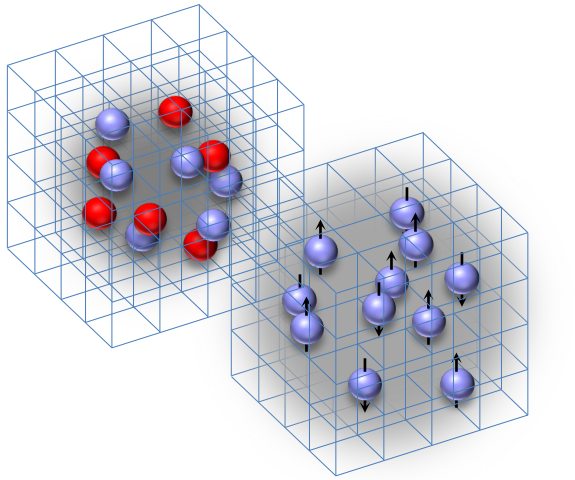
Nuclear Lattice Simulations and FRIB Science

Dean Lee
Facility for Rare Isotope Beams
Michigan State University
Nuclear Lattice EFT Collaboration



Theoretical Justifications and Motivations
for Early High-Profile FRIB Experiments
May 17, 2023

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

Ab initio nuclear thermodynamics

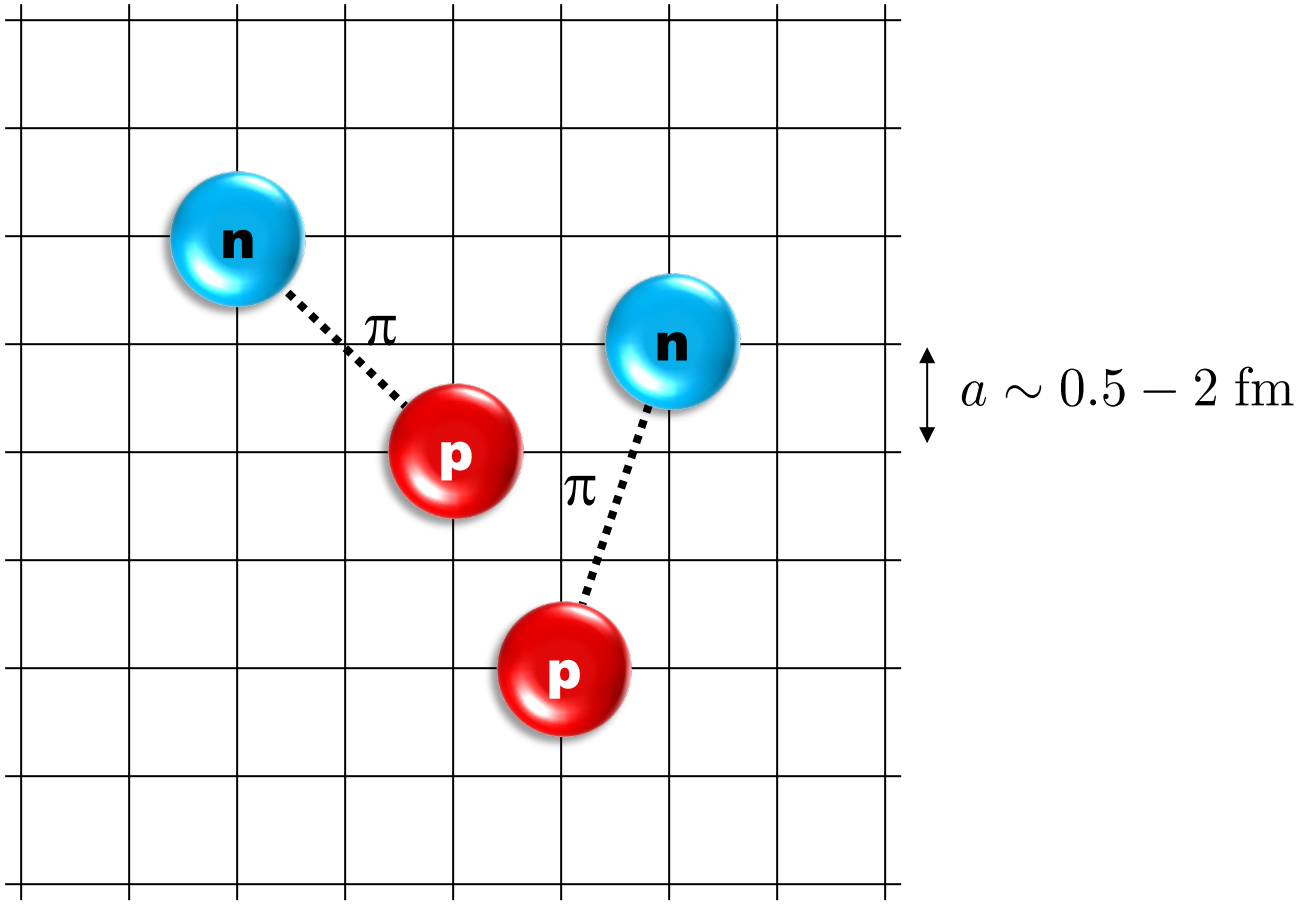
Emergent geometry and duality of ^{12}C

Wave function matching

Neutron driplines and the unitary limit

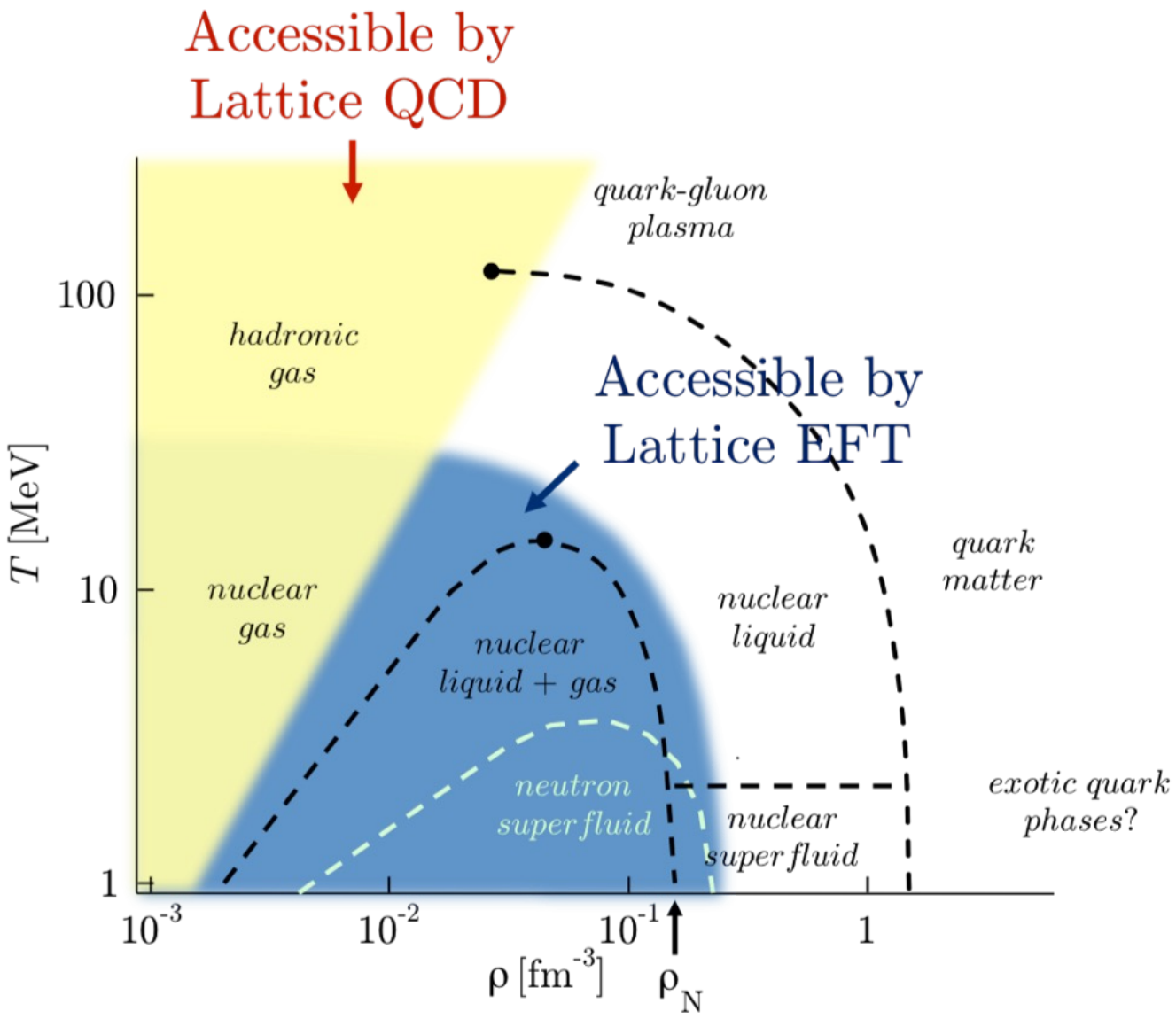
Prospects and challenges

Lattice effective field theory



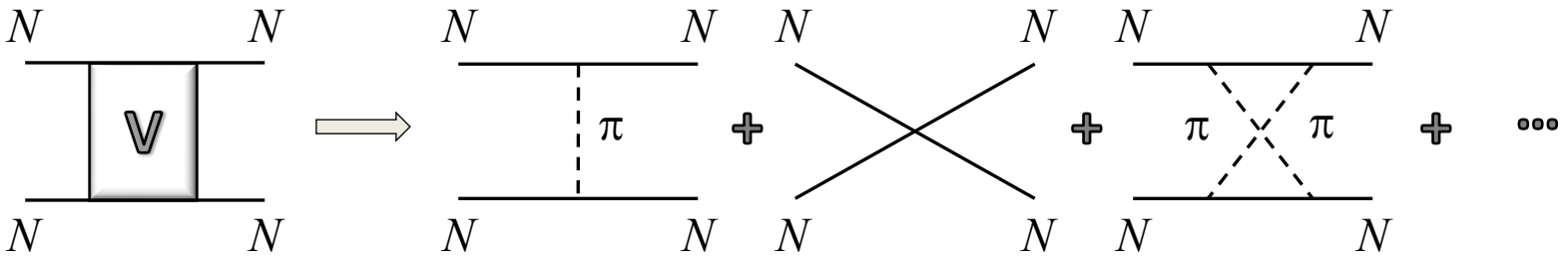
D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

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

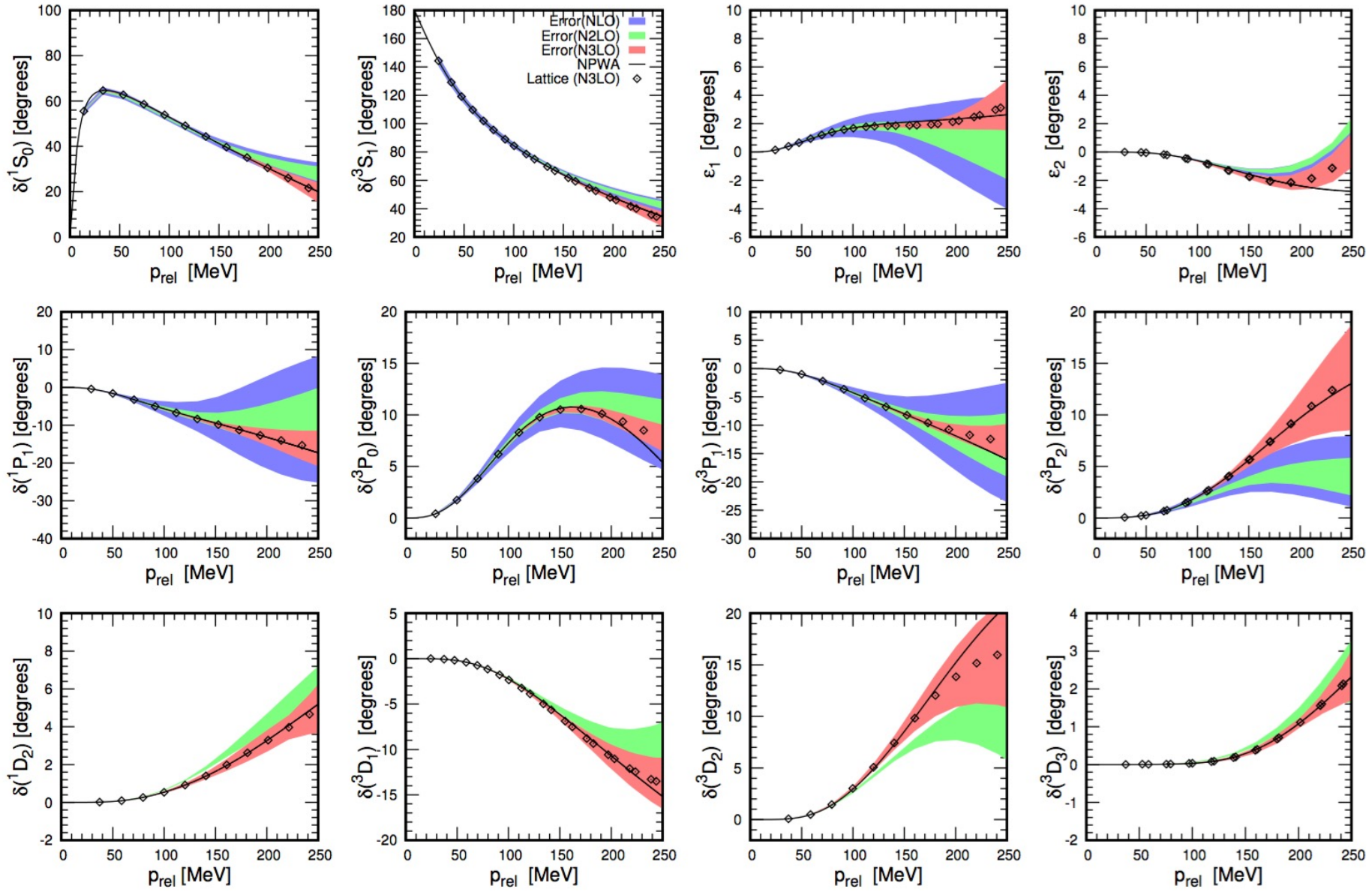
Construct the effective potential order by order



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

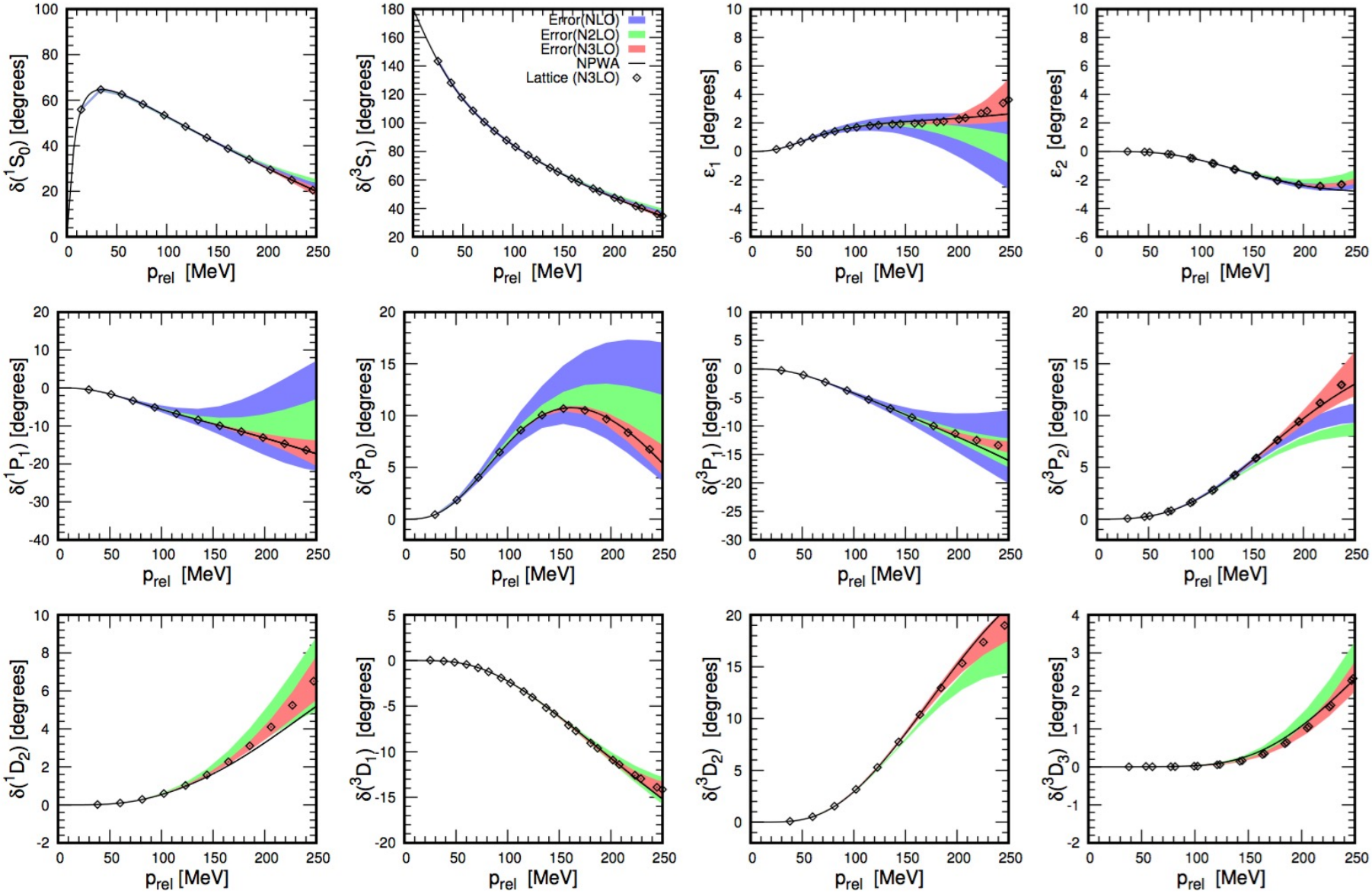
Leading order (LO) Next-to-leading order (NLO)

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

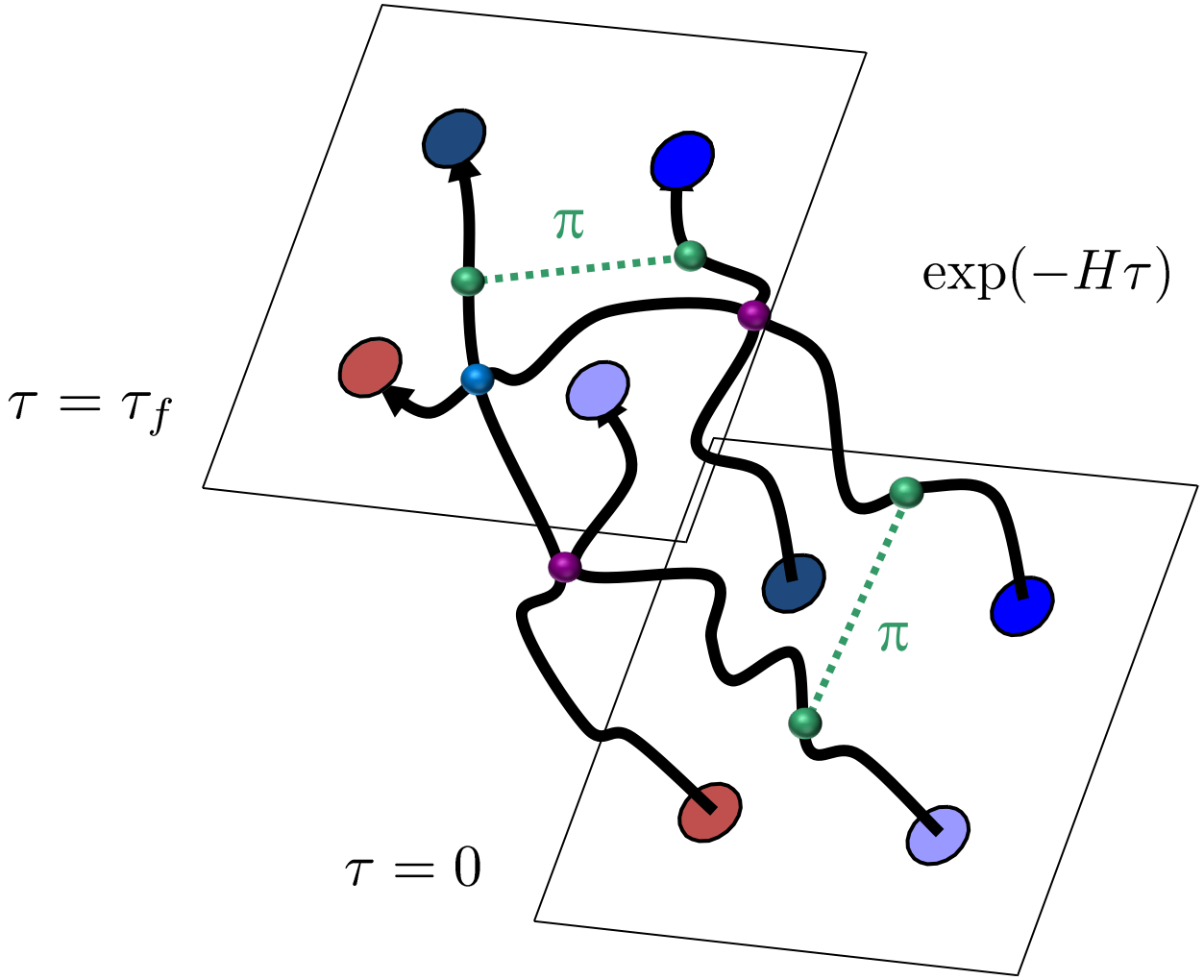


Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, Phys. Rev. C 98, 044002 (2018)

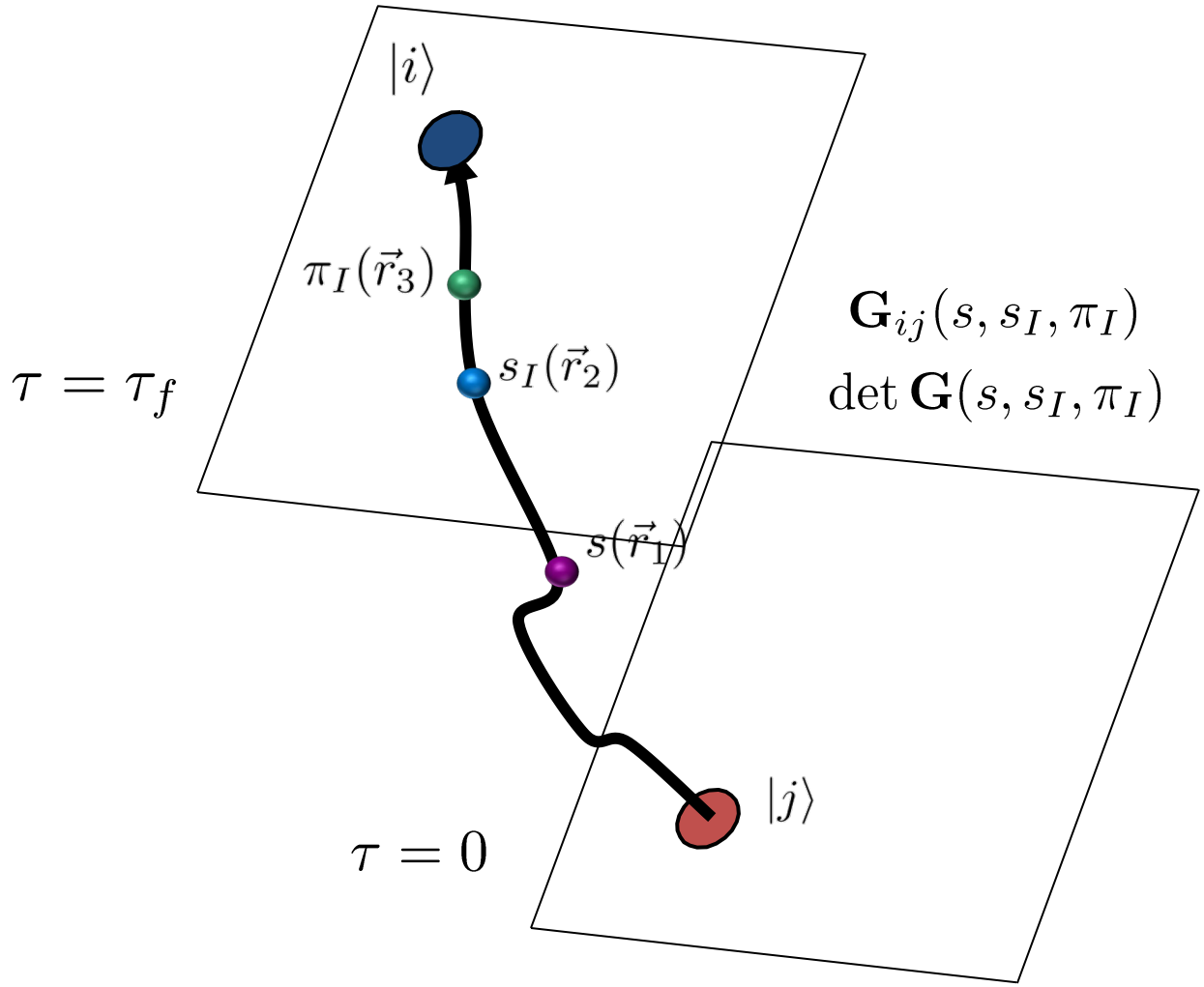
$a = 0.987\,\mathrm{fm}$



Euclidean time projection

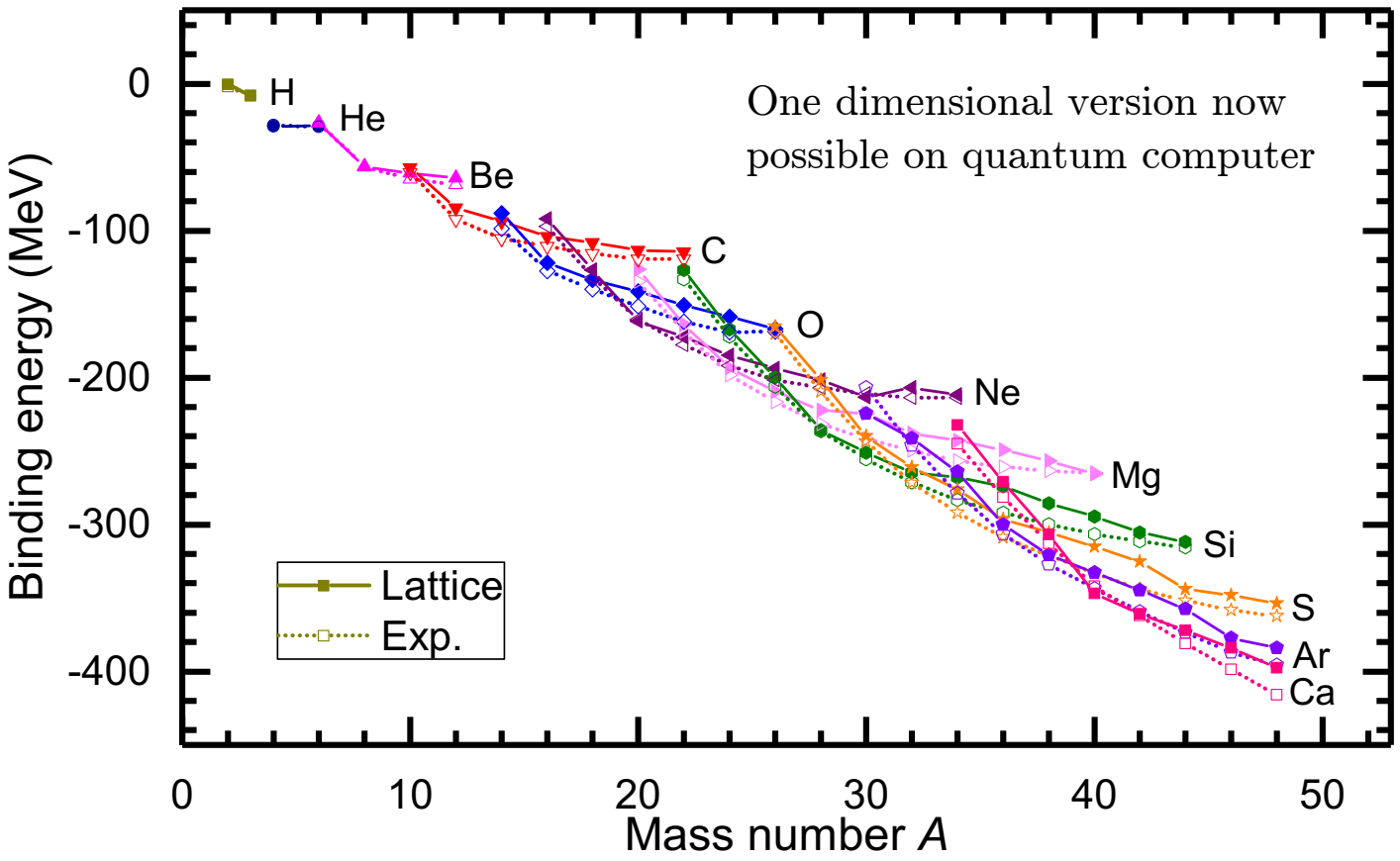


Auxiliary field method



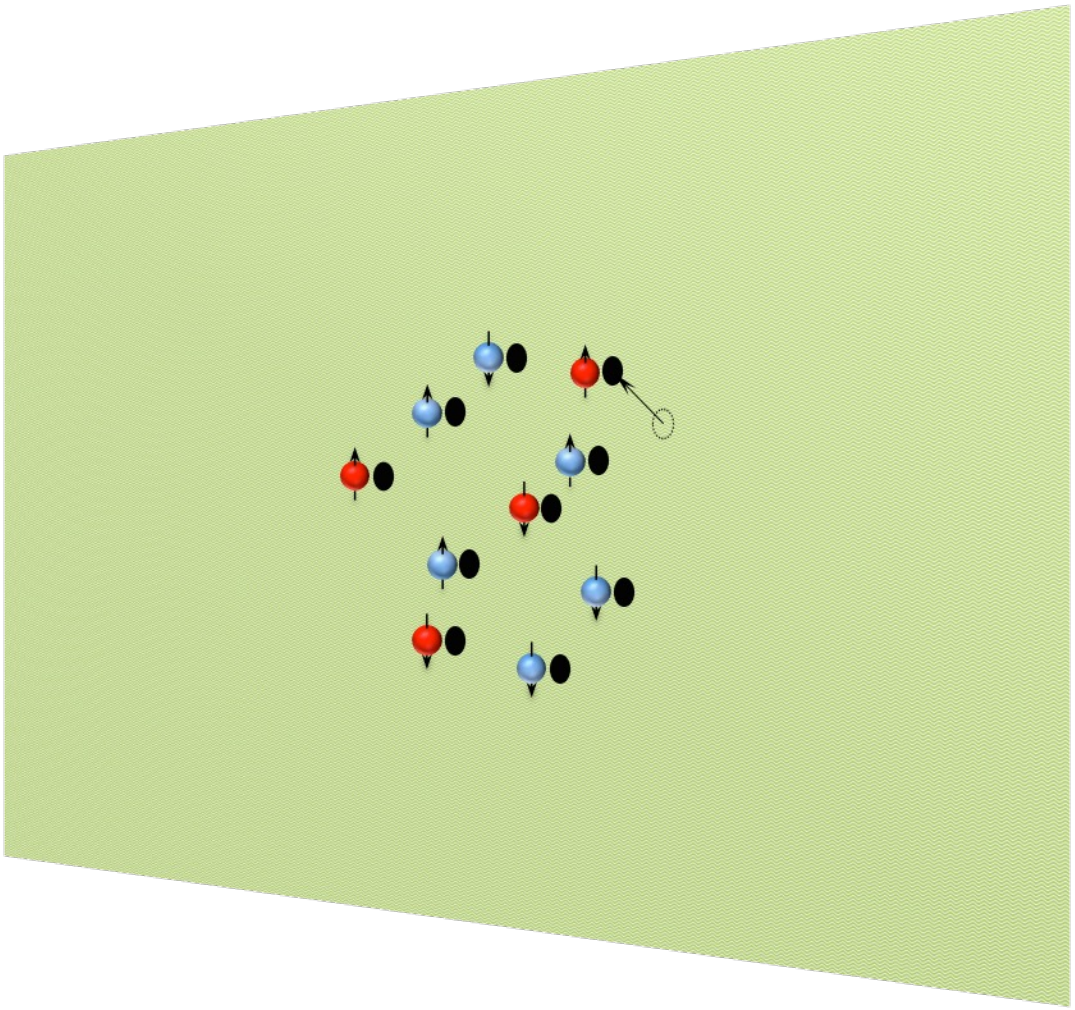
Essential elements for nuclear binding

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

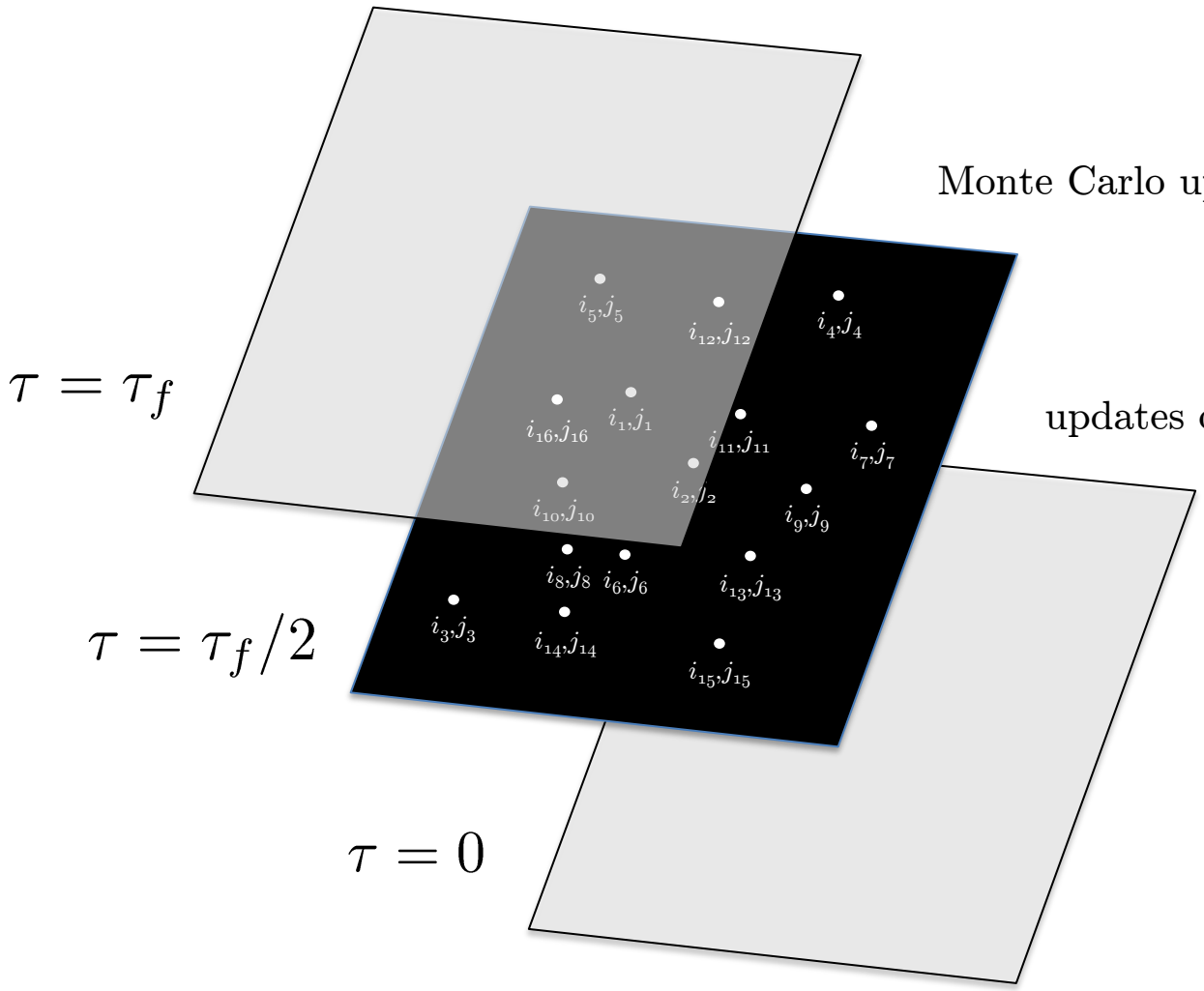


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, Phys. Lett. B 797, 134863 (2019)

Pinhole algorithm



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

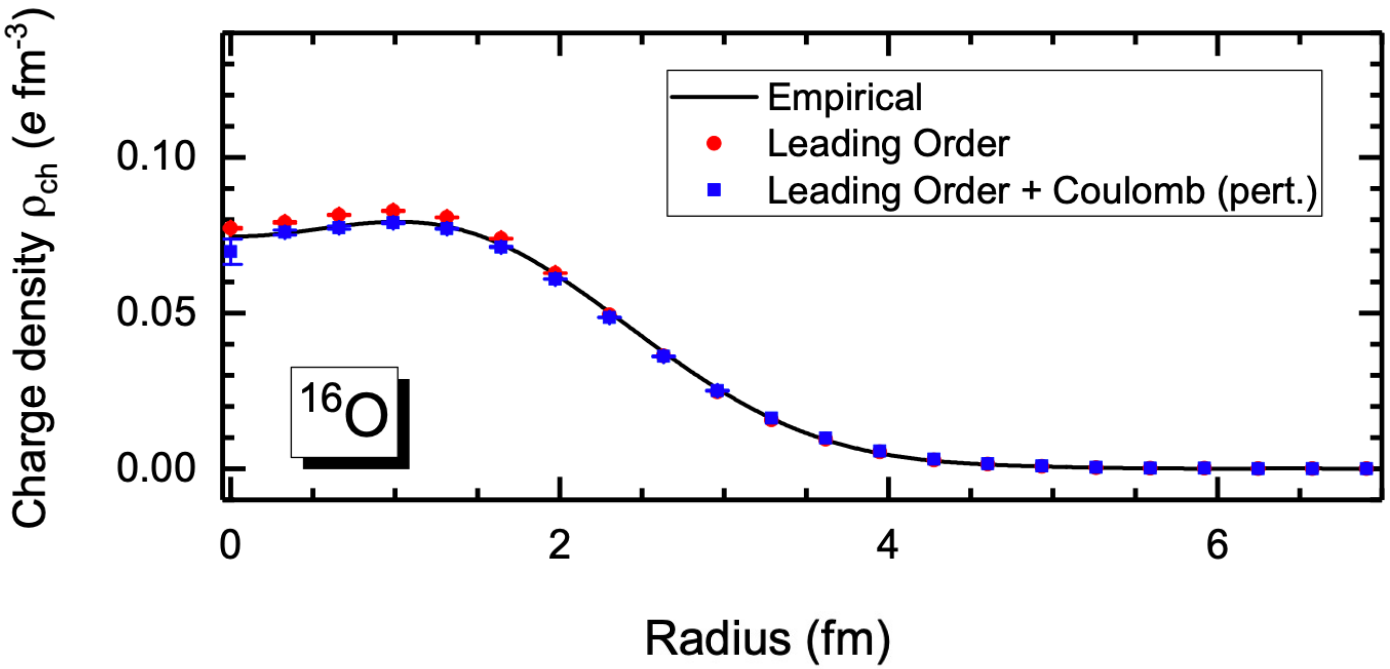


Monte Carlo updates of pinholes

Monte Carlo
updates of auxiliary/pion fields

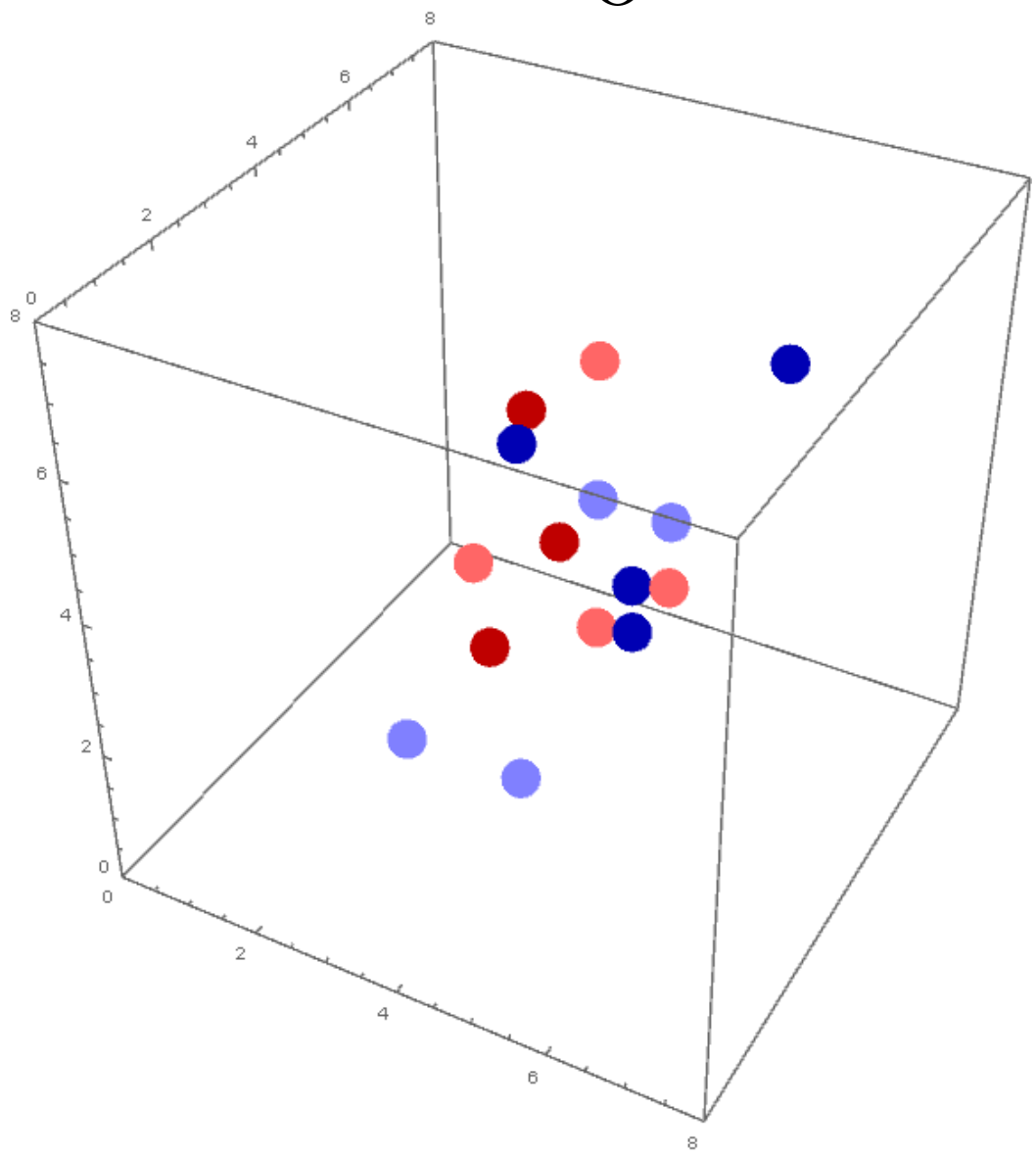
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak,
Phys. Rev. Lett. 119, 222505 (2017)

^{16}O



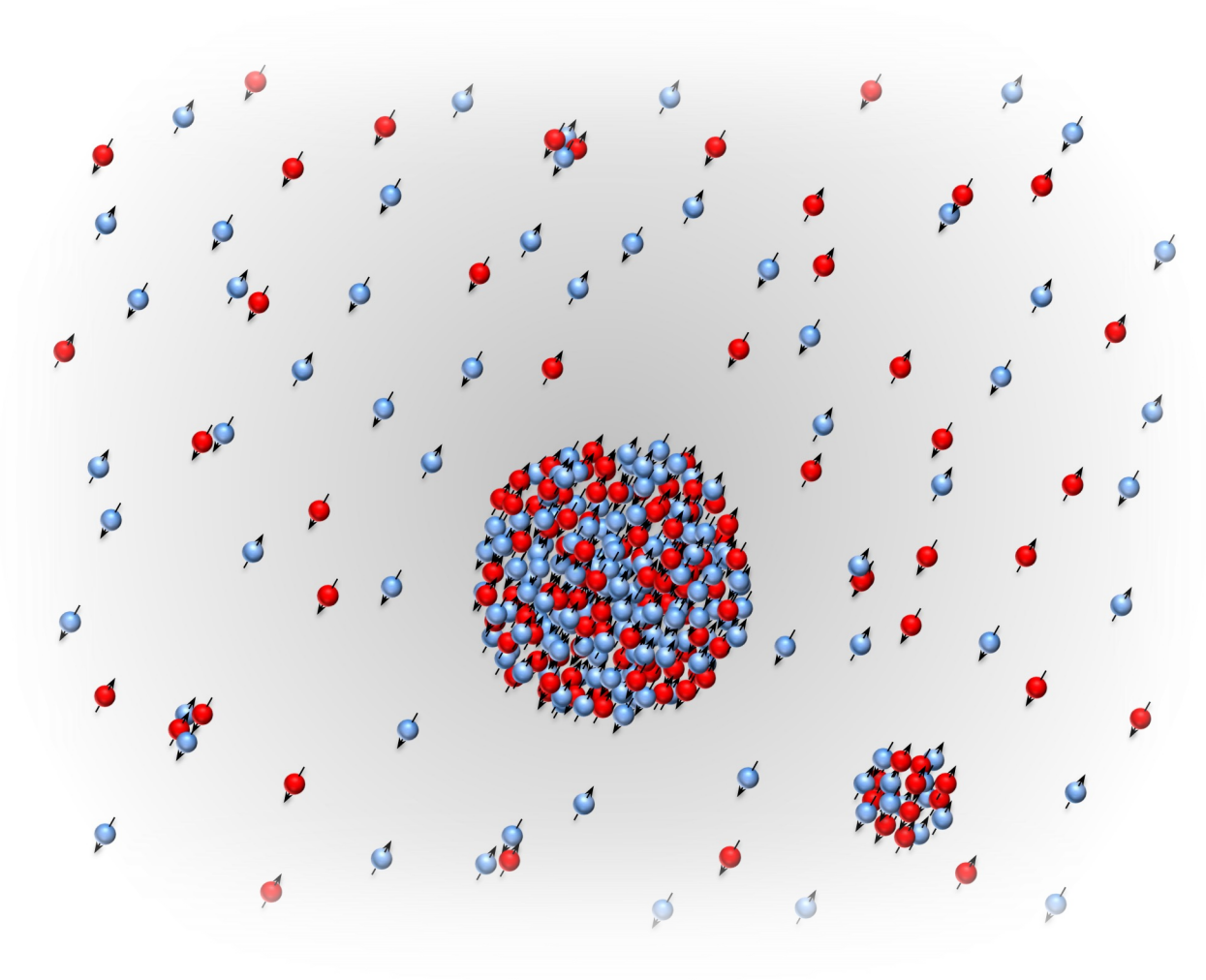
Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, Phys. Lett. B 797, 134863 (2019)

^{16}O



proton up
proton down
neutron up
neutron down

Ab initio nuclear thermodynamics



Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, Phys. Rev. Lett. 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

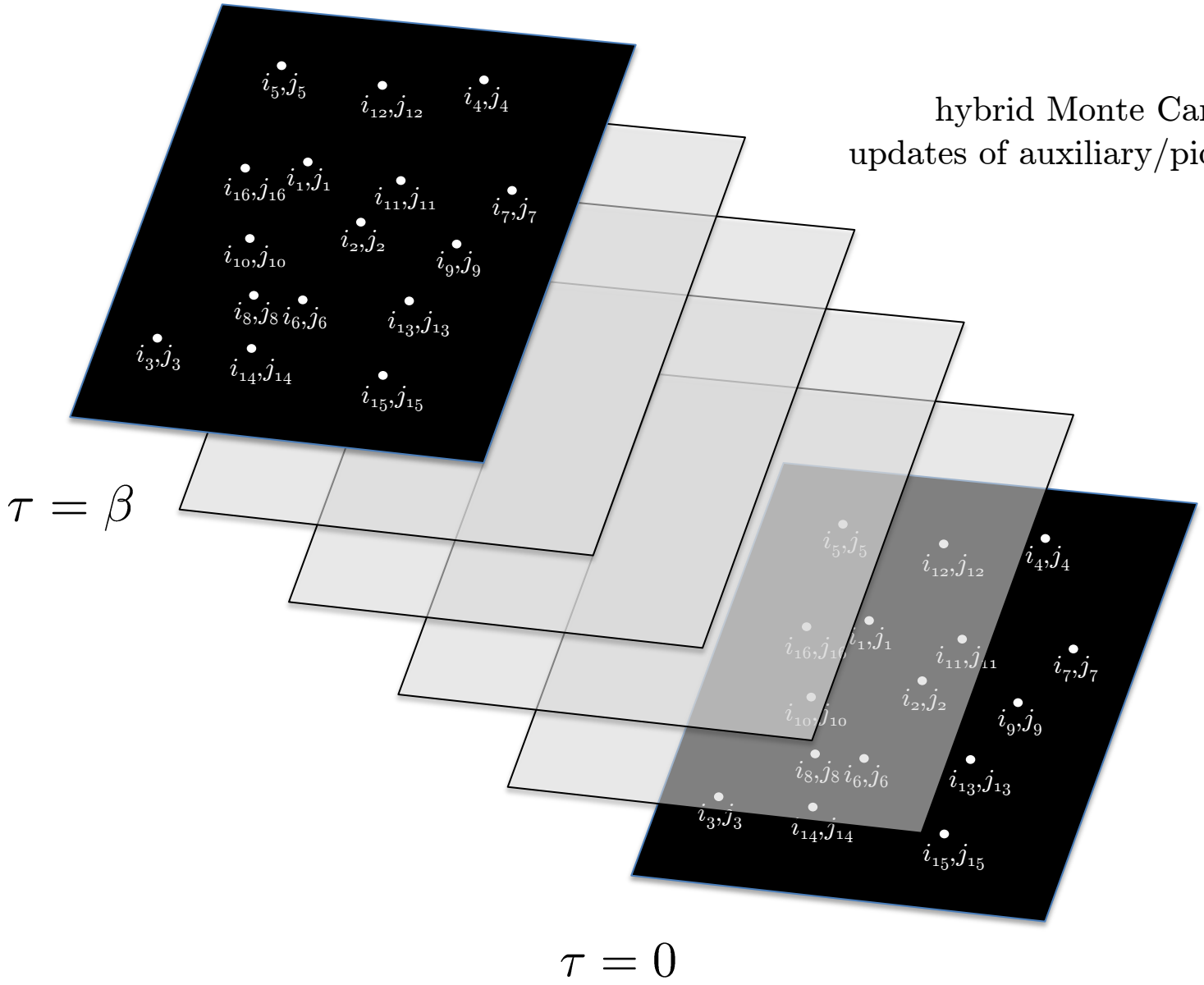
$$\mathrm{Tr}\exp(-\beta H)$$

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

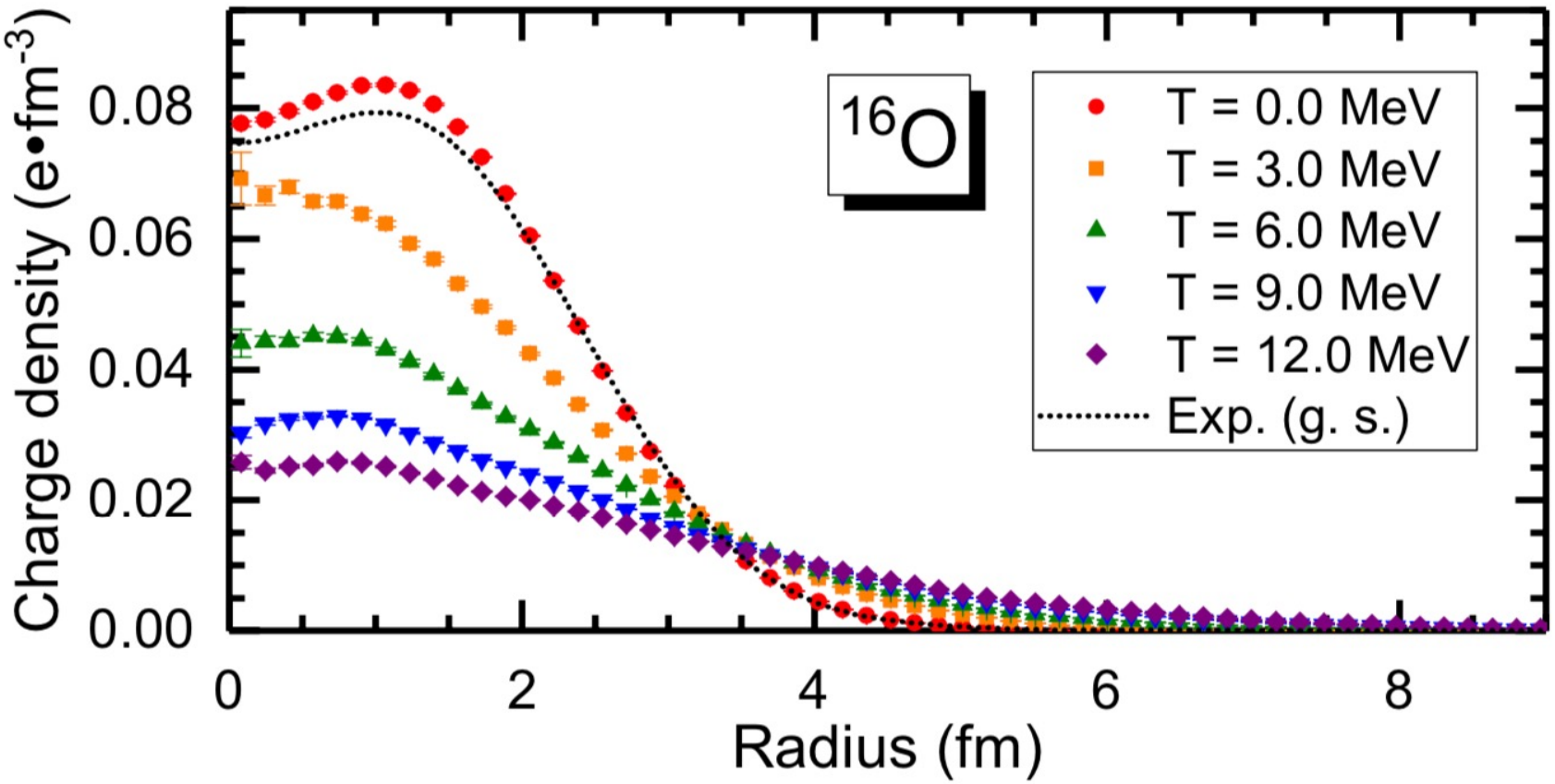
$$\mathrm{Tr}\, O = \frac{1}{A!} \sum_{i_1 \cdots i_A, j_1 \cdots j_A, \mathbf{n}_1 \cdots \mathbf{n}_A} \langle 0 | a_{i_A,j_A}(\mathbf{n}_A) \cdots a_{i_1,j_1}(\mathbf{n}_1)\, O\, a^\dagger_{i_1,j_1}(\mathbf{n}_1) \cdots a^\dagger_{i_A,j_A}(\mathbf{n}_A) | 0 \rangle$$

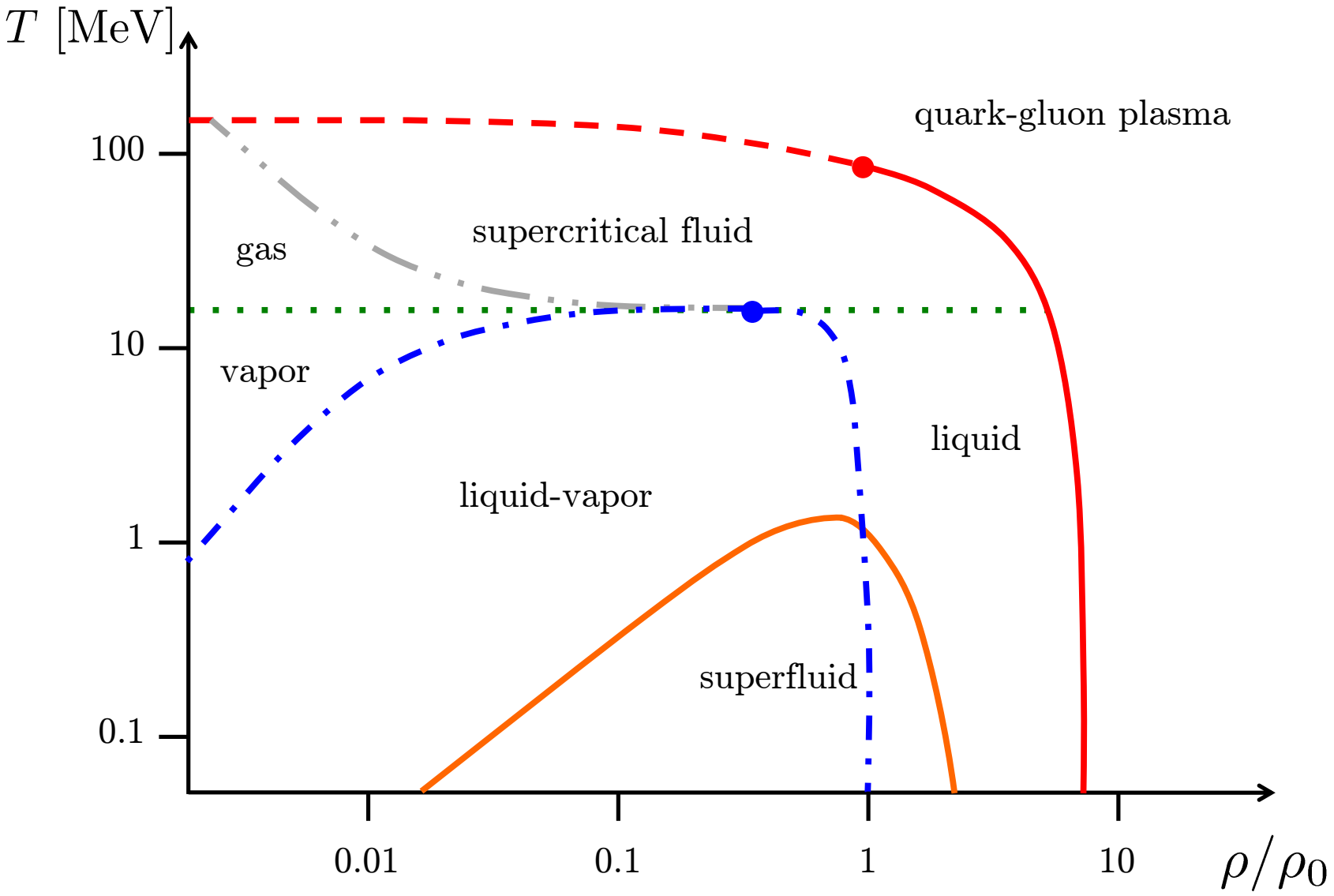
This can be used to calculate the partition function in the canonical ensemble.

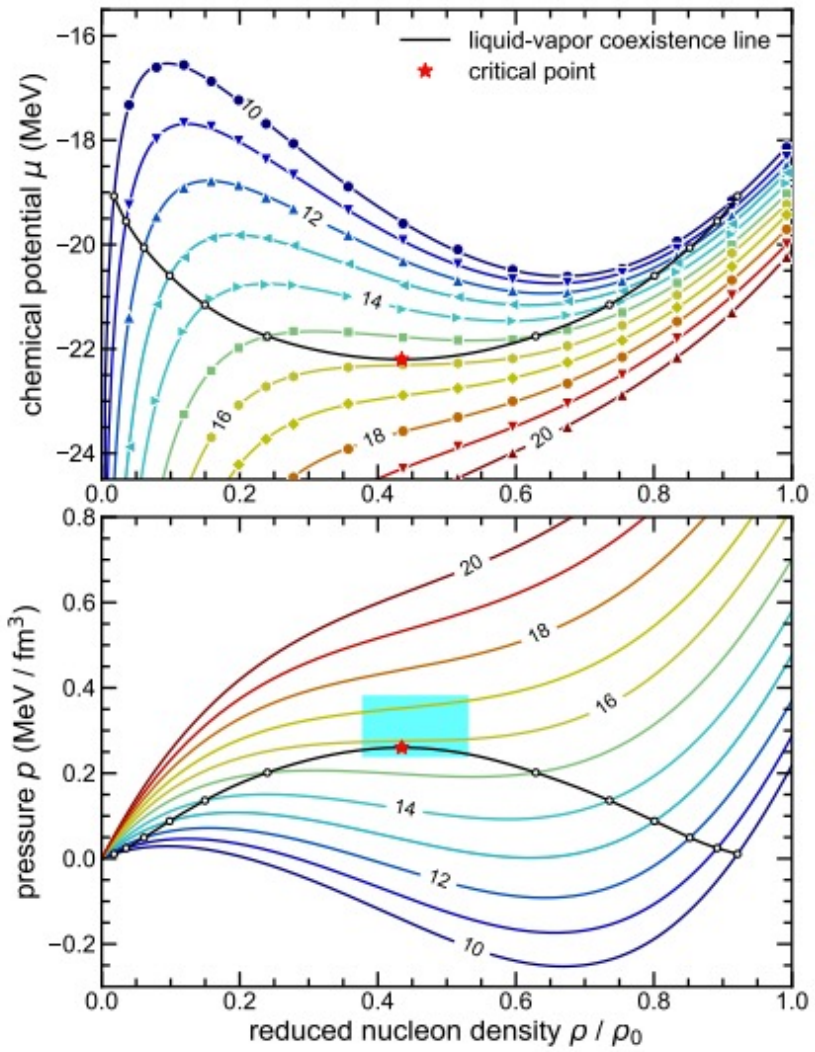
Metropolis updates of pinholes



hybrid Monte Carlo
updates of auxiliary/pion fields


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

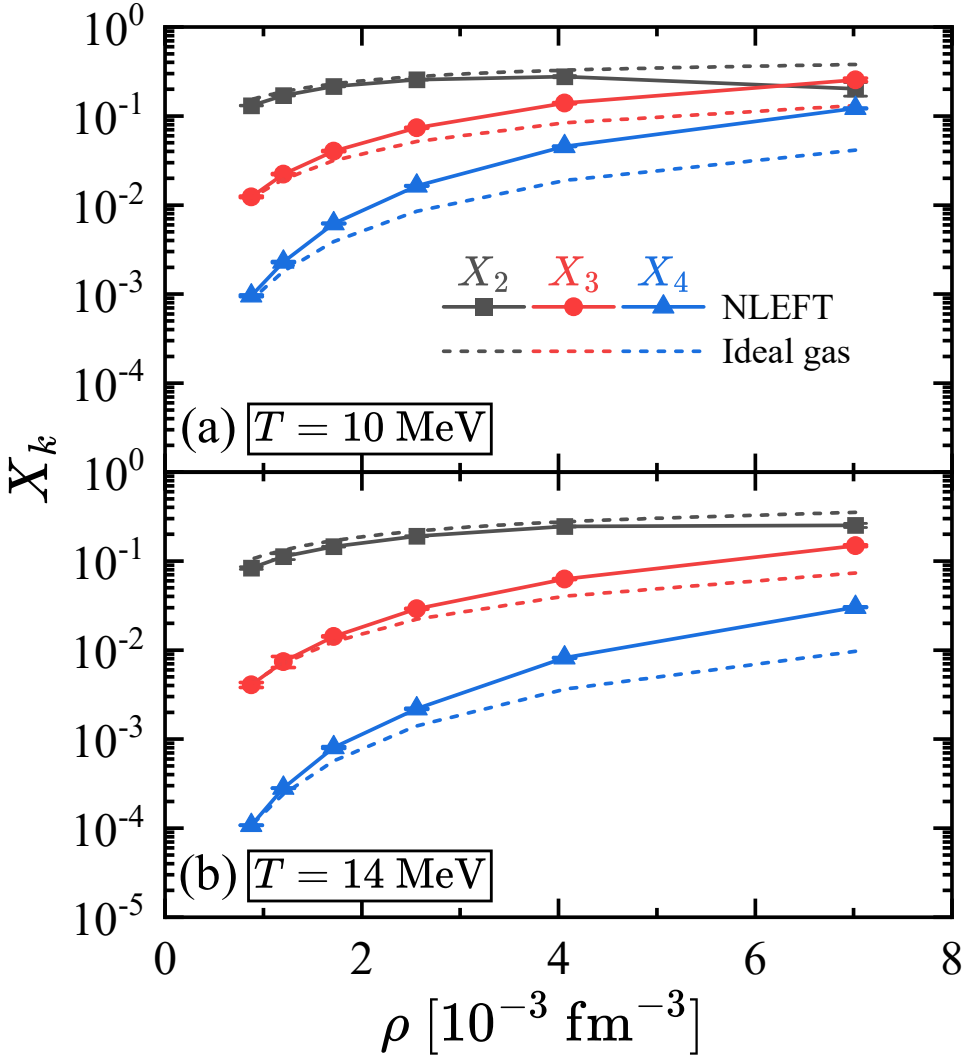

T [MeV]
100
10
1
0.1
quark-gluon plasma
supercritical fluid
gas
vapor
liquid
liquid-vapor
superfluid
0.01
0.1
1
10
ρ/ρ_0



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

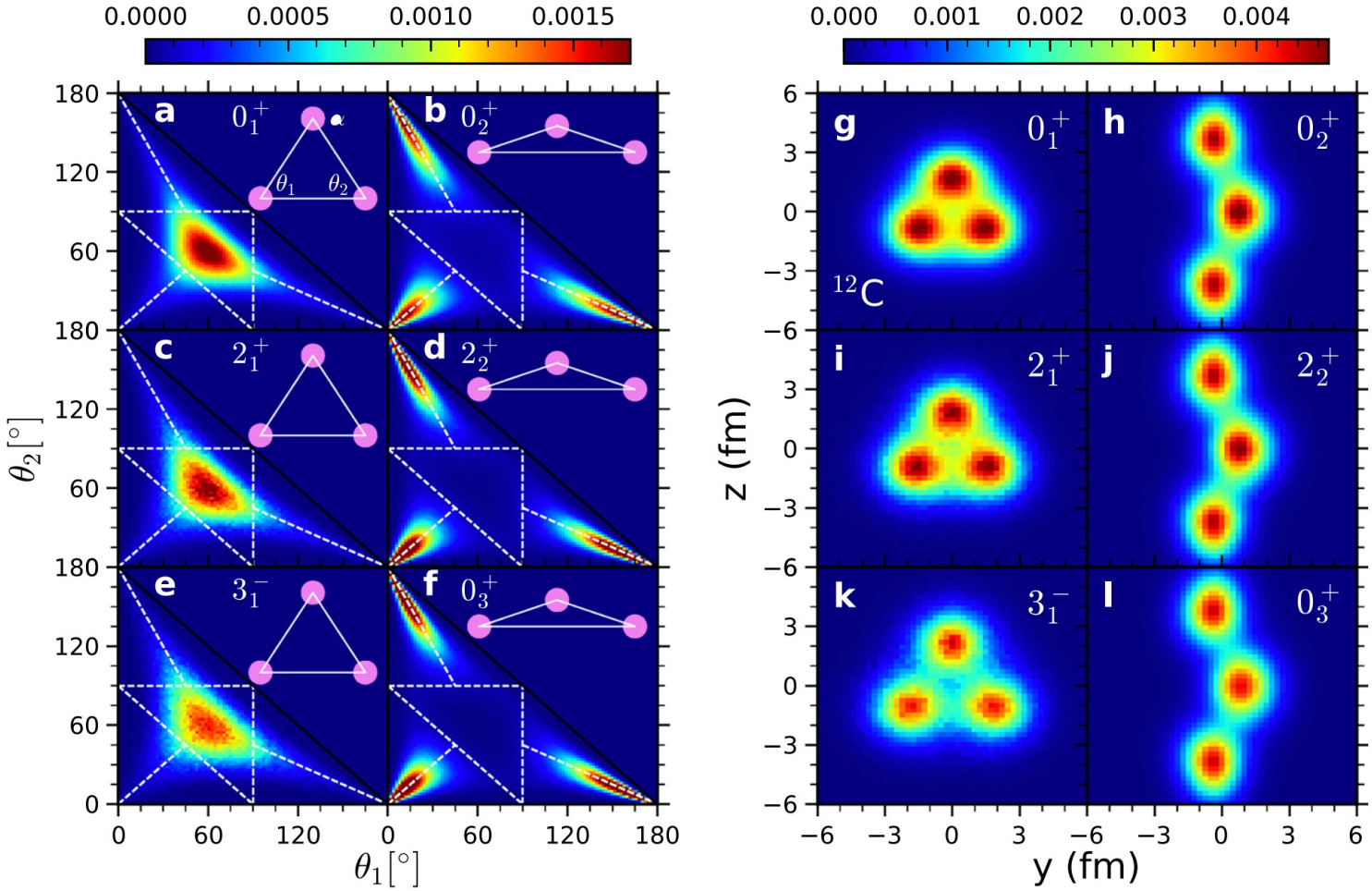
Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, Phys. Rev. Lett. 125, 192502 (2020)

Cluster abundance as function of density and temperature

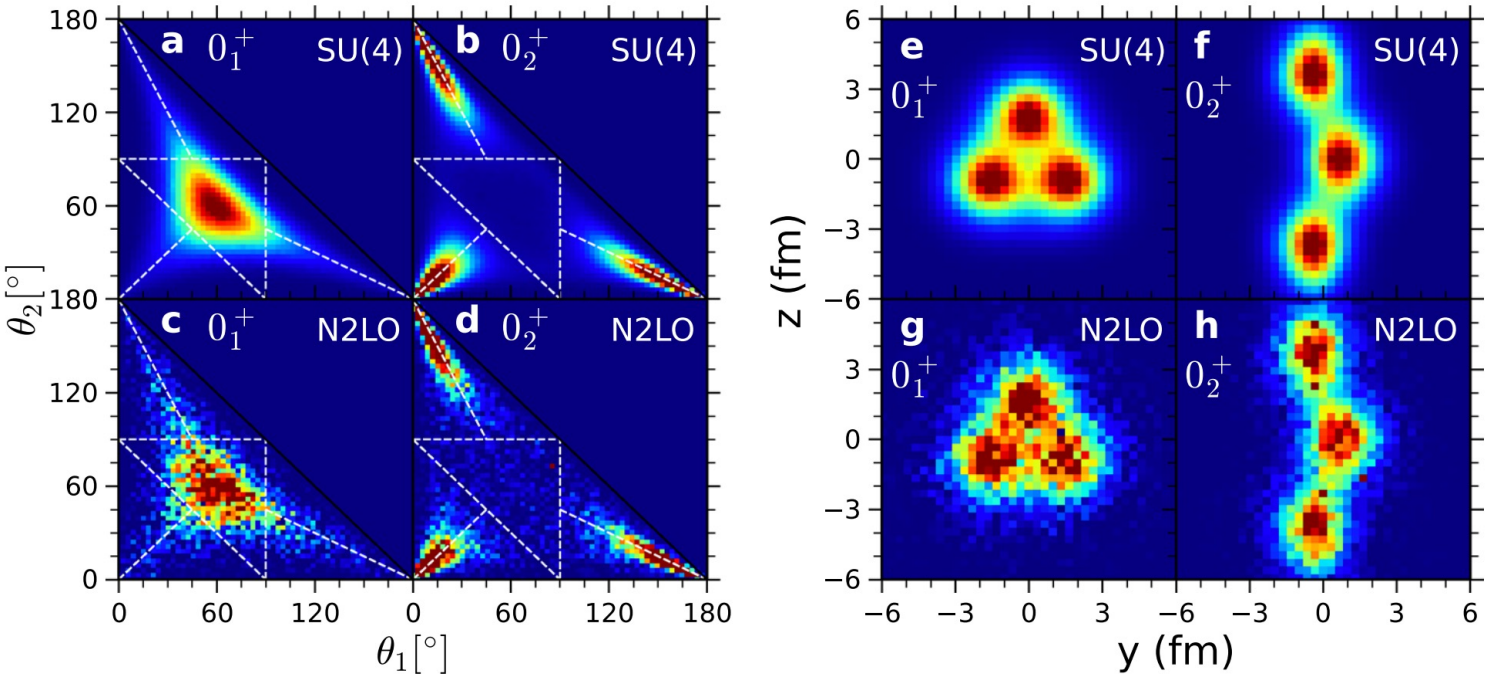


Z. Ren et al., work in progress

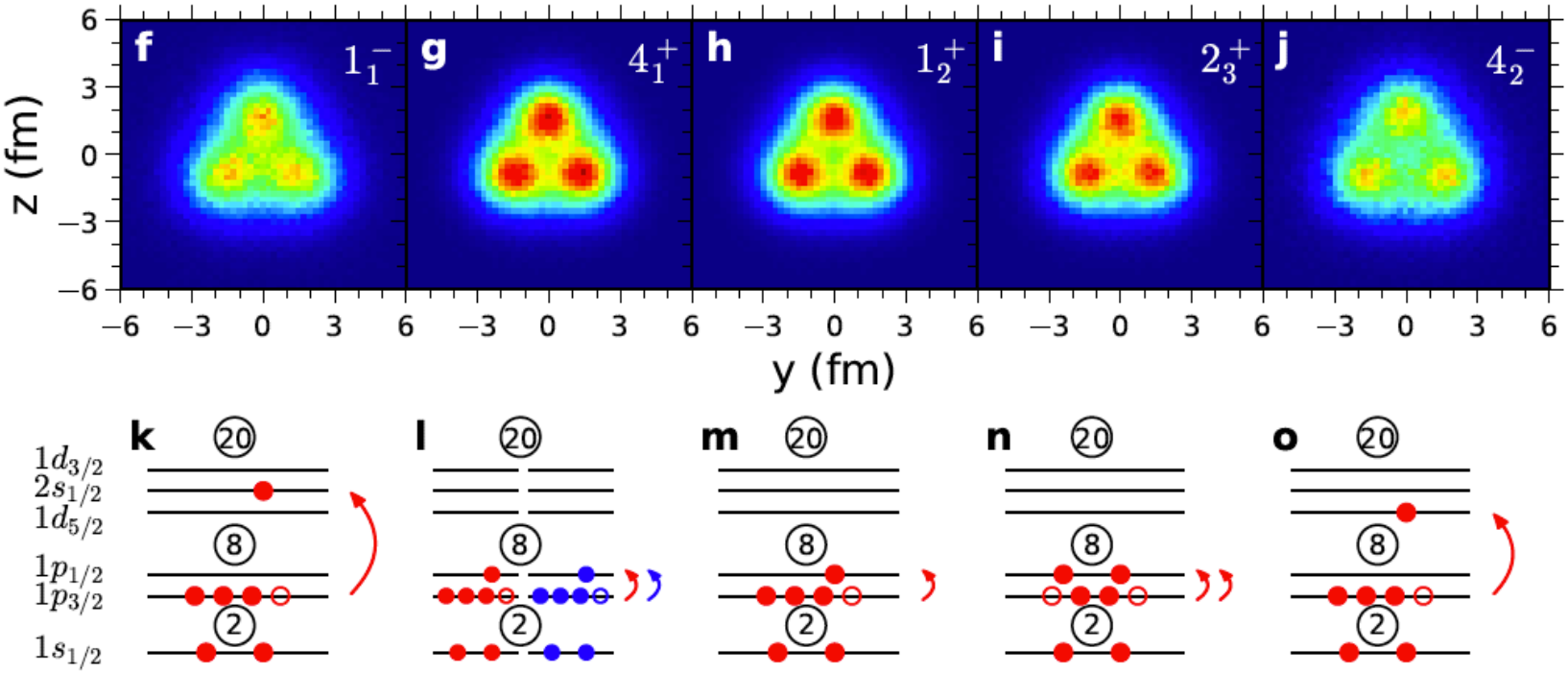
Emergent geometry and duality of ^{12}C

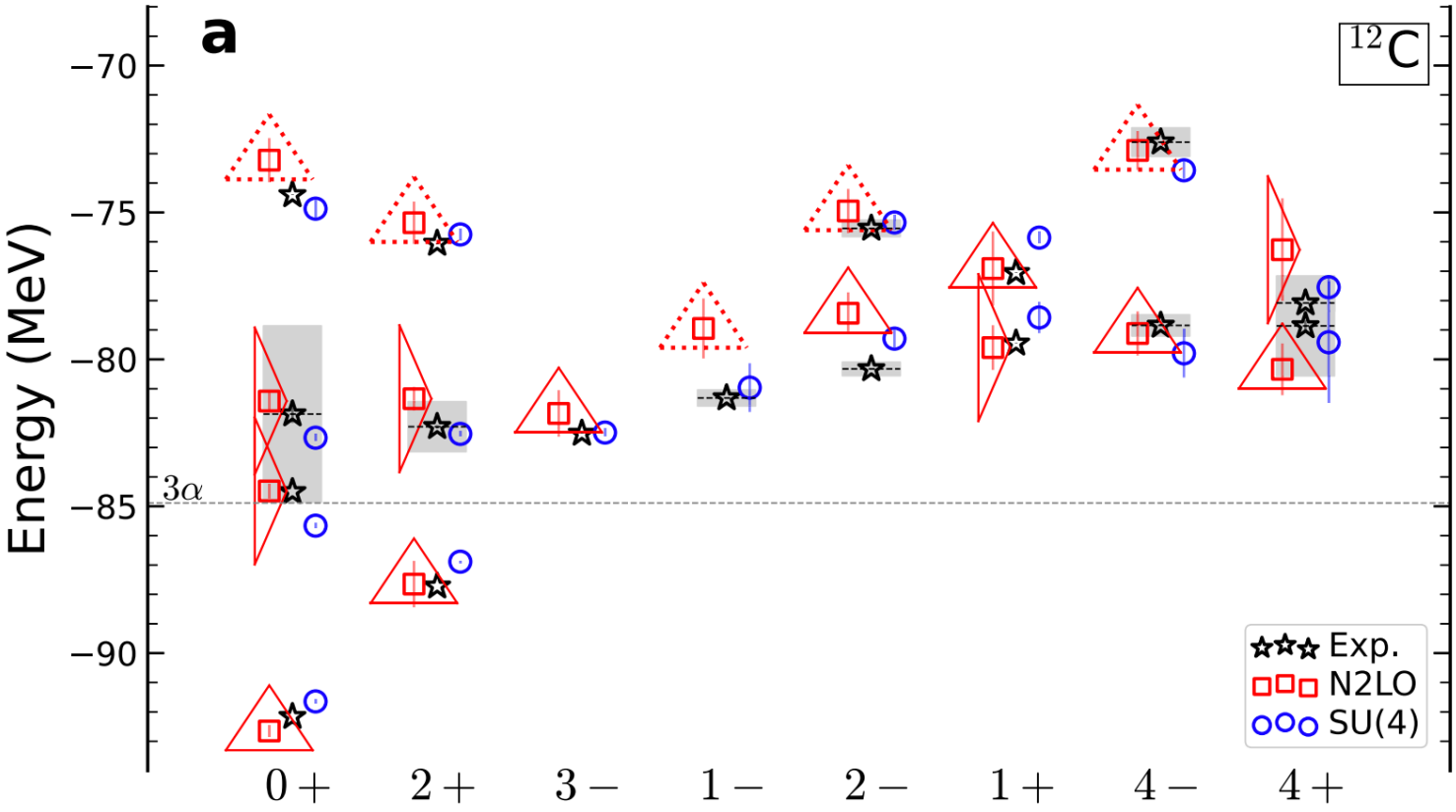


Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



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

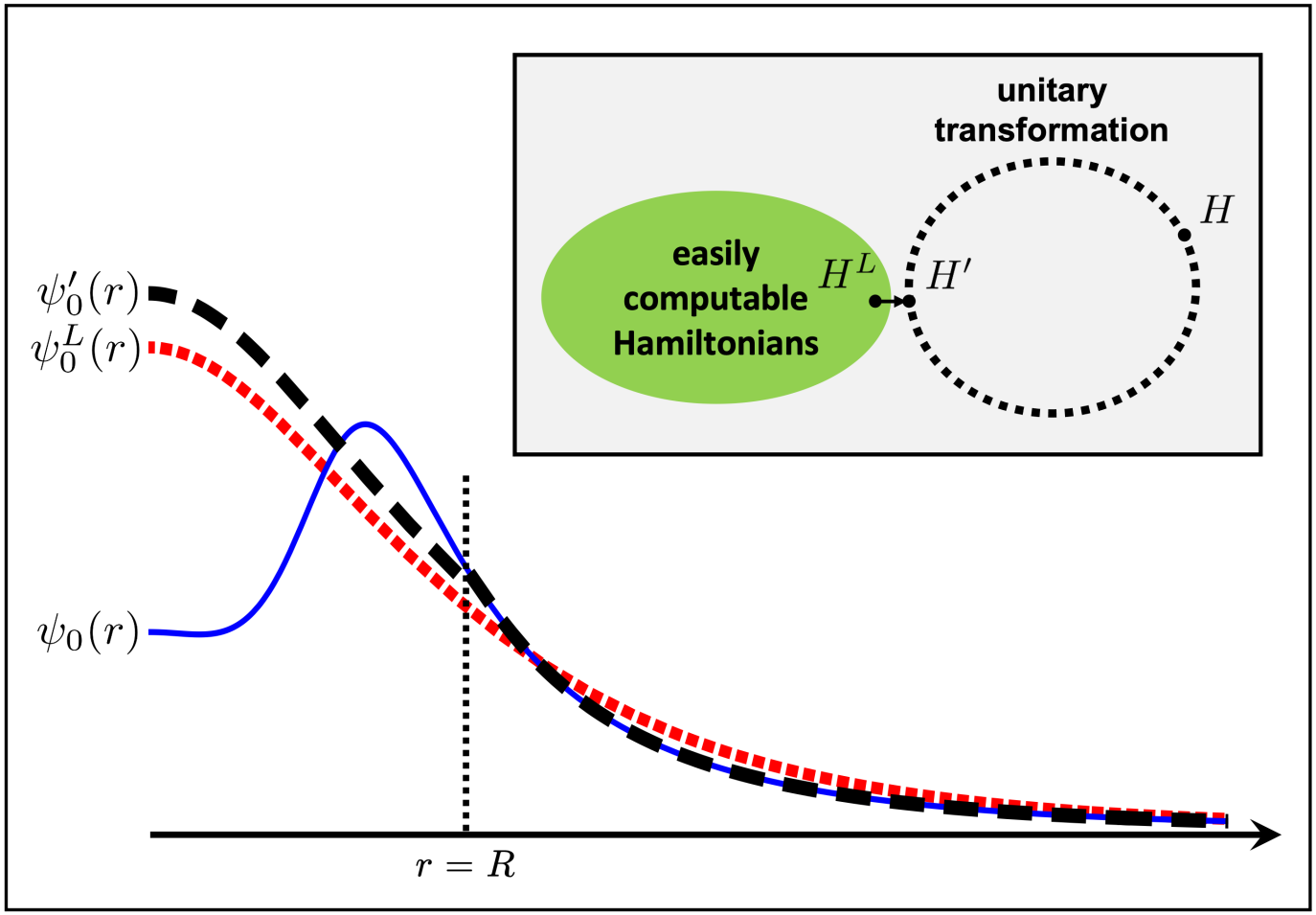

f
1_1^-
g
4_1^+
h
1_2^+
i
2_3^+
j
4_2^-
z (fm)
y (fm)
6
3
0
−3
−6
k
l
m
n
o
20
8
2
$1d_{3/2}$
$2s_{1/2}$
$1d_{5/2}$
$1p_{1/2}$
$1p_{3/2}$
$1s_{1/2}$



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

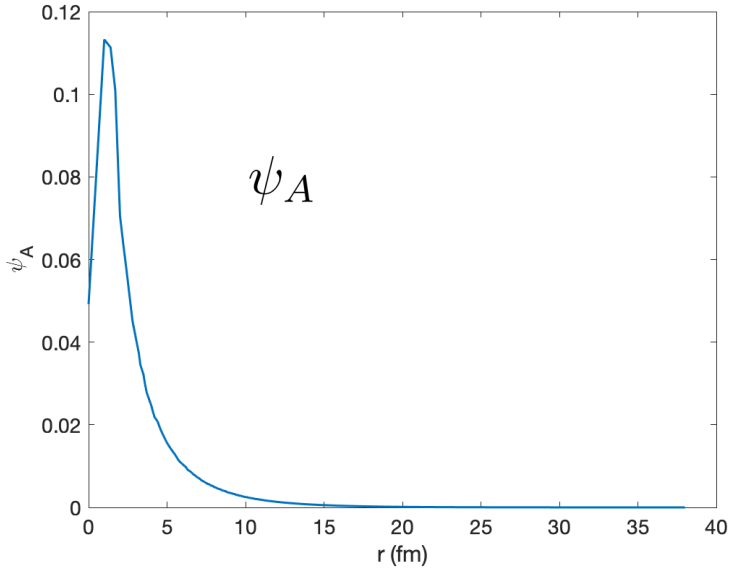
Lattice Monte Carlo simulations can compute highly nontrivial correlations in nuclear many-body systems. Unfortunately, sign oscillations prevent direct simulations using a high-fidelity Hamiltonian based on chiral effective field theory due to short-range repulsion.

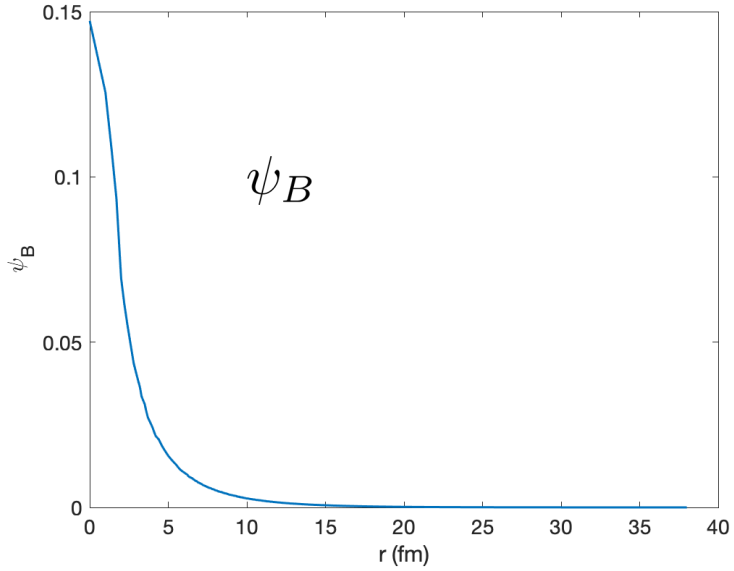
Wave function matching

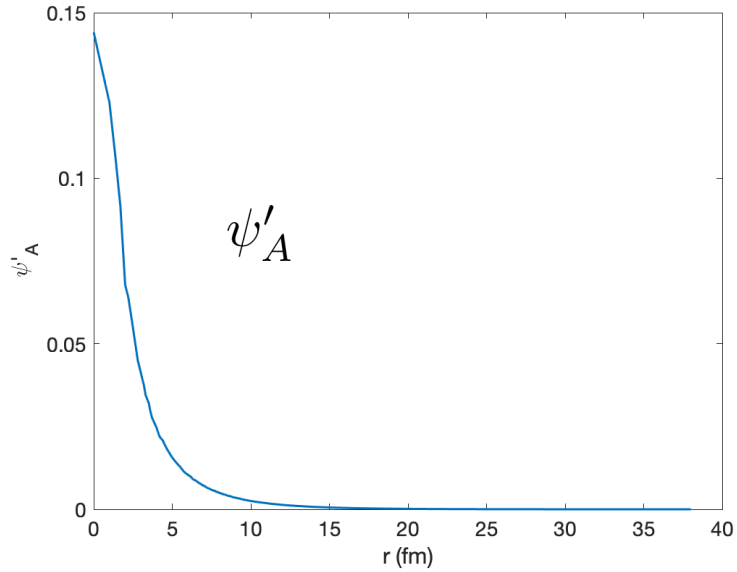


Elhatisari, Bovermann, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Ma, Meißner, Rupak, Shen, Song, Stellin, arXiv: 2210.17488

Ground state wave functions





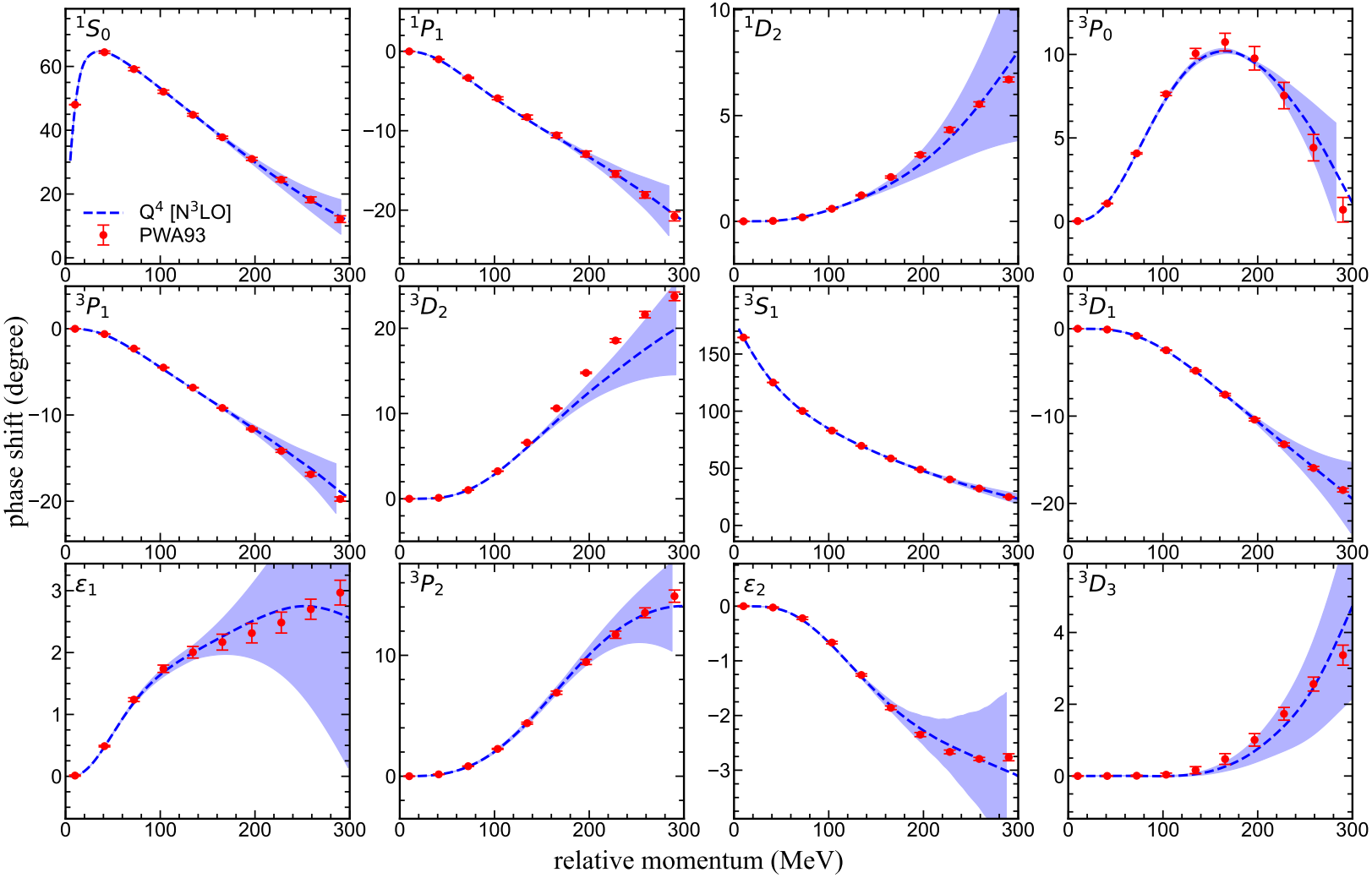


With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of H_B and using first-order perturbation theory.

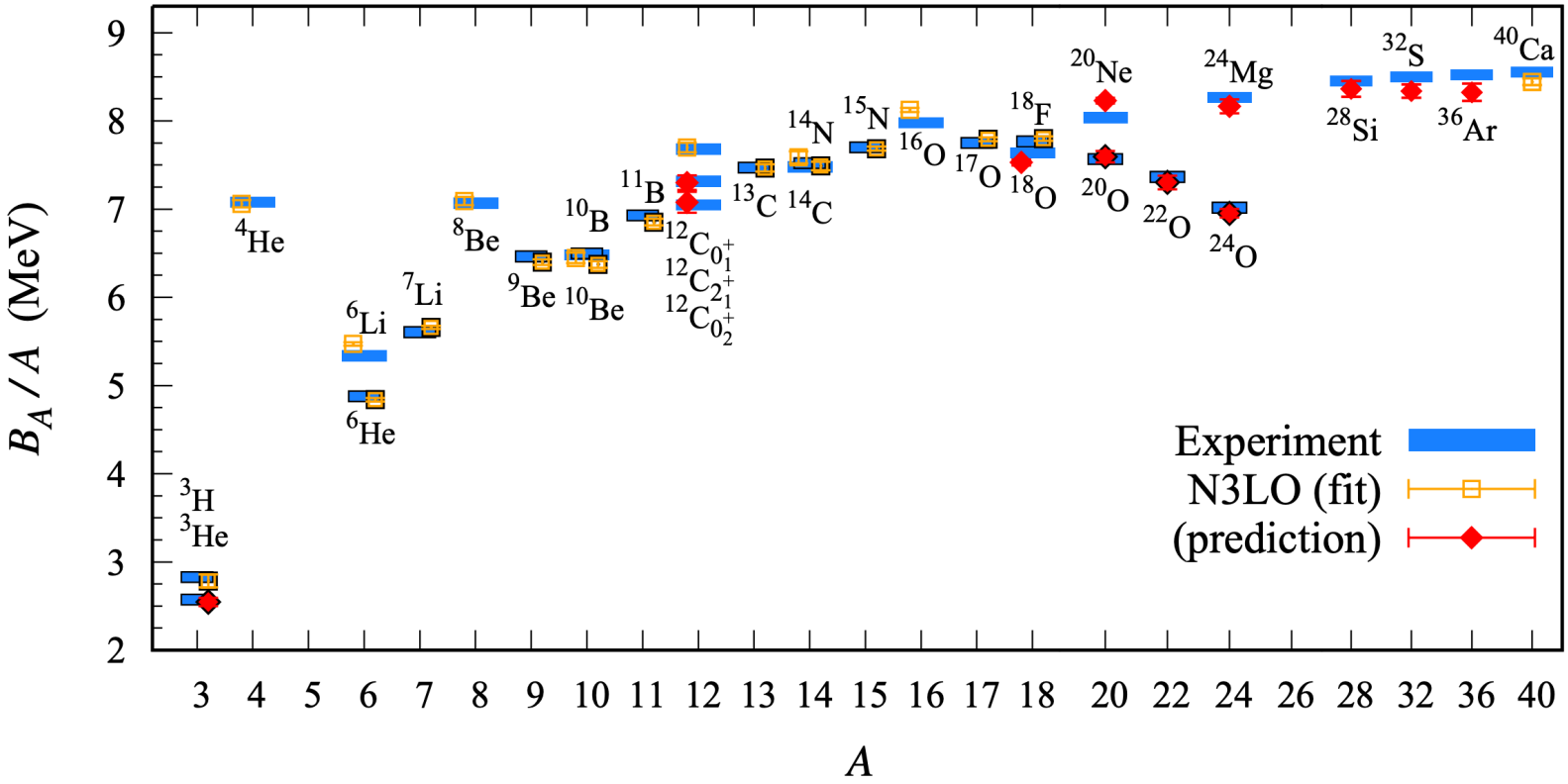
$R = 2.6$ fm

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

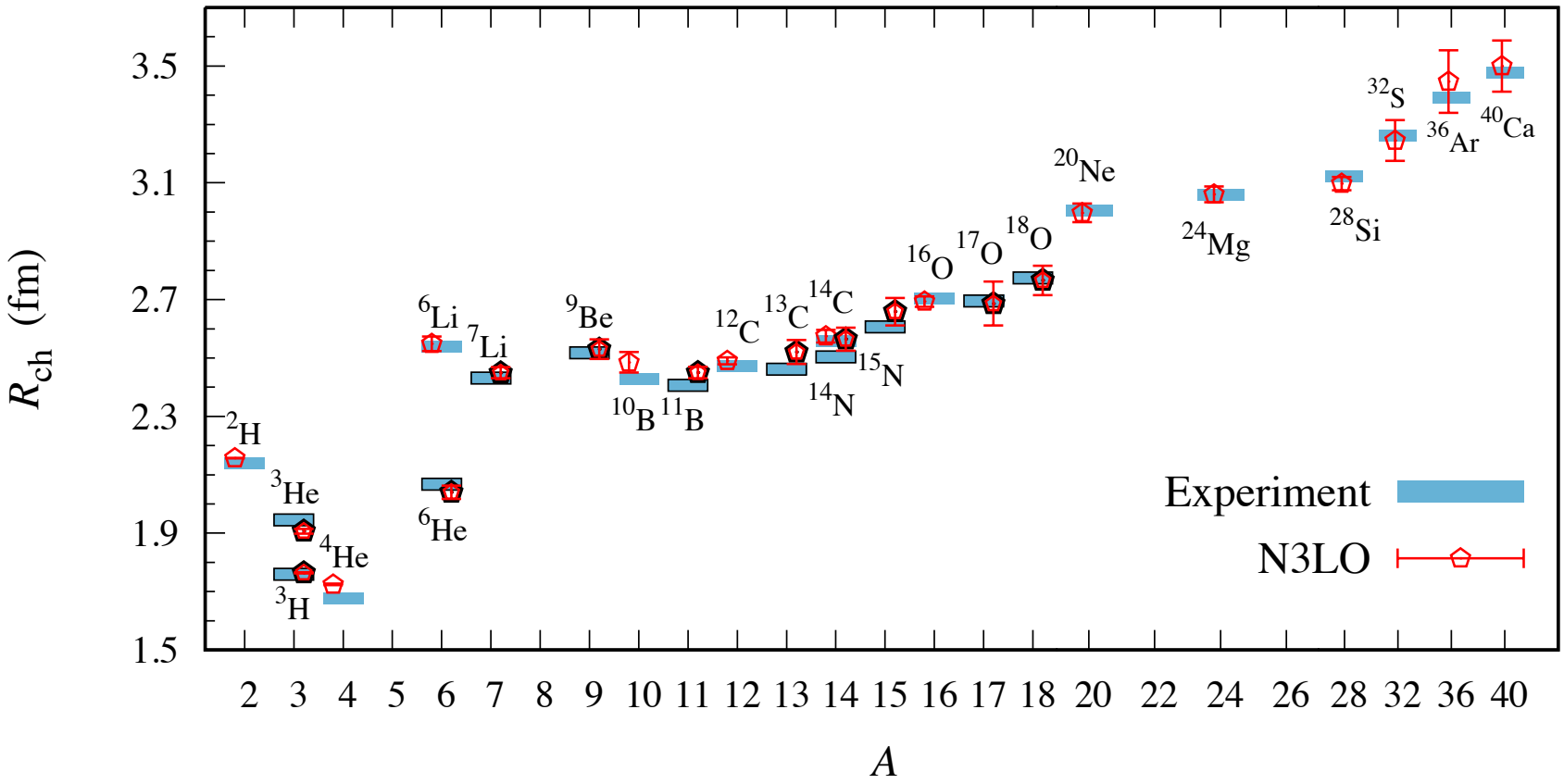


Binding energy per nucleon



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

See Yuanzhuo's talk later today on calculations of charge radii using a more computational efficient technique called the rank-one operator method. He will also present calculations of spin and density correlations in neutron matter relevant for neutrino scattering in core-collapse supernovae.

Neutron and nuclear matter

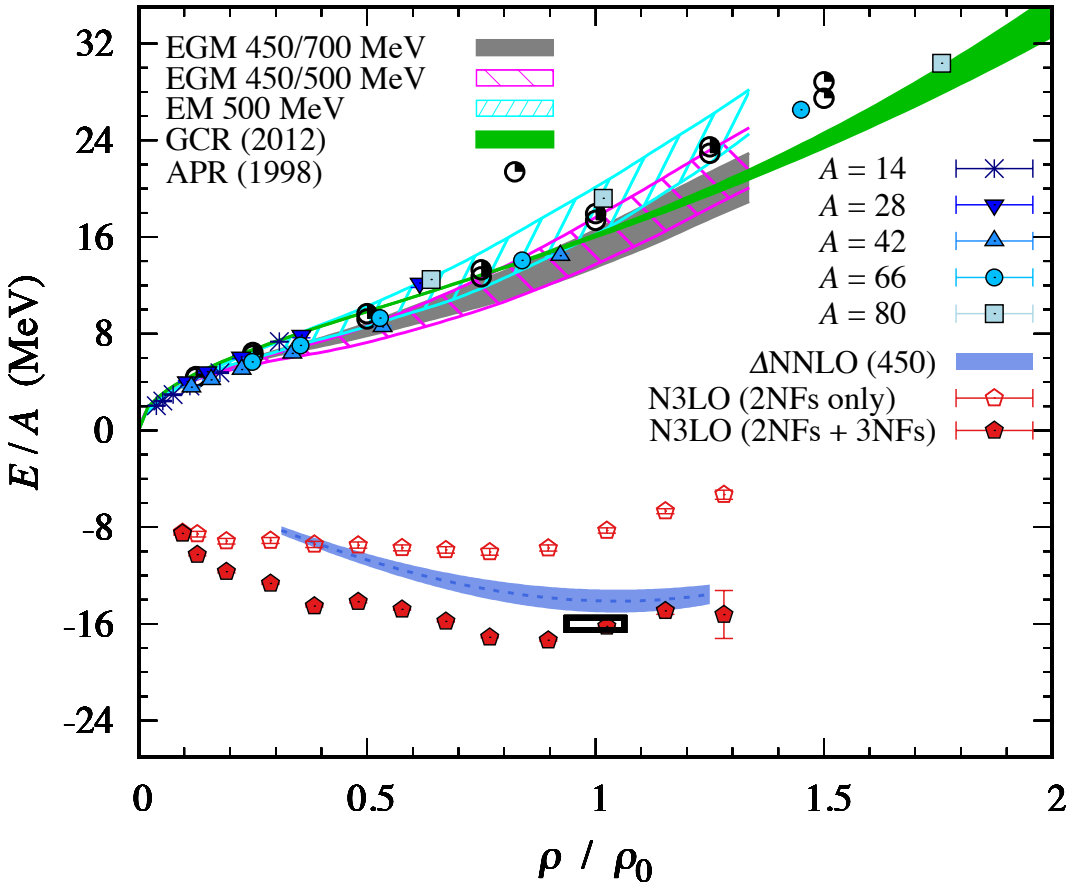
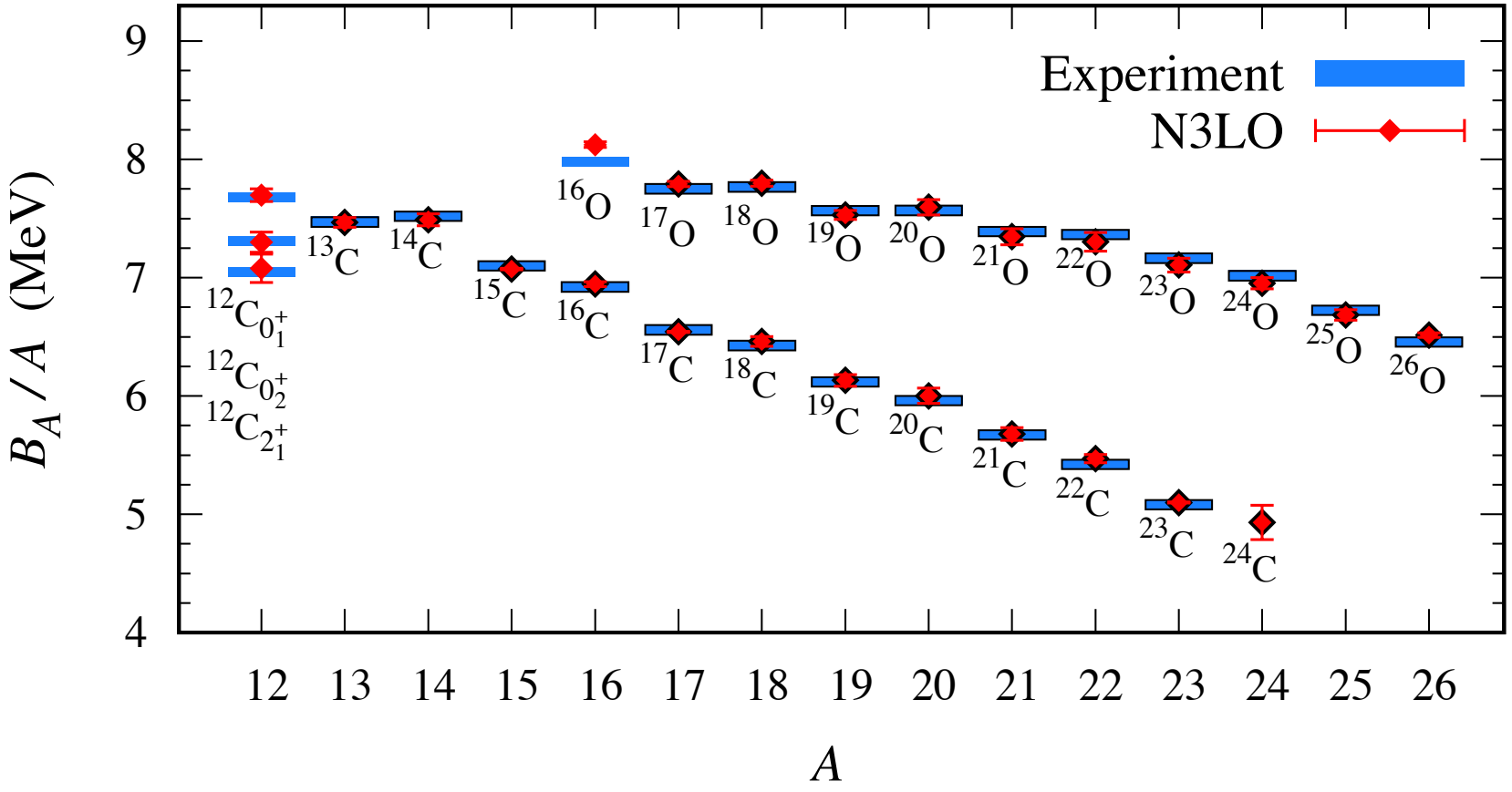


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

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



M. Kim, Y.-H. Song, Y. Kim, et al., work in progress

Unitarity limit

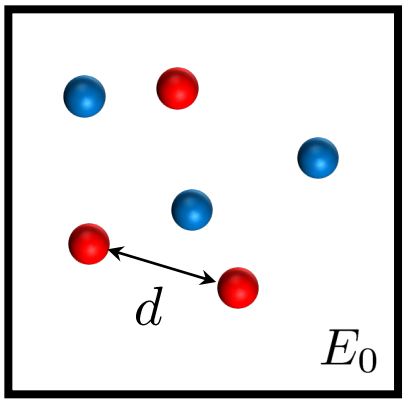
Consider S-wave two-body scattering in three dimensions at low momenta. The scattering amplitude is

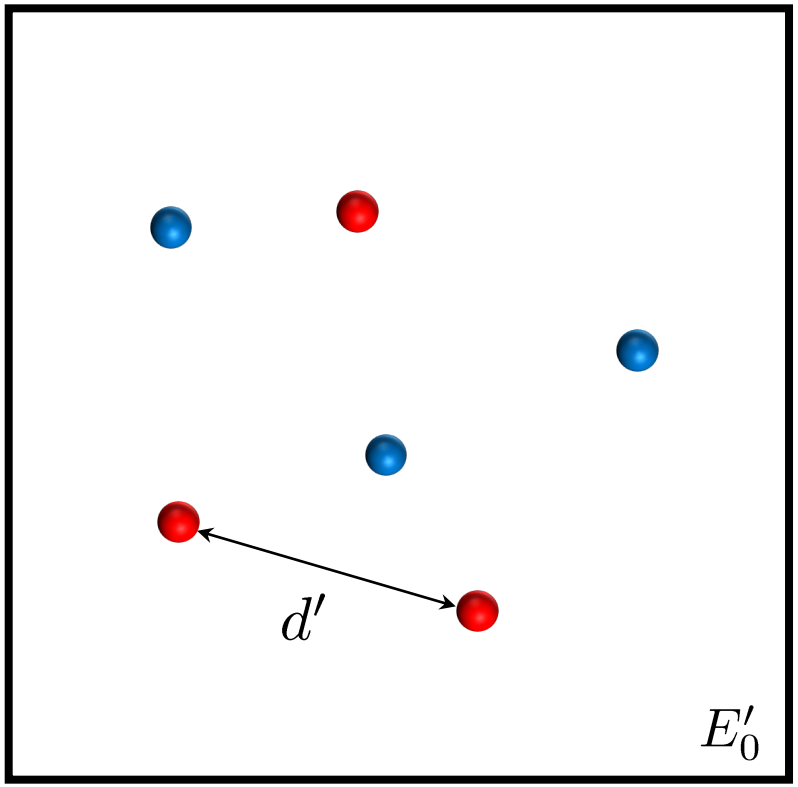
$$f_0(p) \propto \frac{1}{p \cot \delta_0(p) - ip}$$

The effective range expansion: $$p \cot \delta_0(p) = -\frac{1}{a_0} + \frac{1}{2} r_0 p^2 + \cdots$$

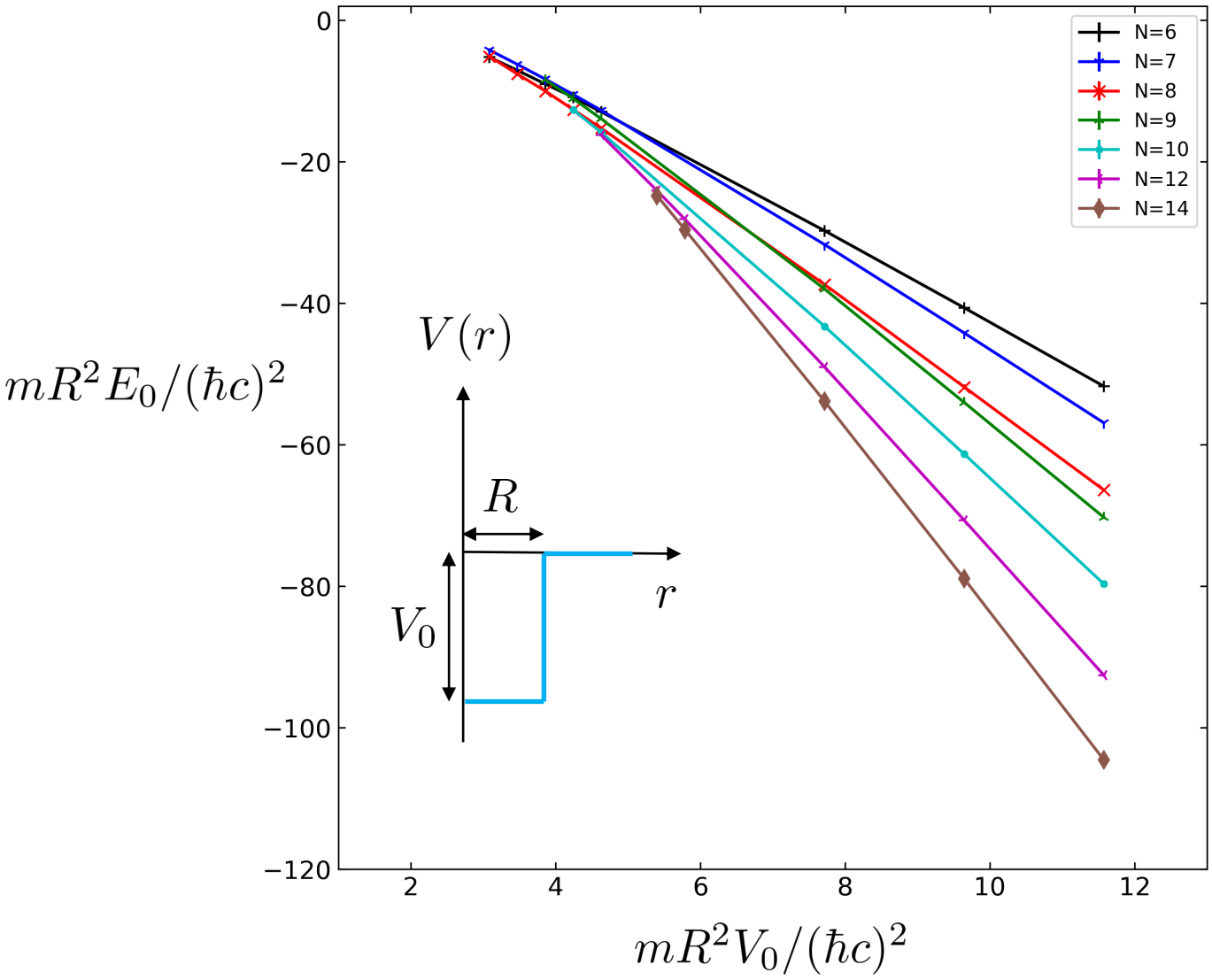
Consider when the scattering length a_0 is infinite. At low momenta, we get

$$p \cot \delta_0(p) \approx 0 \qquad f_0(p) \propto \frac{i}{p} \qquad \text{scale invariant physics}$$





$$E_0 d^2 = E_0' d'^2$$



M. Kim, Y.-H. Song, Y. Kim, et al., work in progress

Prospects and challenges

Nuclear physics is the materials science of subatomic particles. We are likely only scratching the surface of what is interesting and exciting. Breakthroughs are possible if we ask deep questions and inquire on the source of even small experimental deviations from our current theoretical understanding.

In the time remaining, the rest of this presentation is an informal oral summary of some future directions of the Nuclear Lattice Effective Field Theory Collaboration and connections with early high-profile experiments at FRIB.