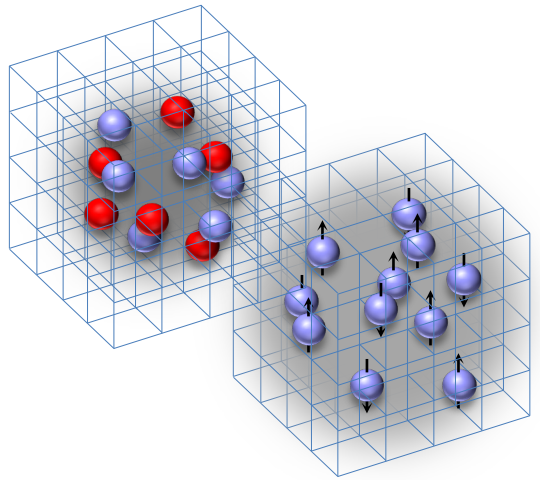
Nuclear Lattice Simulations

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

X$^{\text{th}}$ Tastes of Nuclear Physics
University of Western Cape
November 30 – December 4, 2020



FRIB

MICHIGAN STATE UNIVERSITY

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

JÜLICH FORSCHUNGSZENTRUM

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Outline

From nuclear forces to nuclear structure

Lattice effective field theory

A tale of two interactions

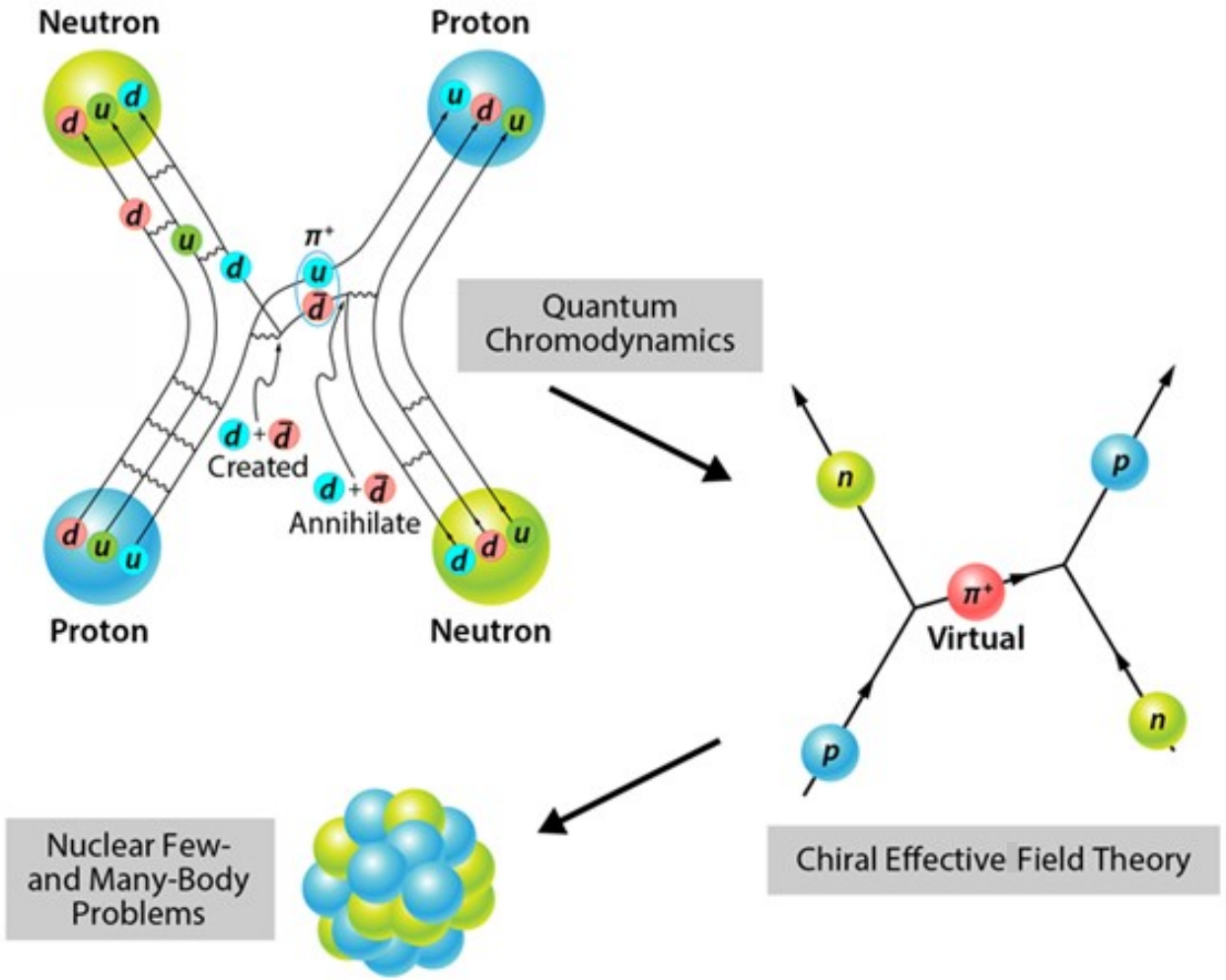
Essential elements for nuclear binding

Nuclear thermodynamics

Eigenvector continuation

Summary and outlook

Nuclear forces and nuclear structure



Effective field theories and energy scales

Lattice quantum chromodynamics

Chiral effective field theory

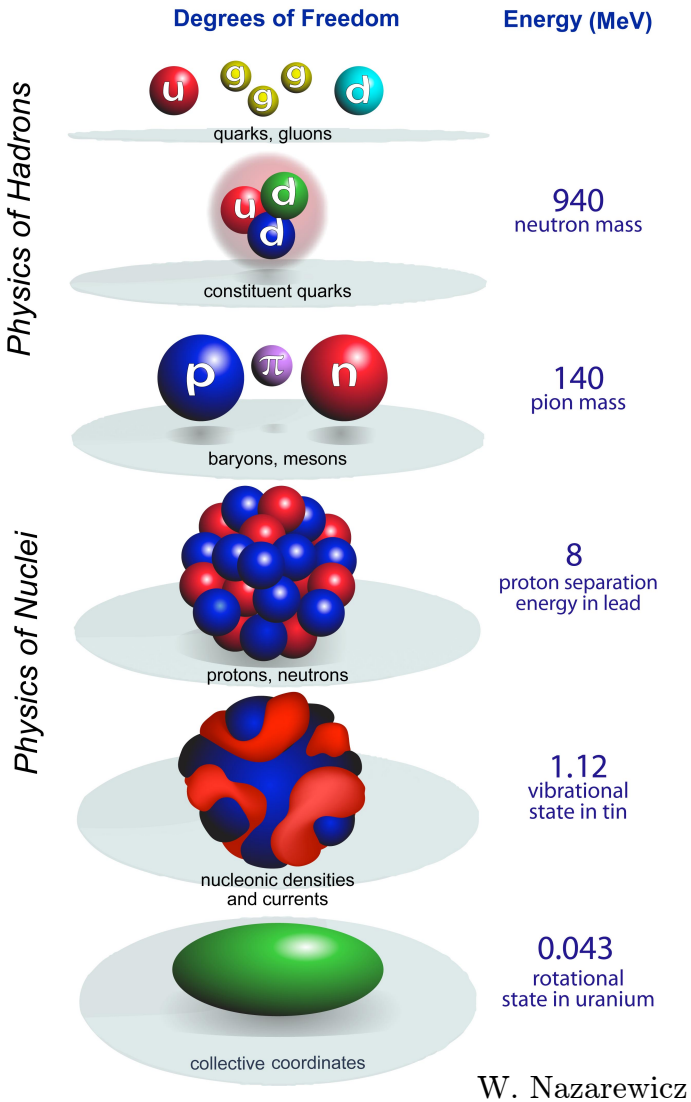
Microscopic A-body methods

Configuration interactions

Density functional methods

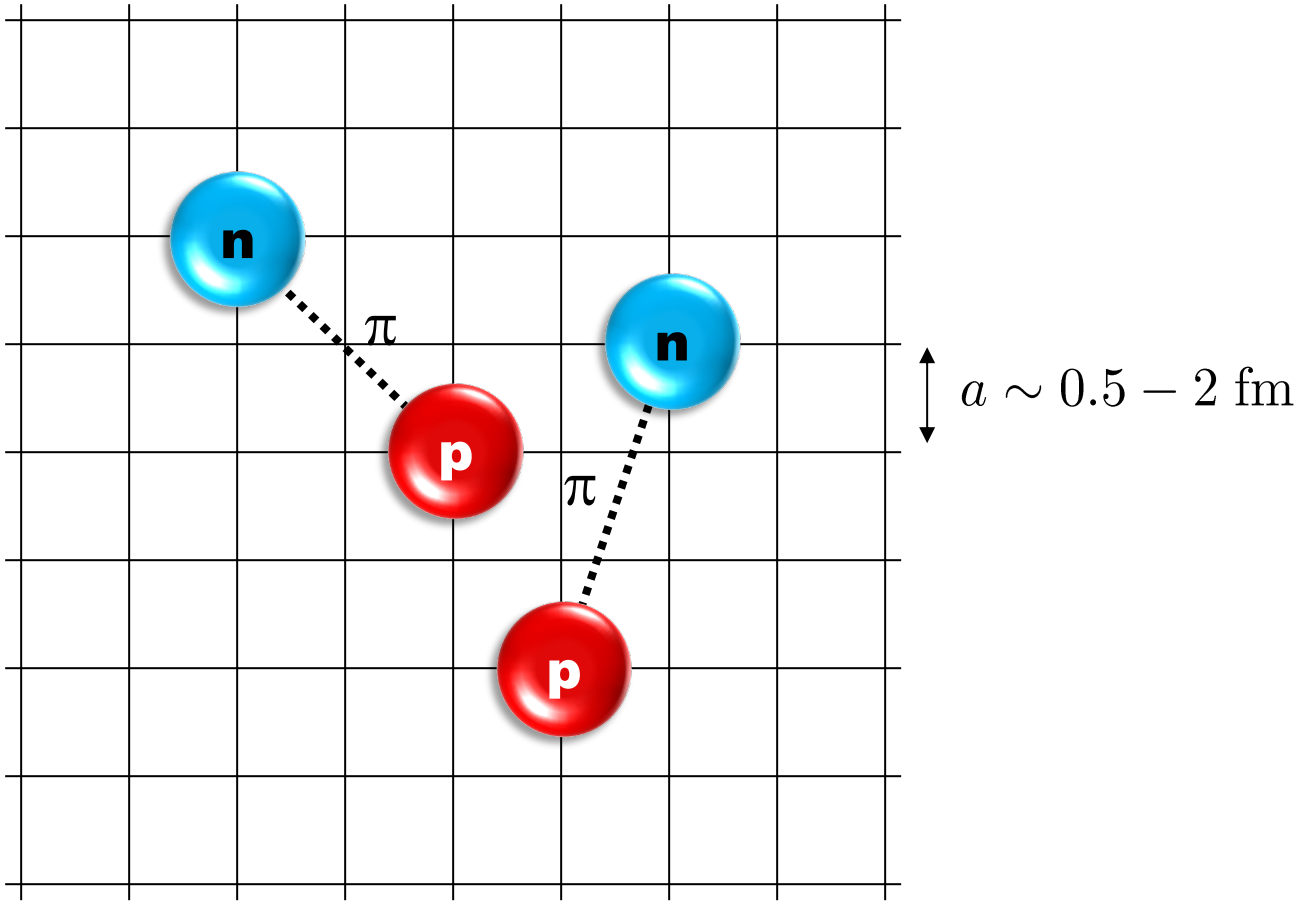
Mean field methods

Effective theory of collective modes

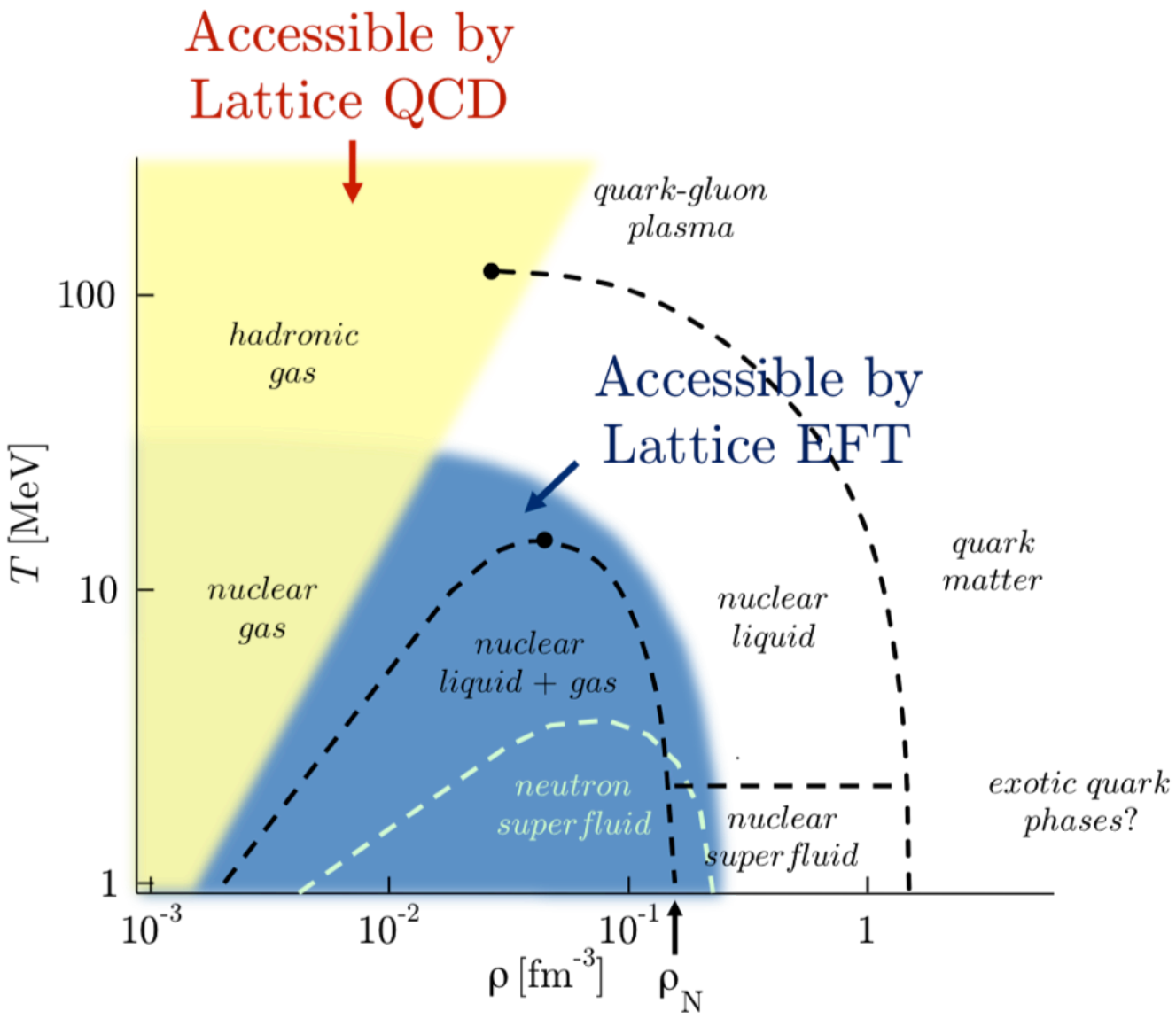


W. Nazarewicz

Lattice effective field theory

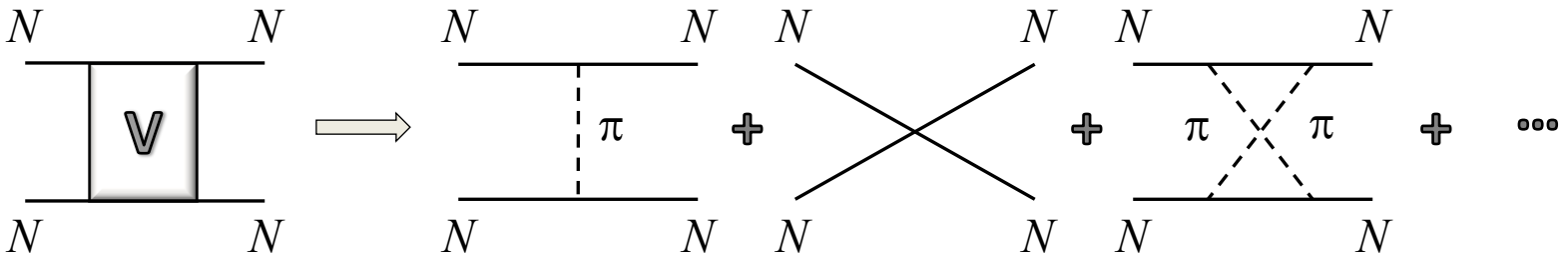


Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)


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

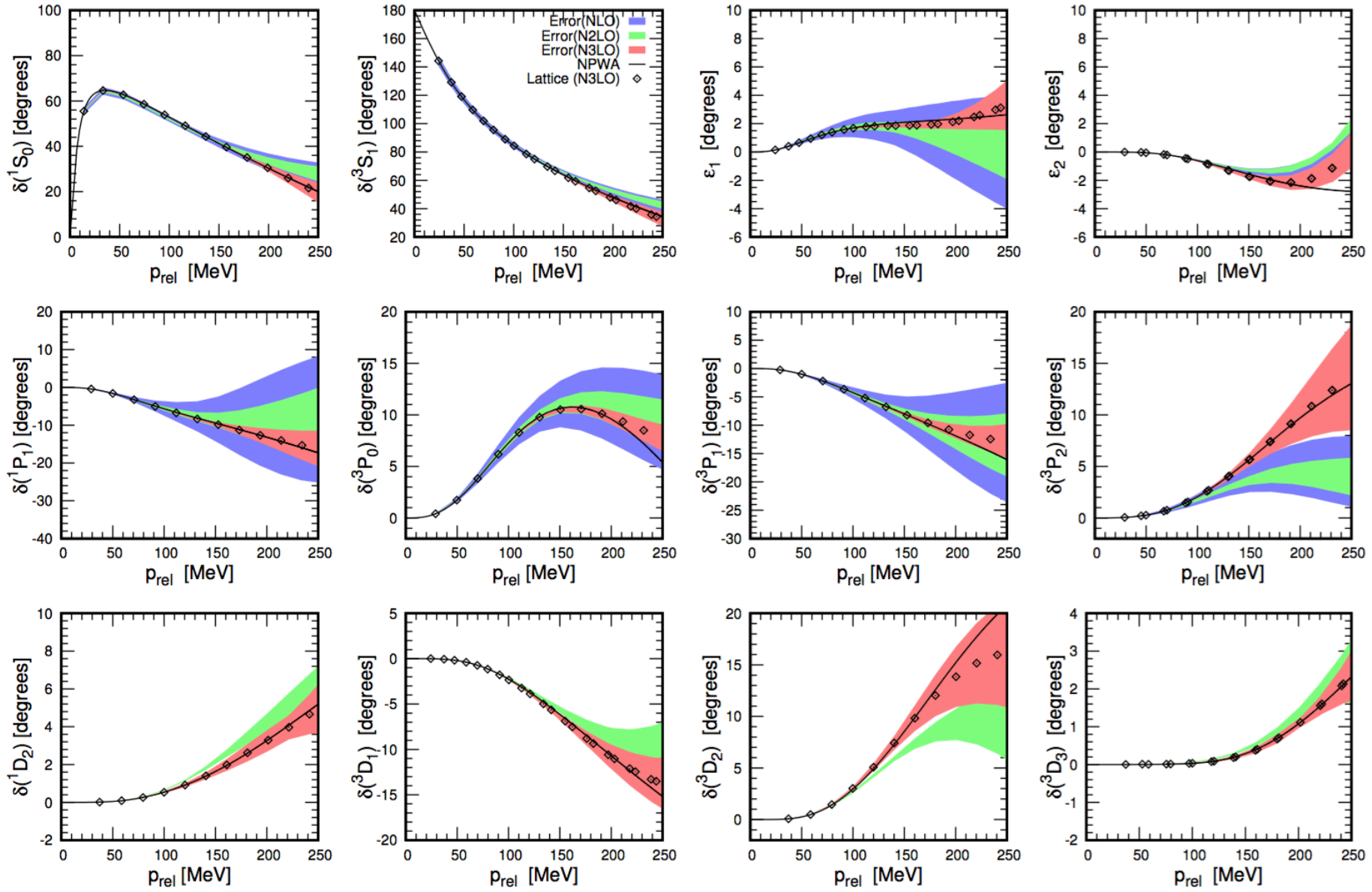
Construct the effective potential order by order



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

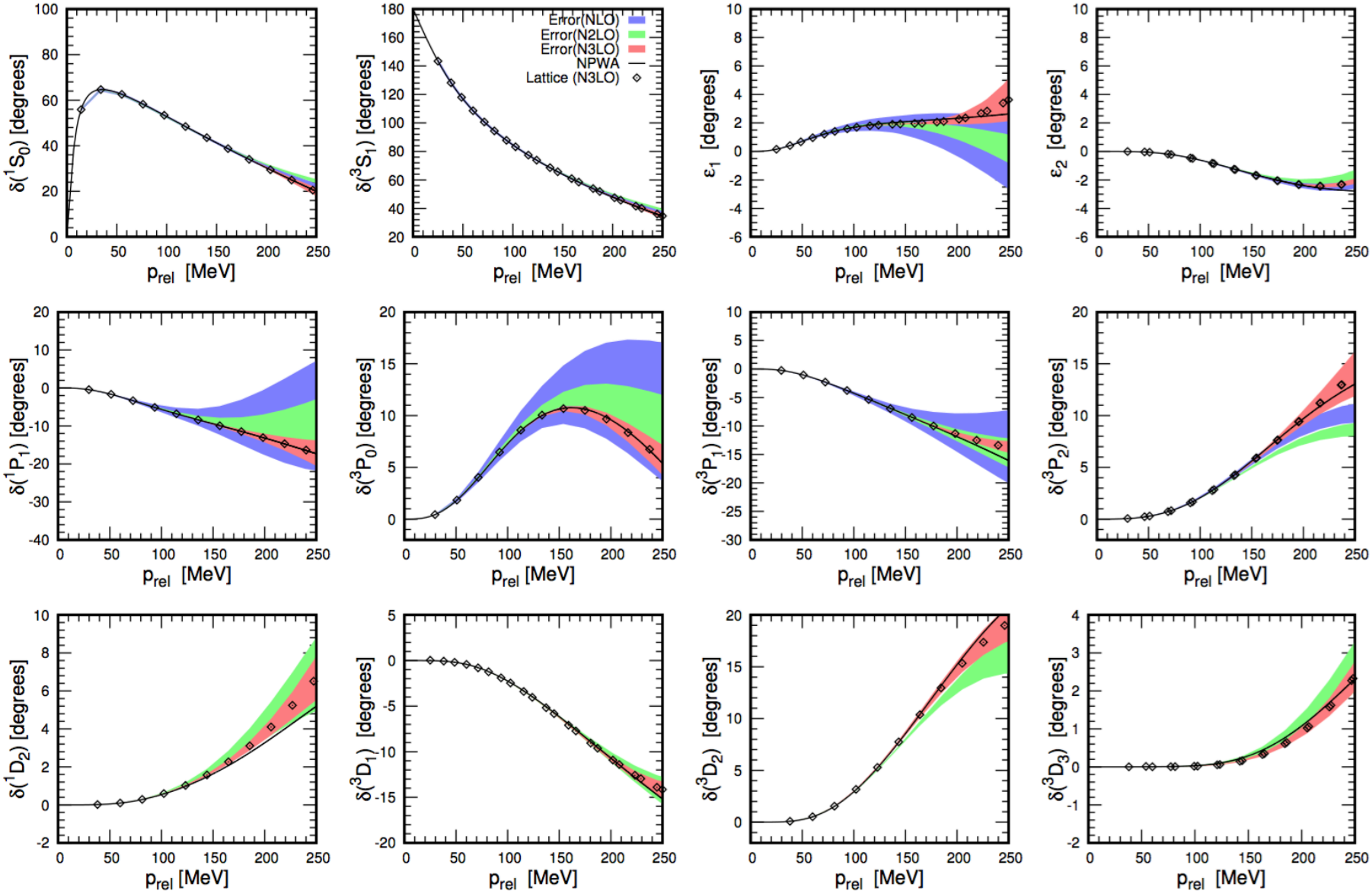
Leading order (LO) Next-to-leading order (NLO)

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



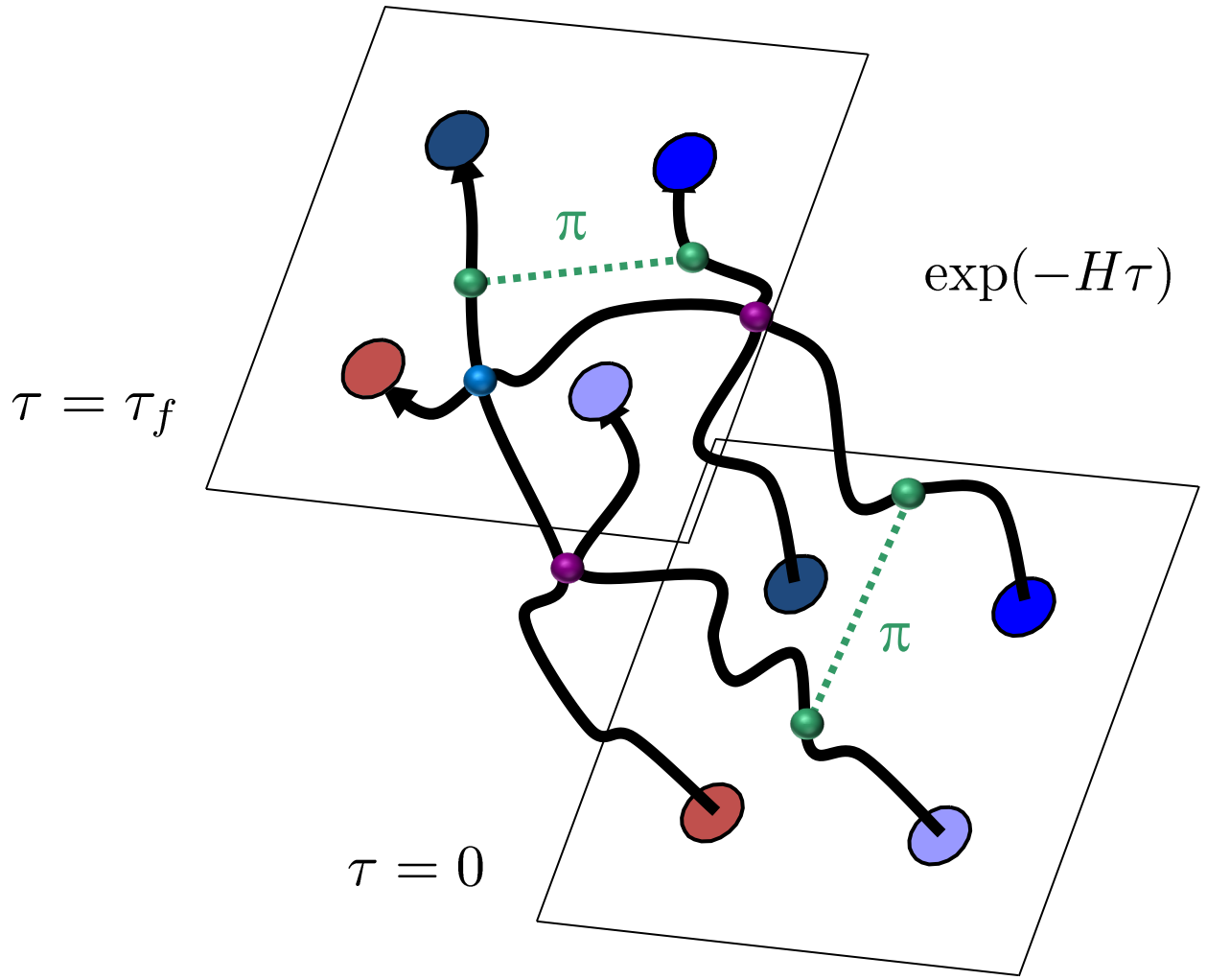
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

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



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

Euclidean time projection



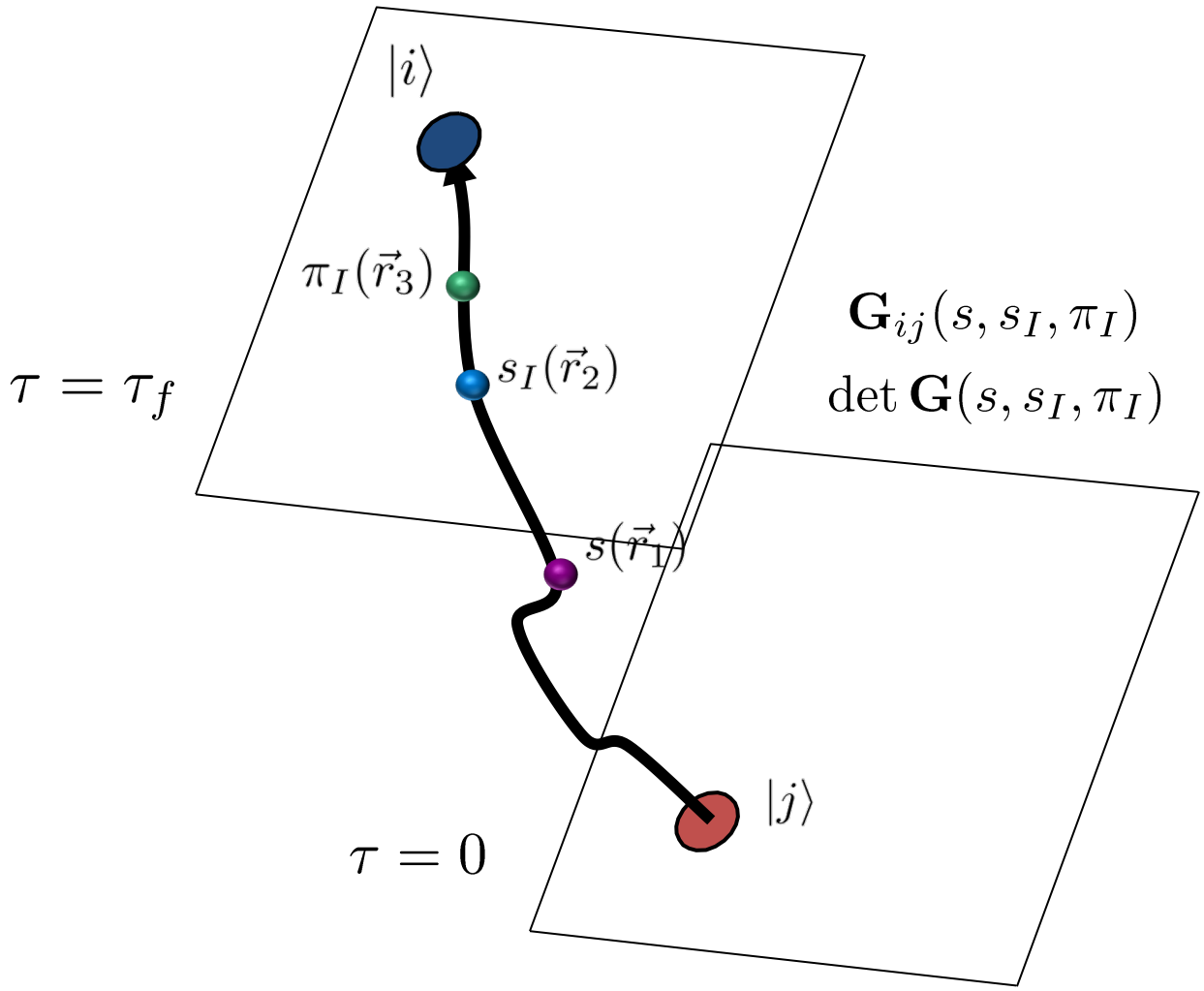
Auxiliary field method

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

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

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

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

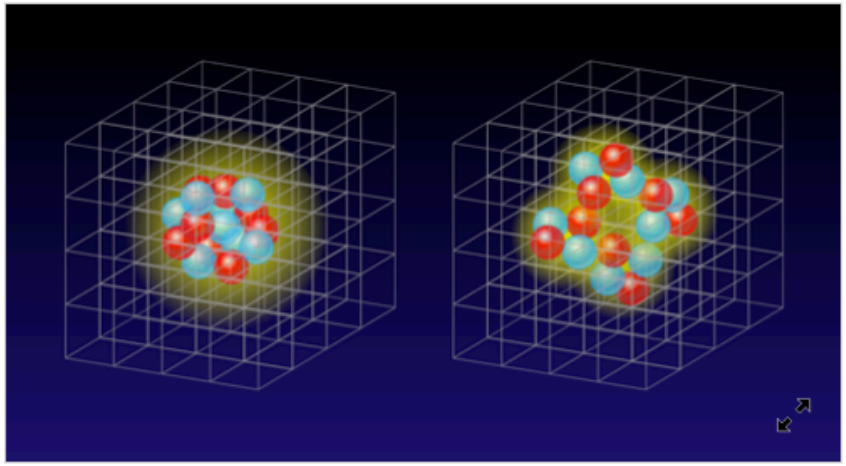

$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = \tau_f$
$\tau = 0$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{G}(s, s_I, \pi_I)$

Viewpoint: Uncovering a Quantum Phase Transition in Nuclei

David J. Dean, Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

September 19, 2016 • *Physics* 9, 106

Simulations predict that the ground states of certain light nuclei lie near a quantum phase transition between a liquid-like phase and a phase involving clusters of alpha particles.



APS/Alan Stonebraker

Figure 1: Lee and colleagues performed simulations of a nucleus in which they tweaked the interaction between nucleons (protons and neutrons) [1]. They found that, depending on the form of the interaction, the nucleus lay on either side of a quantum phase transition. The transition is between (left) a phase in which protons and neutrons are evenly distributed (a Fermi liquid) to (right) a phase in which the protons and neutrons cluster into alpha particles. **Show less**

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)

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

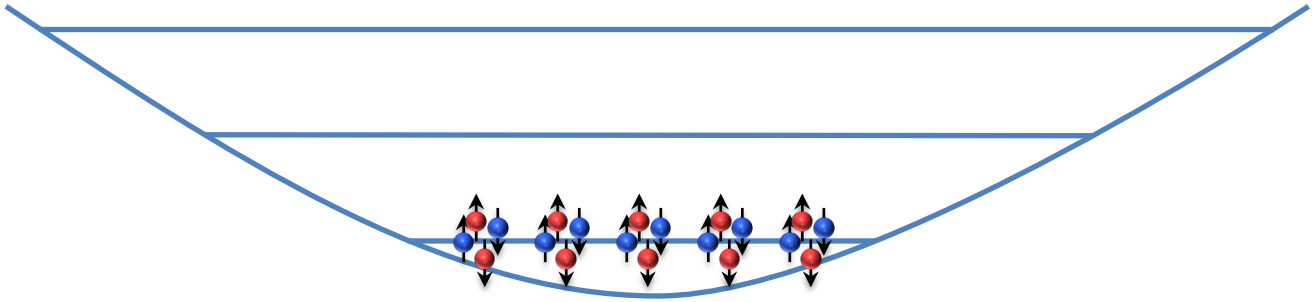
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

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

Bose condensate of alpha particles!



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

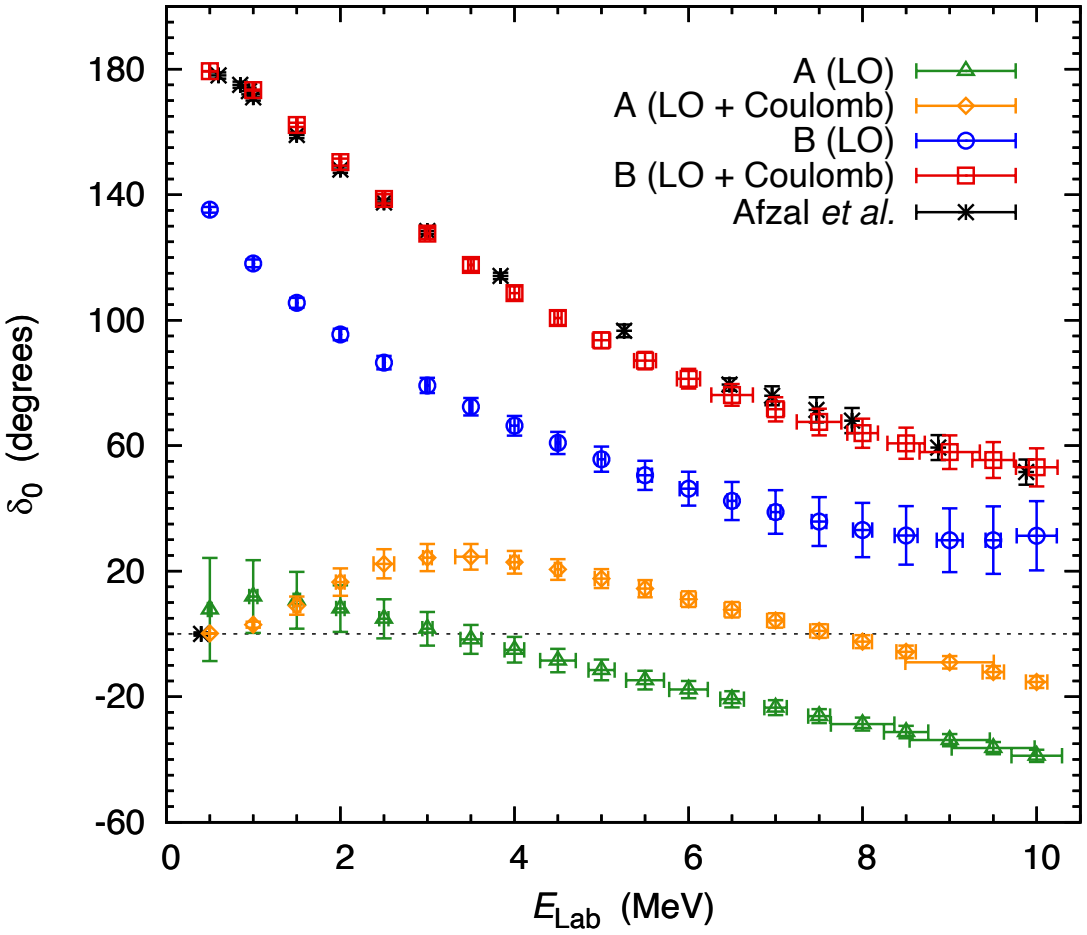
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

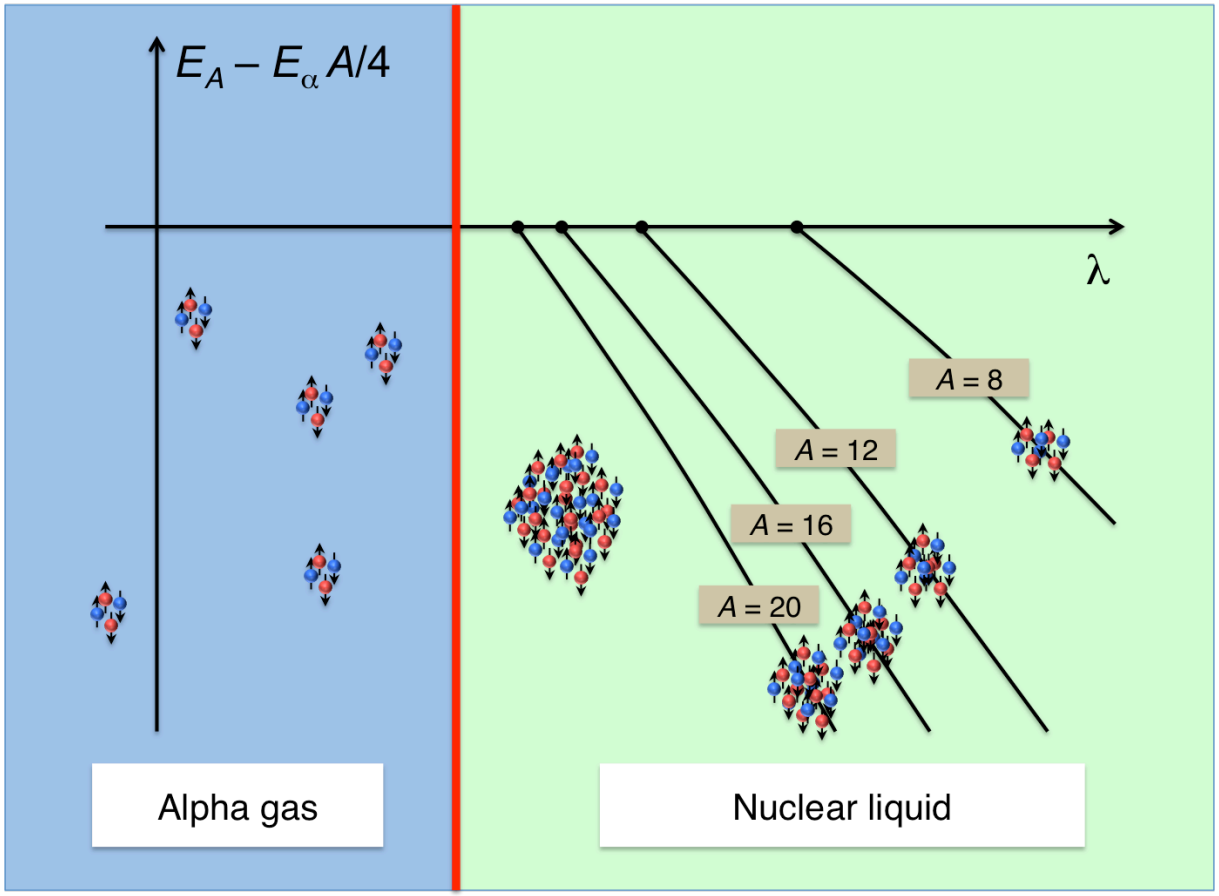
$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^{4}\mathrm{He}}} = 5.03(3)$$

Alpha-alpha scattering



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

Control parameters: Sensitivity to interaction range and locality



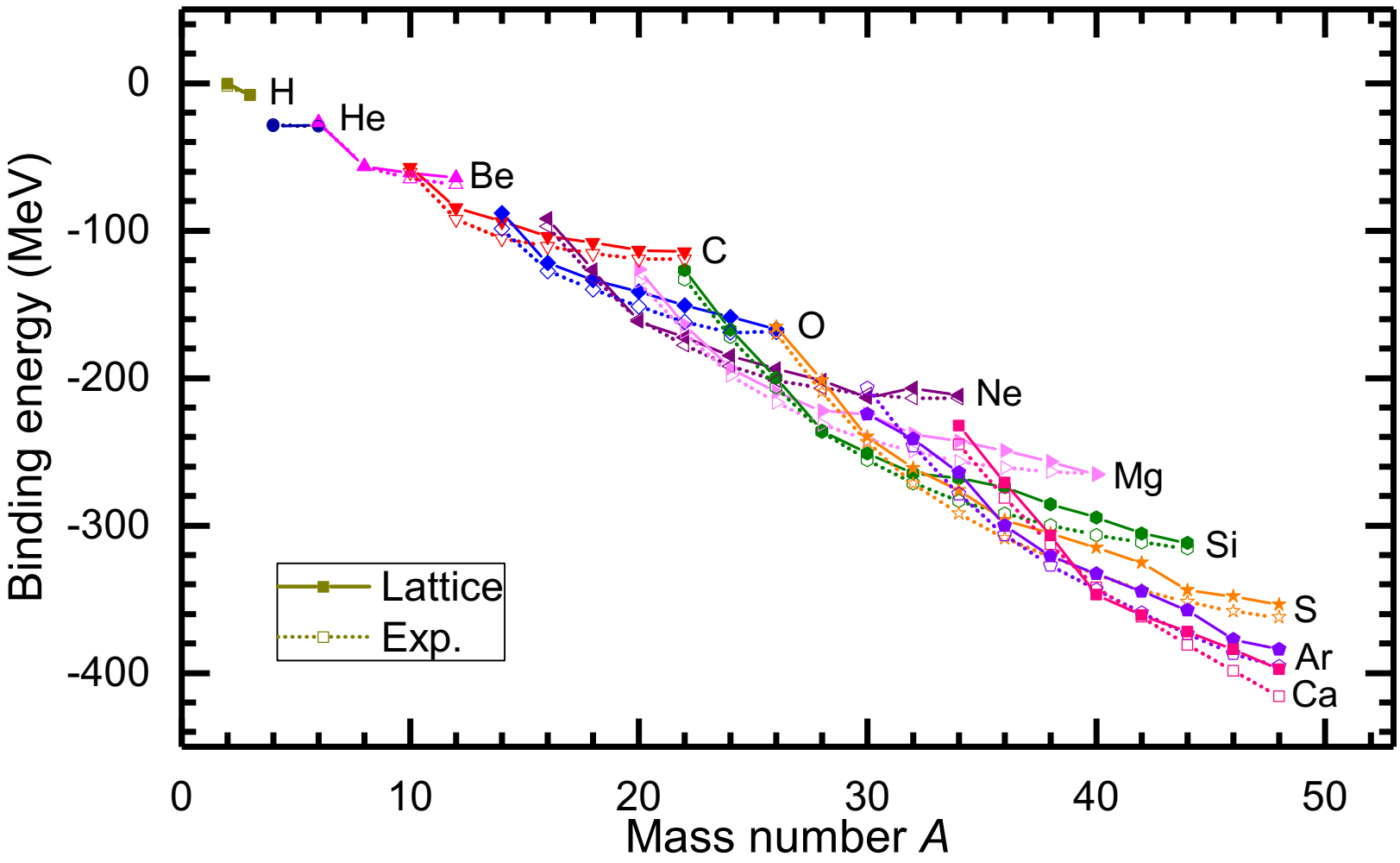
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

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

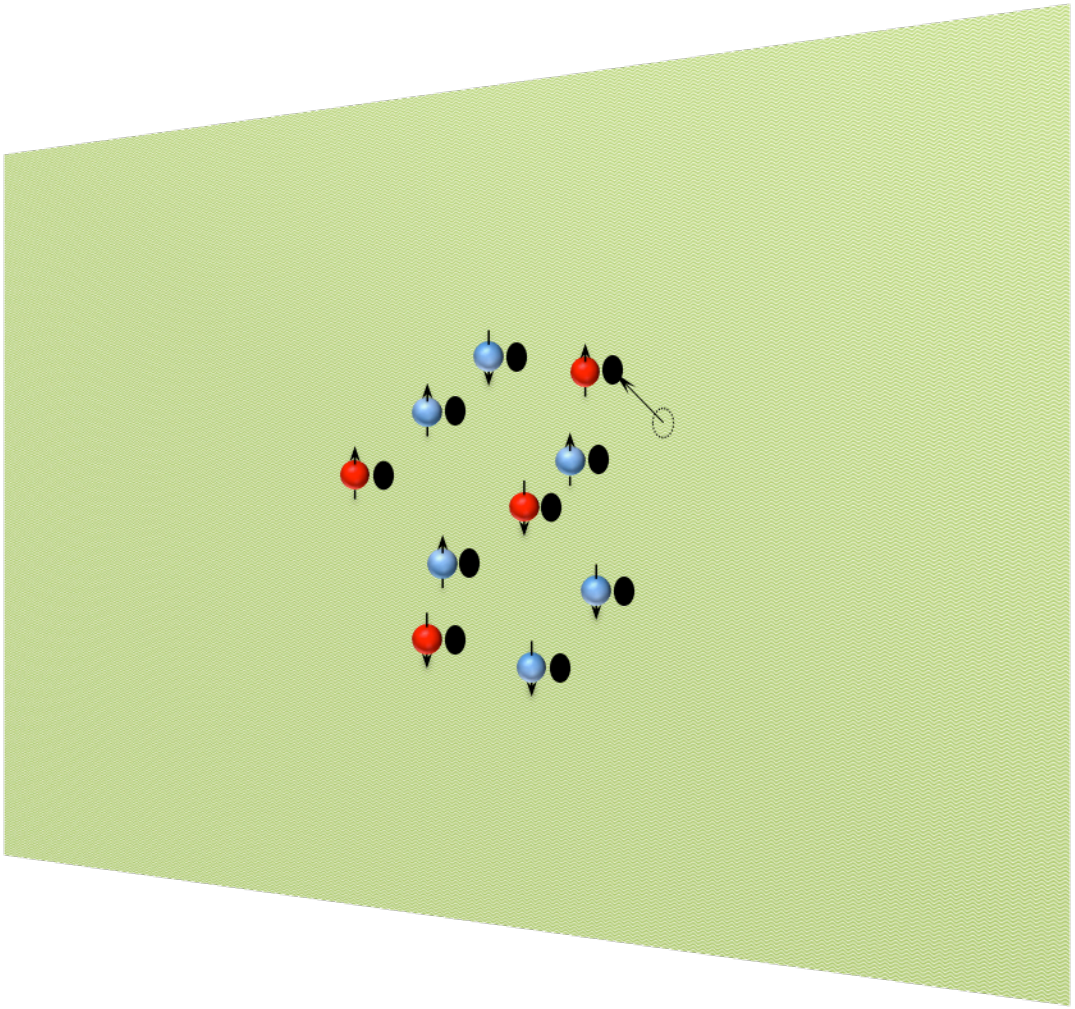


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

	B	Exp.	$R_{\rm ch}$	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

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

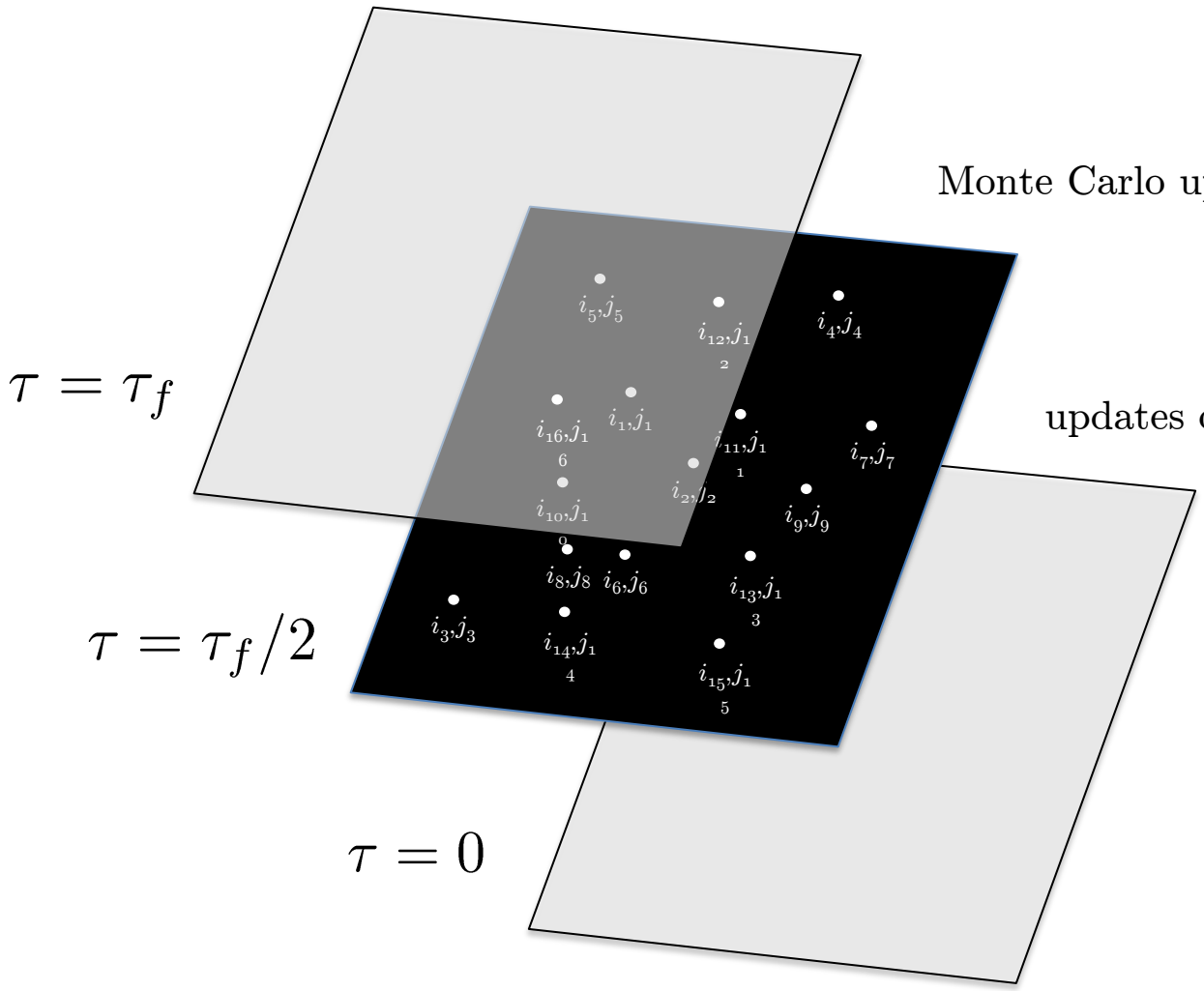
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

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

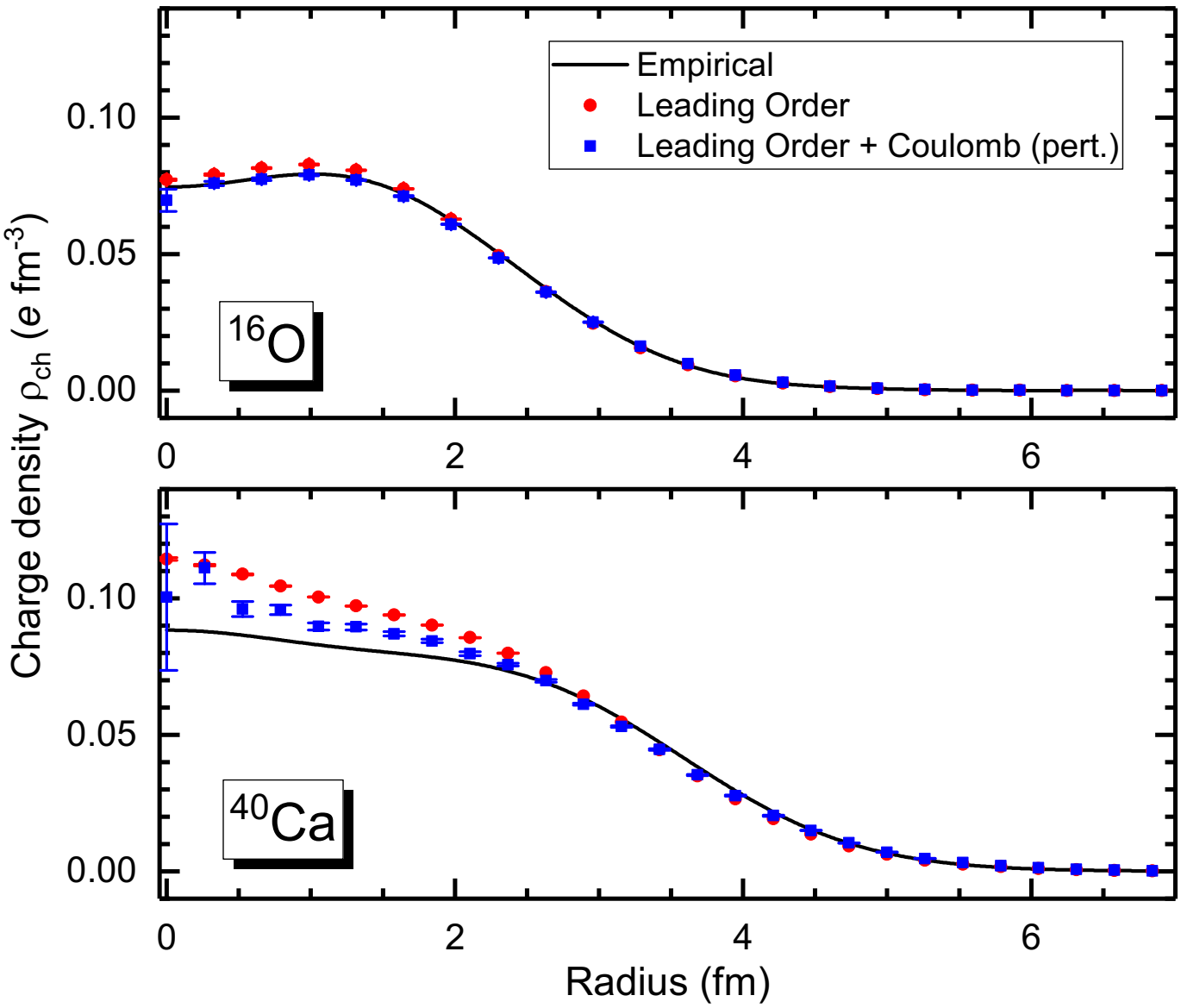
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$



Monte Carlo updates of pinholes

Monte Carlo
updates of auxiliary/pion fields

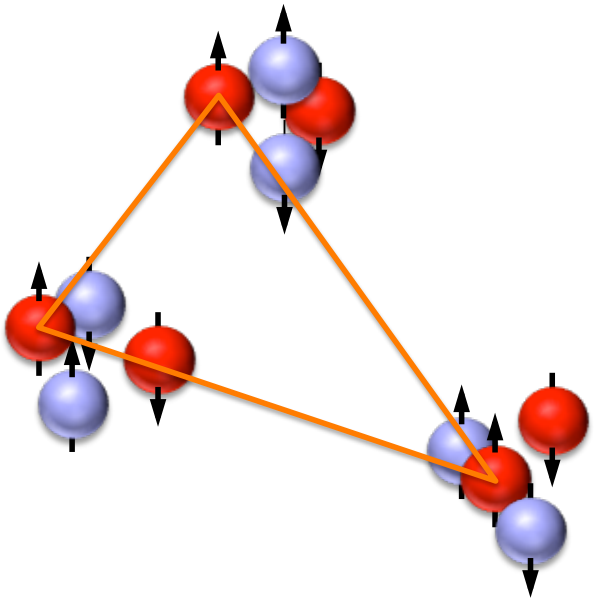
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



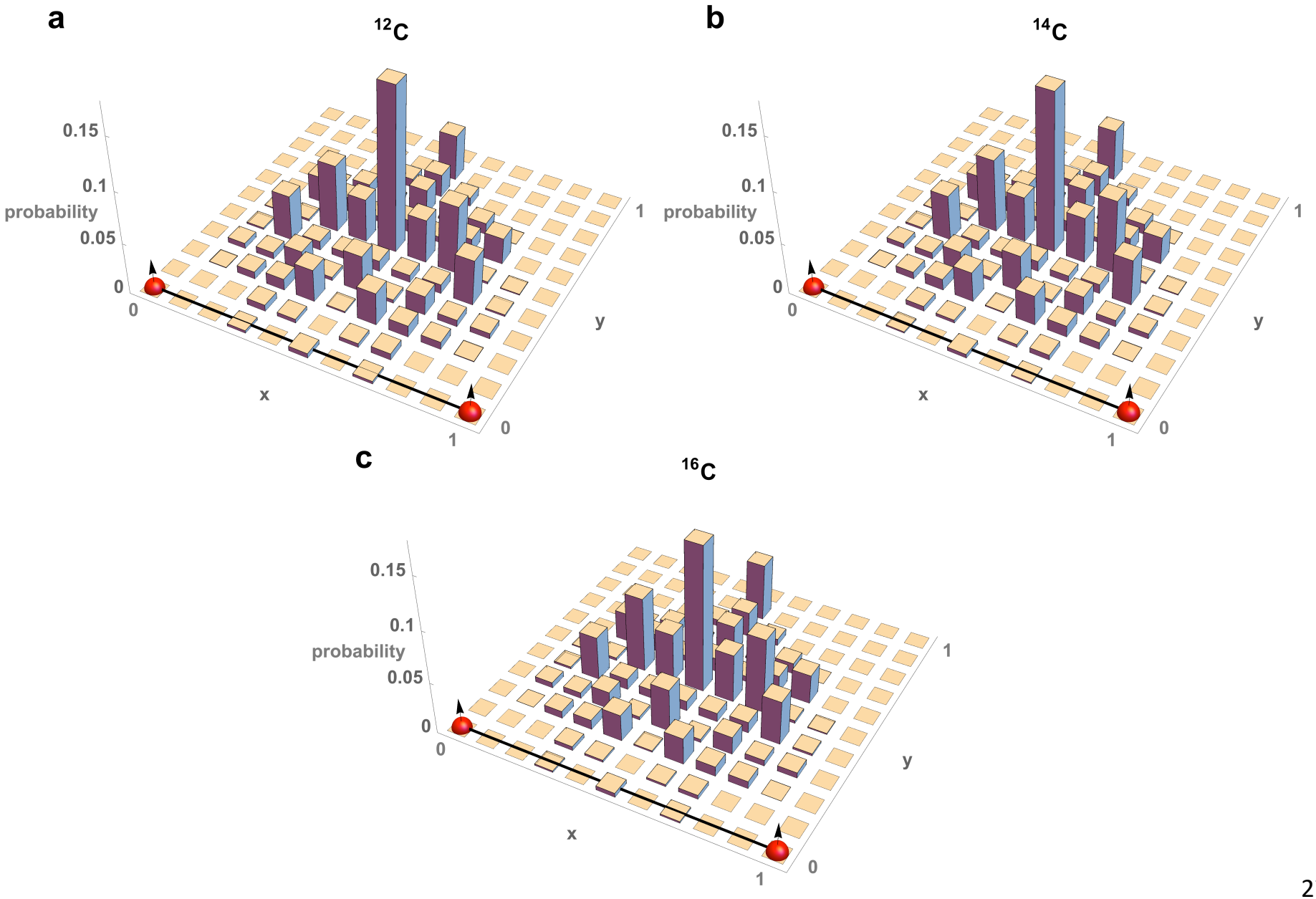
Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

Model-independent measure of alpha cluster geometry

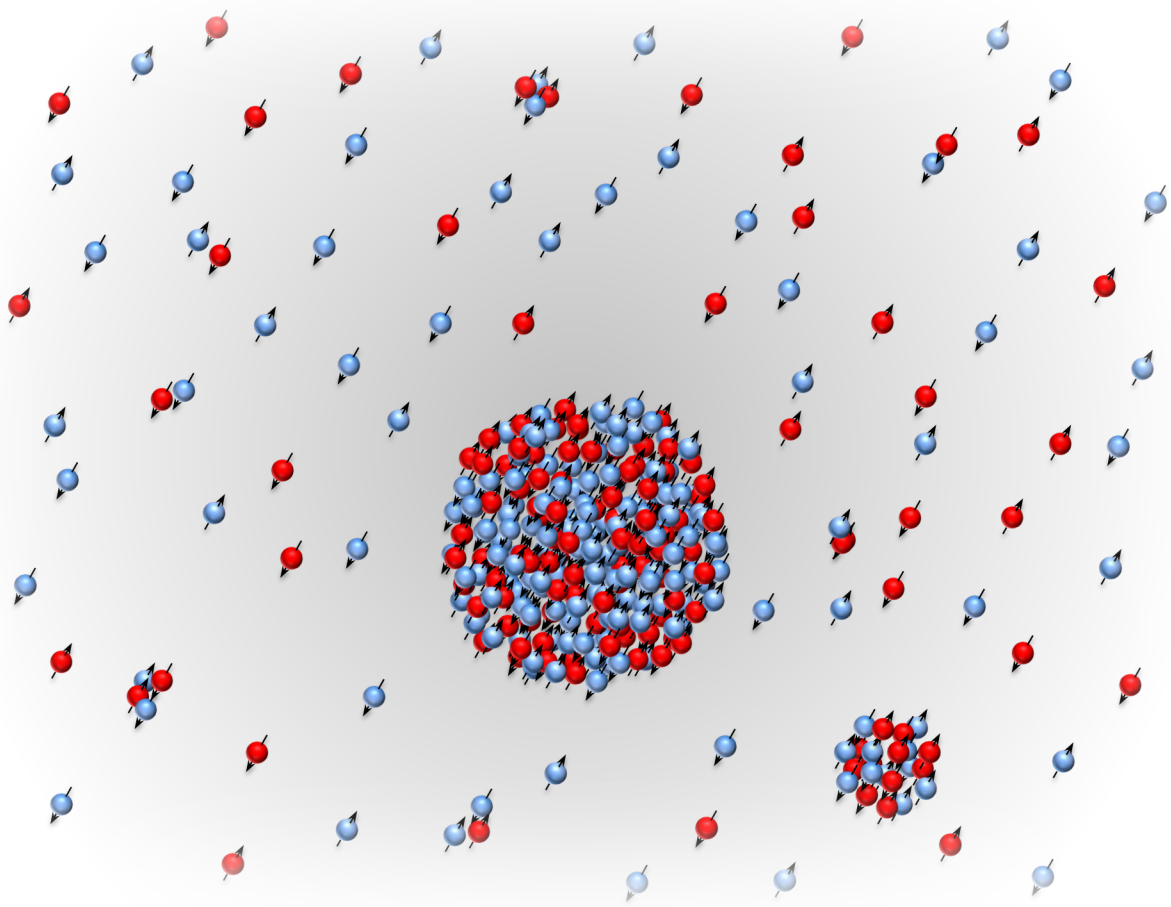
For the carbon isotopes, we can map out the alpha cluster geometry by computing the density correlations of the three spin-up protons. We compute these density correlations using the pinhole algorithm.



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


a
^{12}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
b
^{14}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
c
^{16}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1

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

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

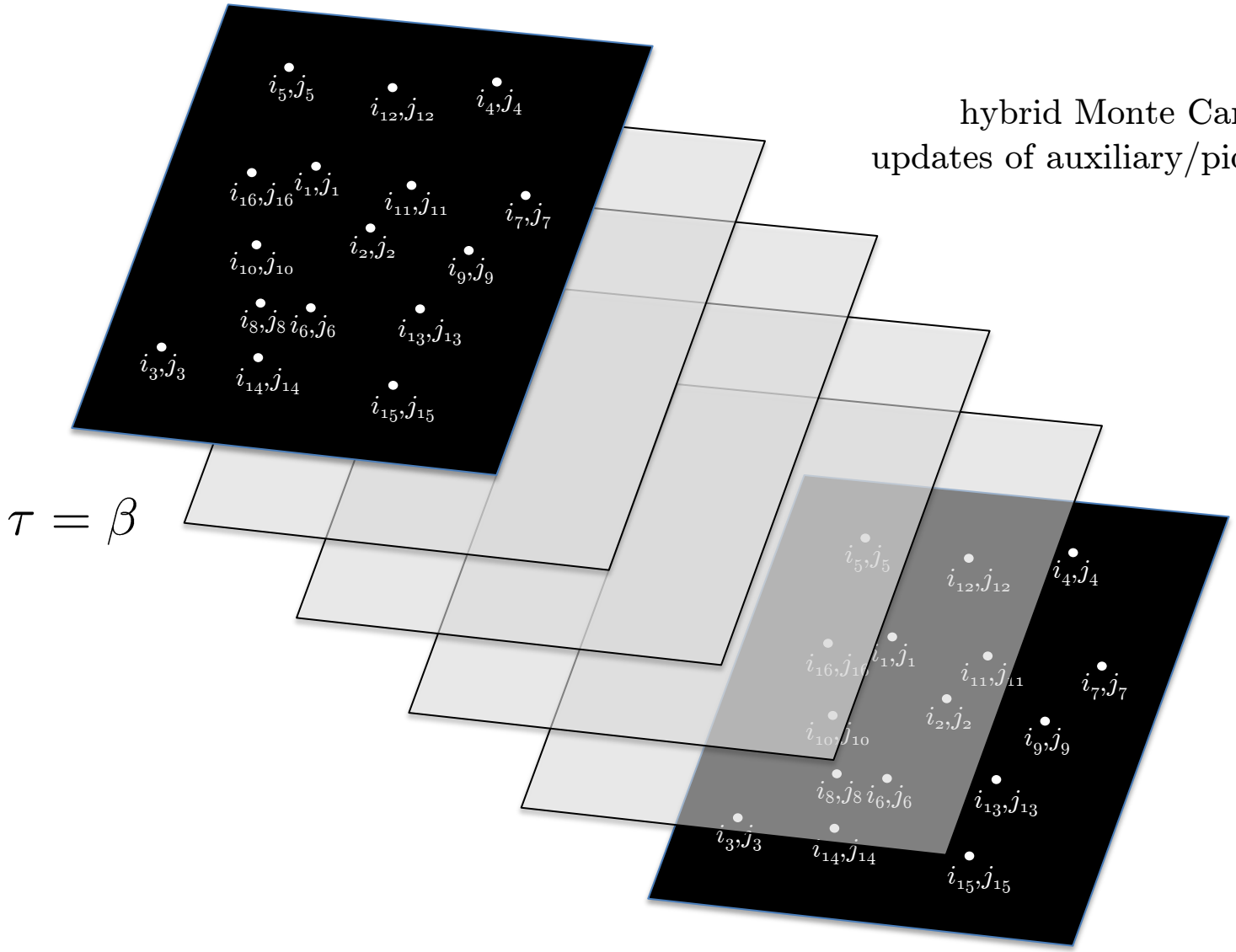
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

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

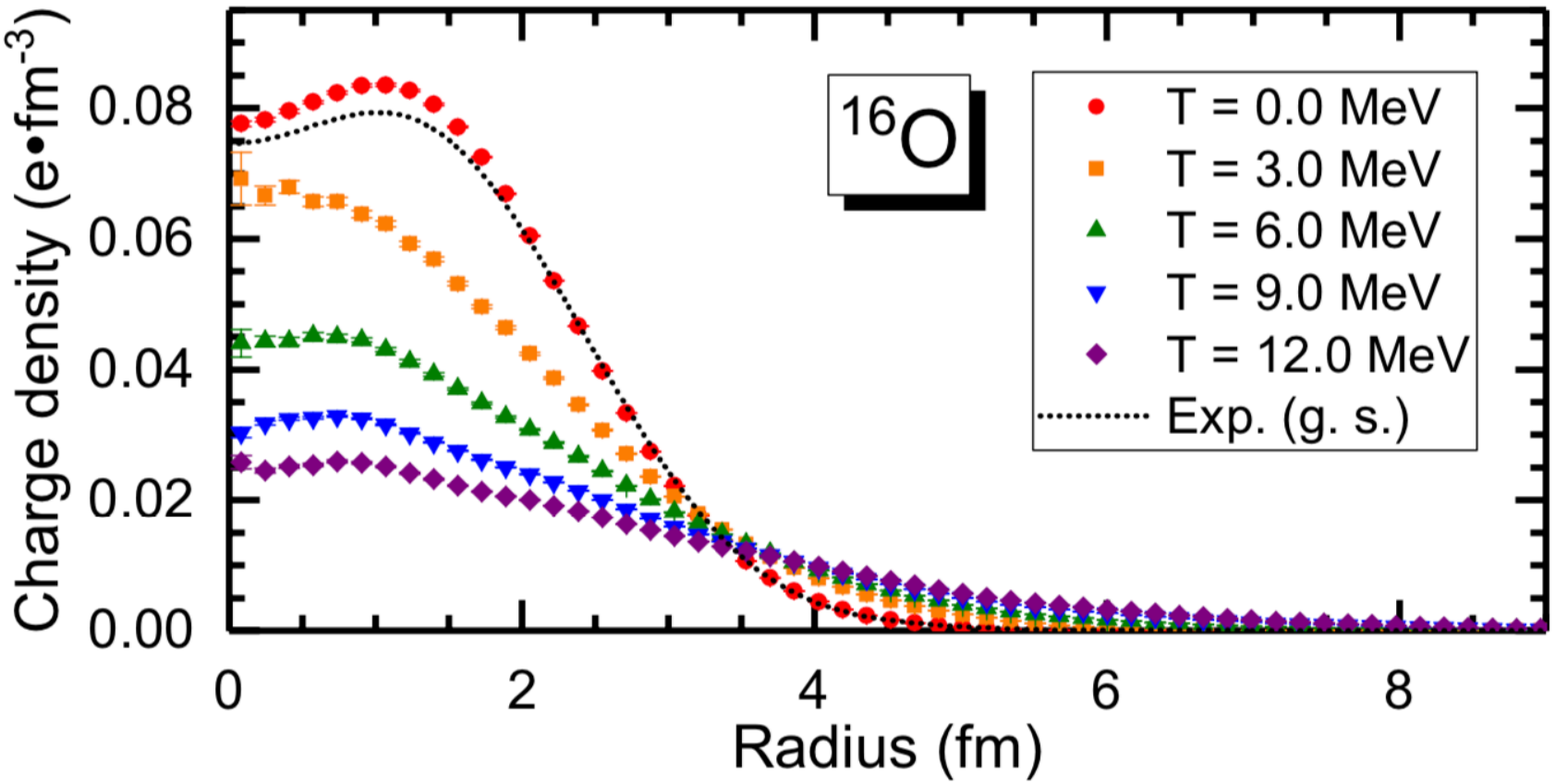
This can be used to calculate the partition function in the canonical ensemble.

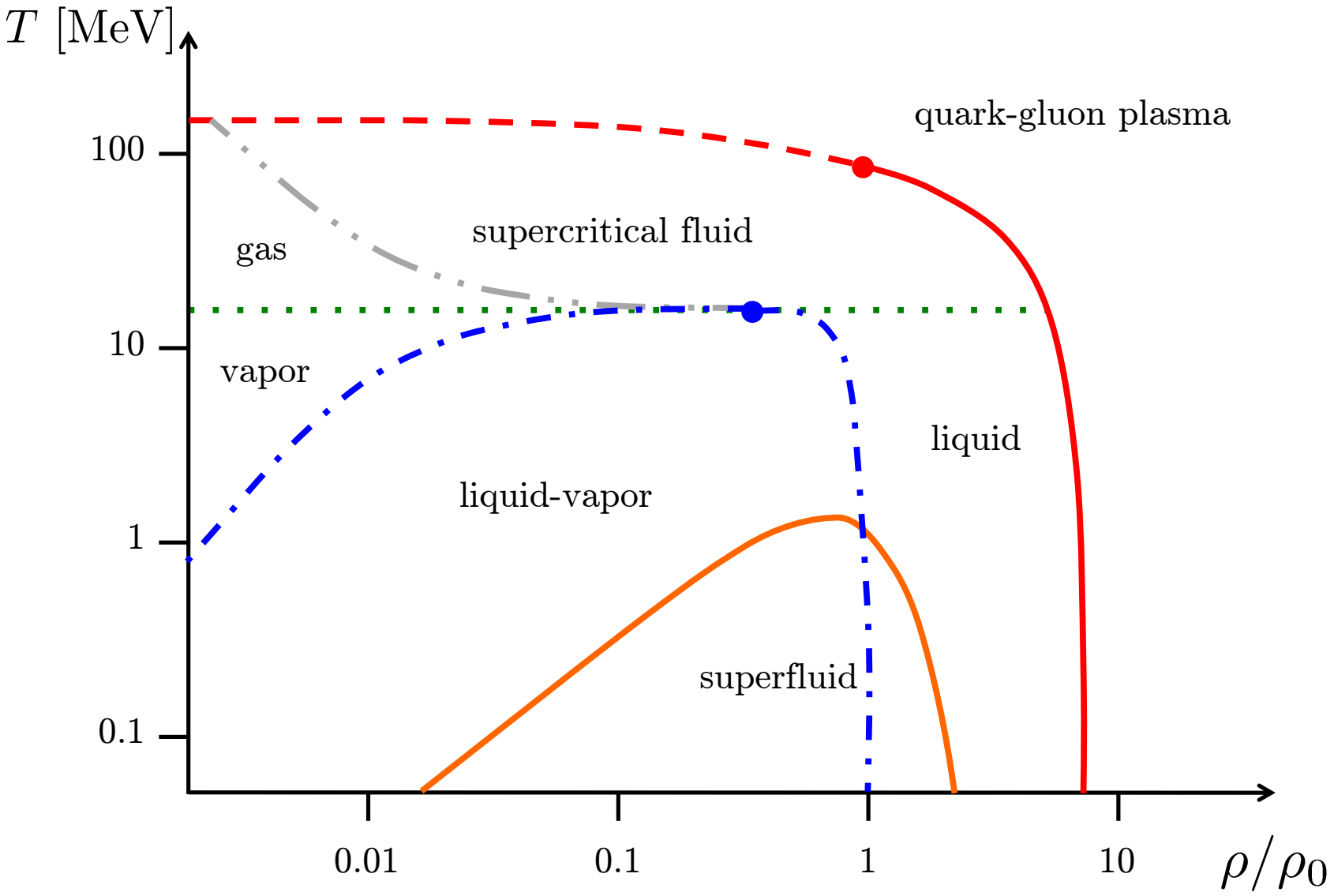
Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

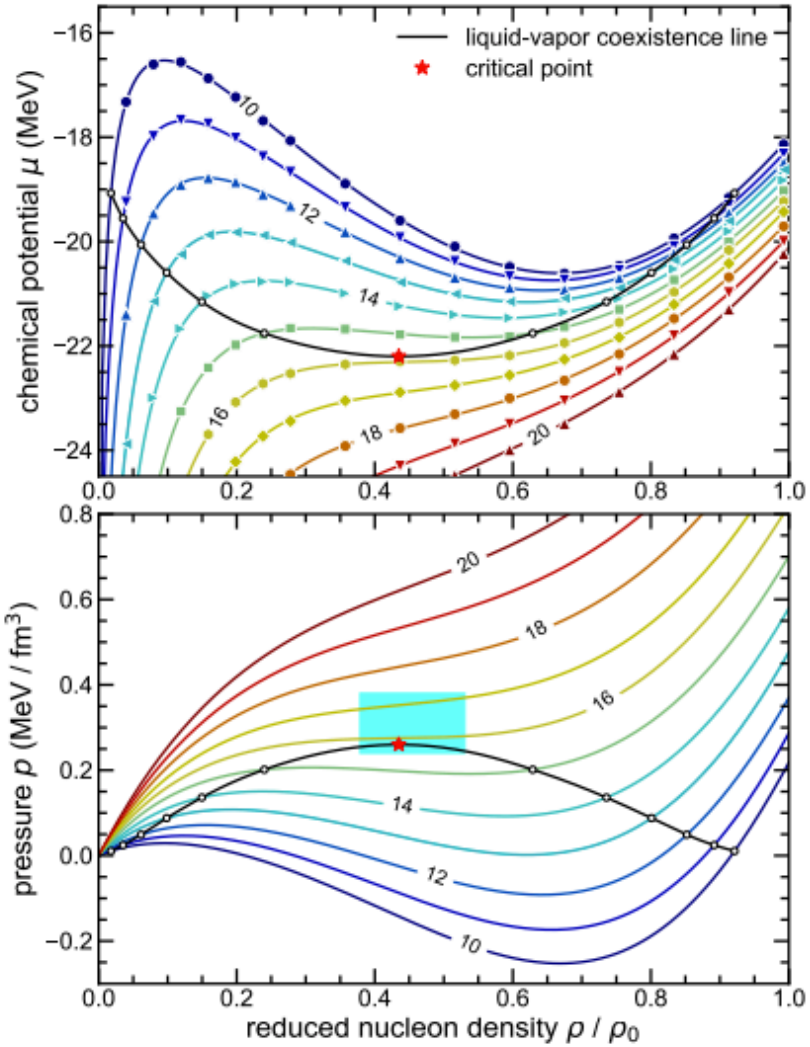
Metropolis updates of pinholes



hybrid Monte Carlo
updates of auxiliary/pion fields

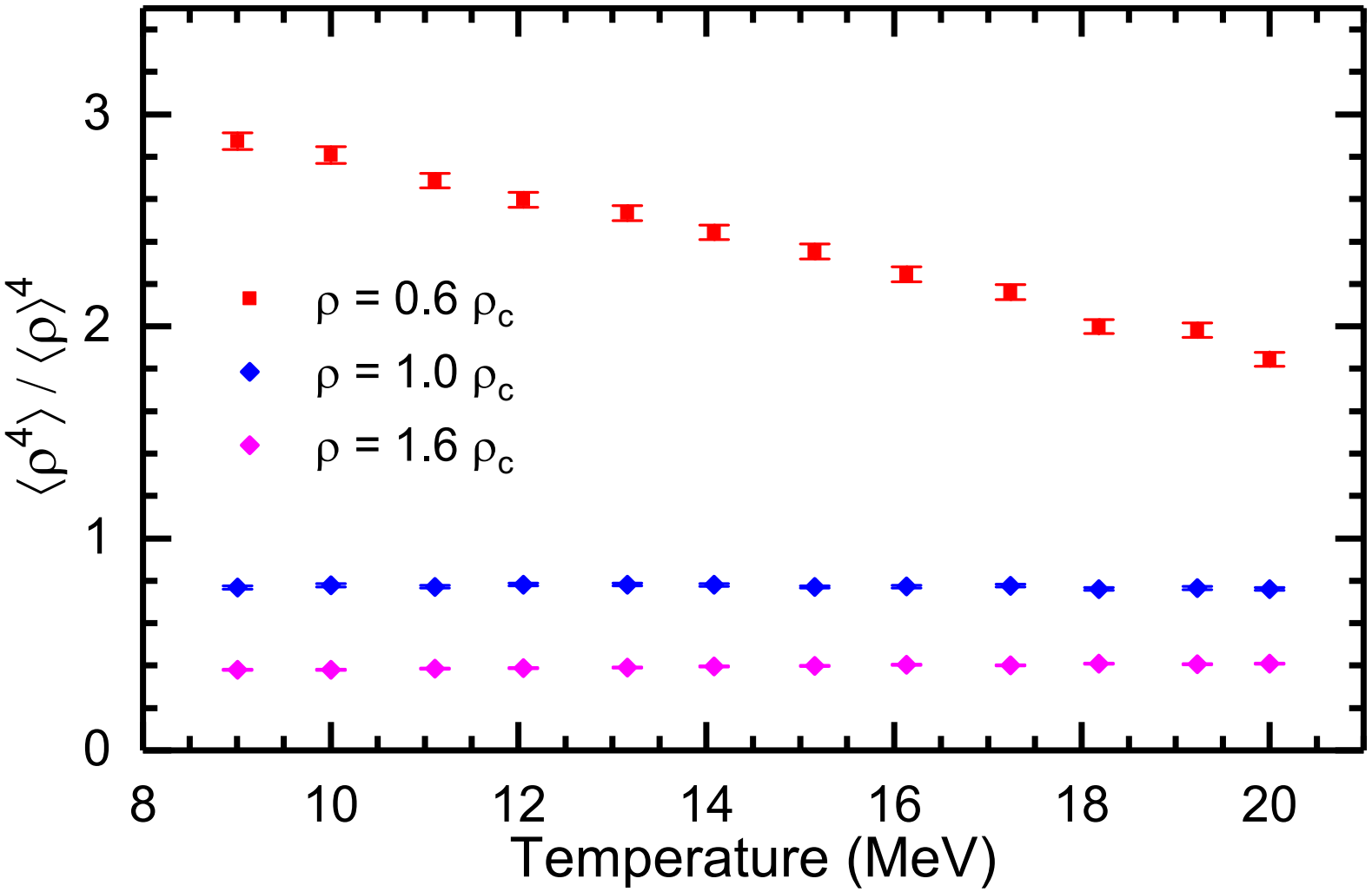

Charge density (e•fm^{-3})
0.00
0.02
0.04
0.06
0.08
0
2
4
6
8
Radius (fm)
^{16}O
T = 0.0 MeV
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV
Exp. (g. s.)


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

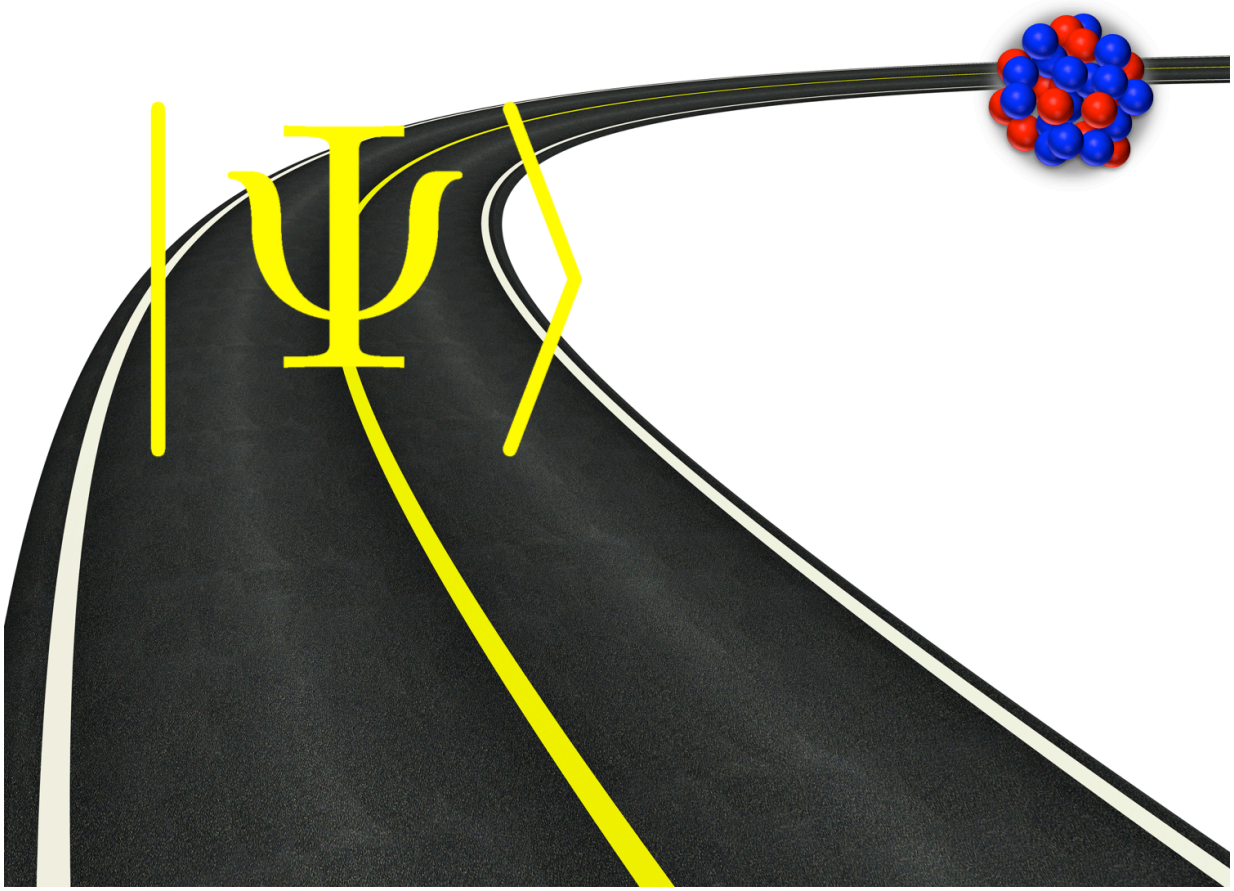


$$T_c = 15.80(0.32)(1.60)\,\mathrm{MeV}$$
$$\rho_c = 0.089(04)(18)\,\mathrm{fm}^{-3}$$
$$\mu_c = -22.20(0.44)(2.20)\,\mathrm{MeV}$$
$$P_c = 0.260(05)(30)\,\mathrm{MeV\ fm}^{-3}$$

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


$\langle\rho^4\rangle / \langle\rho\rangle^4$
0
1
2
3
8
10
12
14
16
18
20
Temperature (MeV)
$\rho = 0.6\ \rho_c$
$\rho = 1.0\ \rho_c$
$\rho = 1.6\ \rho_c$

Eigenvector continuation



D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121 (2018) 032501

Eigenvector continuation

We demonstrate that when a control parameter in the Hamiltonian matrix is varied smoothly, the extremal eigenvectors do not explore the large dimensionality of the linear space. Instead they trace out trajectories with significant displacements in only a small number of linearly-independent directions.

We can prove this empirical observation using analytic function theory and the principles of analytic continuation.

Since the eigenvector trajectory is a low-dimensional manifold embedded in a very large space, we can find the desired eigenvector using a variational subspace approximation.

D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121 (2018) 032501

Consider a one-parameter family of Hamiltonian matrices of the form

$$H(c) = H_0 + cH_1$$

where H_0 and H_1 are Hermitian. Let the eigenvalues and eigenvectors be

$$H(c)|\psi_j(c)\rangle = E_j(c)|\psi_j(c)\rangle$$

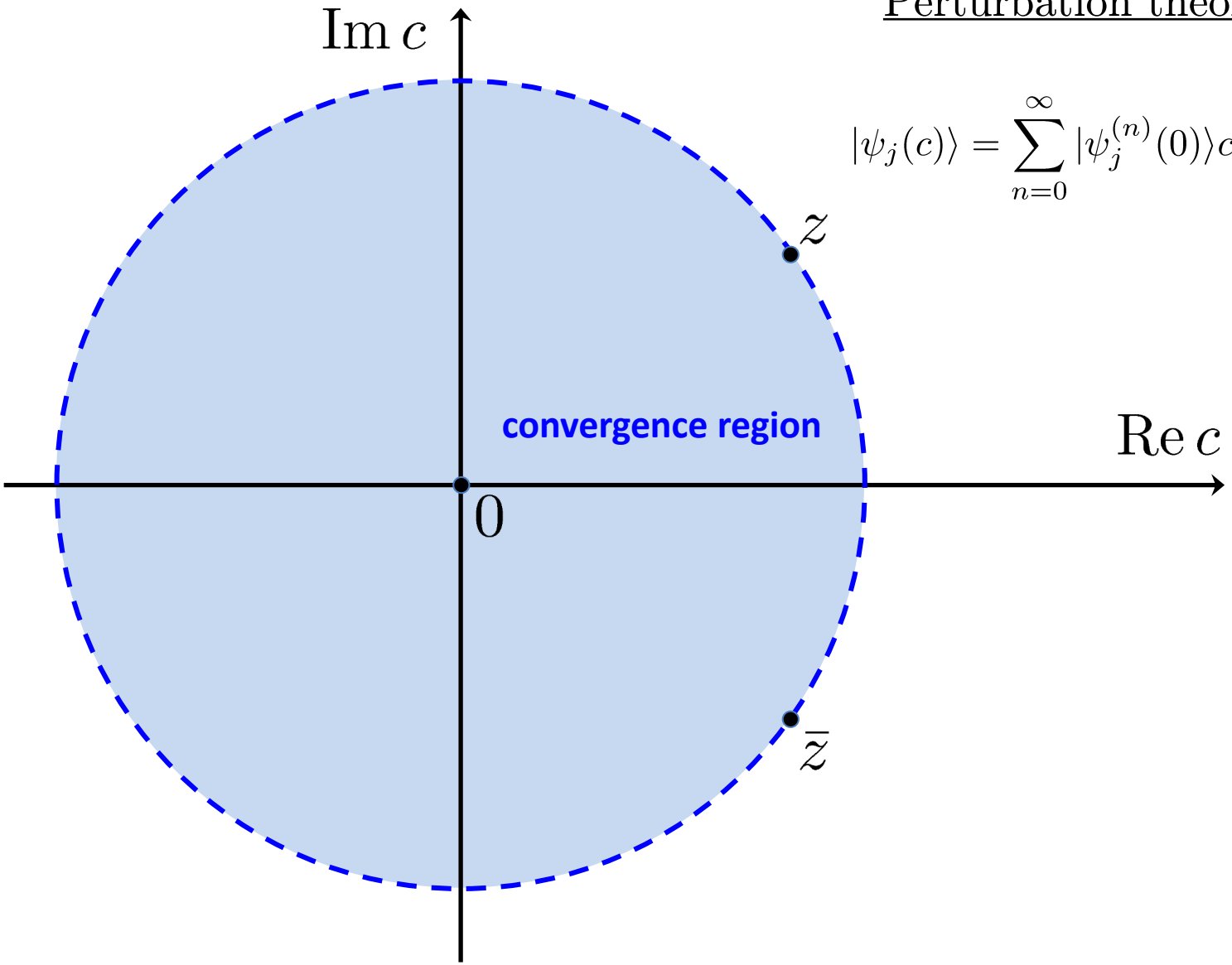
We can perform series expansions around the point $c = 0$.

$$E_j(c) = \sum_{n=0}^{\infty} E_j^{(n)}(0)c^n/n!$$
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

This is the strategy of perturbation theory. We can compute each term in the series when the eigenvalues and eigenvectors of H_0 are known or computable.

Perturbation theory

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$



Bose-Hubbard model

In order to illuminate our discussion with a concrete example, we consider a quantum Hamiltonian known as the Bose-Hubbard model in three dimensions. It describes a system of identical bosons on a three-dimensional cubic lattice.

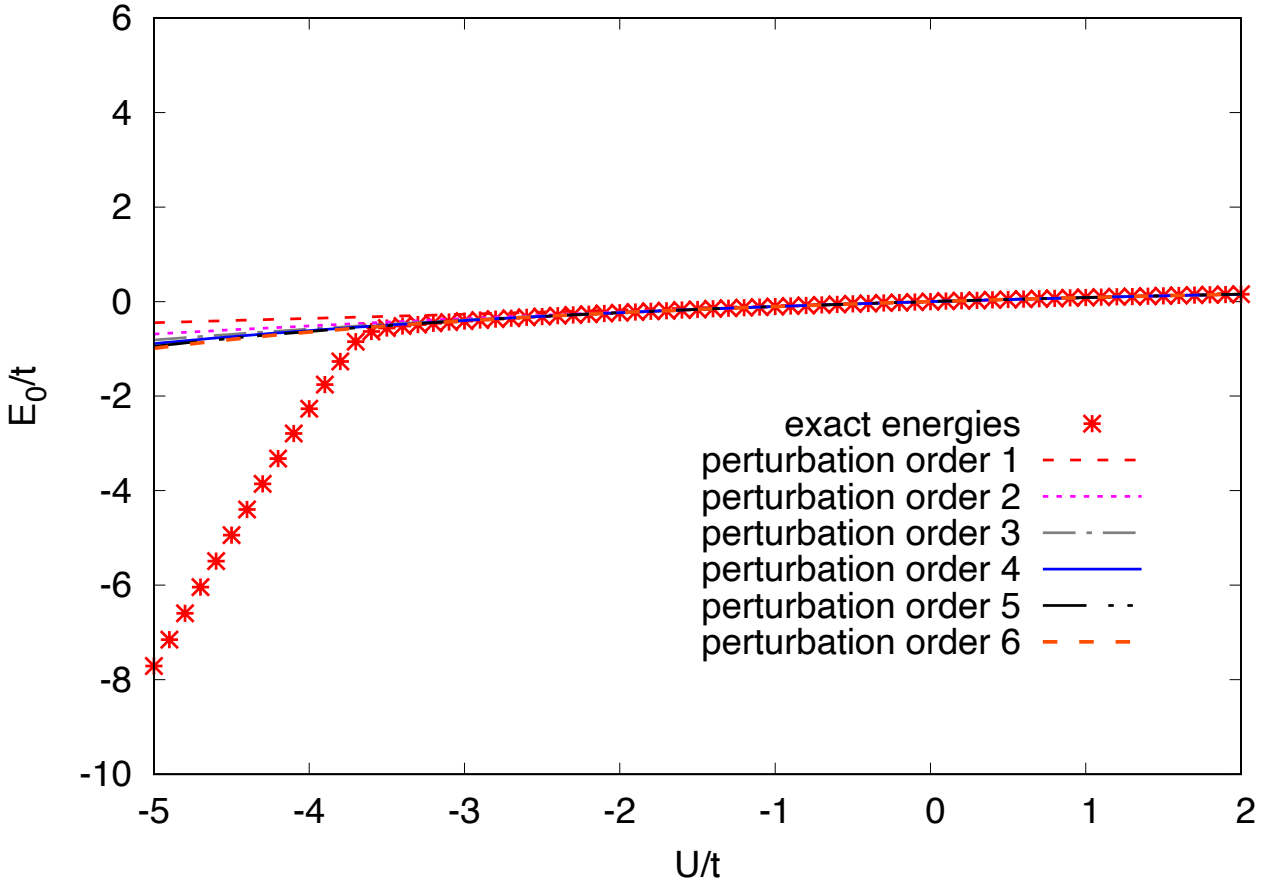
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

$$\rho(\mathbf{n}) = a^\dagger(\mathbf{n}) a(\mathbf{n})$$

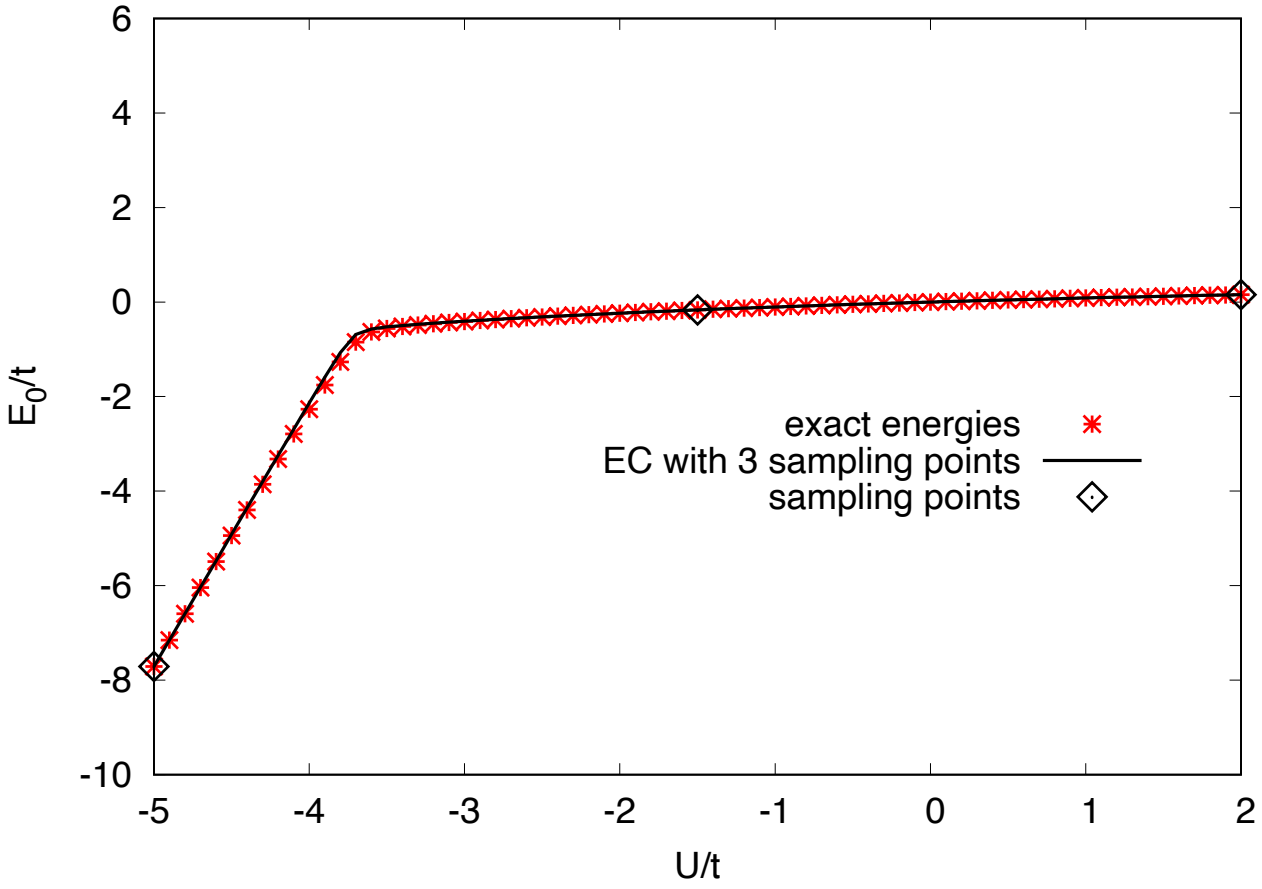
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

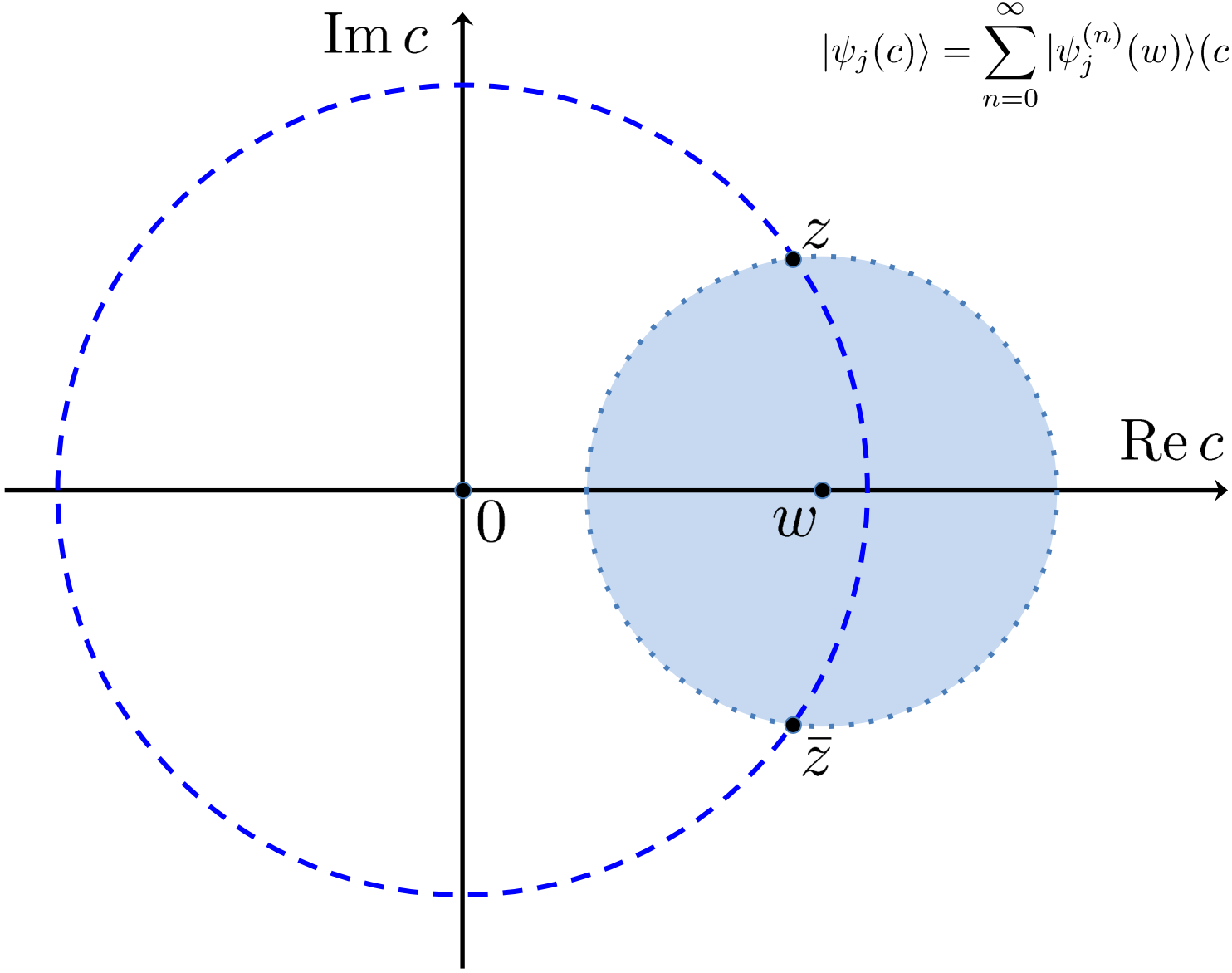
Perturbation theory fails at strong attractive coupling

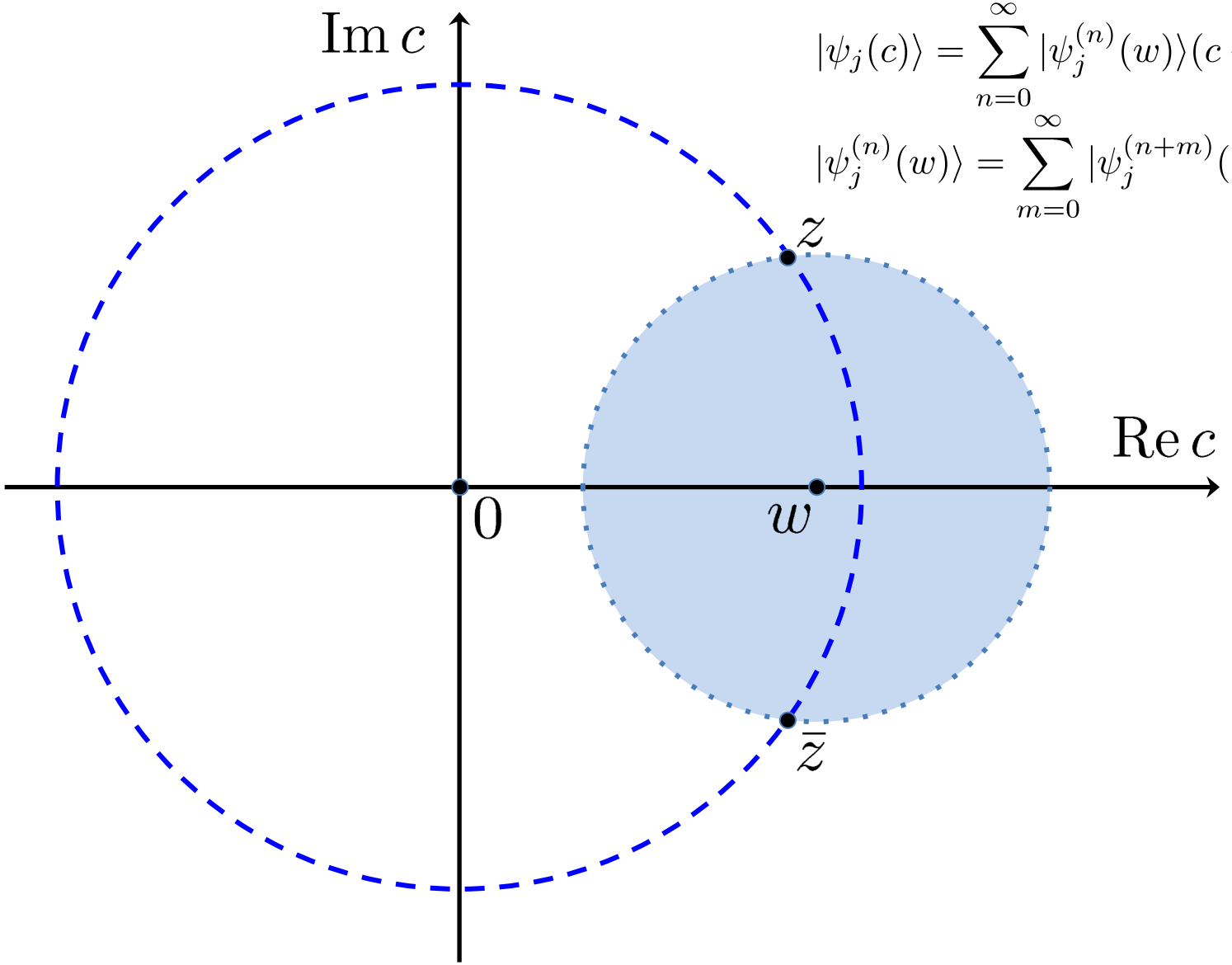


Restrict the linear space to the span of three vectors



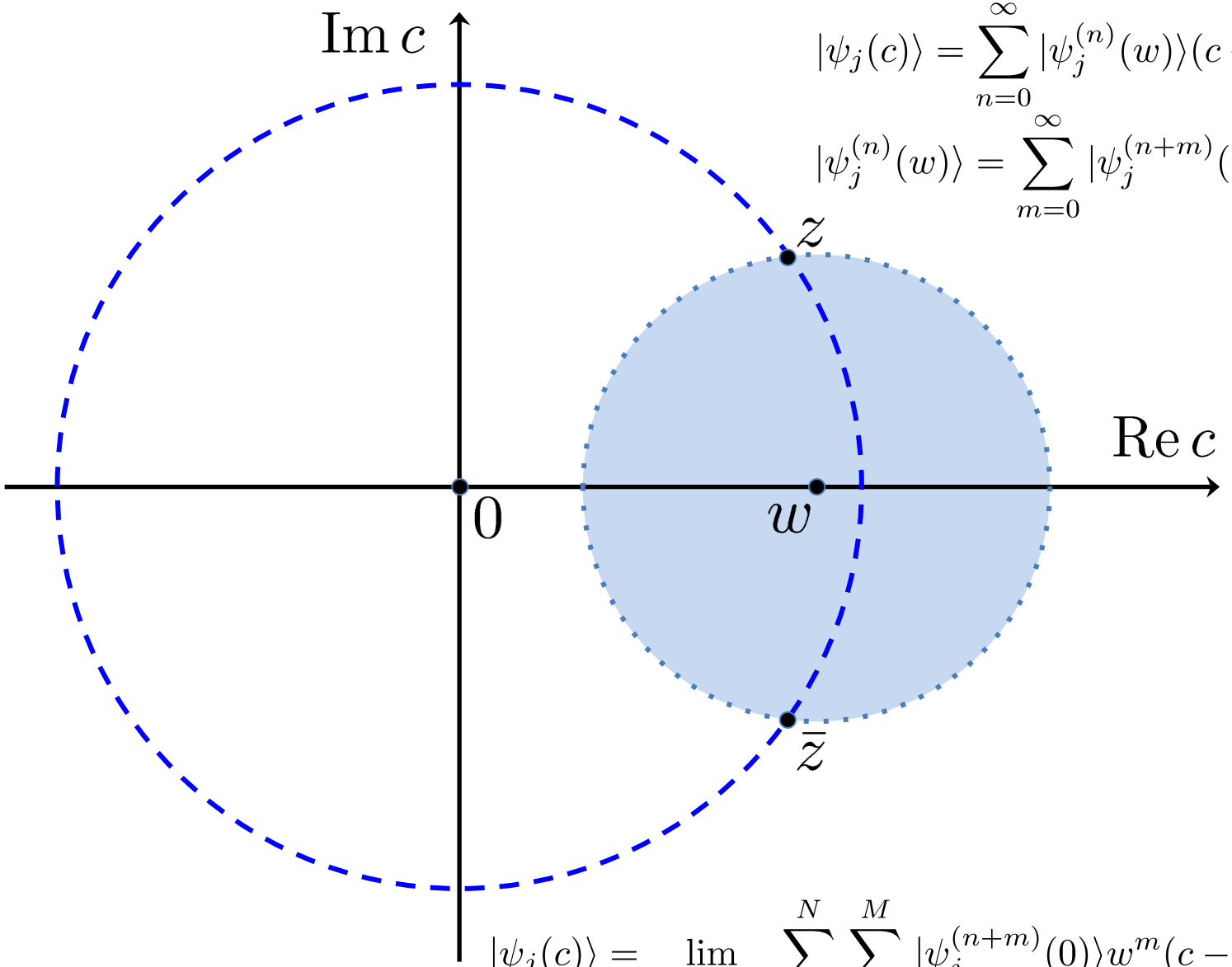
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

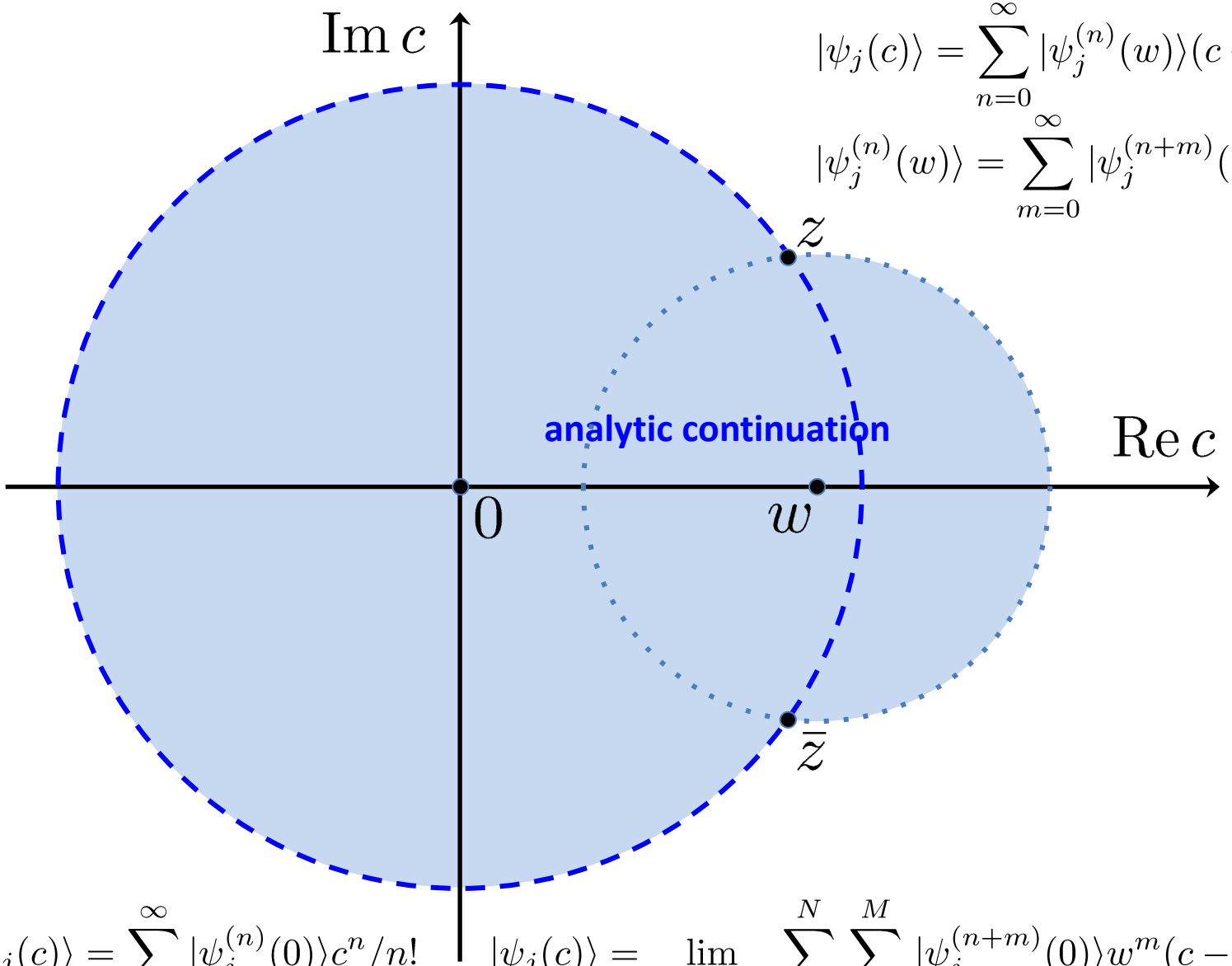
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

The eigenvector can be well approximated as a linear combination of a few vectors, using either the original series expansion

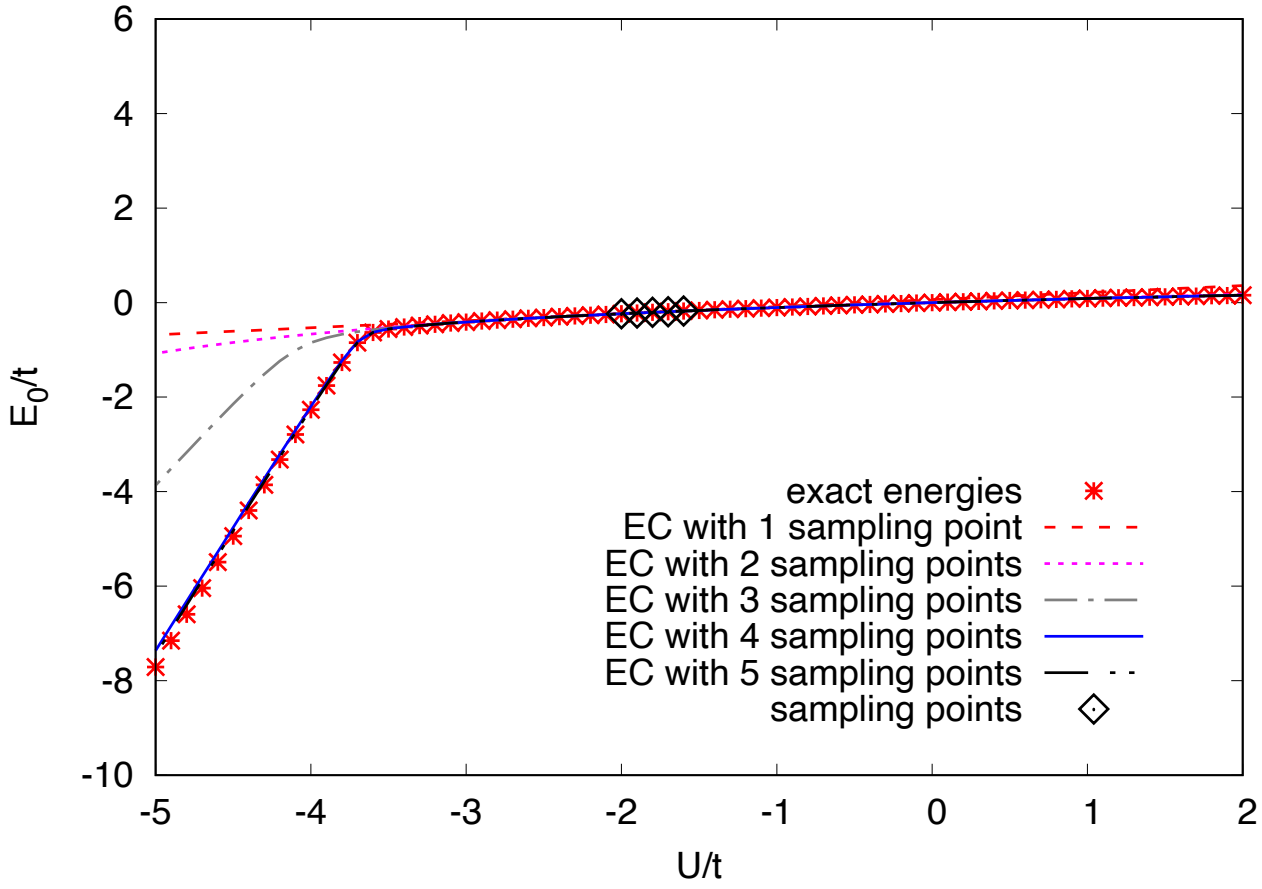
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

or the rearranged multi-series expansion we obtained through analytic continuation

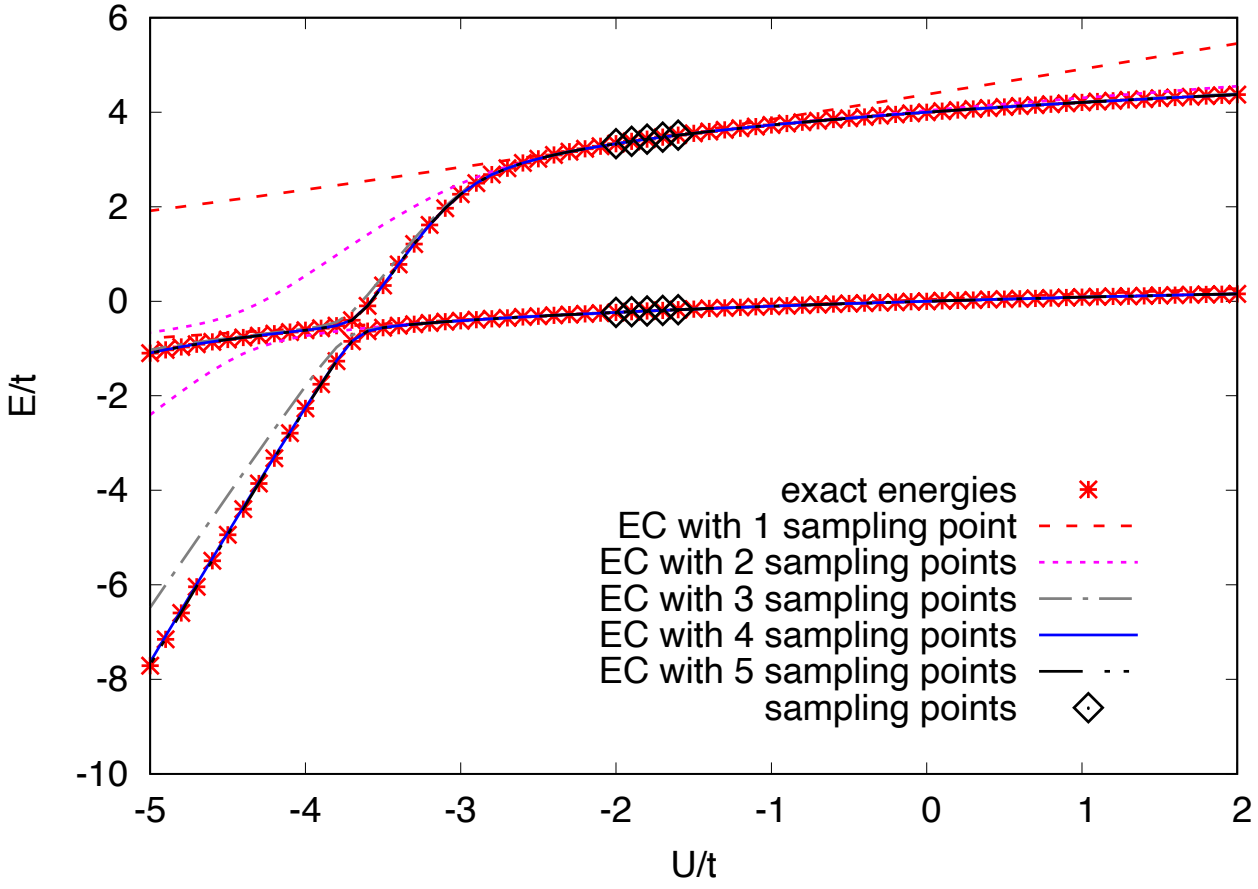
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

We can “learn” the eigenvector trajectory in one region and perform eigenvector continuation to another region



Applying eigenvector continuation to more than one eigenvector at a time accelerates convergence near avoided level crossings.



Physics Letters B
Volume 810, 10 November 2020, 135814

Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification

S. König [a, b, c], A. Ekström [d], K. Hebeler [a, b], D. Lee [e], A. Schwenk [a, b, f]

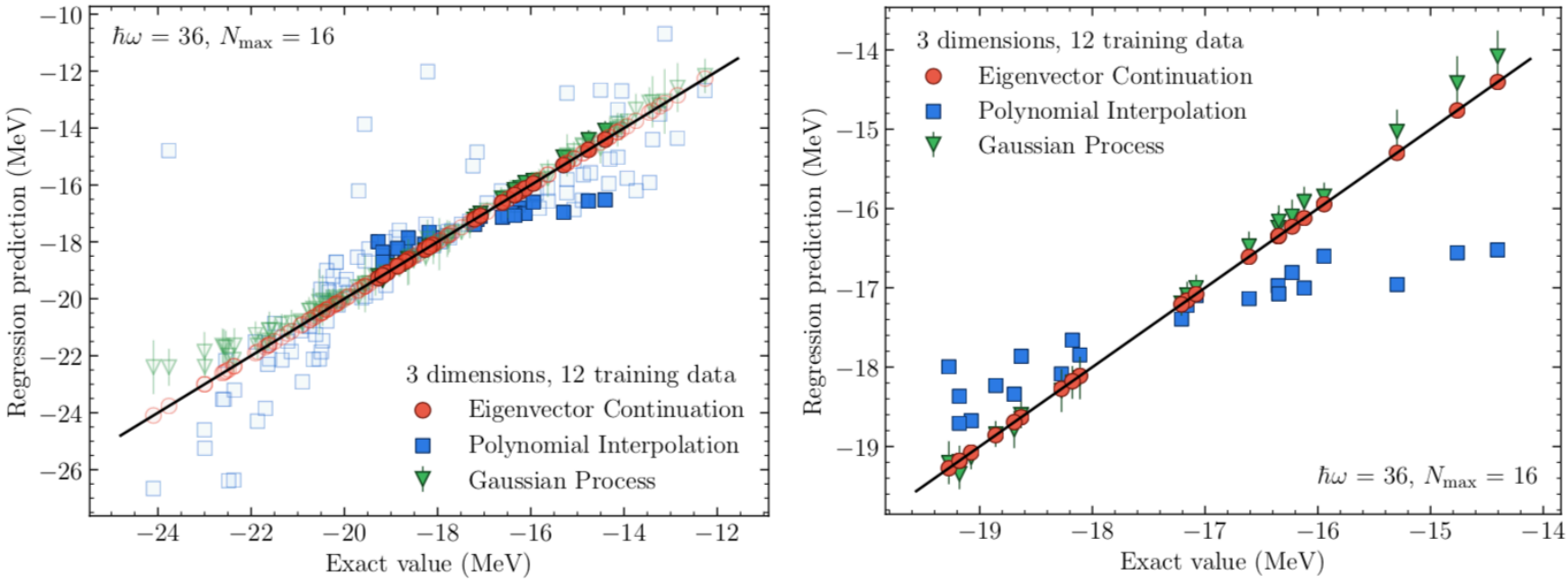


Figure 1. Comparison of different emulators for the ^{4}He ground-state energy using 12 training data points to explore a space where three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols). See main text on how these are defined. The right panel shows the same data restricted to interpolation samples (note the smaller axis range).

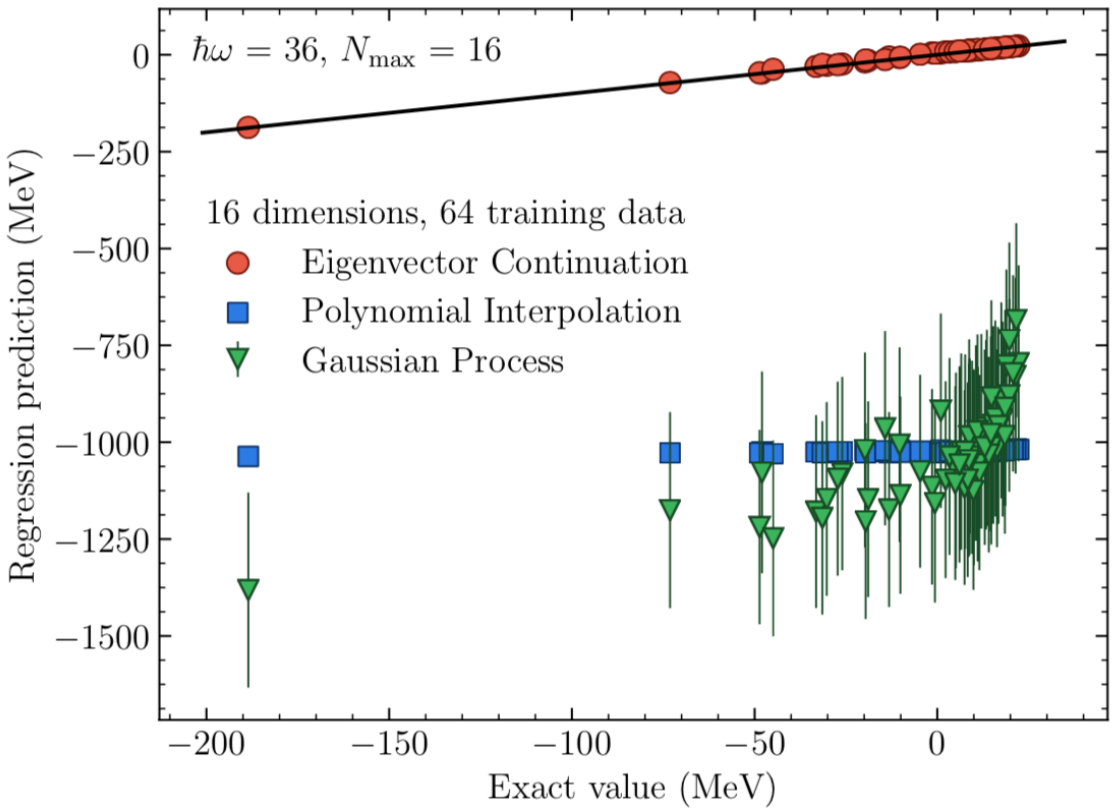


Figure 2. Comparison of different emulators for the ^{4}He ground-state energy using 64 training data points to explore a space where all 16 LECs are varied.

1. arXiv:2007.03635 [pdf, other] nucl-th cond-mat.mtrl-sci hep-lat hep-ph nucl-ex doi 10.1016/j.physletb.2020.135719

Efficient emulators for scattering using eigenvector continuation

Authors: R. J. Furnstahl, A. J. Garcia, P. J. Millican, Xilin Zhang

Abstract: **Eigenvector continuation** EC has been shown to accurately and efficiently reproduce ground states for targeted sets of Hamiltonian parameters. It uses as variational basis vectors the corresponding ground-state eigensolutions from selected other sets of parameters. Here we extend the EC approach to scattering using the... ▽ More

Submitted 28 September, 2020; **v1** submitted 7 July, 2020; **originally announced** July 2020.

Comments: Close to the published version; 12 pages, 10 figures, with supplemental material; include more discussions on the computational-cost reduction and Kohn anomalous singularity; several jupyter notebooks for reproducing all the results in the paper can be accessed at https://github.com/buqeye/eigenvector-continuation

2. arXiv:2004.07651 [pdf, other] nucl-th cond-mat.str-el hep-lat hep-ph math.NA

Convergence of Eigenvector Continuation

Authors: Avik Sarkar, Dean Lee

Abstract: **Eigenvector**... ▽ More

Submitted 16 April, 2020; **originally announced** April 2020.

Comments: 5+1 pages (main + supplemental), 6+0 figures (main + supplemental)

3. arXiv:2002.02724 [pdf, other] nucl-th

Bogoliubov many-body perturbation theory under constraint

Authors: Pepijn Demol, Mikael Frosini, Alexander Tichai, Vittorio Somà, Thomas Duguet

Abstract: ...from those obtained via a configuration interaction (CI) diagonalization, the series is shown to eventually diverge. The application of a novel resummation method coined as **eigenvector**... ▽ More

Submitted 7 February, 2020; **originally announced** February 2020.

Comments: 45 pages, 10 figures

4. arXiv:1911.12578 [pdf, other] nucl-th cond-mat.str-el doi 10.1103/PhysRevC.101.041302

Improved many-body expansions from eigenvector continuation

Authors: Pepijn Demol, Thomas Duguet, Andreas Ekström, Mikael Frosini, Kai Hebeler, Sebastian König, Dean Lee, Achim Schwenk, Vittorio Somà, Alexander Tichai

Abstract: ...methods. In large-scale many-body applications such schemes are often of limited use since no a priori analytical knowledge of the expansion is available. We present here **eigenvector continuation** as an alternative resummation tool that is both efficient and reliable because it is based on robust and simple mathematical... ▽ More

Submitted 28 November, 2019; **originally announced** November 2019.

Comments: 6 pages, 2 figures

Journal ref: Phys. Rev. C 101, 041302 (2020)

5. arXiv:1910.02922 [pdf, other] nucl-th doi 10.1103/PhysRevLett.123.252501

Global sensitivity analysis of bulk properties of an atomic nucleus

Authors: Andreas Ekström, Gaute Hagen

Abstract: ...in the next-to-next-to-leading order chiral Hamiltonian with two- and three-nucleon forces. For this purpose we develop a subspace-projected coupled-cluster method using **eigenvector continuation** [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018)]. With this method we compute the binding energy and charge radius of... ▽ More

Submitted 7 October, 2019; **originally announced** October 2019.

Comments: 6 pages, 3 figures, Supplemental Material provided as ancillary material

Journal ref: Phys. Rev. Lett. 123, 252501 (2019)

Summary and outlook

We have found evidence that nature is close to a quantum phase transition between nuclear liquid and Bose gas of alpha particles.

We have constructed a 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 have used the pinhole algorithm to study nucleon densities and clustering.

First principles calculations of nuclear thermodynamics using the pinhole trace algorithm are possible. We have mapped out the nuclear liquid-gas phase diagram and are studying alpha clustering as a function of density and temperature.

We are using eigenvector continuation to perform calculations for systems where Monte Carlo sign oscillations would otherwise make the calculation impossible.

Eigenvector continuation is being used by several different groups for uncertainty quantification, emulators for the quantum many-body problem, emulators for scattering, resummation method for many-body perturbation theory, etc.