Ab initio lattice simulations for nuclear structure and heavy-ion collision initial states

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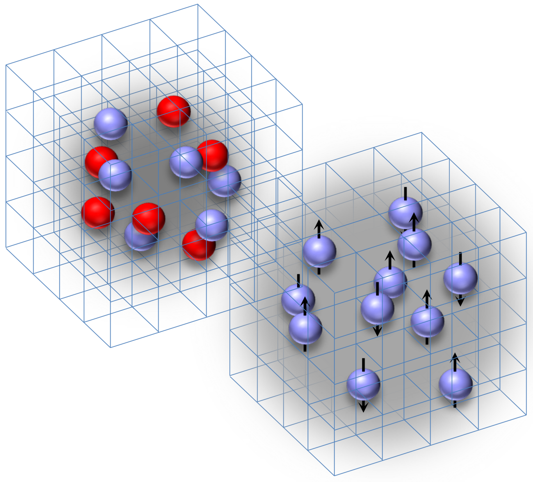

RHIC-BES Online Seminar
May 16, 2023

FRIB
MICHIGAN STATE UNIVERSITY
NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project
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INT PROGRAM INT-23-1A

Intersection of nuclear structure and high-energy nuclear collisions

January 23, 2023 - February 24, 2023

HIGH-RESOLUTION IMAGES

VIEW SCHEDULE

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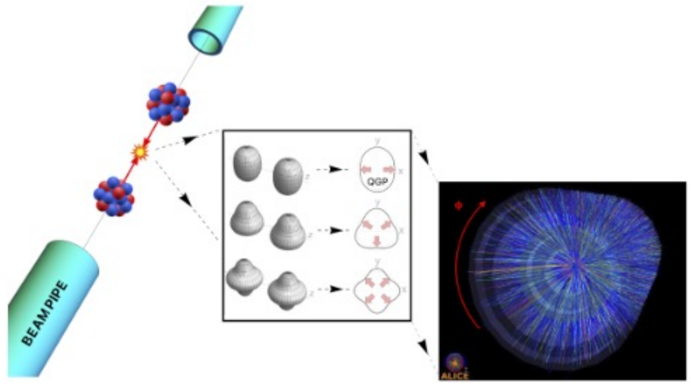


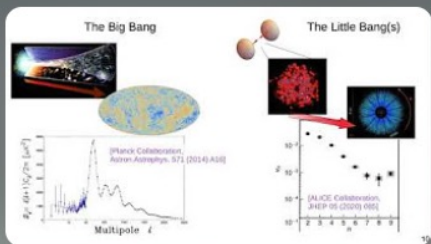
High-energy heavy-ion collisions producing a quark gluon plasma whose energy density profile reflects the collective structure of the colliding ions

OVERVIEW

Note to applicants: This a 5-week "hybrid" program with a one-week "hybrid" workshop embedded (however see disclaimer below). Please specify in the COMMENTS section of the Application Form either [In-Person], [Virtual] or [Either] to reflect your preferred mode of attendance. Please be aware that all in-person participants must show proof of vaccination against COVID-19 upon arrival to the INT.

Disclaimer: Please be aware that due to ongoing concerns regarding the COVID-19 pandemic, this program may be changed from in-person to hybrid, or to online-only if necessary.

Until now, the communities of high-energy heavy-ion physics and of low-energy nuclear structure physics have been largely disconnected. To model and understand the evolution of the quark-gluon plasma (QGP), heavy-ion physics requires some input from nuclear structure physics that is typically simplified or assumed to be well-known. However, over the past decade both our understanding of the evolution of the QGP and the quality of the experimental data have become good enough to grant sensitivity to the details of the geometry of the colliding ions, and thus challenge the nuclear structure input. Measurements from collisions of ^{238}U or ^{129}Xe nuclei at high energy, for instance, can only be understood via the inclusion of



INT Program 23-1a

by The Institute for Nuclear Theory

59 videos 299 views Last updated on Mar 21, 2023

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INT Program 23-1a, "Intersection of nuclear structure and high-energy nuclear collisions", took place from January 23rd to February 24th, 2023 at the Institute for Nuclear Theory in Seattle, WA.

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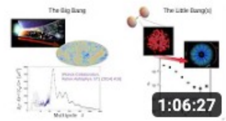

INT 23-1a: G. Giacalone, "Nuclear structure for high-energy nuclear physics"
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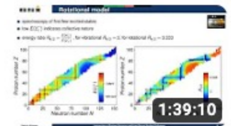

INT 23-1a: K. Wimmer, "Overview of nuclear deformation in low-energy experiments"
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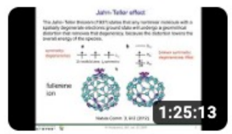

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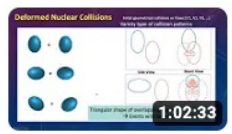

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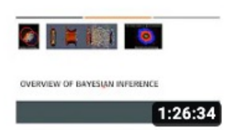

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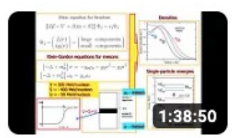

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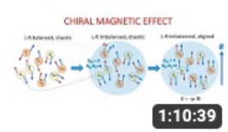

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Outline

Ab initio methods

Lattice effective field theory

Essential elements for nuclear binding

^{16}O ^{16}O collisions at RHIC and LHC energies

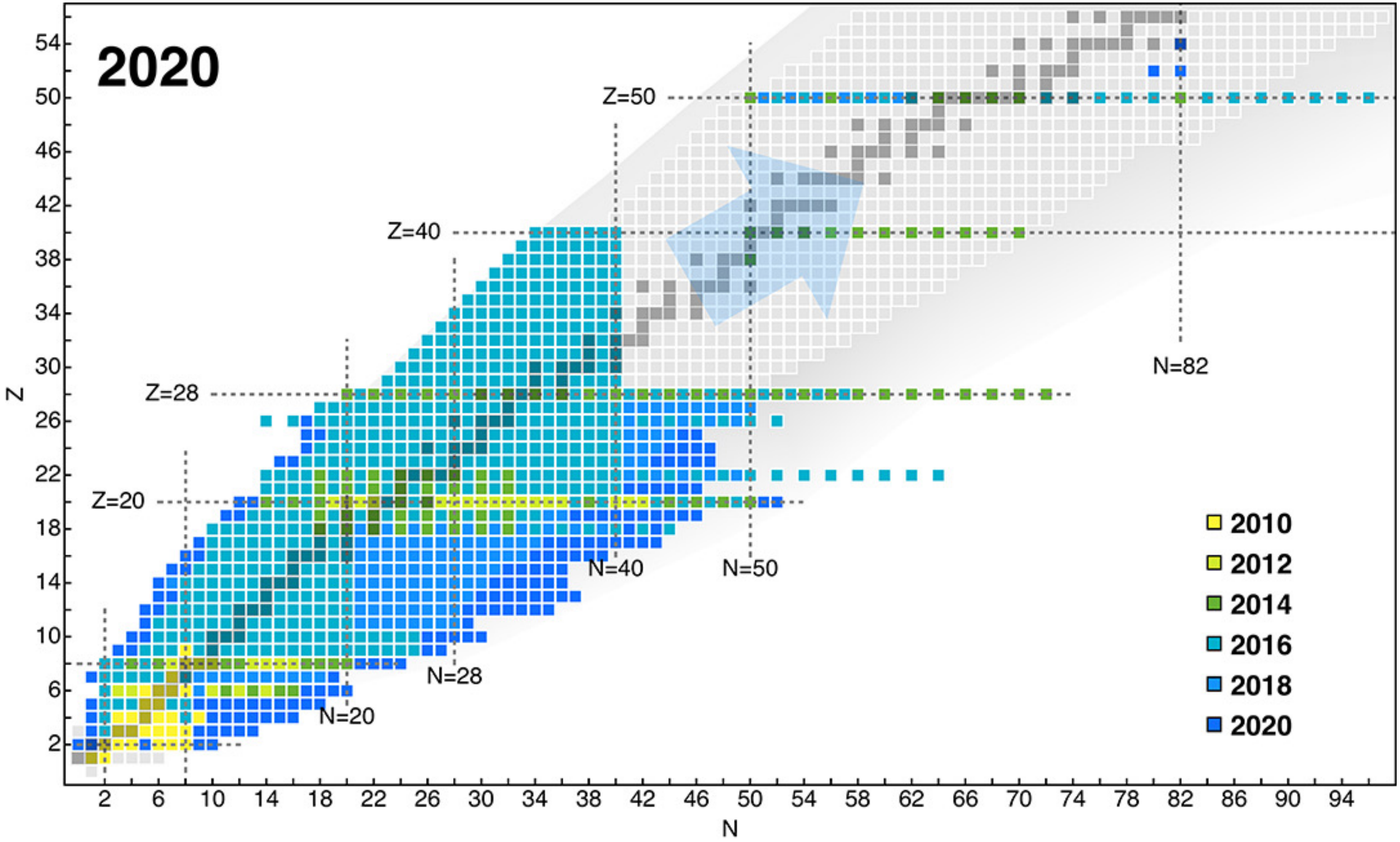
Ab initio nuclear thermodynamics

Structure and spectrum of ^{12}C

Wave function matching

Outlook

Ab initio methods



[Hergert, Front. Phys. 8, 379 (2020)]

Many-Body Perturbation Theory

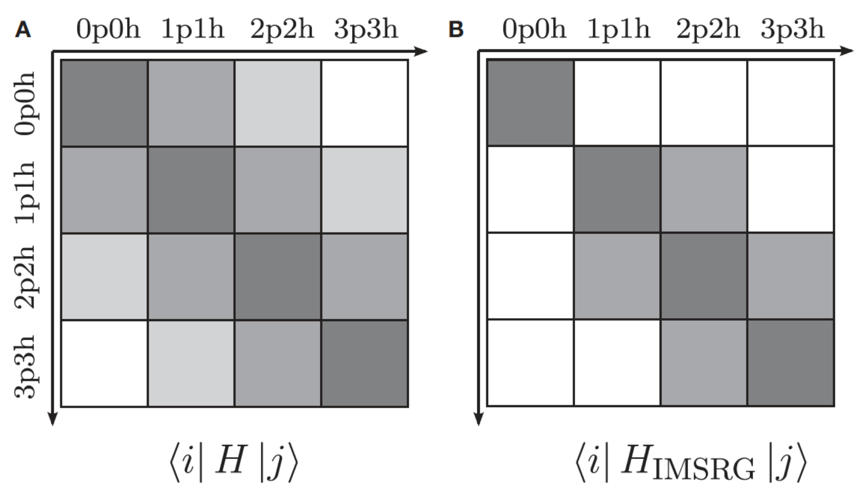
[Roth et al., Phys. Lett. B683, 272 (2010); Tichai et al., Phys. B756, 283 (2016)]

$$|\Psi\rangle = |\Phi\rangle + \sum_{n=1}^{\infty} \left(\frac{1}{H_0 - E^{(0)}} H_I \right)^n |\Phi\rangle$$

$$E = E^{(0)} + \langle\Phi| \sum_{n=1}^{\infty} H_I \left(\frac{1}{H_0 - E^{(0)}} H_I \right)^n |\Phi\rangle$$

In-Medium Similarity Renormalization Group

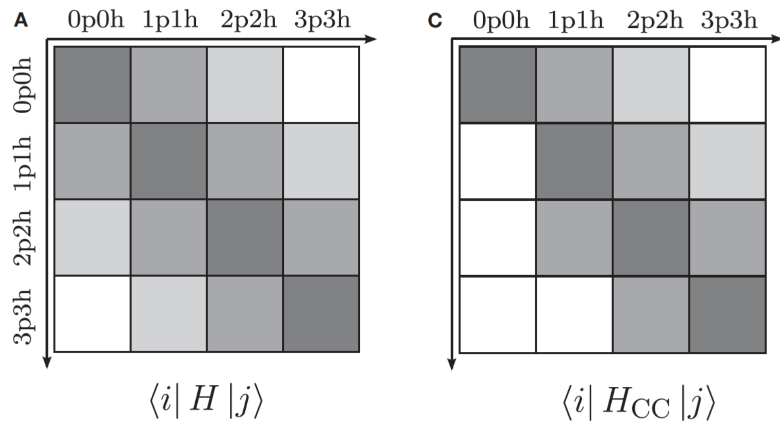
[Hergert et al., Phys. Rev. 621, 165 (2016); Stroberg et al., Phys. Rev. Lett. 118, 032502 (2017)]



[Hergert, Front. Phys. 8, 379 (2020)]

Coupled Cluster Methods

[Hagen et al., Rept. Prog. Phys. 77, 096302 (2014); Duguet et al., Phys. Rev. C 91, 064320 (2015)]



Self-Consistent Green's Functions

[Dickhoff et al., Prog. Part. Nucl. Phys. 52, 377 (2004), Soma et al. Phys. Rev. C 101, 014318 (2020)]

$$g_{pq\cdots rs} = \langle \Psi_0^A | \, T \left[a_p(t_p) a_q(t_q) \cdots a_s^\dagger(t_s) a_r^\dagger(t_r) \right] | \Psi_0^A \rangle$$

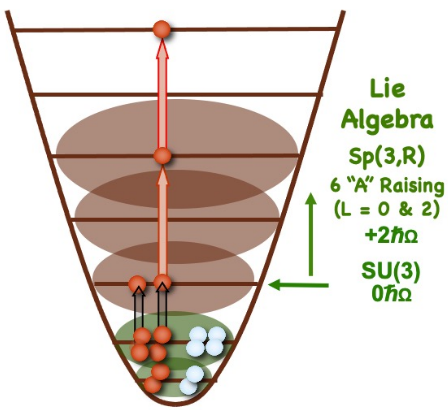
No-Core Configuration Interaction

[Barrett et al., Prog. Part. Nucl. Phys. 69, 131 (2013); Navratil et al., Phys. Scripta. 91 053002, (2016)]

$$|\Psi\rangle = |\Psi\rangle_{\text{core}} \otimes |\Psi\rangle_{\text{valence}} \rightarrow |\Psi\rangle_{\text{all valence}}$$

Symmetry-Adapted No-Core Configuration Interaction

[Launey et al., Prog. Part. Nucl. Phys. 89, 101 (2016); Dytrych et al. Phys. Rev. Lett. 124, 042501 (2020)]



Projected Generator Coordinate Method

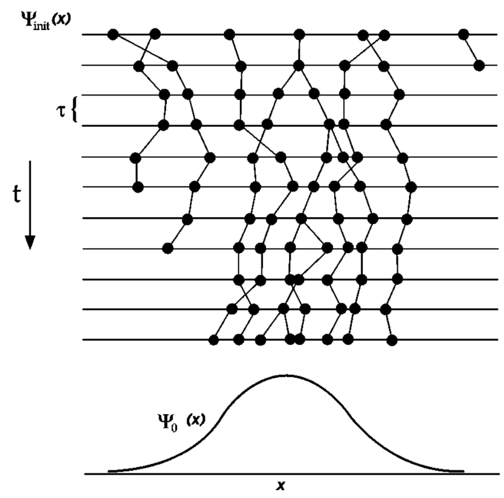
[Otsuka et al., Prog. Part. Nucl. Phys. 47, 319 (2001); Shimizu, Phys. Scripta. 92, 063001 (2017); Frosini et al. Eur. Phys. J. A 58, 63 (2022)]

$$|\Phi_i(J,M,\pi)\rangle = \sum_{K=-J}^{J} g_K P^J_{M,K} P^\pi |\phi_i\rangle$$

$$|\Psi(J,M,\pi)\rangle = \sum_{i=1}^{N_{\rm basis}} f_i |\Phi_i(J,M,\pi)\rangle$$

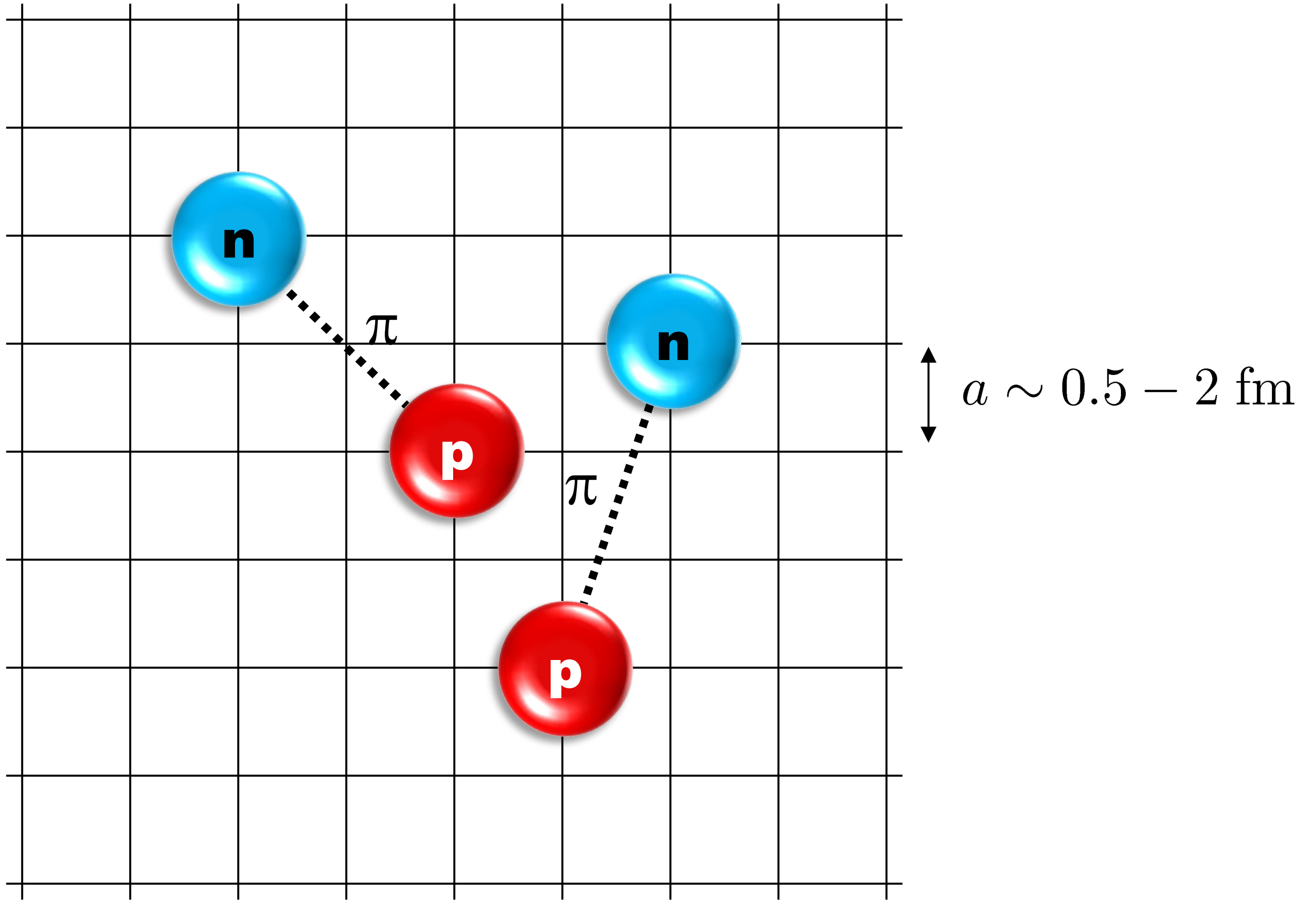
Quantum Monte Carlo

[Carlson et al., Rev. Mod. Phys. 87, 1067 (2015); Gandolfi et al, Front. Phys. 8, 117 (2020)]



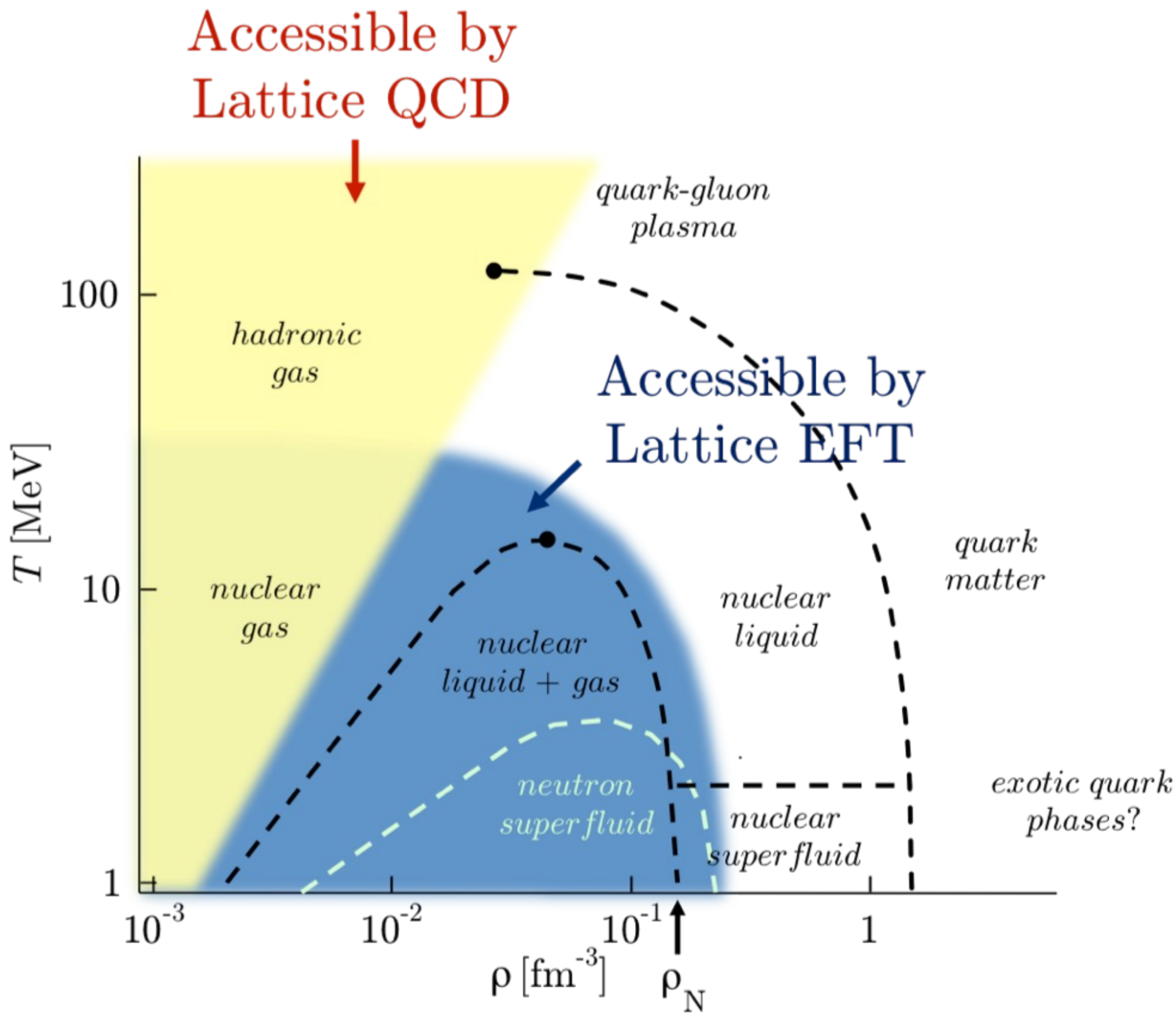
[Foulkes et al., Rev. Mod. Phys. 73, 1 (2001)]

Lattice effective field theory



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

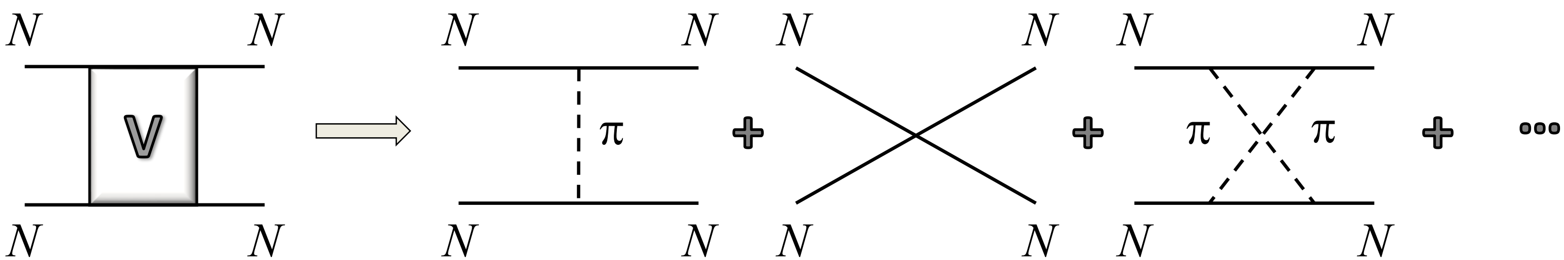
[Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer]



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

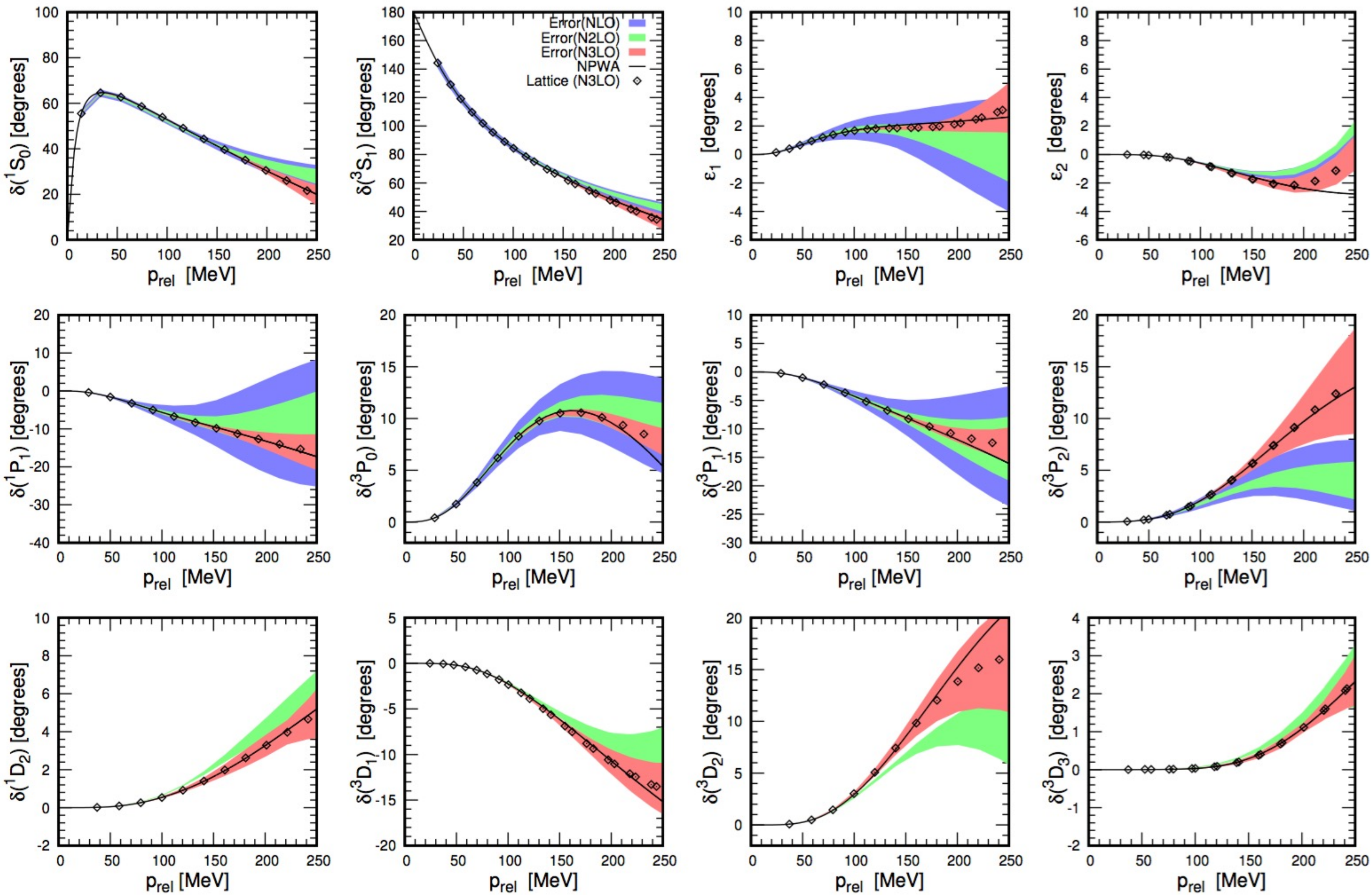
Construct the effective potential order by order



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

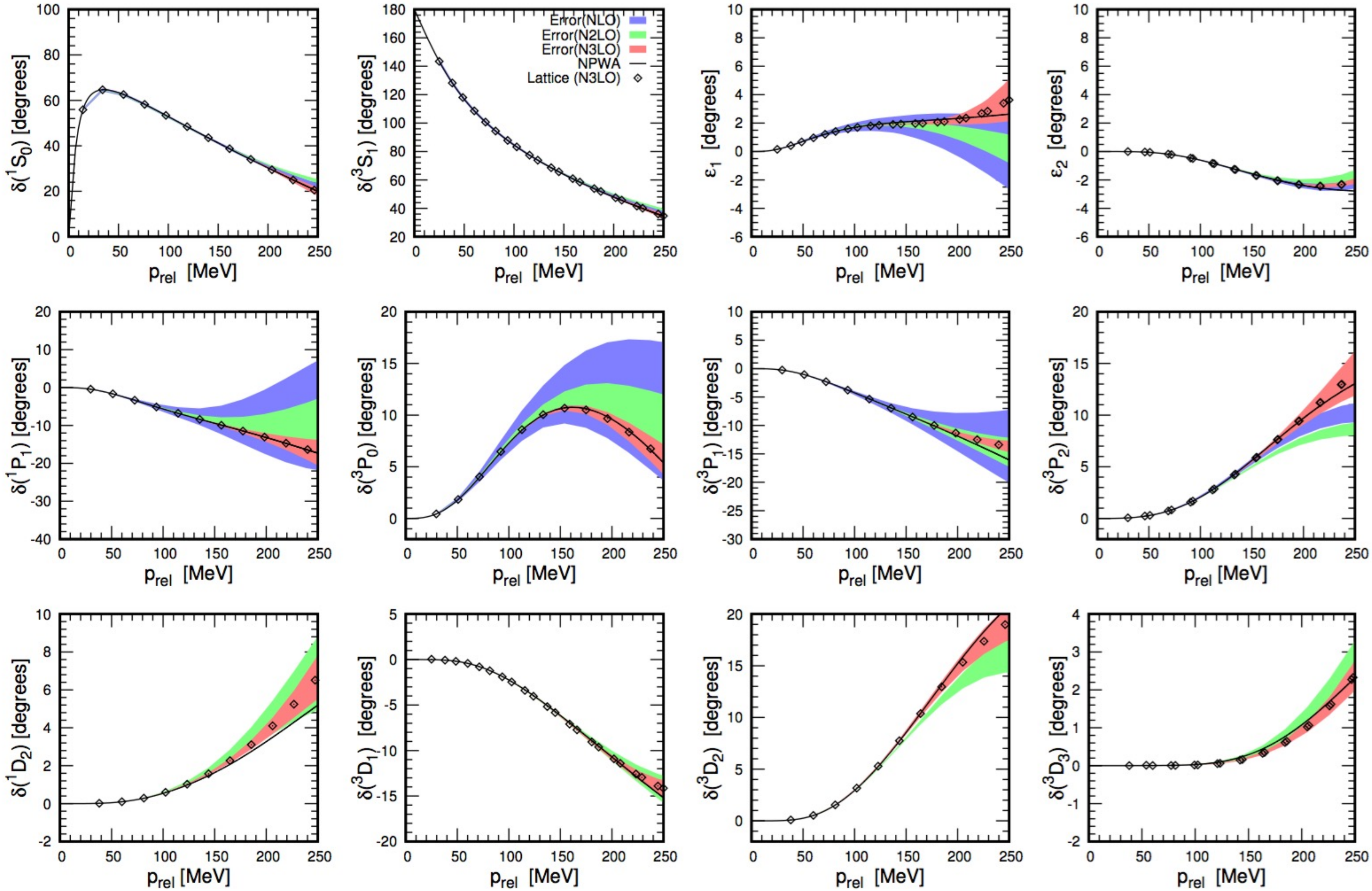
Leading order (LO) Next-to-leading order (NLO)

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

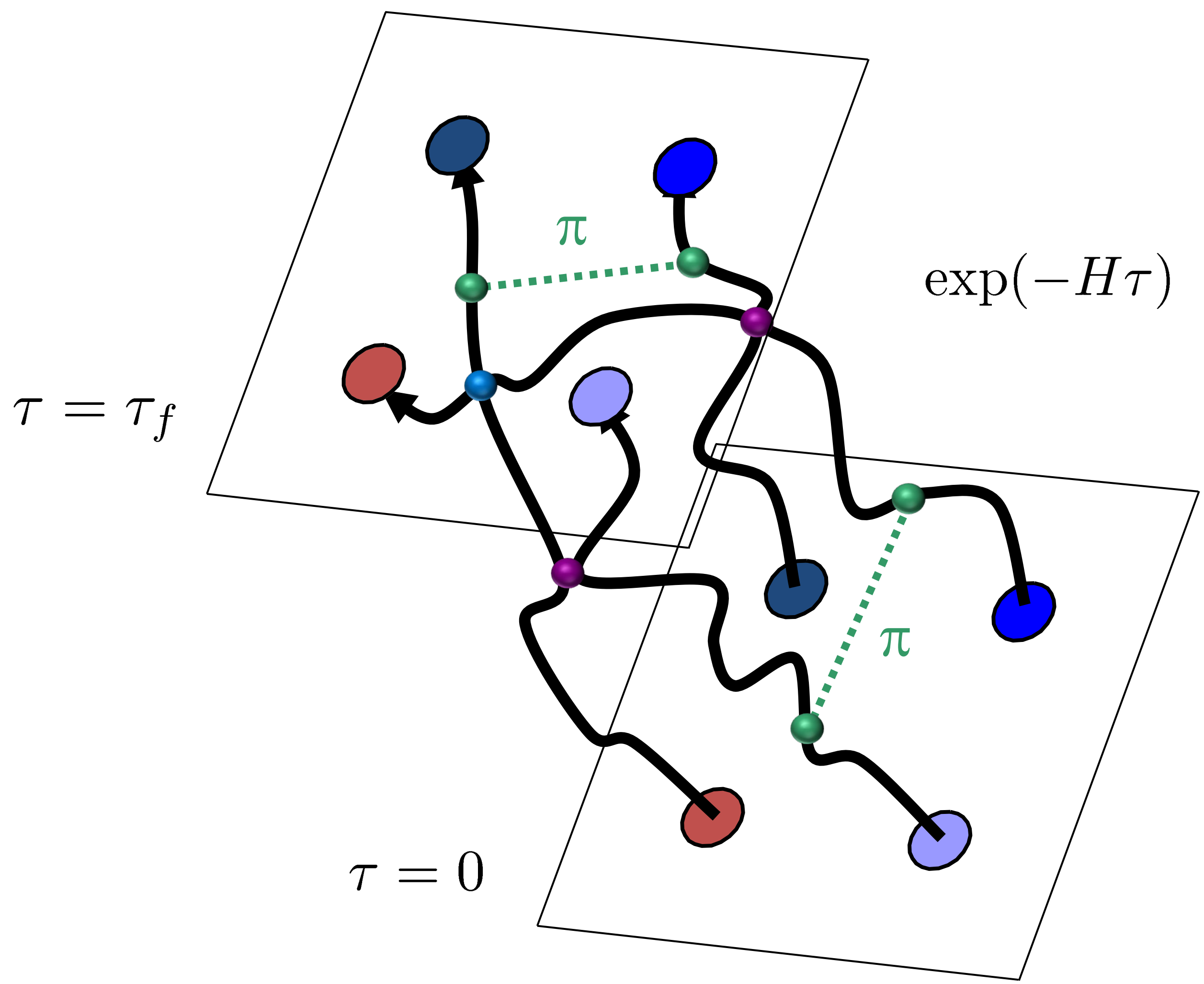


[Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)]

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



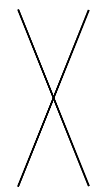
Euclidean time projection



Auxiliary field method

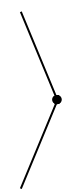
We can write exponentials of the interaction using a Gaussian integral identity

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



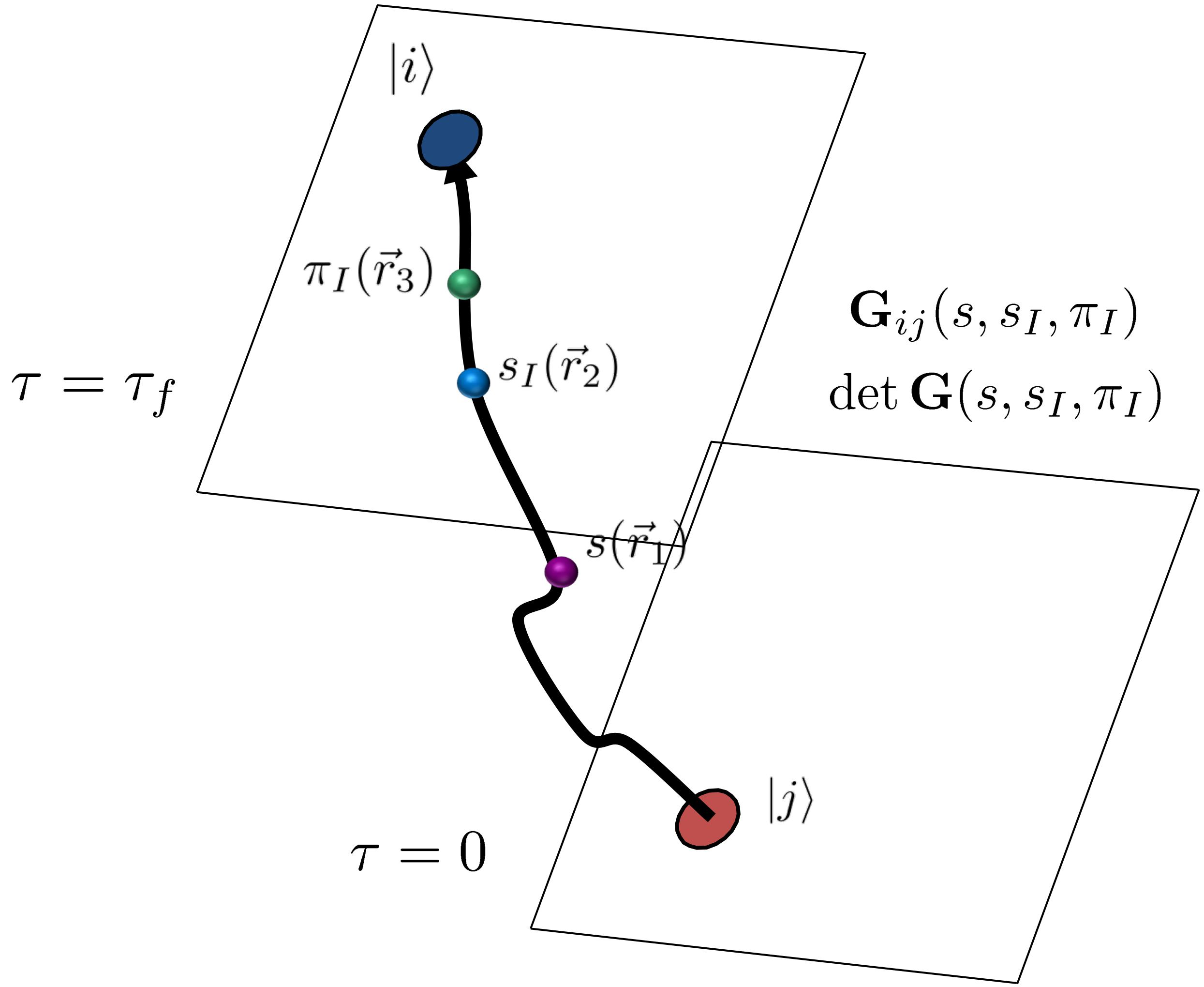
$(N^{\dagger}N)^{2}$

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



$sN^{\dagger}N$

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



$\mathbf{G}_{ij}(s, s_I, \pi_I)$

$\det \mathbf{G}(s, s_I, \pi_I)$

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?

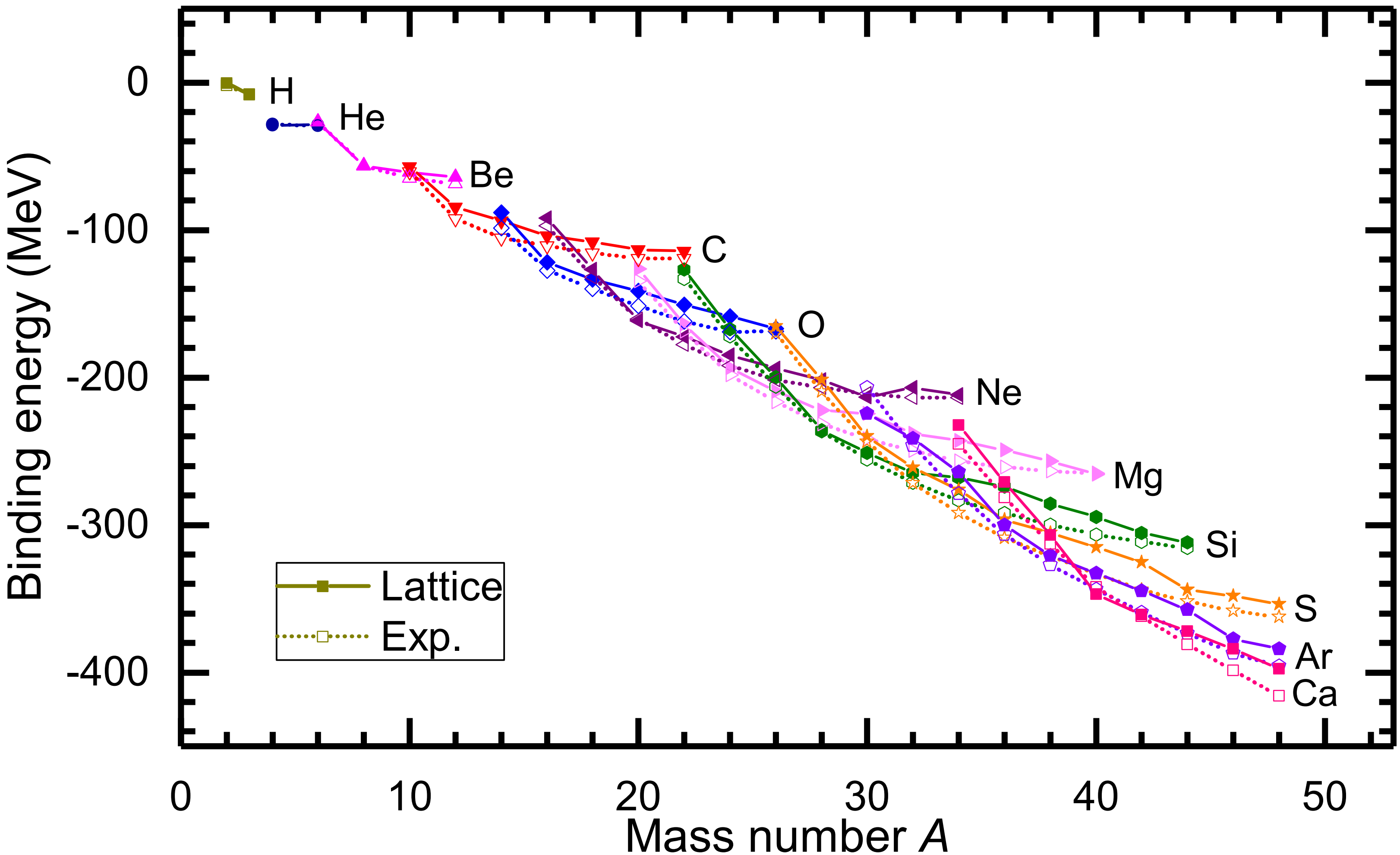
We construct an interaction with only four parameters.

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

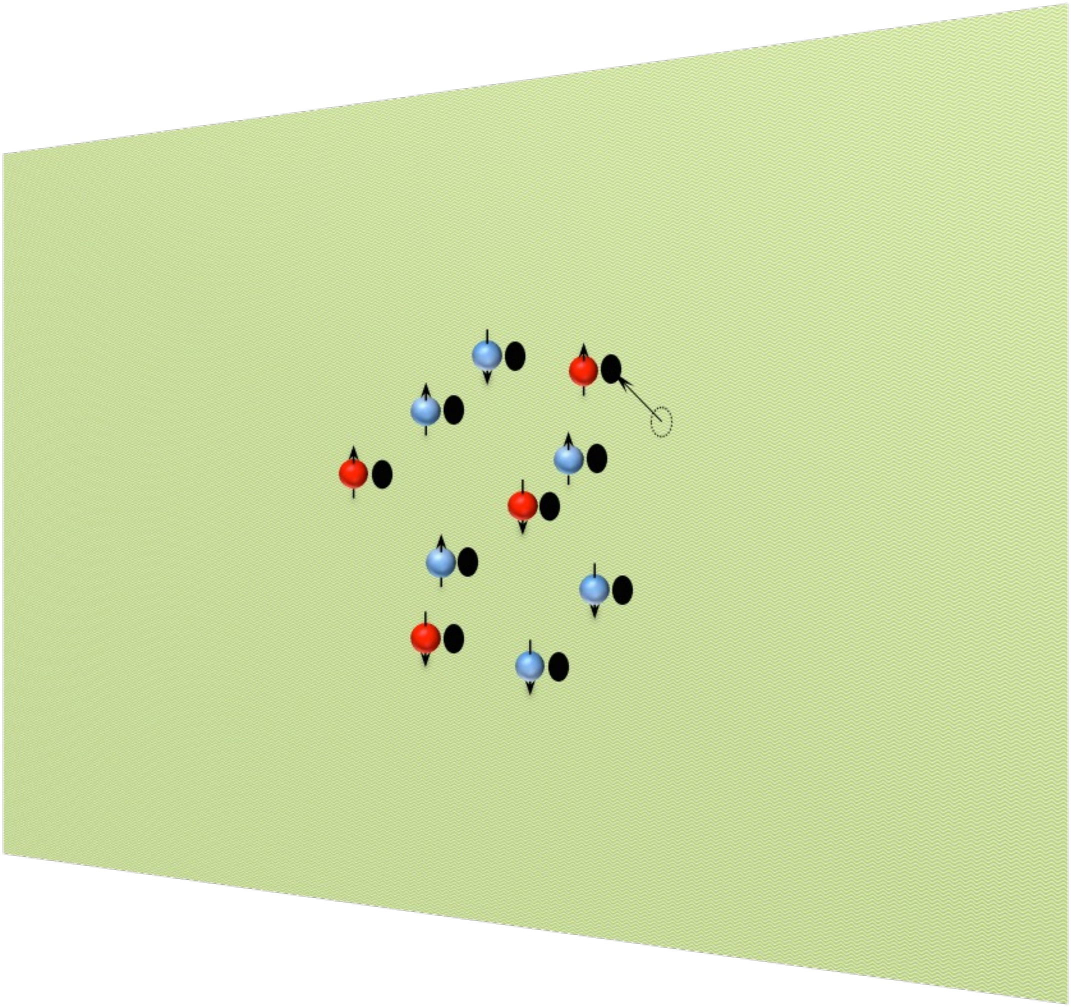
fit to $A > 3$



[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

Pinhole algorithm



Seeing Structure with Pinholes

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

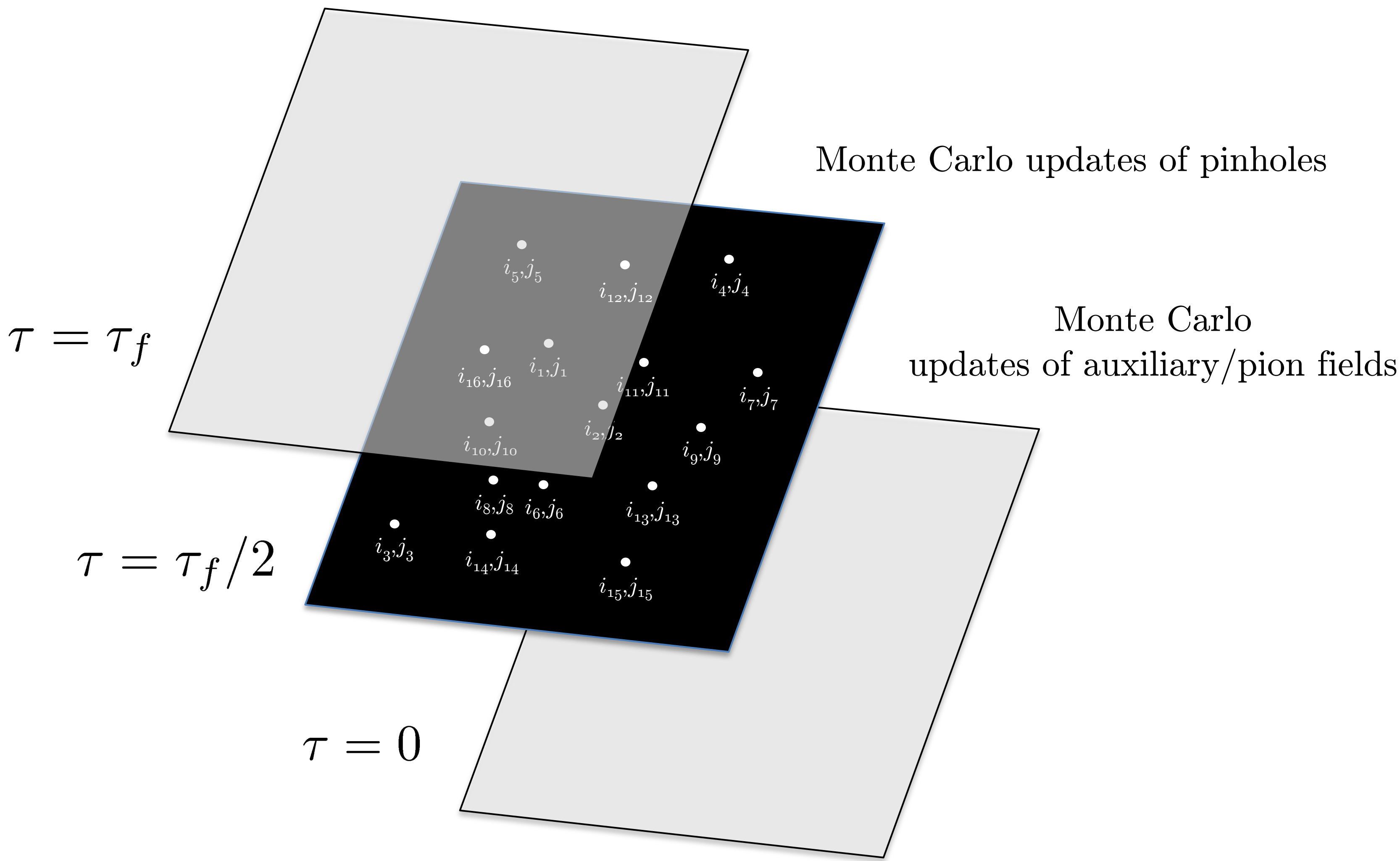
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

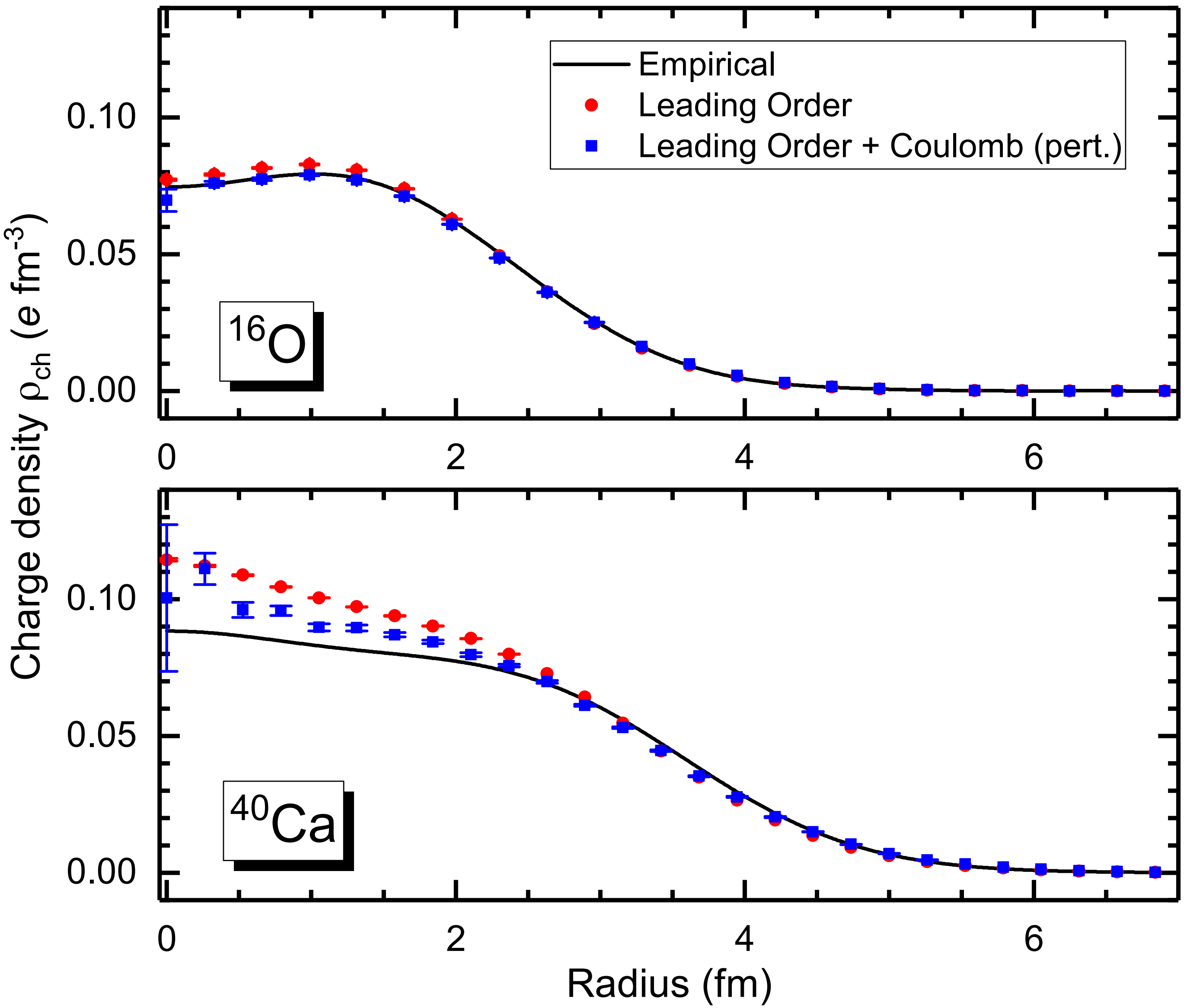
$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = \,:\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

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

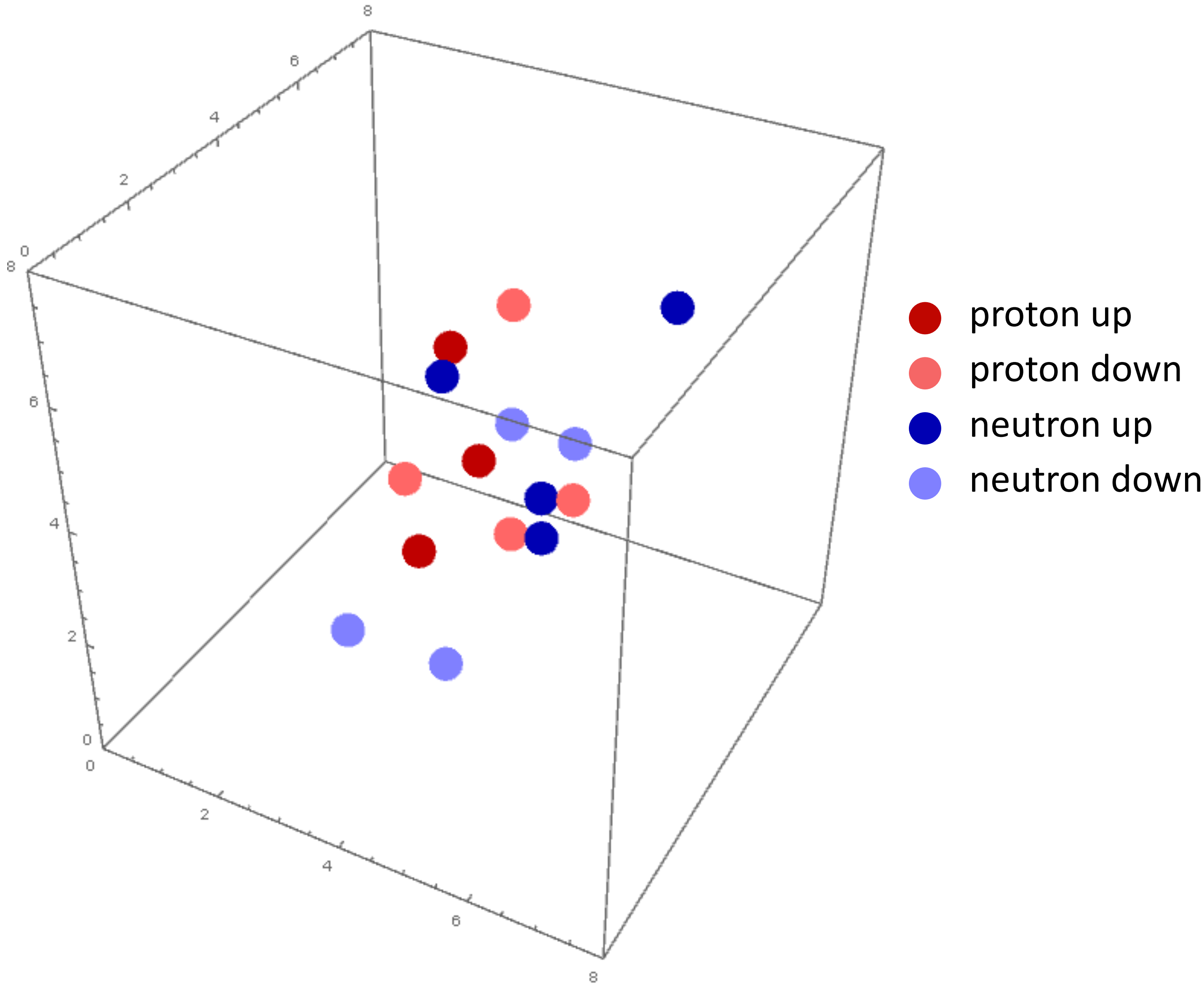


]Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)]



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

^{16}O



^{16}O ^{16}O collisions at RHIC and LHC energies

[Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins PRC 104, L041901 (2021)]

^{16}O ^{16}O collisions have been proposed at LHC to probe dependence on initial states of intermediate size, where alpha clustering is expected to be significant.

For ^{16}O ^{16}O collisions, the system is quite small, and we are pushing the limits of hydrodynamics. We use the Duke Bayesian tune of iEBE-VISHNU package to pPb and PbPb collisions at the LHC.
[Bernhard et al., Nat. Phys. 15 1113 (2019), Moreland et al., Phys. Rev. C 101, 024911 (2020)]

We use the T$_{\mathrm{R}}$ENTo model to general the initial entropy distribution.
[Moreland et al., Phys. Rev. C 92, 044903 (2015)]

The initial entropy distribution is then passed through a free-streaming phase of duration 0.37 fm/c and used to initialize the hydrodynamics evolution.

We compute the following cumulants of the flow harmonics v_n:

$$v_n\{2\} = \left[\left\langle v_n^2 \right\rangle\right]^{\frac{1}{2}}$$
$$v_n\{4\} = \left[2\left\langle v_n^2 \right\rangle^2 - \left\langle v_n^4 \right\rangle\right]^{\frac{1}{4}}$$

We first compute results taking the initial density as a Woods-Saxon potential with density, radius, and diffusivity fitted to empirical values. We then consider the same Woods-Saxon potential, taking into account the quark substructure of the nucleons. We then use the nucleon distributions from the lattice effective field theory calculations. This incorporates correlations such as alpha clustering.

[Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins PRC 104, L041901 (2021)]

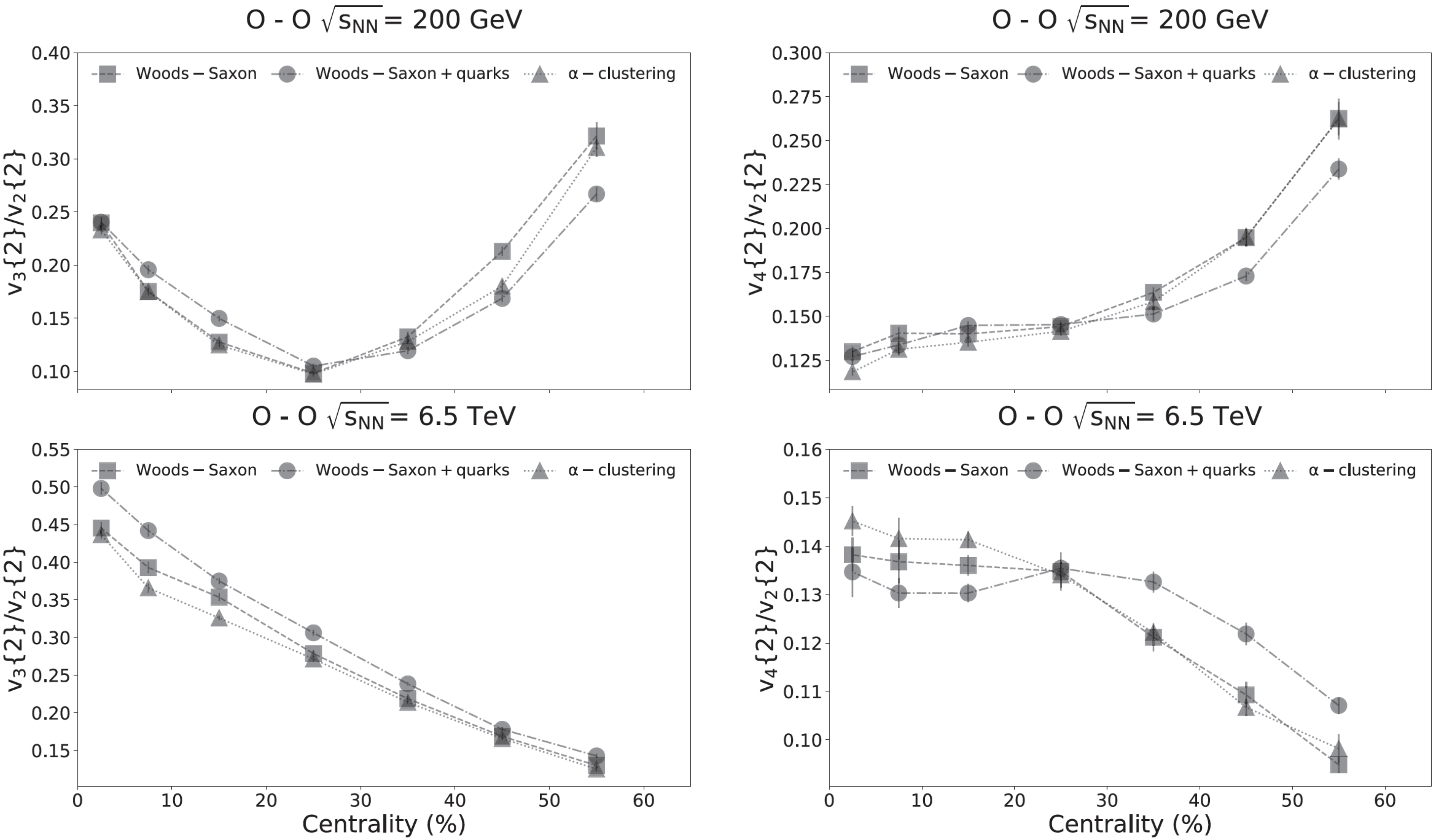
How much alpha clustering?

$$\langle \rho^2 \rangle_{^{16}\mathrm{O}} = 4.59(11)\, \langle \rho^2 \rangle_{^{4}\mathrm{He}}$$

$$\langle \rho^3 \rangle_{^{16}\mathrm{O}} = 4.67(23)\, \langle \rho^3 \rangle_{^{4}\mathrm{He}}$$

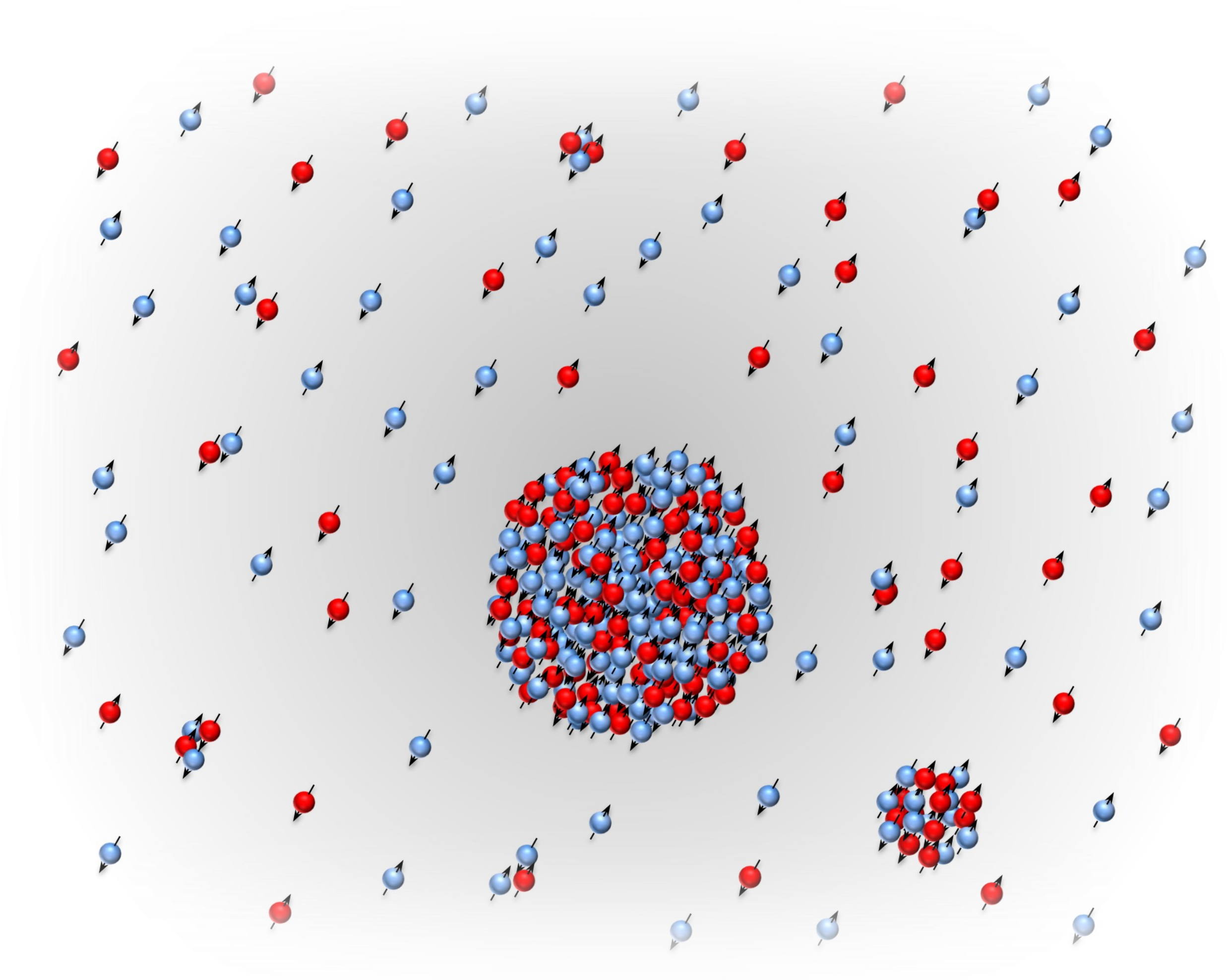
$$\langle \rho^4 \rangle_{^{16}\mathrm{O}} = 4.44(27)\, \langle \rho^4 \rangle_{^{4}\mathrm{He}}$$

About 10% greater than the simple tensor product of four alpha clusters. The excess is due to entanglement of the alpha cluster wave functions.



[Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins PRC 104, L041901 (2021)]

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

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

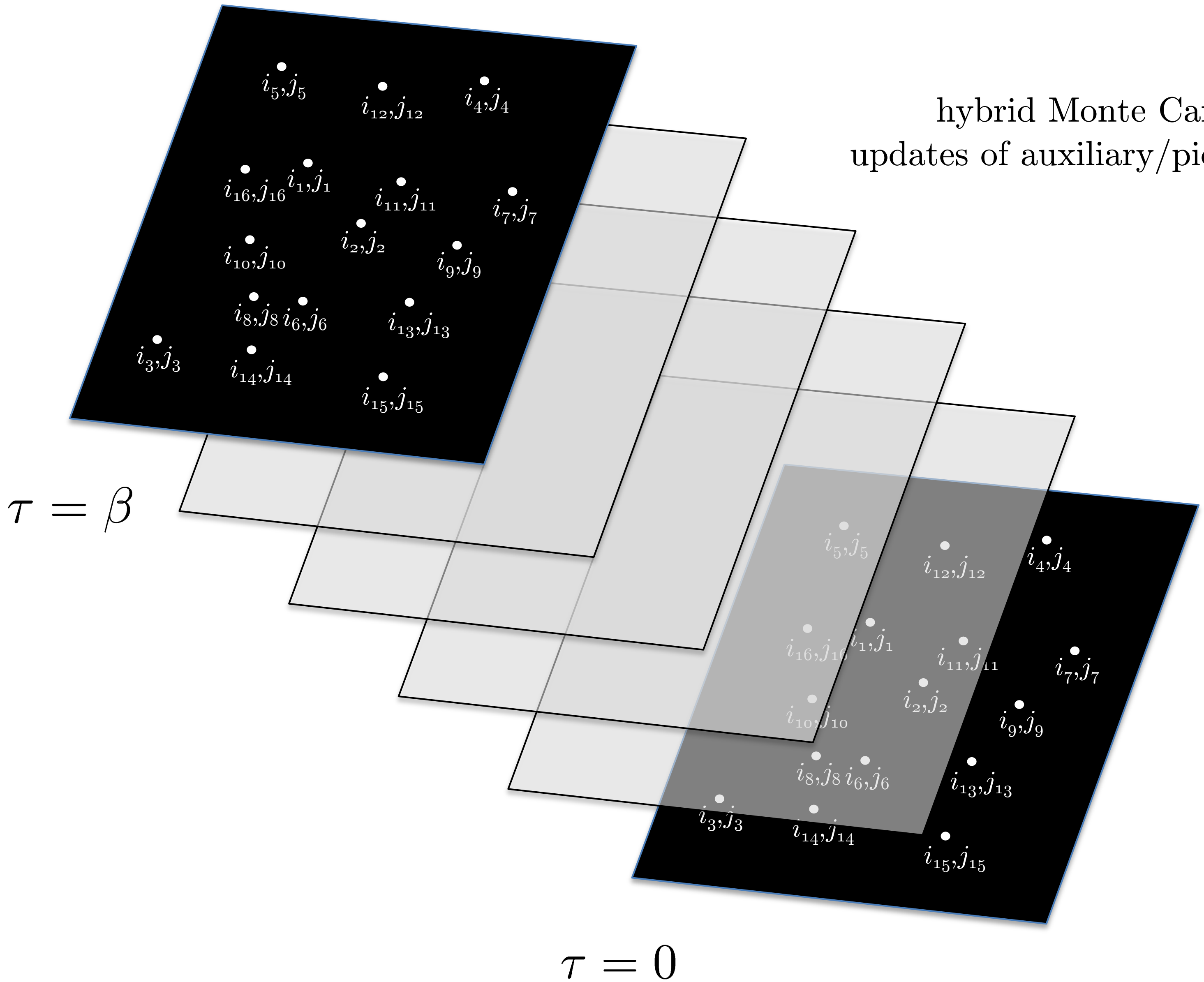
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

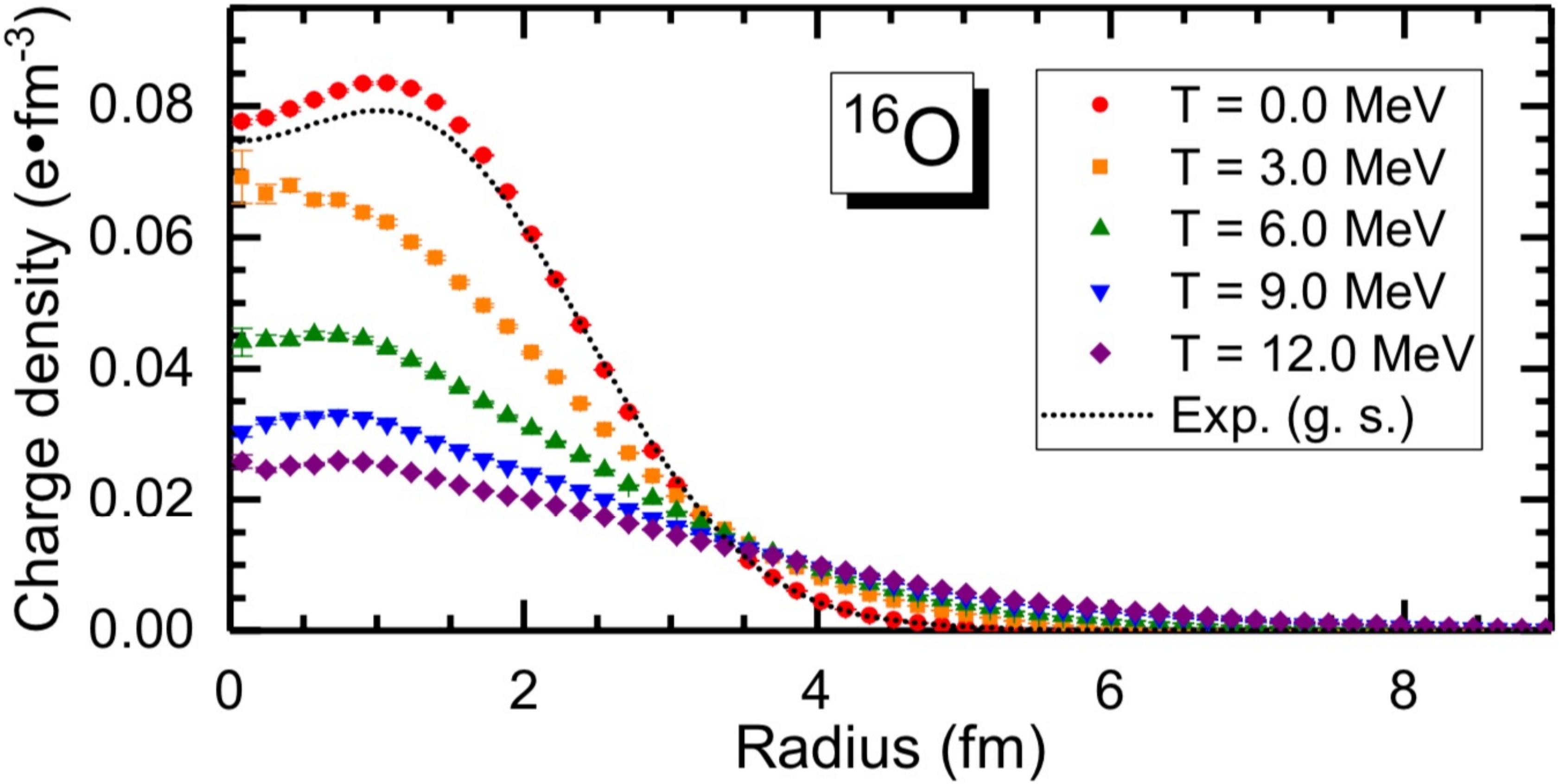
$$\mathrm{Tr}\, O$$
$$= \frac{1}{A!} \sum_{i_1 \cdots i_A, j_1 \cdots j_A, \mathbf{n}_1 \cdots \mathbf{n}_A} \langle 0 | a_{i_A,j_A}(\mathbf{n}_A) \cdots a_{i_1,j_1}(\mathbf{n}_1)\, O\, a^{\dagger}_{i_1,j_1}(\mathbf{n}_1) \cdots a^{\dagger}_{i_A,j_A}(\mathbf{n}_A) | 0 \rangle$$

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

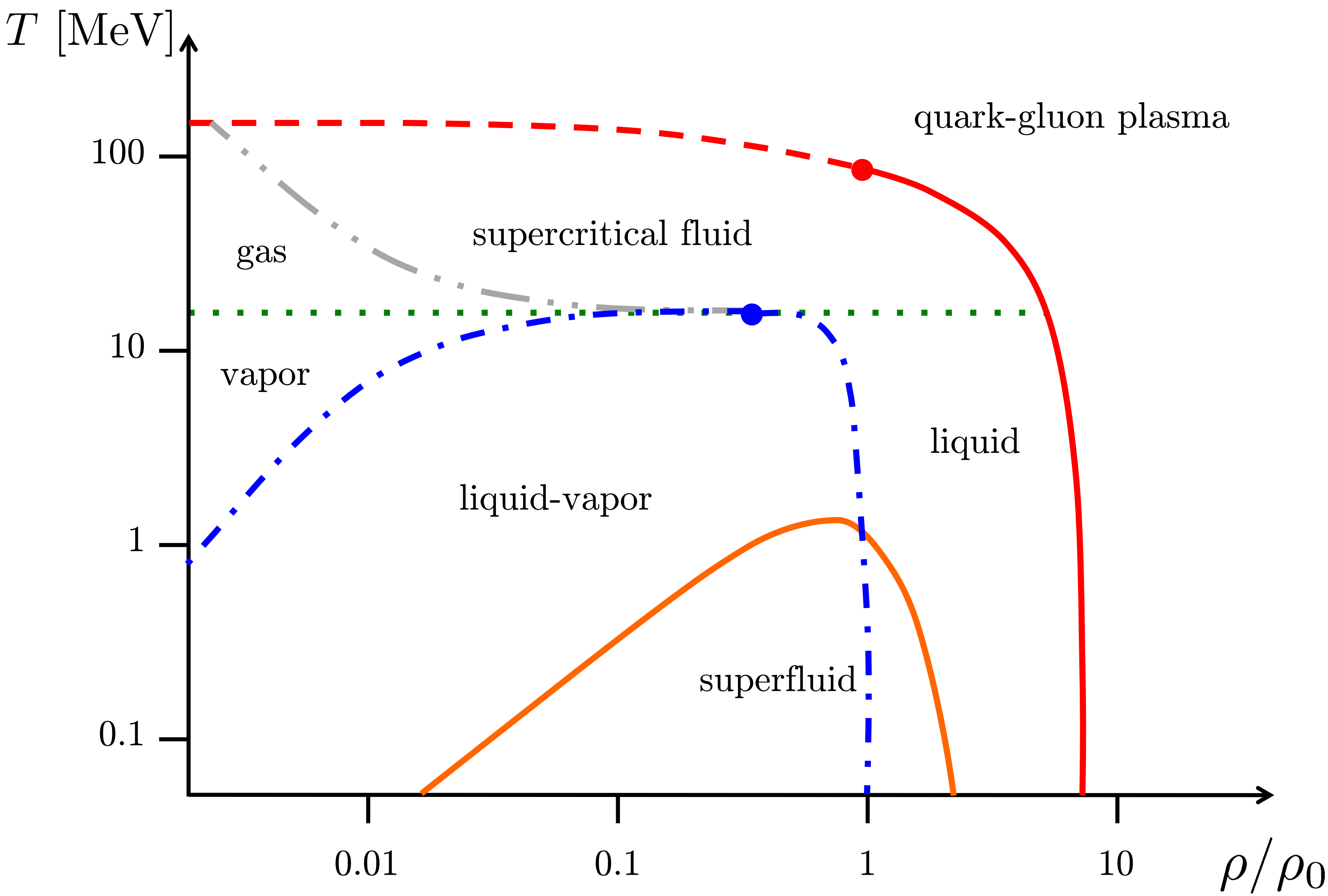
Metropolis updates of pinholes

hybrid Monte Carlo
updates of auxiliary/pion fields

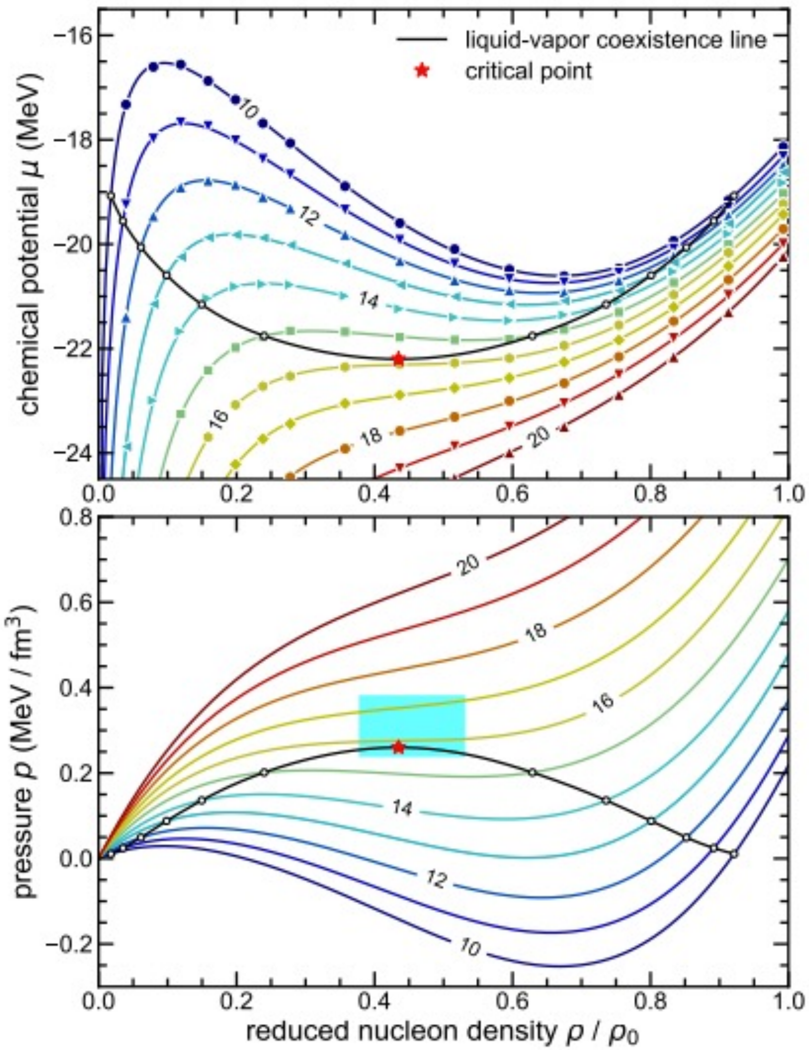




Charge density (e•fm^-3)
0.08
0.06
0.04
0.02
0.00
0
2
4
6
8
Radius (fm)
16O
T = 0.0 MeV
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV
Exp. (g. s.)



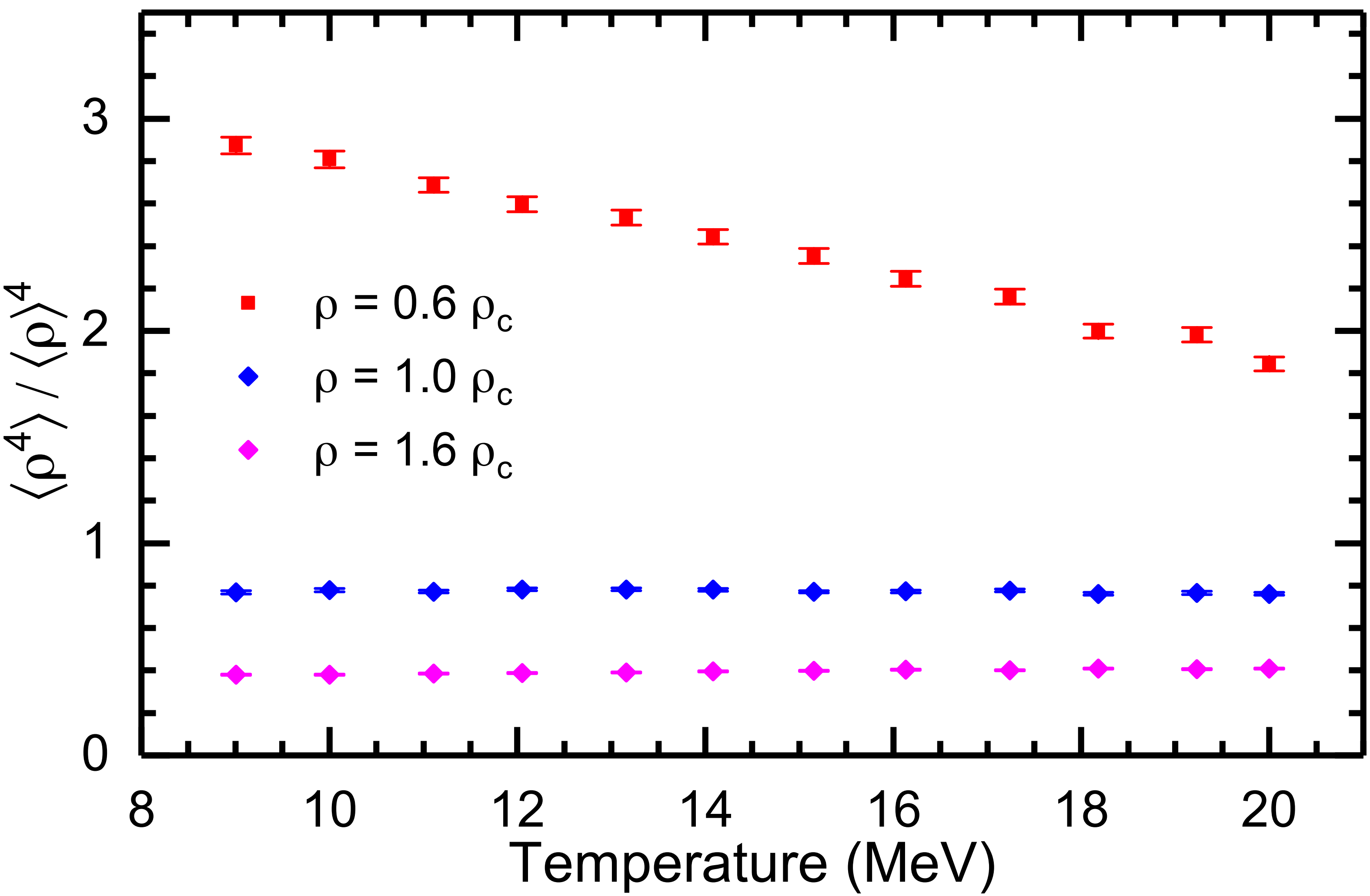
T [MeV]
100
10
1
0.1
0.01
0.1
1
10
ρ/ρ_0
quark-gluon plasma
supercritical fluid
gas
vapor
liquid
liquid-vapor
superfluid



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

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

Alpha clustering as function of density and temperature



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

Structure and spectrum of ^{12}C

nature communications

Article https://doi.org/10.1038/s41467-023-38391-y

Emergent geometry and duality in the carbon nucleus

Received: 31 March 2022

Accepted: 28 April 2023

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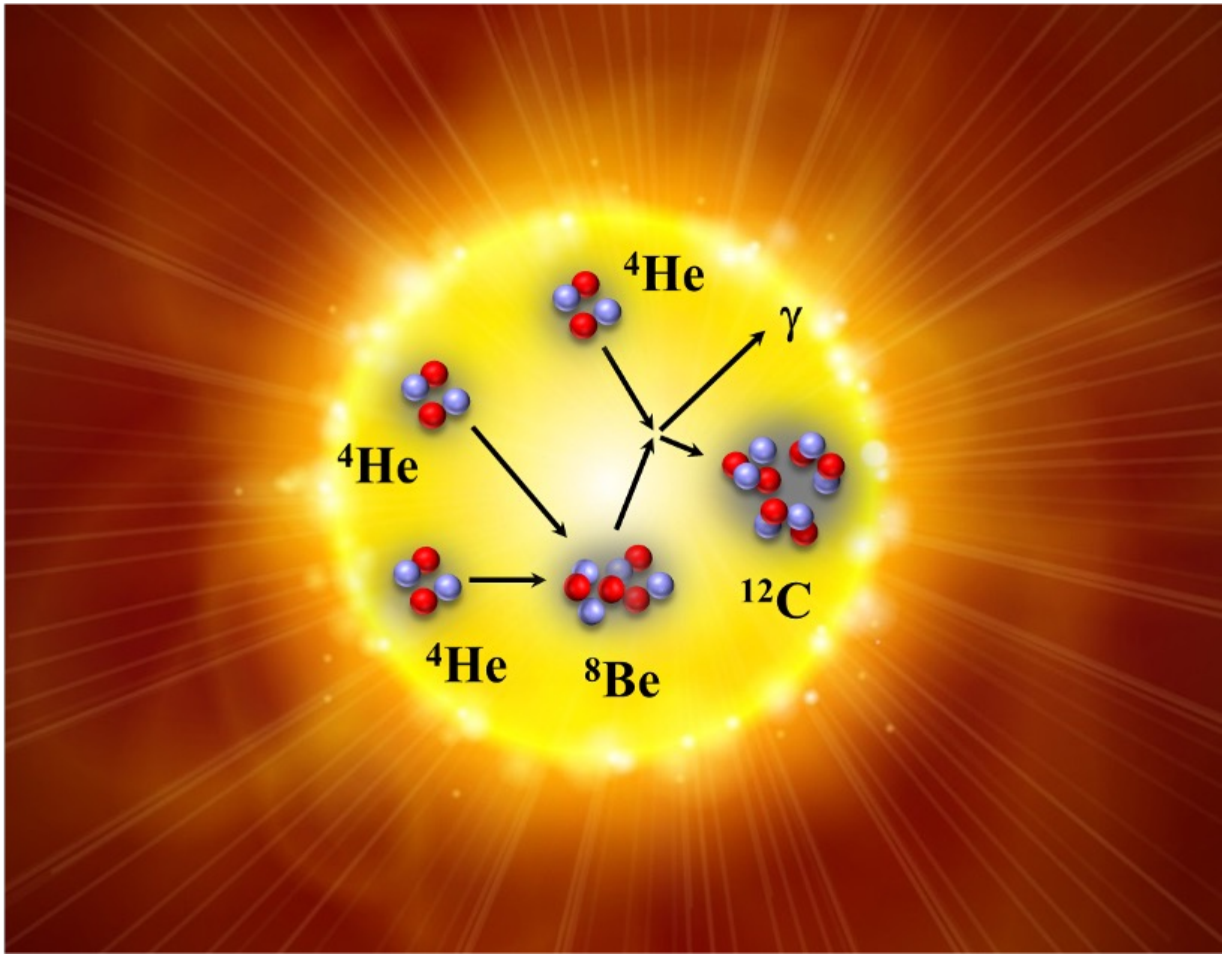
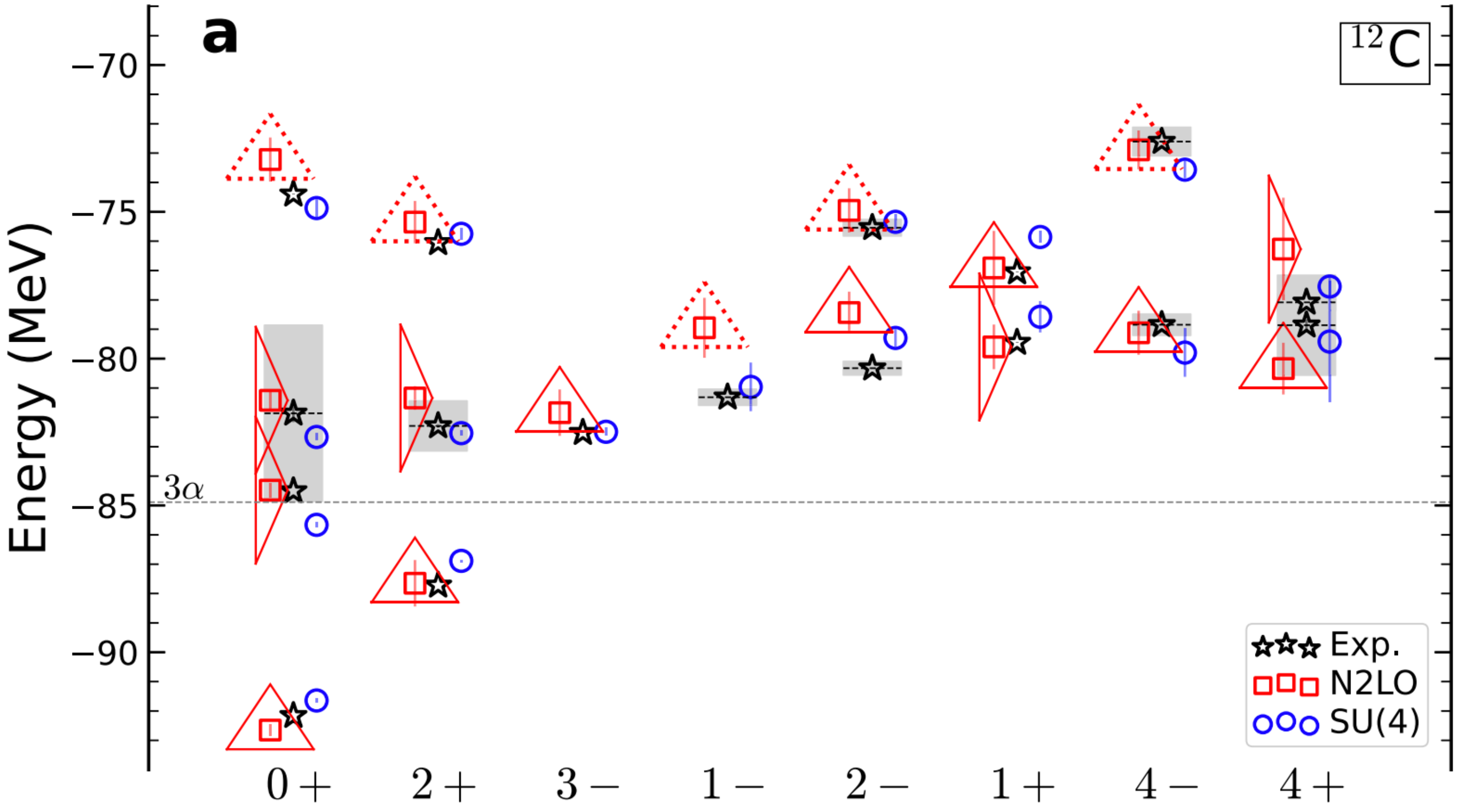
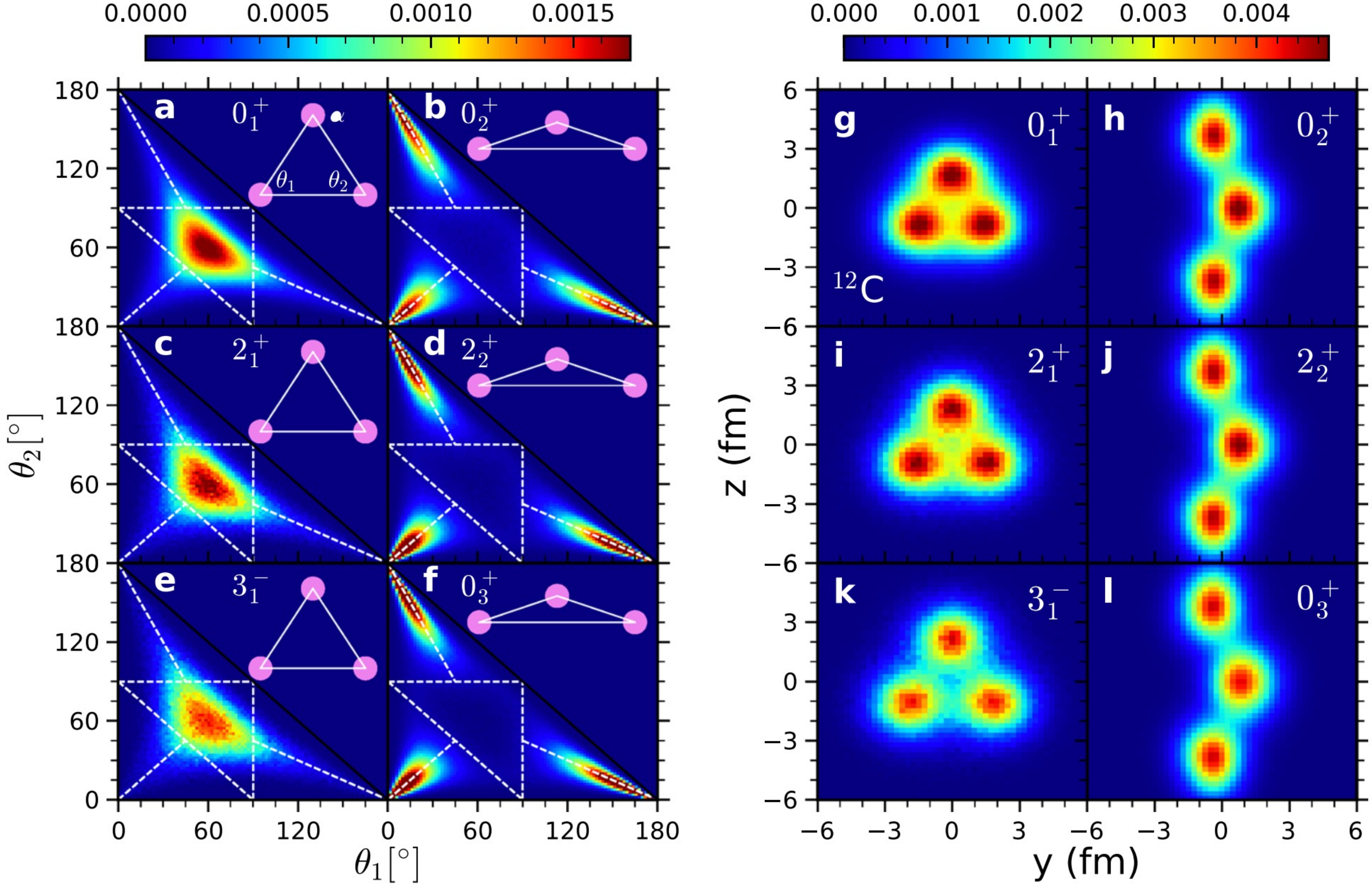

^{4}He
γ
^{4}He
^{4}He
^{8}Be
^{12}C



[Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)]



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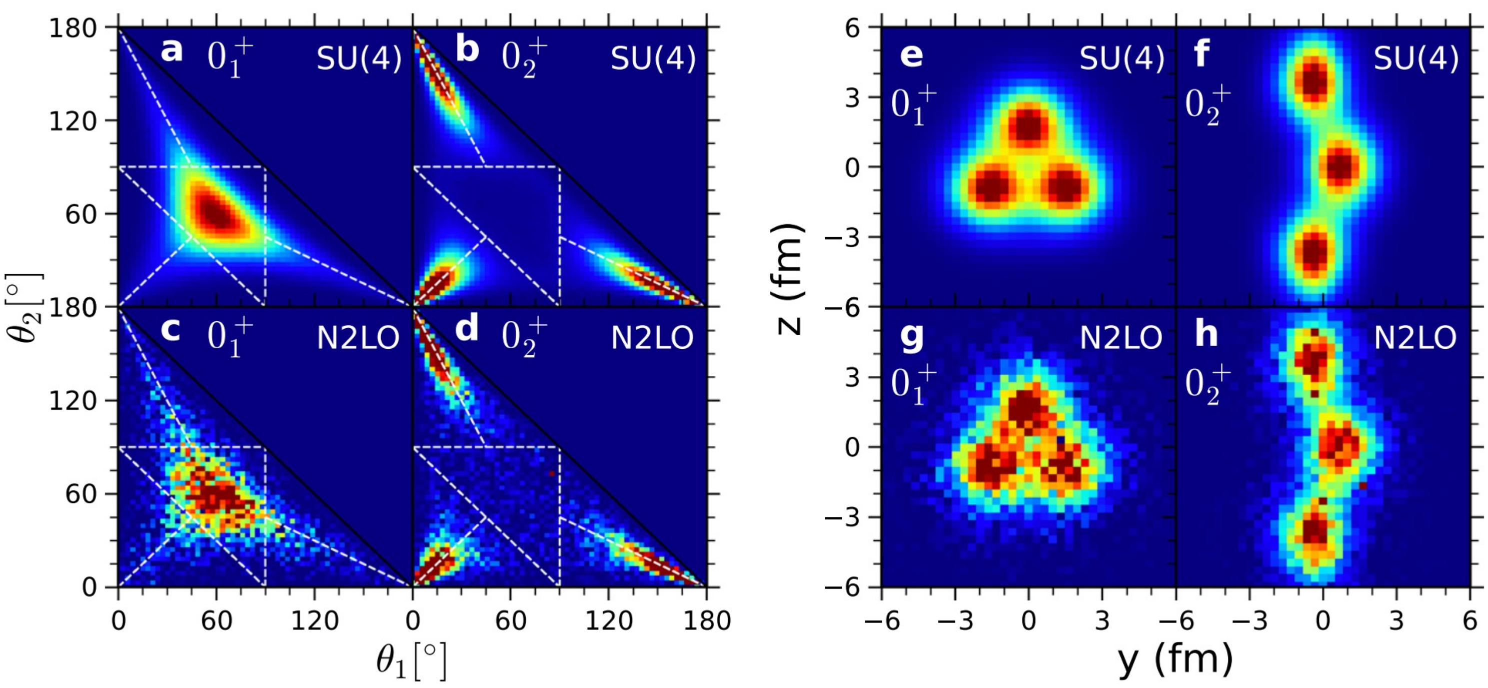
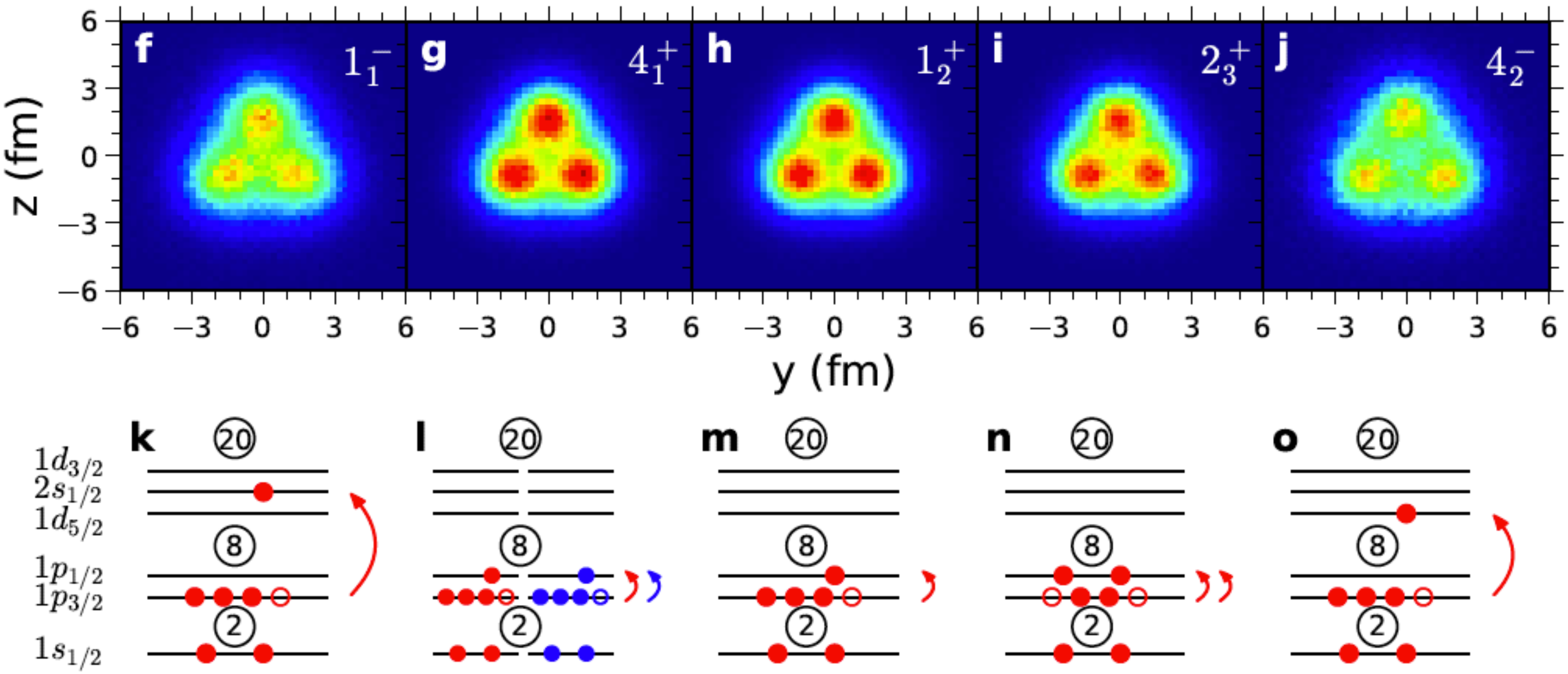


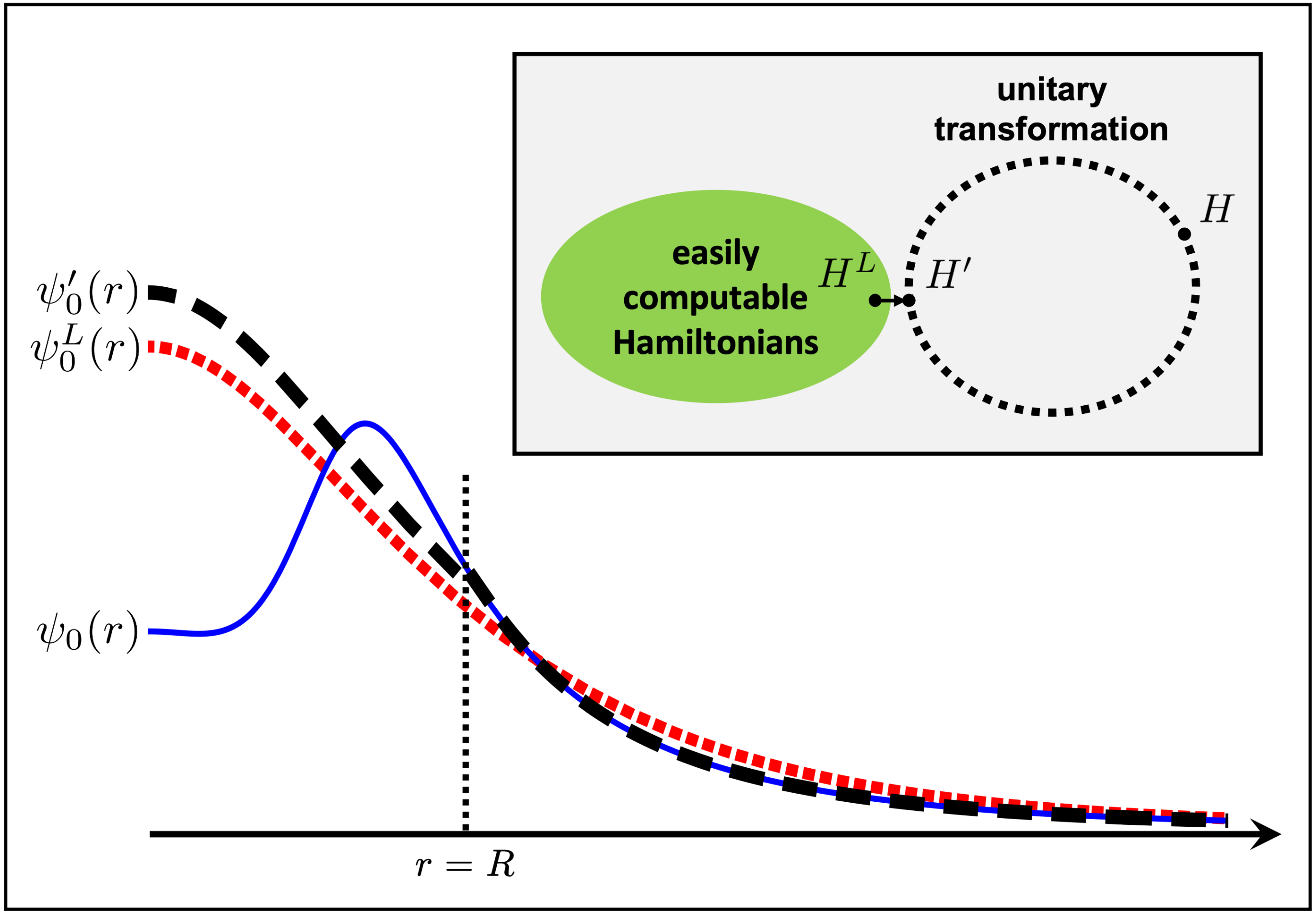
[Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)]



f
1_1^-
g
4_1^+
h
1_2^+
i
2_3^+
j
4_2^-
z (fm)
y (fm)
k
l
m
n
o
20
8
2
$1d_{3/2}$
$2s_{1/2}$
$1d_{5/2}$
$1p_{1/2}$
$1p_{3/2}$
$1s_{1/2}$

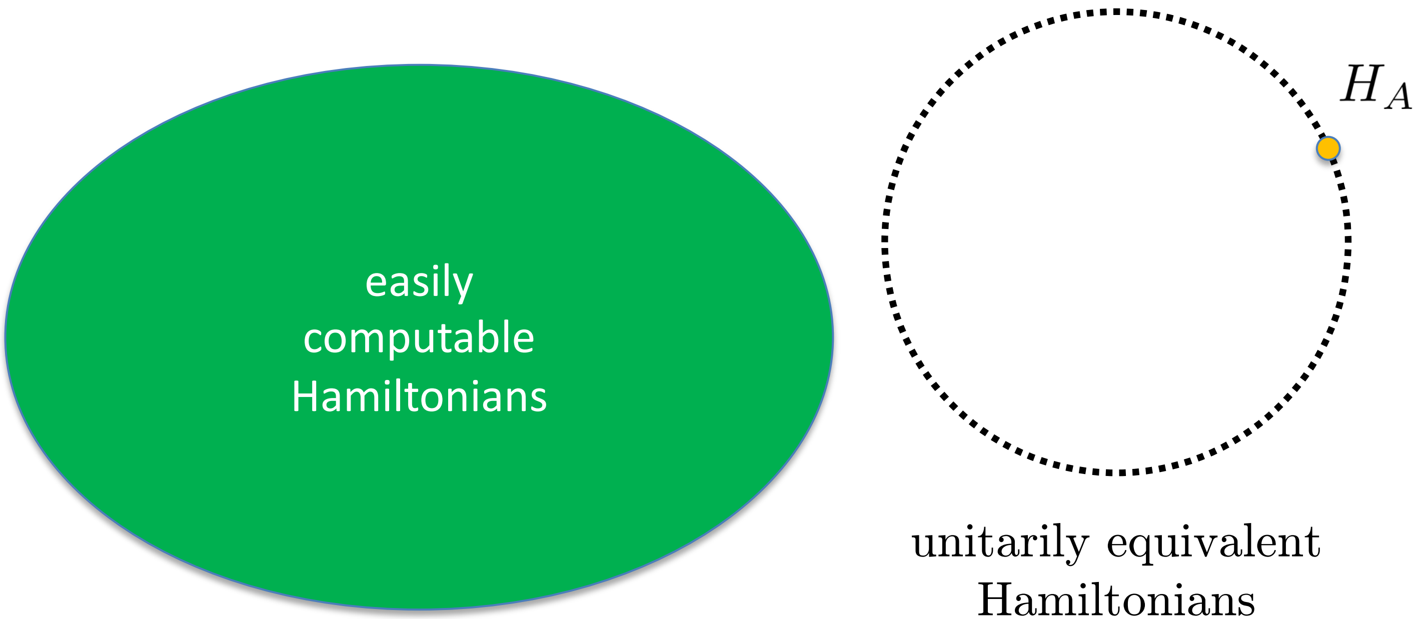
Lattice Monte Carlo simulations can compute highly nontrivial correlations in nuclear many-body systems. Unfortunately, sign oscillations prevent direct simulations using a high-fidelity Hamiltonian based on chiral effective field theory due to short-range repulsion.

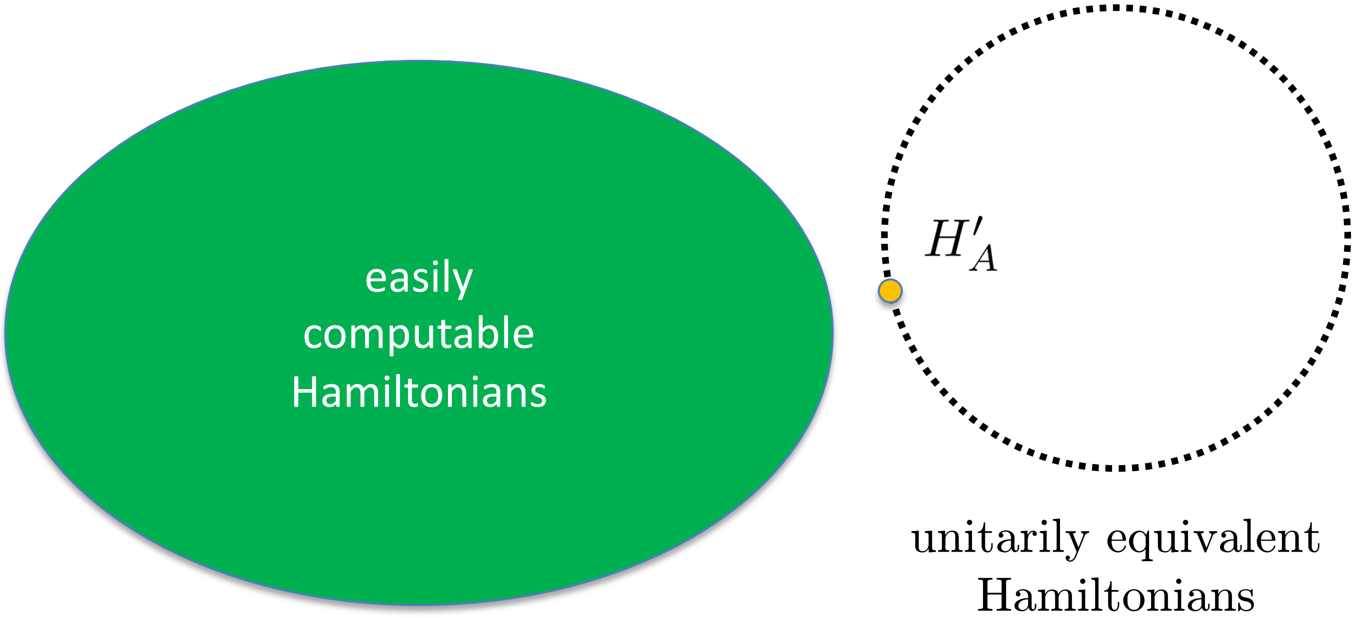
Wave function matching



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

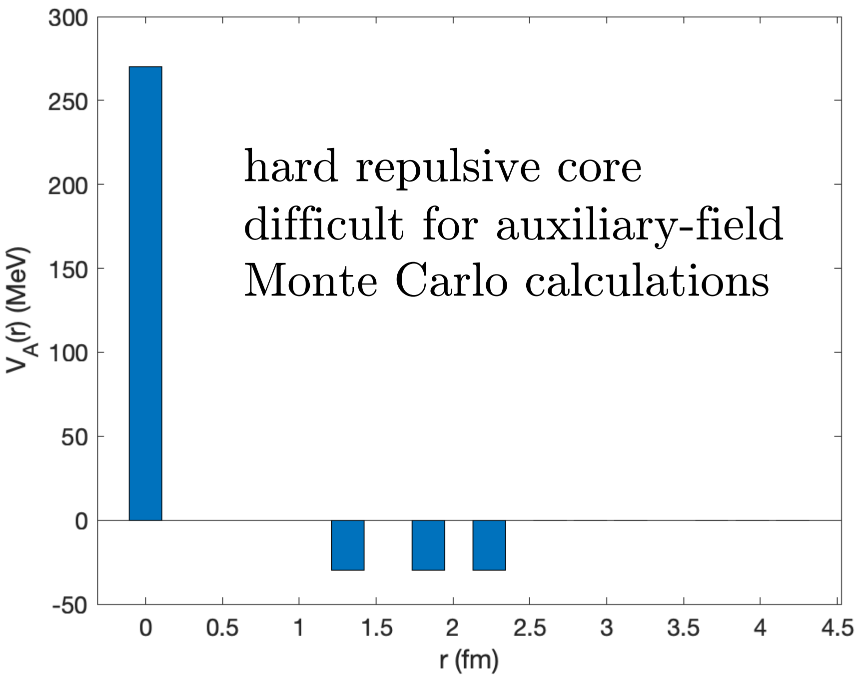

easily
computable
Hamiltonians
H_A


easily
computable
Hamiltonians
H_A
unitarily equivalent
Hamiltonians

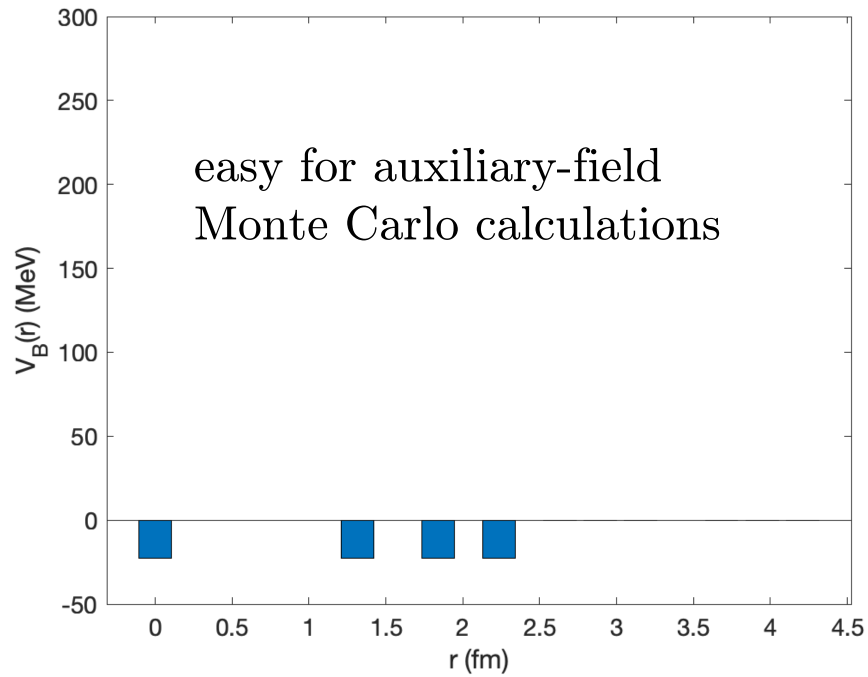

easily
computable
Hamiltonians
H'_A
unitarily equivalent
Hamiltonians

Wave function matching

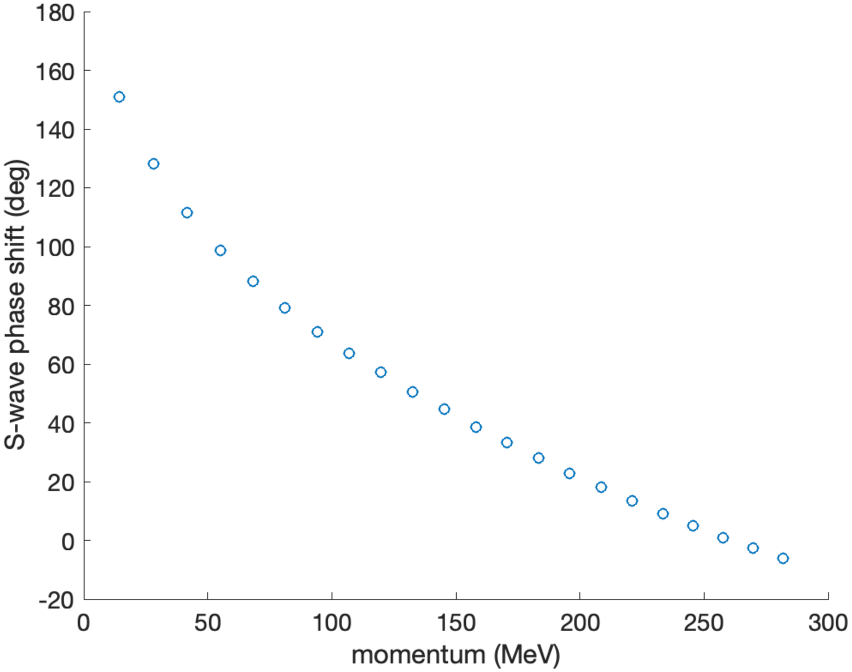
$V_A(r)$



$V_B(r)$

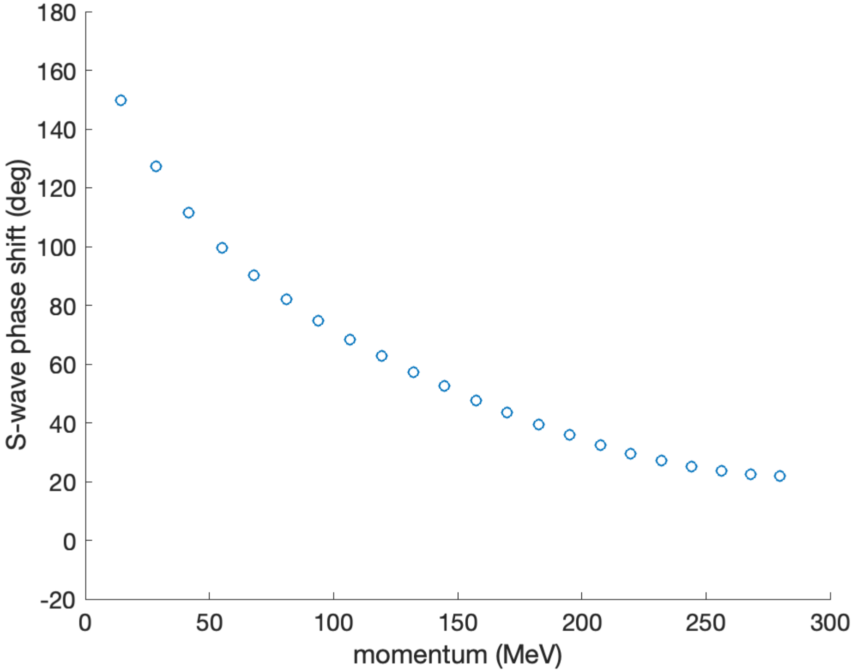


$V_A(r)$



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

$V_B(r)$



S-wave phase shift (deg)
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 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

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

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

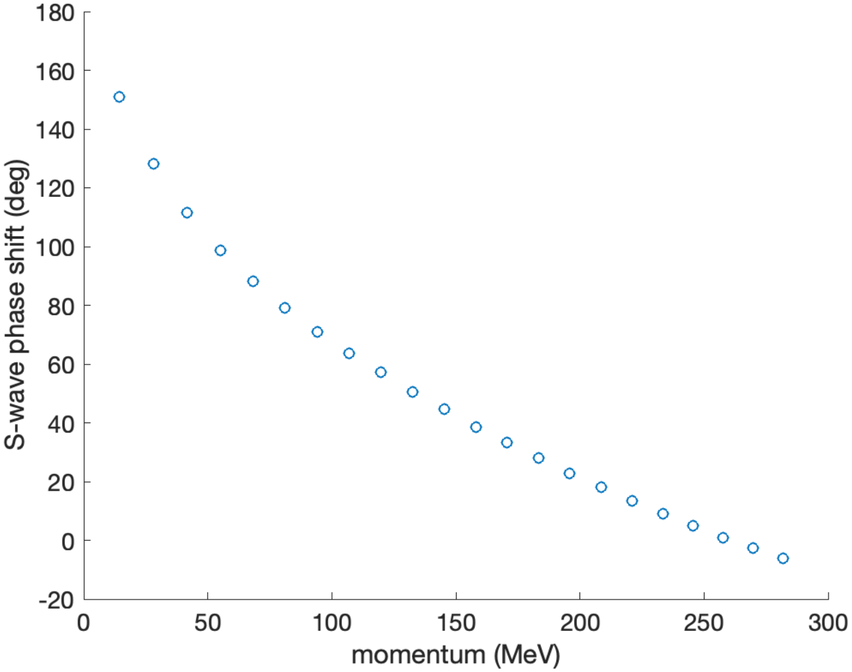
$$U : H_A \to H'_A = U^\dagger H_A U$$

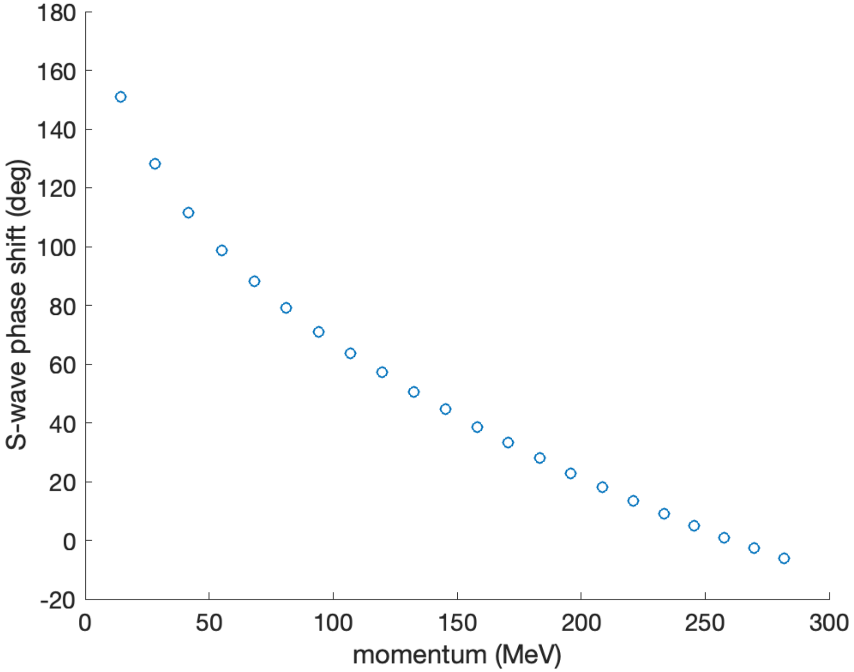
and the resulting nonlocal interaction is

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

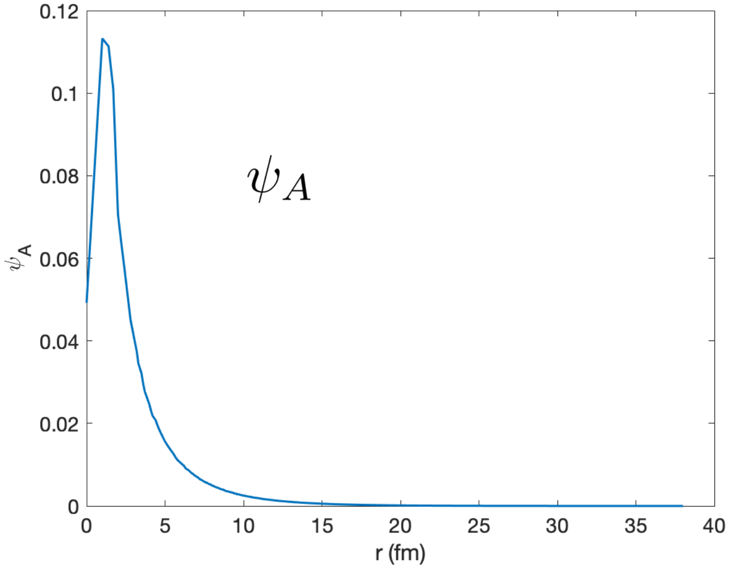
Since they are unitarily equivalent, the phase shifts are exactly the same

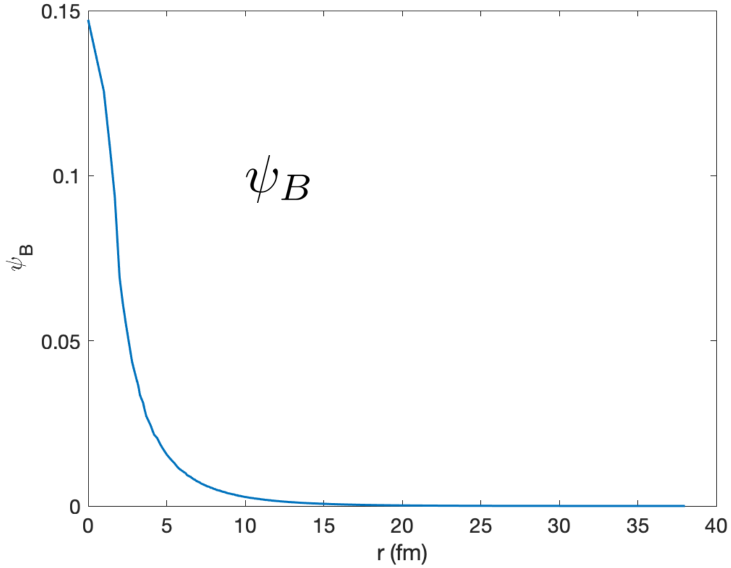
$$V_A(r) \qquad\qquad V'_A(r, r')$$

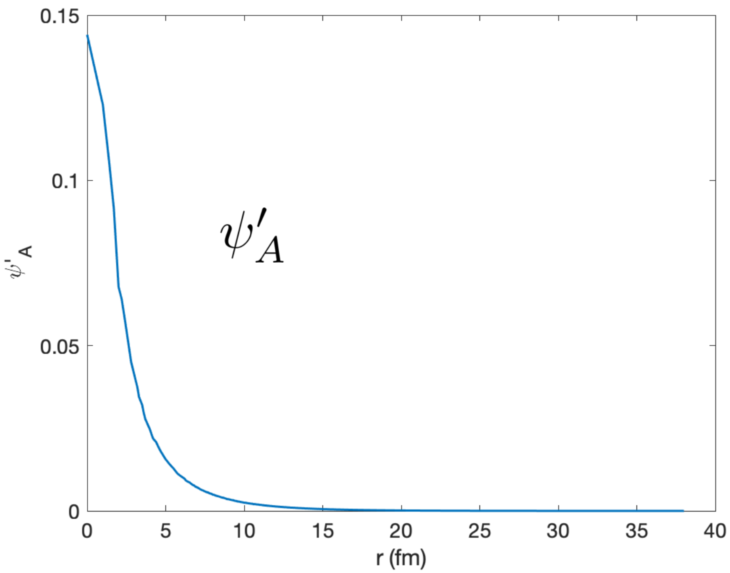




Ground state wave functions





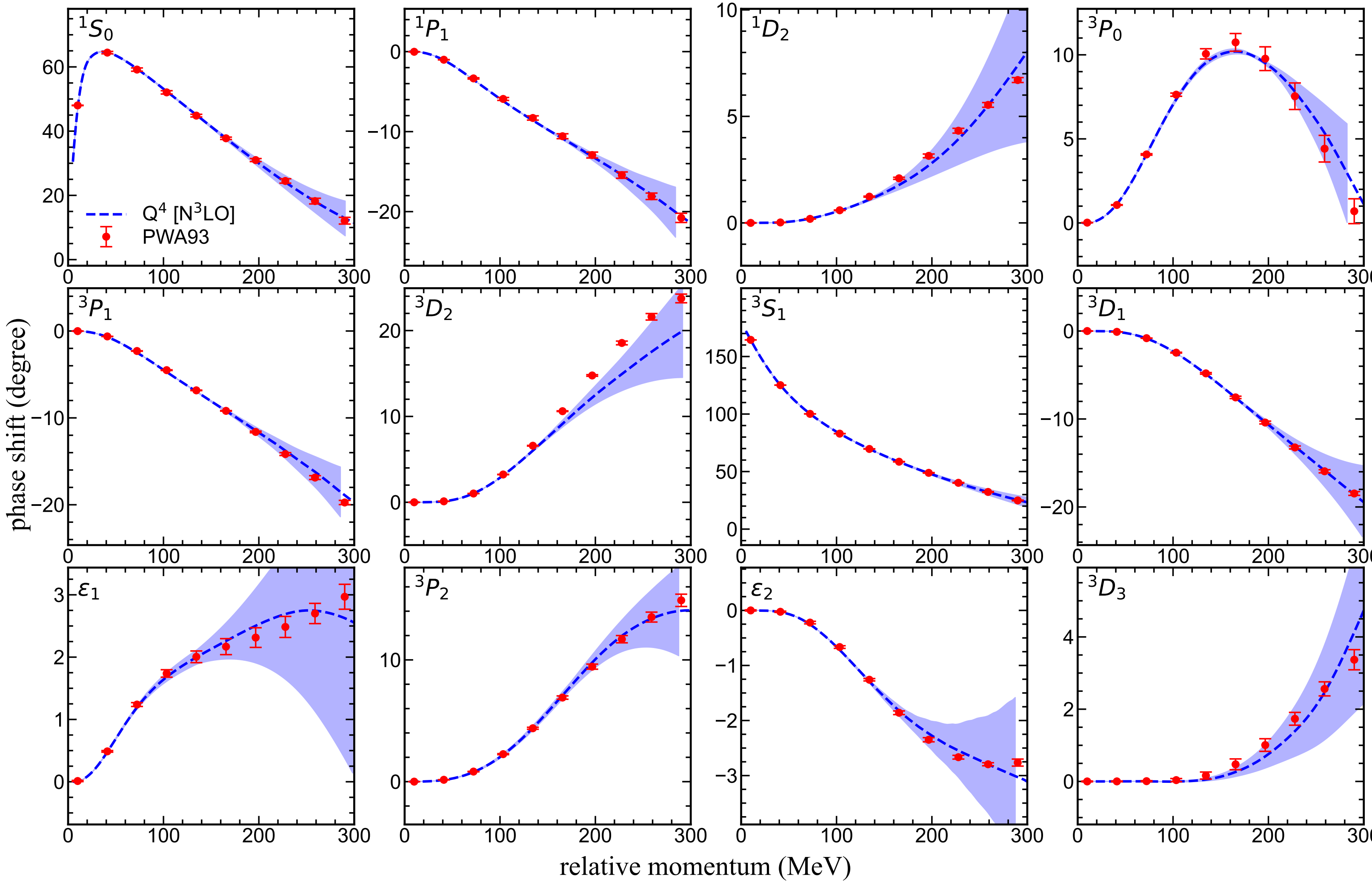


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

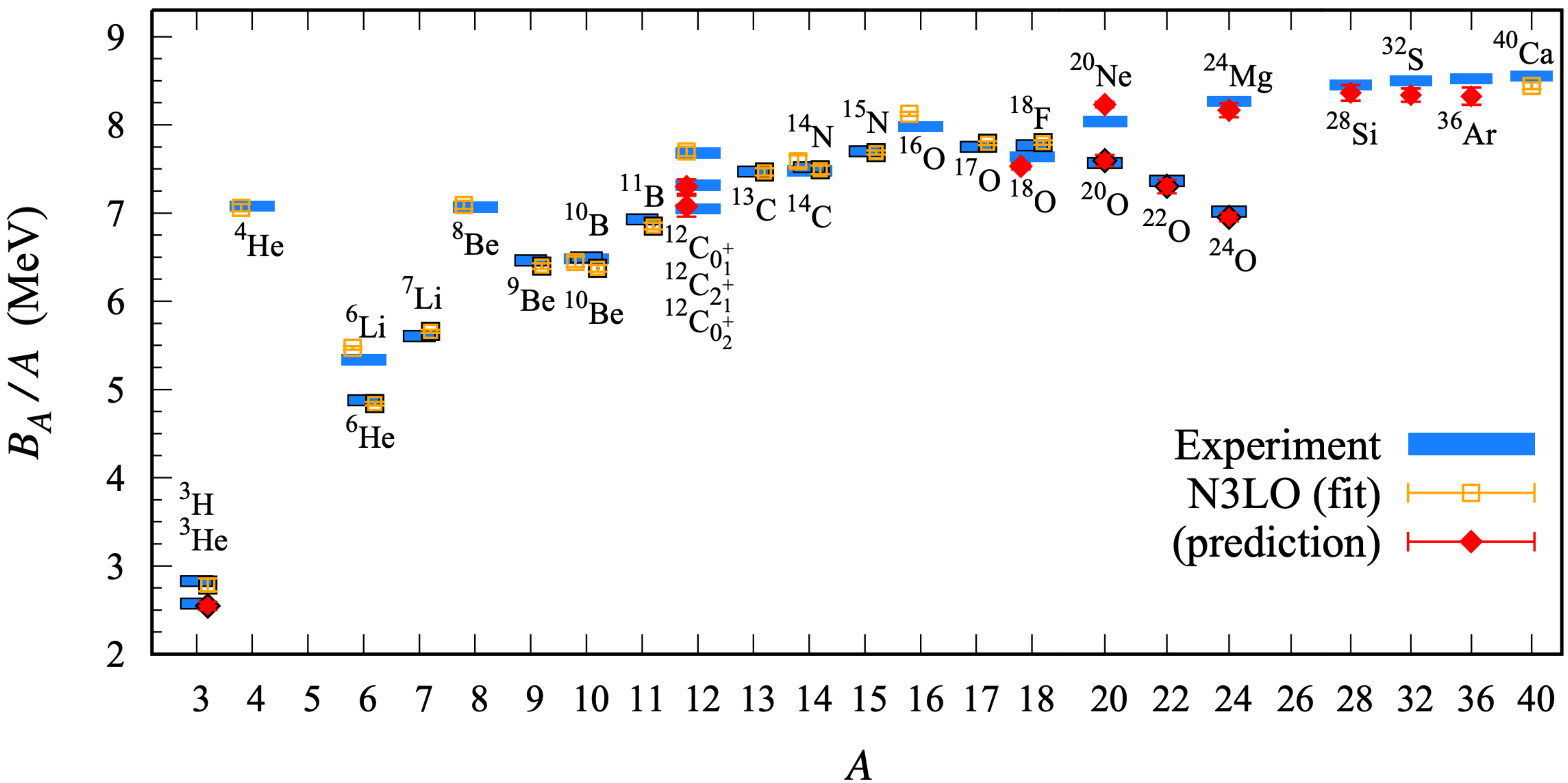
$R = 2.6$ fm

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

N3LO chiral effective field theory interaction

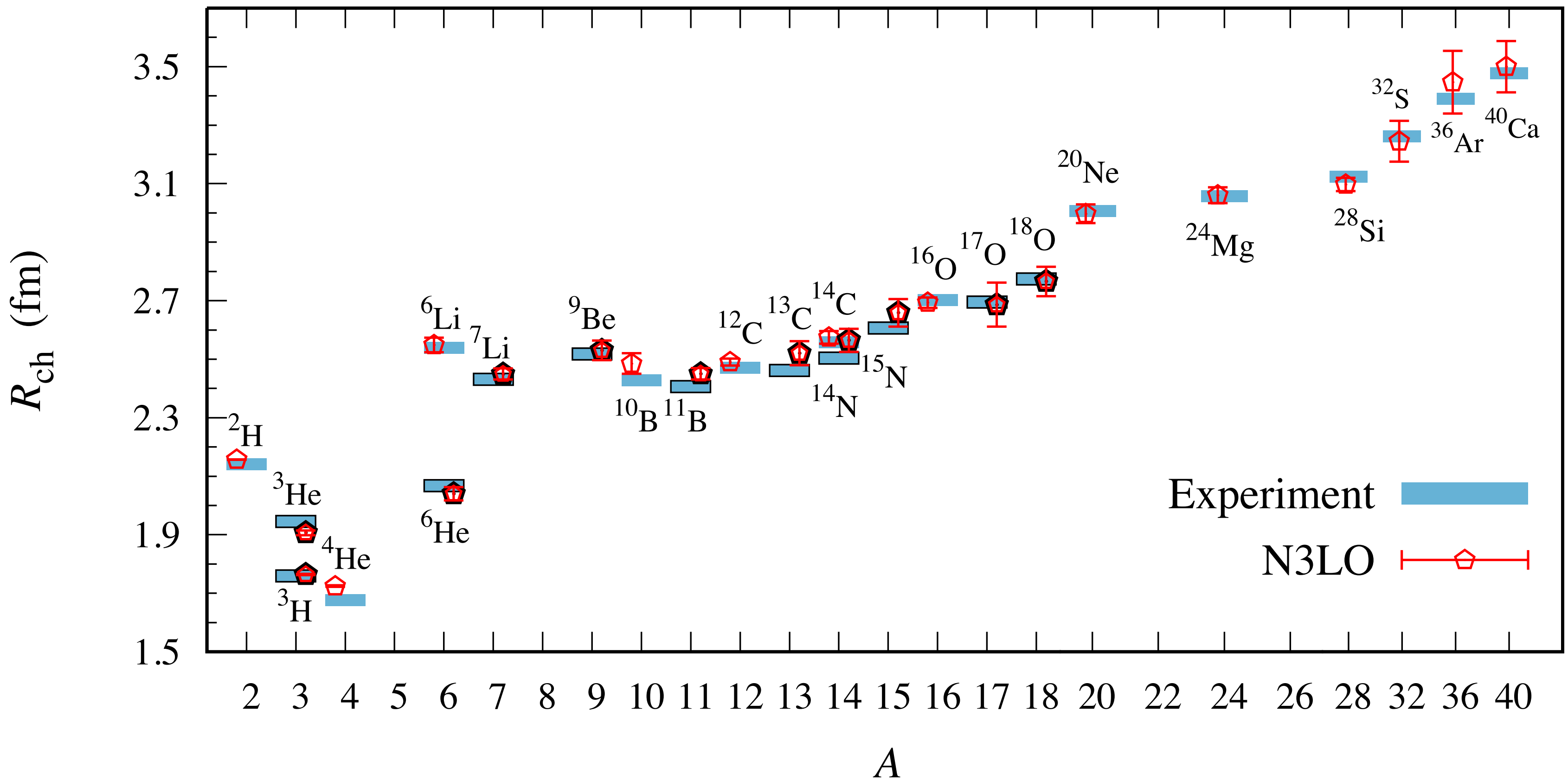


Binding energy per nucleon



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



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Neutron and nuclear matter

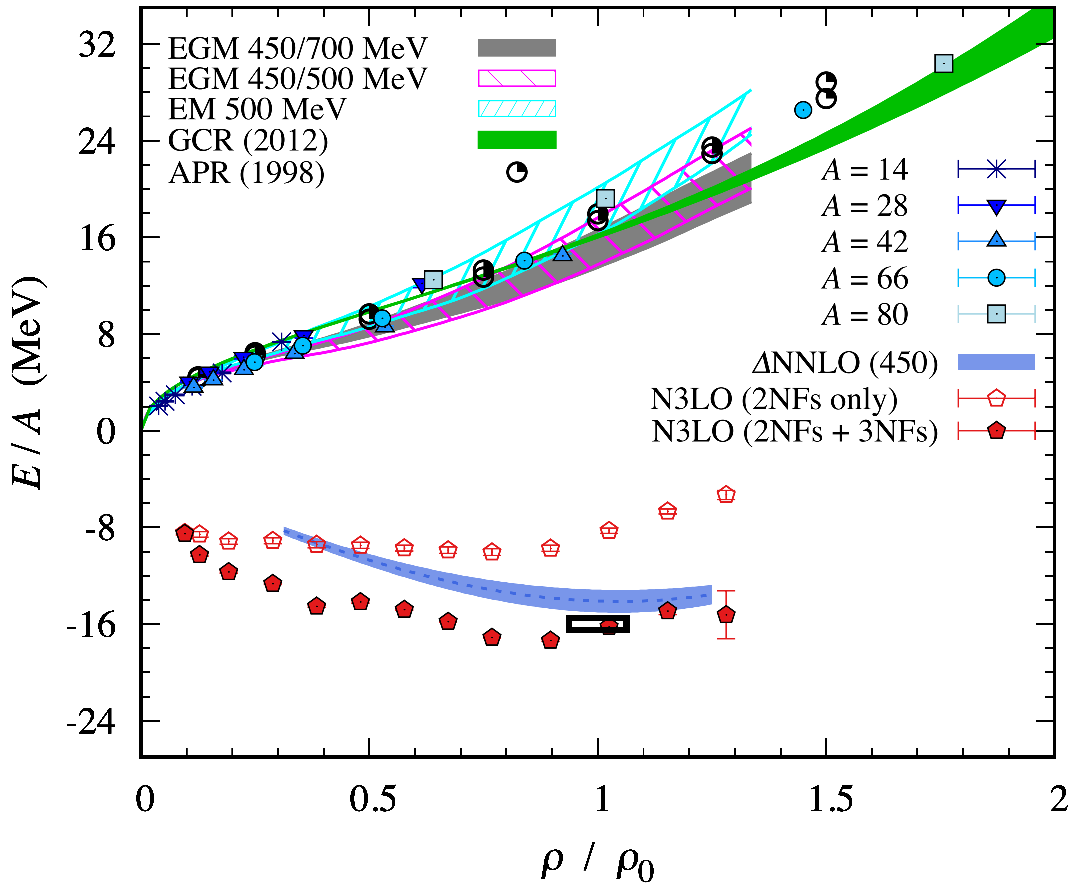

Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

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

Outlook

This was an overview of some current capabilities for *ab initio* nuclear structure calculations and how they can interface with studies of relativistic heavy ion collisions.

Over the next decade, it will likely be possible to do *ab initio* calculations of nuclear states across the entire nuclear chart. What interesting problems can the nuclear structure community and the relativistic heavy-ion community address together in the future?