Nuclear Lattice Simulations

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Facility for Rare Isotope Beams
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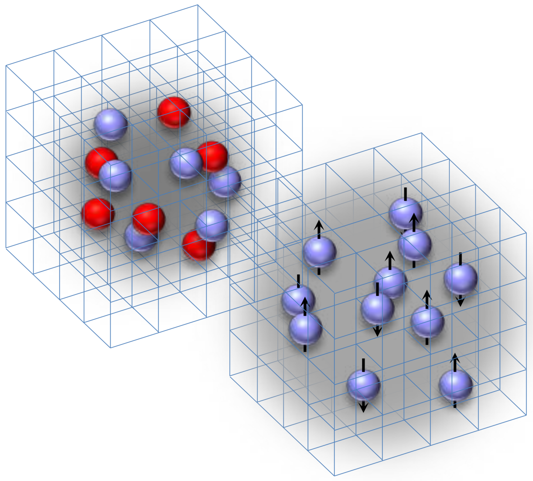
Nuclear Lattice EFT Collaboration



Theoretical Physics Colloquium
Arizona State University
September 1, 2021

FRIB
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Nuclear Computational Low-Energy Initiative
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Outline

Lattice effective field theory

A tale of two interactions

Hidden spin-isospin exchange symmetry

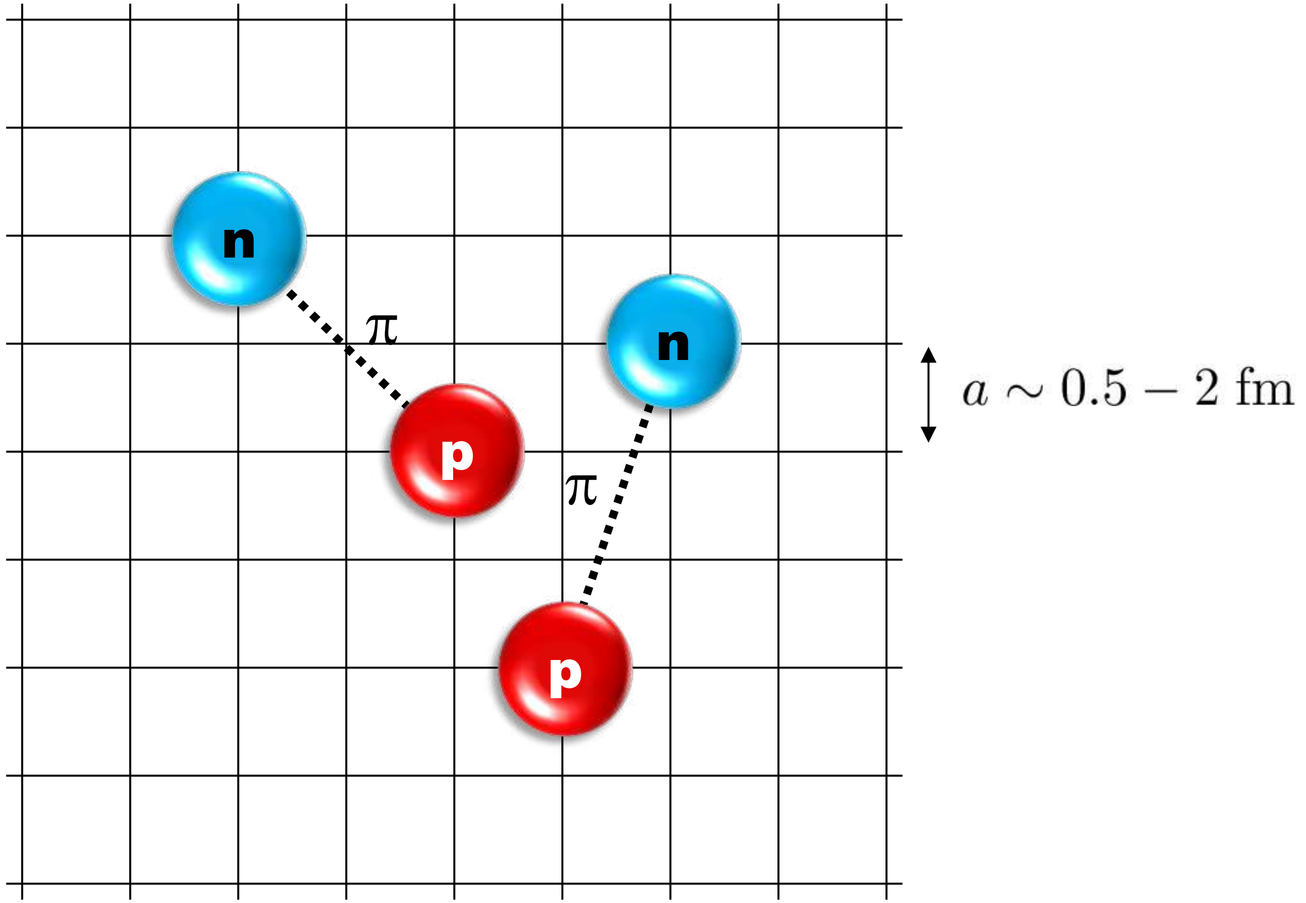
Essential elements for nuclear binding

Nuclear thermodynamics

Wave function matching

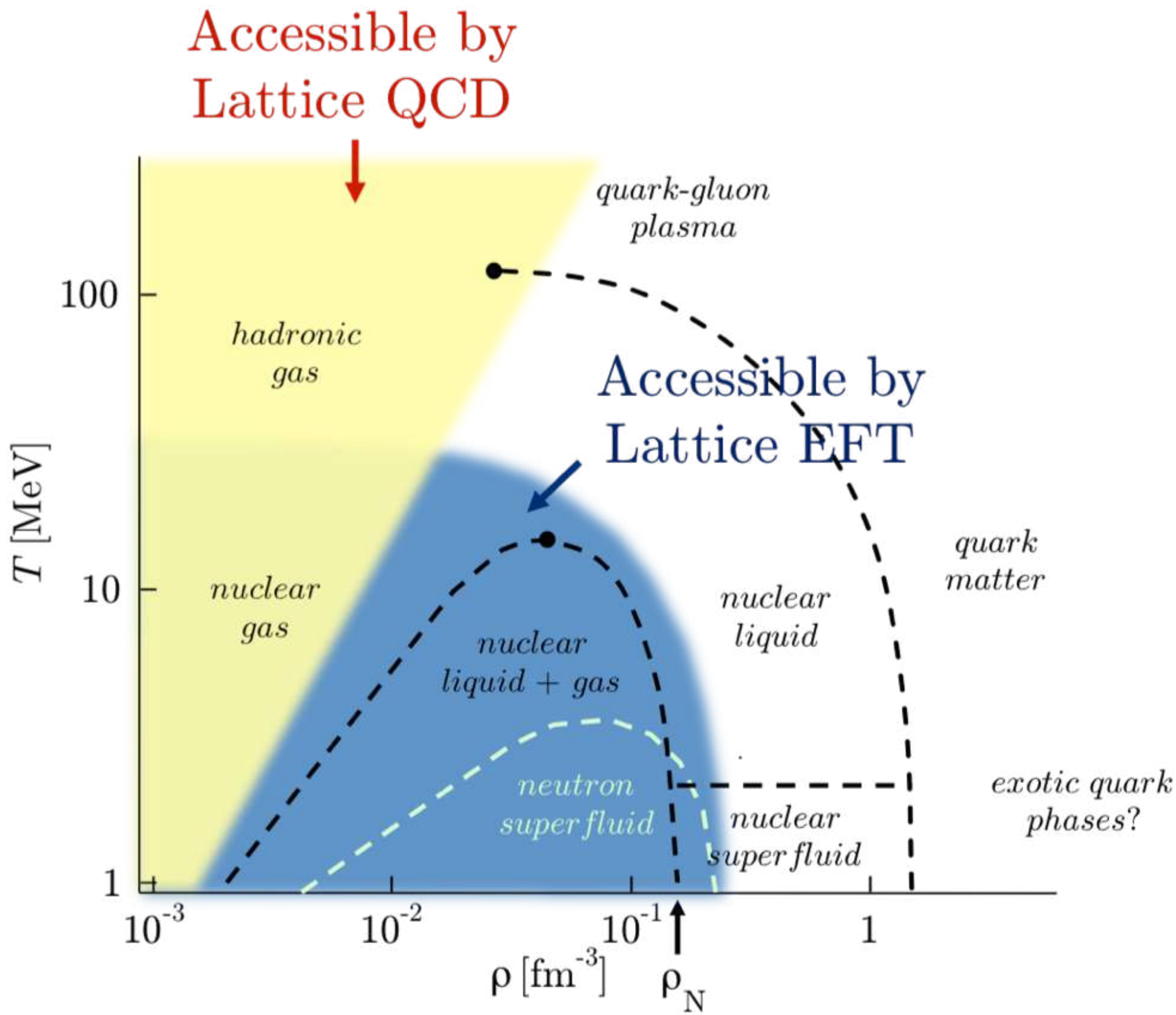
Summary

Lattice effective field theory



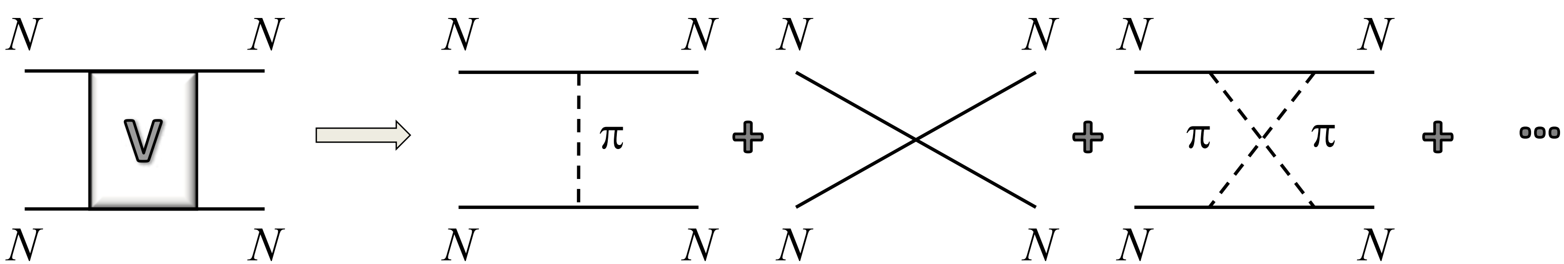
D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

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


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

Chiral effective field theory

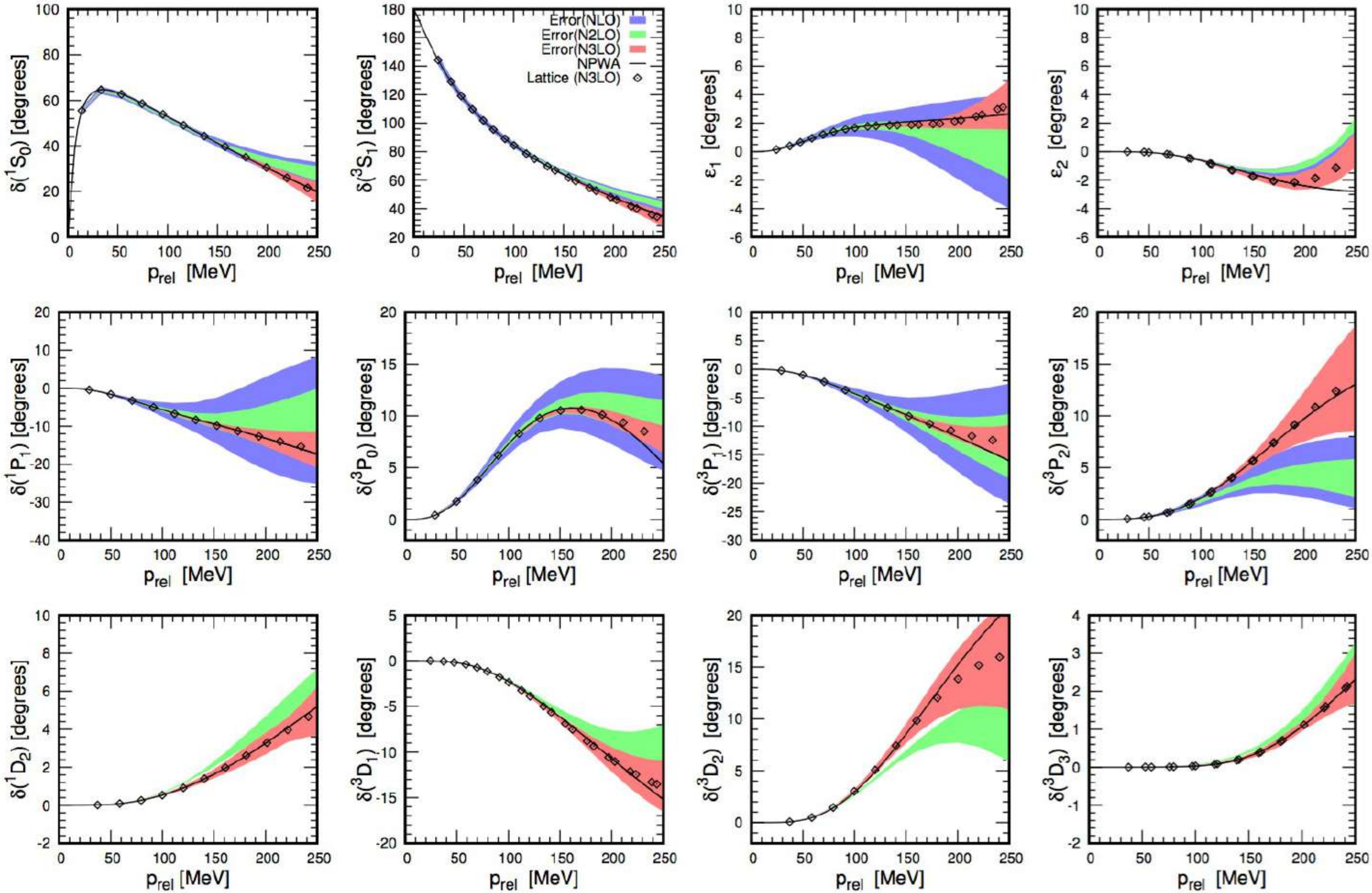
Construct the effective potential order by order



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

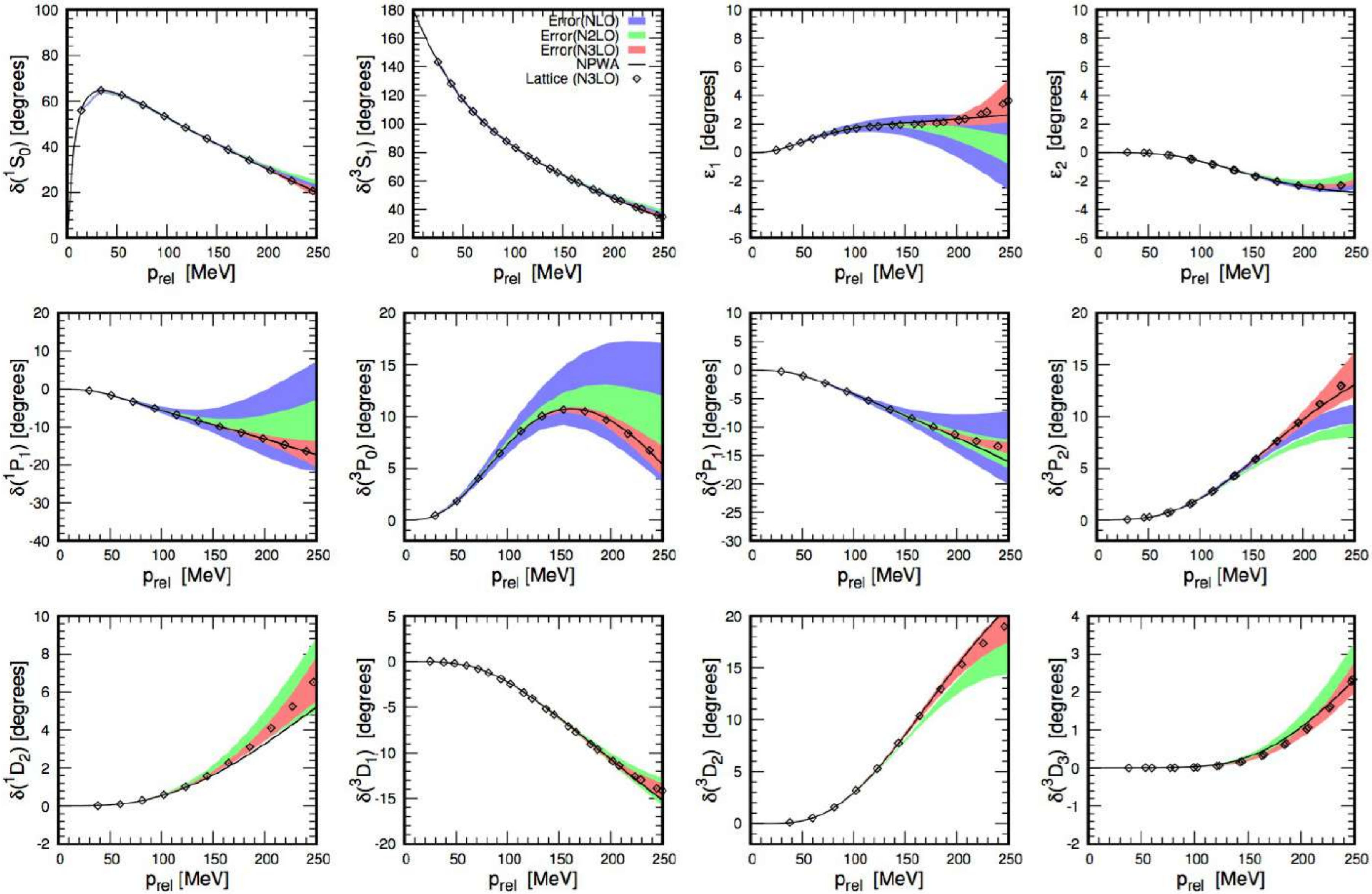
Leading order (LO) — Next-to-leading order (NLO)

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



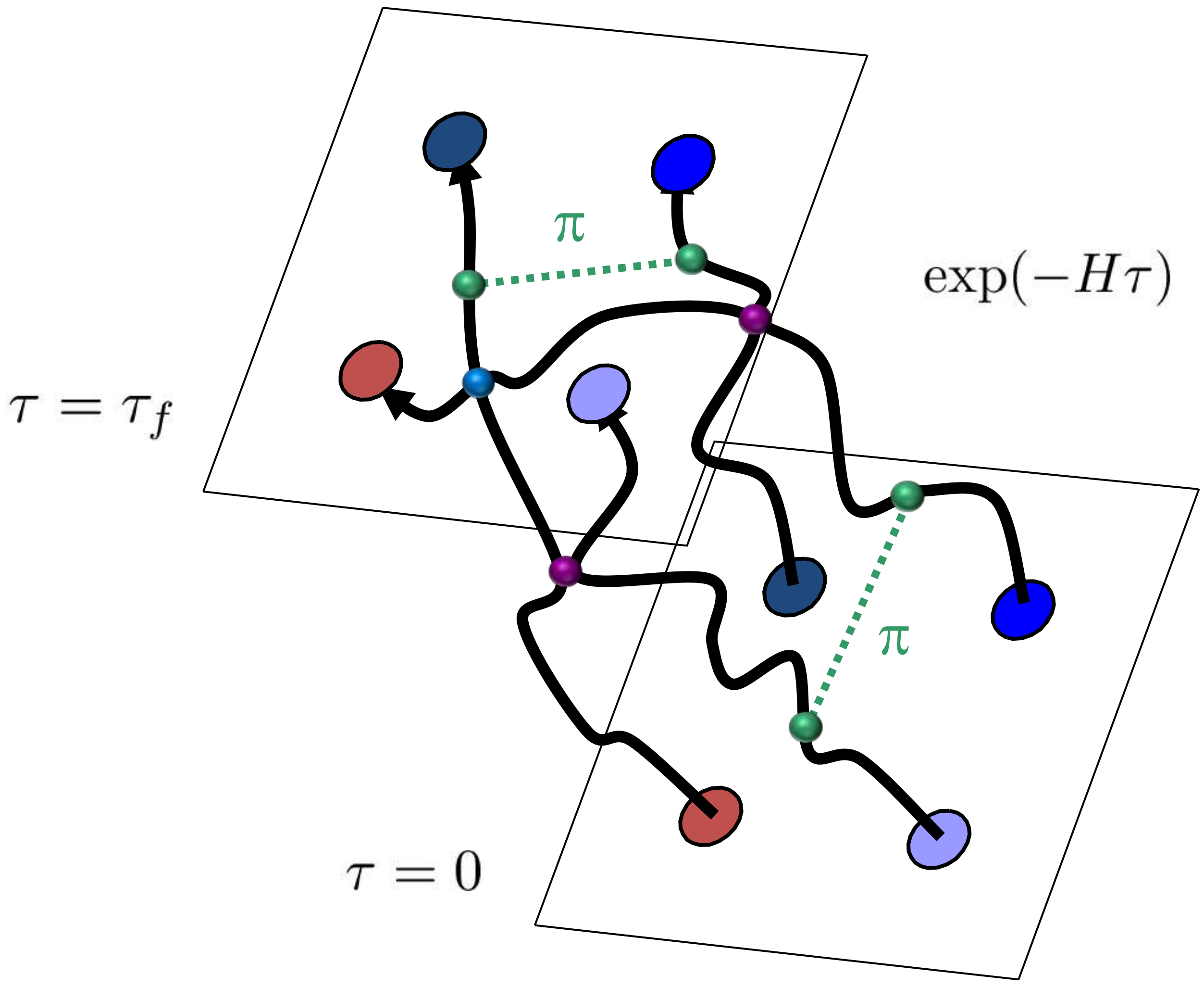
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

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



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

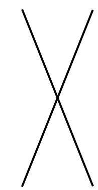
Euclidean time projection



Auxiliary field method

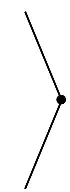
We can write exponentials of the interaction using a Gaussian integral identity

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



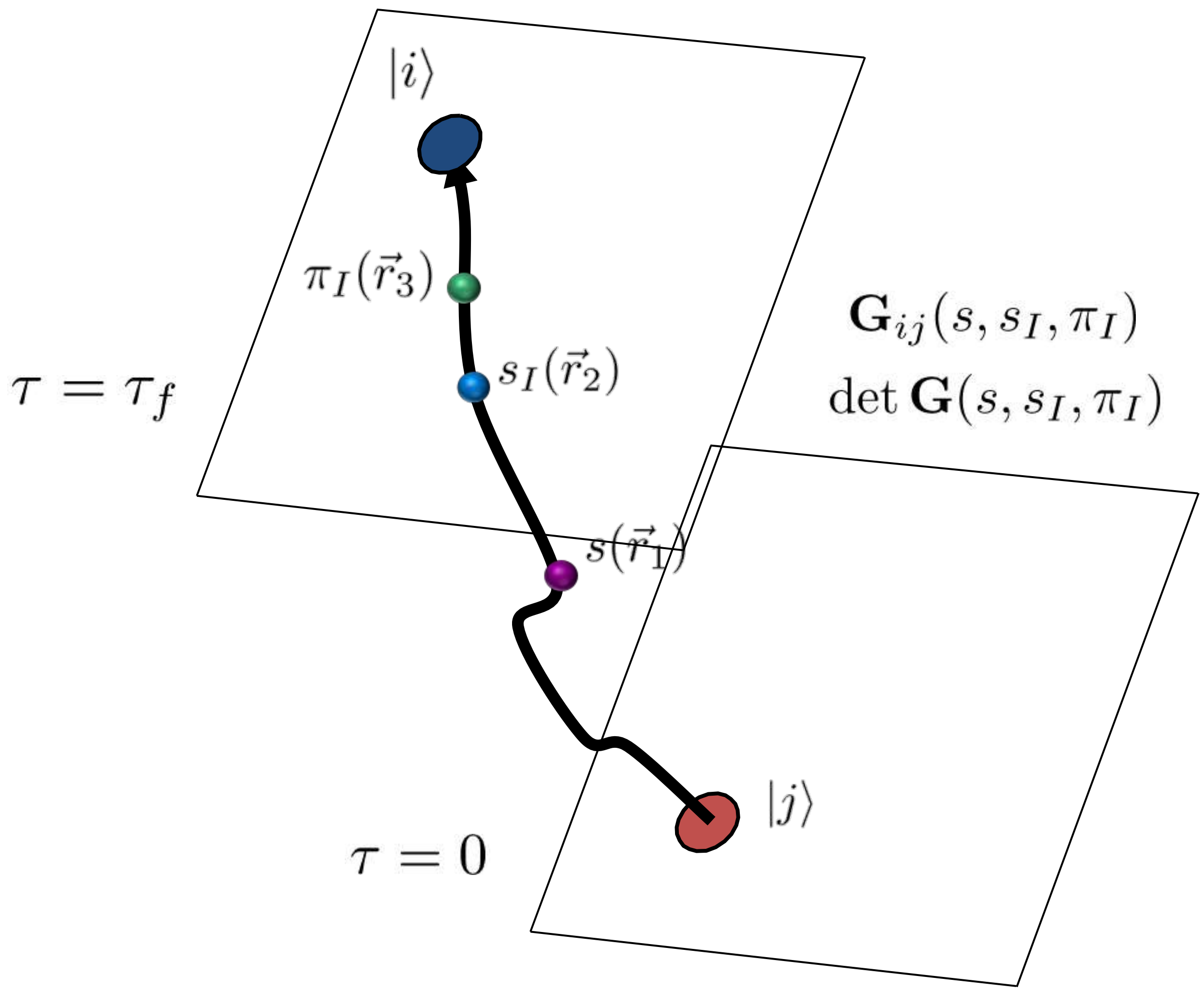
$(N^\dagger N)^2$

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



$sN^\dagger N$

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


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

A tale of two interactions

Two LO interactions, A and B, have nearly identical nucleon-nucleon phase shifts and well as three- and four-nucleon bound states

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{8}Be	−58.61(14)	−59.73(6)	−56.51(14)	−57.29(7)	−56.591
^{12}C	−88.2(3)	−95.0(5)	−84.0(3)	−89.9(5)	−92.162
^{16}O	−117.5(6)	−135.4(7)	−110.5(6)	−126.0(7)	−127.619
^{20}Ne	−148(1)	−178(1)	−137(1)	−164(1)	−160.645

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

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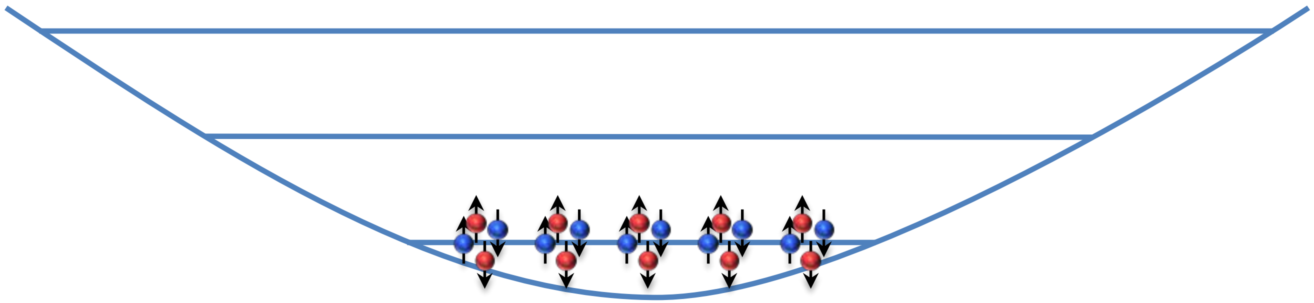
$$\frac{E_{^8\mathrm{Be}}}{E_{^4\mathrm{He}}} = 1.997(6)$$

$$\frac{E_{^{12}\mathrm{C}}}{E_{^4\mathrm{He}}} = 3.00(1)$$

$$\frac{E_{^{16}\mathrm{O}}}{E_{^4\mathrm{He}}} = 4.00(2)$$

$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^4\mathrm{He}}} = 5.03(3)$$

Bose condensate of alpha particles!



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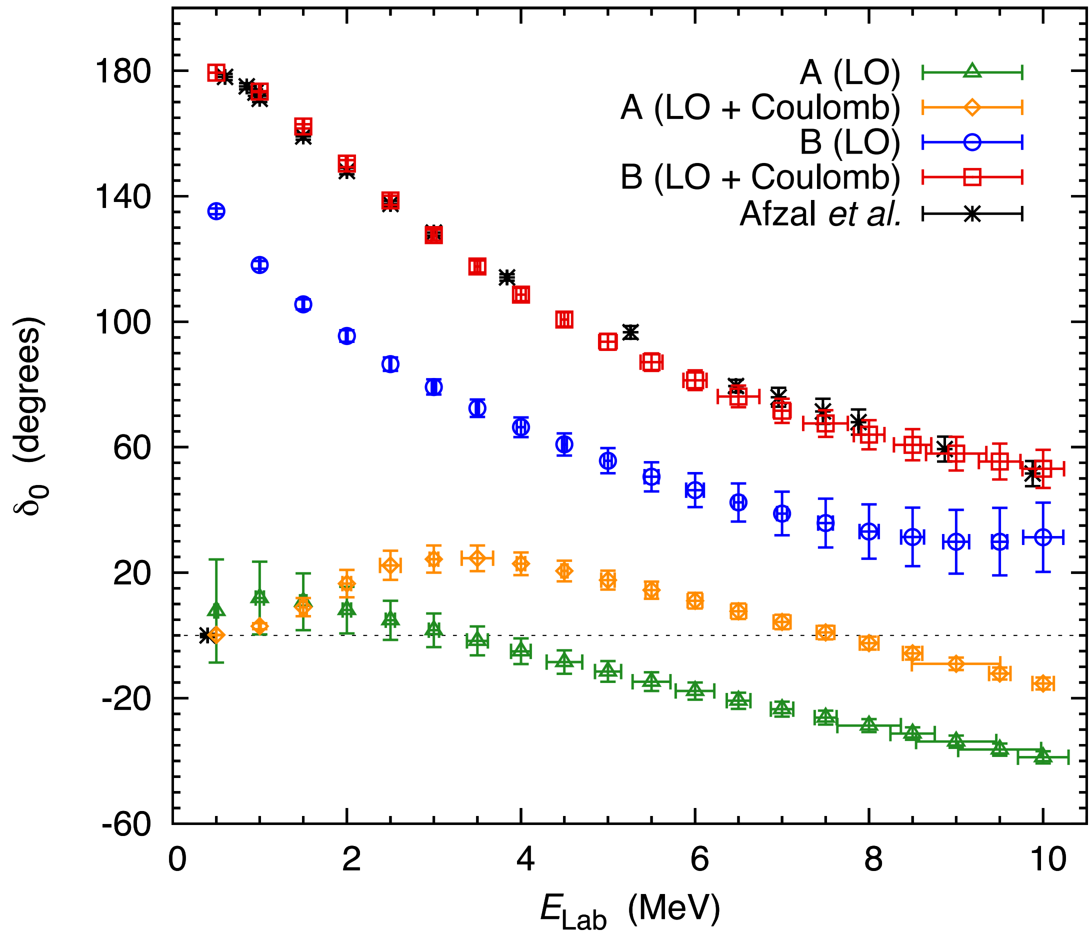
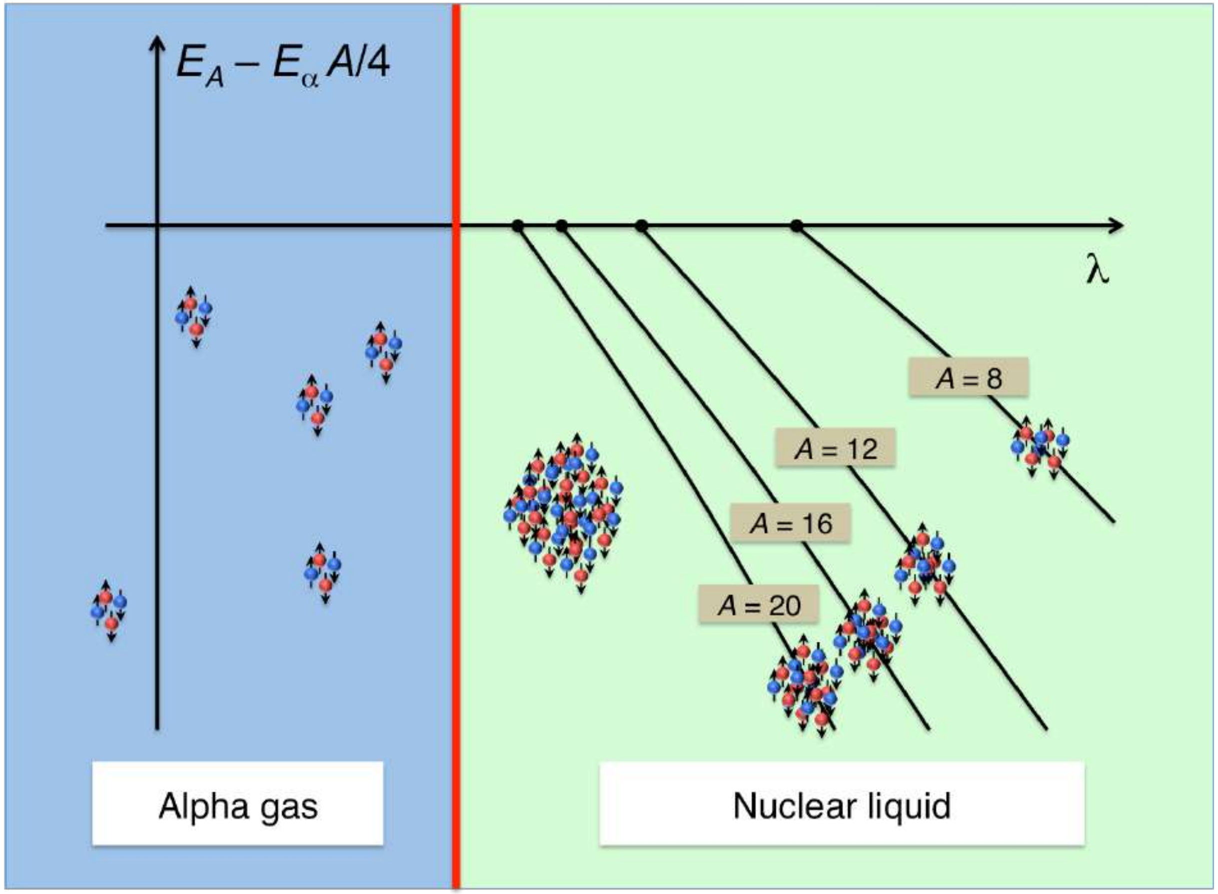
Alpha-alpha scattering



Alpha-alpha interaction not uniquely determined by low-energy few-body data

Control parameters: Sensitivity to interaction range and locality



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

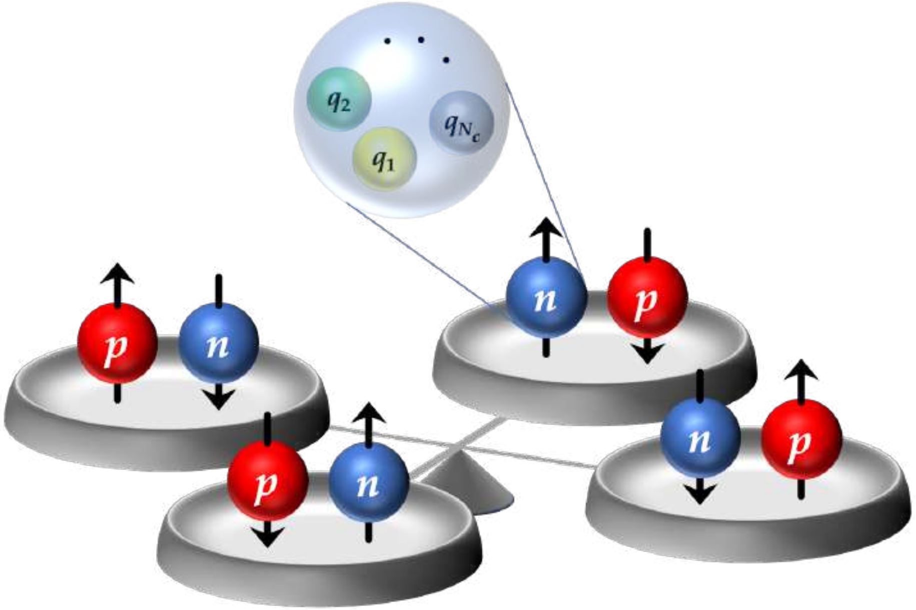
Hidden spin-isospin exchange symmetry

Kaplan, Savage, PLB 365, 244 (1996)

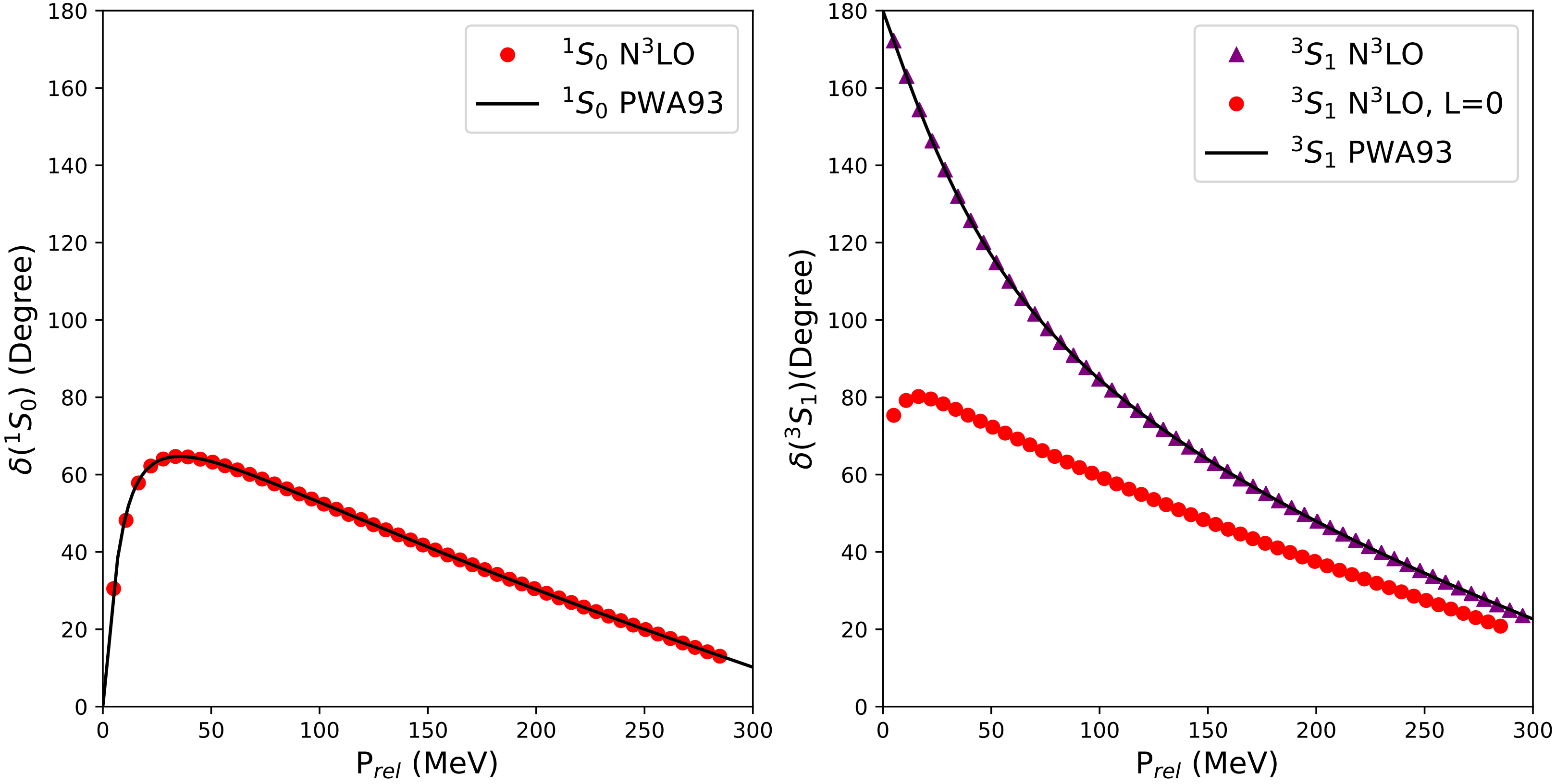
Kaplan, Manohar, PRC 56, 76 (1997)

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

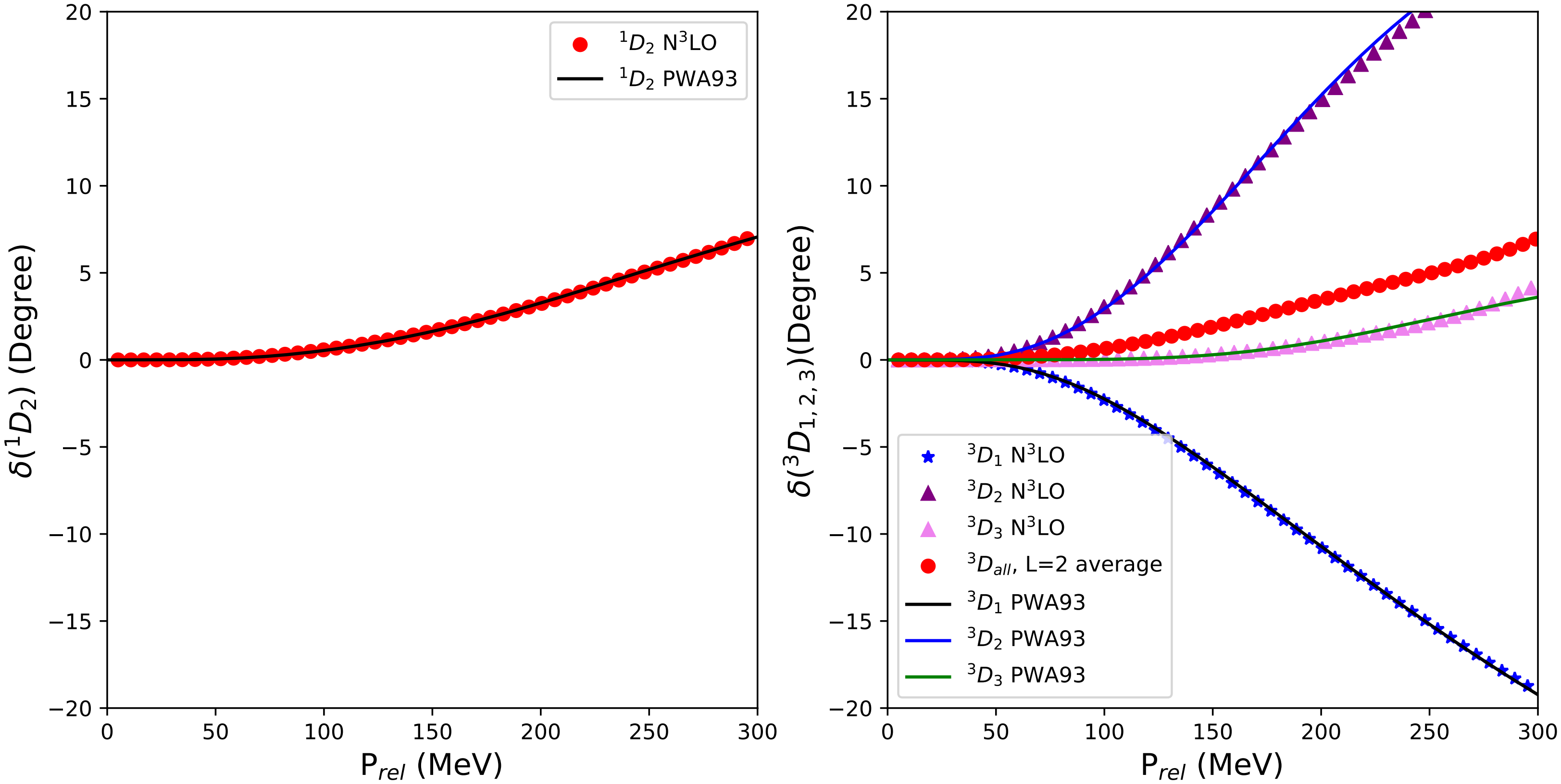
$$V^{2N}_{\mathrm{large}-N_c} = V_C + \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 W_S + (3\hat{r} \cdot \vec{\sigma}_1 \hat{r} \cdot \vec{\sigma}_2 - \vec{\sigma}_1 \cdot \vec{\sigma}_2) \vec{\tau}_1 \cdot \vec{\tau}_2 W_T$$



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



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



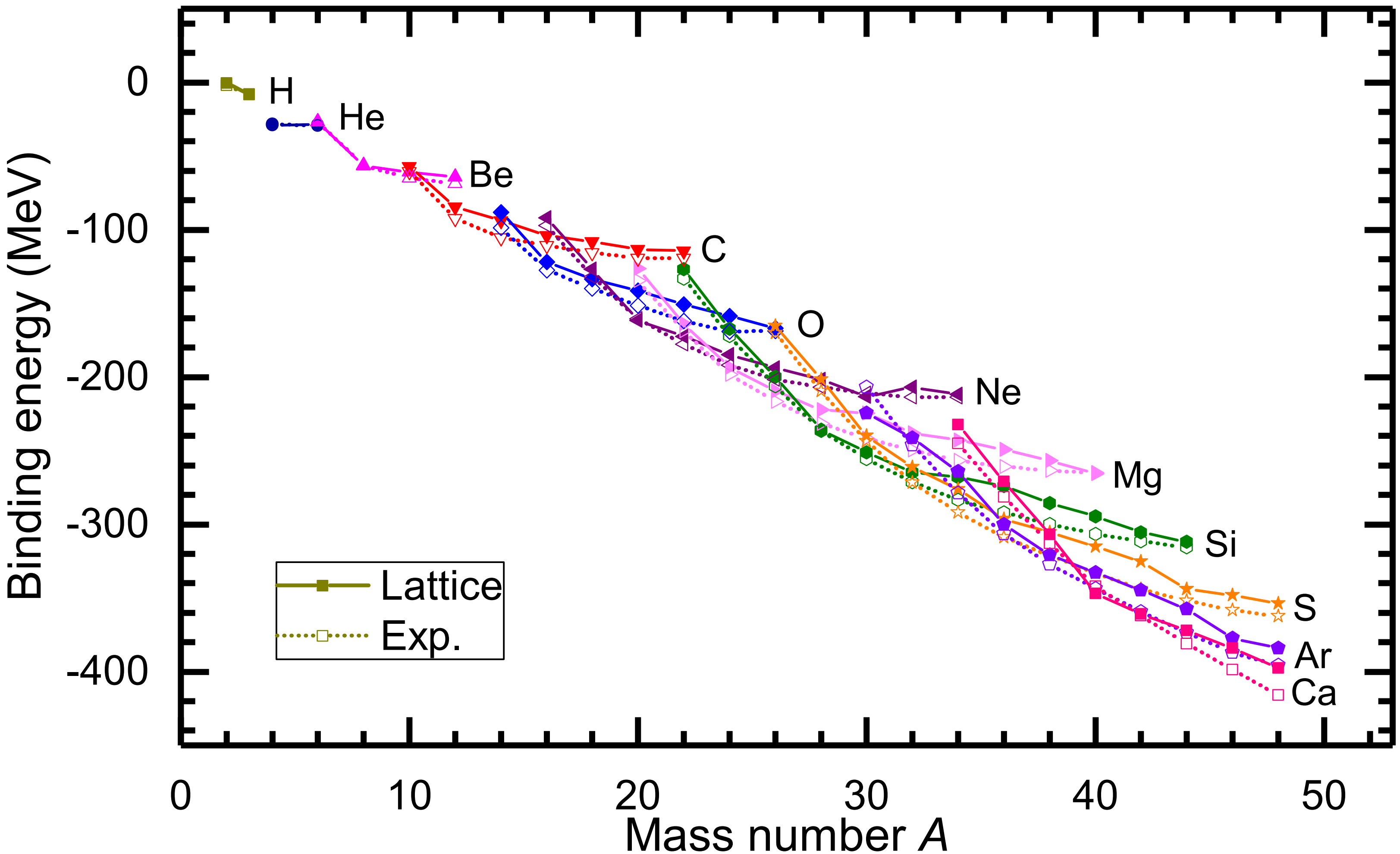
D.L., Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, Meißner, PRL 127, 062501 (2021)

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

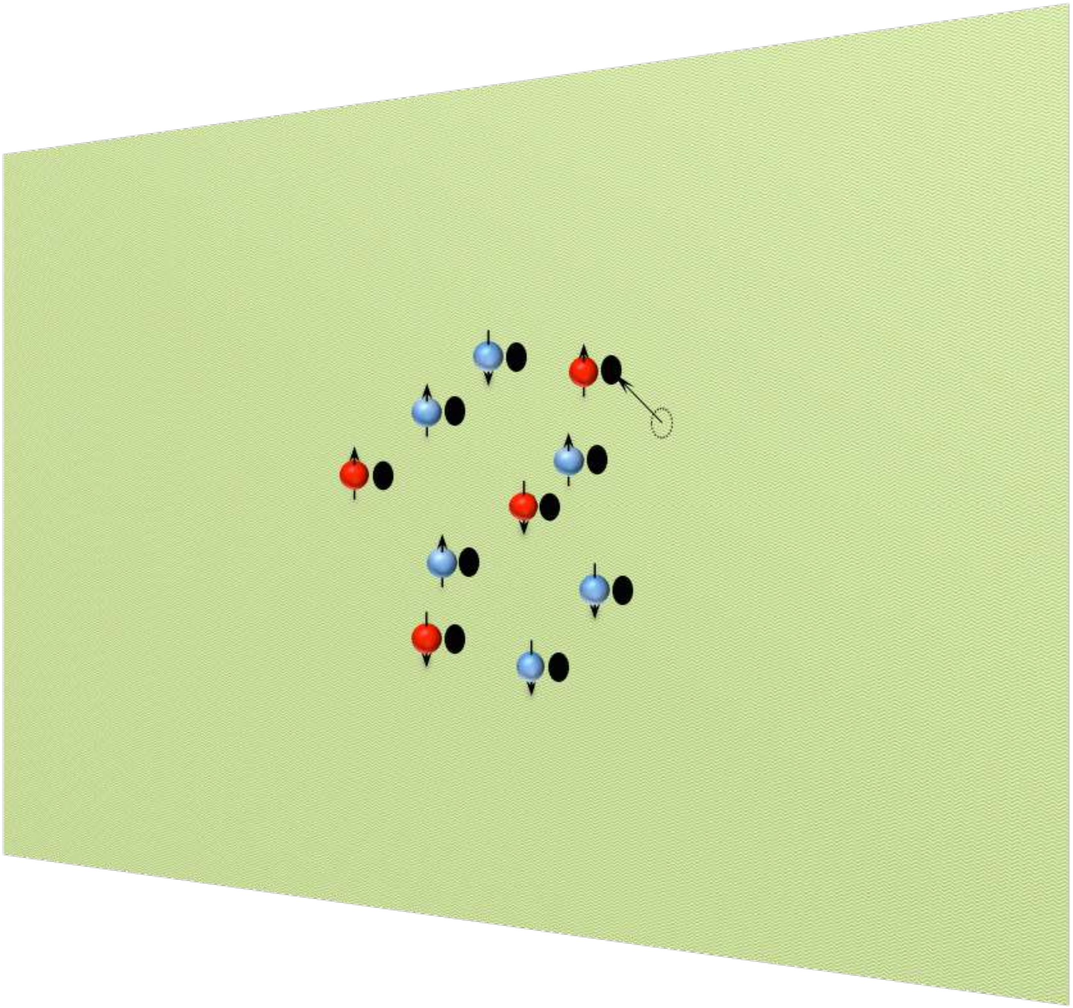


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

	B	Exp.	R_{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)

Pinhole algorithm



Seeing Structure with Pinholes

Consider the density operator for nucleon with spin i and isospin j

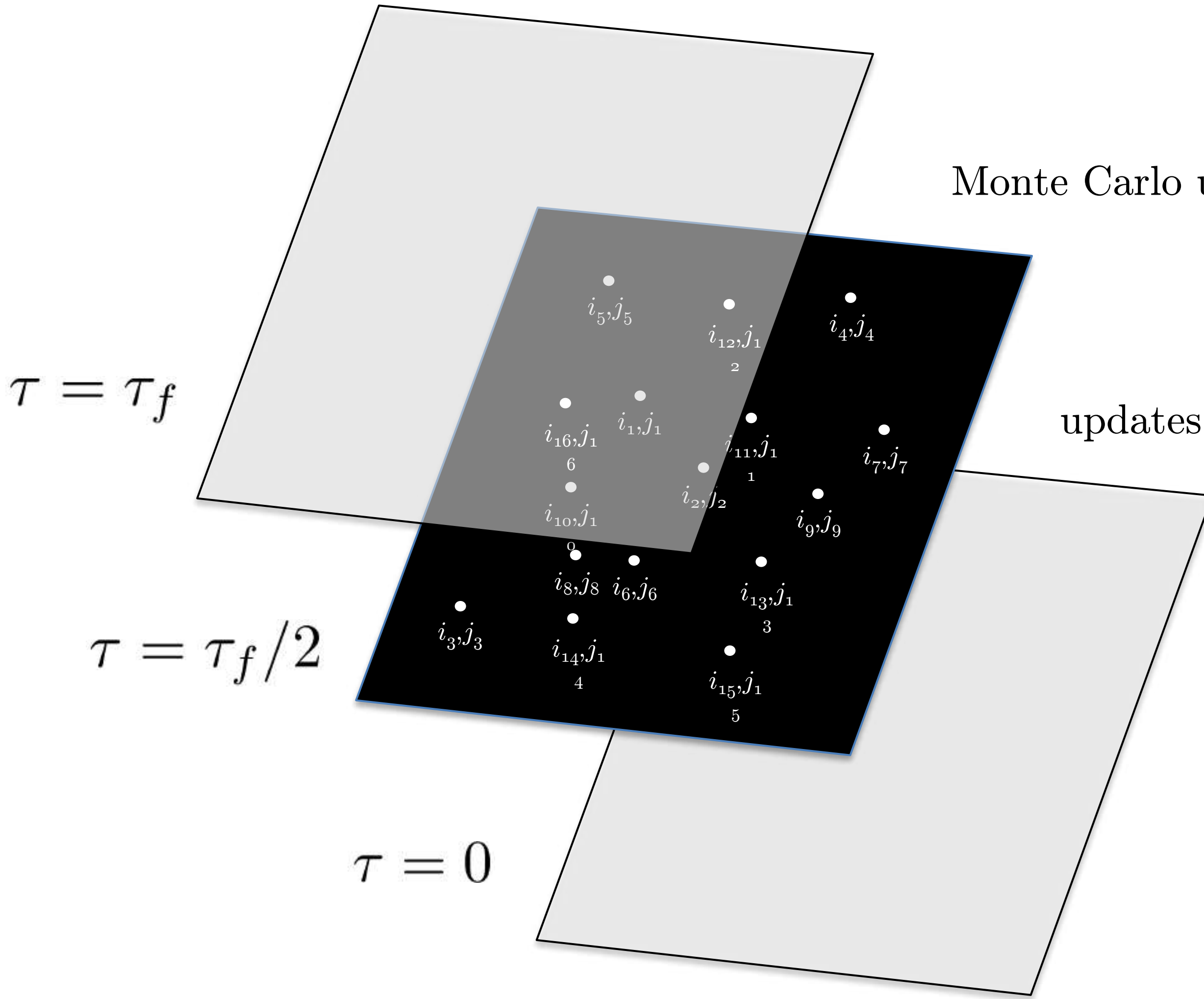
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = : \rho_{i_1,j_1}(\mathbf{n}_1)\cdots \rho_{i_A,j_A}(\mathbf{n}_A) :$$

In the simulations we do Monte Carlo sampling of the amplitude

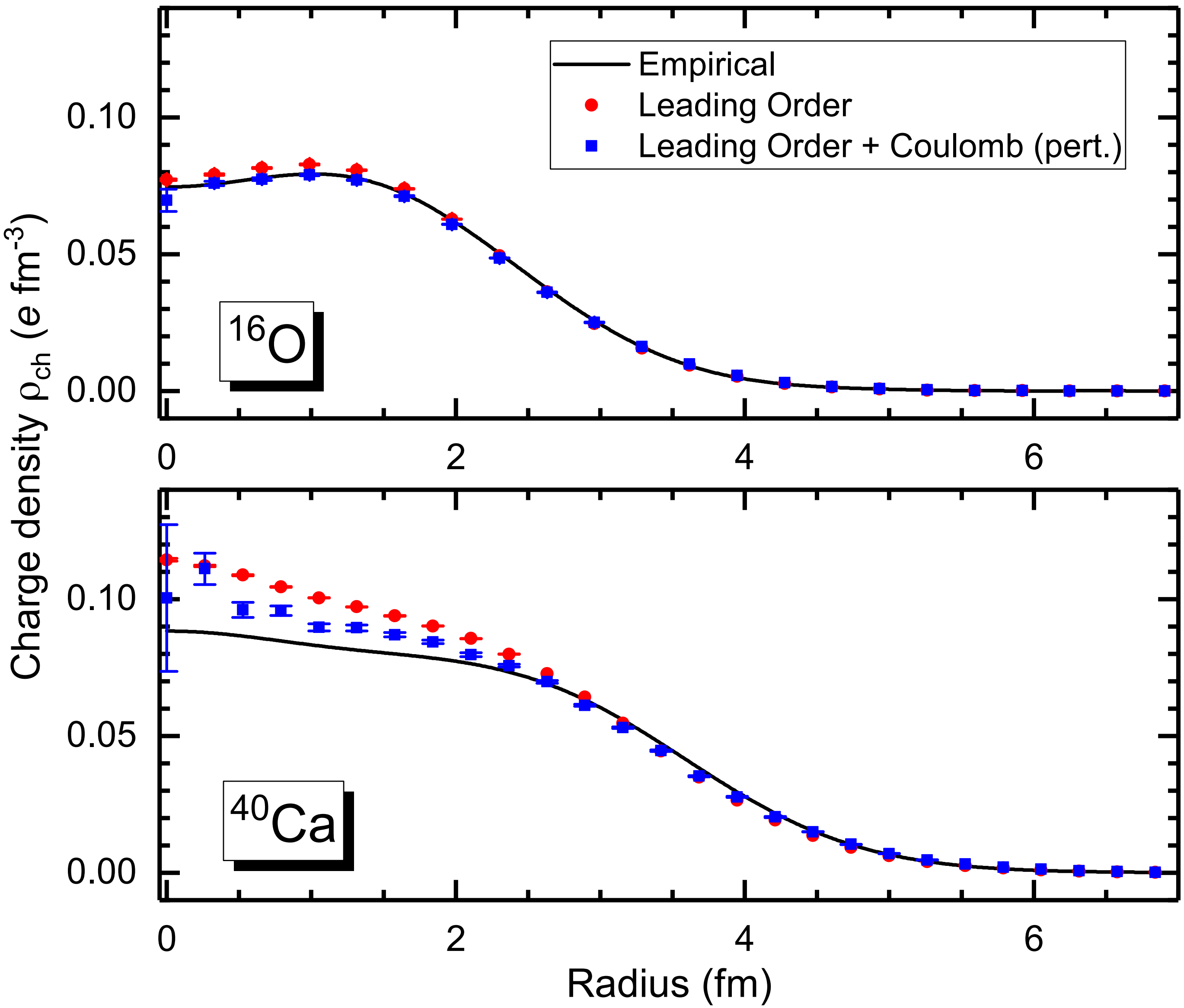
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A, t) = \langle \Psi_I | e^{-Ht/2} \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) e^{-Ht/2} | \Psi_I \rangle$$



Monte Carlo updates of pinholes

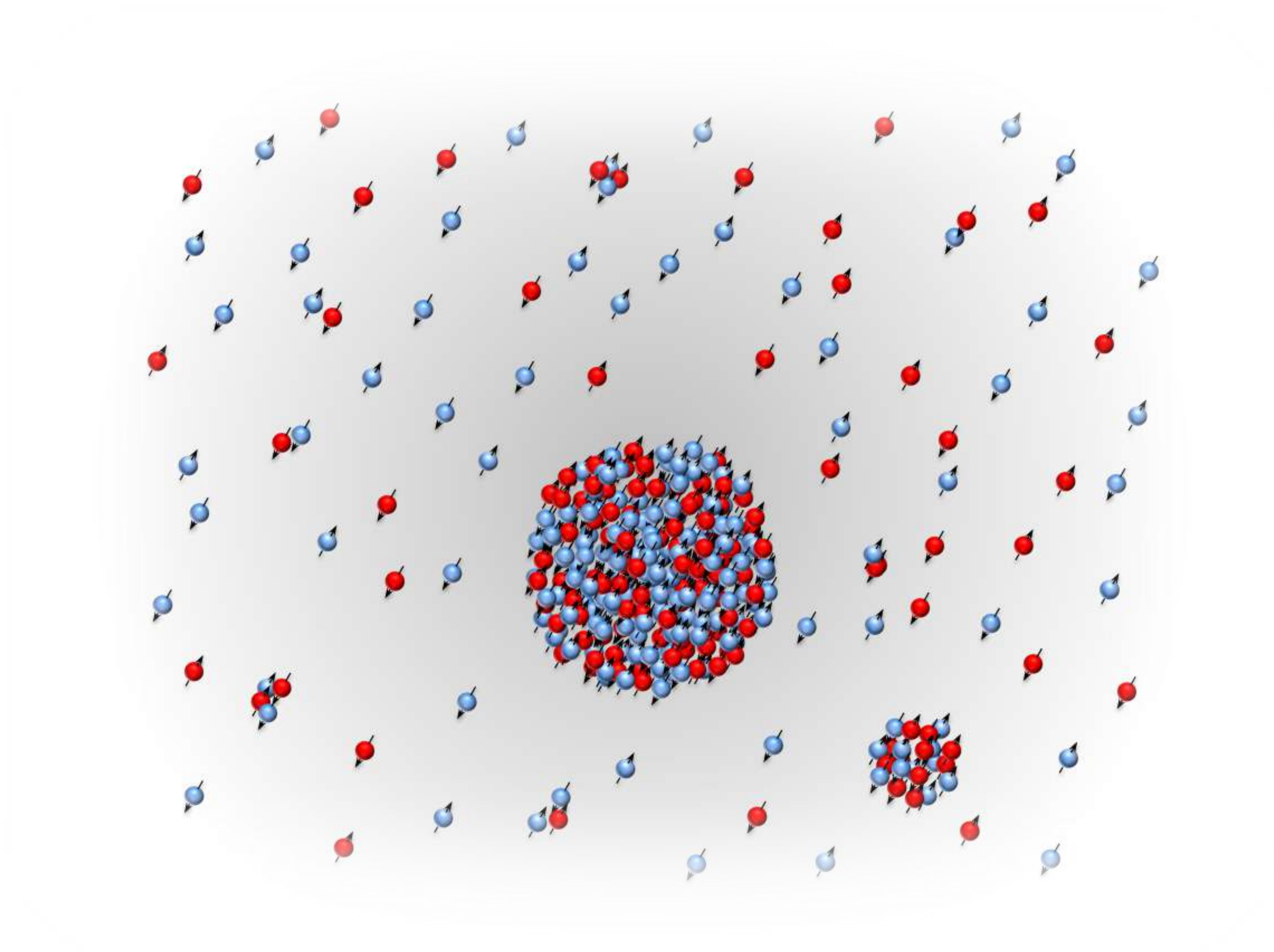
Monte Carlo
updates of auxiliary/pion fields

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



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

Ab initio nuclear thermodynamics



Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

Ab initio nuclear thermodynamics

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

$$\mathrm{Tr}\exp(-\beta H)$$

We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

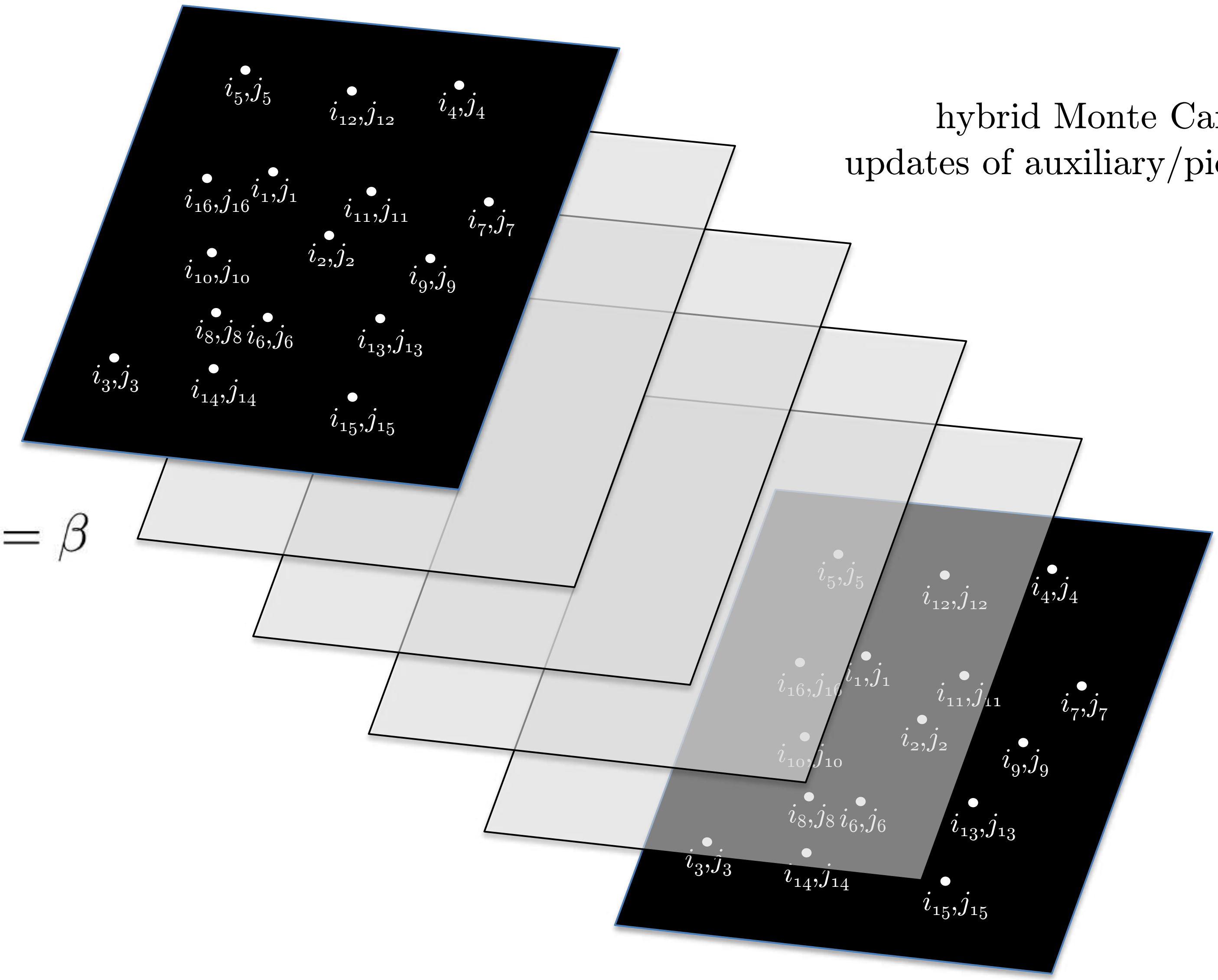
$$\begin{aligned}&\mathrm{Tr}\,O\\ &= \frac{1}{A!}\sum_{i_1\cdots i_A, j_1\cdots j_A, \mathbf{n}_1\cdots\mathbf{n}_A} \langle 0|a_{i_A,j_A}(\mathbf{n}_A)\cdots a_{i_1,j_1}(\mathbf{n}_1)\,O\,a^\dagger_{i_1,j_1}(\mathbf{n}_1)\cdots a^\dagger_{i_A,j_A}(\mathbf{n}_A)|0\rangle\end{aligned}$$

This can be used to calculate the partition function in the canonical ensemble.

Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

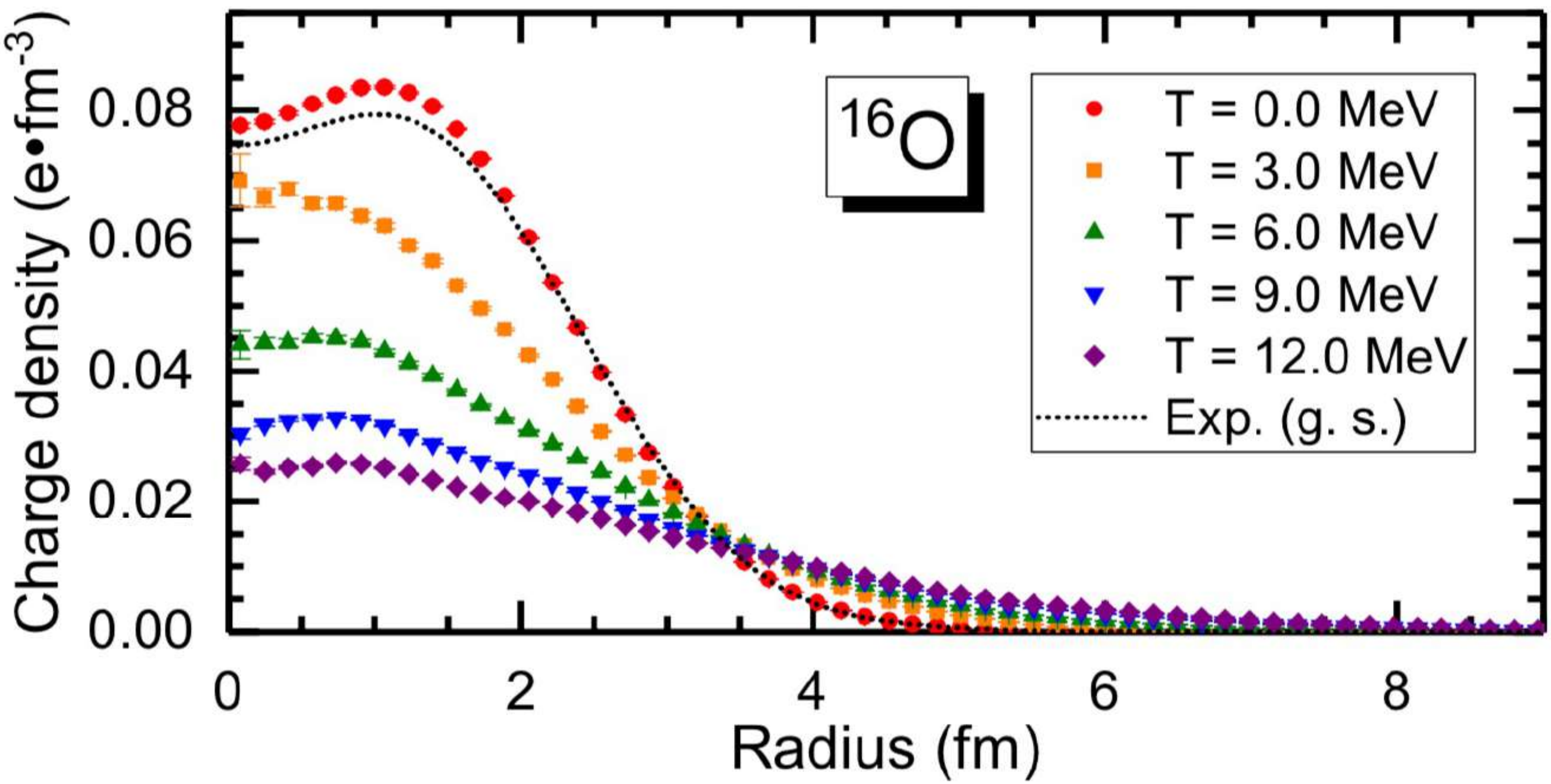
Metropolis updates of pinholes

hybrid Monte Carlo
updates of auxiliary/pion fields

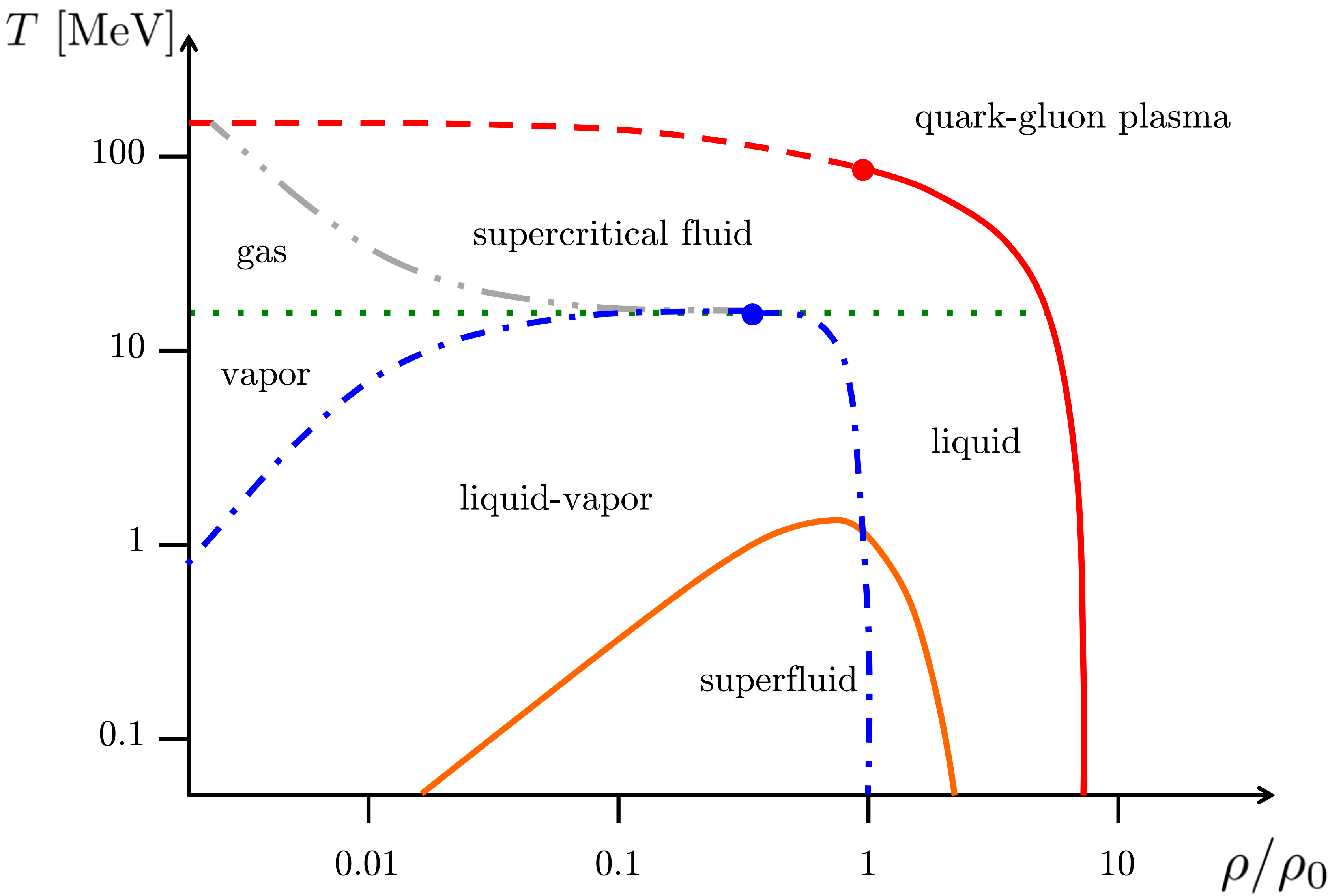


$\tau = \beta$

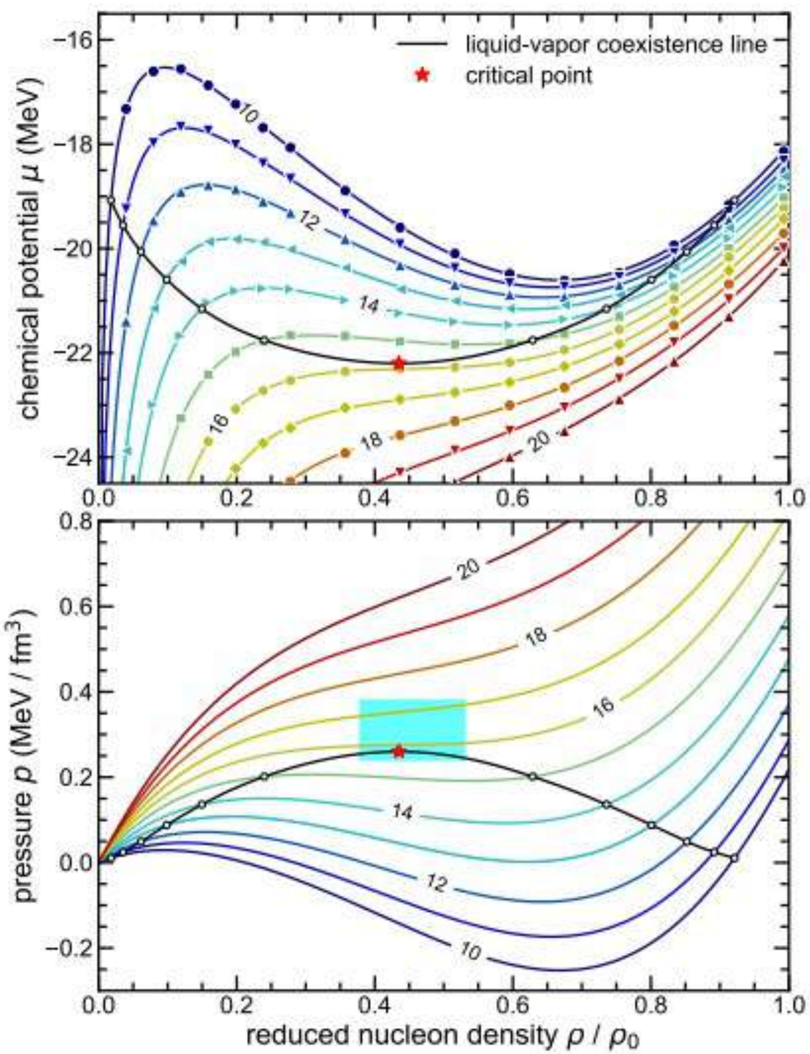
$\tau = 0$



Charge density (e•fm⁻³)
0.08
0.06
0.04
0.02
0.00
0
2
4
6
8
Radius (fm)
16O
T = 0.0 MeV
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV
Exp. (g. s.)

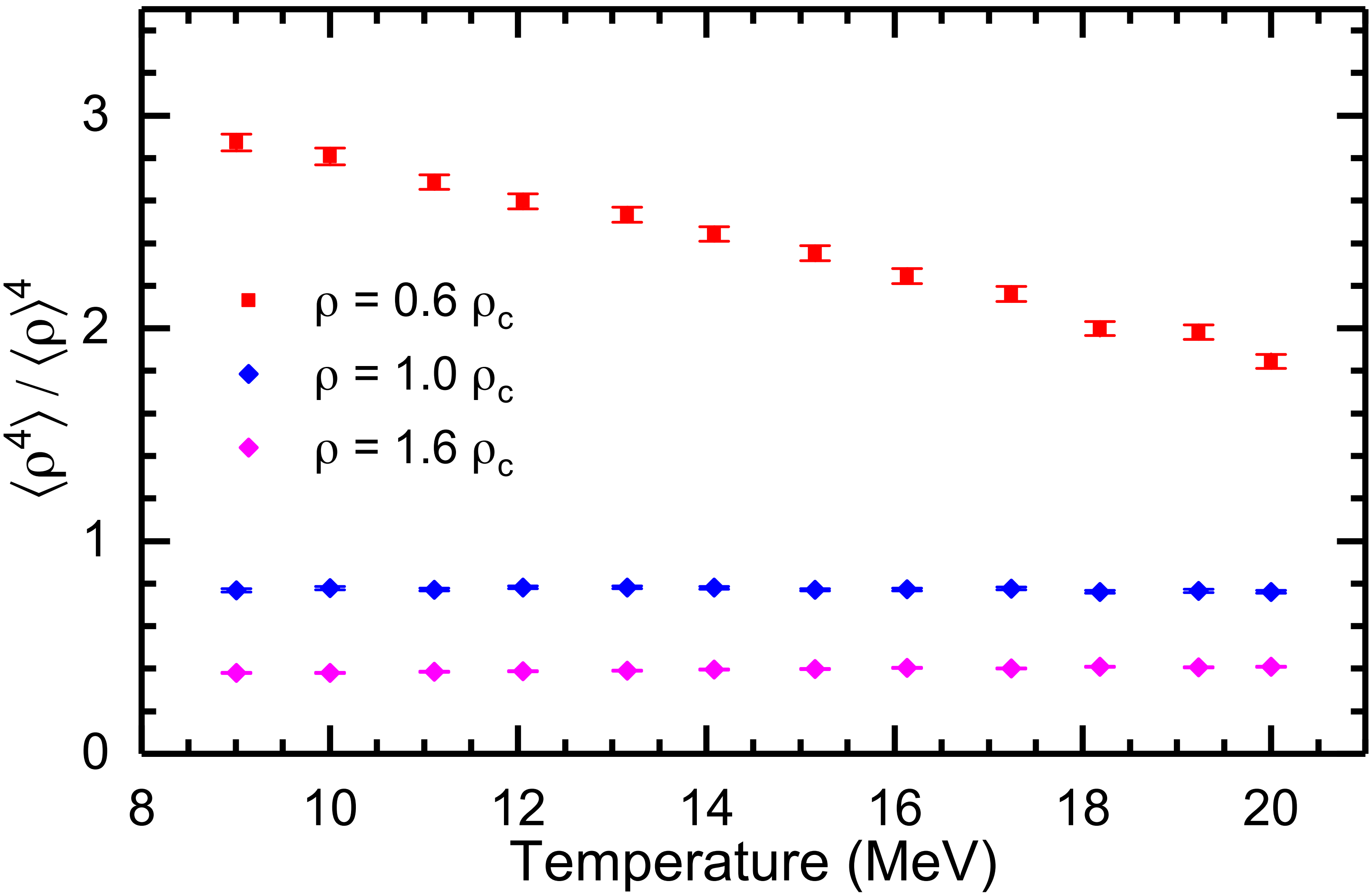


T [MeV]
100
10
1
0.1
quark-gluon plasma
supercritical fluid
gas
vapor
liquid
liquid-vapor
superfluid
0.01
0.1
1
10
ρ/ρ_0



$$T_c = 15.80(0.32)(1.60)\,\mathrm{MeV}$$
$$\rho_c = 0.089(04)(18)\,\mathrm{fm}^{-3}$$
$$\mu_c = -22.20(0.44)(2.20)\,\mathrm{MeV}$$
$$P_c = 0.260(05)(30)\,\mathrm{MeV\ fm}^{-3}$$

Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)



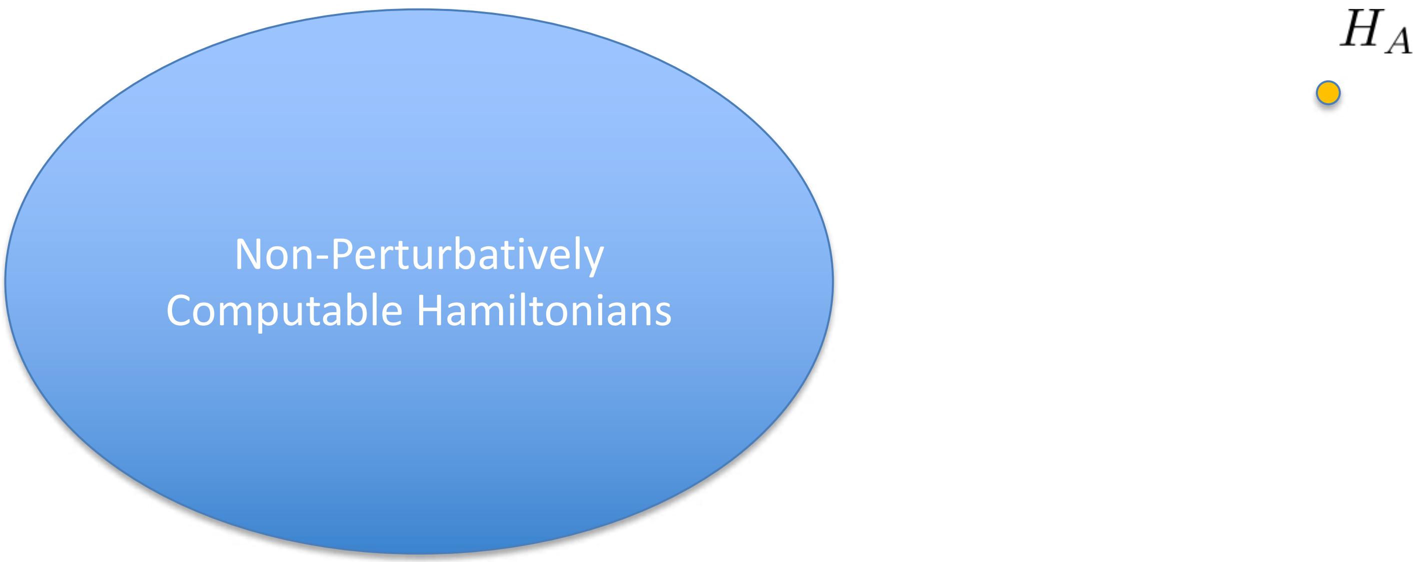
Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

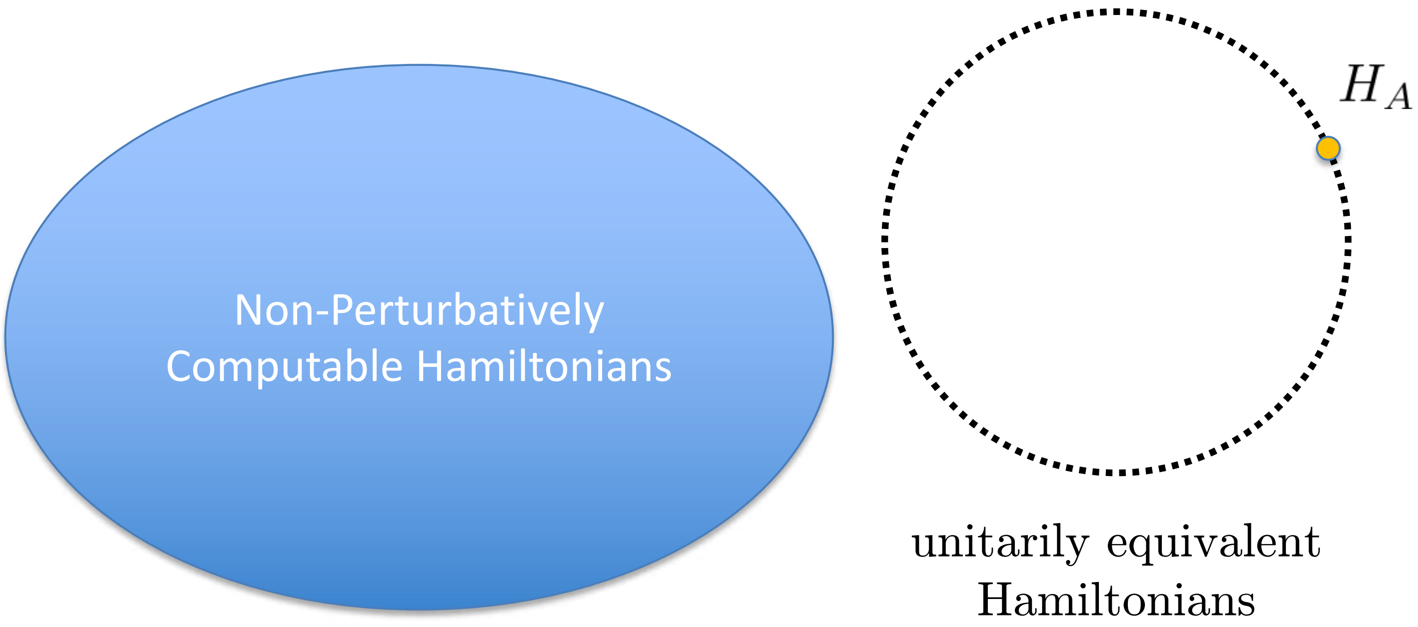
Wave function matching

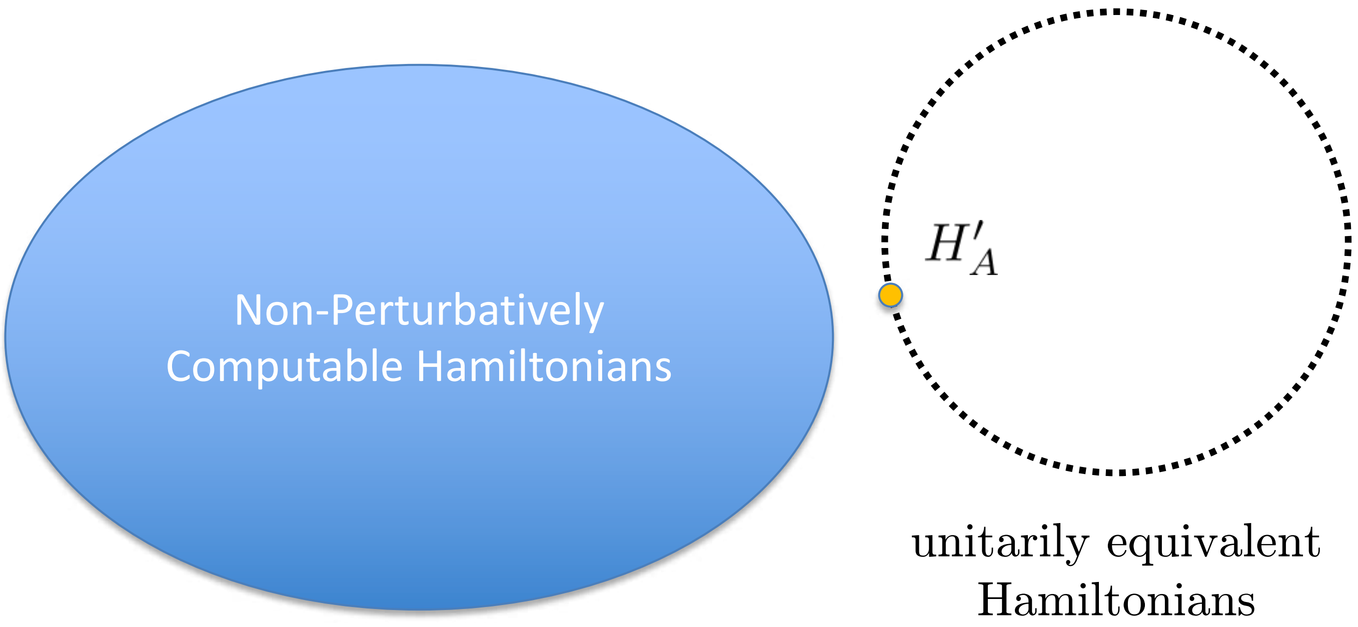
Work in progress: Elhatisari et al.

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.

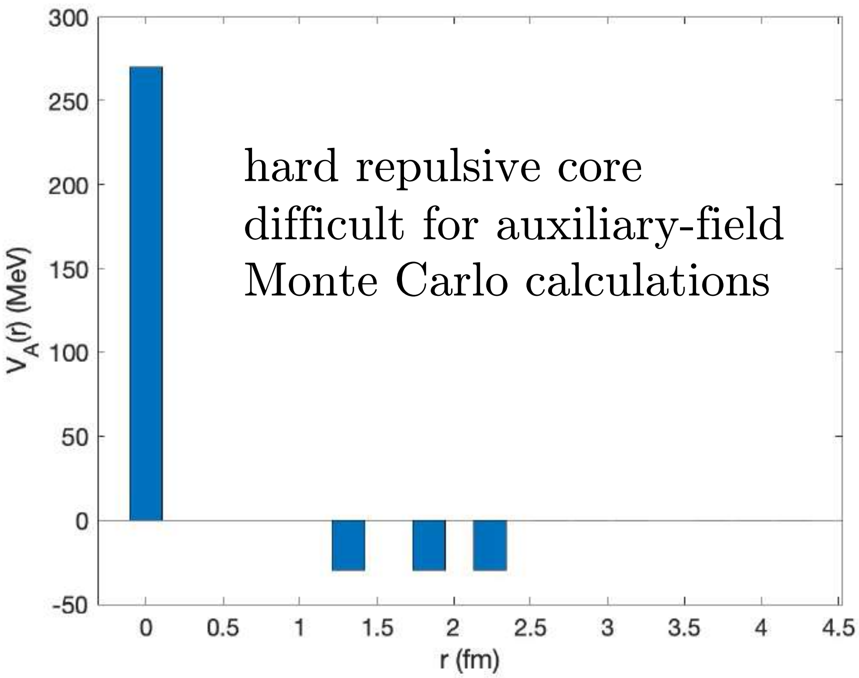

Non-Perturbatively
Computable Hamiltonians
H_A


Non-Perturbatively
Computable Hamiltonians
H_A
unitarily equivalent
Hamiltonians

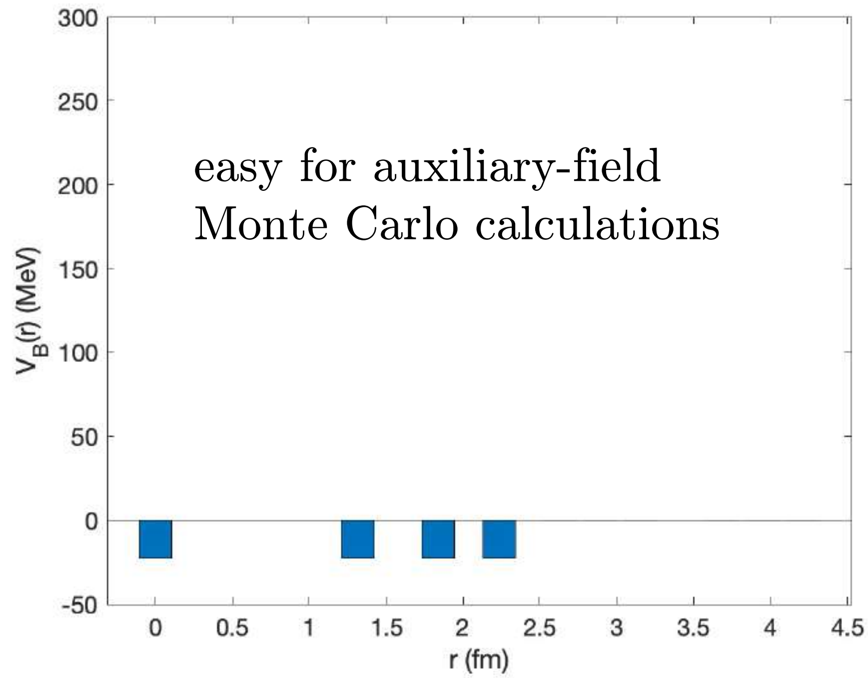

Non-Perturbatively
Computable Hamiltonians
H'_A
unitarily equivalent
Hamiltonians

Wave function matching

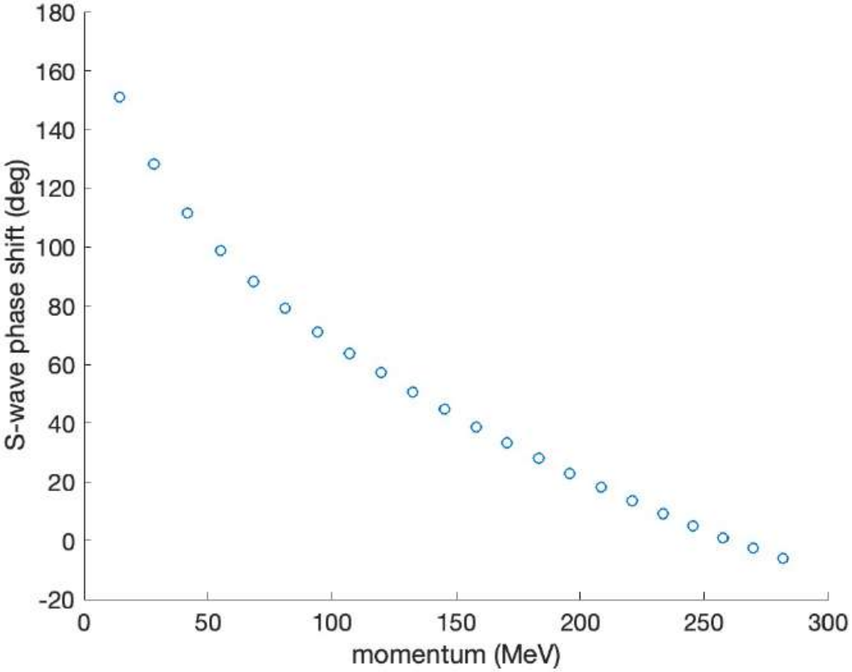
$V_A(r)$



$V_B(r)$

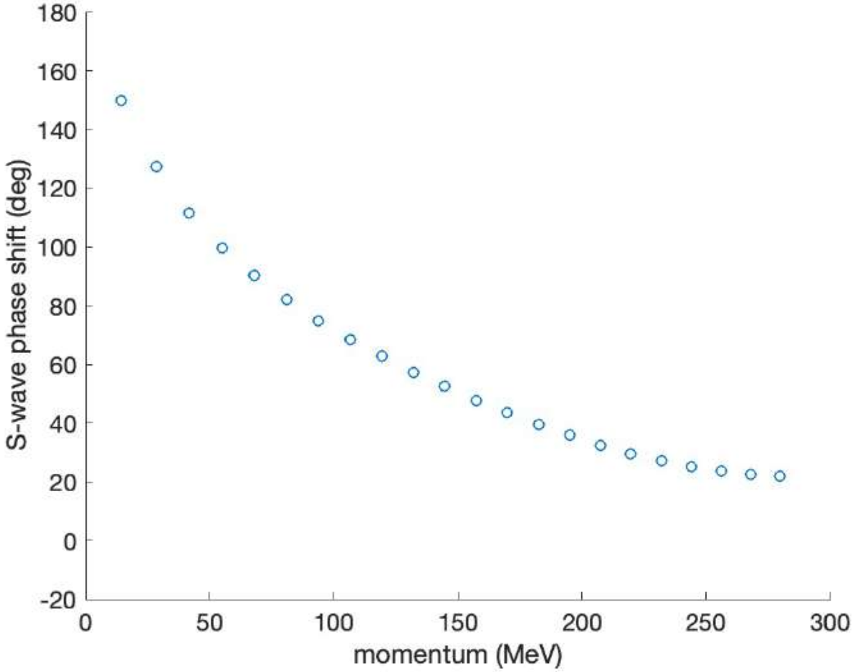


$V_A(r)$



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

$V_B(r)$



180
160
140
120
100
80
60
40
20
0
-20
S-wave phase shift (deg)
0
50
100
150
200
250
300
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)	$\langle\psi_{B,n}\|H_A\|\psi_{B,n}\rangle$ (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

$$U : P \left|\psi_A^0\right\rangle / \| P \left|\psi_A^0\right\rangle \| \to P \left|\psi_B^0\right\rangle / \| P \left|\psi_B^0\right\rangle \|$$

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

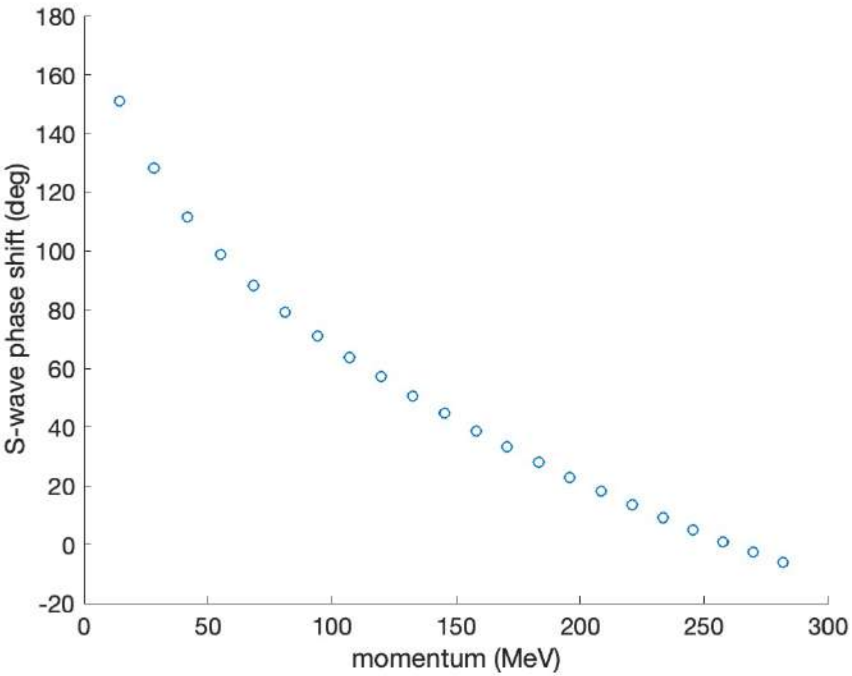
$$U : H_A \to H'_A = U^\dagger H_A U$$

and the resulting nonlocal interaction is

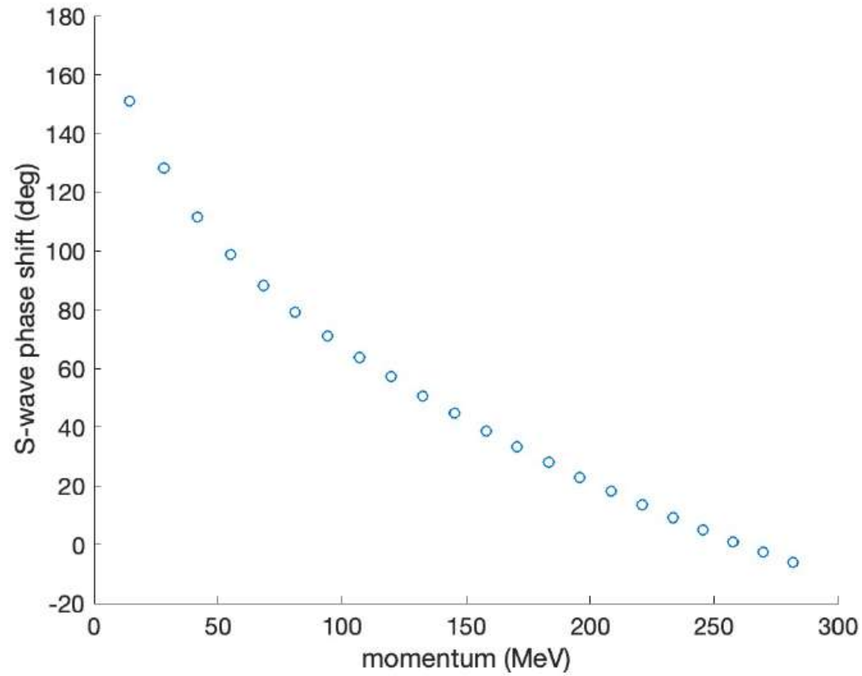
$$V'_A = H'_A - K = U^\dagger H_A U - K$$

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

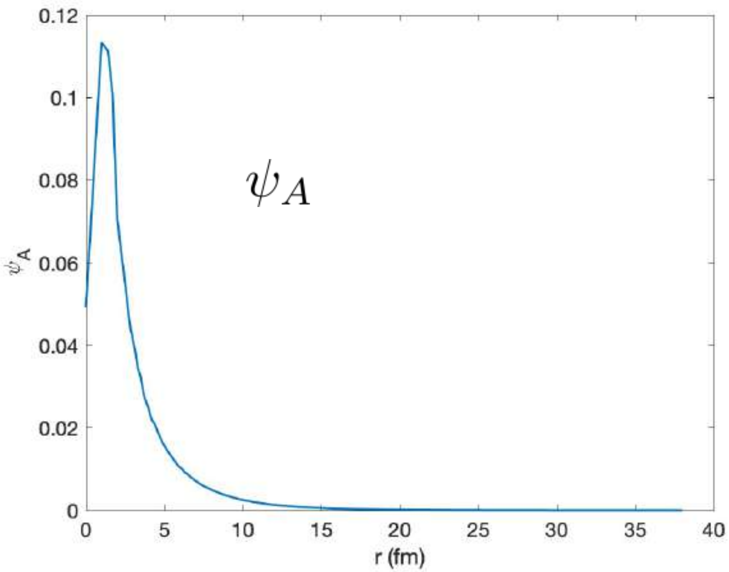
$V_A(r)$

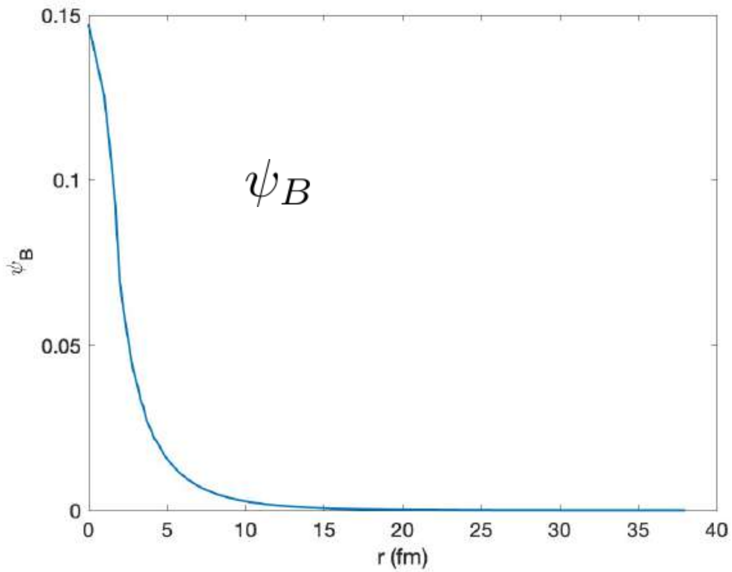


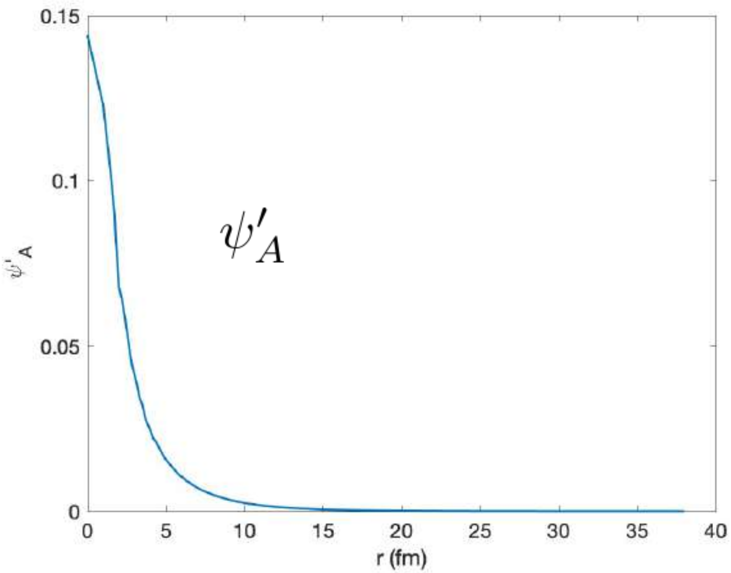
$V'_A(r, r')$



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.

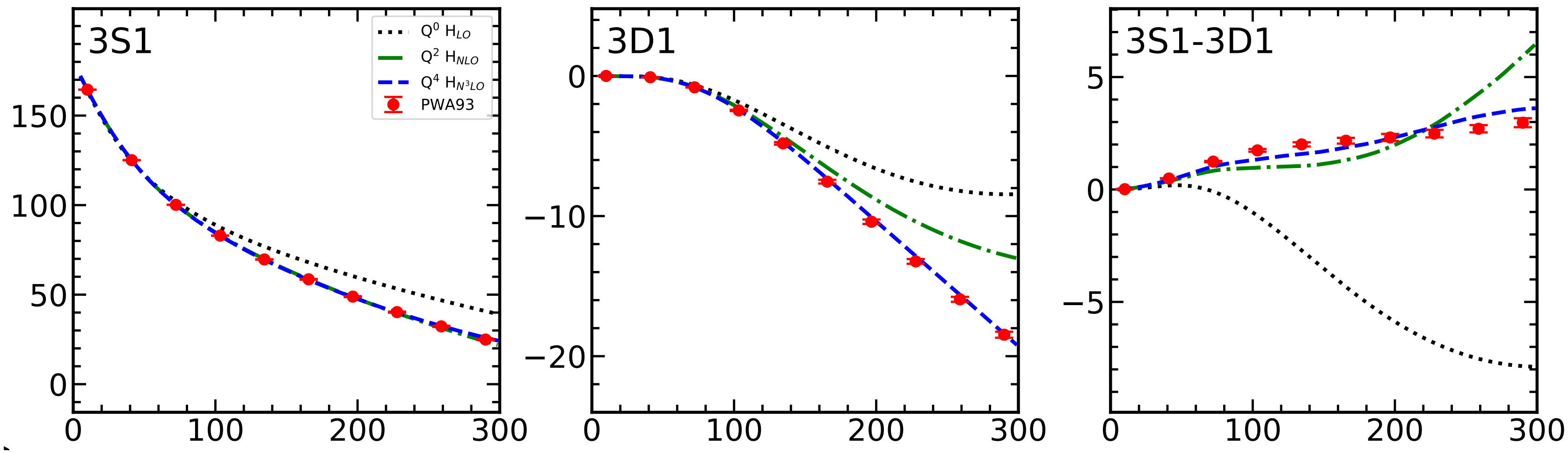
$R = 1.3$ fm

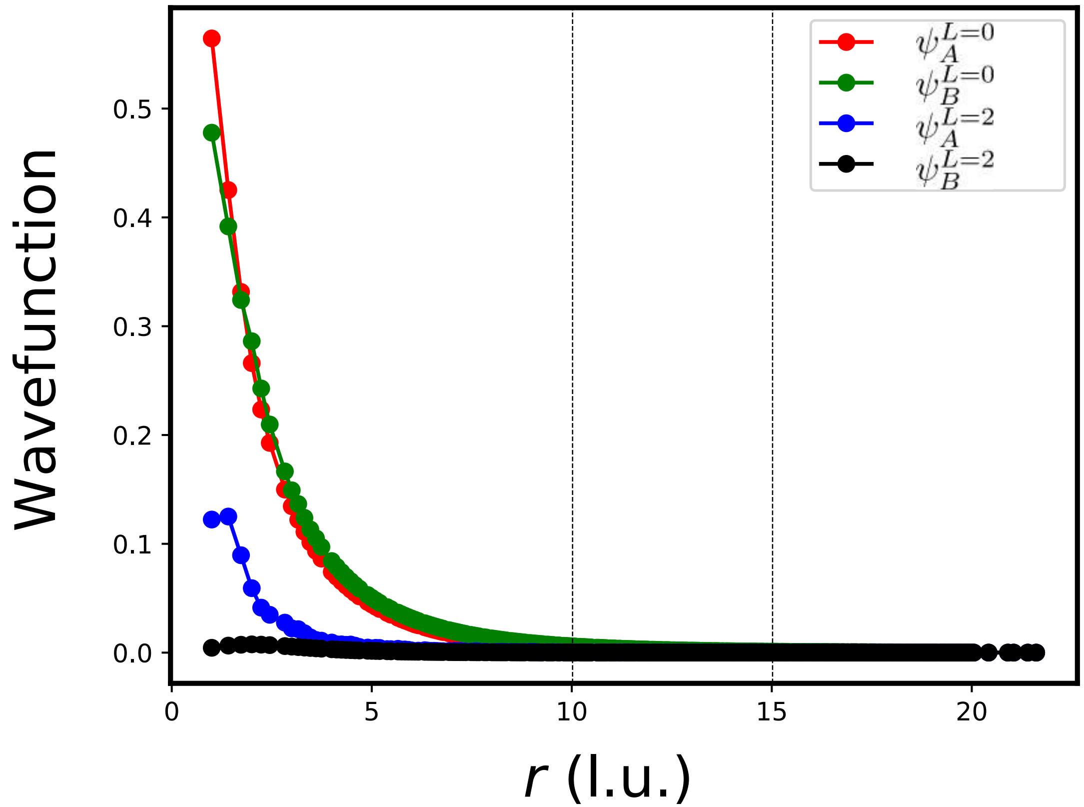
$E_{A,n} = E'_{A,n}$ (MeV)	$\langle \psi_{B,n} \vert H_A \vert \psi_{B,n} \rangle$ (MeV)	$\langle \psi_{B,n} \vert H'_A \vert \psi_{B,n} \rangle$ (MeV)
-1.2186	3.0088	-0.5134
0.2196	0.3289	0.2377
0.8523	1.1275	0.8982
1.8610	2.2528	1.9270
3.2279	3.6991	3.3083
4.9454	5.4786	5.0378
7.0104	7.5996	7.1146
9.4208	10.0674	9.5379
12.1721	12.8799	12.3039
15.2669	16.0458	15.4170

$R = 2.6$ fm

$E_{A,n} = E'_{A,n}$ (MeV)	$\langle \psi_{B,n} \vert H_A \vert \psi_{B,n} \rangle$ (MeV)	$\langle \psi_{B,n} \vert H'_A \vert \psi_{B,n} \rangle$ (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

Application of wave function matching to the 3S1-3D1 chiral interaction at N3LO.





$E_{A,n} = E'_{A,n}$ (MeV)	$\langle \psi_{B,n} \vert H_A \vert \psi_{B,n} \rangle$ (MeV)	$\langle \psi_{B,n} \vert H'_A \vert \psi_{B,n} \rangle$ (MeV)
-2.2234	0.9104	-2.1380
0.7188	1.3362	0.8344

Work in progress: Elhatisari et al.

Summary

We began with an introduction to lattice effective field theory. We then presented evidence that nature is close to a quantum phase transition between nuclear liquid and Bose gas of alpha particles.

We discussed a hidden spin-isospin symmetry of the nucleonic interactions that can be derived in the large-N_c limit.

We constructed a minimal nuclear interaction that can reproduce the ground state properties of light nuclei, medium-mass nuclei, and neutron matter.

We presented first principles calculations of nuclear thermodynamics using the pinhole trace algorithm and probed the nuclear liquid-gas phase diagram and alpha clustering as a function of density and temperature.

We introduced wave function matching method. By using unitary transformations, we construct a high-fidelity Hamiltonian that can be reached by perturbation theory from a Hamiltonian without a sign problem.