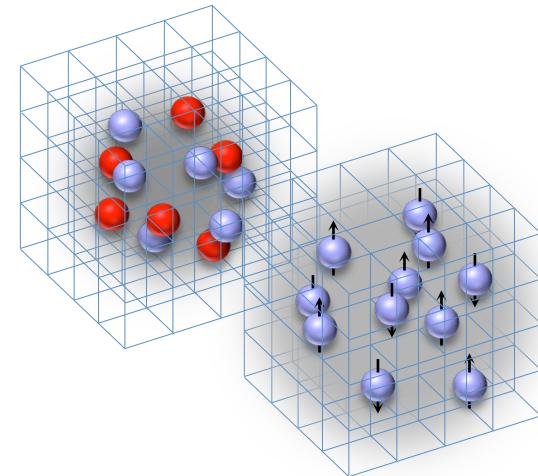


Nuclear Lattice Simulations

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

Pusan National University
Department of Physics
December 20, 2019



Outline

From nuclear forces to nuclear structure

Lattice effective field theory

A tale of two interactions

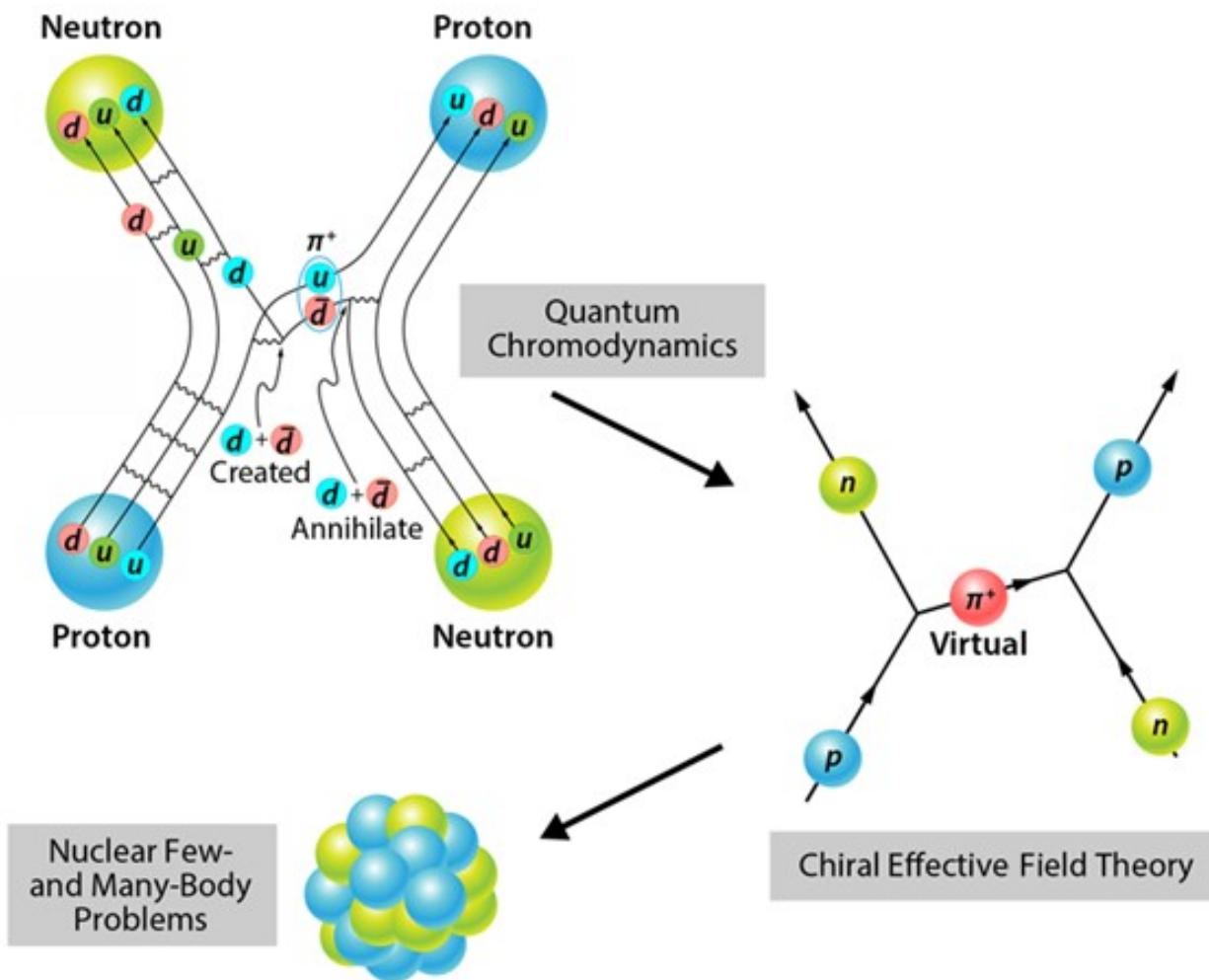
Essential elements for nuclear binding

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

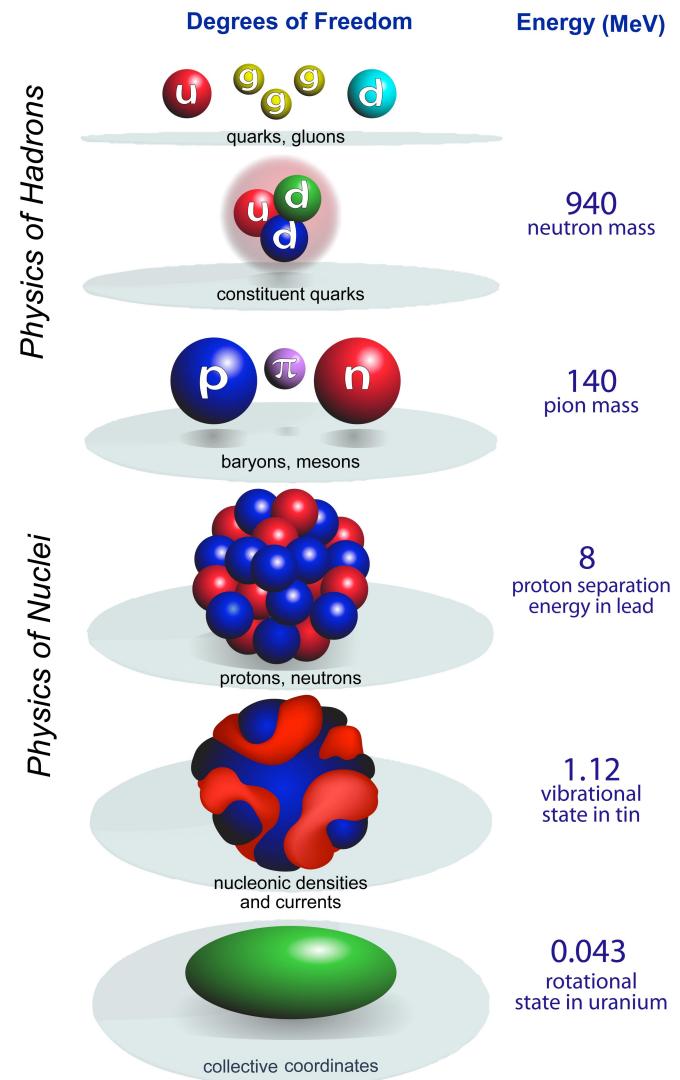
Microscopic A -body methods

Configuration interactions

Density functional methods

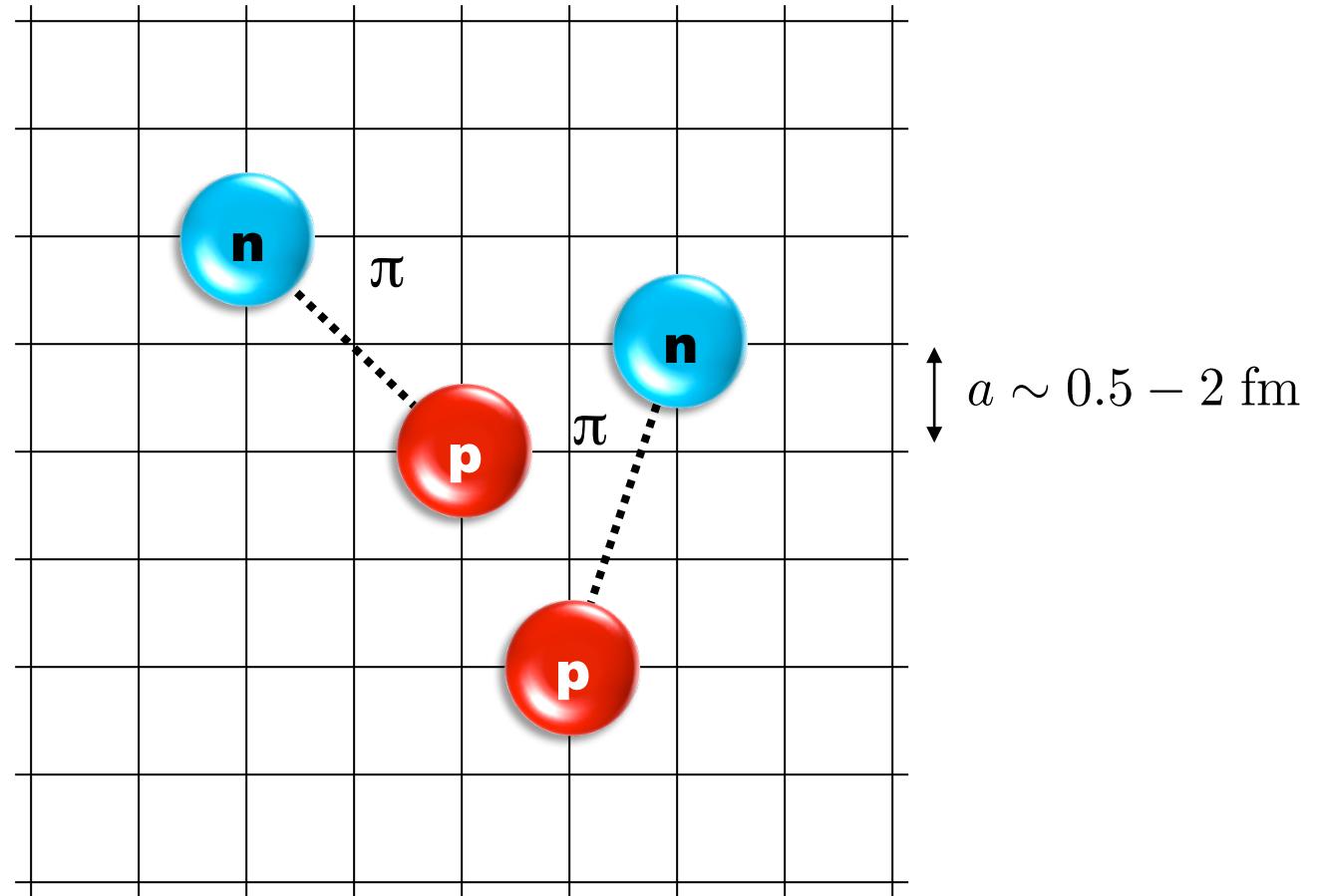
Mean field methods

Effective theory of collective modes



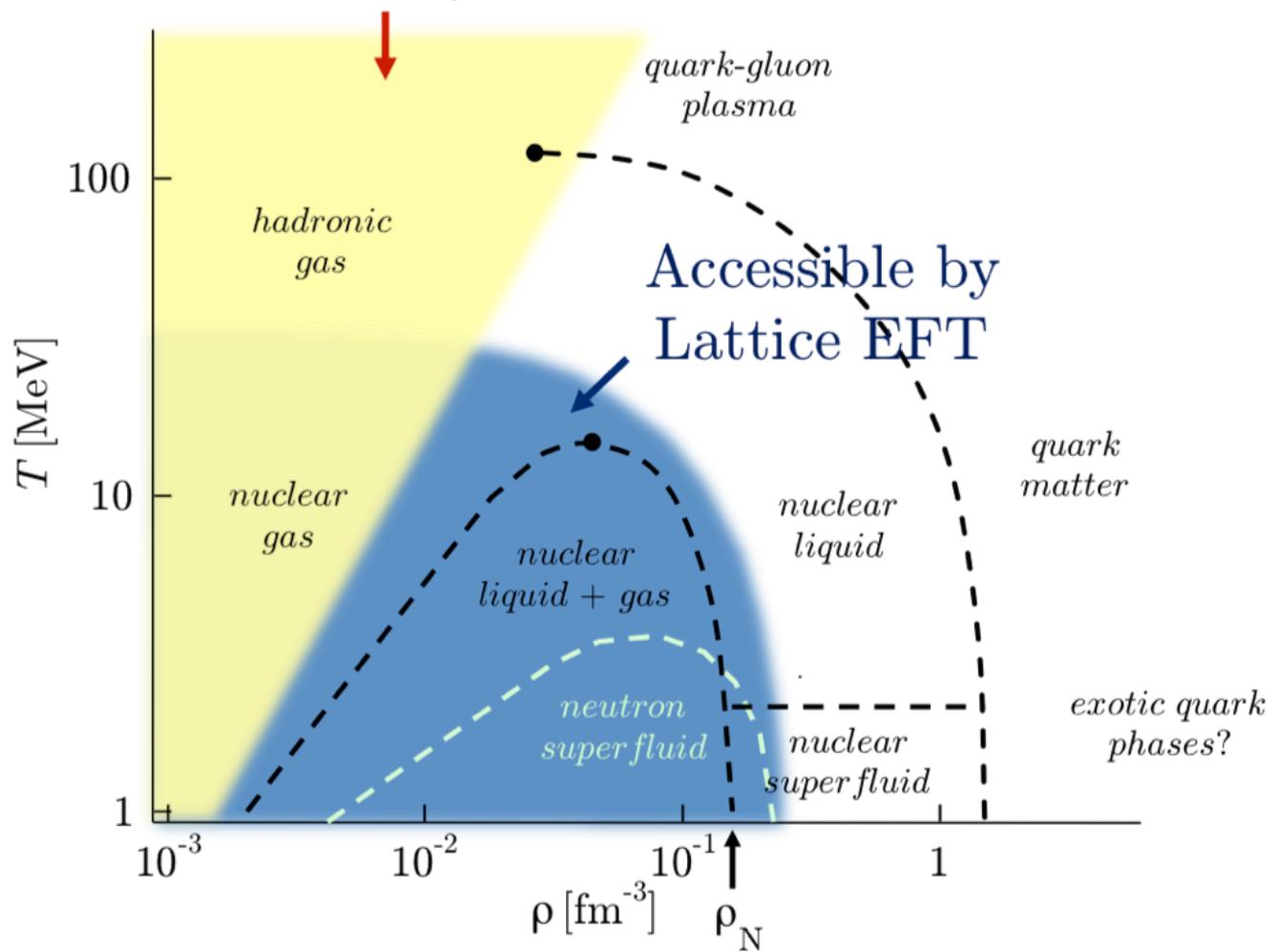
W. Nazarewicz

Lattice effective field theory



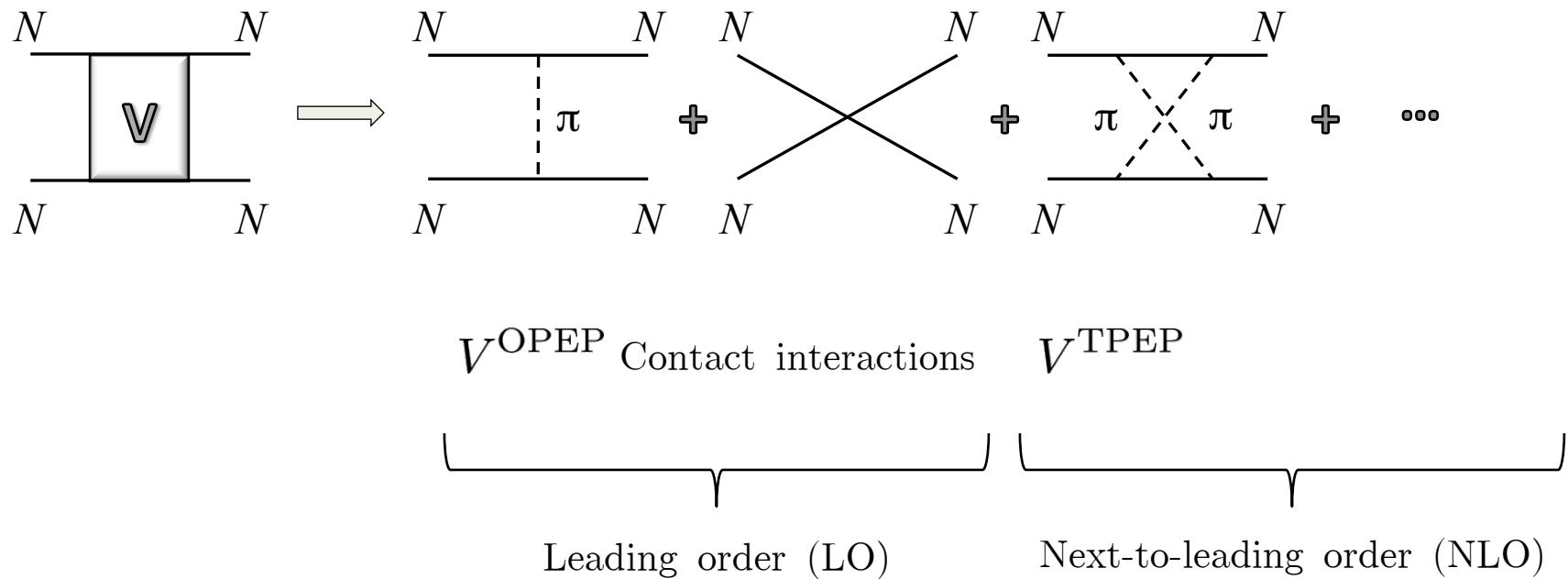
Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Accessible by Lattice QCD

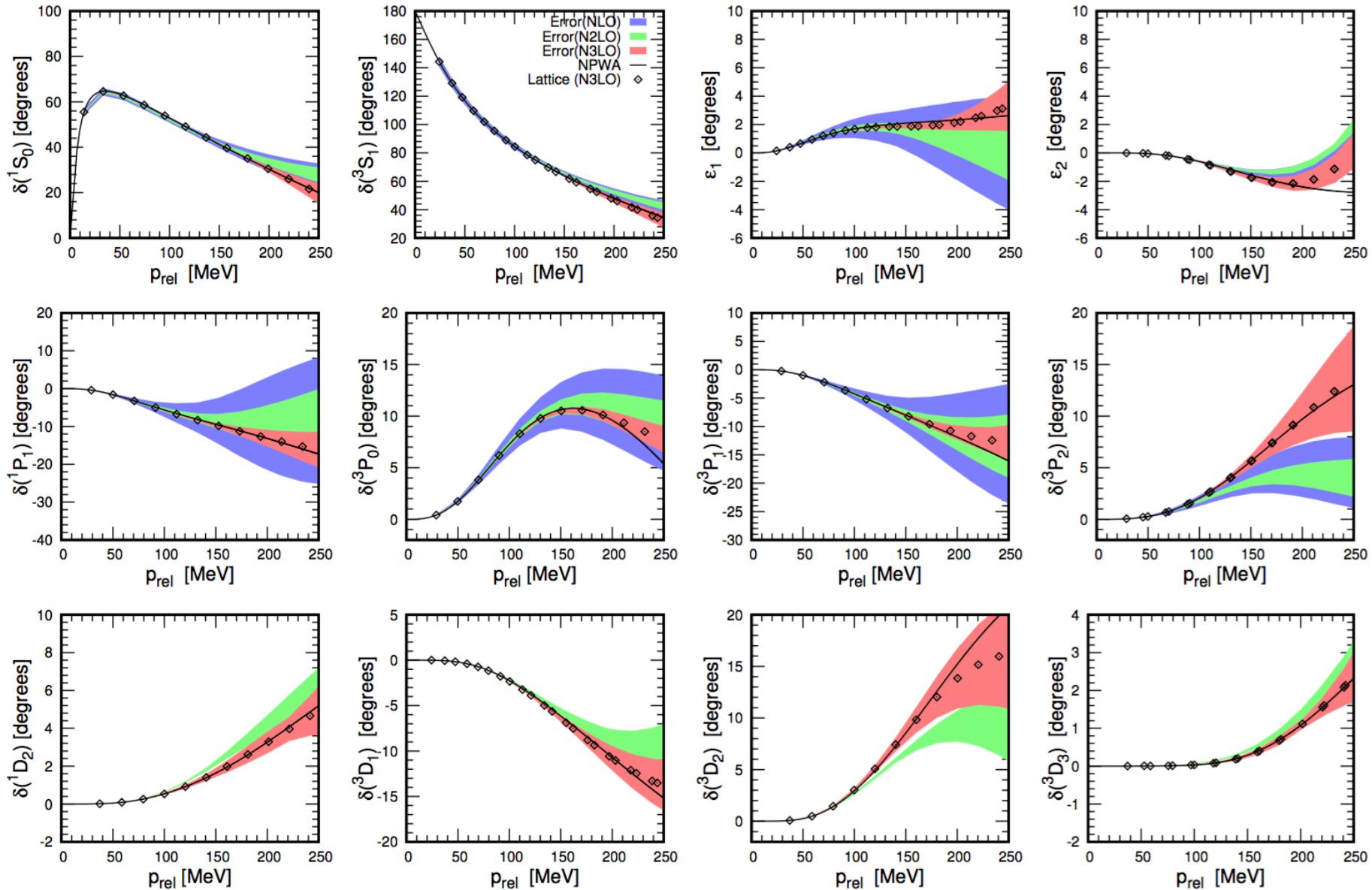


Chiral effective field theory

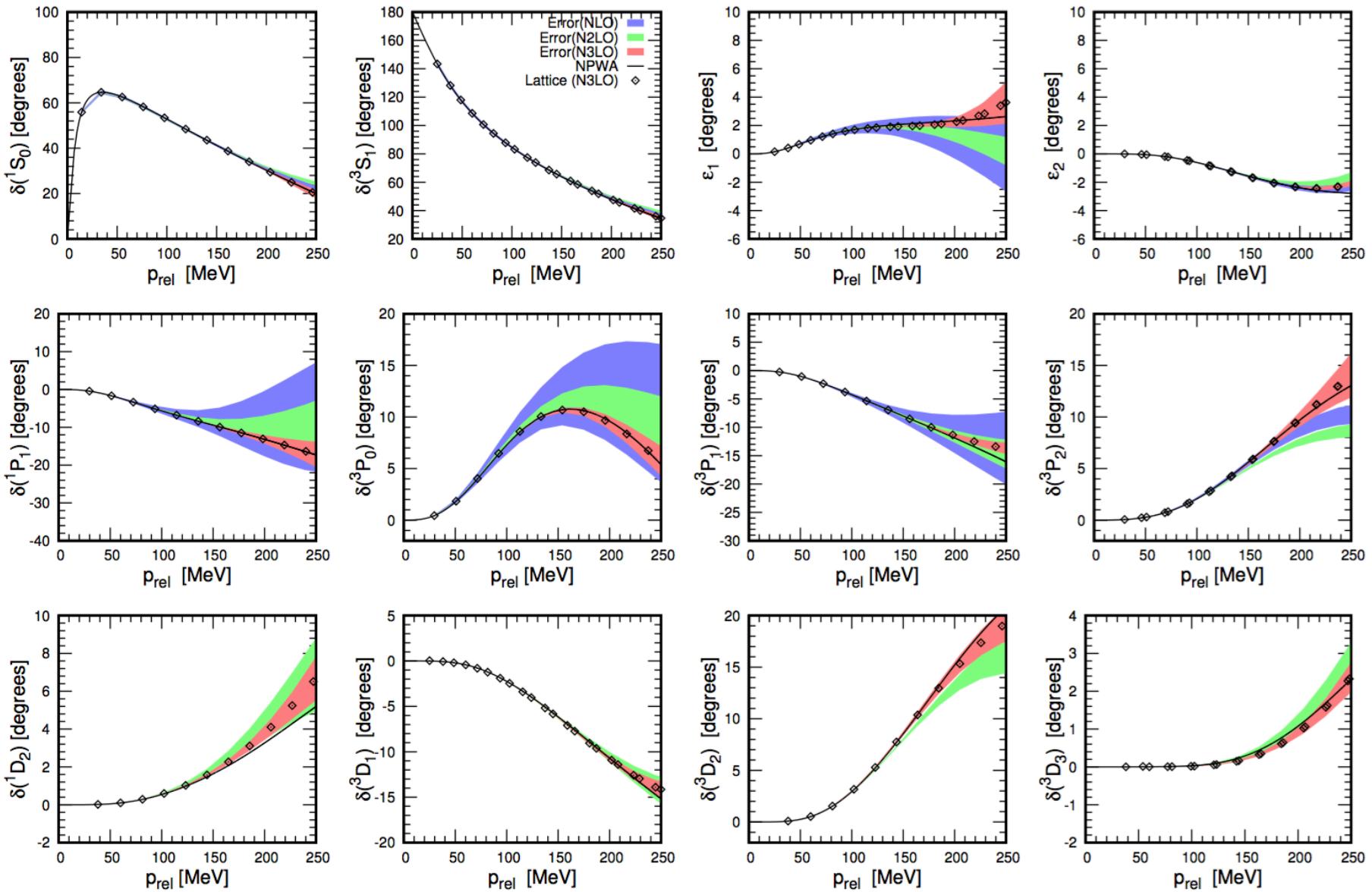
Construct the effective potential order by order



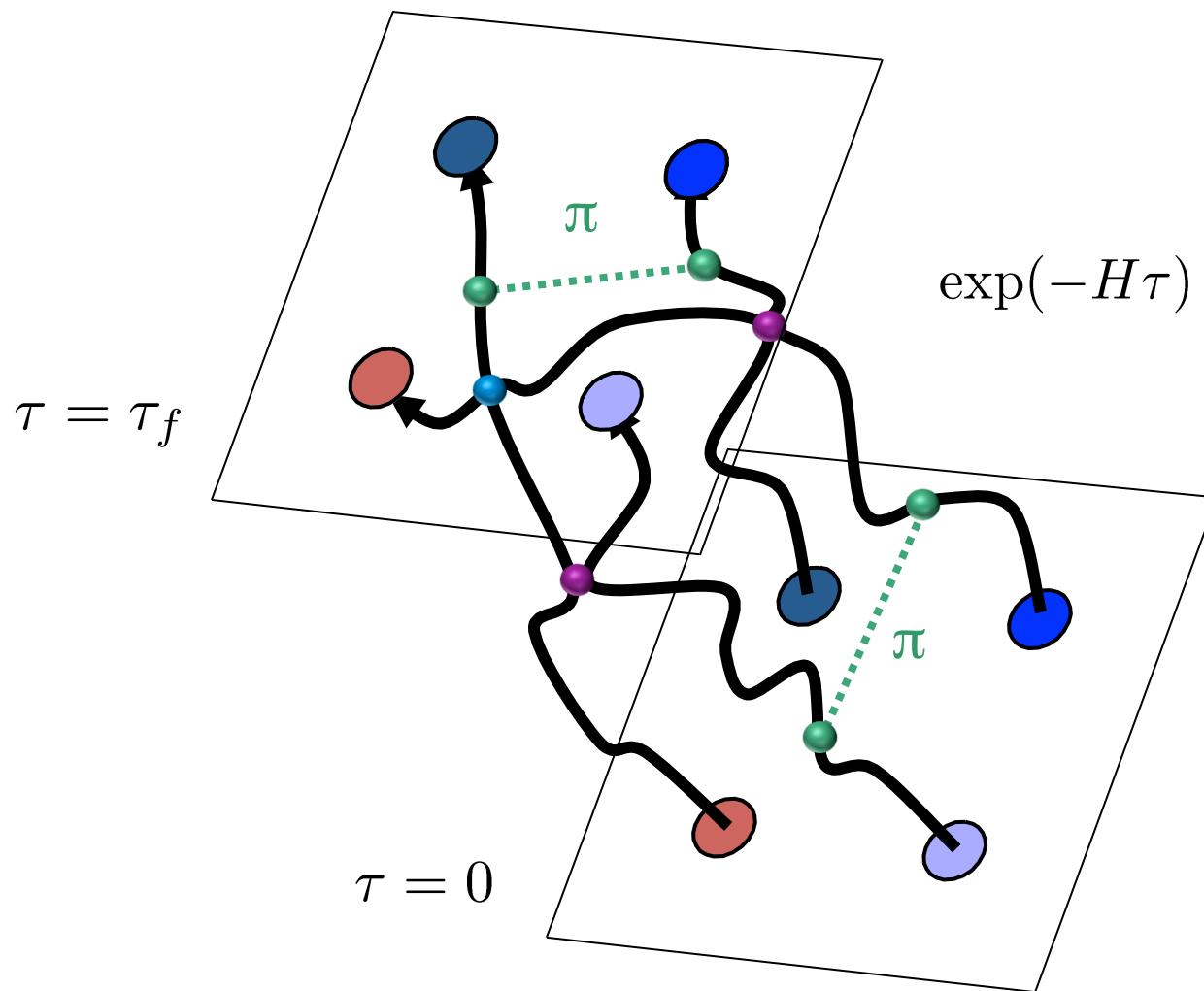
$$a = 1.315 \text{ fm}$$



$$a = 0.987 \text{ fm}$$



Euclidean time projection

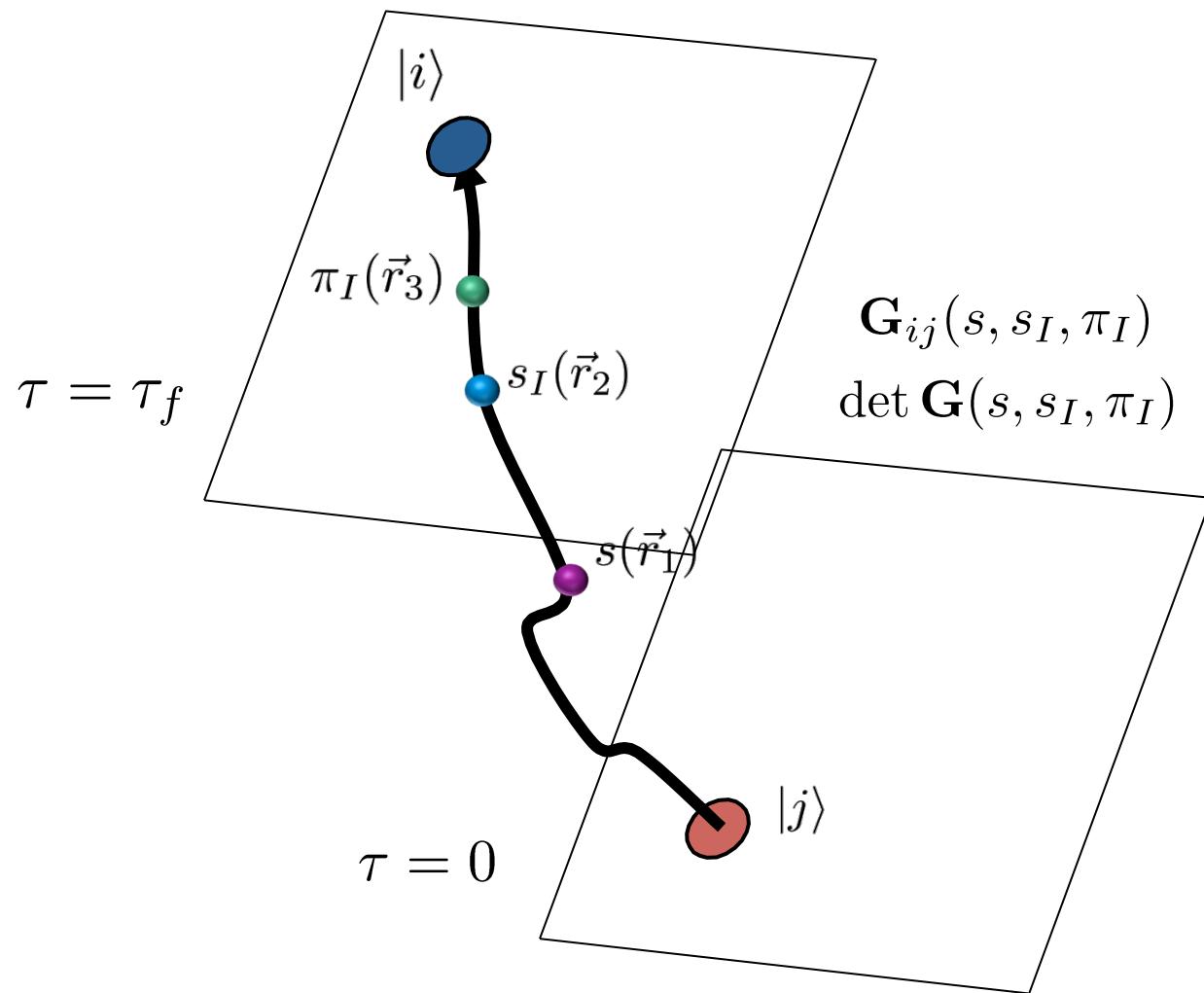


Auxiliary field method

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

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

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



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.

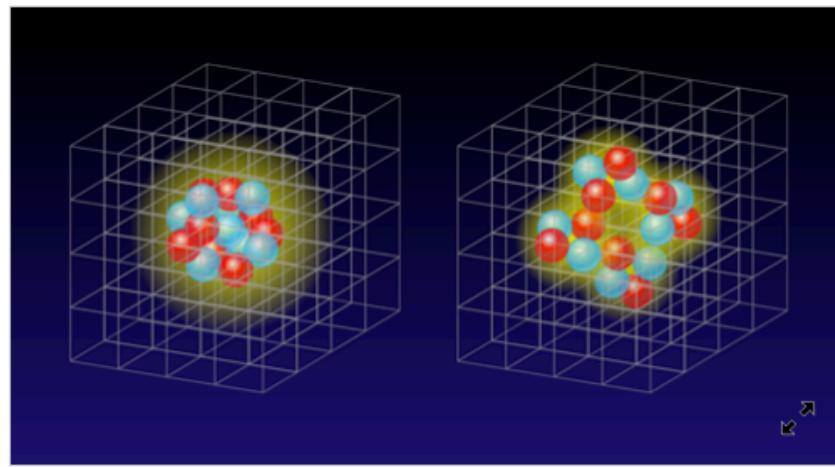


Figure 1: Lee and colleagues performed simulations of a nucleus in which they tweaked the interaction between nucleons (protons and neutrons) [1]. They found that, depending on the form of the interaction, the nucleus lay on either side of a quantum phase transition. The transition is between (left) 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
^8Be	-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

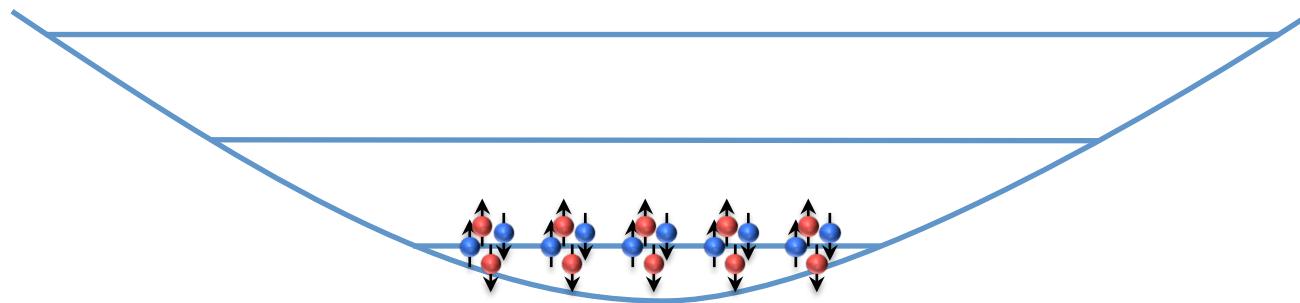
$$\frac{E_{\text{8 Be}}}{E_{\text{4 He}}} = 1.997(6)$$

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

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

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

Bose condensate of alpha particles!



Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^8Be	-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

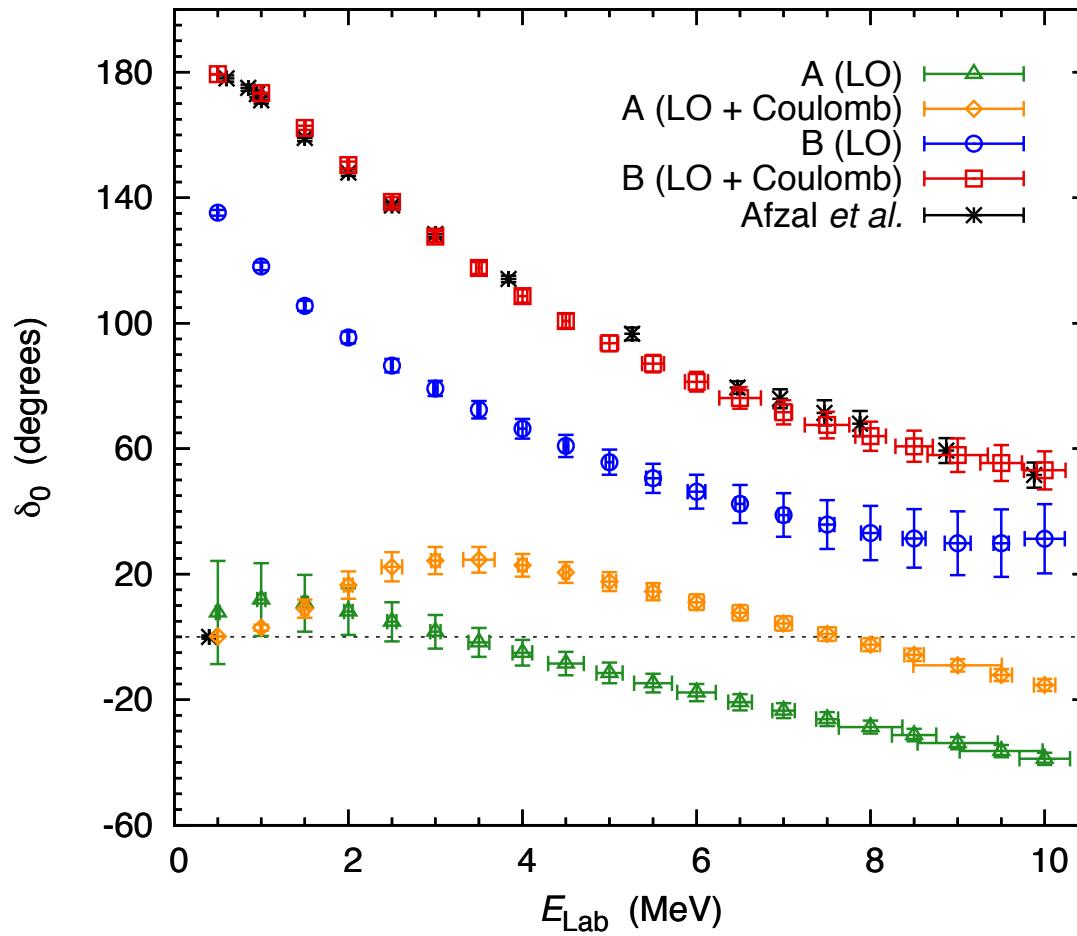
$$\frac{E_{^8\text{Be}}}{E_{^4\text{He}}} = 1.997(6)$$

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

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

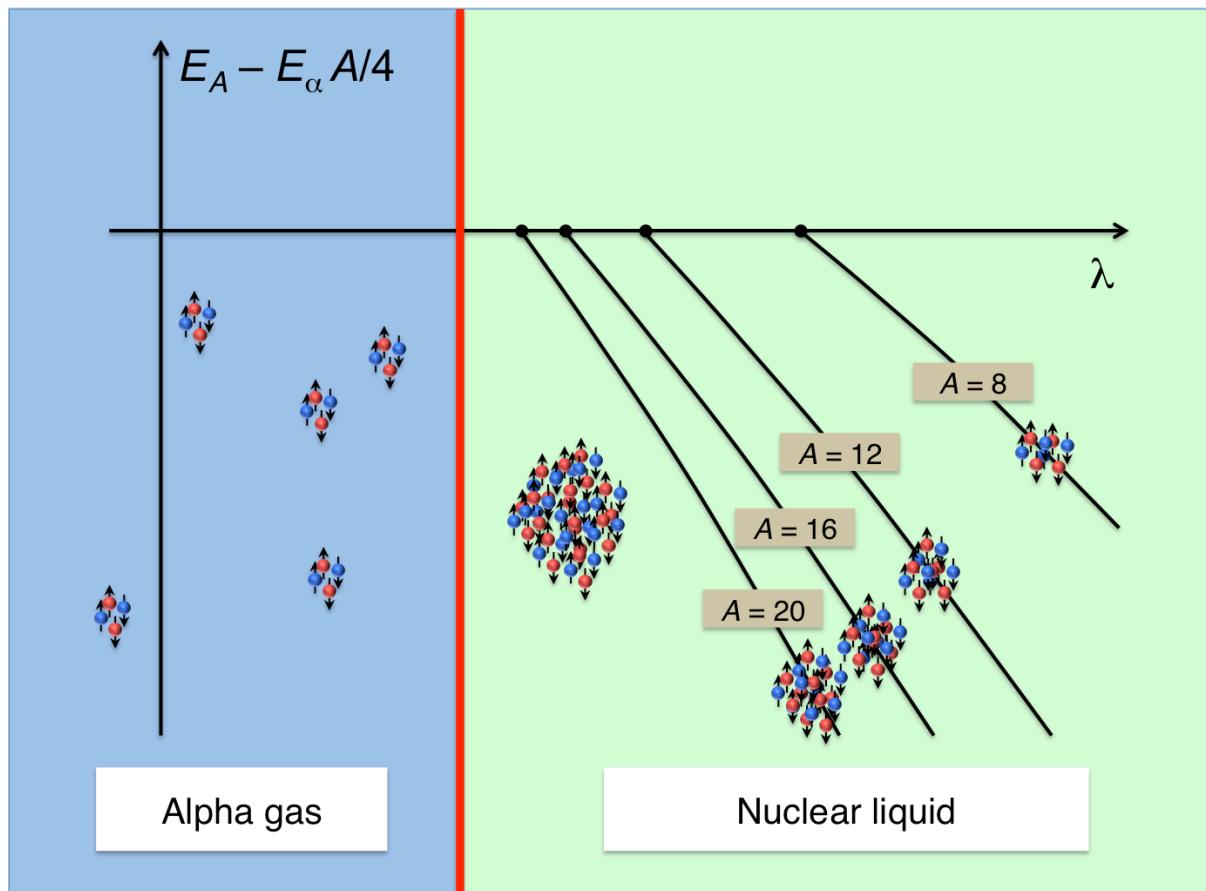
$$\frac{E_{^{20}\text{Ne}}}{E_{^4\text{He}}} = 5.03(3)$$

Alpha-alpha scattering



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

Control parameters: Sensitivity to interaction range and locality



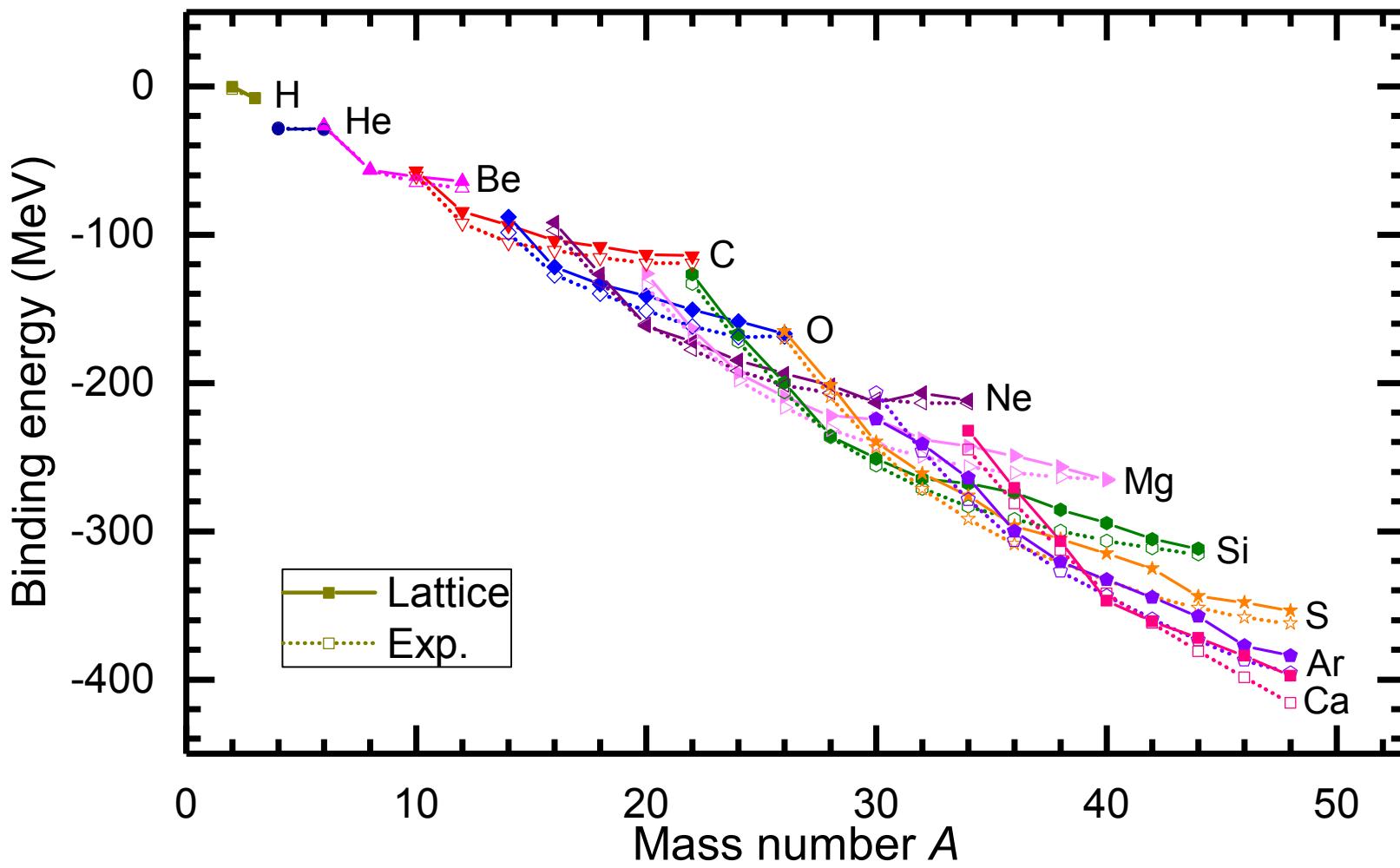
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L.,
Rupak, PRL 117, 132501 (2016)

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



	<i>B</i>	Exp.	<i>R</i> _{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

Seeing Structure with Pinholes

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

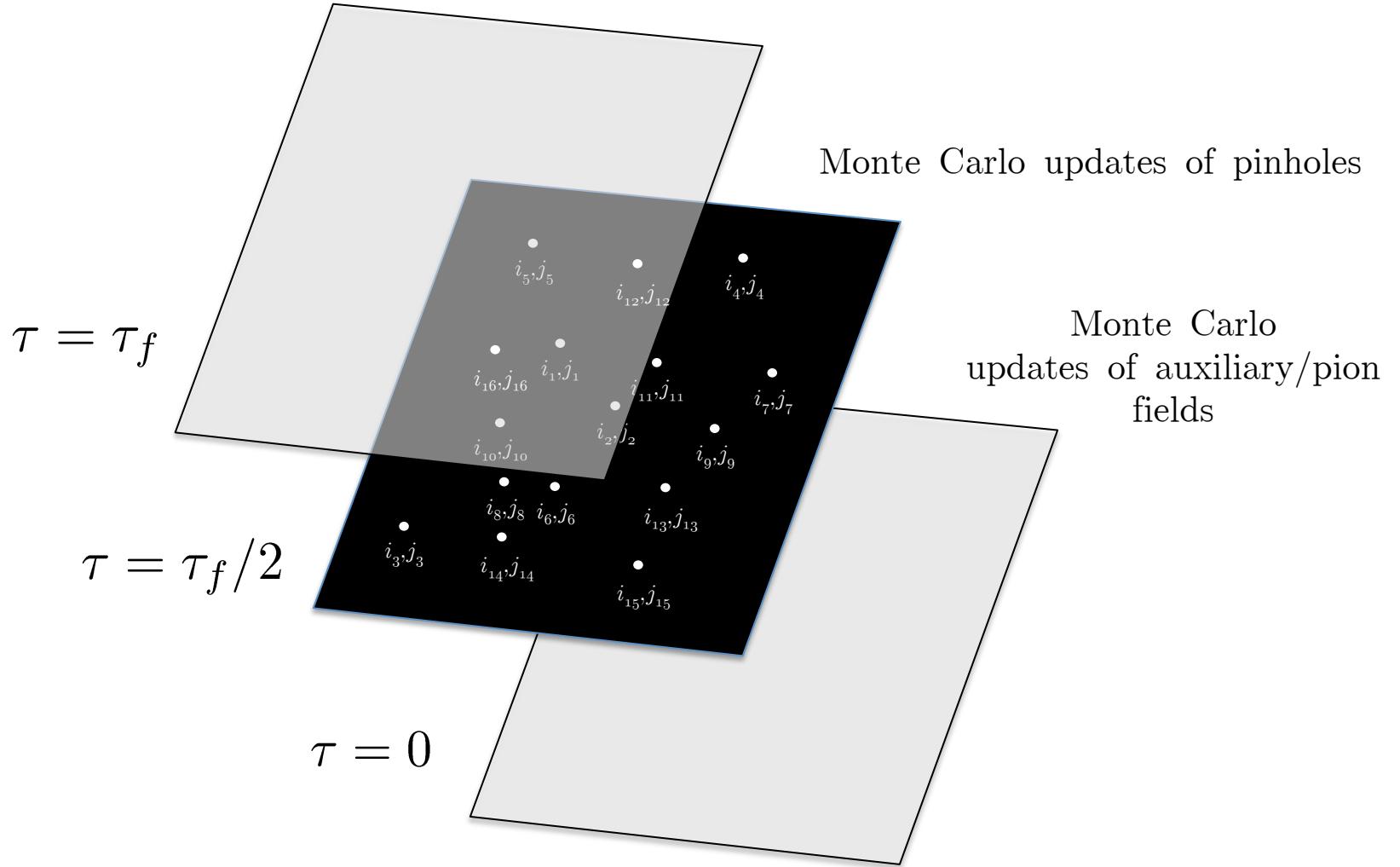
$$\rho_{i,j}(\mathbf{n}) = a_{i,j}^\dagger(\mathbf{n})a_{i,j}(\mathbf{n})$$

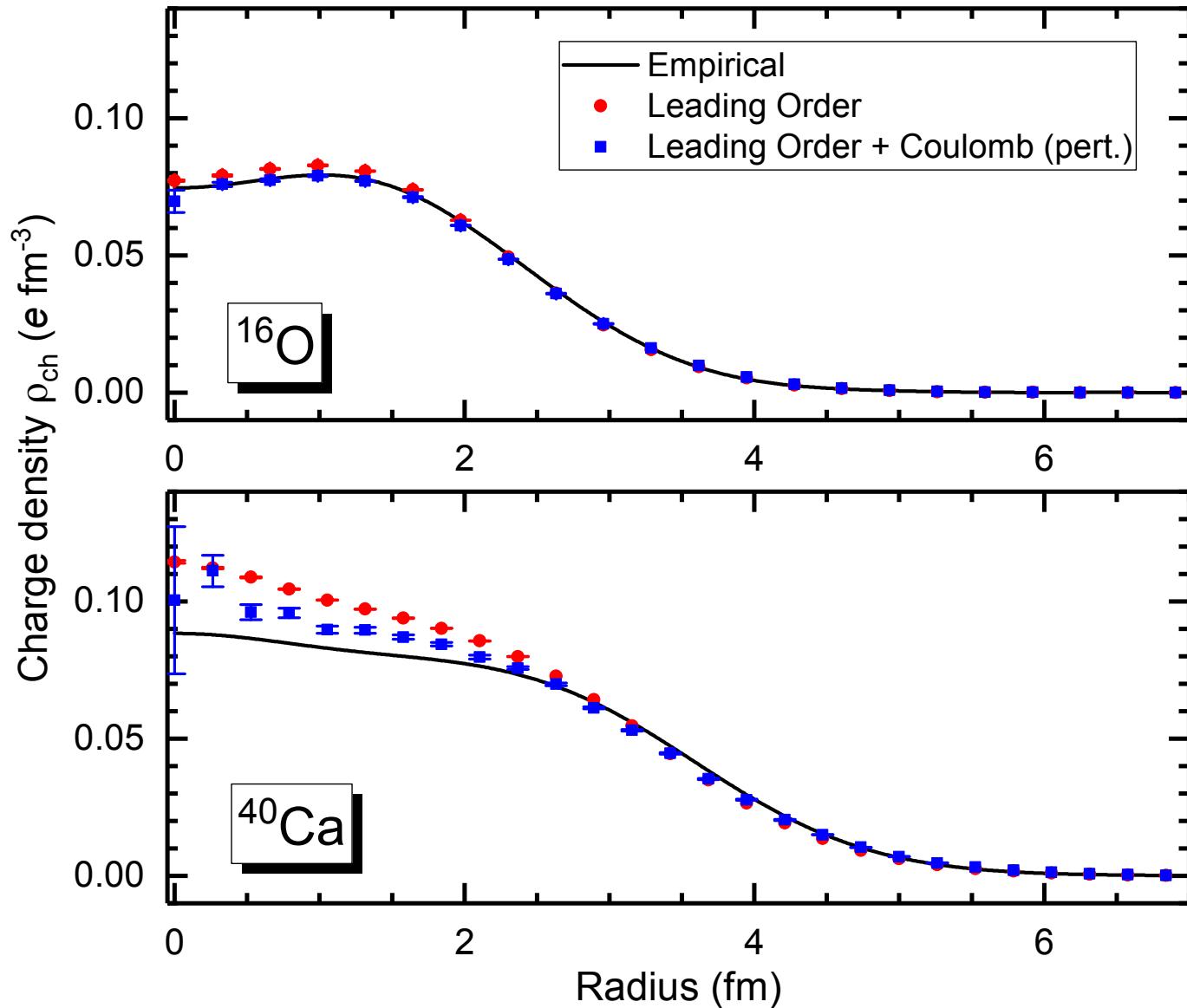
We construct the normal-ordered A -body density operator

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

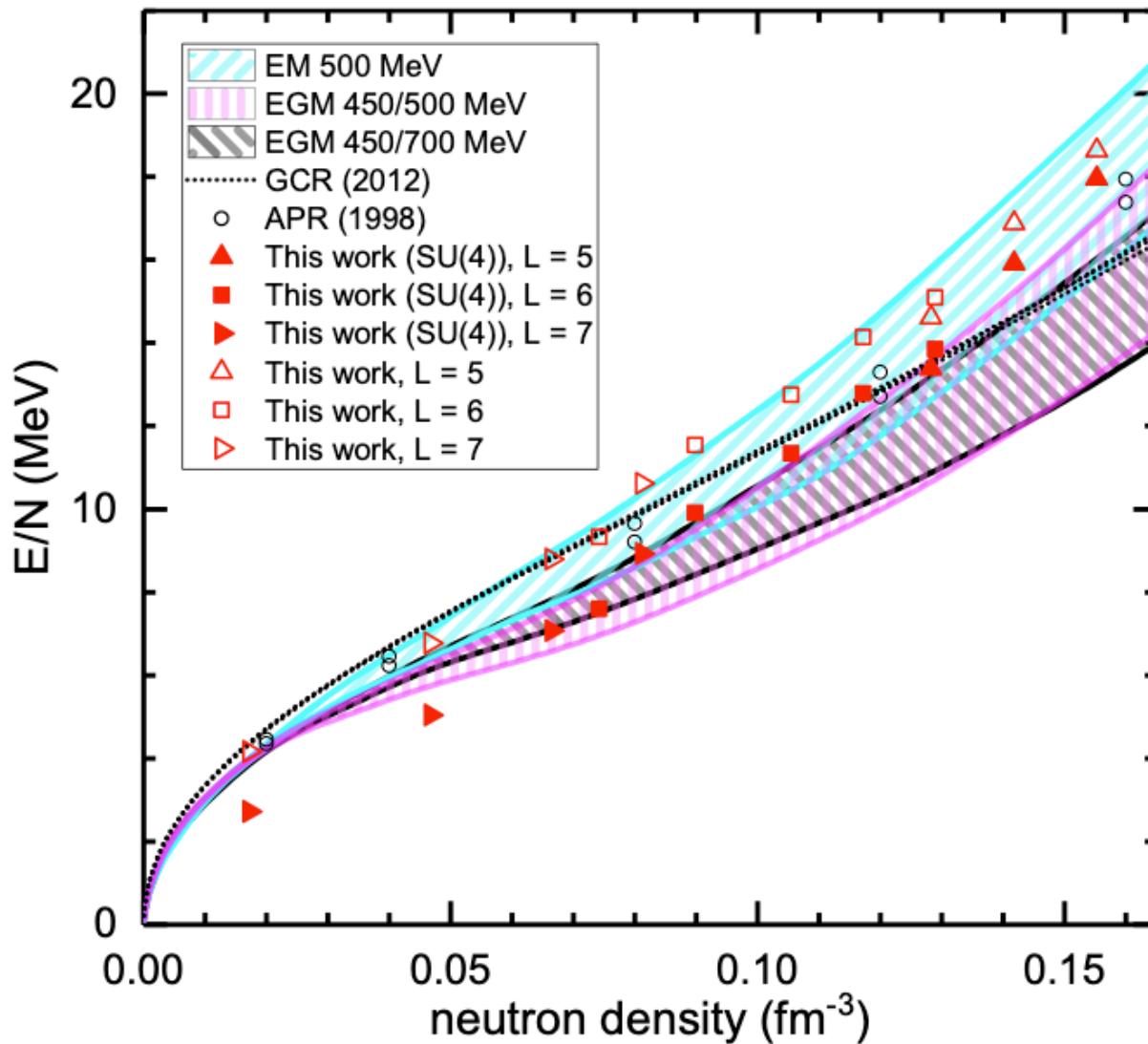
In the simulations we do Monte Carlo sampling of the amplitude

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





Pure neutron matter



Nuclear thermodynamics

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

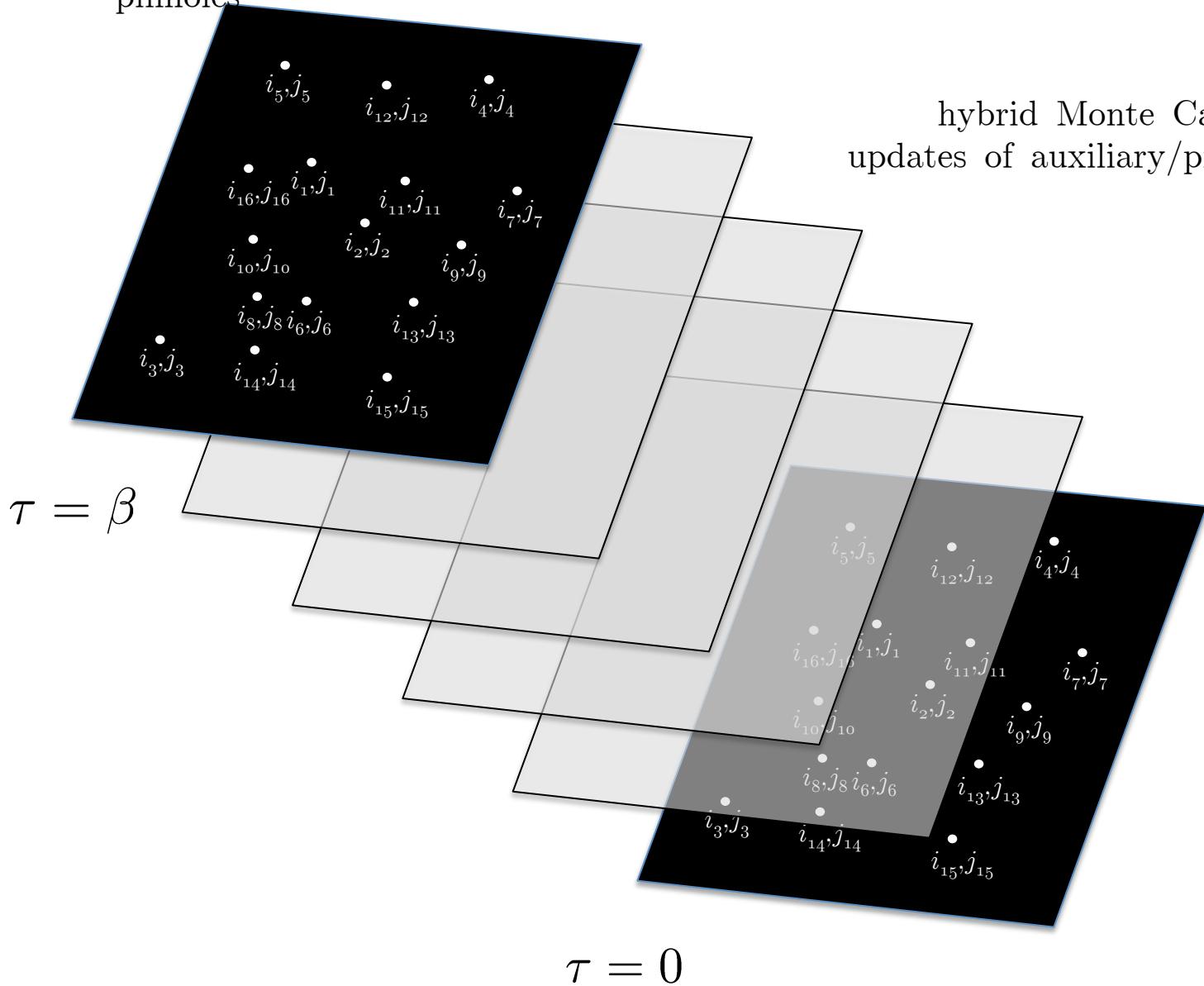
$$\text{Tr} \exp(-\beta H)$$

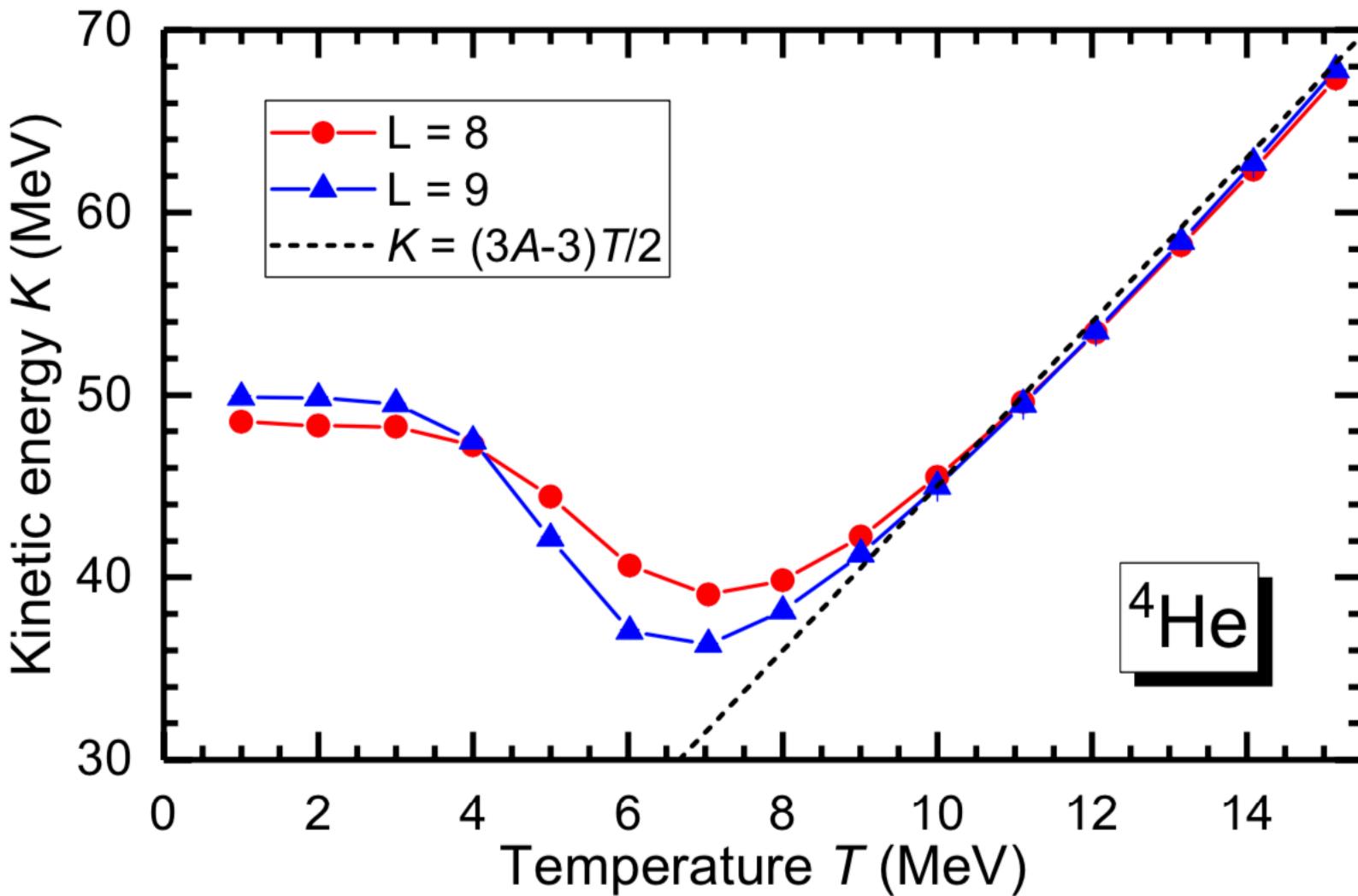
We compute the quantum mechanical trace over A -nucleon states by summing over pinholes (position eigenstates) for the initial and final states

$$\begin{aligned} & \text{Tr } O \\ &= \frac{1}{A!} \sum_{i_1 \dots i_A, j_1 \dots j_A, \mathbf{n}_1 \dots \mathbf{n}_A} \langle 0 | a_{i_A, j_A}(\mathbf{n}_A) \cdots a_{i_1, j_1}(\mathbf{n}_1) O a_{i_1, j_1}^\dagger(\mathbf{n}_1) \cdots a_{i_A, j_A}^\dagger(\mathbf{n}_A) | 0 \rangle \end{aligned}$$

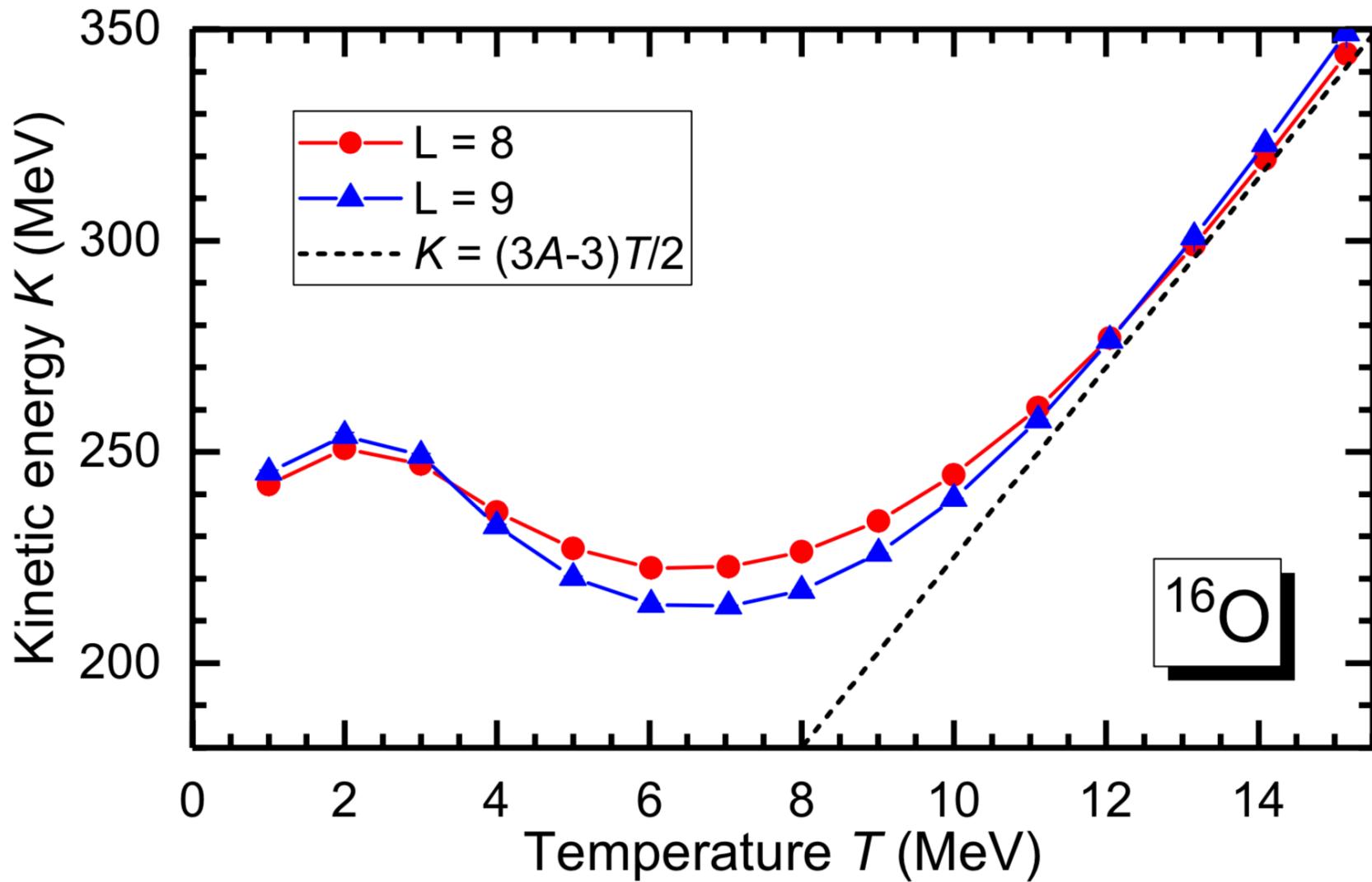
This can be used to calculate the partition function in the canonical ensemble.

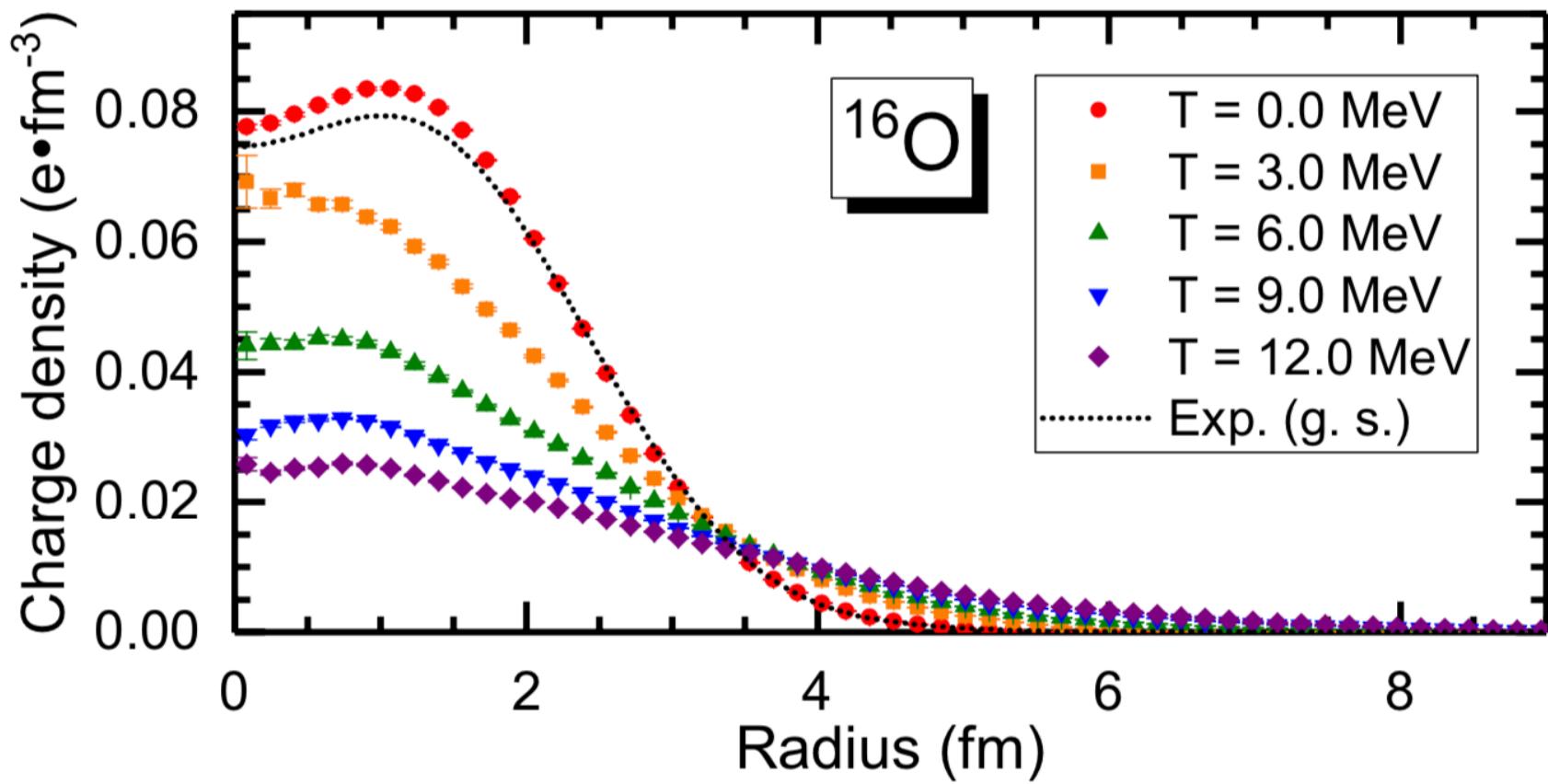
Metropolis updates of
pinholes

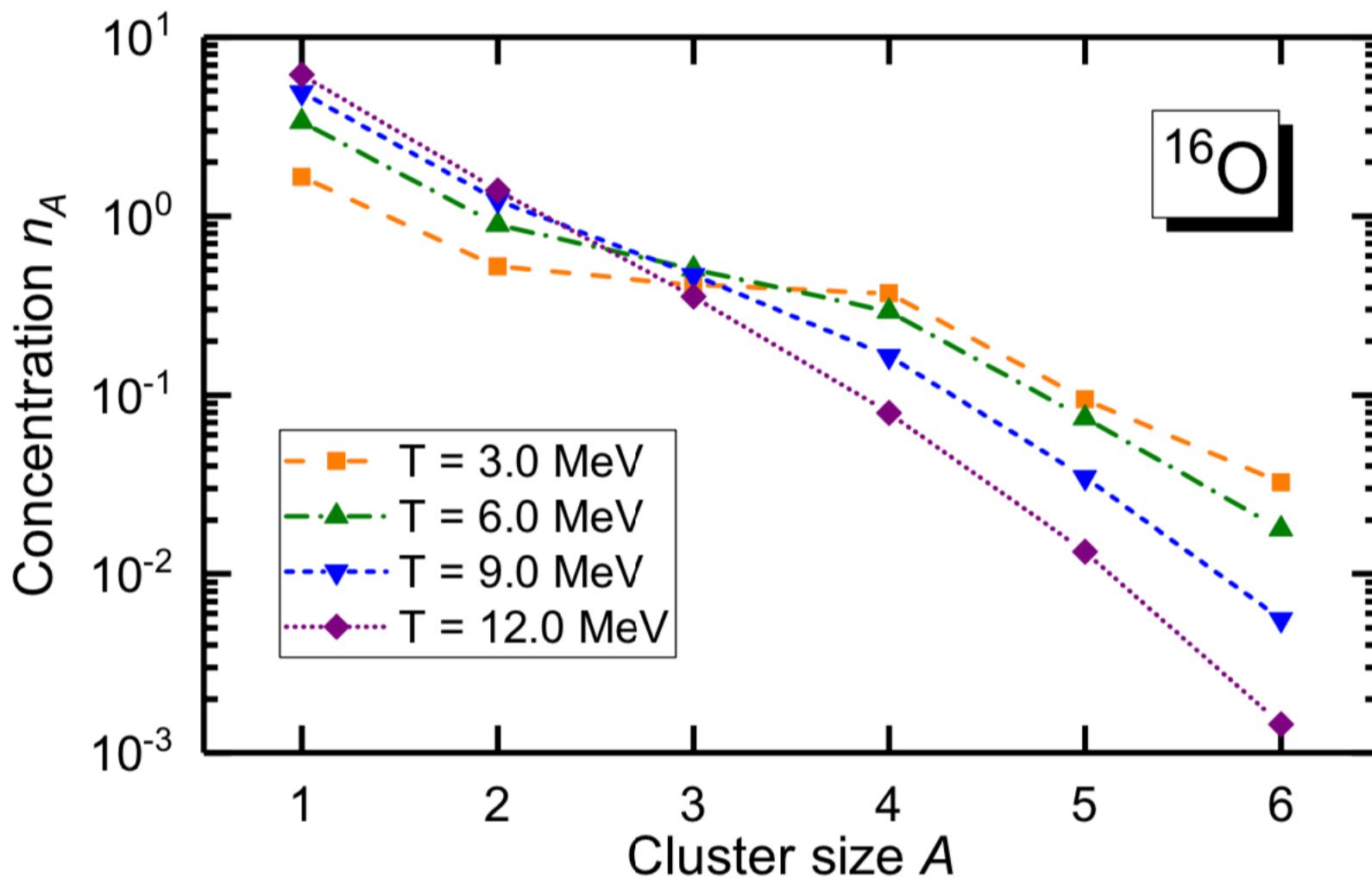


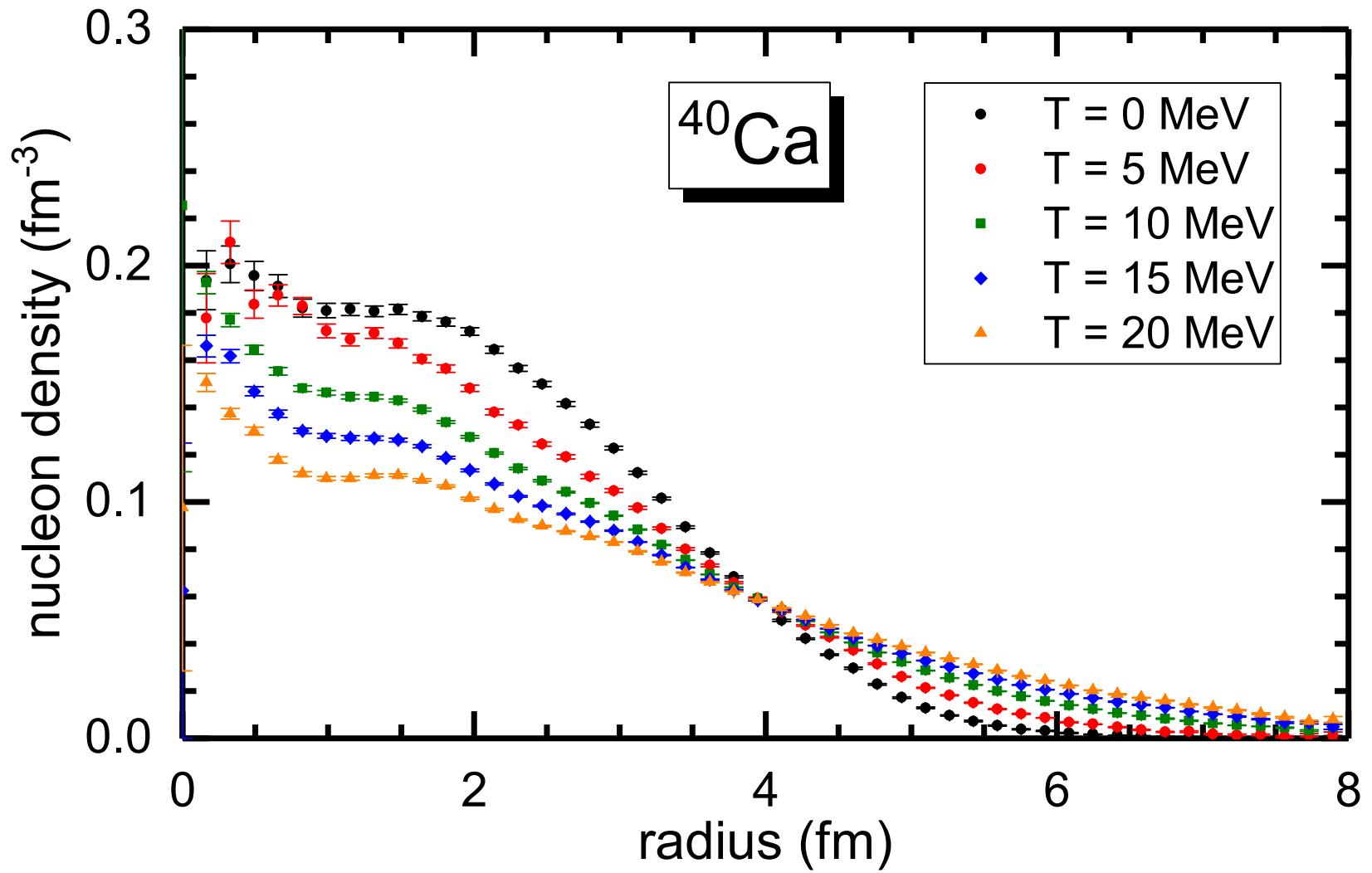


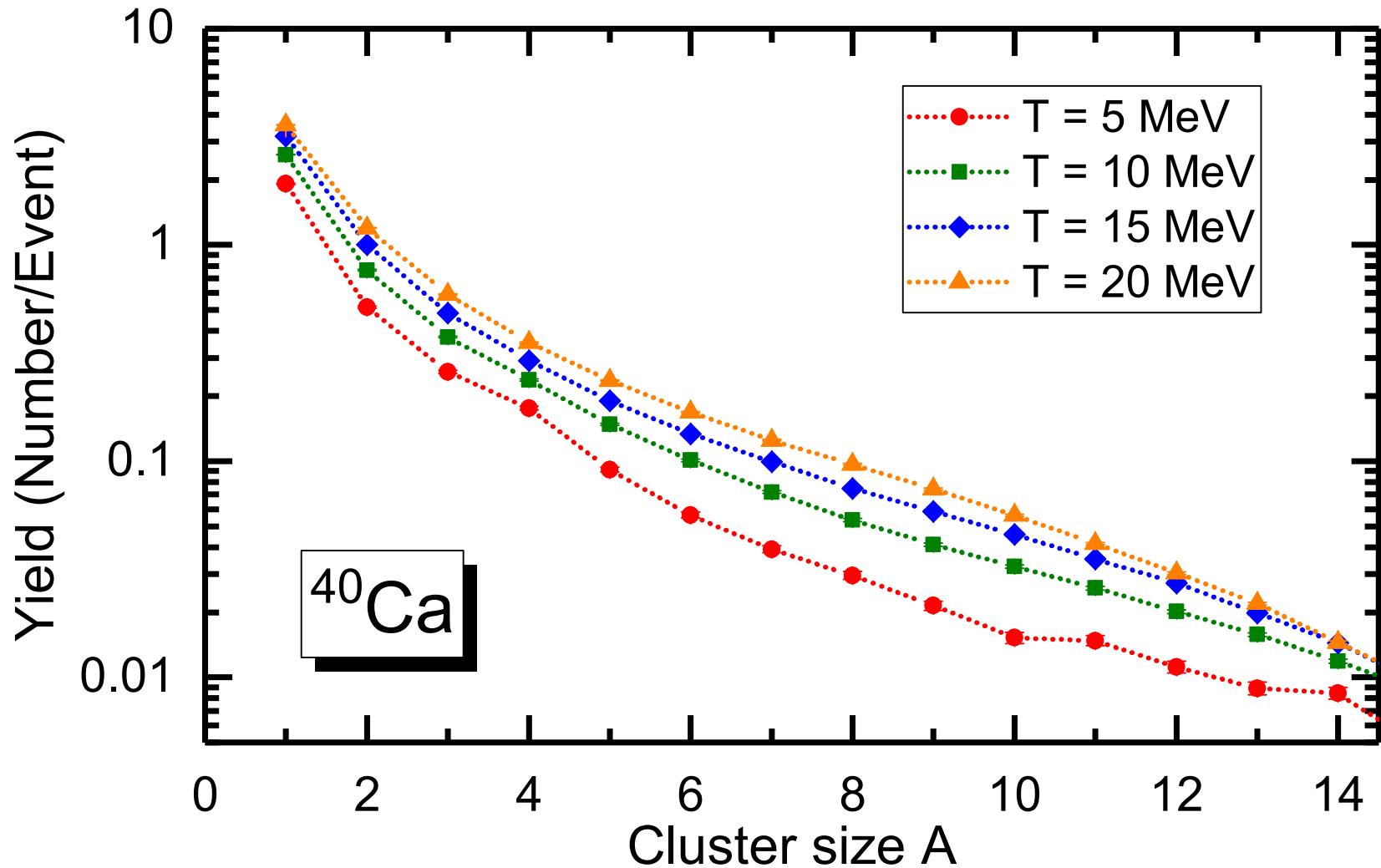
Figures by Bing-Nan Lu

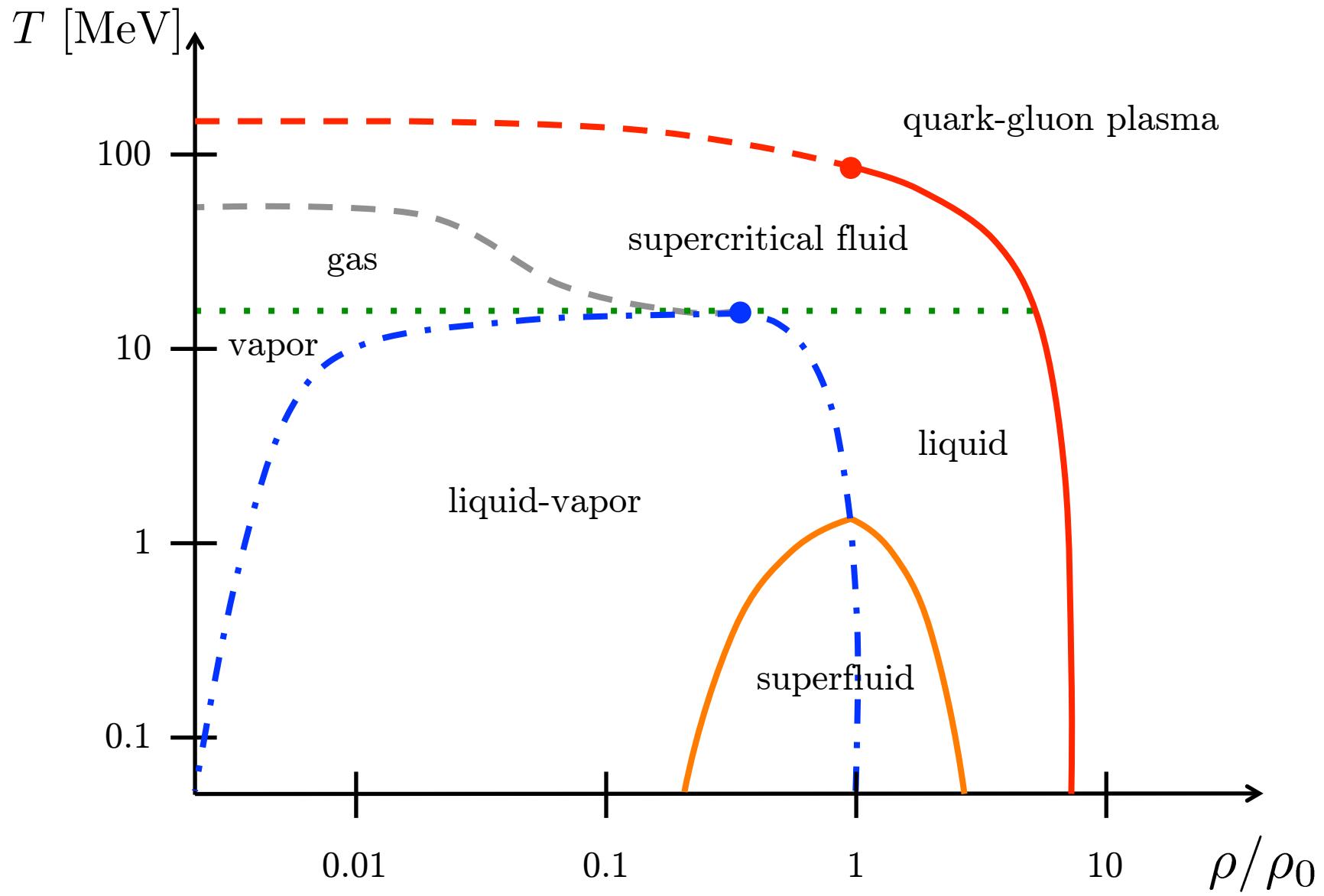


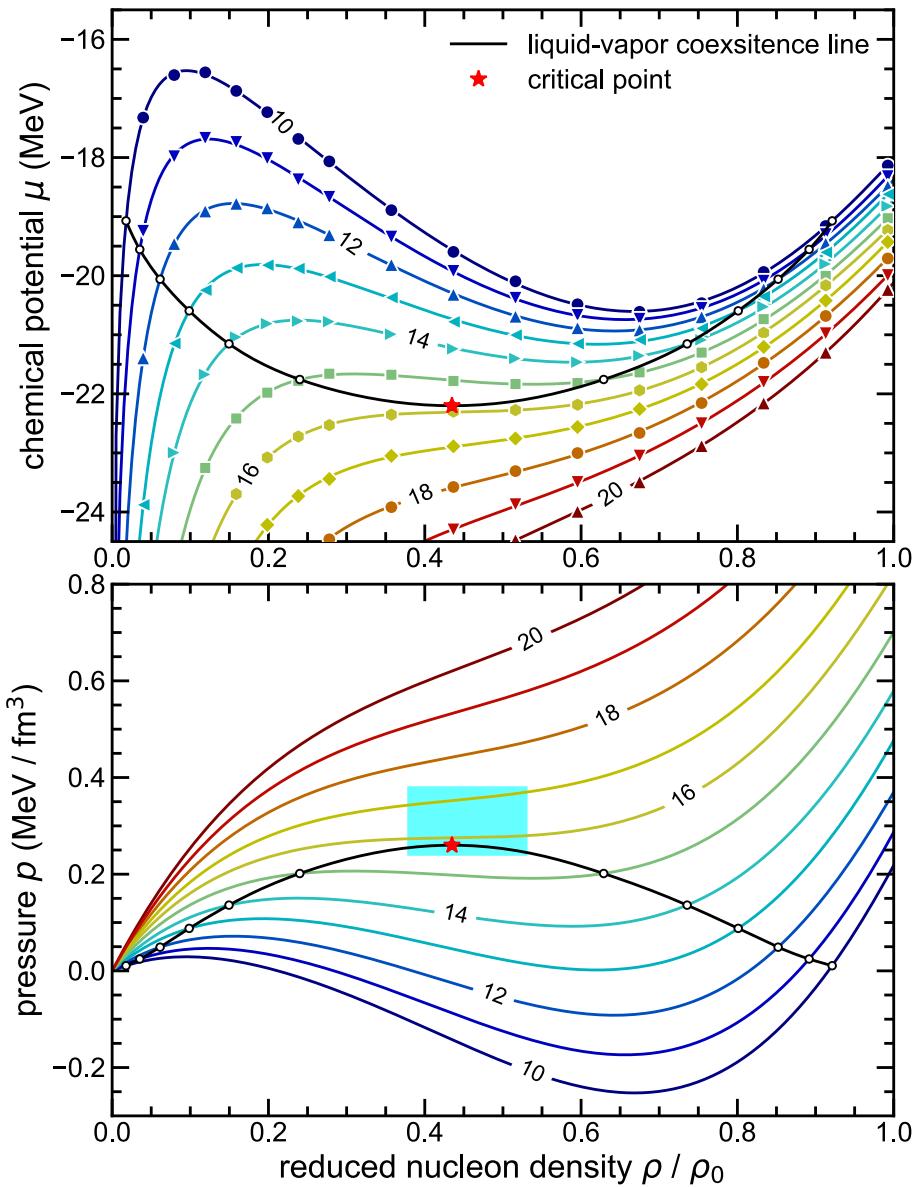












$$T_c = 15.80(3) \text{ MeV}$$

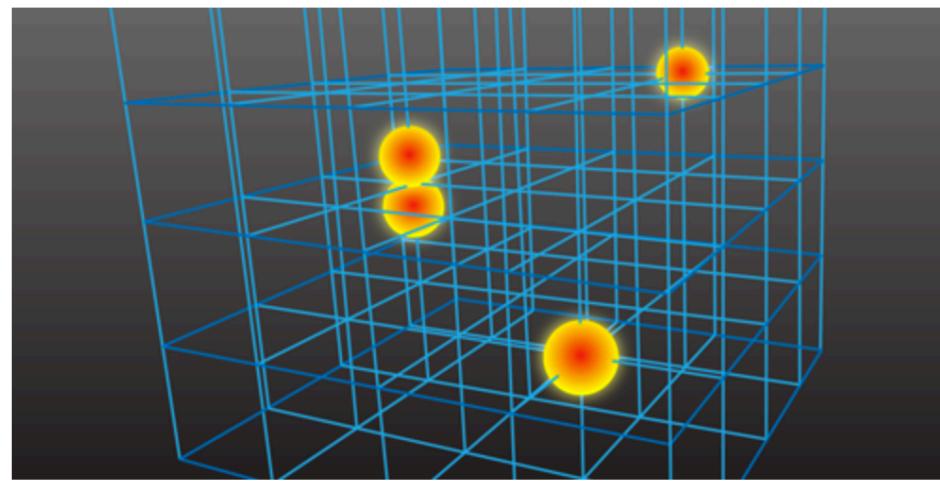
$$\rho_c = 0.089(1) \text{ fm}^{-3}$$

$$P_c = 0.260(3) \text{ MeV/fm}^3$$

Synopsis: Making Quantum Computations Behave

July 17, 2018

A new computational method tackles many-body quantum calculations that have defied a suite of existing approaches.



APS/Alan Stonebraker

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

Bose-Hubbard model

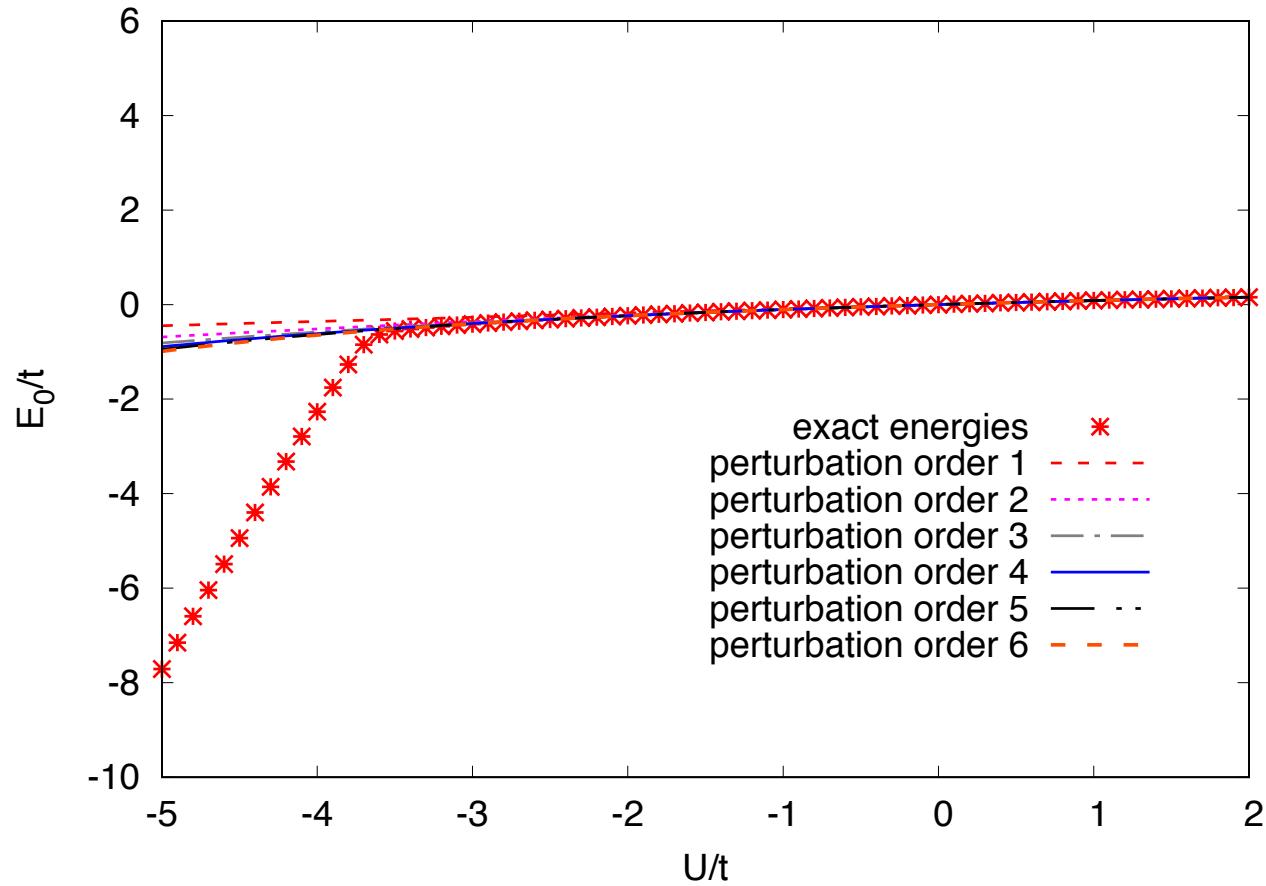
In order to illuminate our discussion with a concrete example, we consider a quantum Hamiltonian known as the Bose-Hubbard model in three dimensions. It describes a system of identical bosons on a three-dimensional cubic lattice.

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

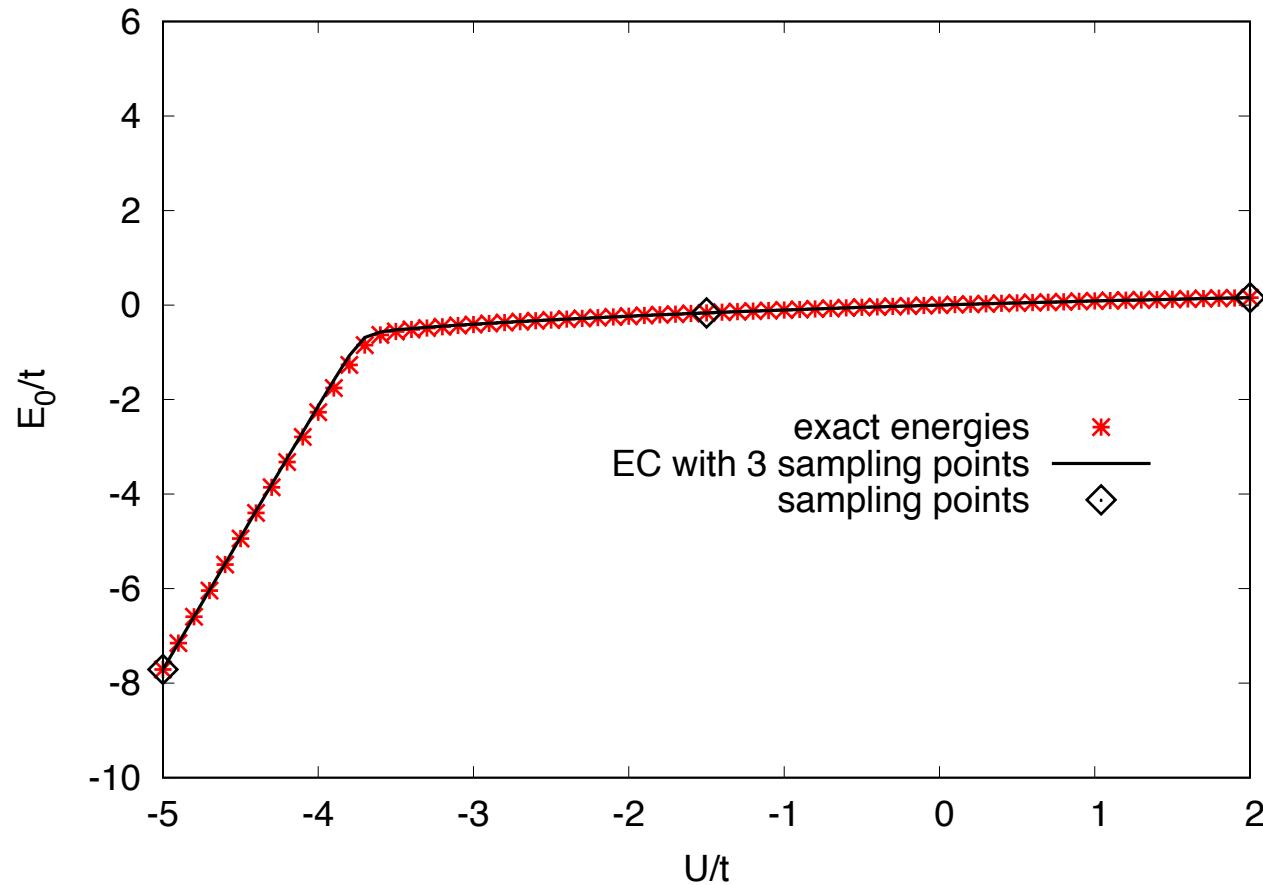
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

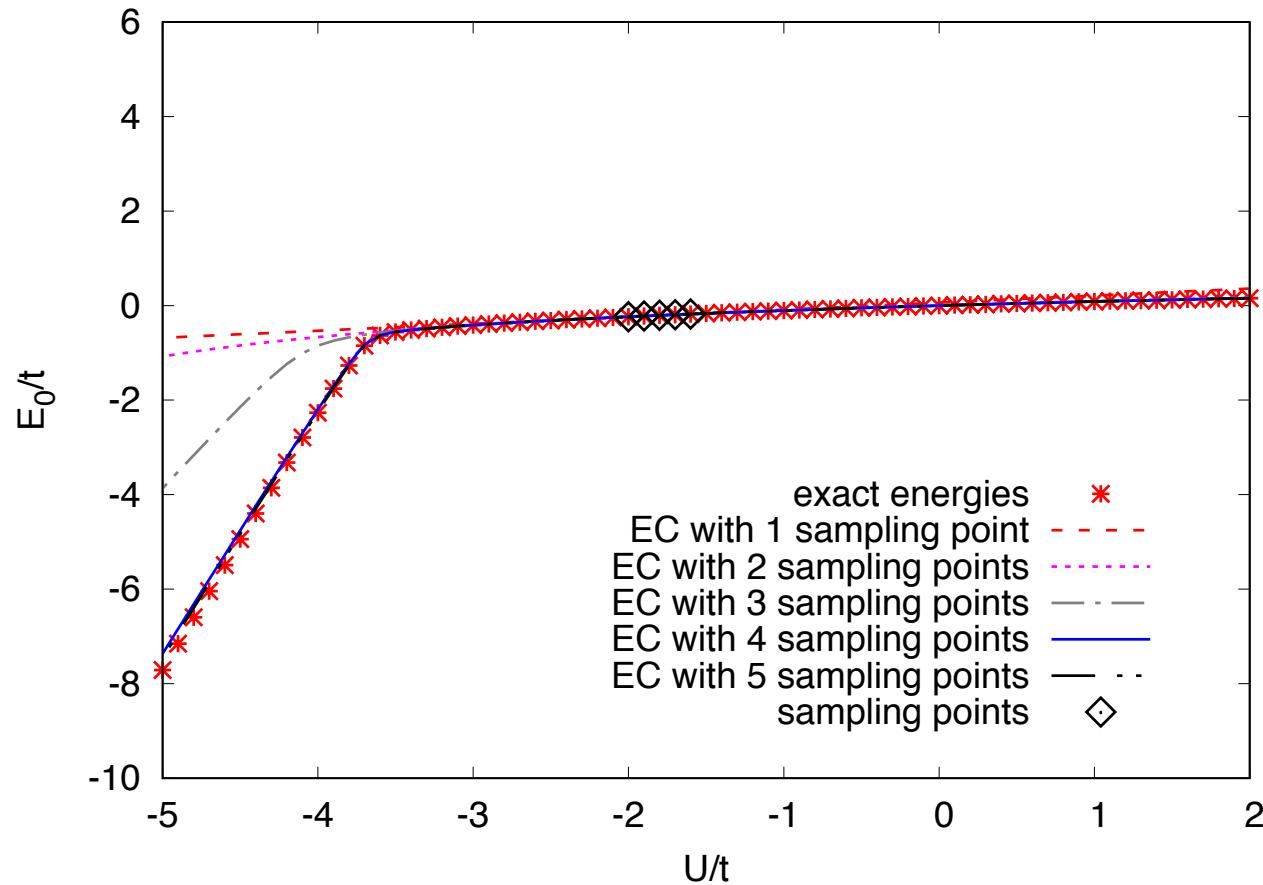
Perturbation theory fails at strong attractive coupling



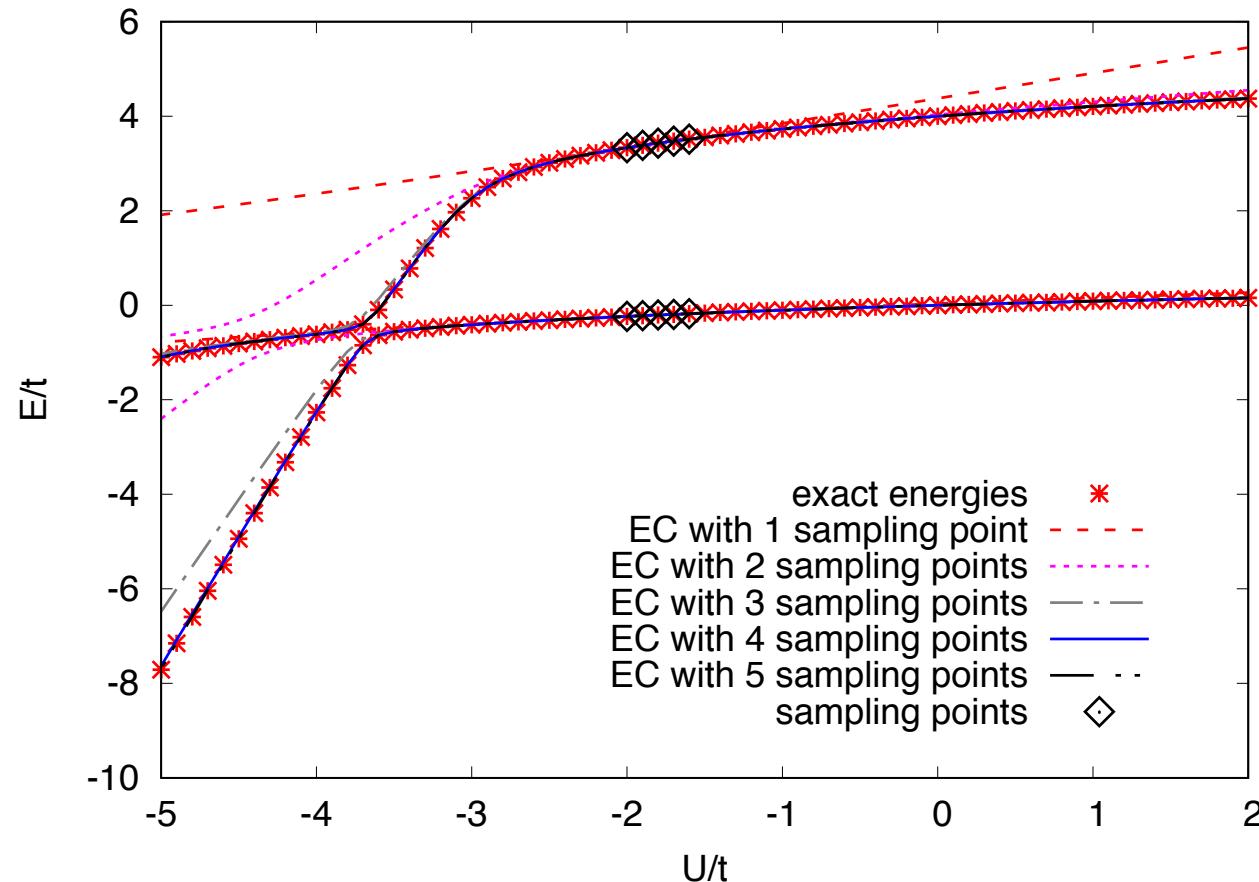
Restrict the linear space to the span of three vectors



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.



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.

First principles calculations of nuclear thermodynamics using the pinhole trace algorithm are now possible. We have mapped out the nuclear liquid-gas phase diagram.

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 research groups for uncertainty quantification. It is also being used as a resummation method for many-body perturbation theory.