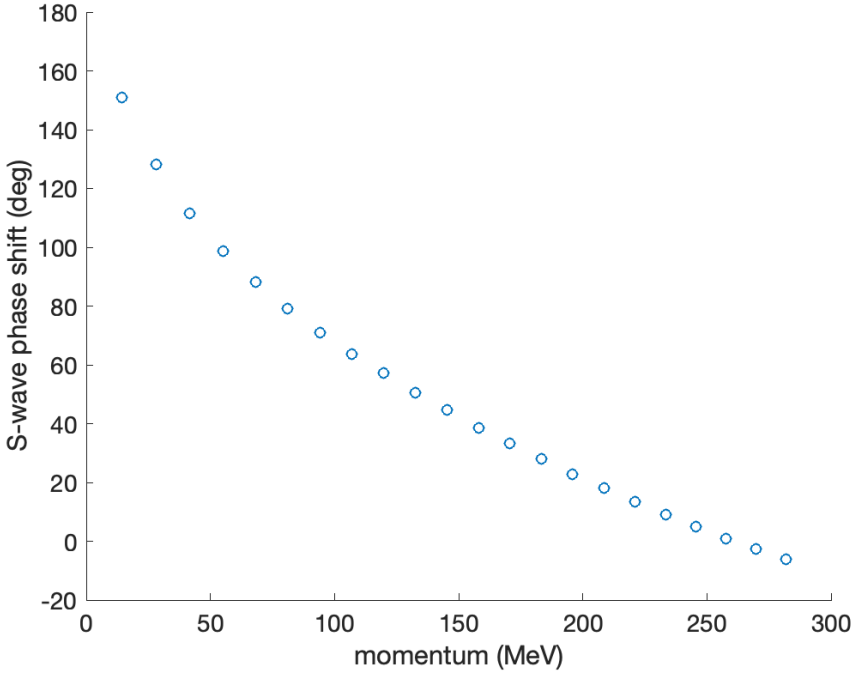
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

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

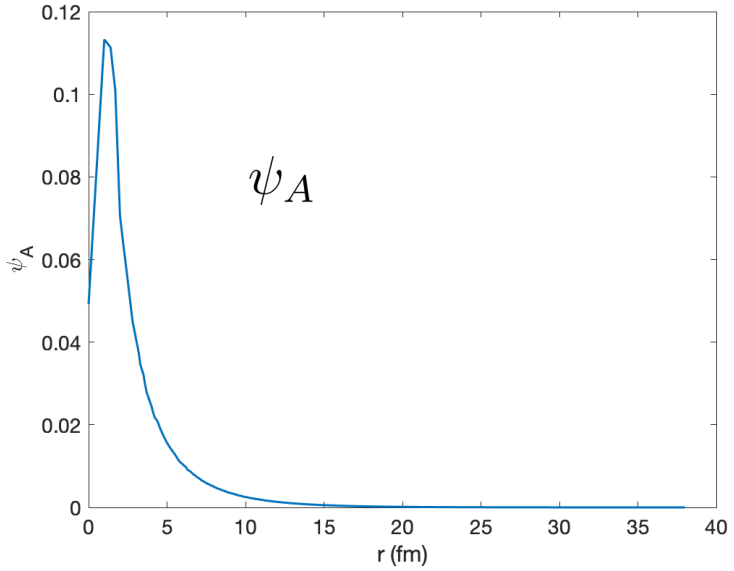
$V_A(r)$

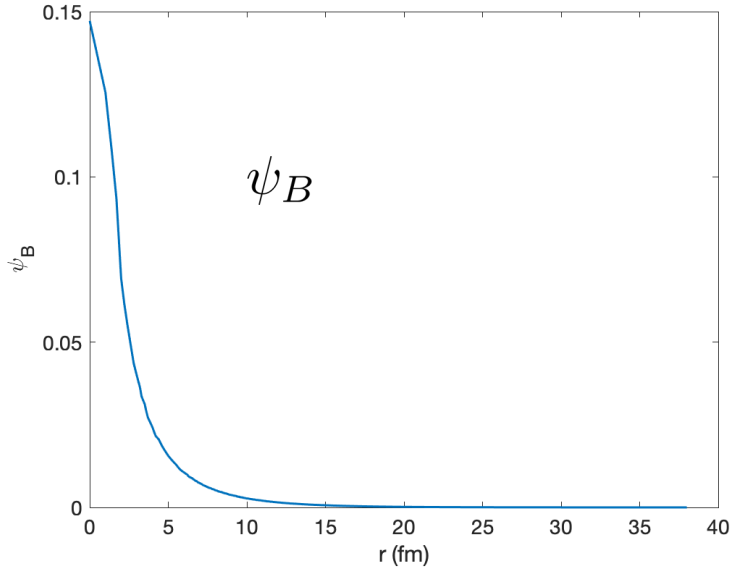

S-wave phase shift (deg)
momentum (MeV)
180
160
140
120
100
80
60
40
20
0
-20
0
50
100
150
200
250
300

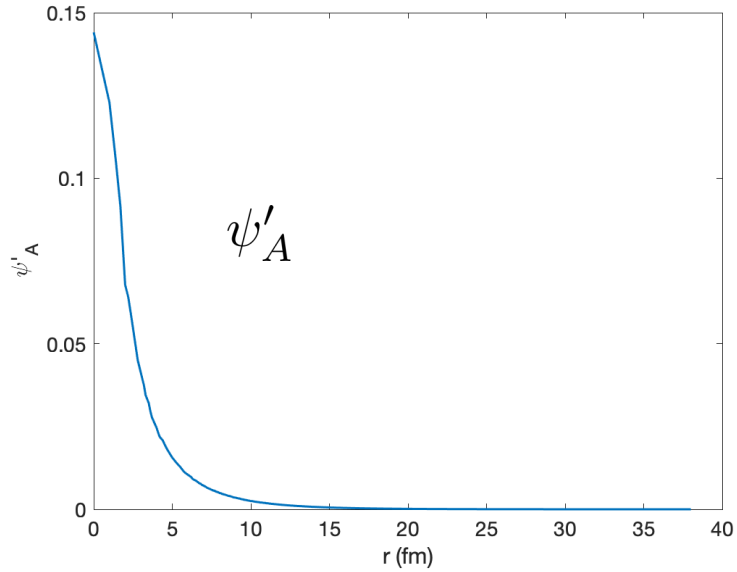
$V'_A(r, r')$


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

Ground state wave functions





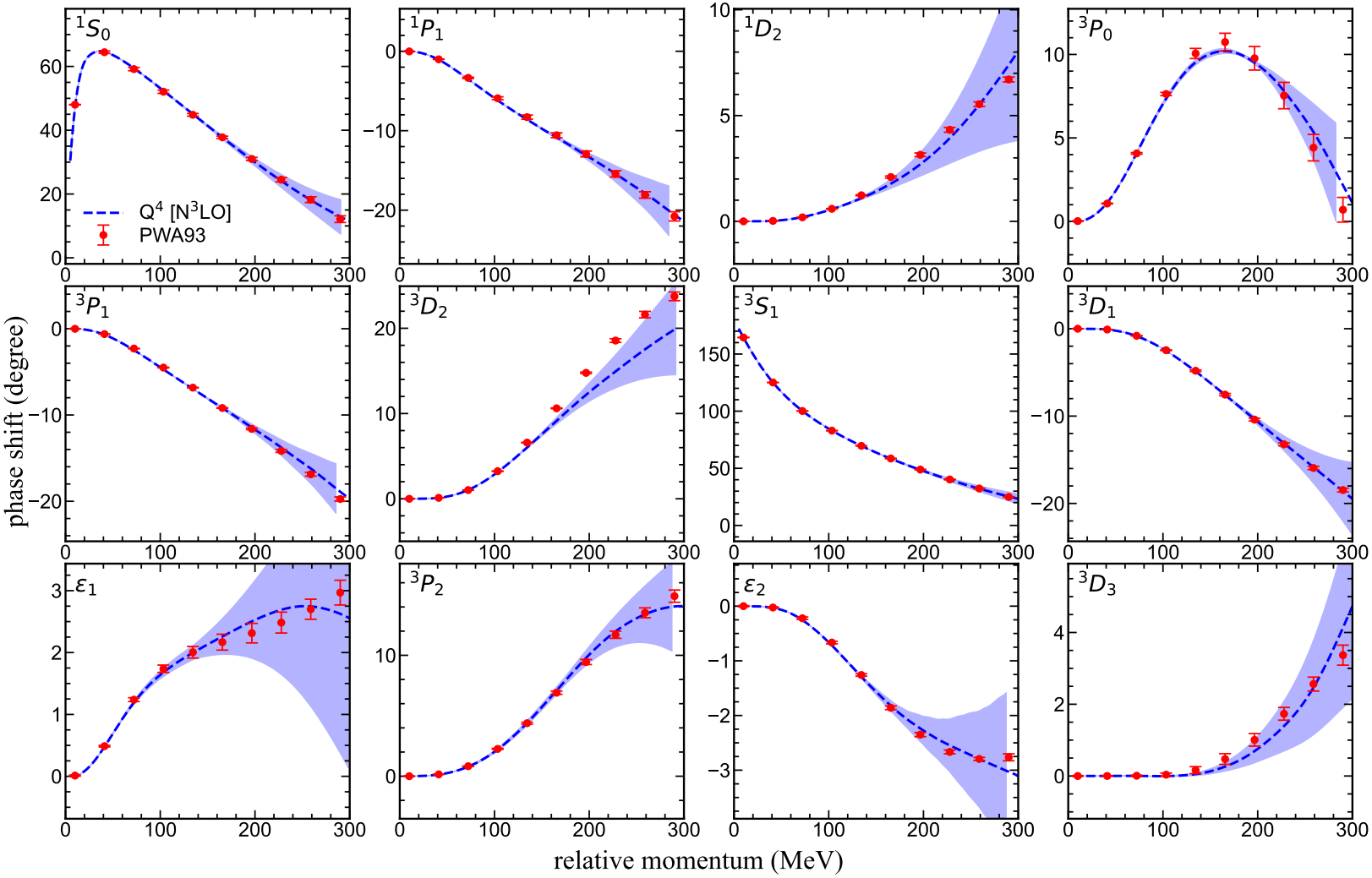


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

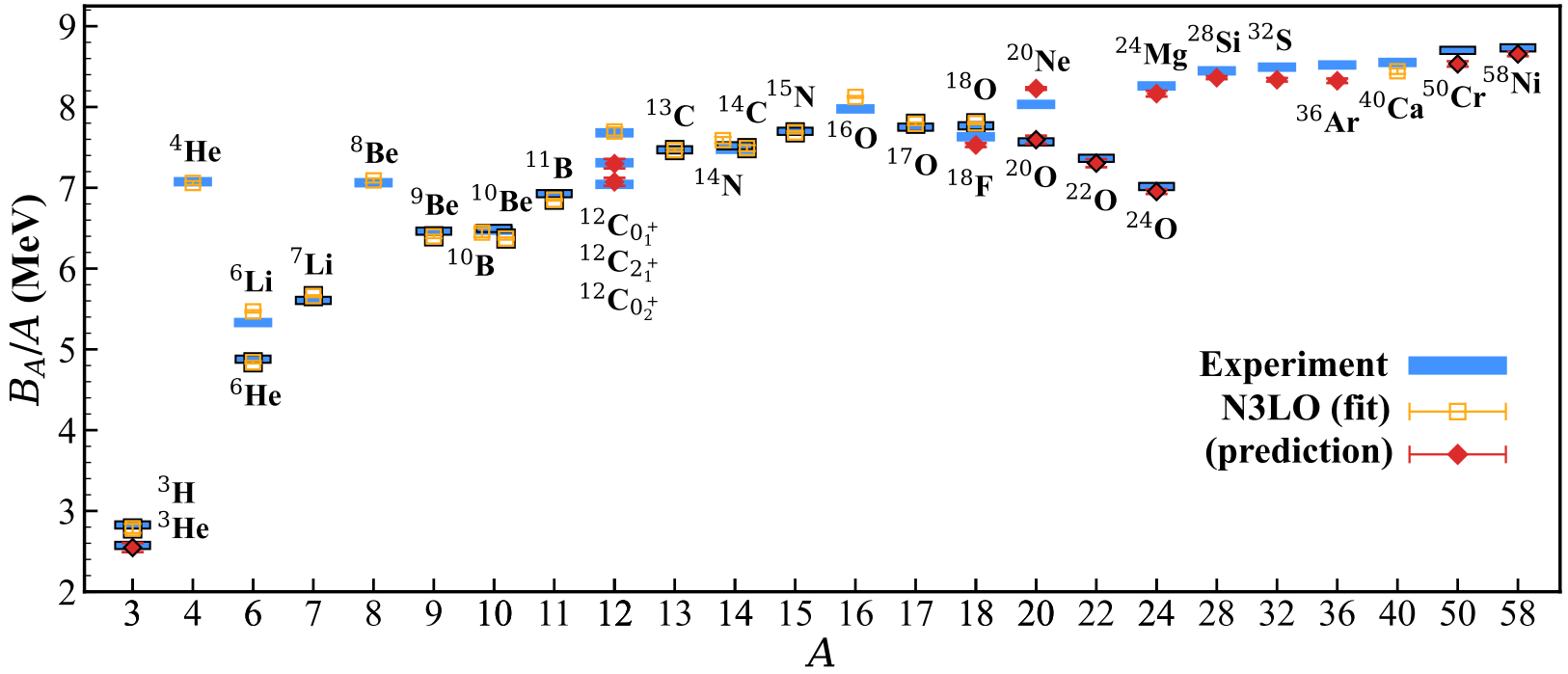
$R = 2.6$ fm

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

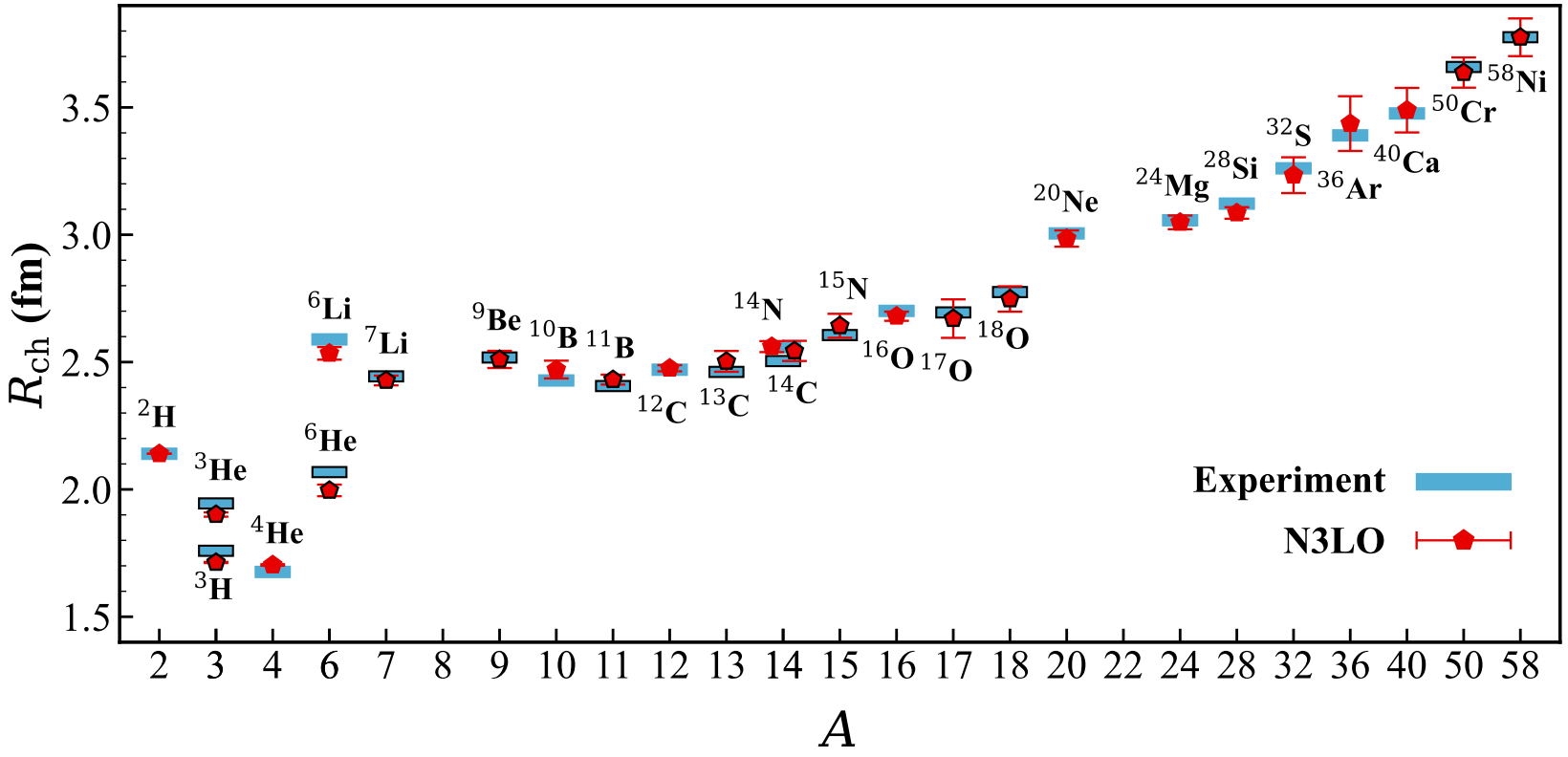


Binding energy per nucleon



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

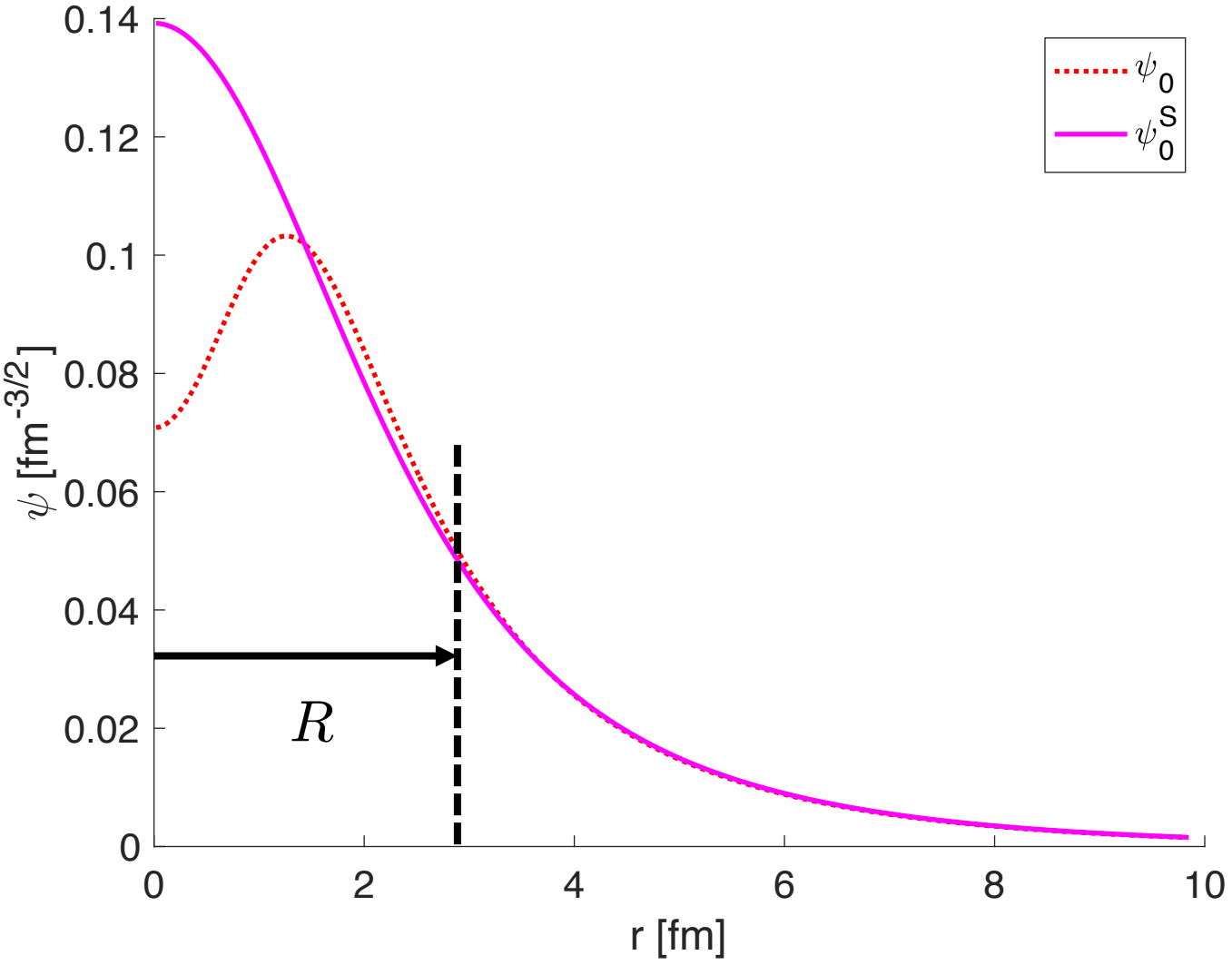
Charge radius



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

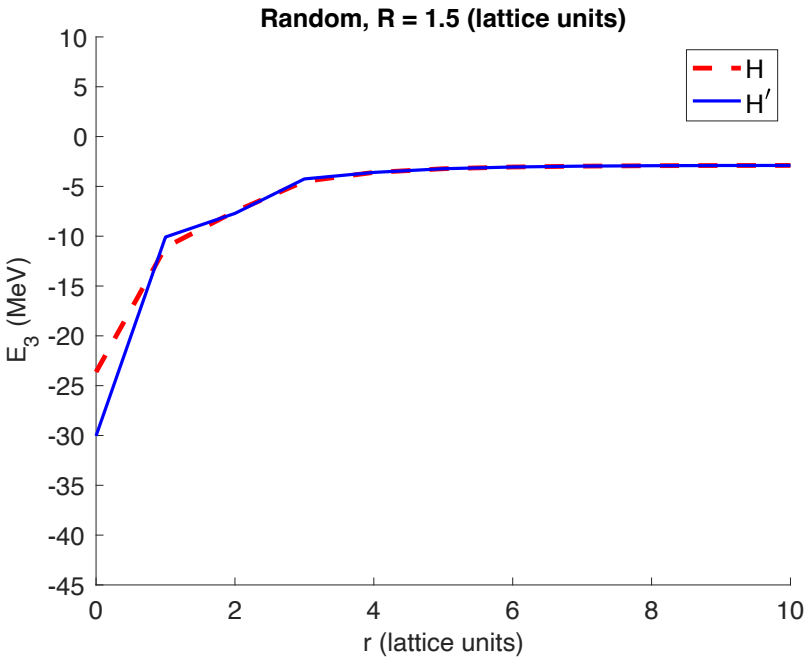
Is wave function matching qualitatively different from the similarity renormalization group, $V_{\text{low-}k}$, or the unitary correlation operator method?

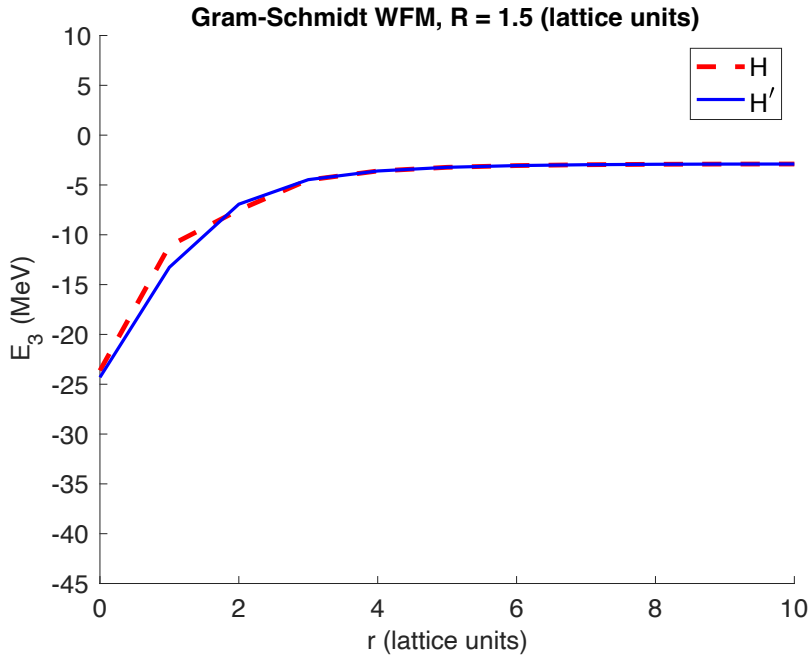
Dependence on wave function matching radius

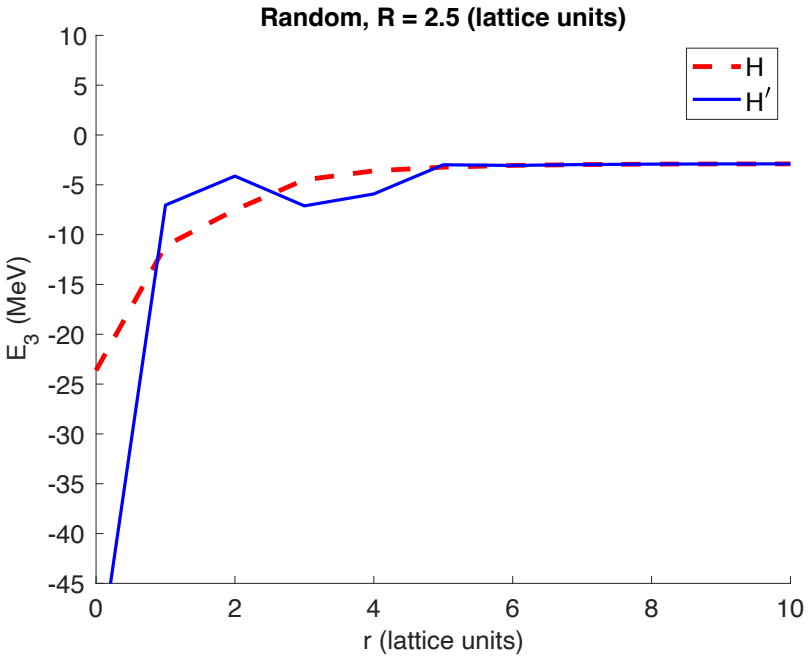


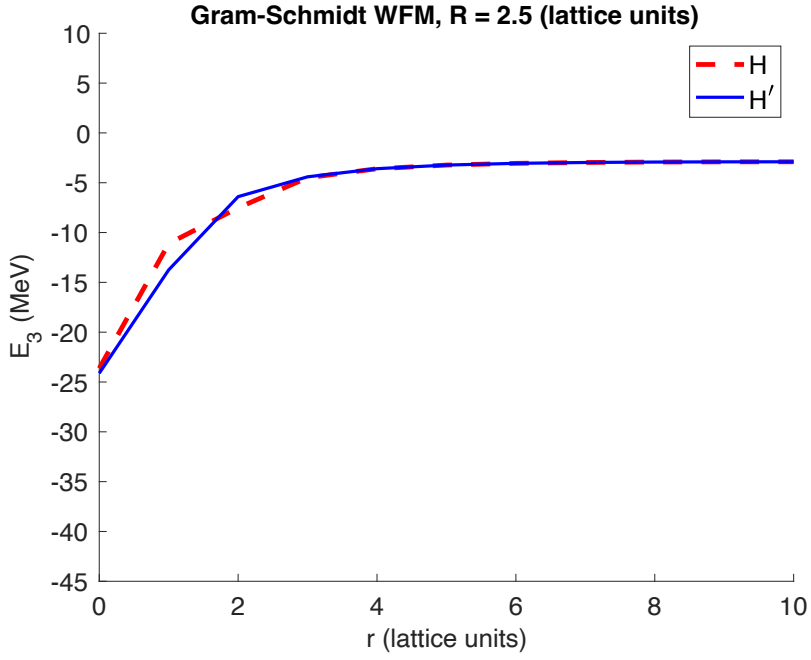
1D system with two infinitely heavy particles and one light particle

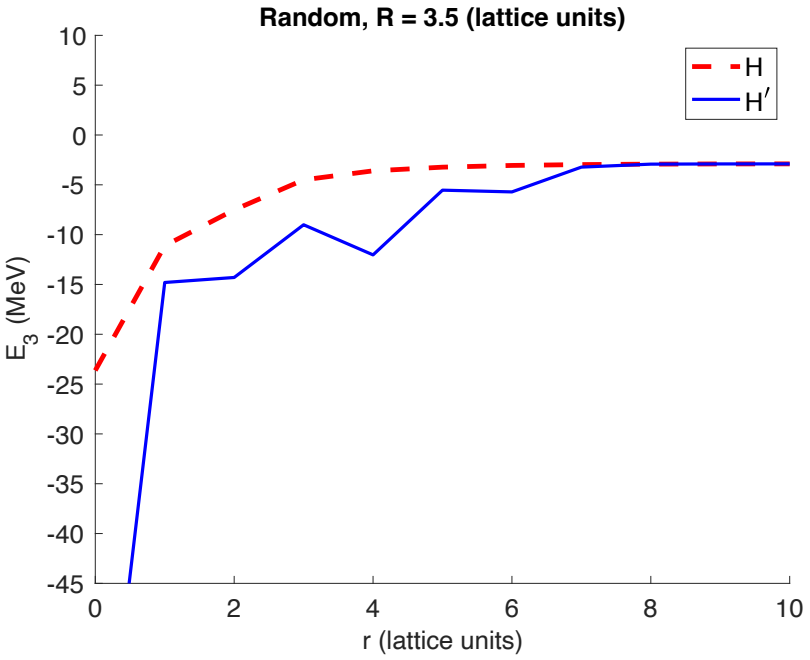
Difference in the three-body ground state energy gives the induced three-body interaction for chosen positions of the infinitely heavy particles.

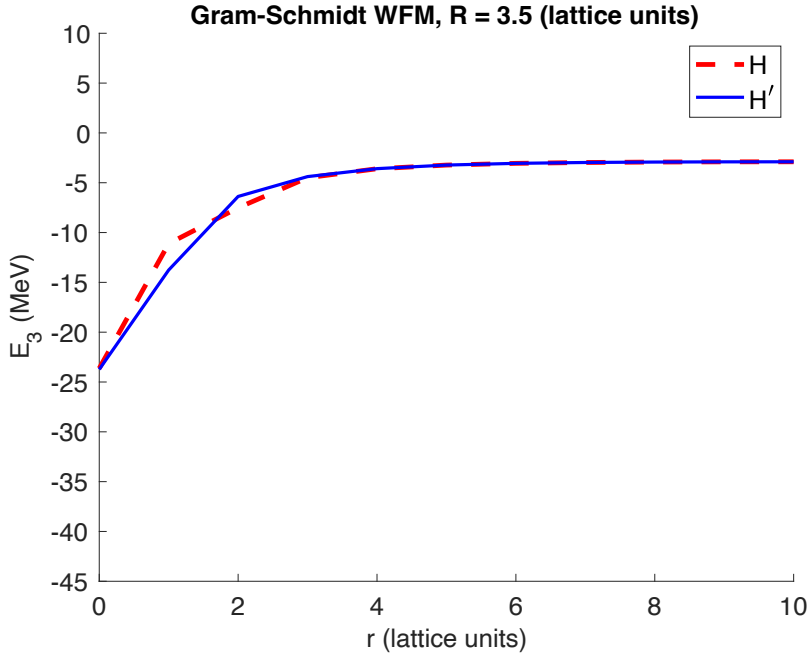


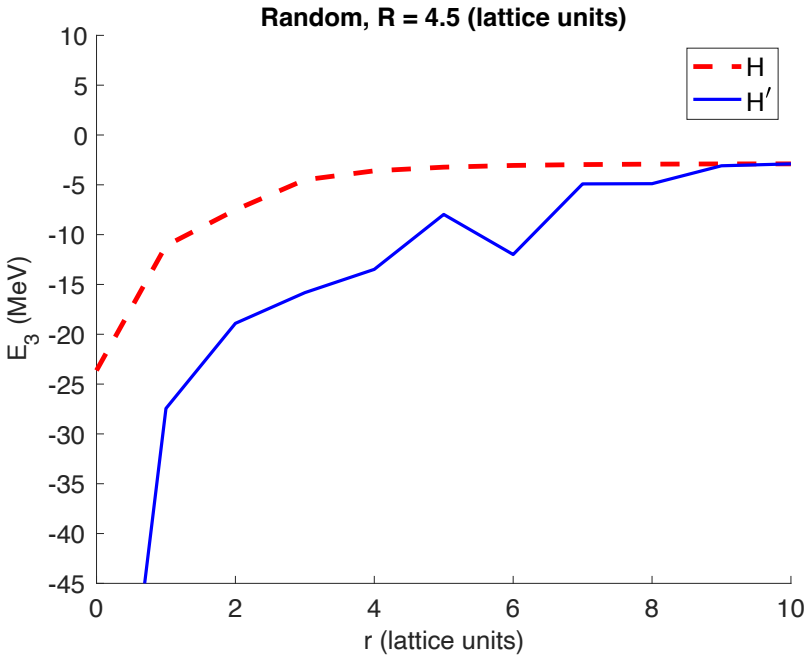


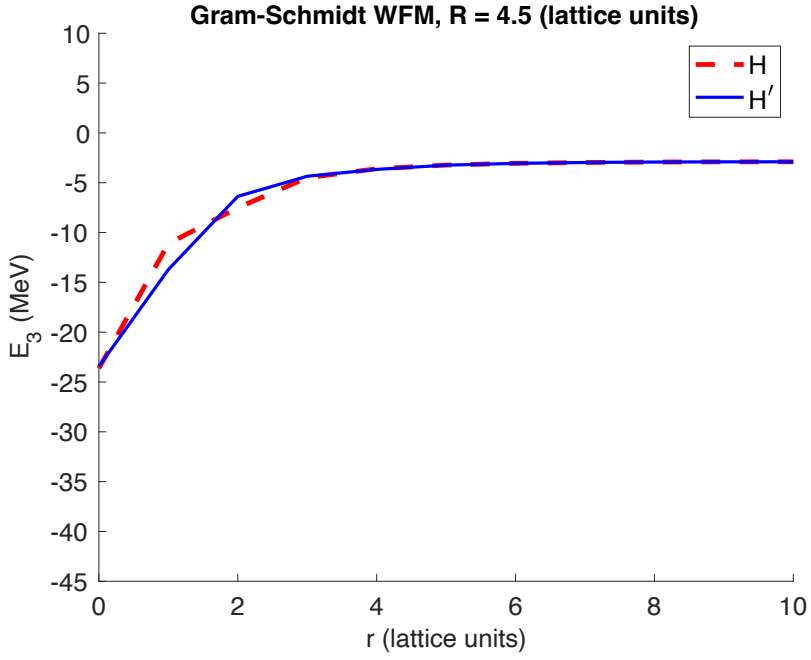

Random, R = 2.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10

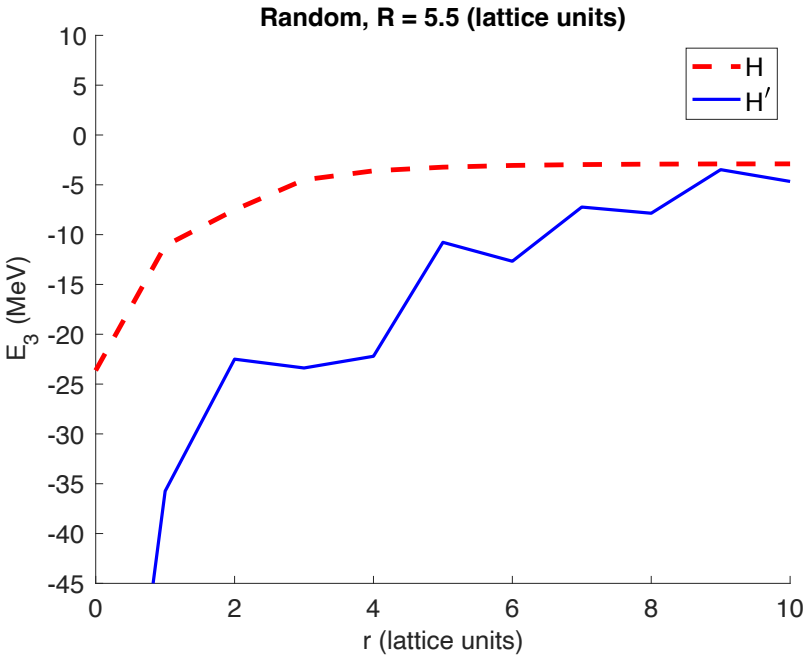

Gram-Schmidt WFM, R = 2.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10

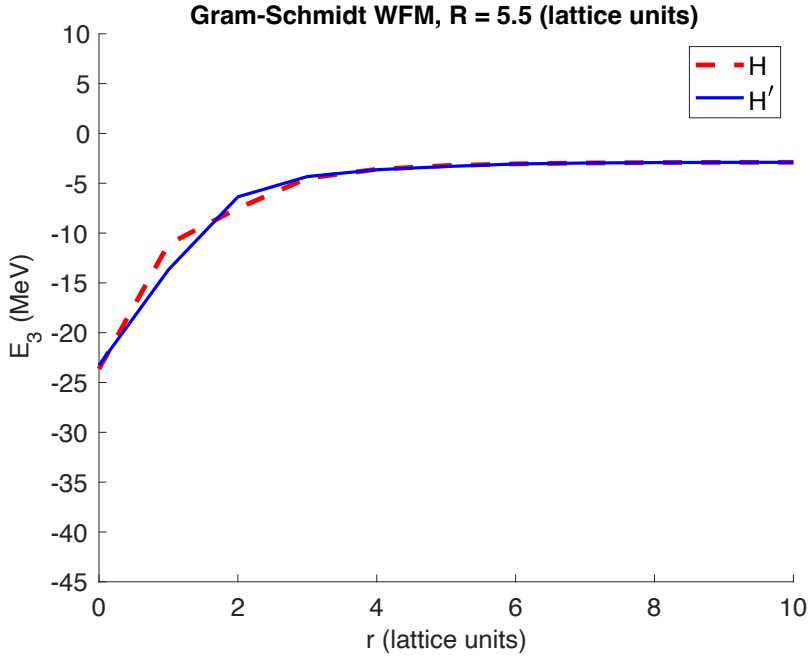

Random, R = 3.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10

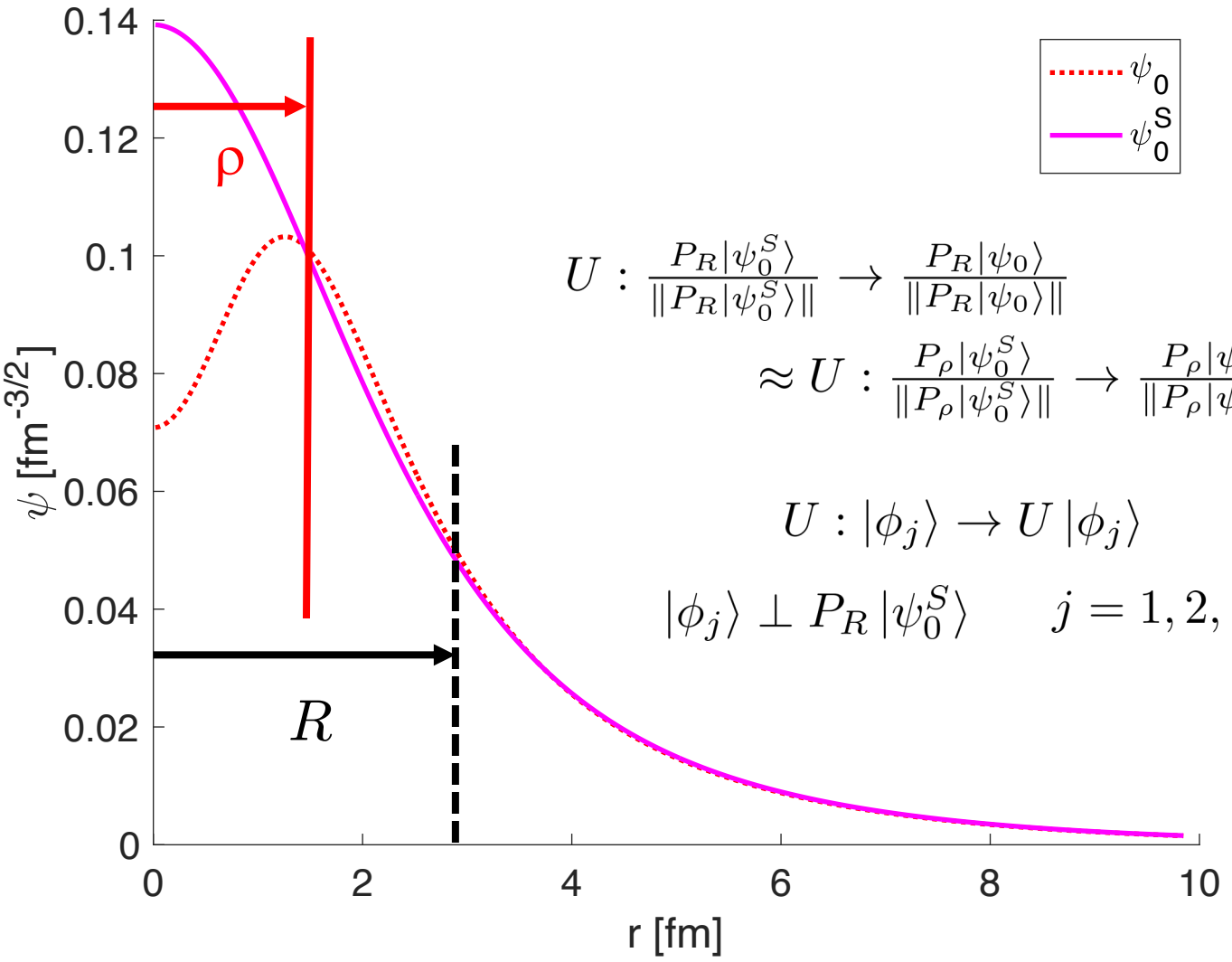

Gram-Schmidt WFM, R = 3.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10


Random, R = 4.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10


Gram-Schmidt WFM, R = 4.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10


Random, R = 5.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10


Gram-Schmidt WFM, R = 5.5 (lattice units)
H
H′
E3 (MeV)
r (lattice units)
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
0
2
4
6
8
10



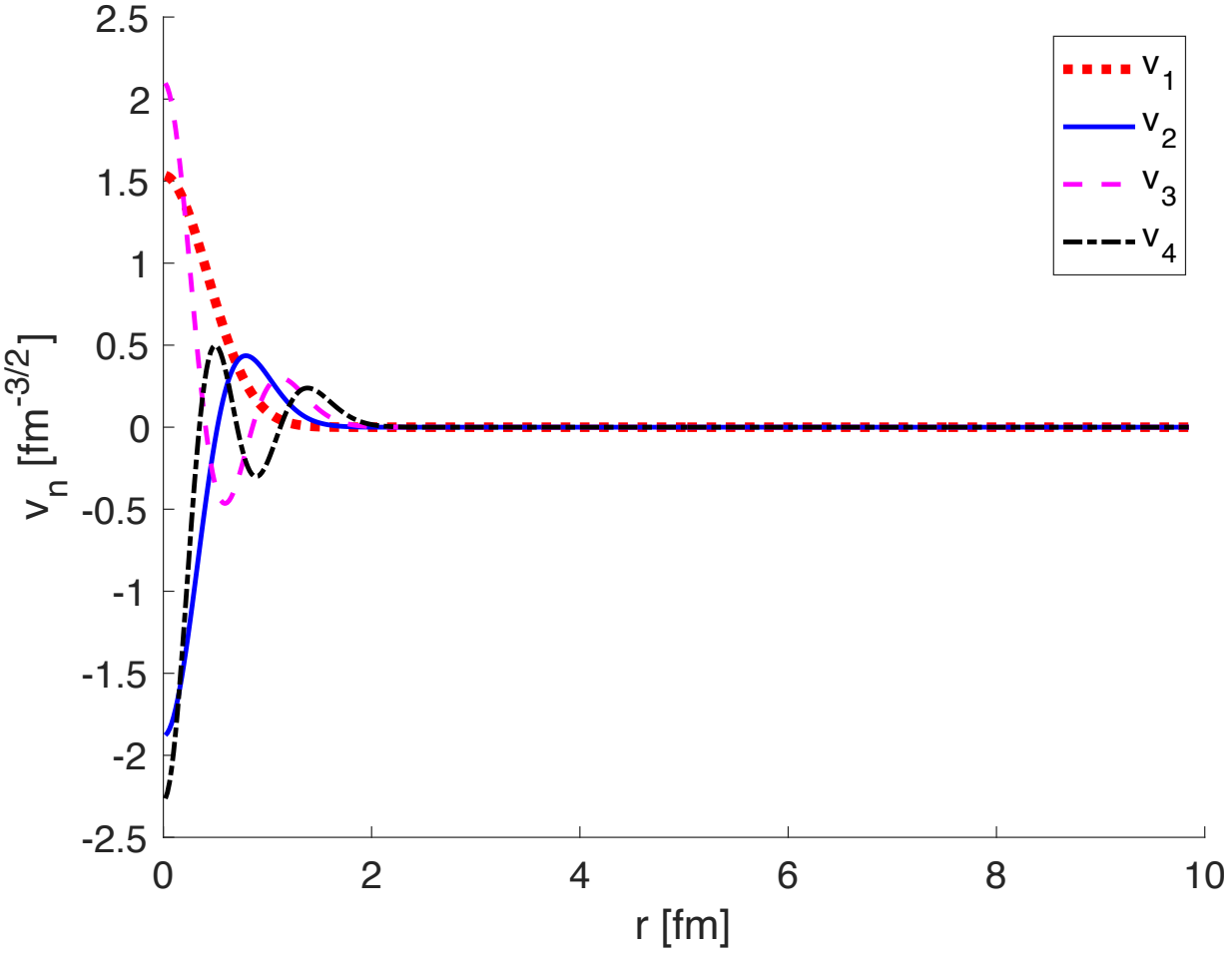
$$U : \frac{P_R|\psi_0^S\rangle}{\|P_R|\psi_0^S\rangle\|} \rightarrow \frac{P_R|\psi_0\rangle}{\|P_R|\psi_0\rangle\|}$$

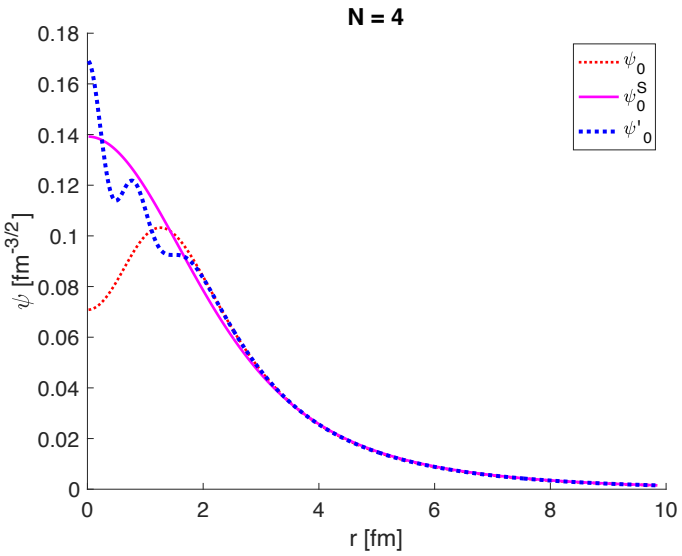
$$\approx U : \frac{P_\rho|\psi_0^S\rangle}{\|P_\rho|\psi_0^S\rangle\|} \rightarrow \frac{P_\rho|\psi_0\rangle}{\|P_\rho|\psi_0\rangle\|}$$

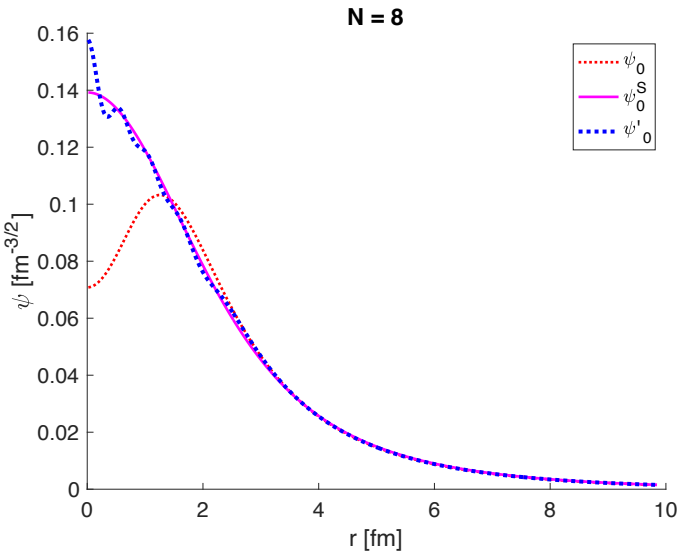
$$U : |\phi_j\rangle \rightarrow U\,|\phi_j\rangle$$

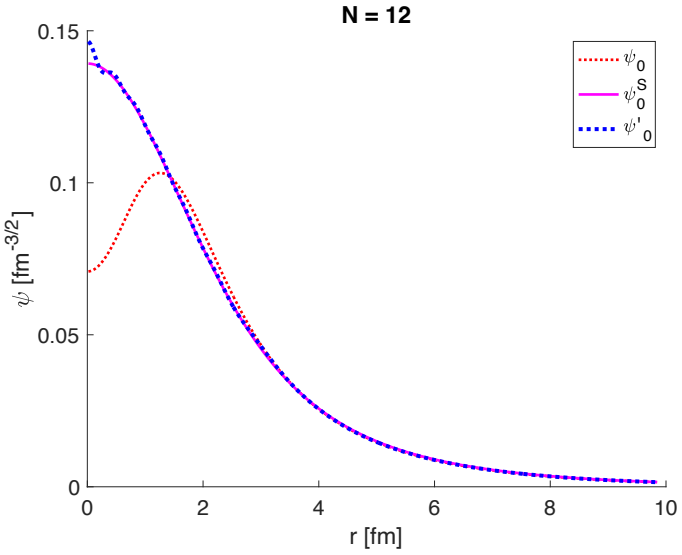
$$|\phi_j\rangle \perp P_R\,|\psi_0^S\rangle \qquad j = 1, 2, \cdots$$

Wave function matching in continuous space




N = 4
ψ_0
ψ_0^S
ψ'_0
ψ [fm$^{-3/2}$]
r [fm]
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
2
4
6
8
10


N = 8
ψ_0
ψ_0^S
ψ'_0
ψ [fm$^{-3/2}$]
r [fm]
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
2
4
6
8
10


N = 12
ψ_0
ψ_0^S
ψ'_0
ψ [fm$^{-3/2}$]
r [fm]
0.15
0.1
0.05
0
0
2
4
6
8
10

Summary

After an introduction to lattice effective field theory, we presented the floating block method for quantum Monte Carlo simulations. The floating block method allows one to calculate the inner product between eigenvectors of different Hamiltonians. We then discussed wave function matching. After this, 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 and described how it can be applied in the continuum.