Ab initio nuclear structure theory and connections to heavy-ion collisions

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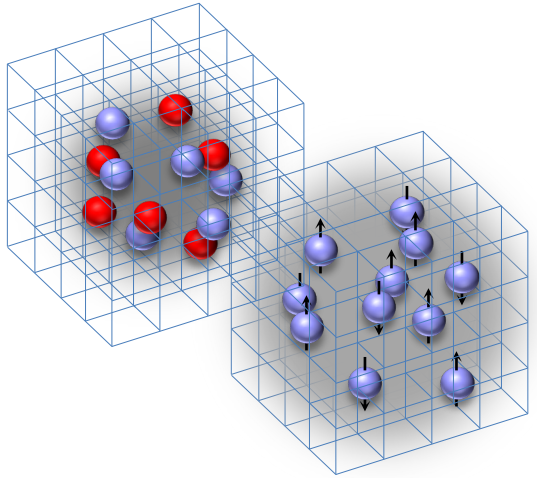

RBRC Workshop:
Physics Opportunities from the RHIC Isobar Run
January 25 – 28, 2022

FRIB

MICHIGAN STATE UNIVERSITY

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project

JÜLICH FORSCHUNGSZENTRUM

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

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Ab initio methods

Lattice effective field theory

Hidden spin-isospin exchange symmetry

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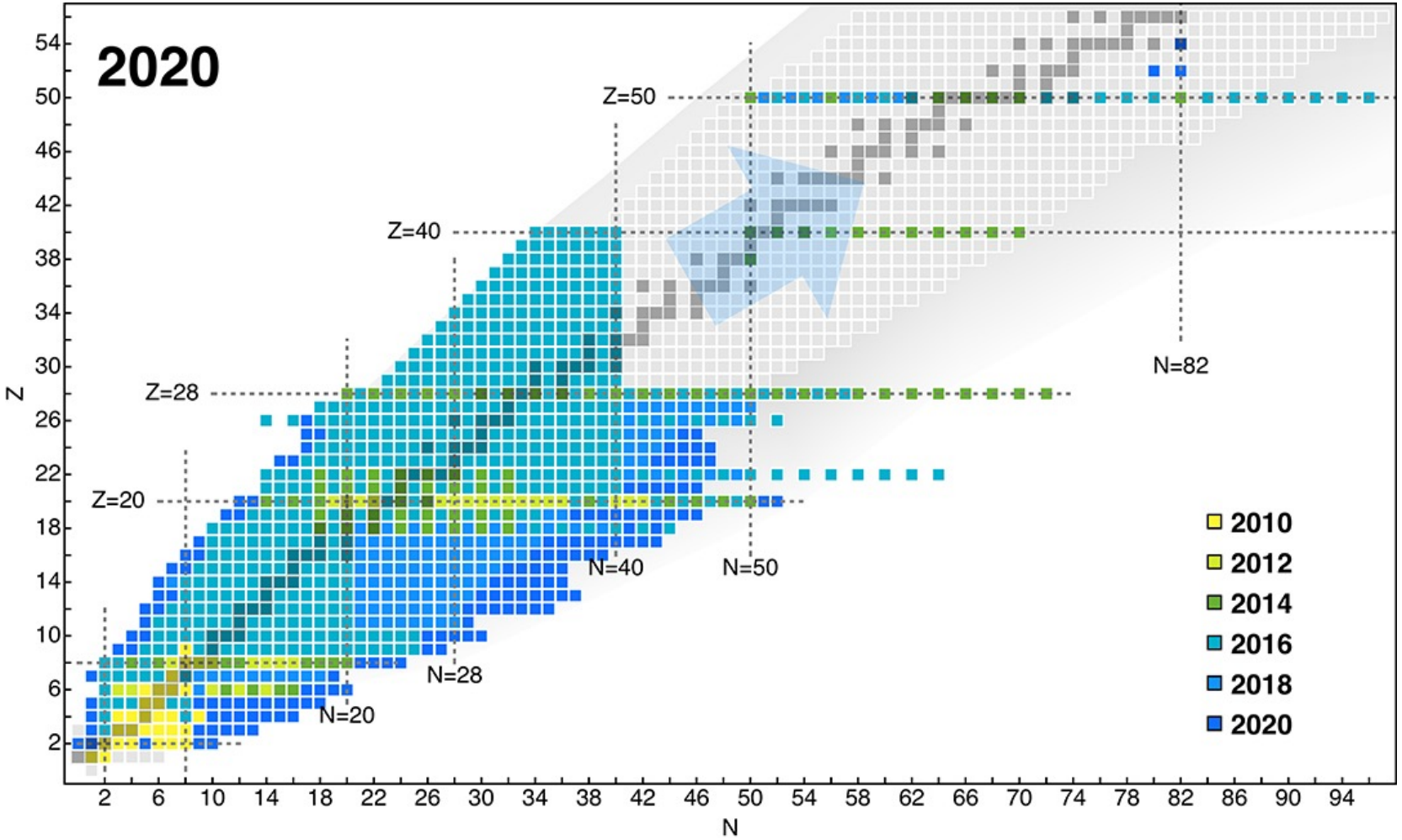
Ab initio methods



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

Many-Body Perturbation Theory

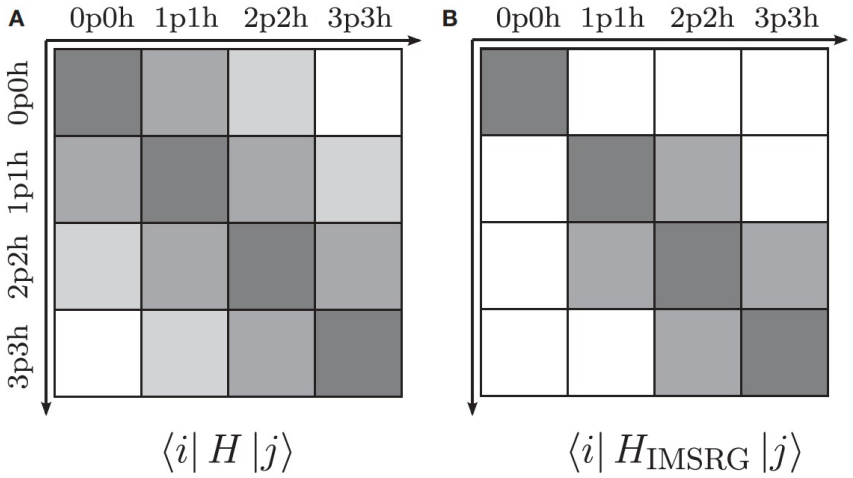
[Roth et al., Phys. Lett. B683, 272 (2010); Tichai et al., Phys. B756, 283 (2016)]

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

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

In-Medium Similarity Renormalization Group

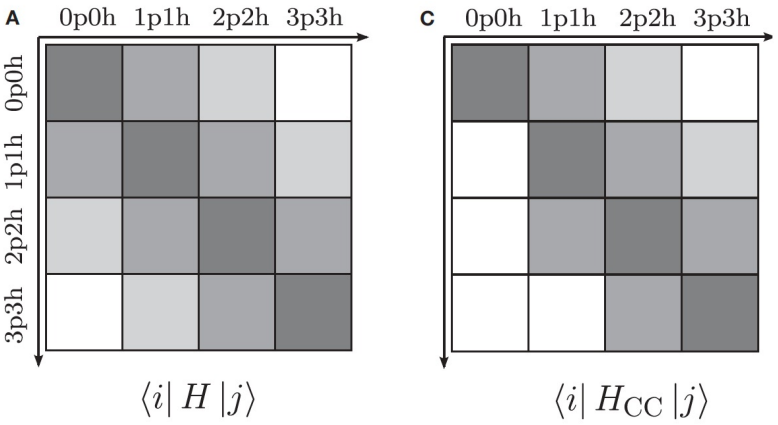
[Hergert et al., Phys. Rev. 621, 165 (2016); Stroberg et al., Phys. Rev. Lett. 118, 032502 (2017)]



[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)]

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

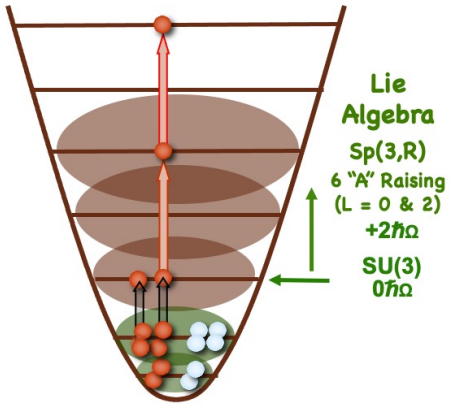
No-Core Configuration Interaction

[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)]



[From Jerry Draayer's talk]

Monte Carlo Shell Model

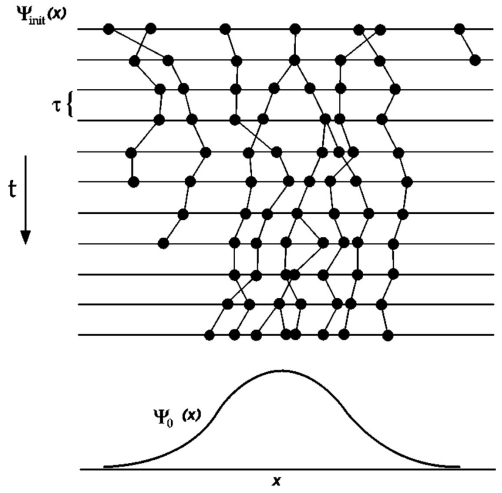
[Otsuka et al., Prog. Part. Nucl. Phys. 47, 319 (2001), Shimizu Phys. Scripta. 92, 063001 (2017)]

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

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

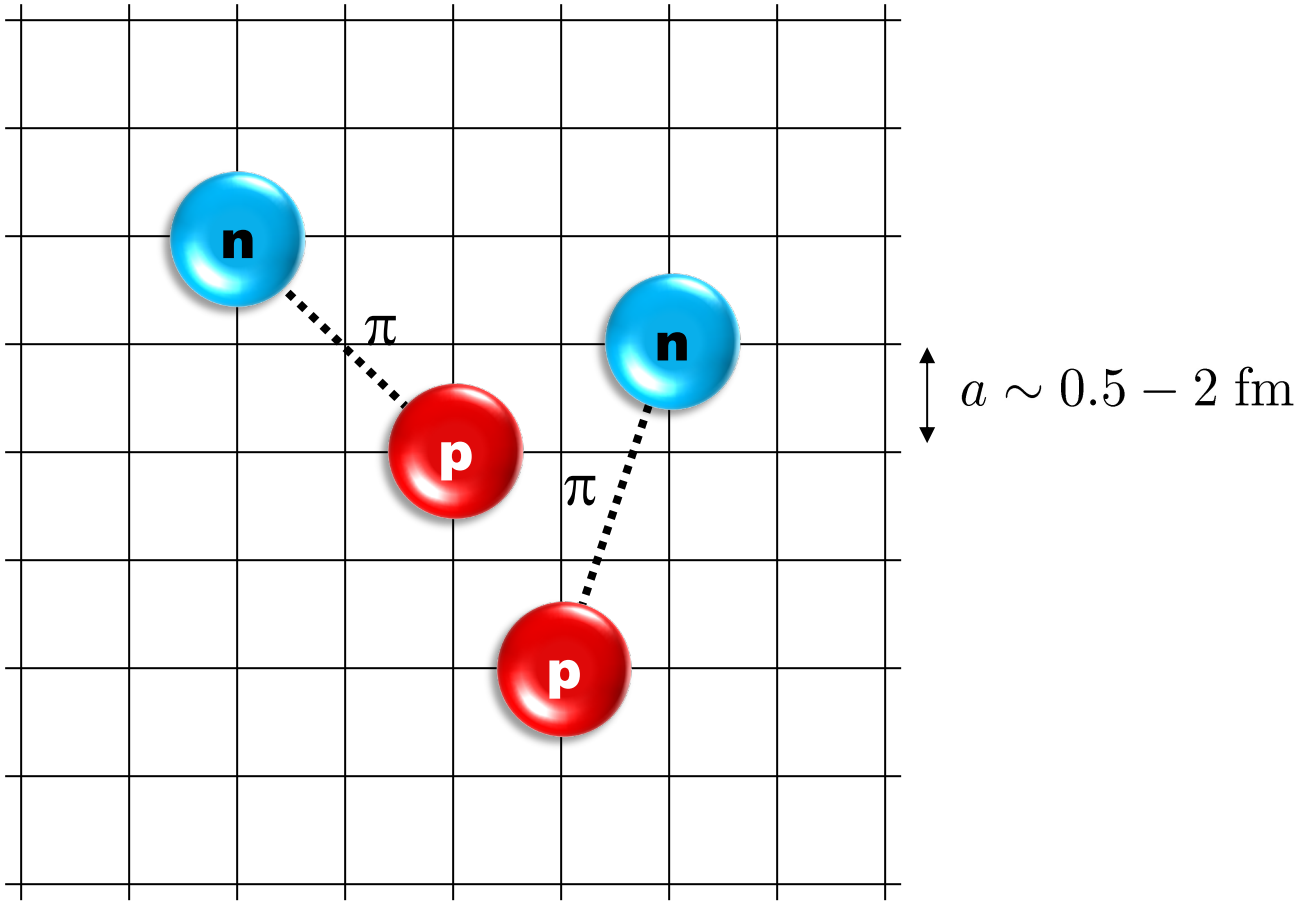
Quantum Monte Carlo

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



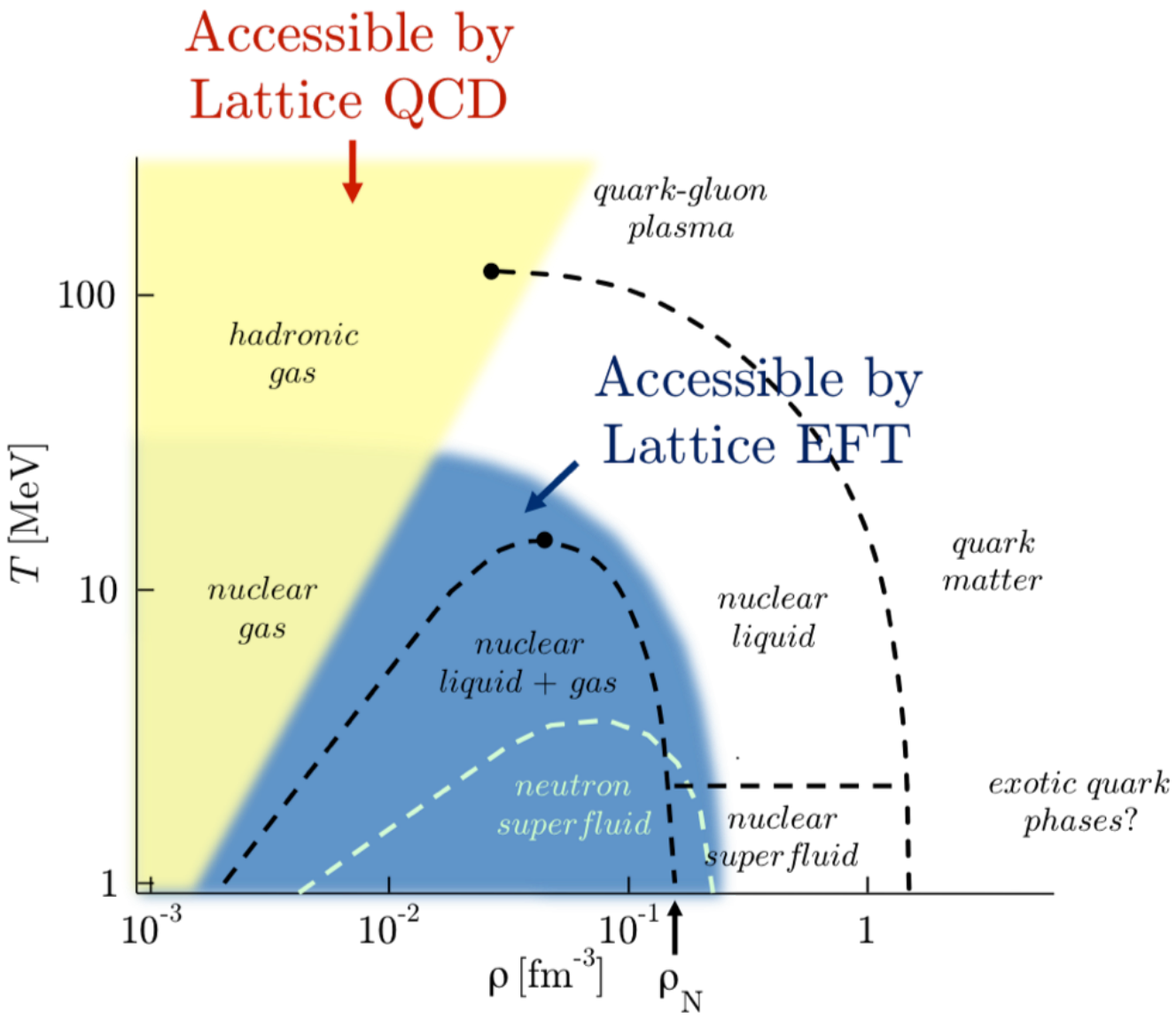
[Foulkes et al., Rev. Mod. Phys. 73, 1 (2001)]

Lattice effective field theory



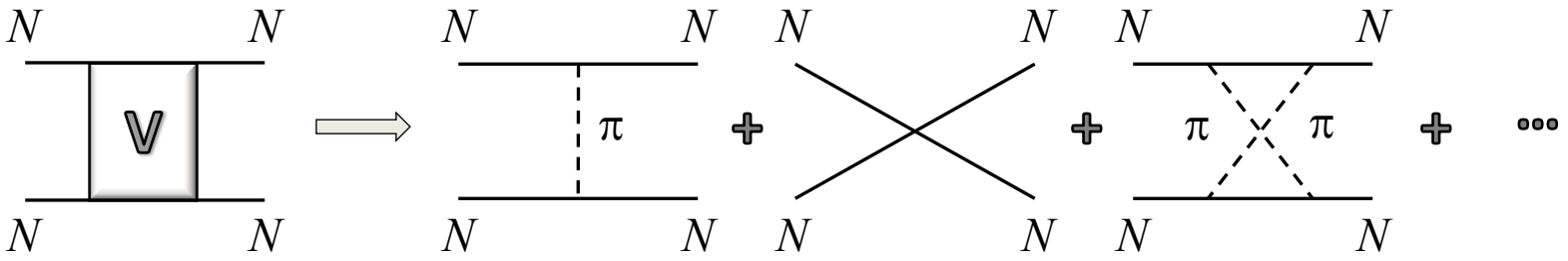
[D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)]

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


Accessible by
Lattice QCD
quark-gluon
plasma
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

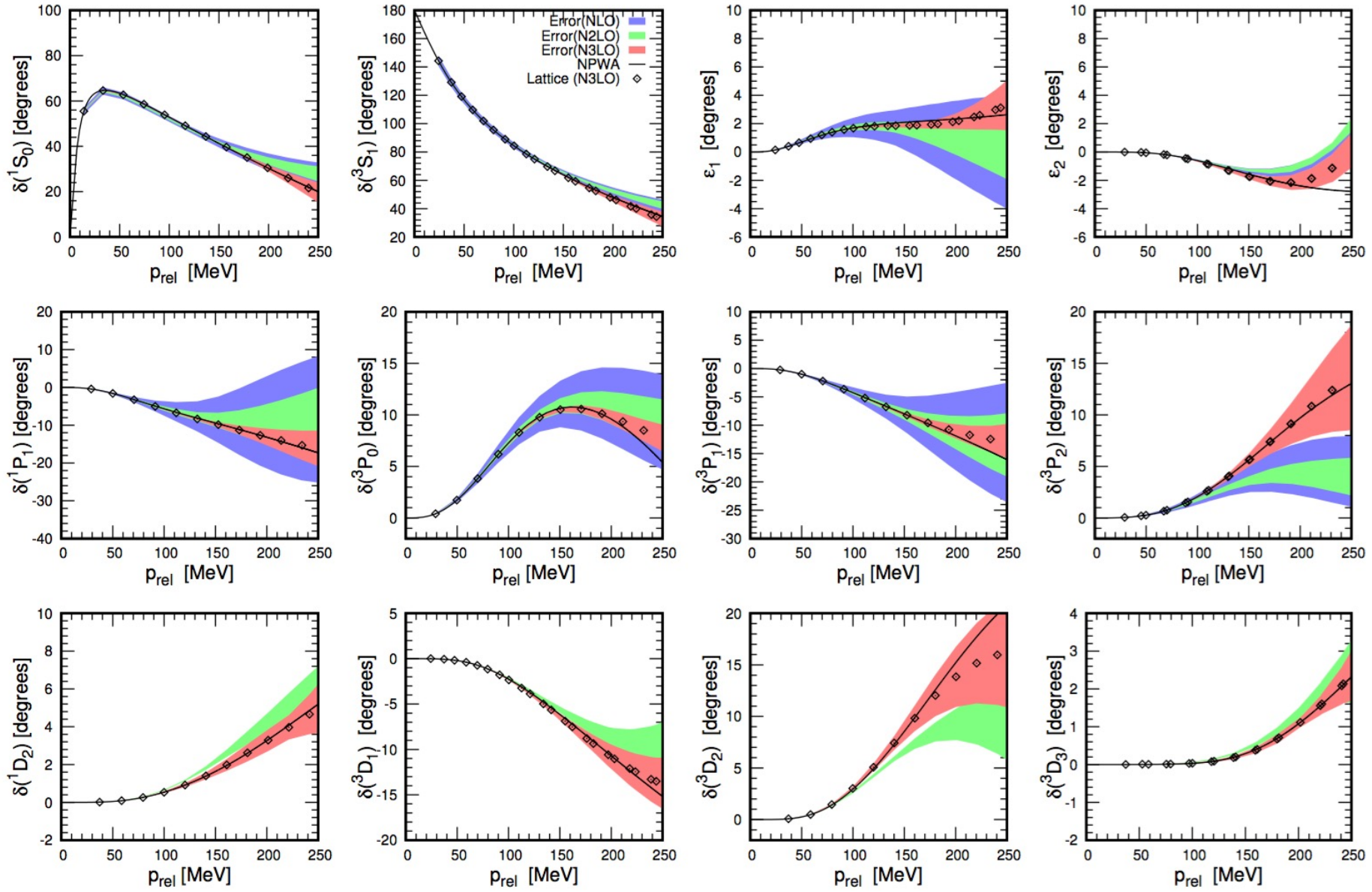
Construct the effective potential order by order



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

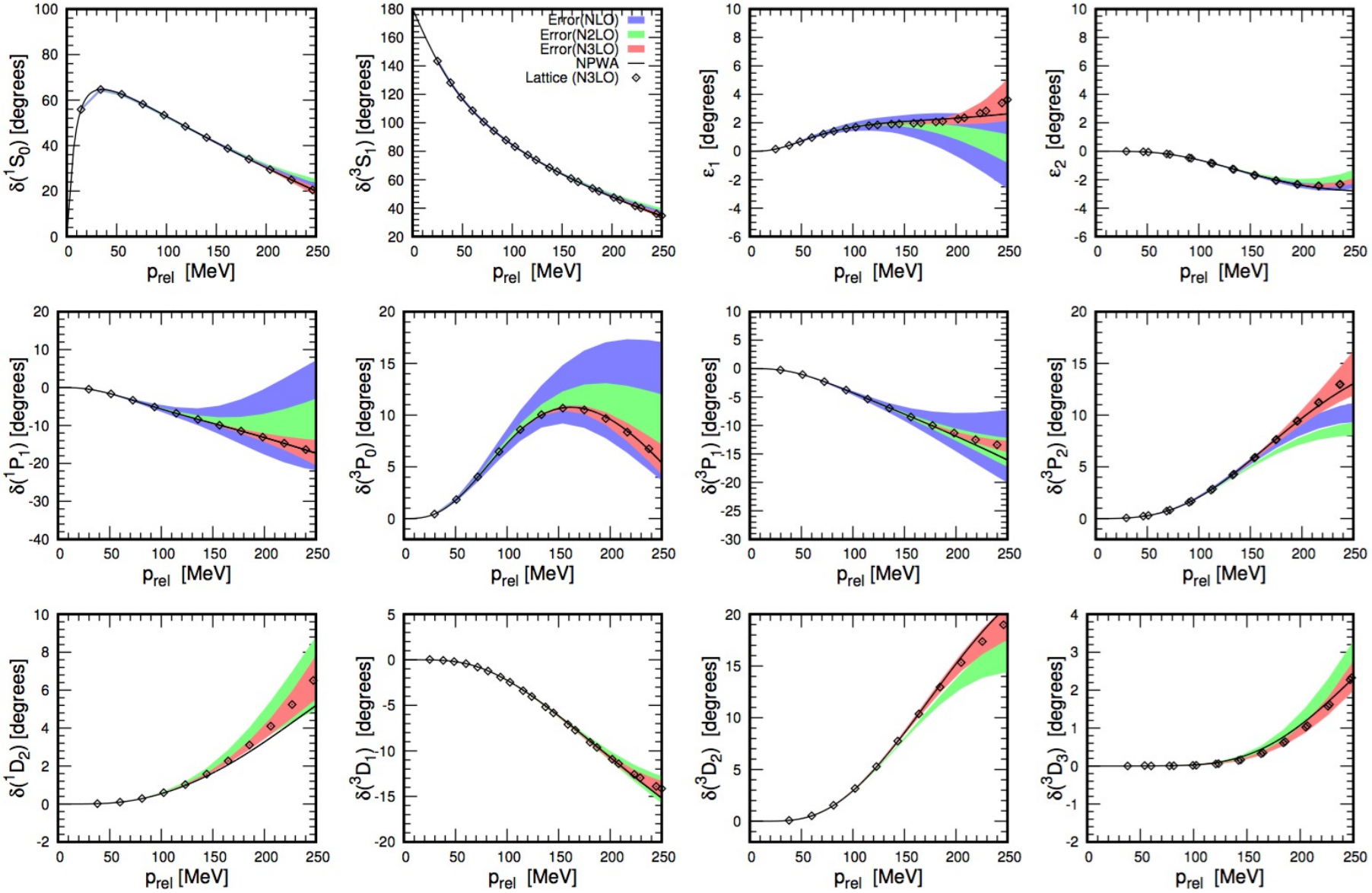
Leading order (LO) Next-to-leading order (NLO)

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

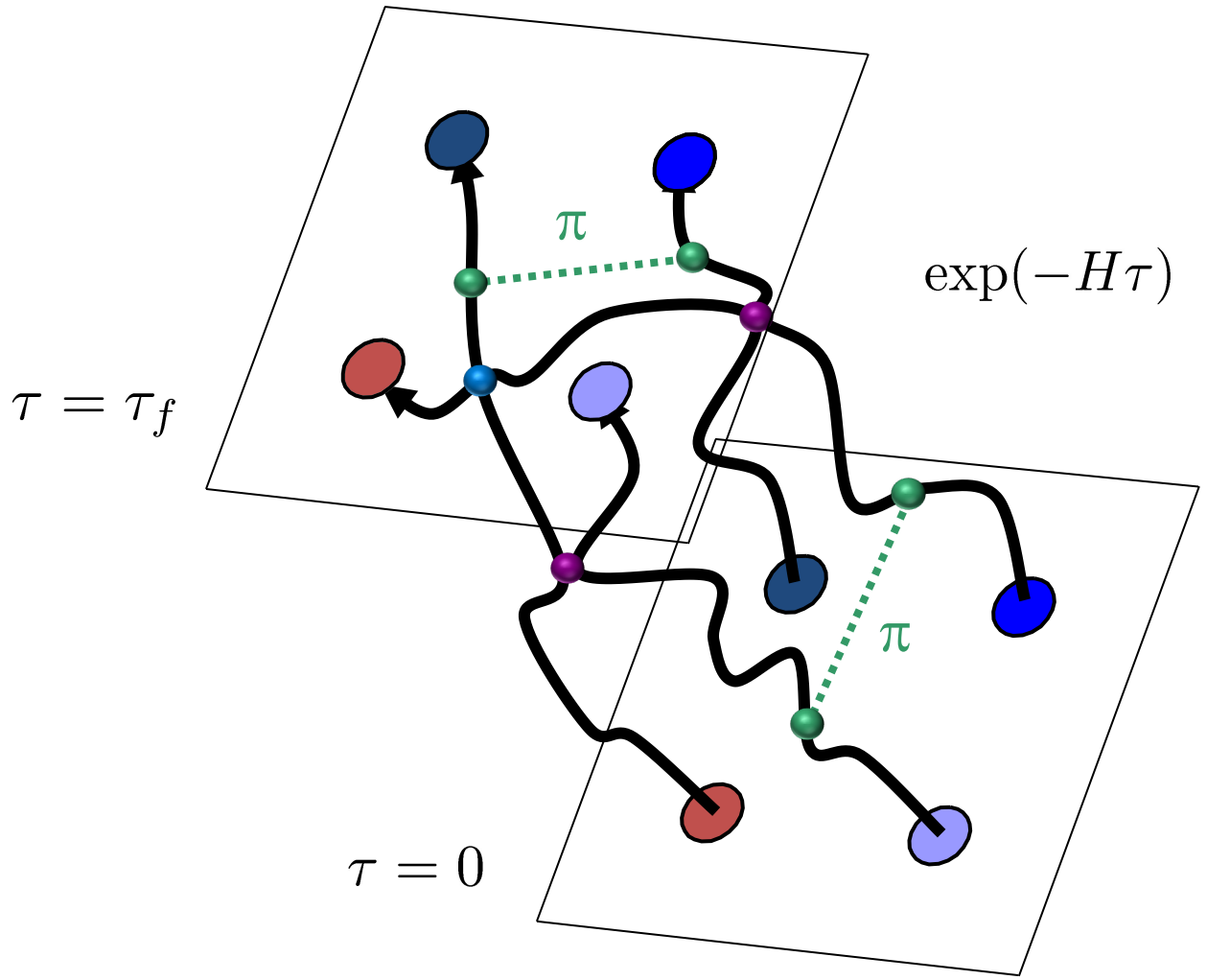


[Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)]

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



Euclidean time projection



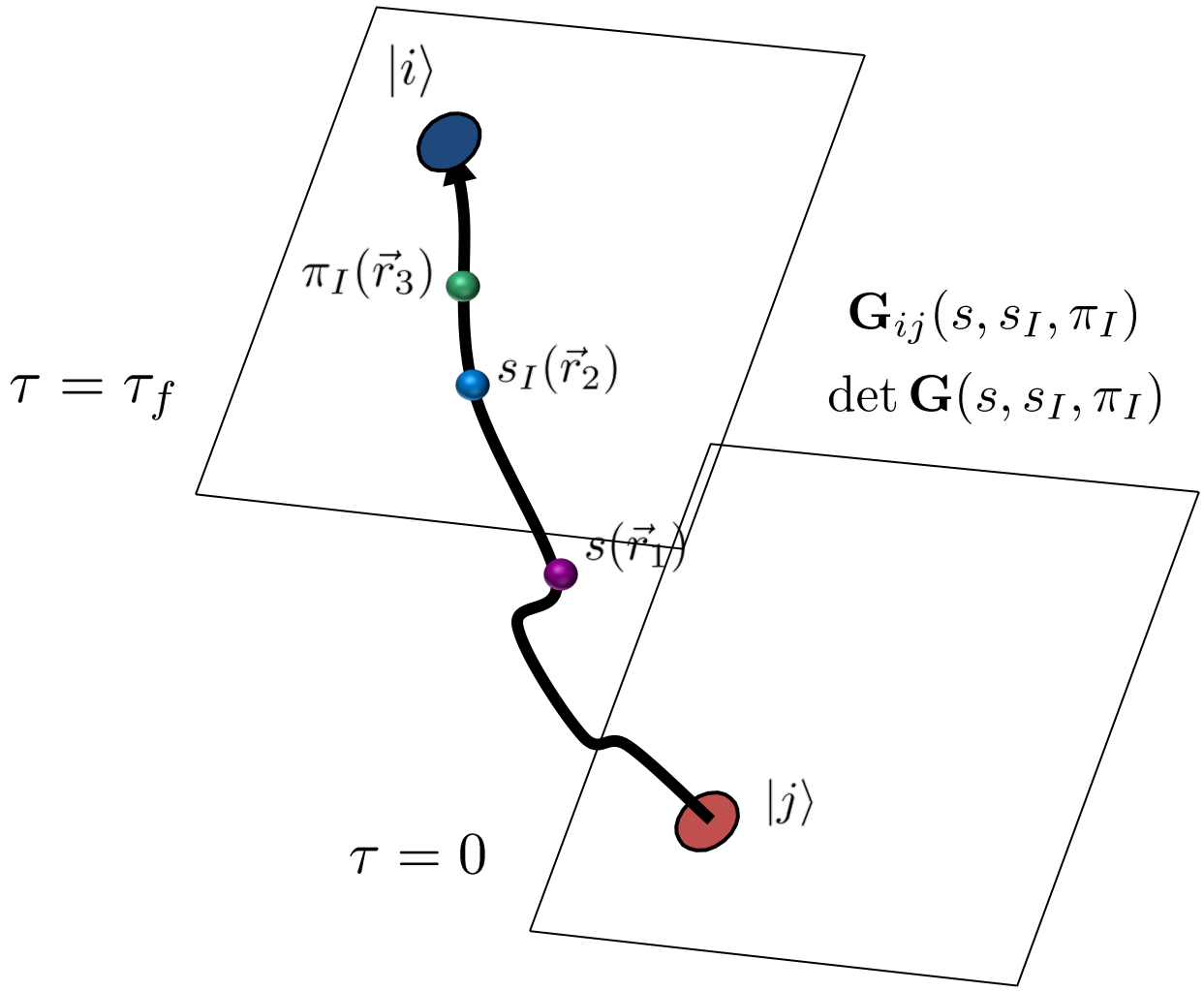
Auxiliary field method

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

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

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

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


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

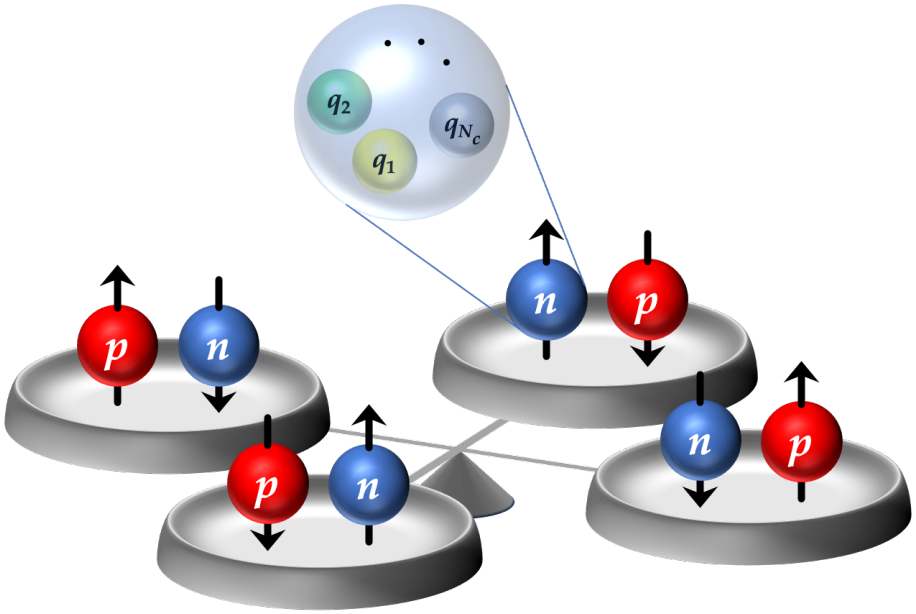
Hidden spin-isospin exchange symmetry

Kaplan, Savage, PLB 365, 244 (1996)

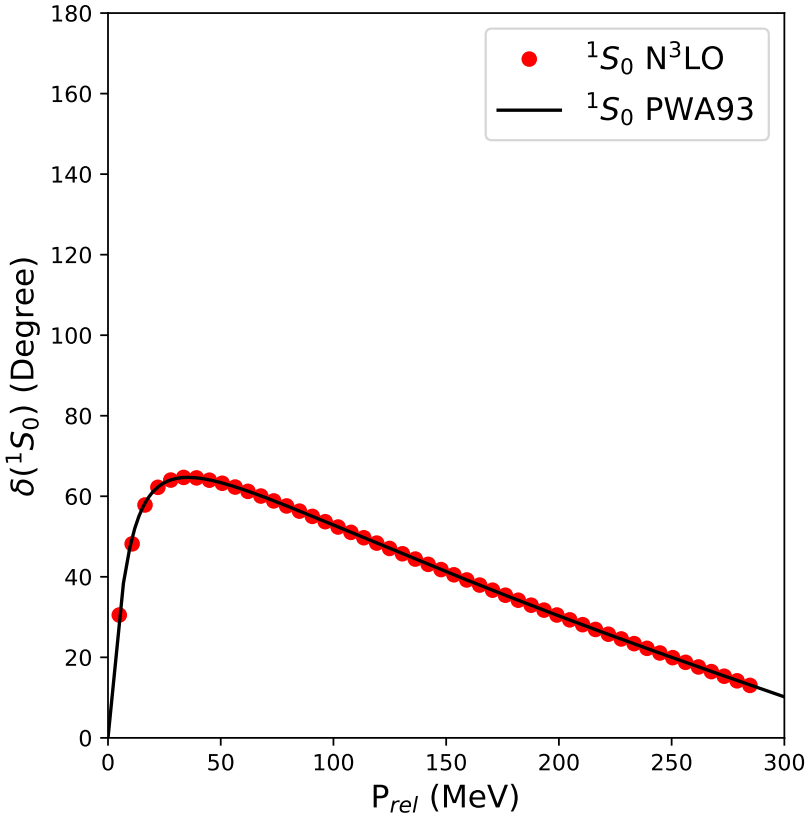
Kaplan, Manohar, PRC 56, 76 (1997)

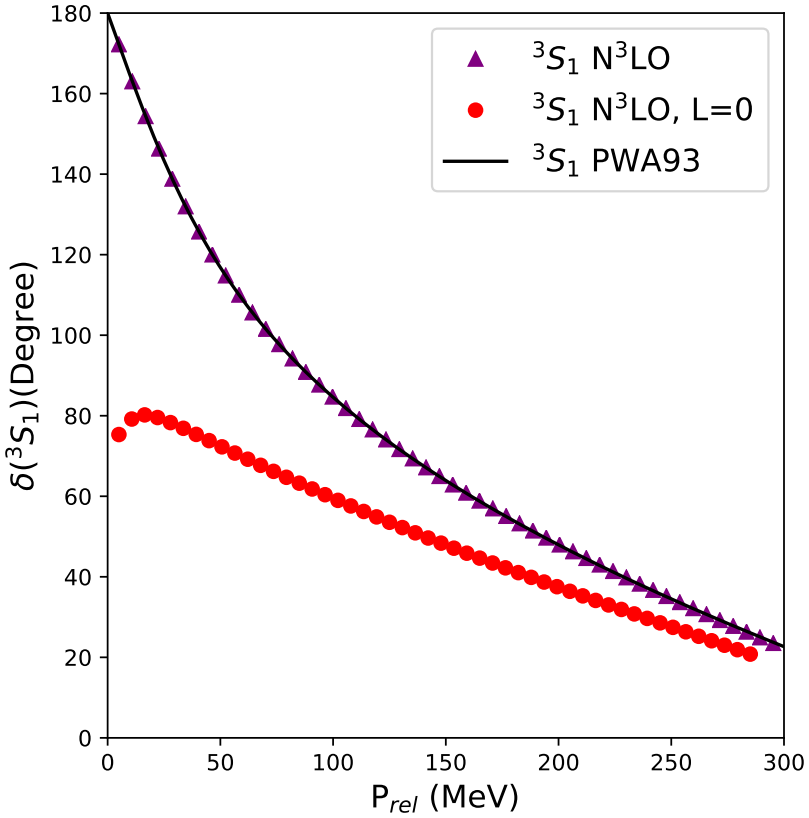
Calle Gordon, Arriola, PRC 80, 014002 (2009)

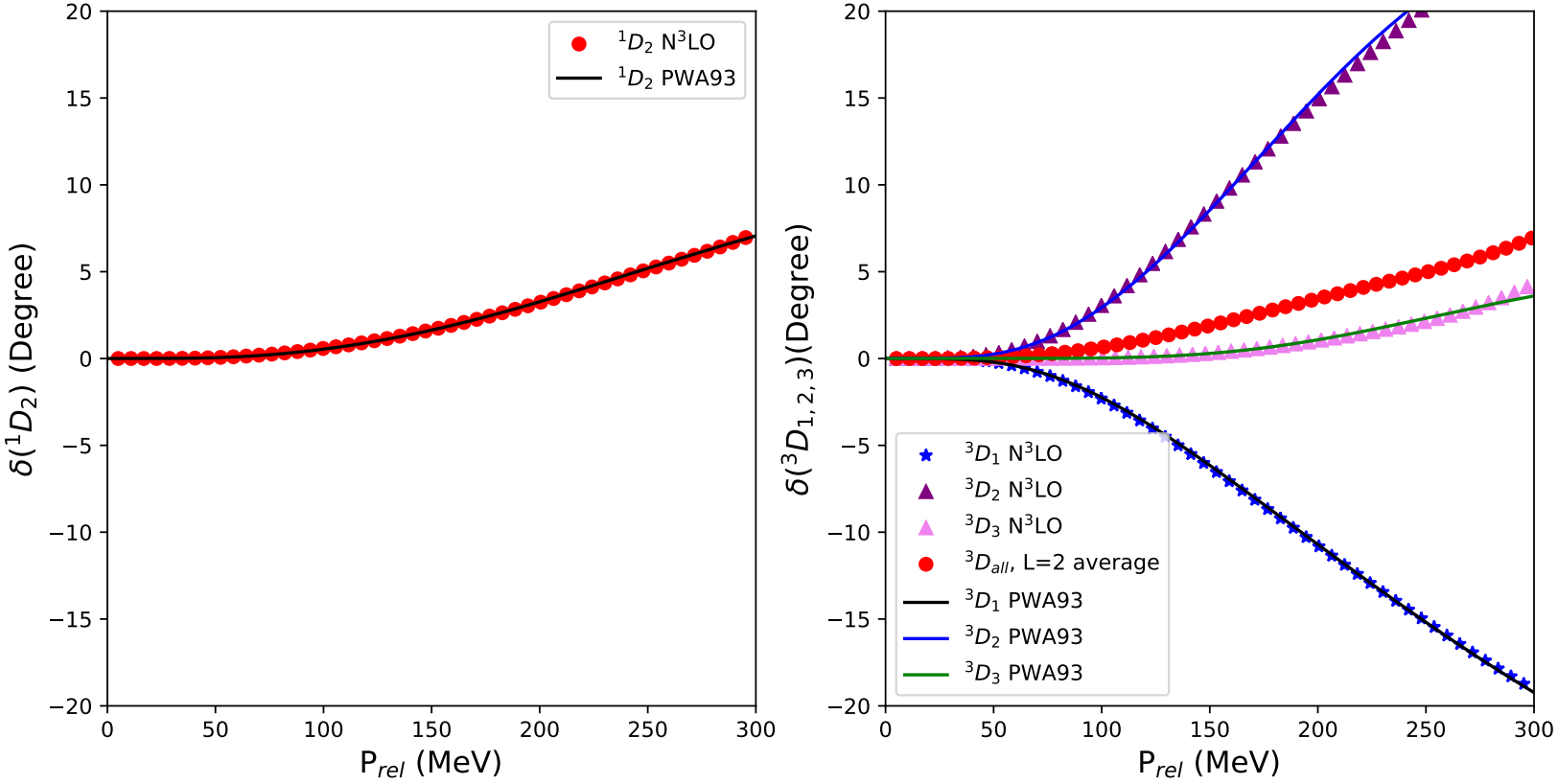
$$V^{2N}_{\text{large}-N_c} = V_C + \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 W_S + (3\hat{r} \cdot \vec{\sigma}_1 \hat{r} \cdot \vec{\sigma}_2 - \vec{\sigma}_1 \cdot \vec{\sigma}_2)\vec{\tau}_1 \cdot \vec{\tau}_2 W_T$$



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


$^1S_0$ N^{3}LO
$^1S_0$ PWA93
$\delta(^1S_0)$ (Degree)
P_{rel} (MeV)
0
20
40
60
80
100
120
140
160
180
0
50
100
150
200
250
300


$^3S_1$ N^{3}LO
$^3S_1$ N^{3}LO, L=0
$^3S_1$ PWA93
$\delta(^3S_1)$(Degree)
P_{rel} (MeV)
0
20
40
60
80
100
120
140
160
180
0
50
100
150
200
250
300



[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?

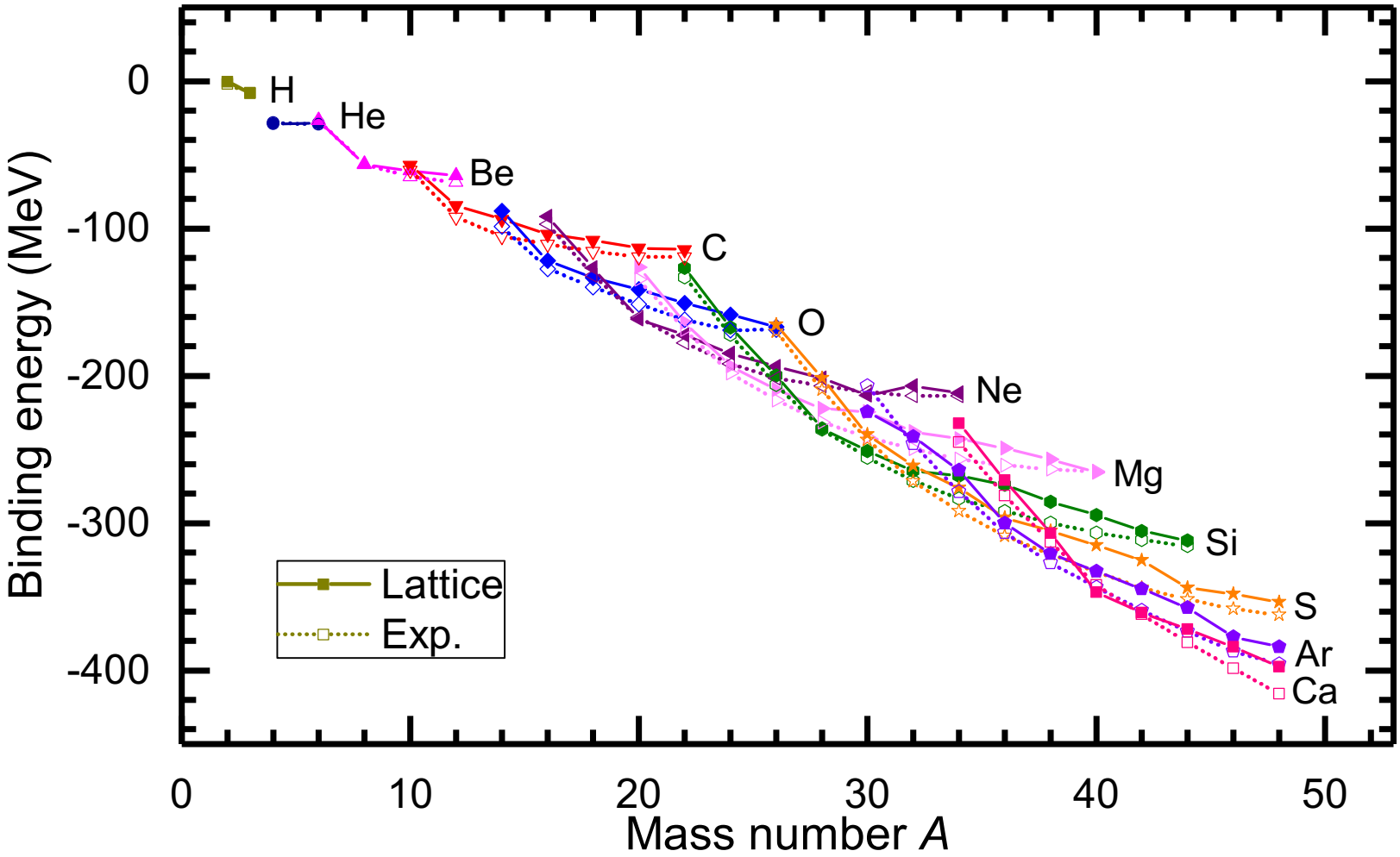
We construct an interaction with only four parameters.

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

fit to $A = 2$, 3 systems

4. Range of the local part of the two-nucleon interaction

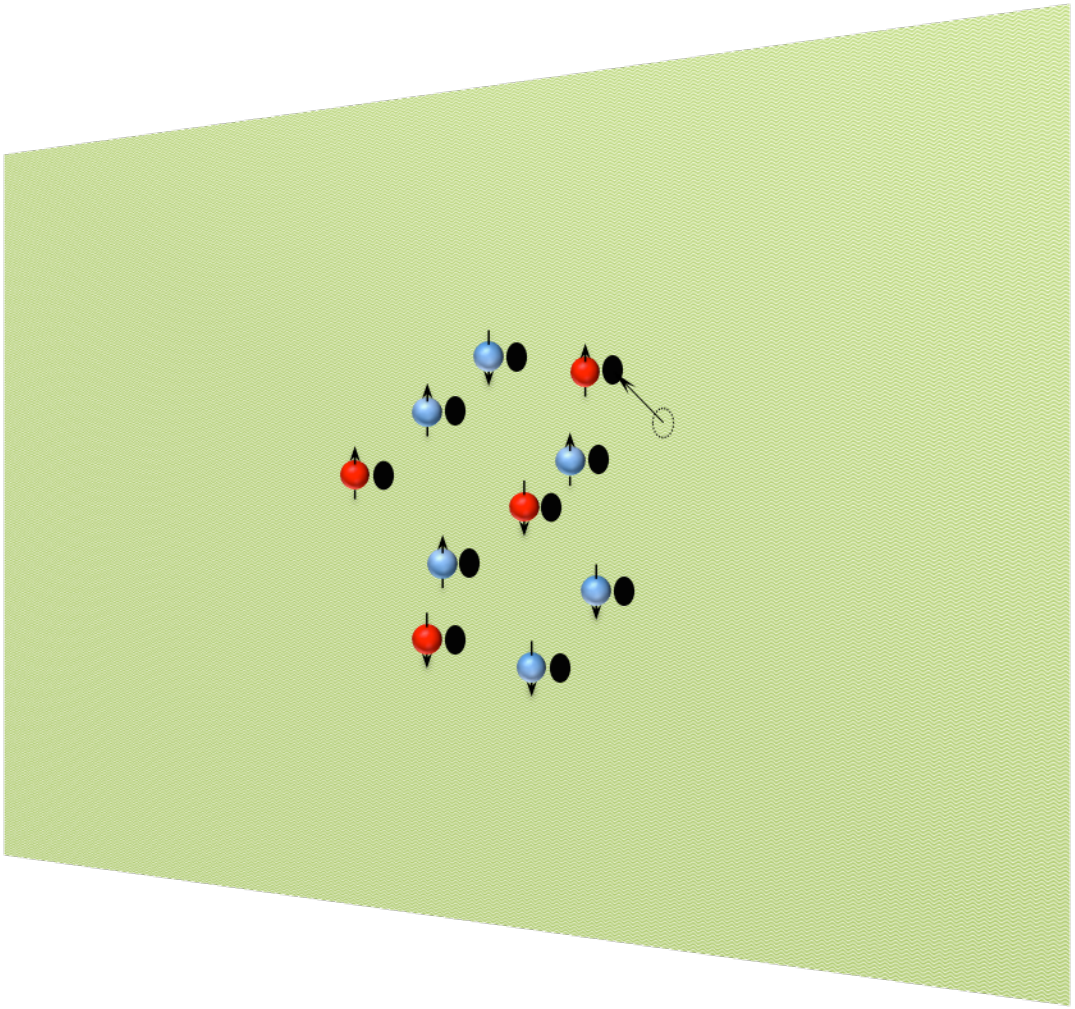
fit to A > 3



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

	B	Exp.	$R_{\rm ch}$	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

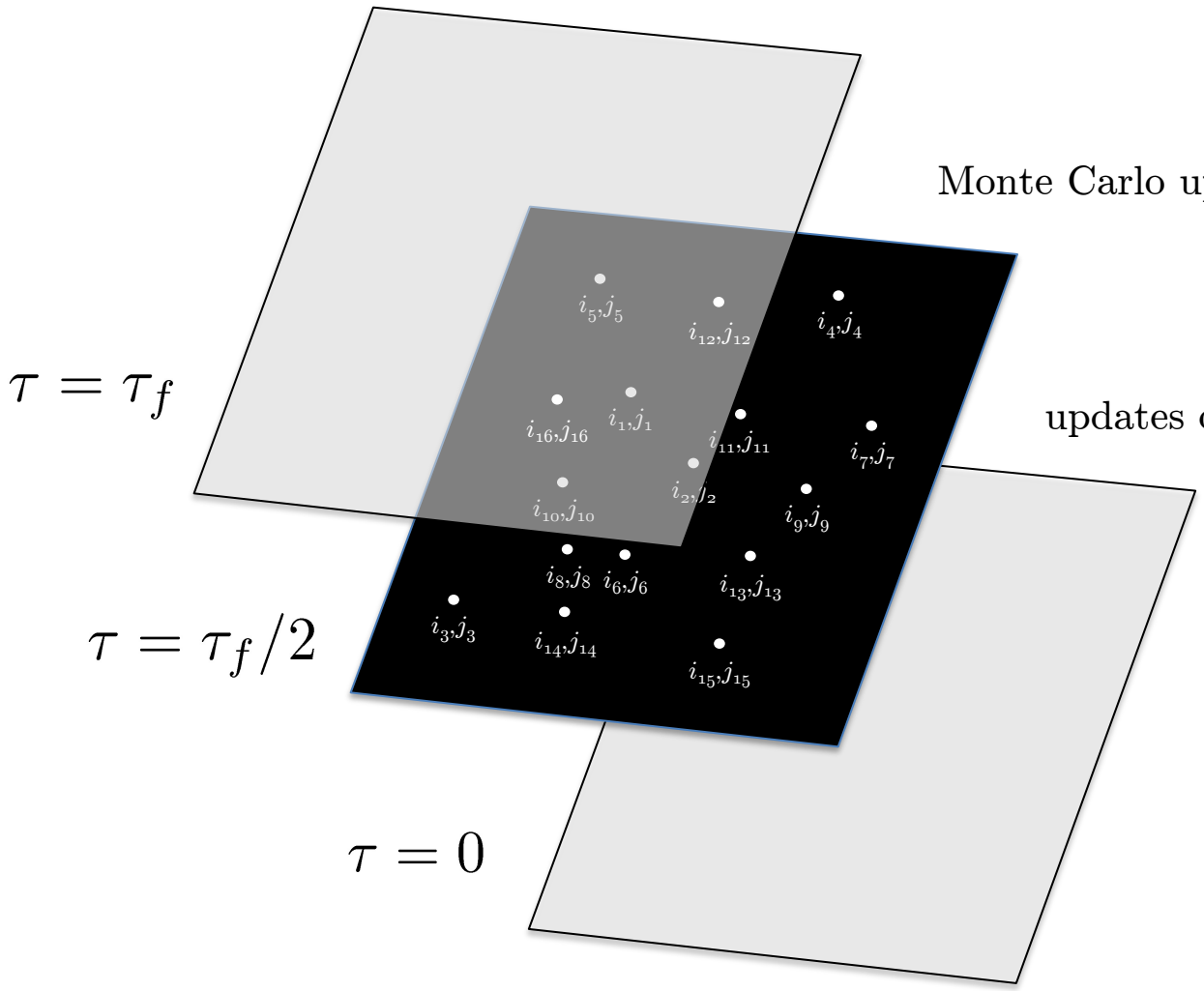
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

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

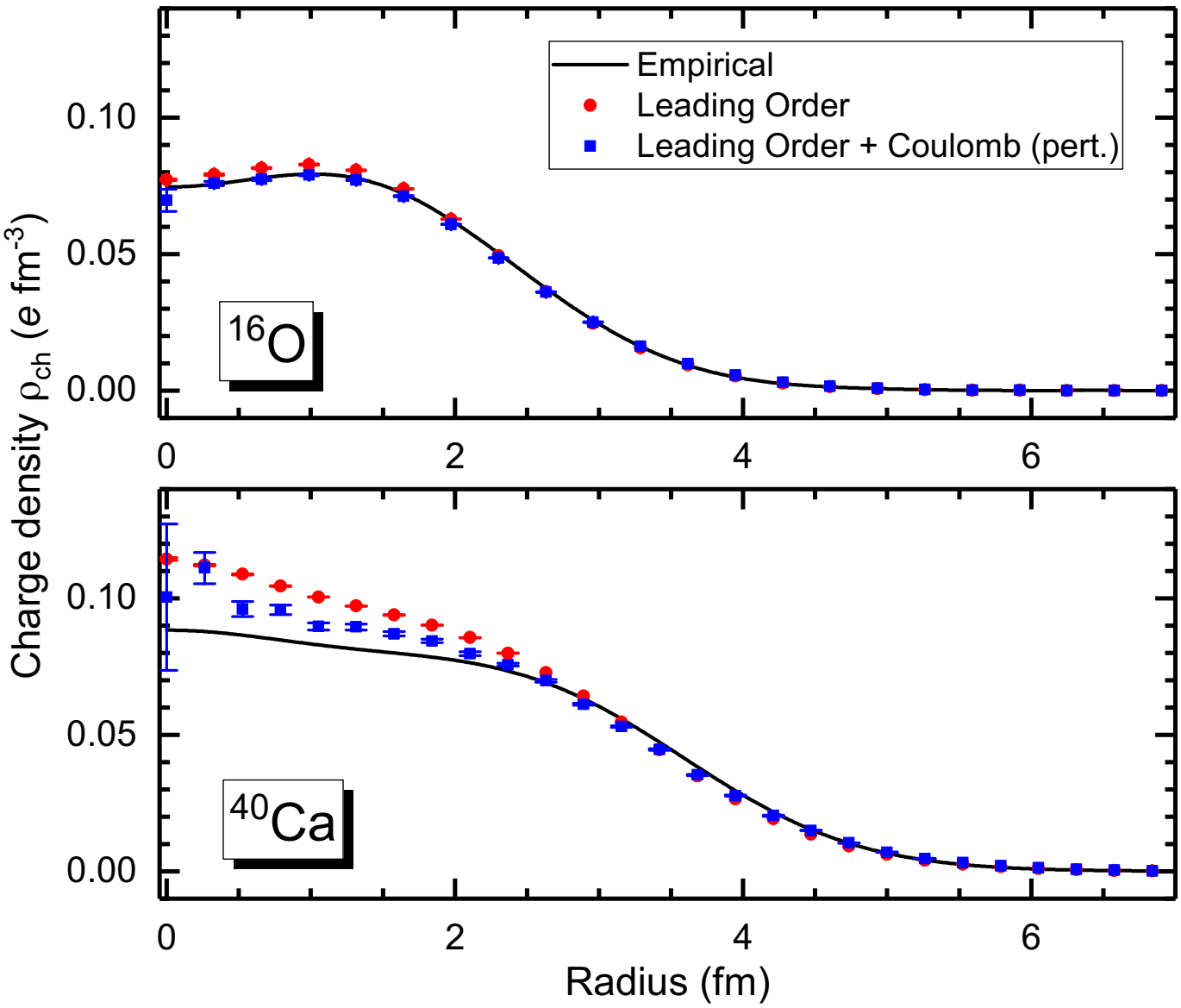
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$



Monte Carlo updates of pinholes

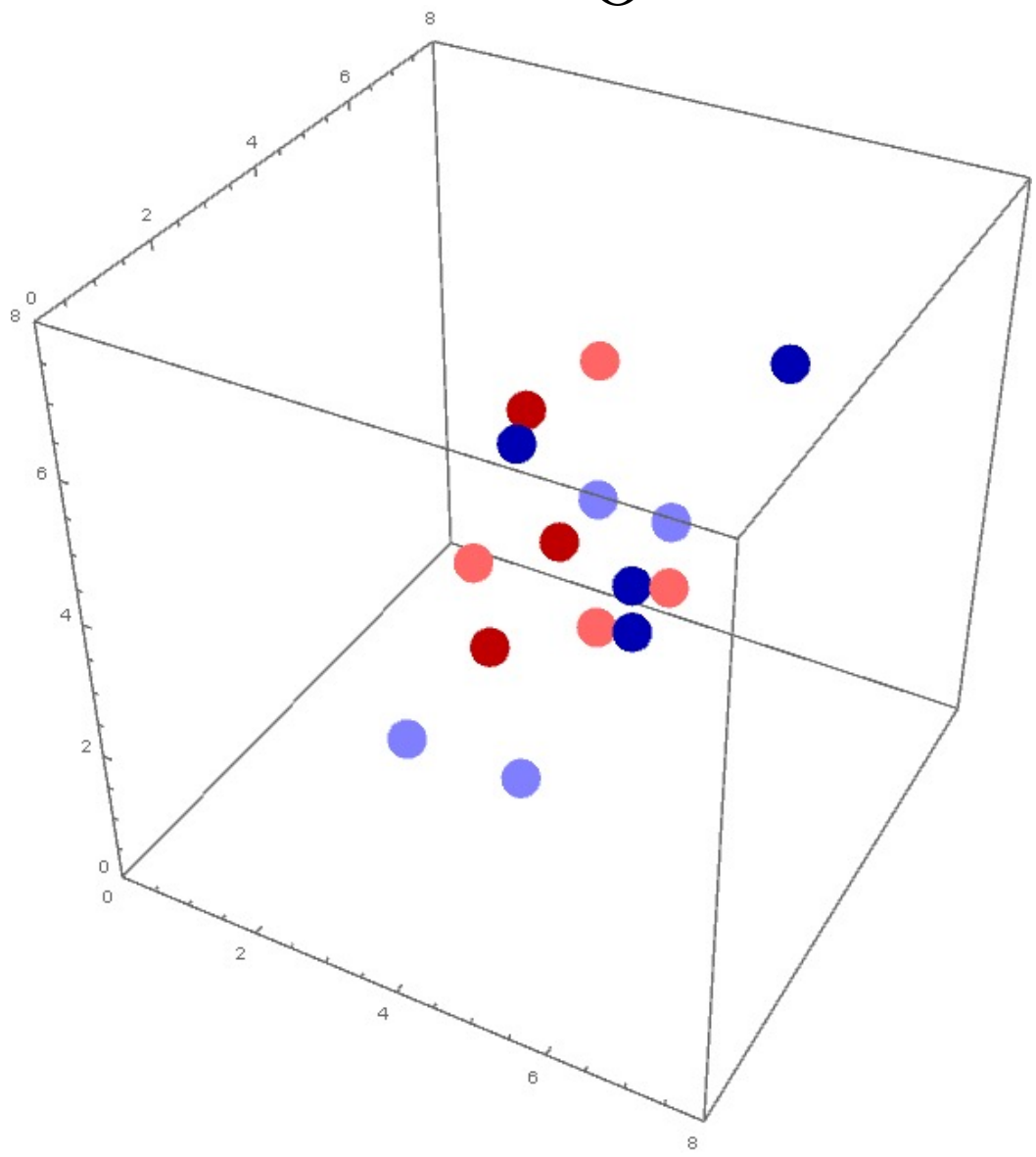
Monte Carlo
updates of auxiliary/pion fields

]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)]

^{16}O



- proton up
- proton down
- neutron up
- neutron down

^{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 RHIC and 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 *p*Pb 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_RENTo 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:

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

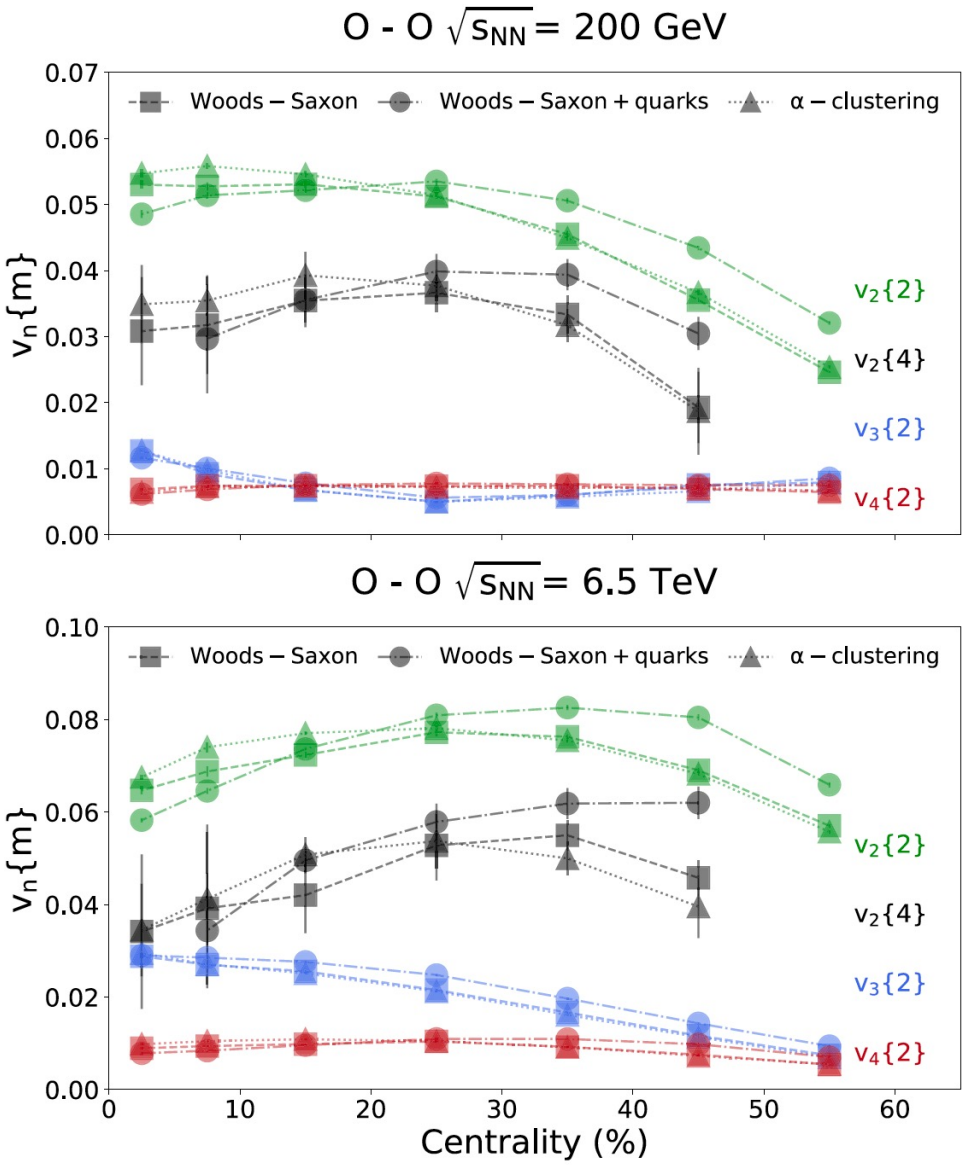
We first compute results taking the initial density as a Woods-Saxon potential with density, radius, and diffusive fitted to empirical values. We then consider the same Woods-Saxon potential, taking into account the quark substructure of the nucleons. Lastly, we consider using the nucleon distribution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

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

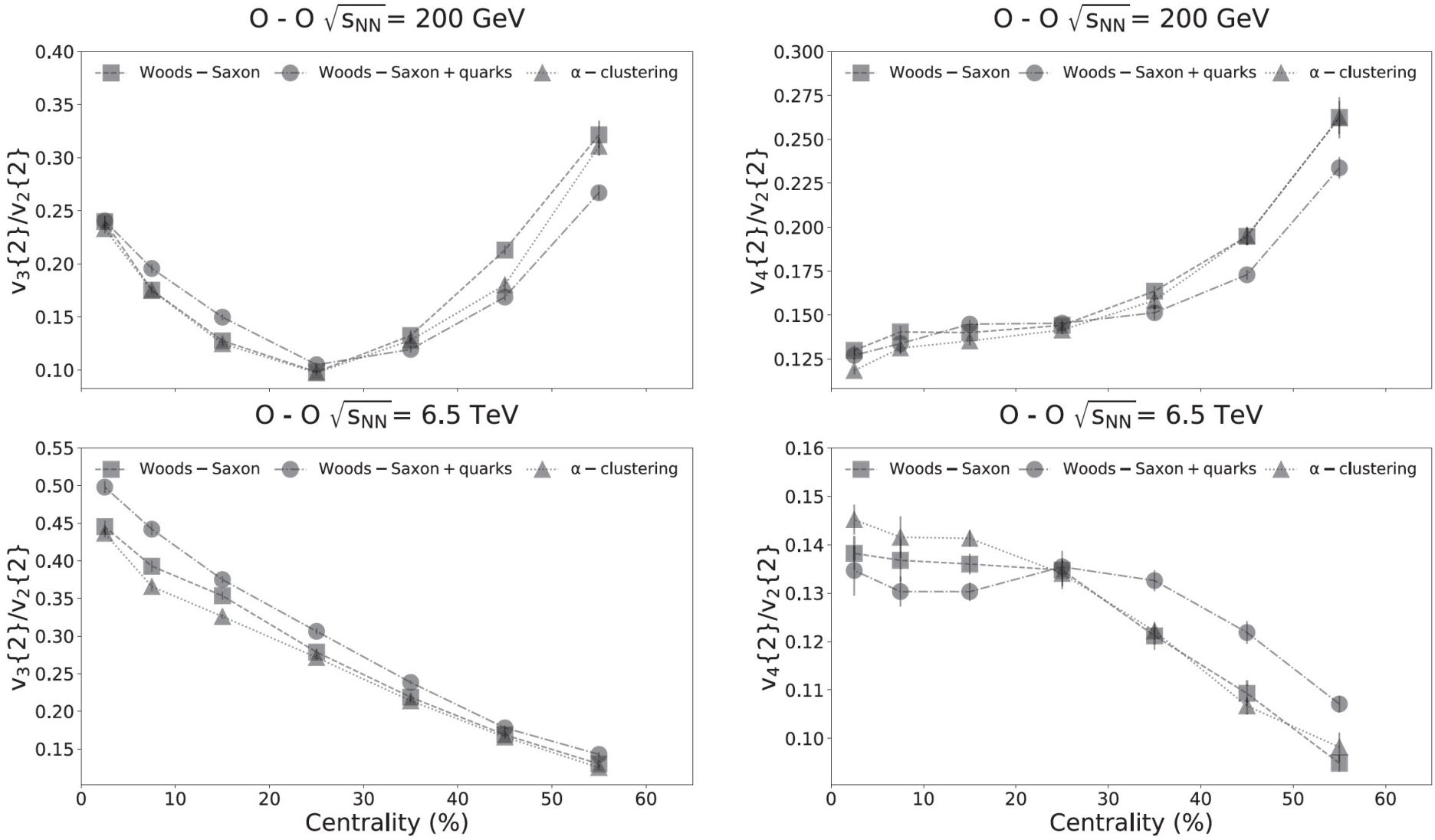
How much alpha clustering?

$$\left\langle \rho^2 \right\rangle_{^{16}\mathrm{O}} = 4.59(11) \left\langle \rho^2 \right\rangle_{^{4}\mathrm{He}}$$
$$\left\langle \rho^3 \right\rangle_{^{16}\mathrm{O}} = 4.67(23) \left\langle \rho^3 \right\rangle_{^{4}\mathrm{He}}$$
$$\left\langle \rho^4 \right\rangle_{^{16}\mathrm{O}} = 4.44(27) \left\langle \rho^4 \right\rangle_{^{4}\mathrm{He}}$$

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

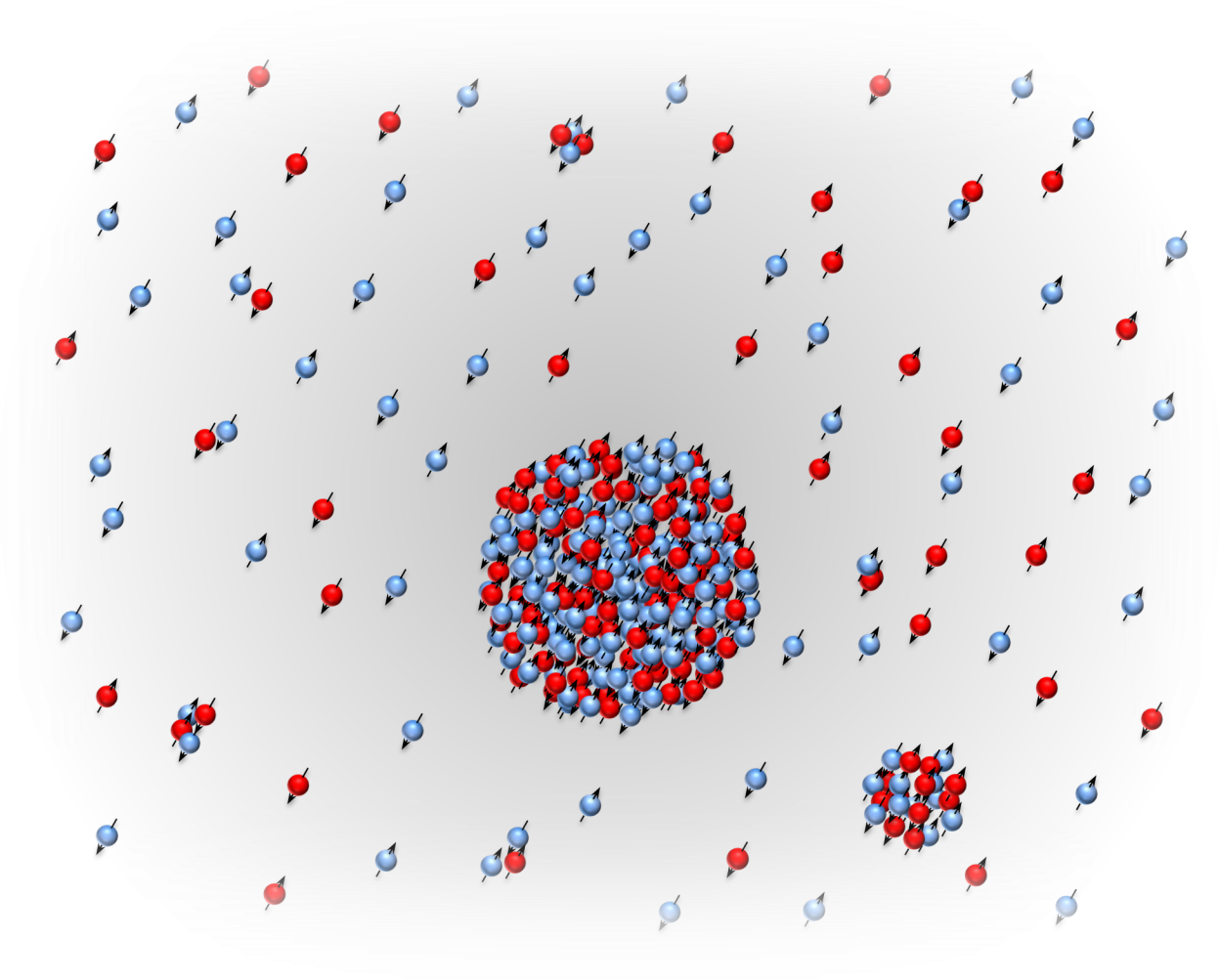


[Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins PRC 104, L041901 (2021)]



[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

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

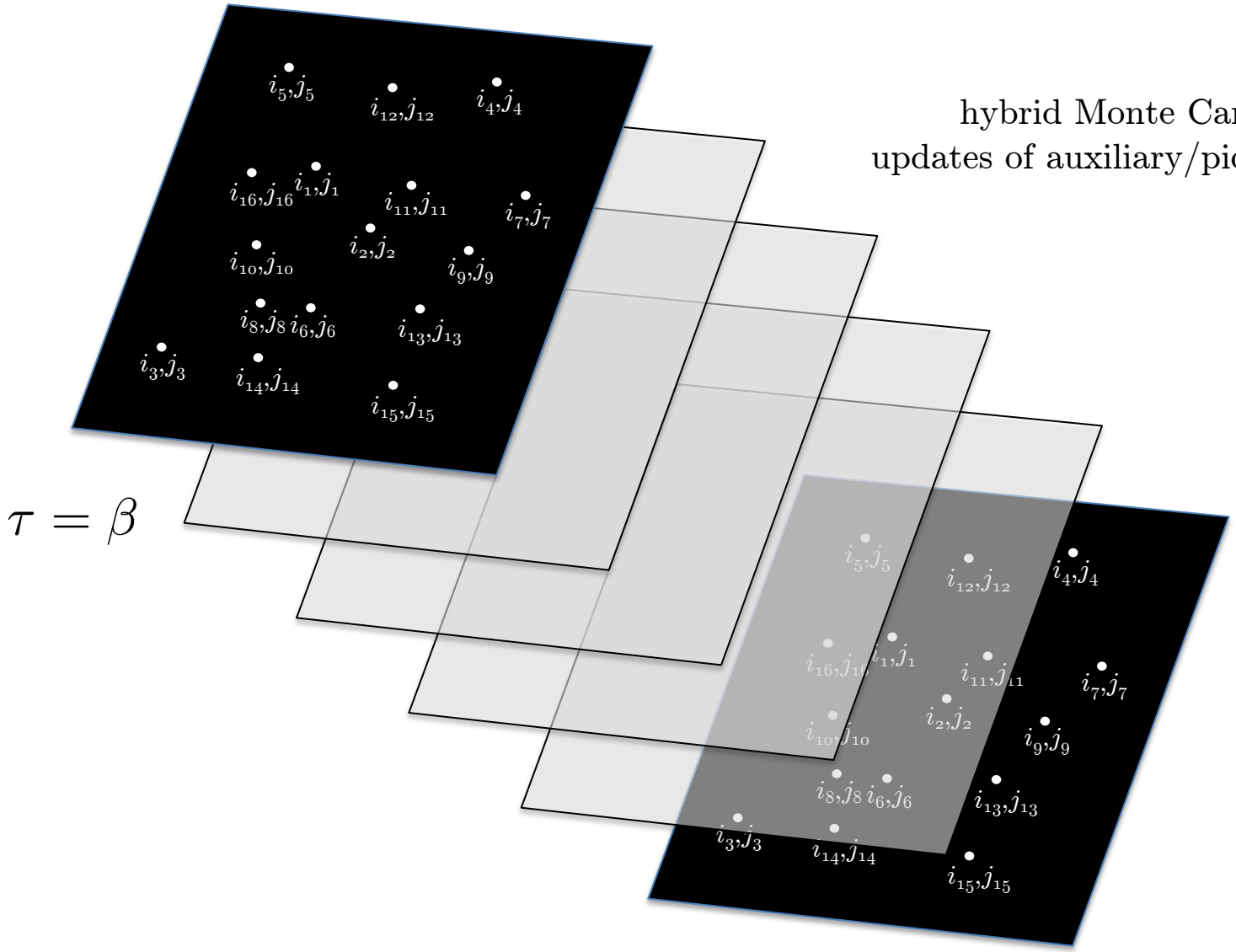
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

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

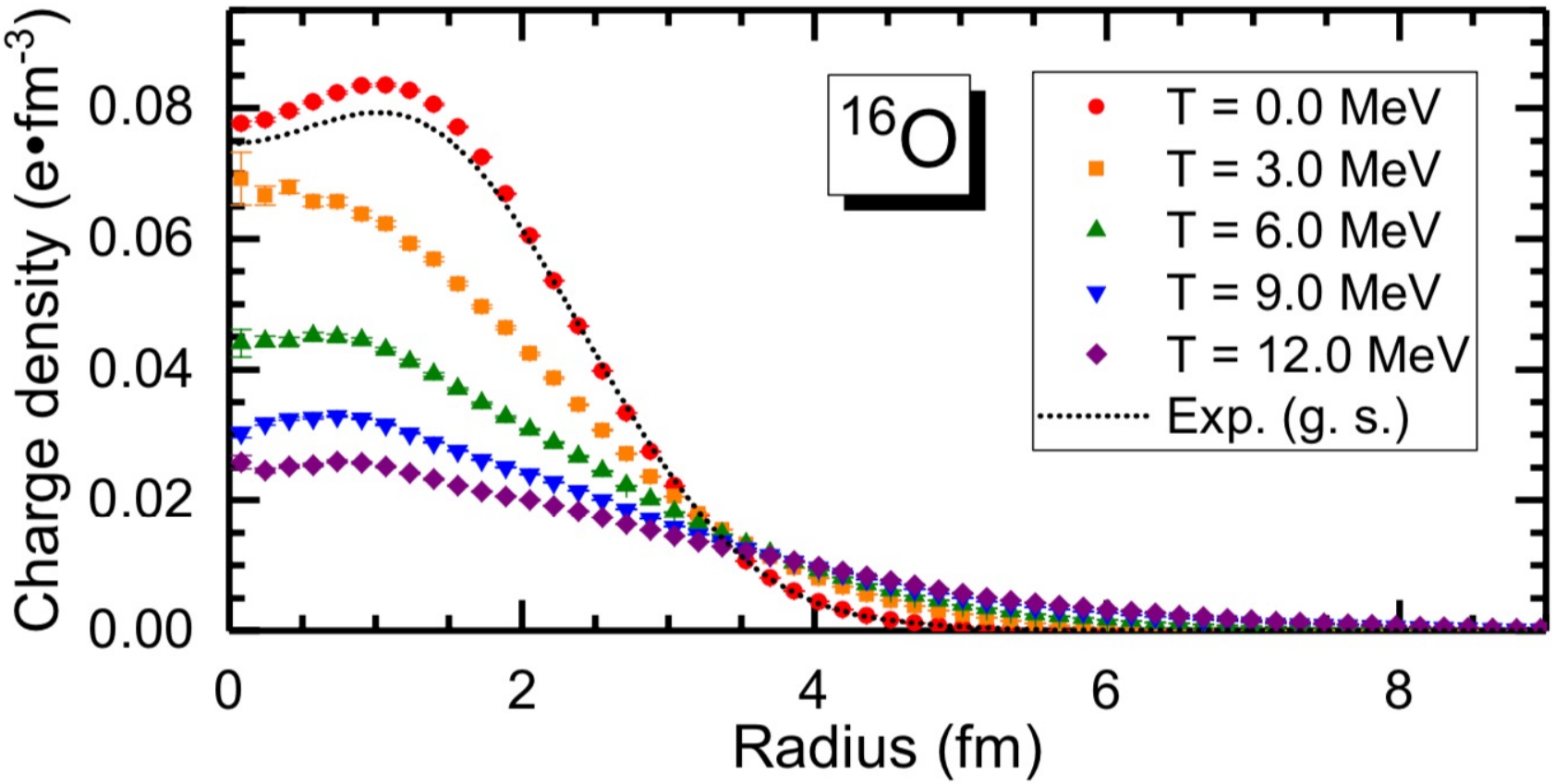
This can be used to calculate the partition function in the canonical ensemble.

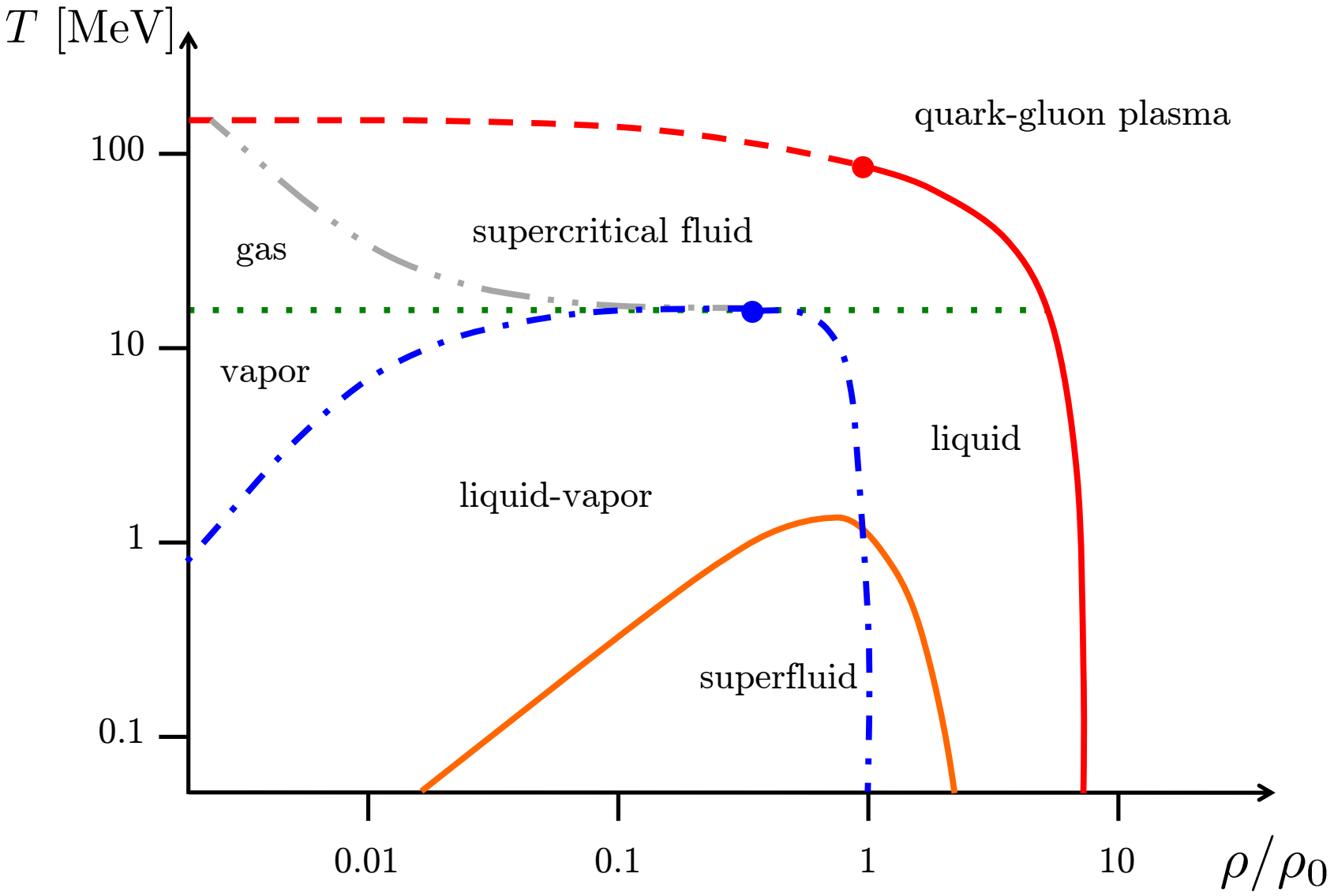
[Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)]

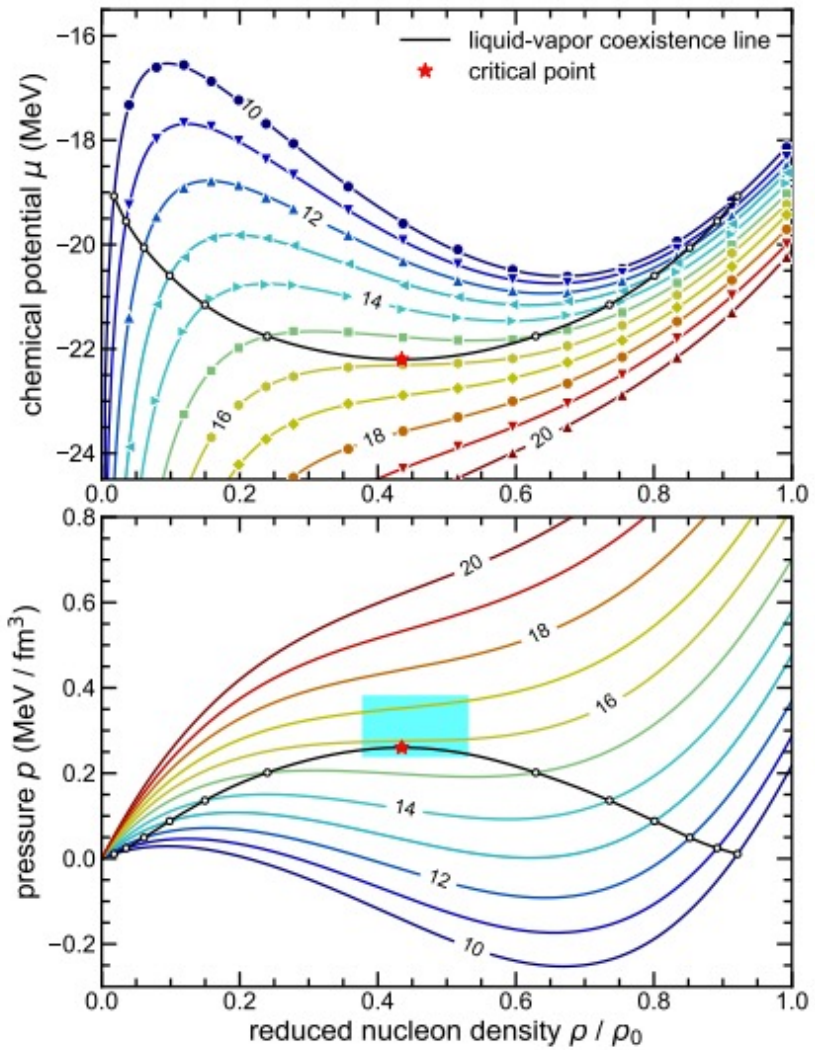
Metropolis updates of pinholes



hybrid Monte Carlo
updates of auxiliary/pion fields


Charge density (e•fm^{-3})
0.08
0.06
0.04
0.02
0.00
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.)

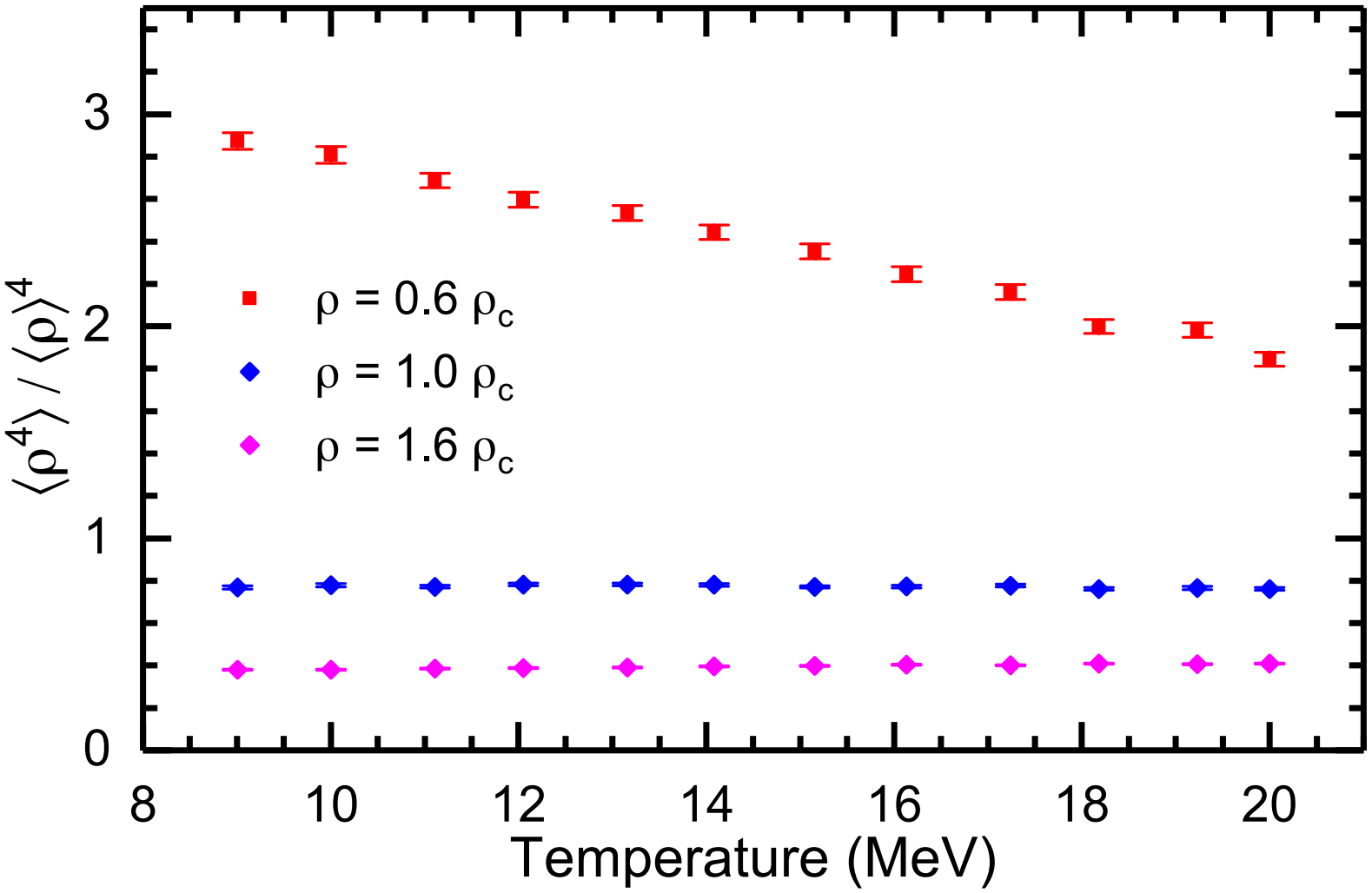

T [MeV]
100
10
1
0.1
quark-gluon plasma
supercritical fluid
gas
vapor
liquid
liquid-vapor
superfluid
0.01
0.1
1
10
ρ/ρ_0



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

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

Alpha clustering as function of density and temperature

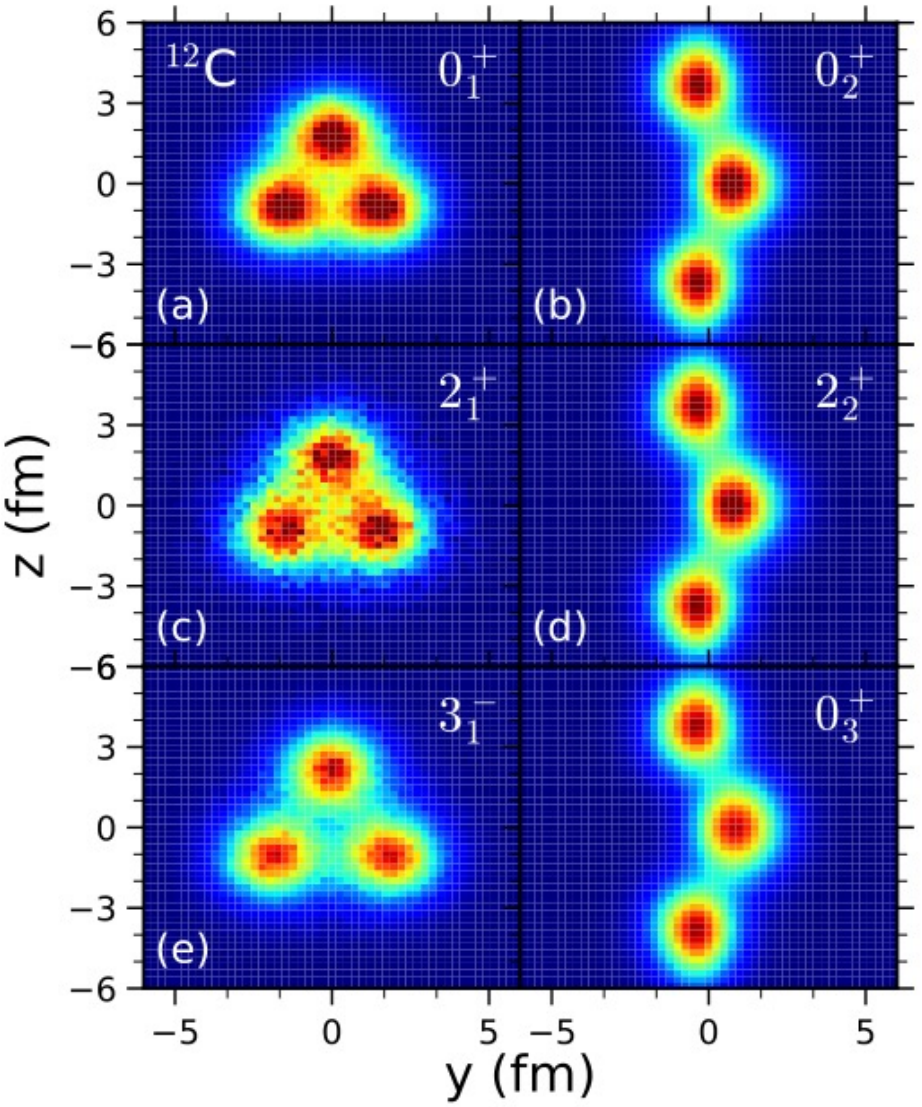


[Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)]

Structure and spectrum of ^{12}C

[Shen, Lähde, D.L. Meißner, EPJA 57, 276 (2021)]

State	$a = 1.97$ fm	$a = 1.64$ fm	Experiment
0_1^+	$-92.15(3)$	$-92.12(4)$	-92.162
2_1^+	$-88.87(4)$	$-88.19(17)$	-87.722
0_2^+	$-85.20(15)$	$-85.23(22)$	-84.508
3_1^-	$-84.9(2)$	$-83.3(5)$	$-82.521(5)$
2_2^+	$-83.5(2)$	$-83.1(5)$	$-82.29(6)$
0_3^+	$-80.0(3)$	$-79.2(6)$	$-81.9(3)$
1_1^-	$-81.5(4)$	$-79.7(4)$	$-81.315(4)$
2_1^-	$-78.6(2)$	$-76.1(2)$	$-80.326(4)$
1_1^+	$-79.67(11)$	$-78.14(24)$	$-79.452(6)$
4_1^-	$-78.1(2)$	$-75.5(5)$	$-78.846(20)$
4_1^+	$-80.99(11)$	$-79.1(6)$	$-78.083(5)$
2_3^+	$-79.9(4)$	$-77.9(2)$	-76.056
0_4^+	$-79.25(11)$	$-76.94(18)$	-74.402



[Work in progress: Shen et al.]

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?