Nuclear Lattice Simulations

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Nuclei in the Laboratory and in Stars
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FRIB
MICHIGAN STATE UNIVERSITY
NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-5 Project
JÜLICH FORSCHUNGSZENTRUM
OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Outline

Lattice effective field theory

Essential elements of nuclear binding

Pinhole algorithm

Emergent geometry and duality of ^{12}C

Wavefunction matching

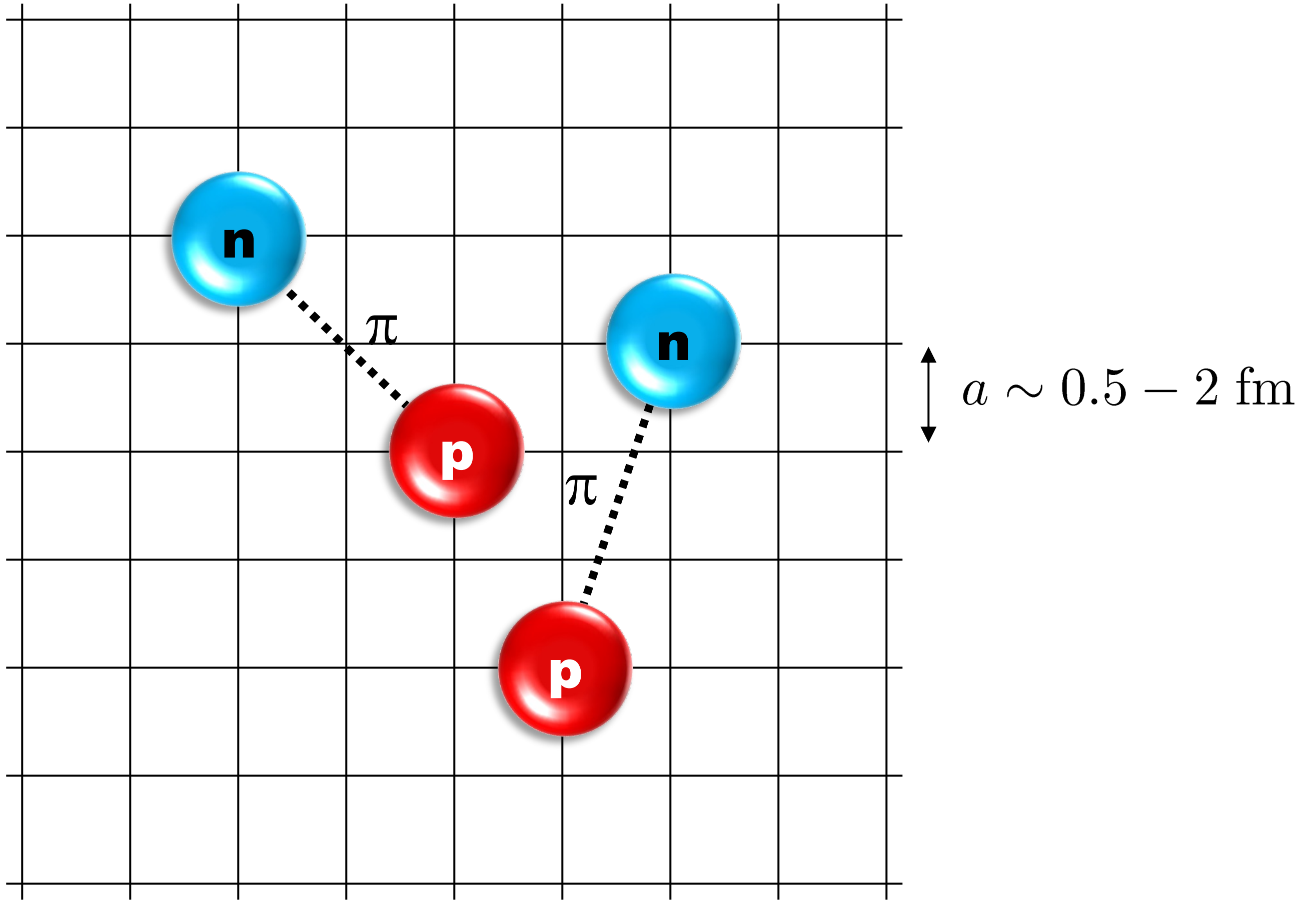
Ab initio nuclear thermodynamics

Structure factors in hot neutron matter

Superfluidity

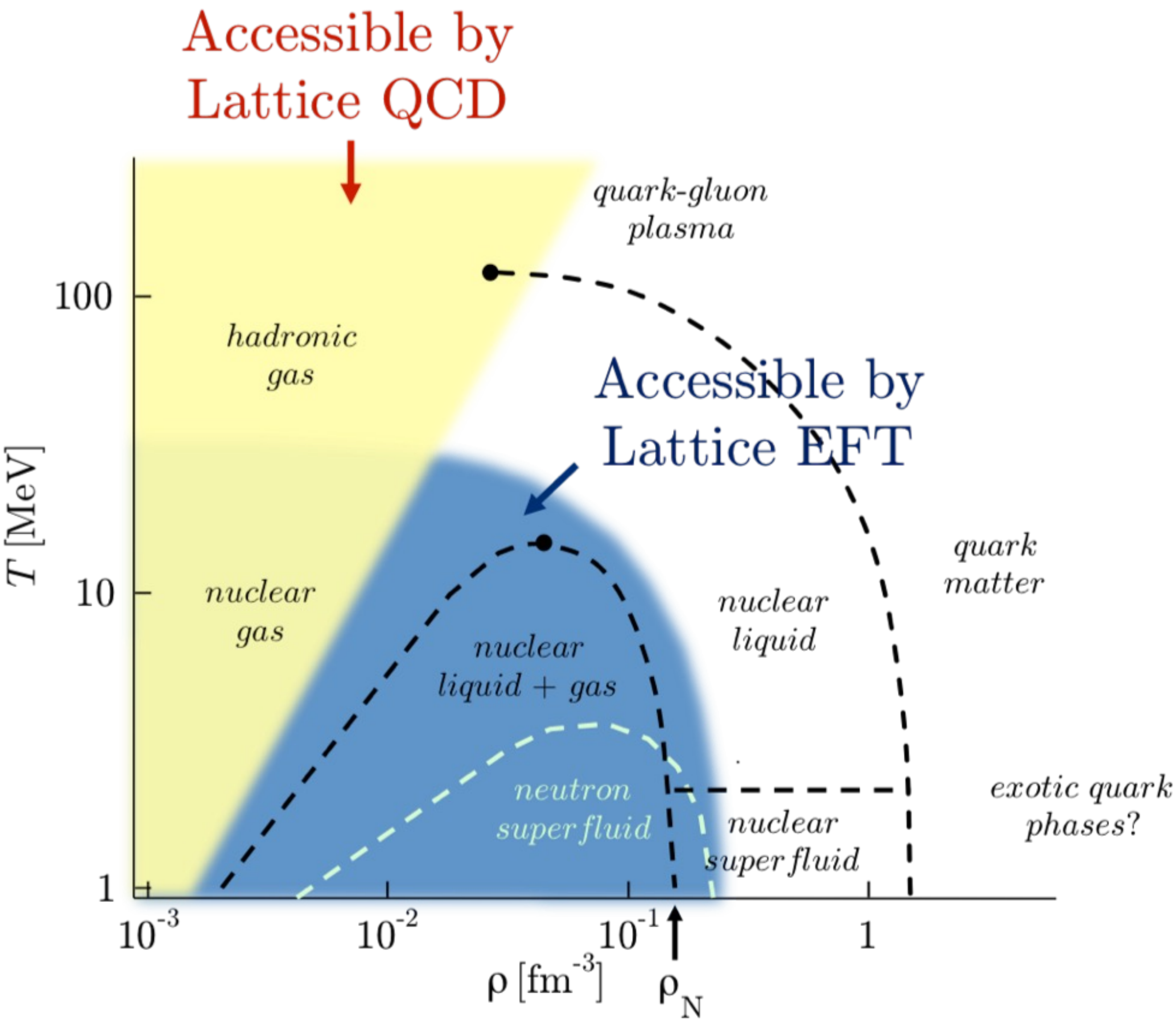
Summary and outlook

Lattice effective field theory



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

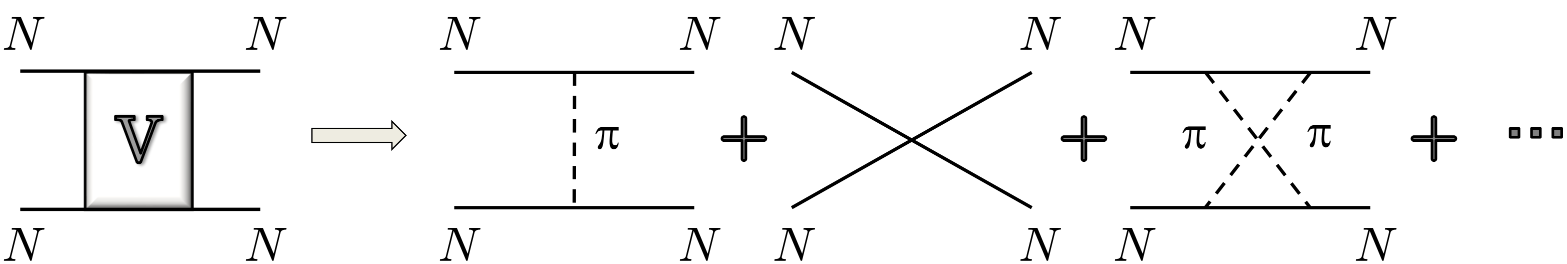
Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer



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

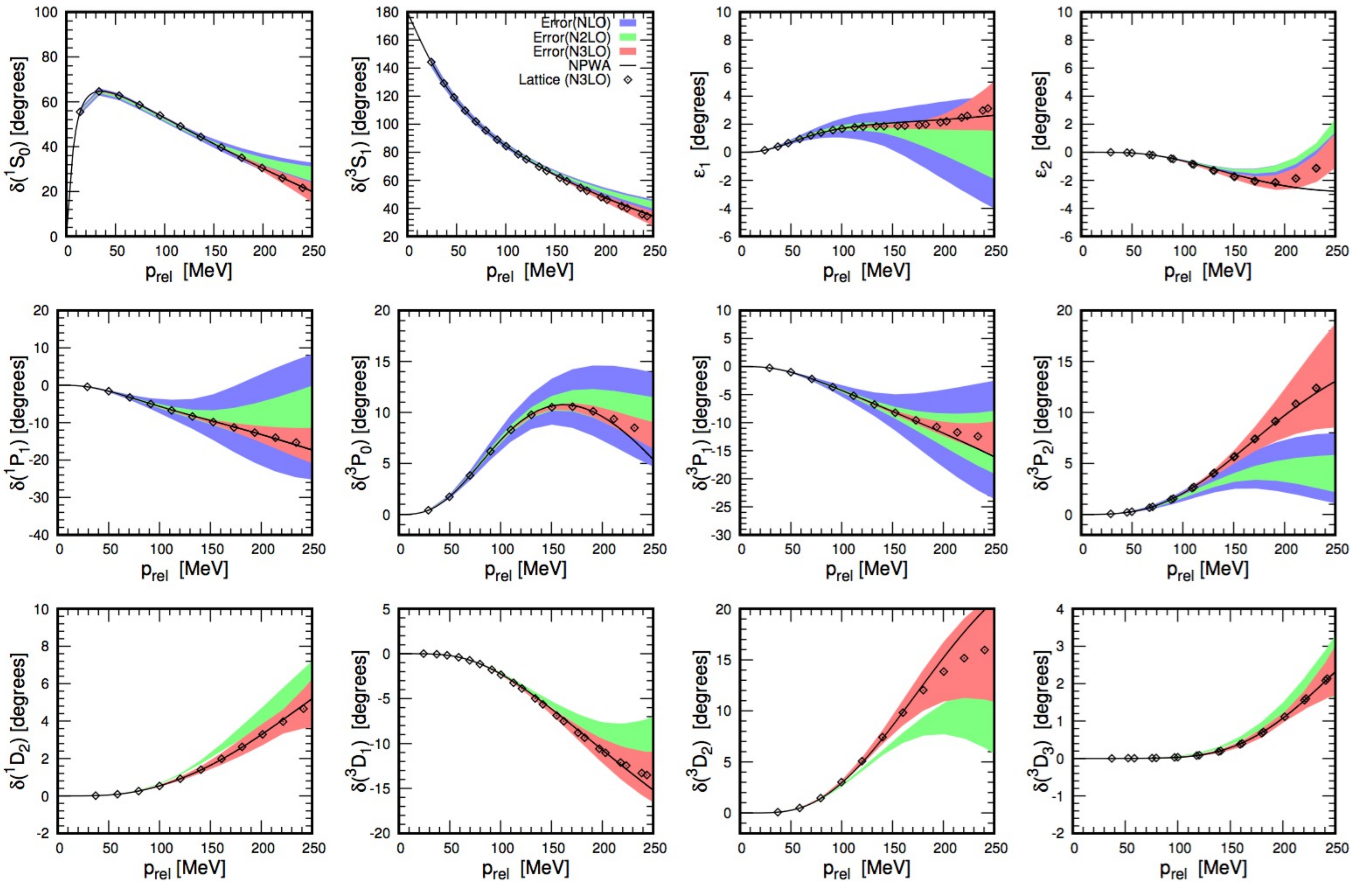
Construct the effective potential order by order



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

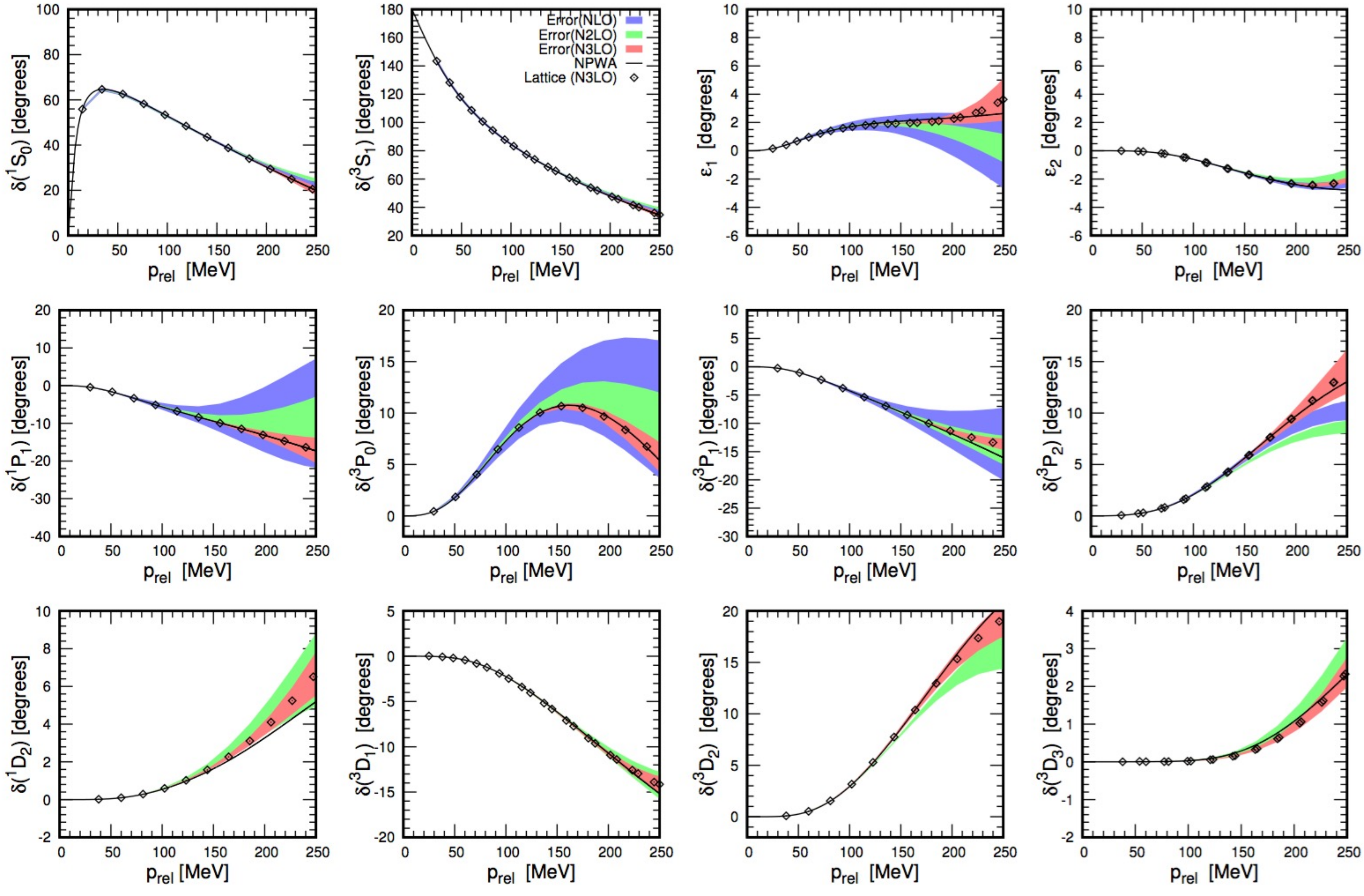
Leading order (LO) Next-to-leading order (NLO)

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

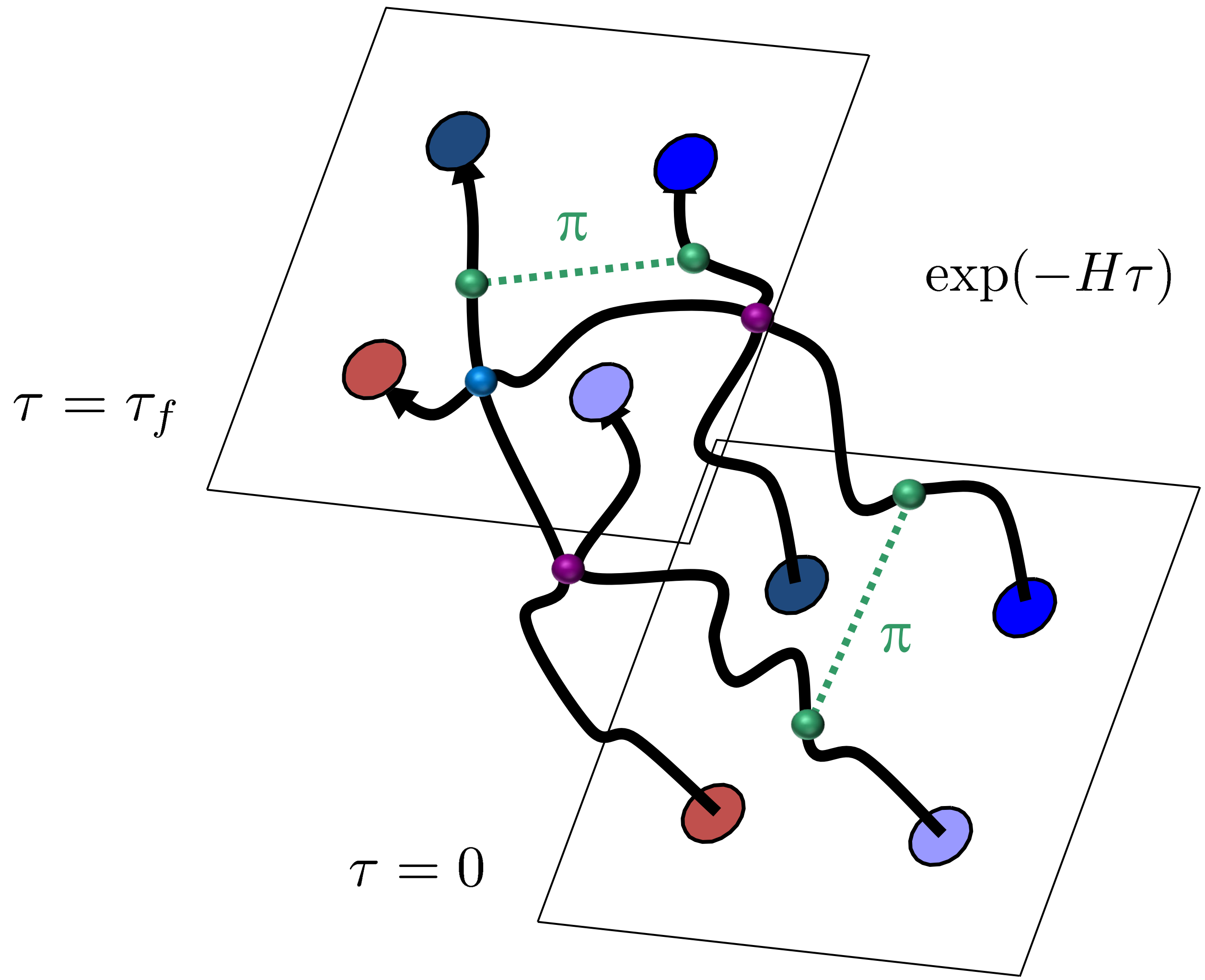


Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

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



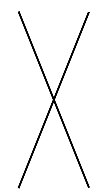
Euclidean time projection



Auxiliary field method

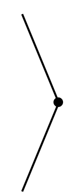
We can write exponentials of the interaction using a Gaussian integral identity

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



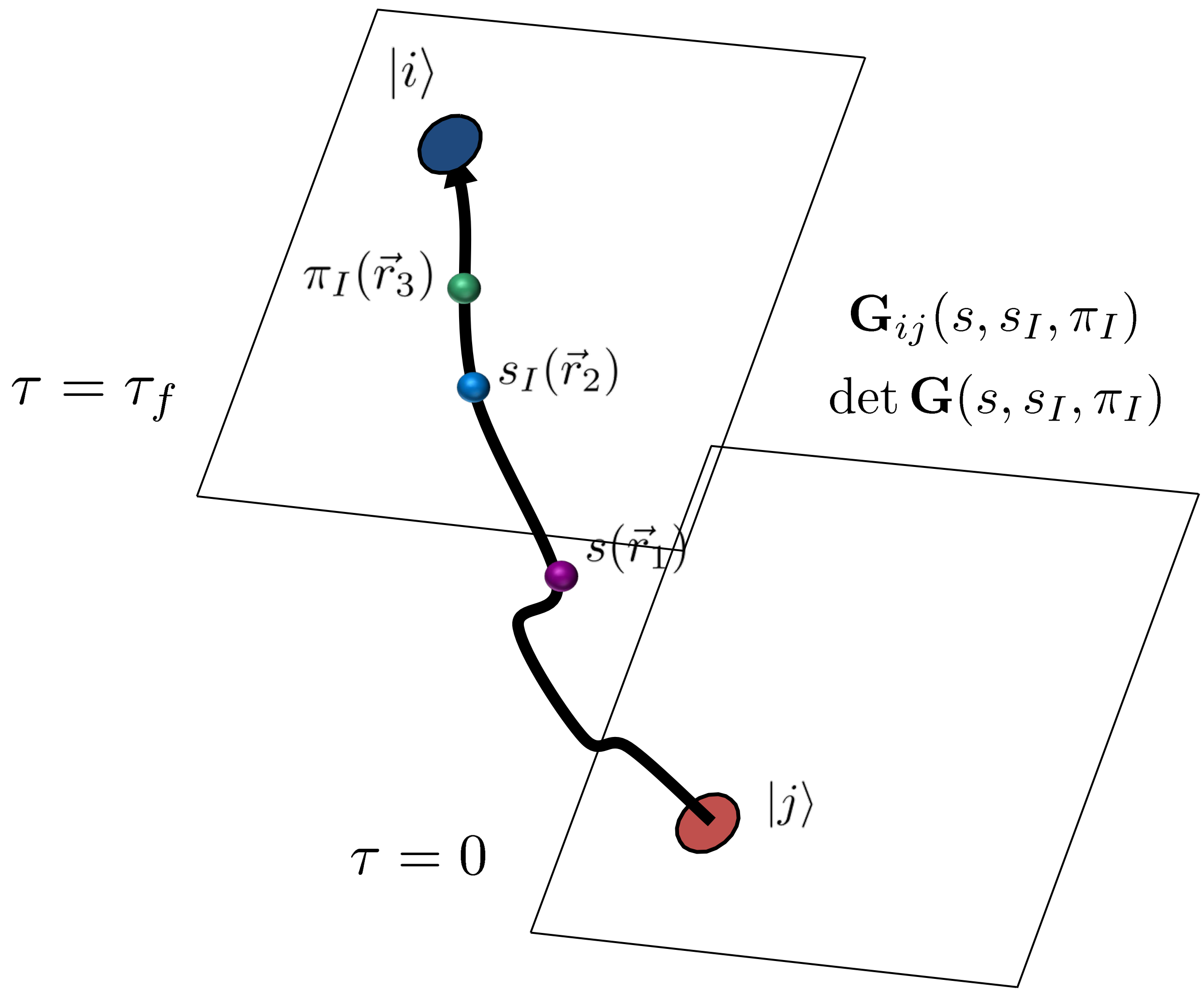
$(N^\dagger N)^2$

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



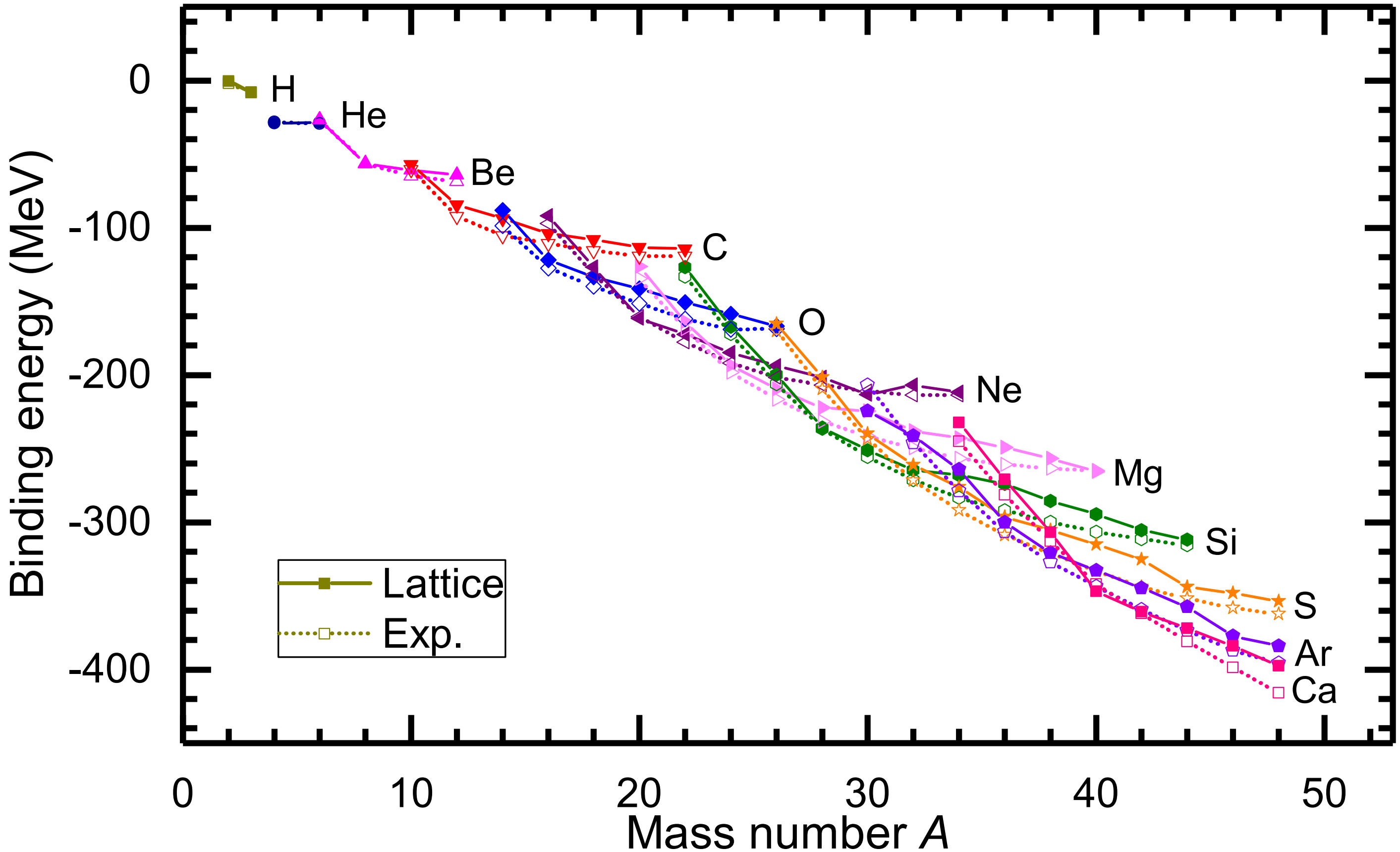
$sN^\dagger N$

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


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

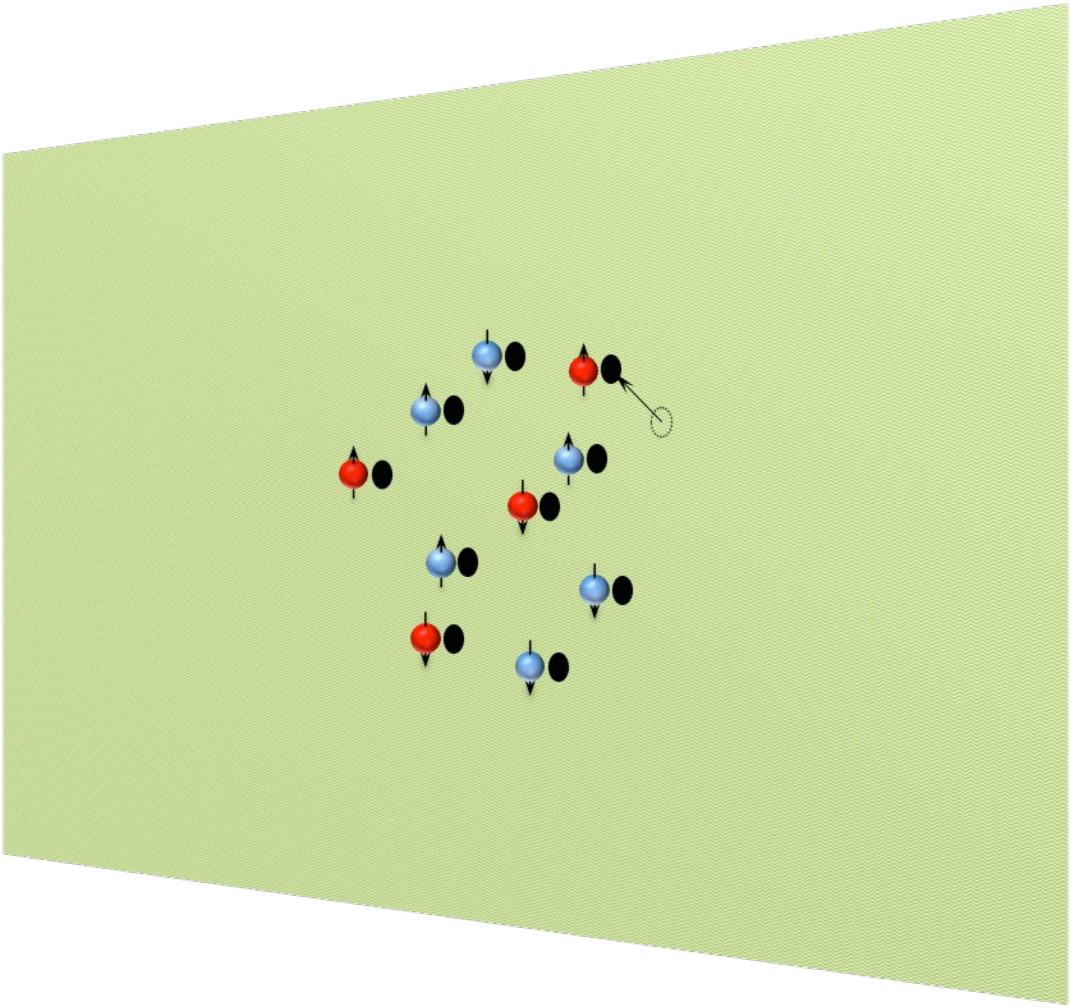
Essential elements for nuclear binding

$$H = H_{\text{free}} + \frac{1}{2!}C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{1}{3!}C_3 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3 + V_{\text{Coulomb}}$$

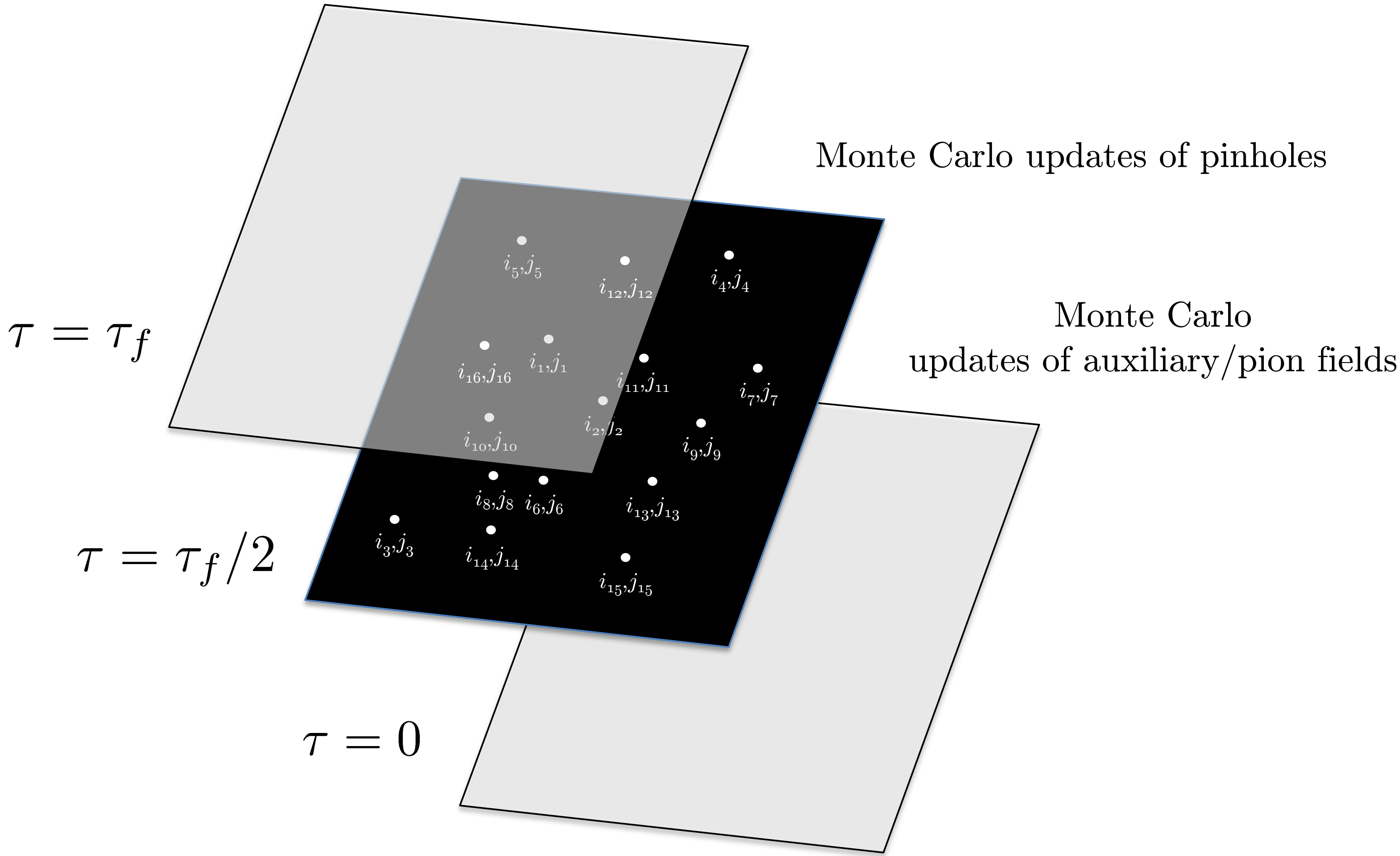


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

Pinhole algorithm

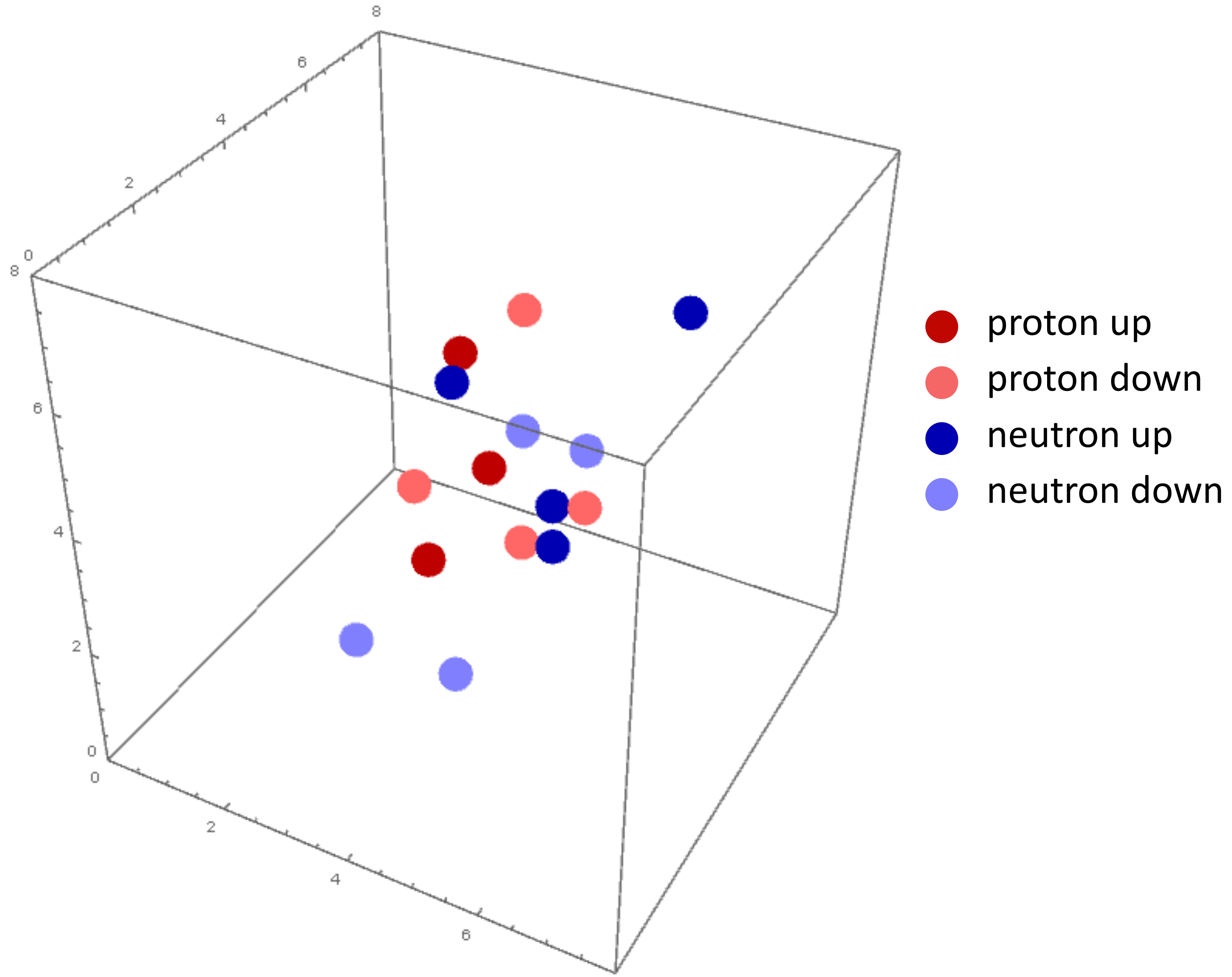


Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



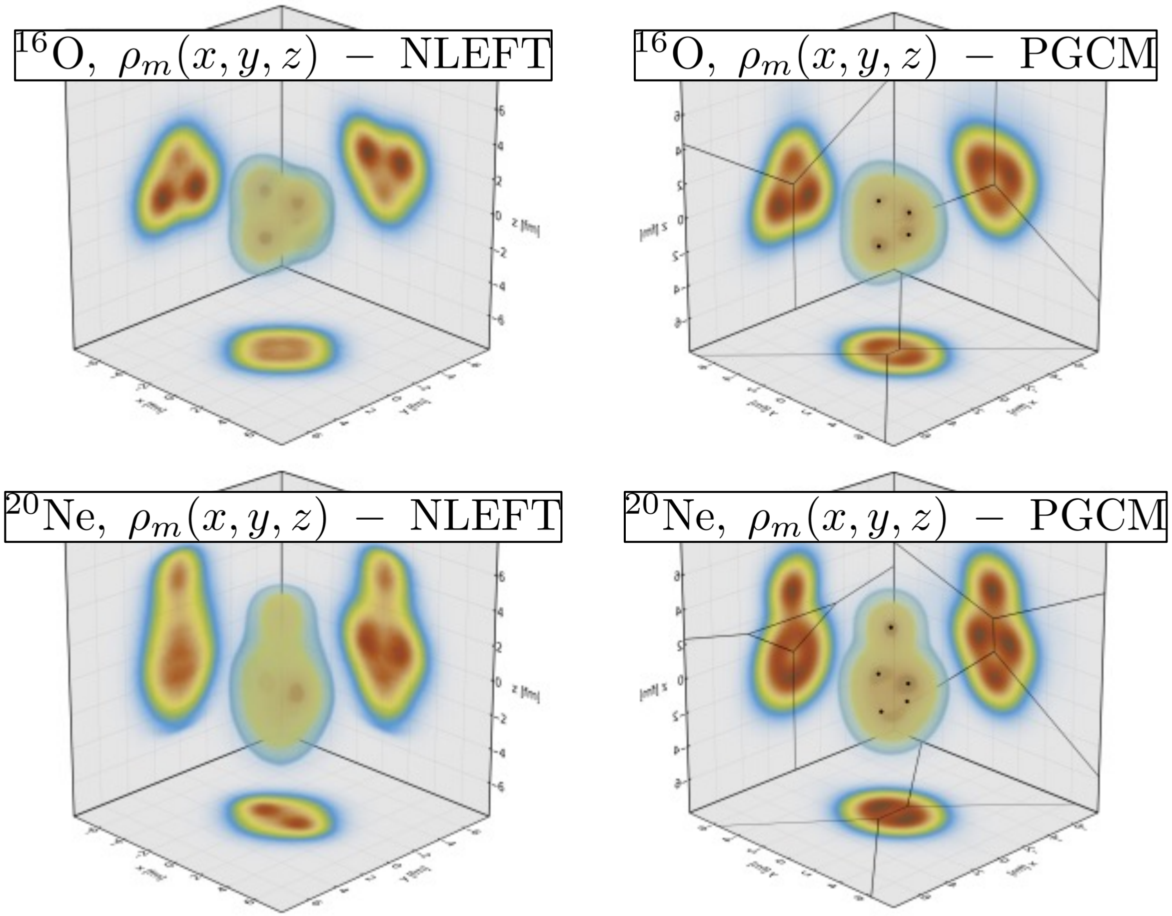
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

^{16}O



Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins, Phys. Rev. C 104 L041901 (2021)

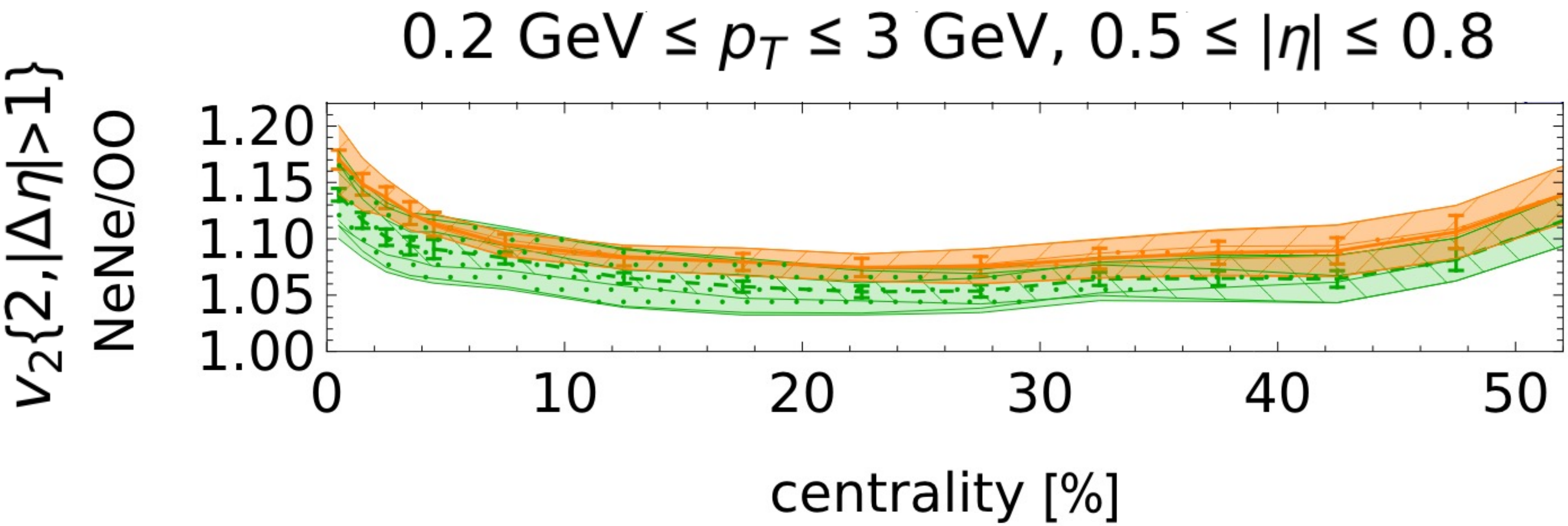
Relativistic heavy collisions: $^{16}O^{16}O$ versus $^{20}Ne^{20}Ne$



Giacalone et al., arXiv:2402.05995

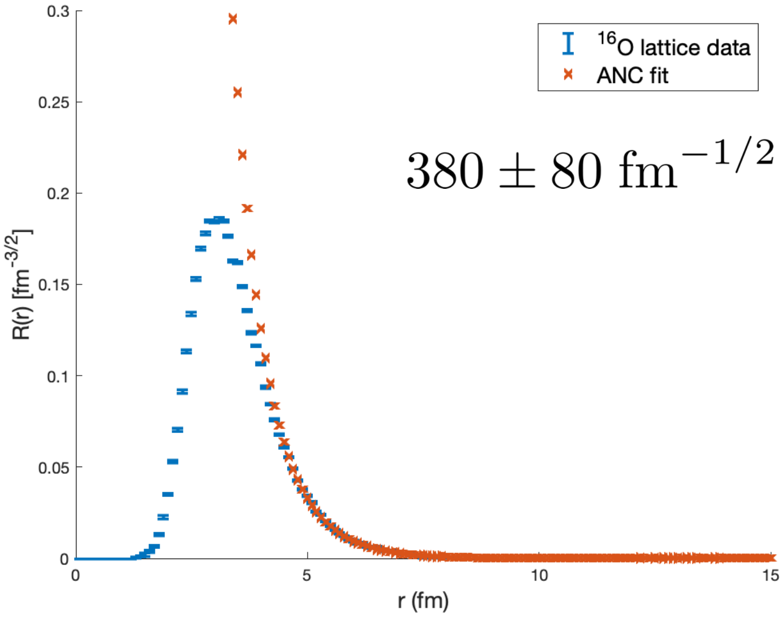
For the 1% most central events, the elliptic flow of ^{20}Ne^{20}Ne collisions relative to ^{16}O^{16}O collisions is enhanced by as much as

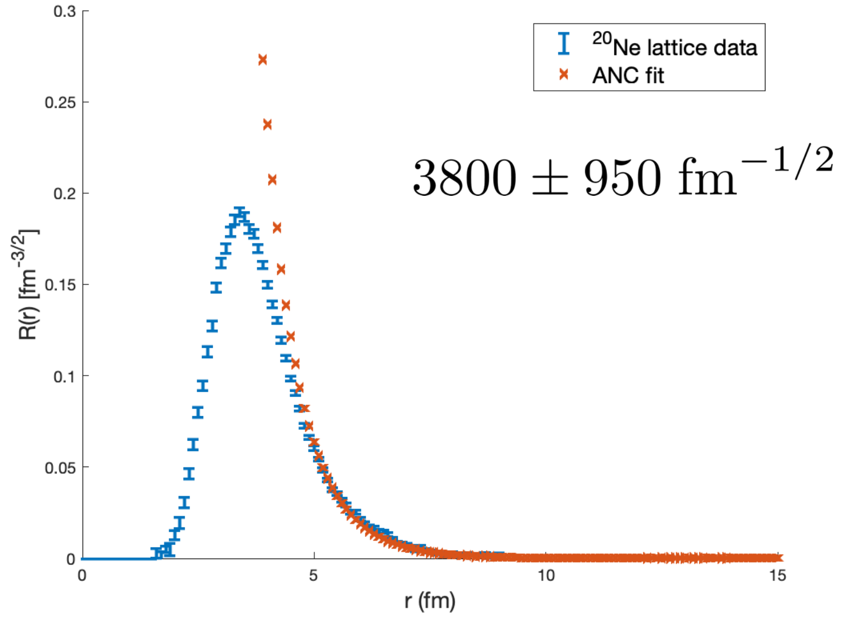
1.170(8)stat.(30)syst. for NLEFT
1.139(6)stat.(39)syst. for PGCM



Giacalone et al., arXiv:2402.05995

Asymptotic normalization coefficients

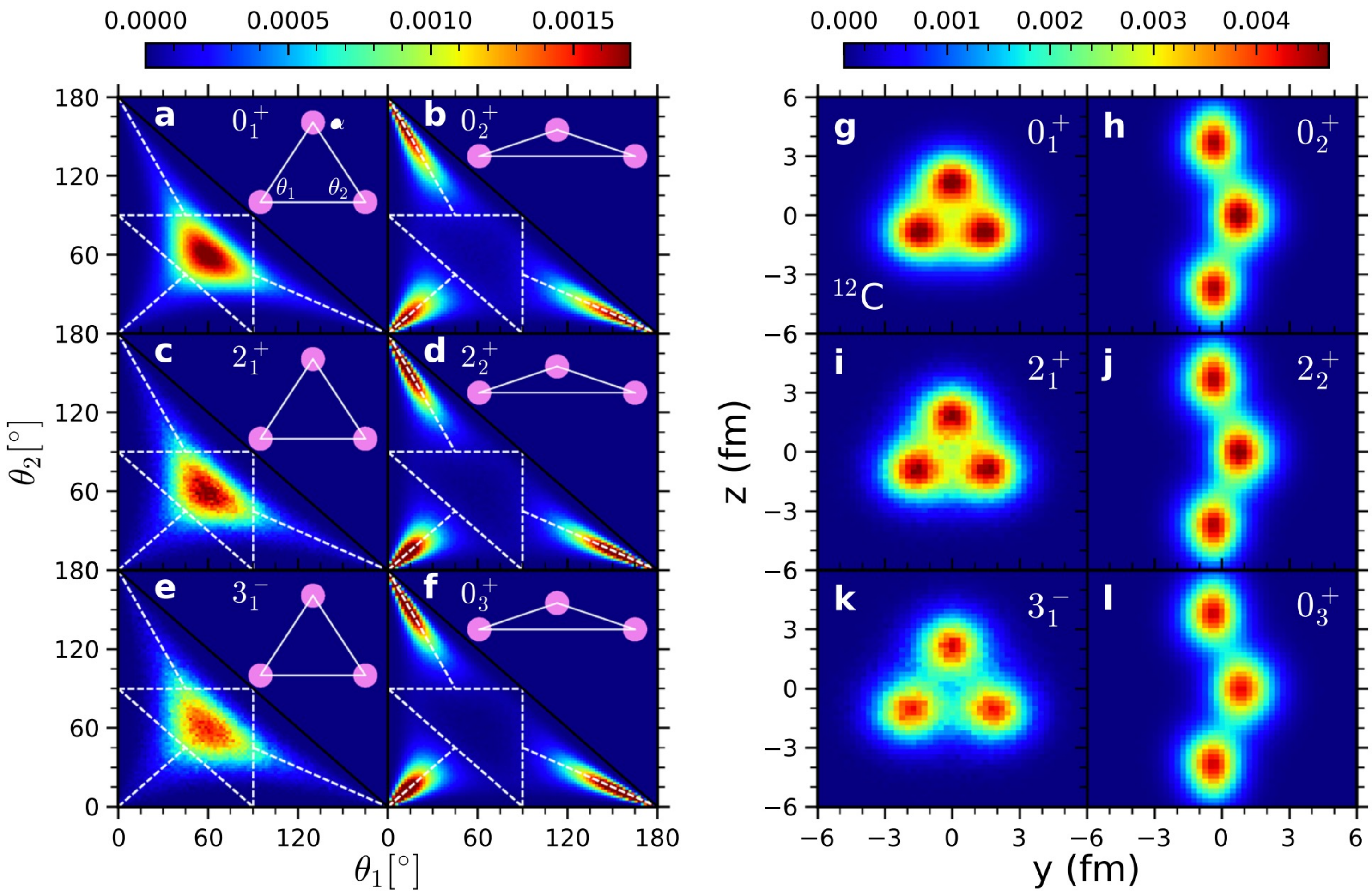




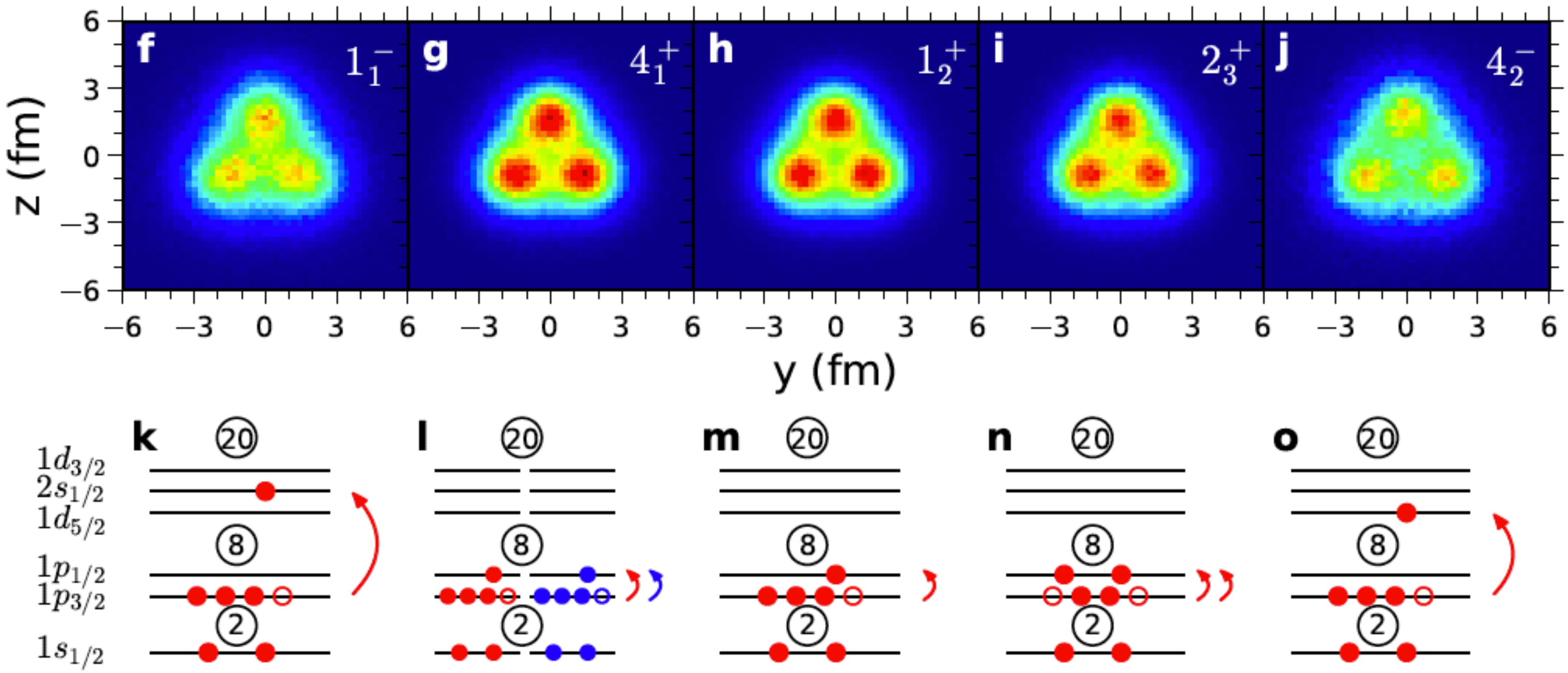
$$^{12}\mathrm{C}\left(^{20}\mathrm{Ne},^{16}\mathrm{O}\right)^{16}\mathrm{O}$$

E. Harris et al., work in progress

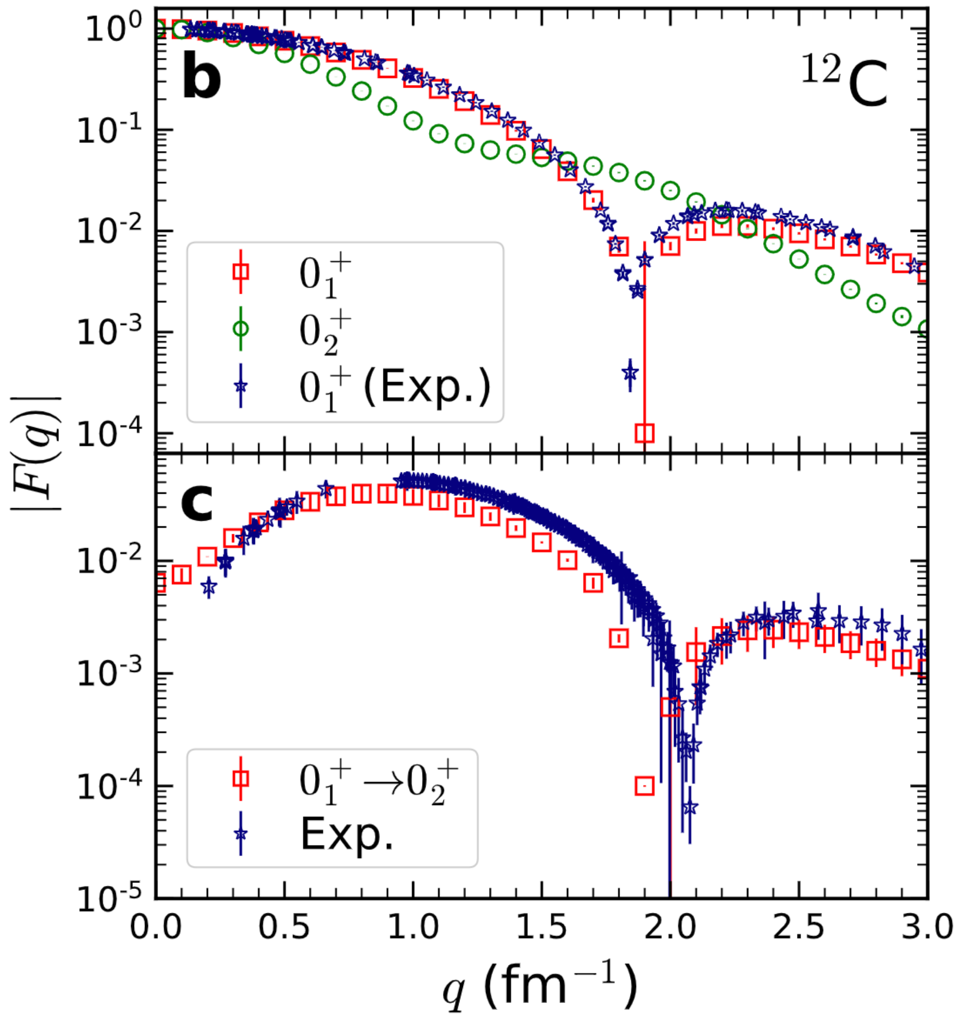
Emergent geometry and duality of ^{12}C



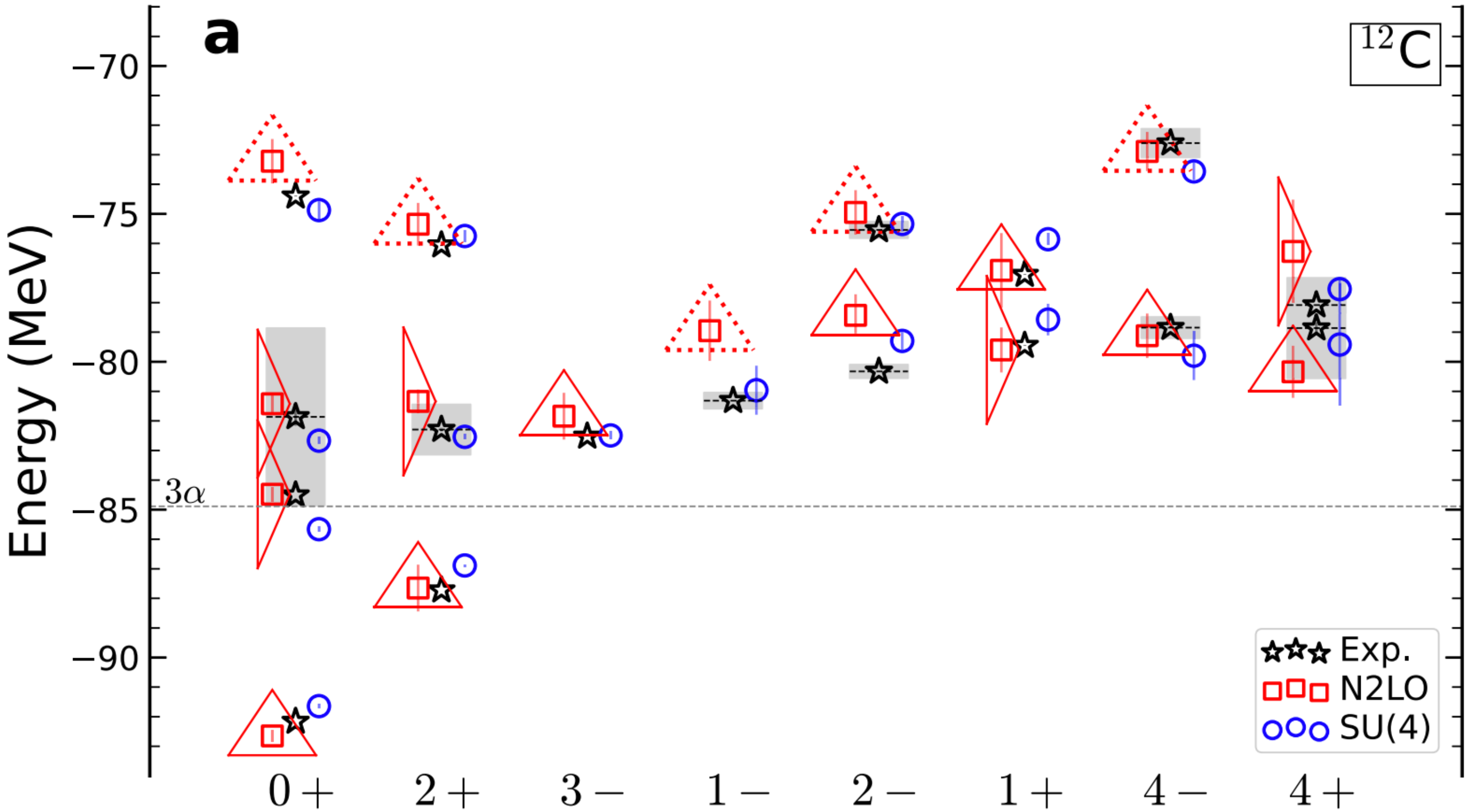
Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



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
$1d_{3/2}$
$2s_{1/2}$
$1d_{5/2}$
$1p_{1/2}$
$1p_{3/2}$
$1s_{1/2}$

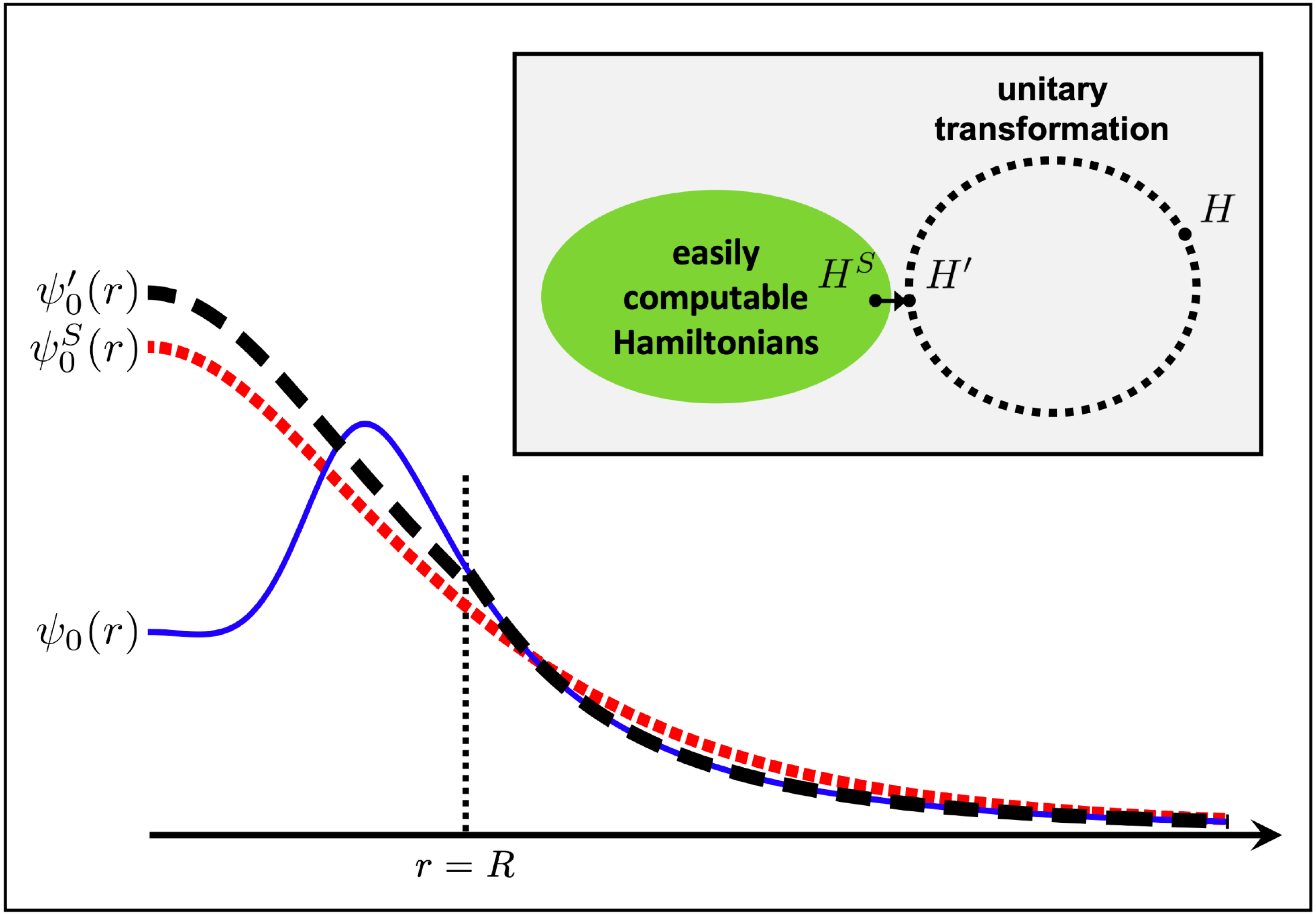


Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



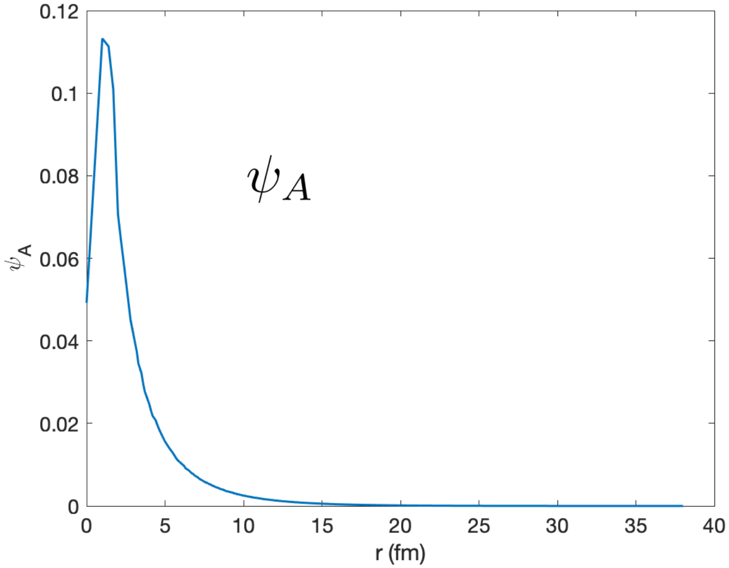
Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)

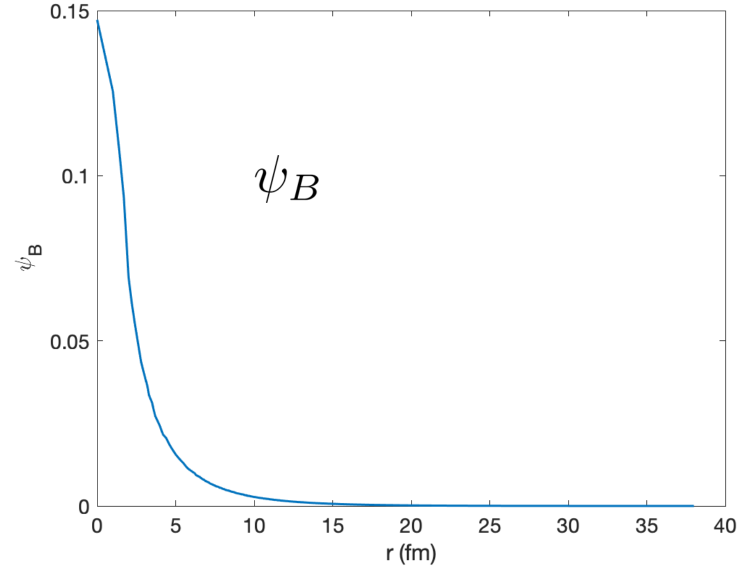
Wavefunction matching

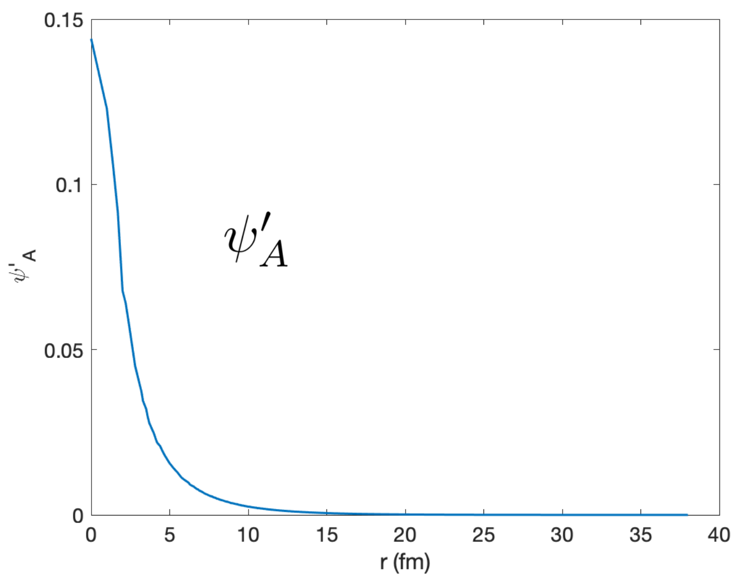


Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Ground state wavefunctions







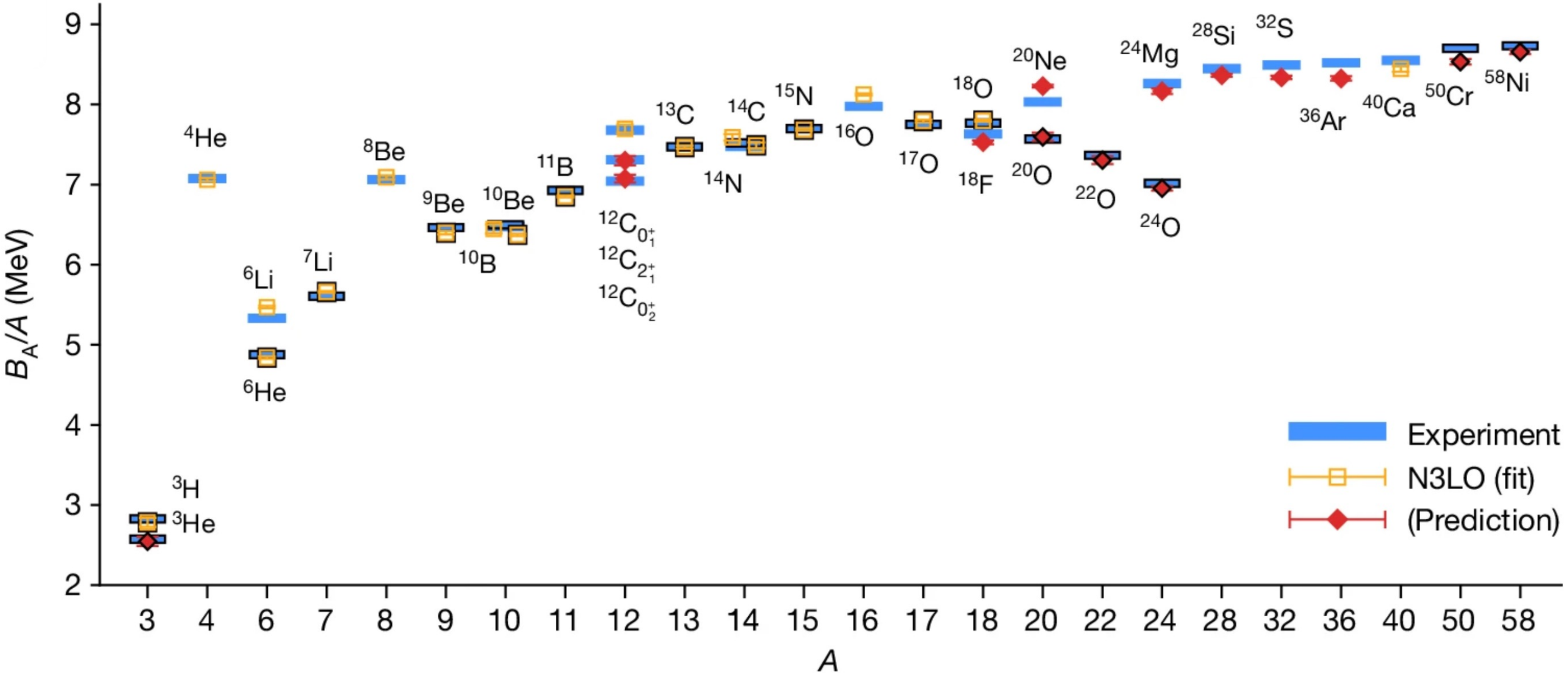
Try to compute the energies of H_A using the eigenfunctions of H_B and first-order perturbation theory. This doesn't work.

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

Use wavefunction matching first to transform the Hamiltonian. Then the convergence of perturbation theory is much faster.

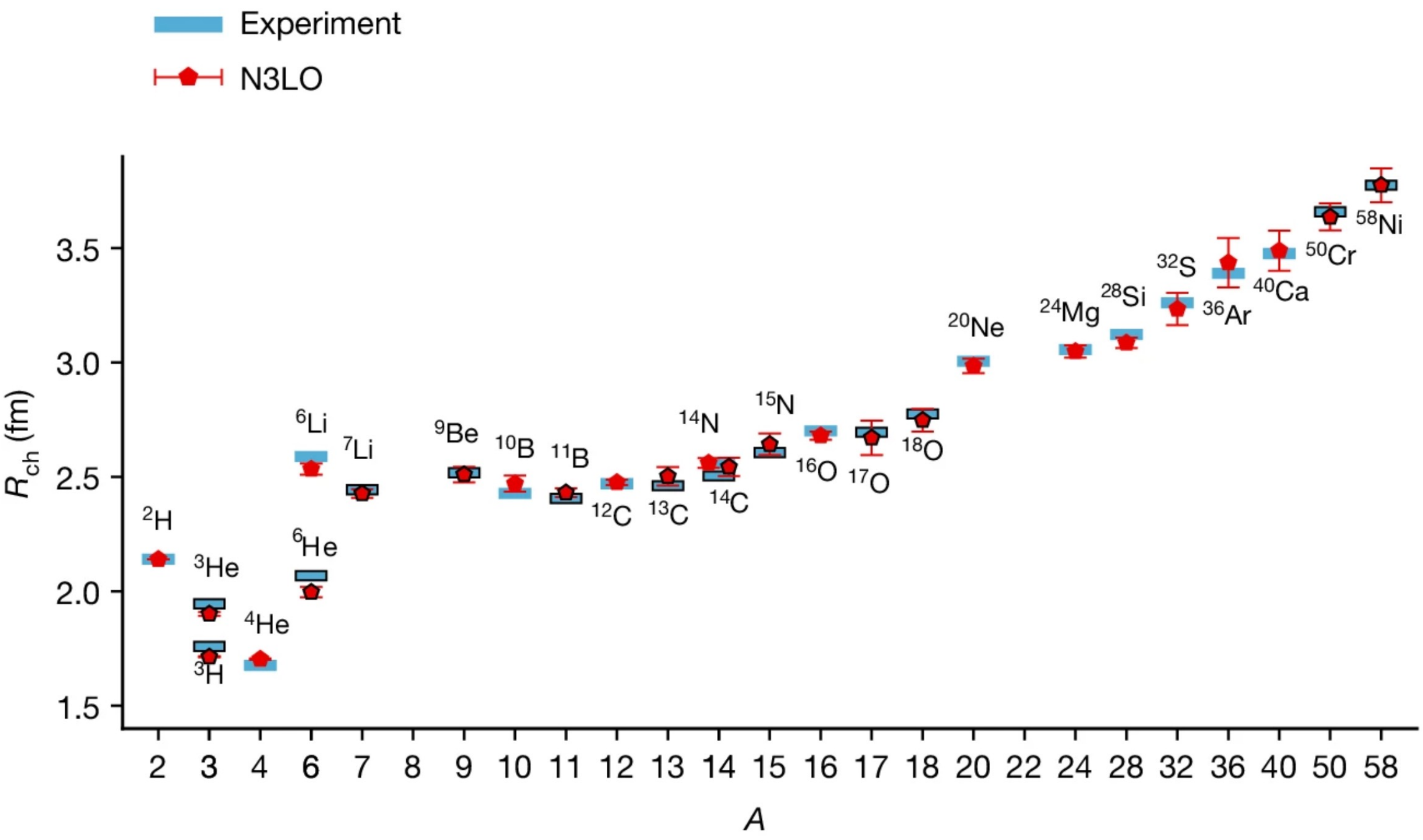
$E_{A,n} = E'_{A,n}$ (MeV)	$\langle \psi_{B,n} \| H_A \| \psi_{B,n} \rangle$ (MeV)	$\langle \psi_{B,n} \| H'_A \| \psi_{B,n} \rangle$ (MeV)
-1.2186	3.0088	-1.1597
0.2196	0.3289	0.2212
0.8523	1.1275	0.8577
1.8610	2.2528	1.8719
3.2279	3.6991	3.2477
4.9454	5.4786	4.9798
7.0104	7.5996	7.0680
9.4208	10.0674	9.5137
12.1721	12.8799	12.3163
15.2669	16.0458	15.4840

Binding energies



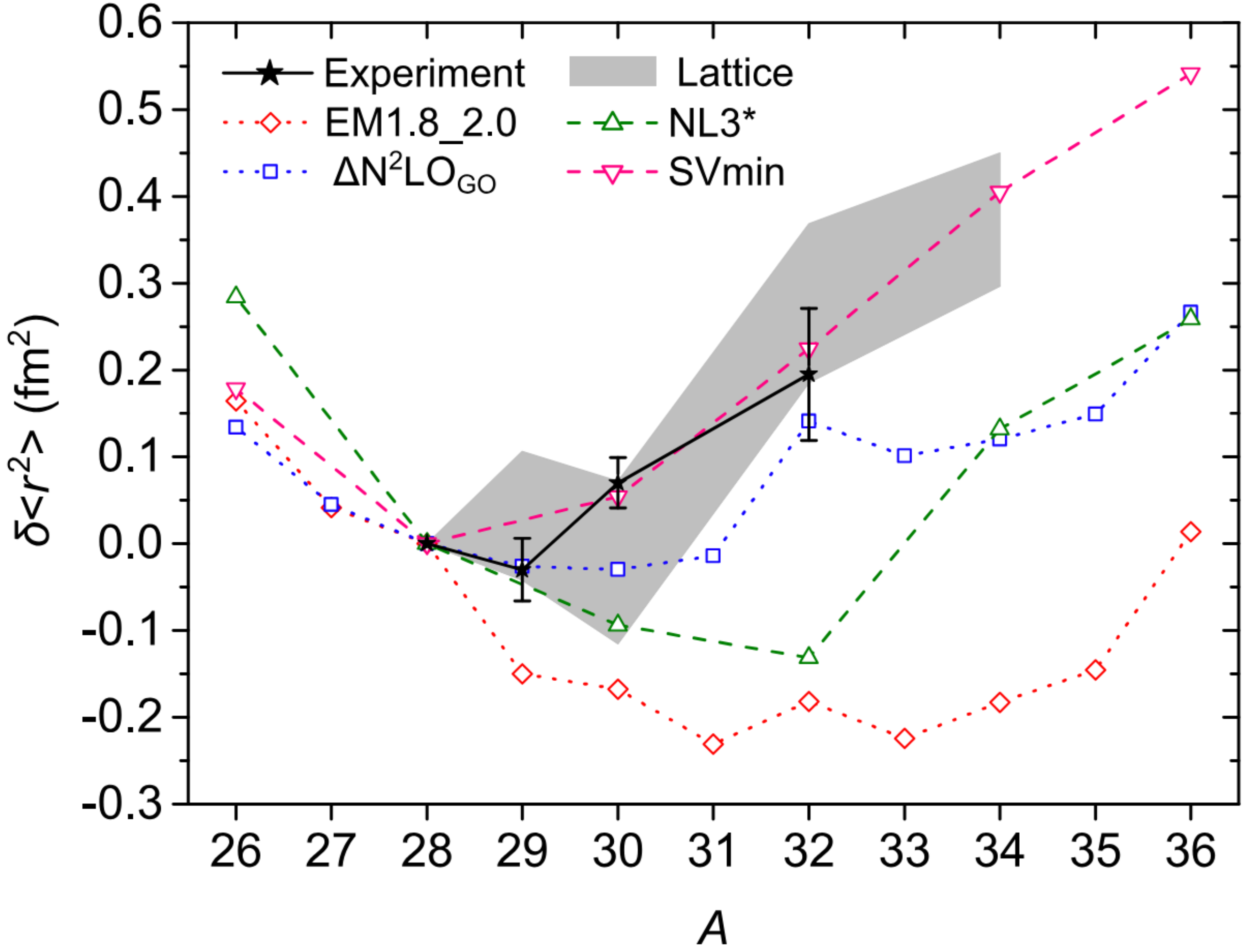
Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Charge radii



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Charge radii of silicon isotopes



K. König et al., PRL 132, 162502 (2024)

Neutron and nuclear matter

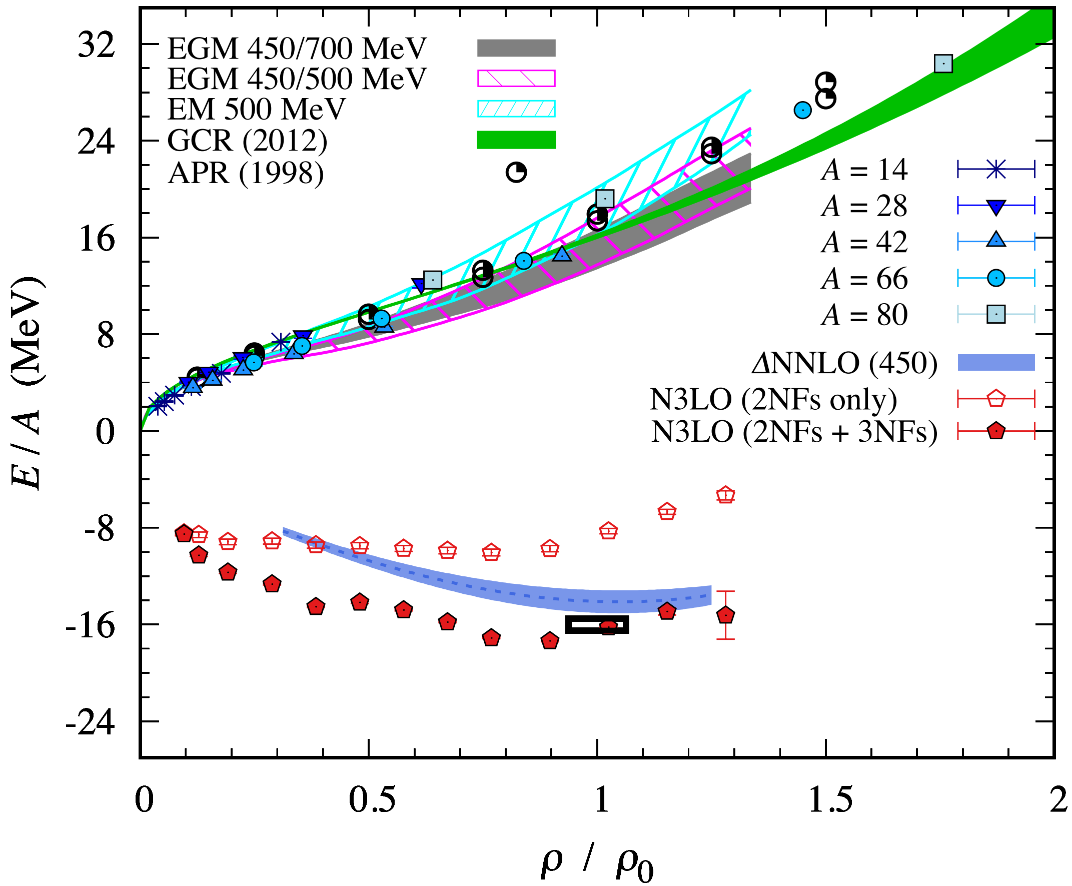
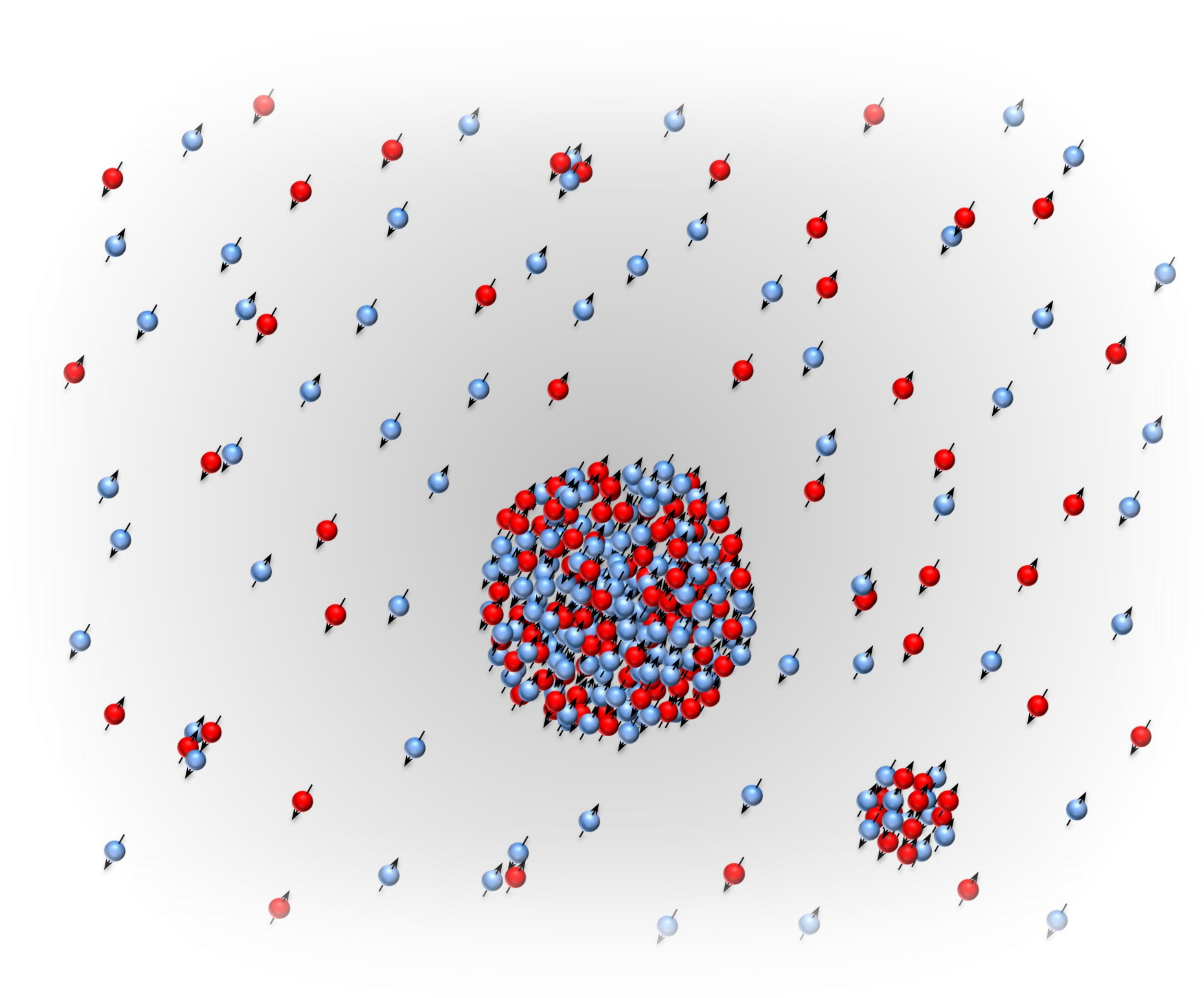


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

<u>*Ab initio* nuclear thermodynamics</u>



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

<u>*Ab initio* nuclear thermodynamics</u>

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

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

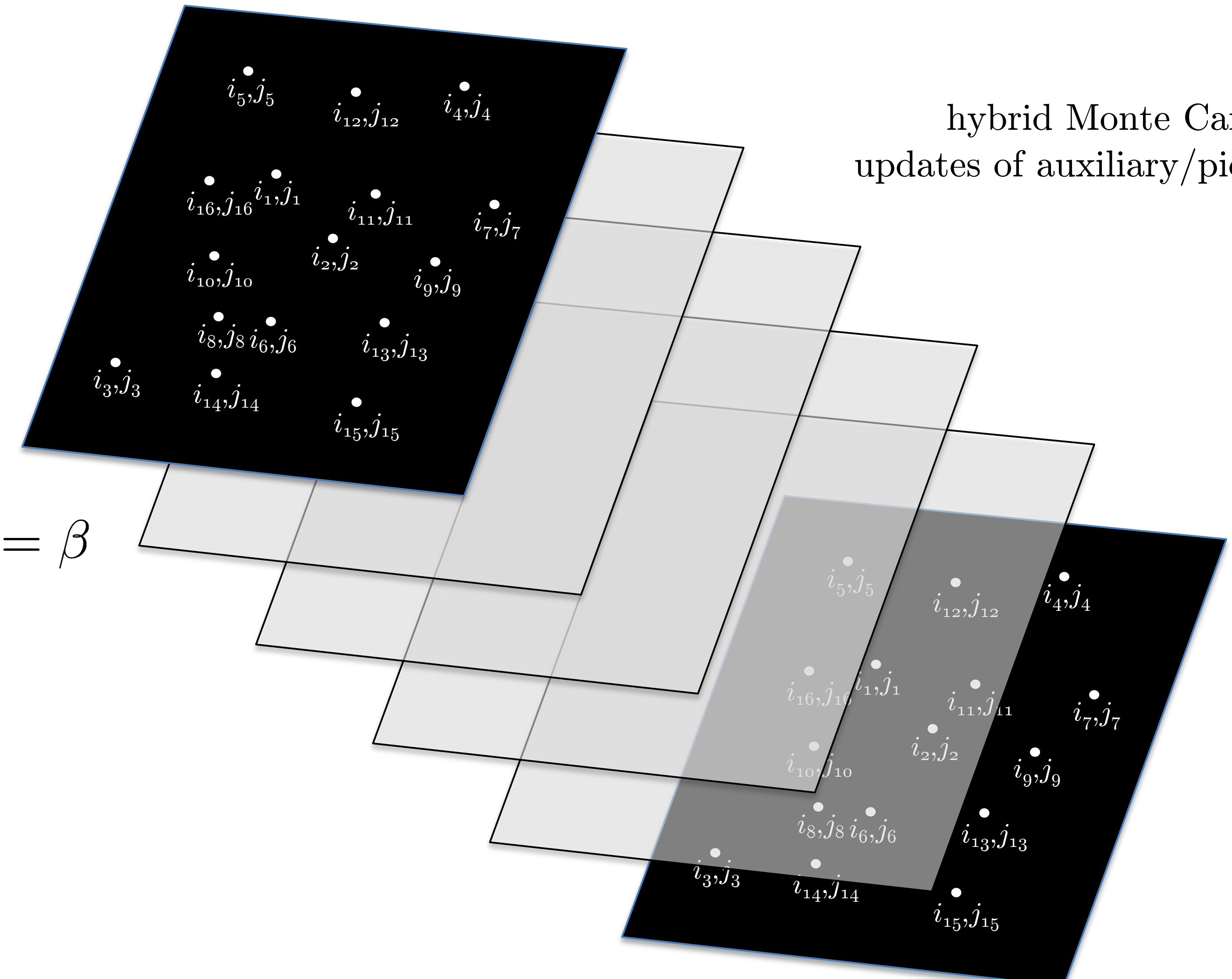
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

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

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



$\tau = \beta$

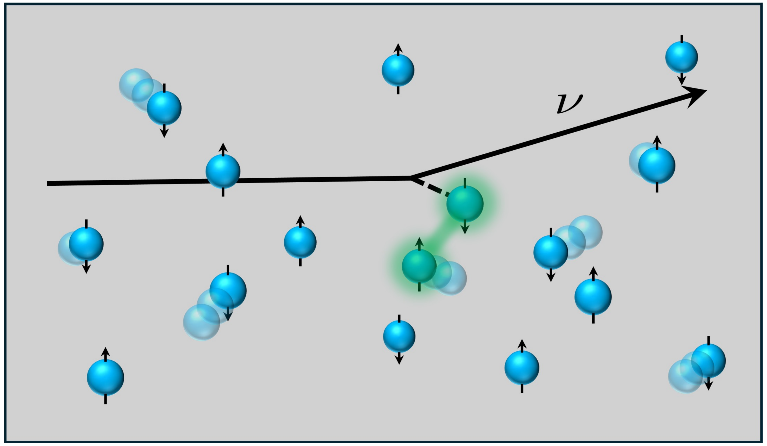
$\tau = 0$

Structure factors for hot neutron matter

$$S_{\rm v}(\boldsymbol{q}) = \frac{1}{L^3}\sum_{\boldsymbol{n}\boldsymbol{n}'} {\rm e}^{-i\boldsymbol{q}\cdot\boldsymbol{n}}\left[\langle\hat{\rho}(\boldsymbol{n}+\boldsymbol{n}')\hat{\rho}(\boldsymbol{n}')\rangle - (\rho^0)^2\right]$$

$$S_{\rm a}(\boldsymbol{q}) = \frac{1}{L^3}\sum_{\boldsymbol{n}\boldsymbol{n}'} {\rm e}^{-i\boldsymbol{q}\cdot\boldsymbol{n}}\left[\langle\hat{\rho}_z(\boldsymbol{n}+\boldsymbol{n}')\hat{\rho}_z(\boldsymbol{n}')\rangle - (\rho_z^0)^2\right]$$

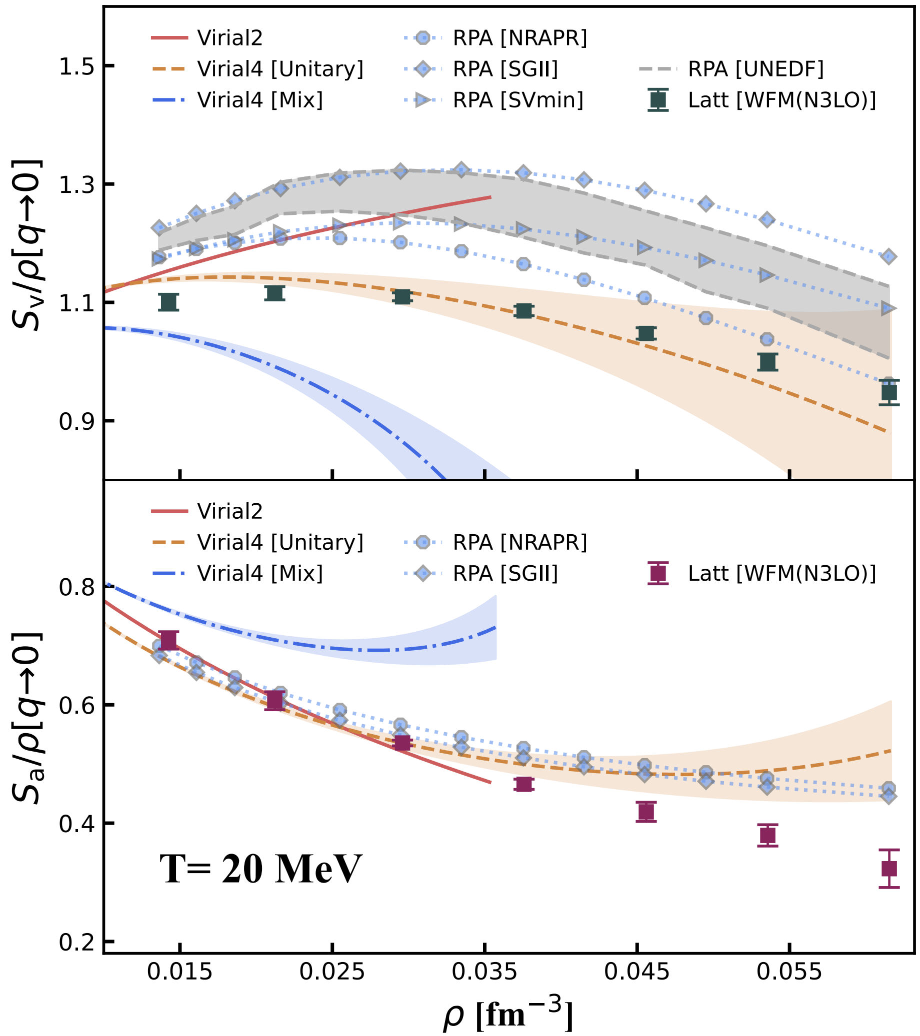
ESA/Hubble/L Calcada



Ma, Lin, Lu, Elhatisari, D.L., Meißner, Steiner, Wang, PRL **132**, 232502 (2024)

See also Alexandru, Bedaque, Berkowitz, Warrington, PRL **126**, 132701 (2021)

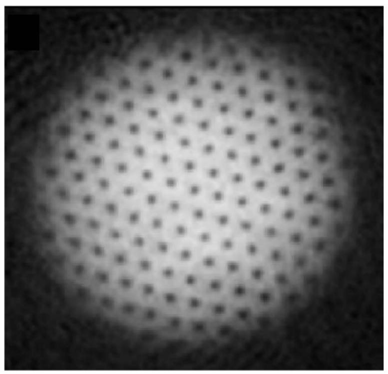
Calculations using high-fidelity chiral EFT interactions



Ma, Lin, Lu, Elhatisari, D.L., Meißner, Steiner, Wang, PRL **132**, 232502 (2024)

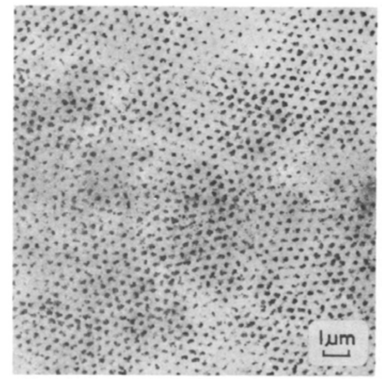
Superfluidity

BEC Theory



Ketterle, Zwierlein,
Ultracold Fermi Gases (2008)

BCS Theory



Essmann, Träuble,
Physics Letters A 27, 3 (1968)

Off-diagonal long-range order

Bosonic superfluidity

$$\langle \Psi_0 | a^\dagger(\mathbf{r}) a(\mathbf{0}) | \Psi_0 \rangle$$

Fermionic superfluidity (S-wave)

$$\langle \Psi_0 | a^\dagger_\downarrow(\mathbf{r}) a^\dagger_\uparrow(\mathbf{r} + \Delta\mathbf{r}) a_\uparrow(\Delta\mathbf{r}) a_\downarrow(\mathbf{0}) | \Psi_0 \rangle$$

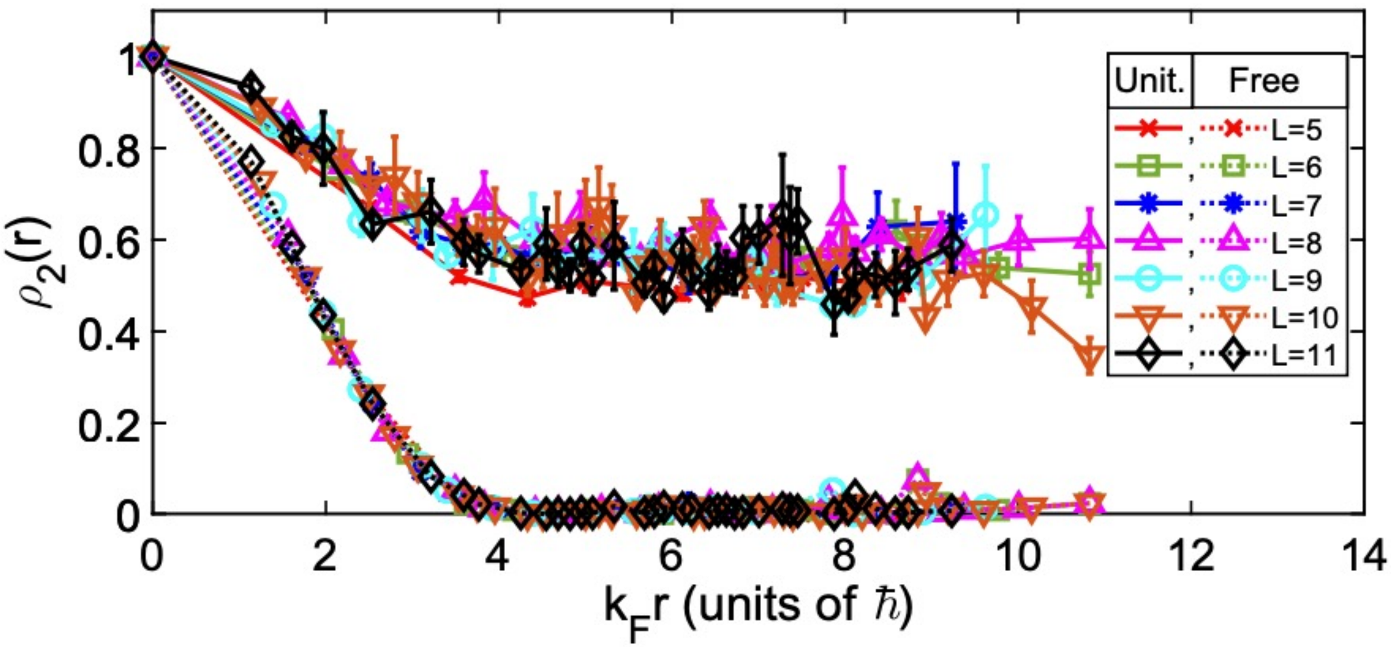
Fermionic superfluidity (P-wave)

$$\langle \Psi_0 | a^\dagger_\uparrow(\mathbf{r}) a^\dagger_\uparrow(\mathbf{r} + \Delta\mathbf{r}) a_\uparrow(\Delta\mathbf{r}) a_\uparrow(\mathbf{0}) | \Psi_0 \rangle$$

Yang, RMP **34**, 694 (1962)

Unitary limit

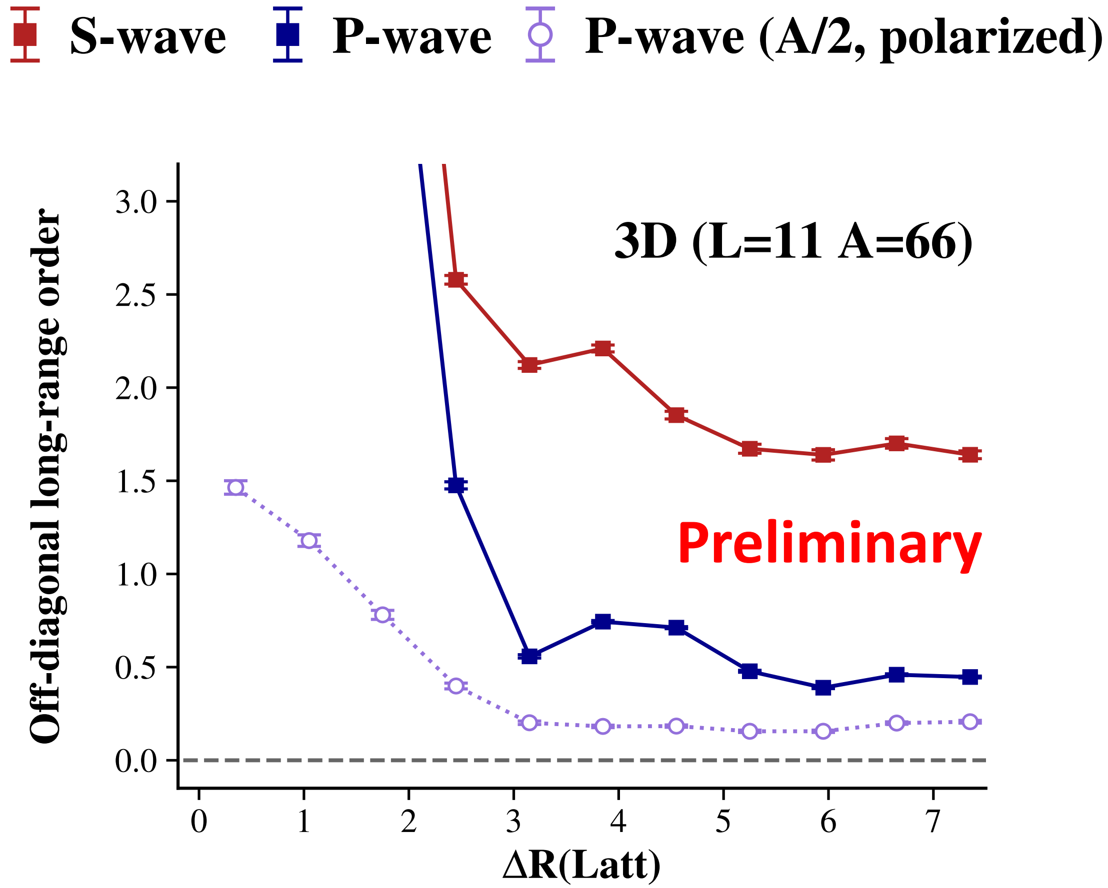
$$H = H_{\text{free}} + \frac{1}{2} C_2 \sum_{\mathbf{n}} \rho(\mathbf{n})^2$$



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

Multimodal superfluidity

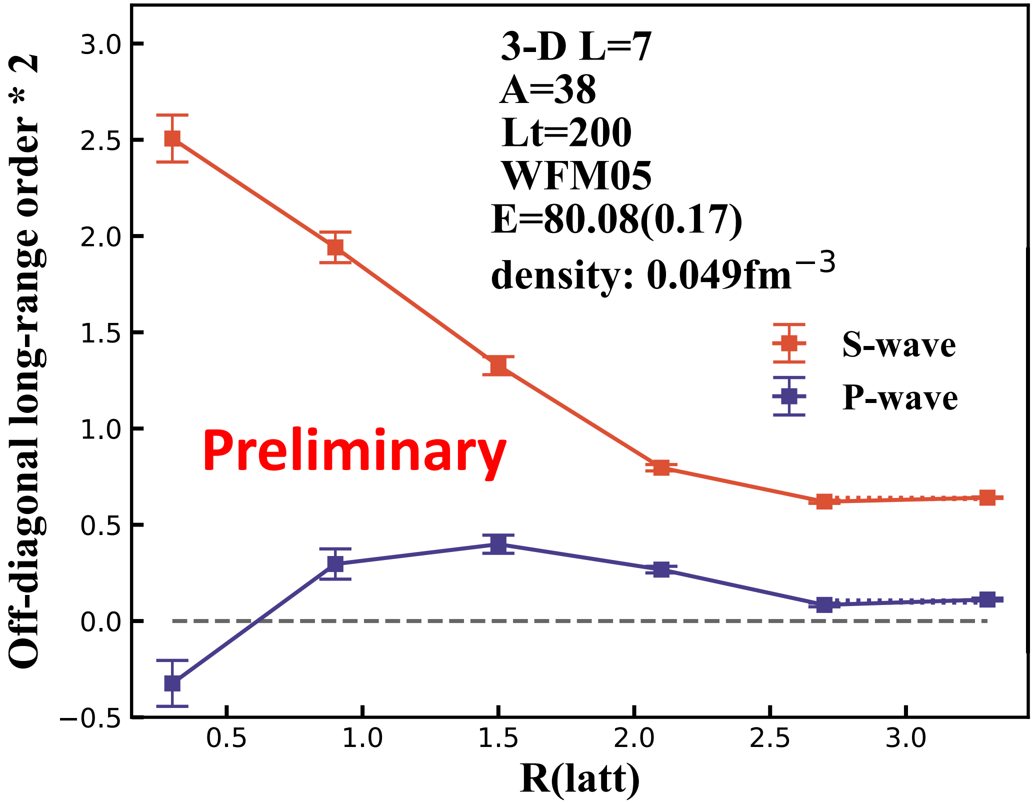
$$H = H_{\text{free}} + \frac{1}{2}C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2$$



Ma *et al.*, work in progress

Multimodal superfluidity in neutron matter

Leading-order chiral EFT interaction



Ma *et al.*, work in progress

Summary and outlook

Nuclear lattice effective field theory is being used to perform *ab initio* calculations of nuclear many-body systems. Wavefunction matching allows for the use of high-fidelity chiral effective field theory interactions, and the lattice simulations provide reliable predictions for experiments as well as deeper insights into the underlying physics. The collaboration is working to produce calculations of nuclear structure, scattering, reactions, thermodynamics, and superfluidity.