Nuclear forces and structure in nuclear lattice simulations

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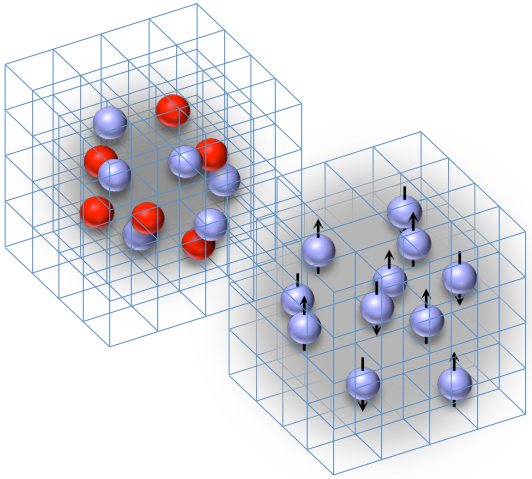
Nuclear Lattice EFT Collaboration

ECT* Workshop on
New Ideas in Constraining Nuclear Forces
Trento – June 4, 2018



Outline

Lattice effective field theory

A tale of two interactions

Effective forces between bound states

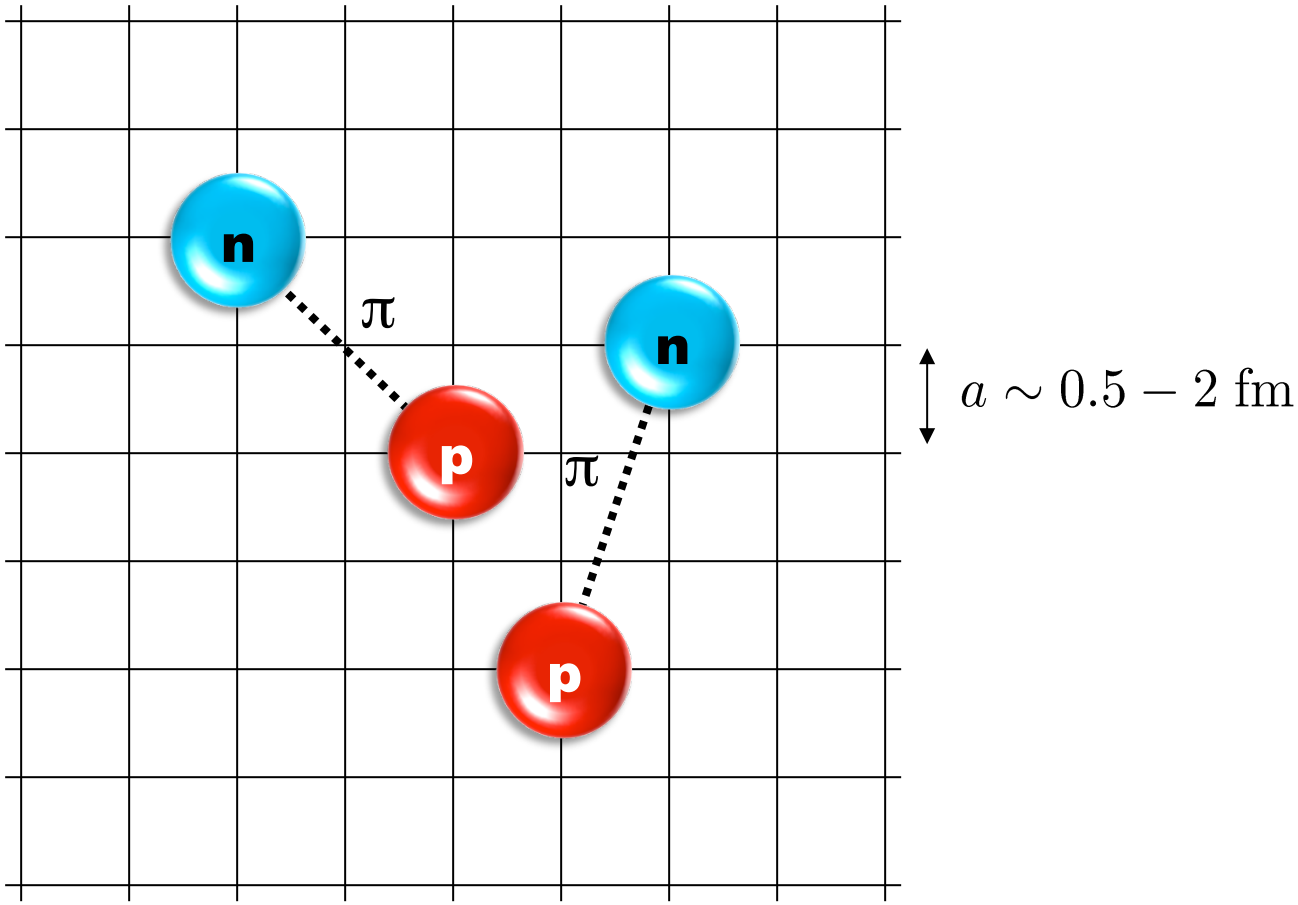
Structure and thermodynamics

Eigenvector continuation

Discussion questions

Summary and outlook

Lattice effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
TALENT summer school lectures: qmc2016.wordpress.ncsu.edu

$a \sim 1.32$ fm

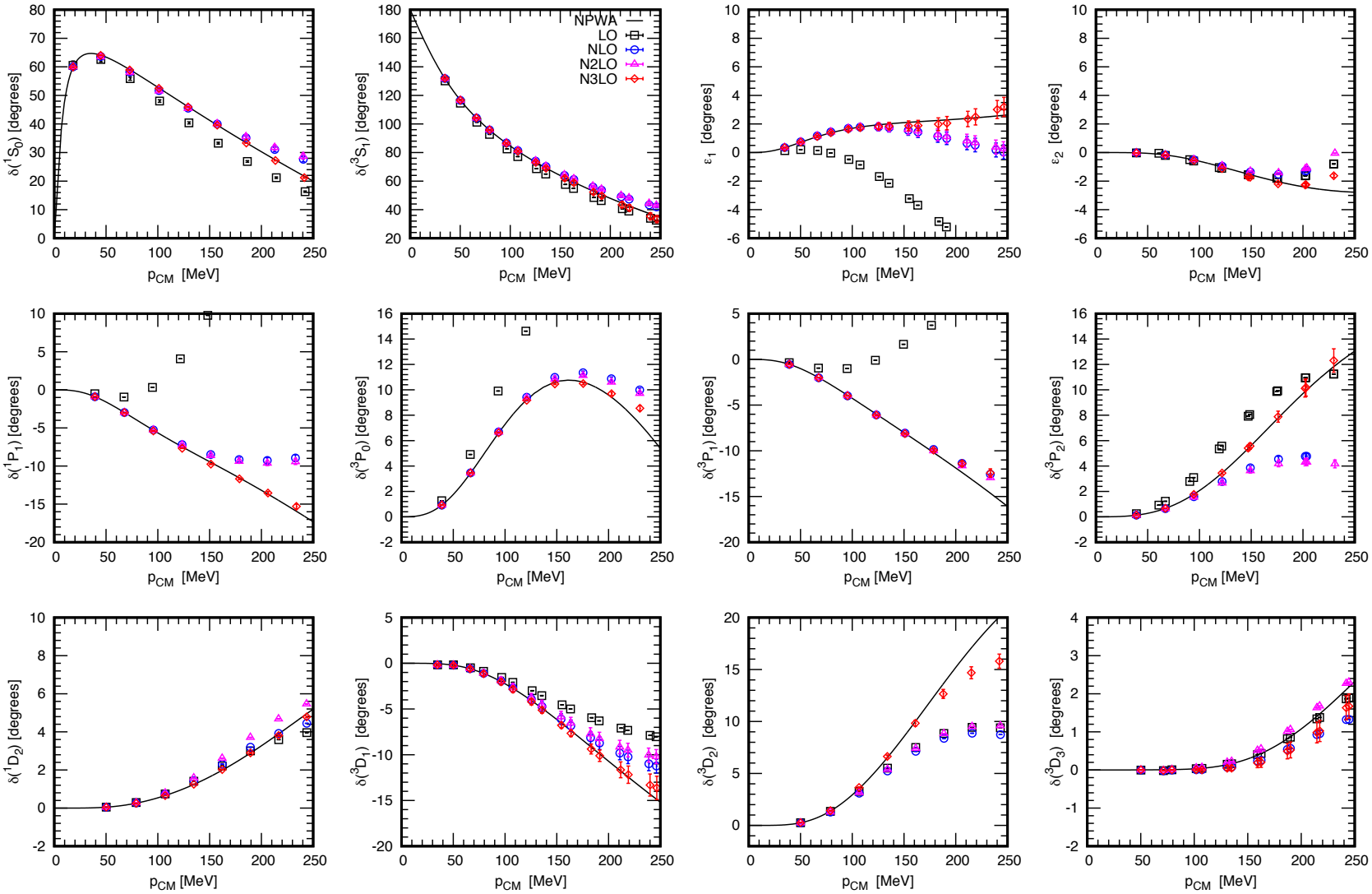


Figure courtesy of Ning Li

$a \sim 0.987$ fm

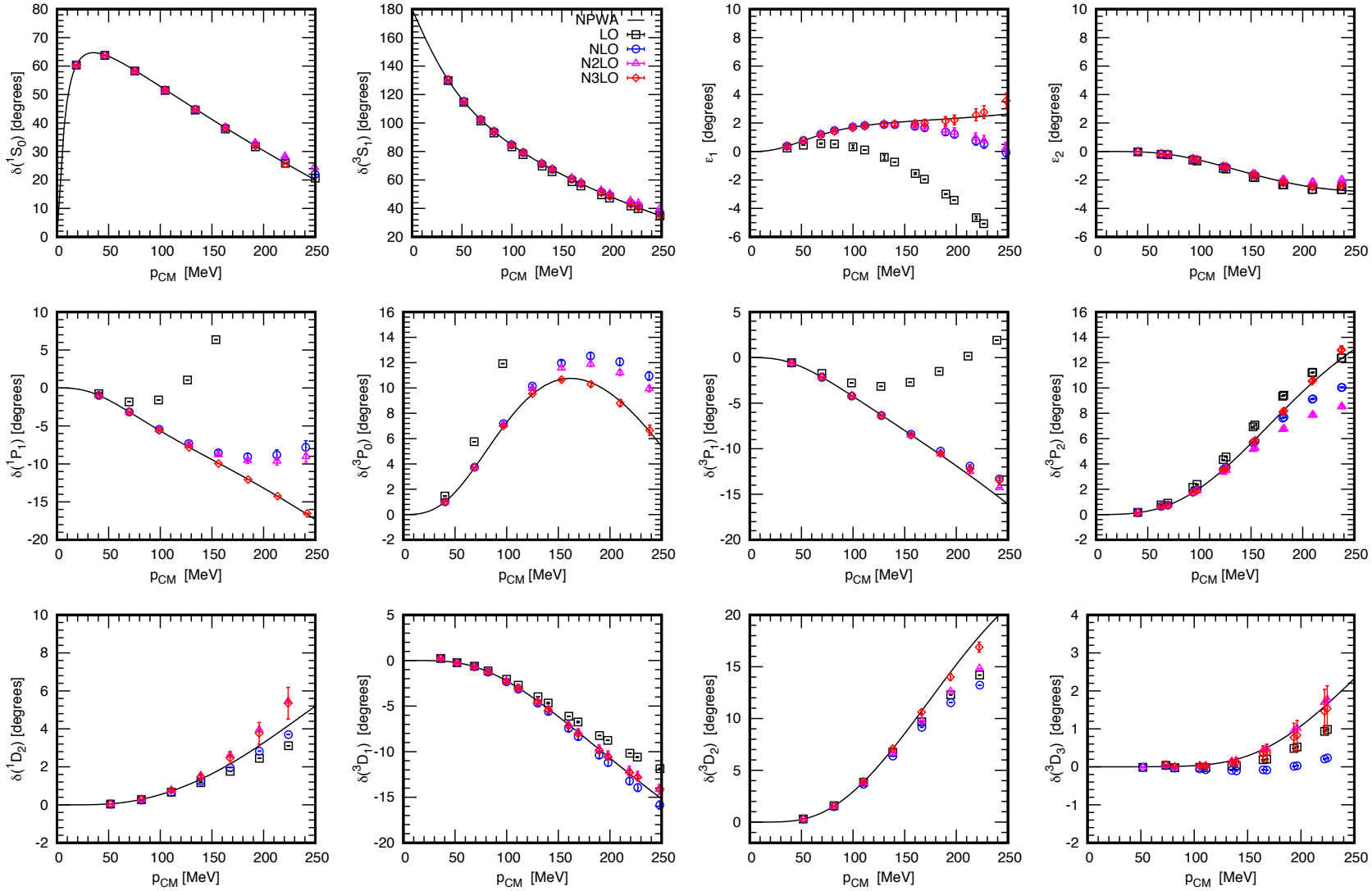
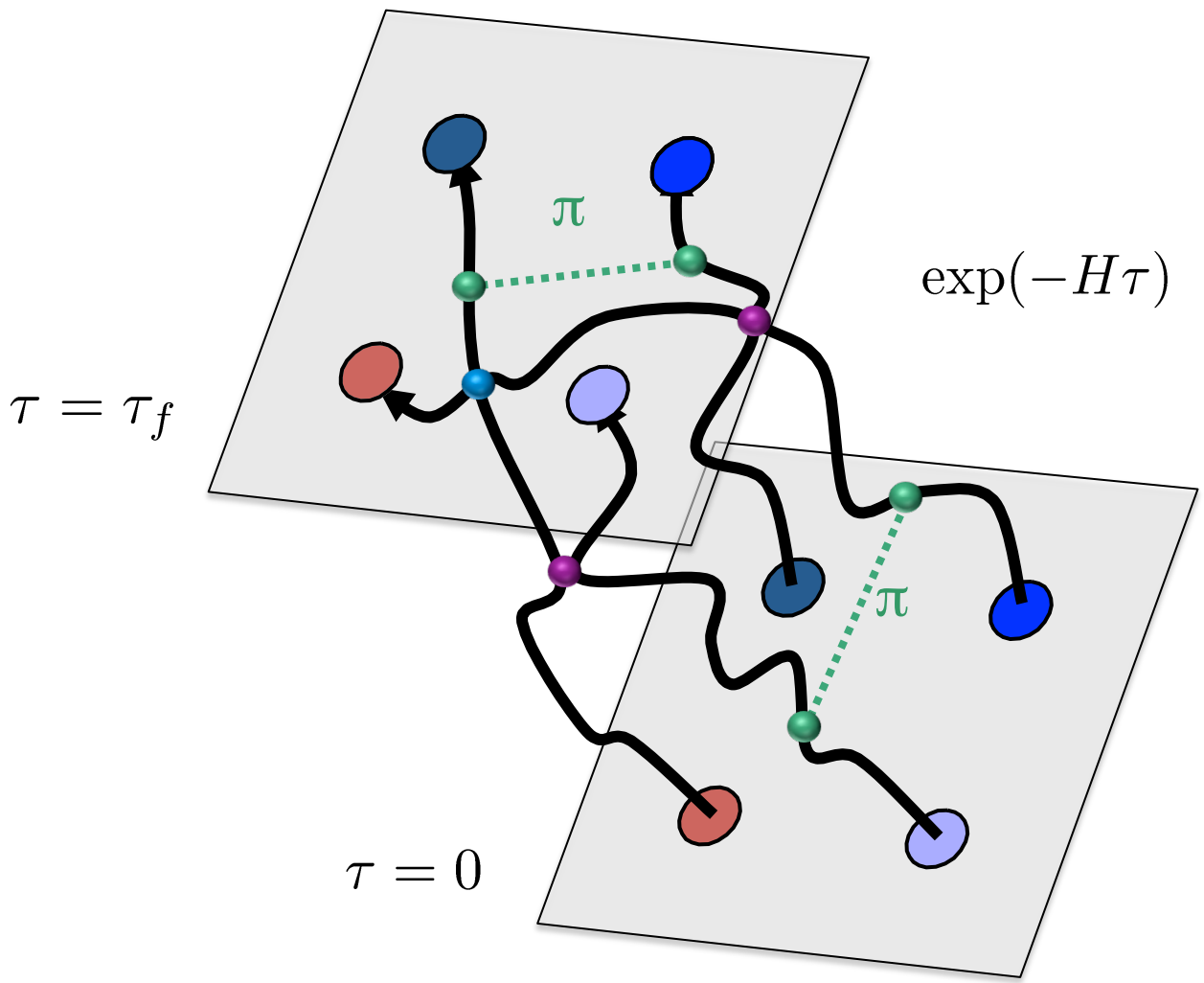
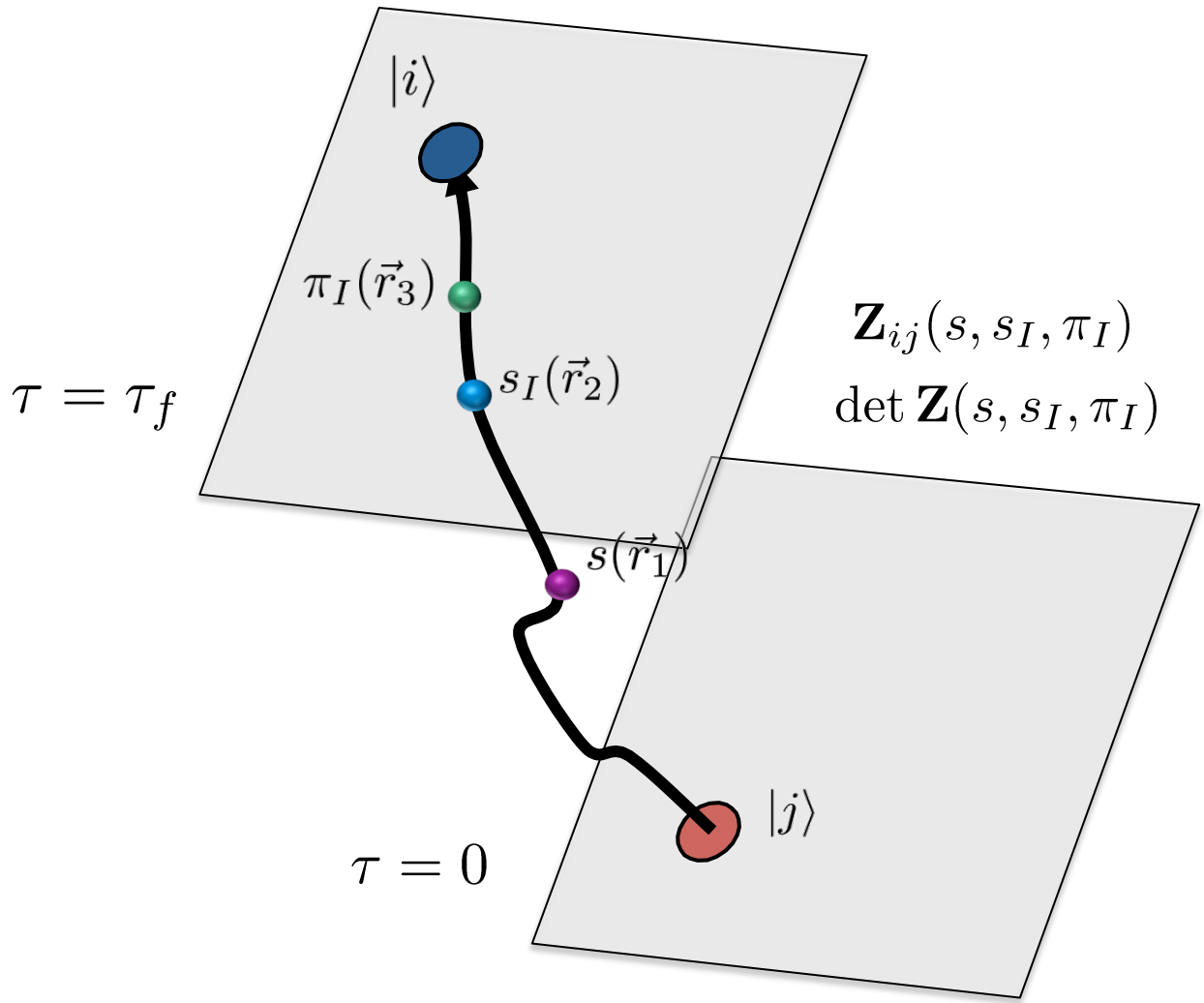


Figure courtesy of Ning Li

Euclidean time projection



Auxiliary field method



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

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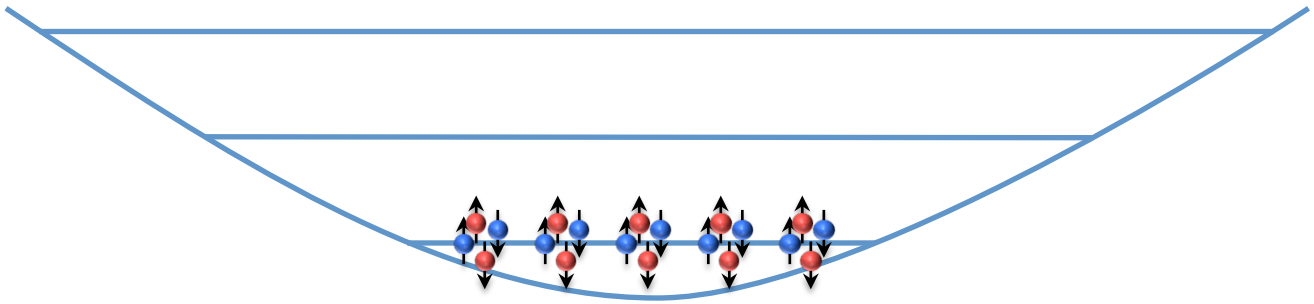
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

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

Bose condensate of alpha particles!



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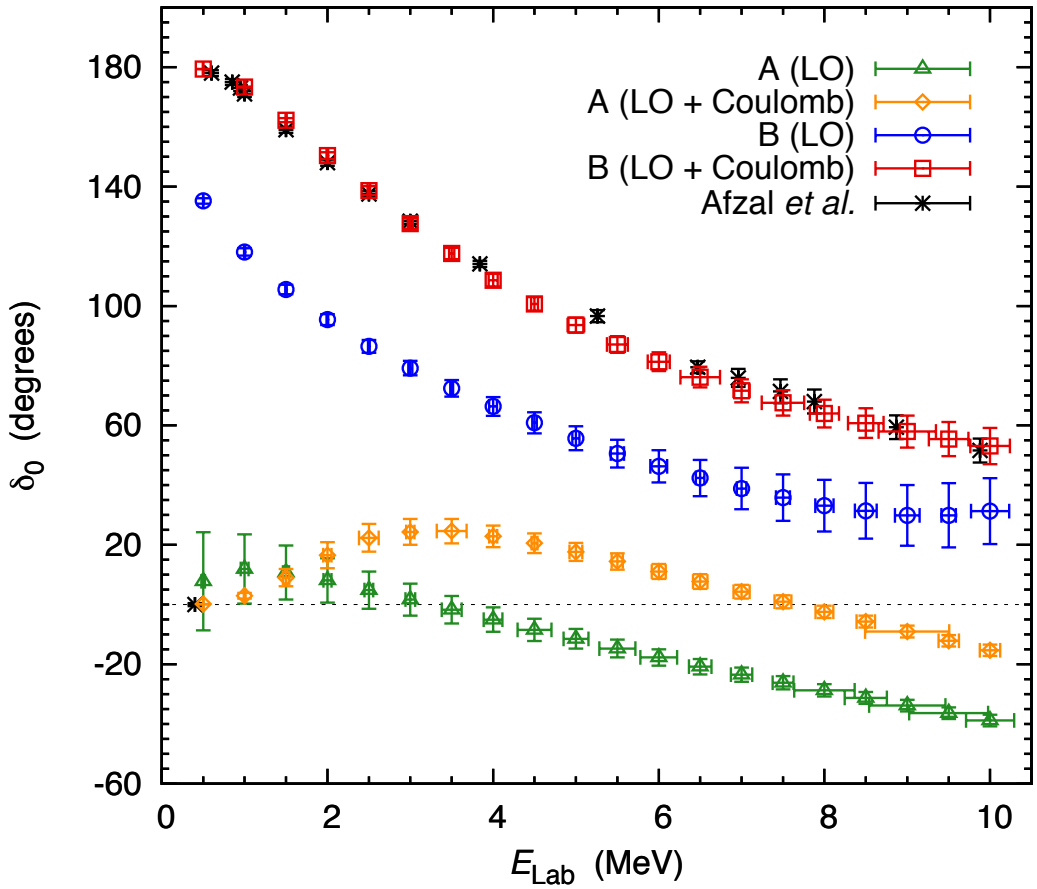
Alpha-alpha interaction

The alpha-alpha scattering phase shift shows a clear difference between the two interactions.

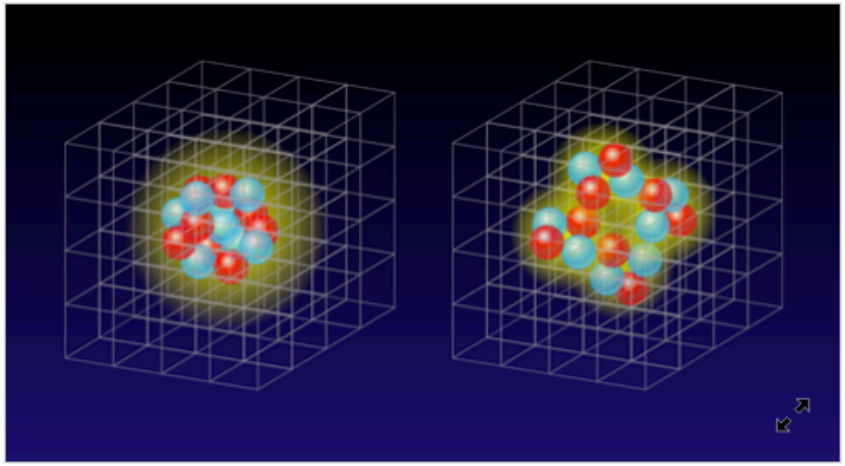


Viewpoint: Uncovering a Quantum Phase Transition in Nuclei

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

September 19, 2016 • *Physics* 9, 106

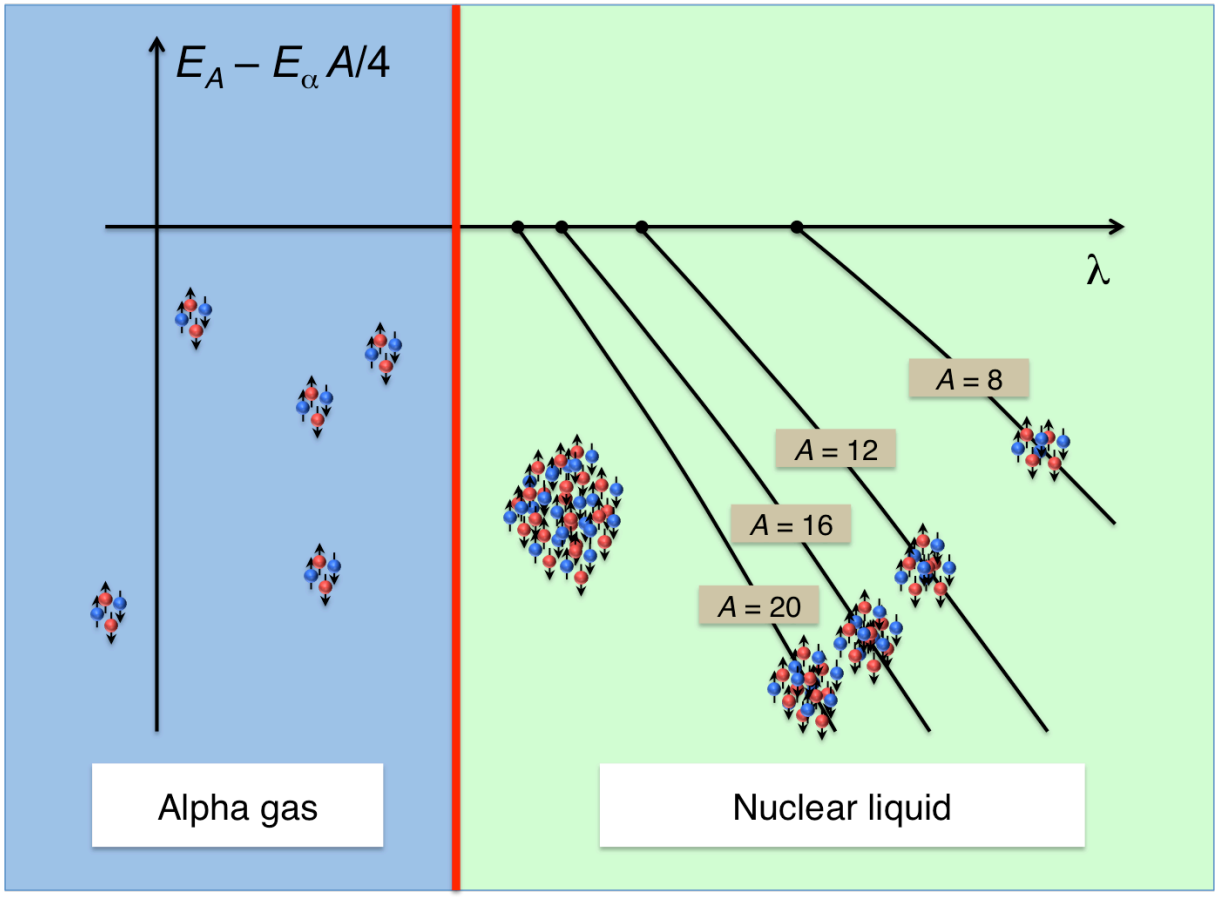
Simulations predict that the ground states of certain light nuclei lie near a quantum phase transition between a liquid-like phase and a phase involving clusters of alpha particles.



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**

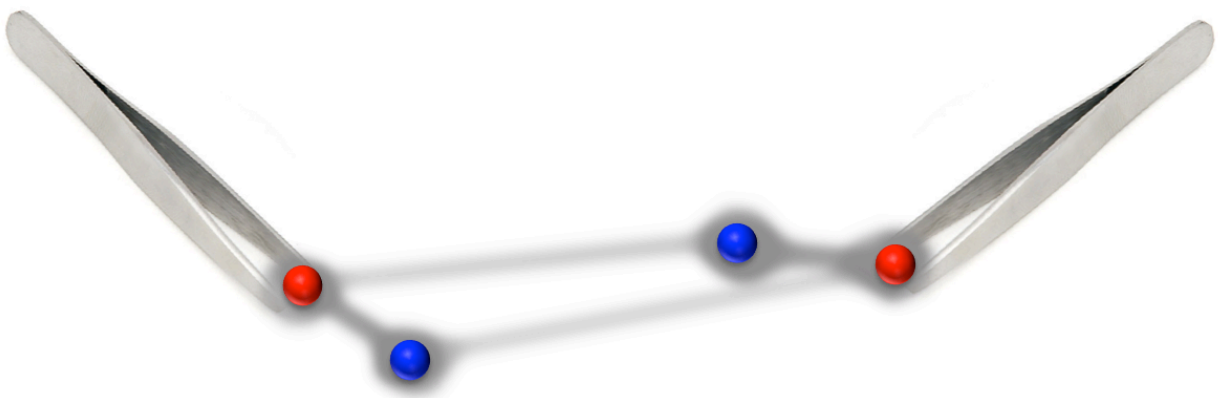
Control parameters: Sensitivity to interaction range and locality



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

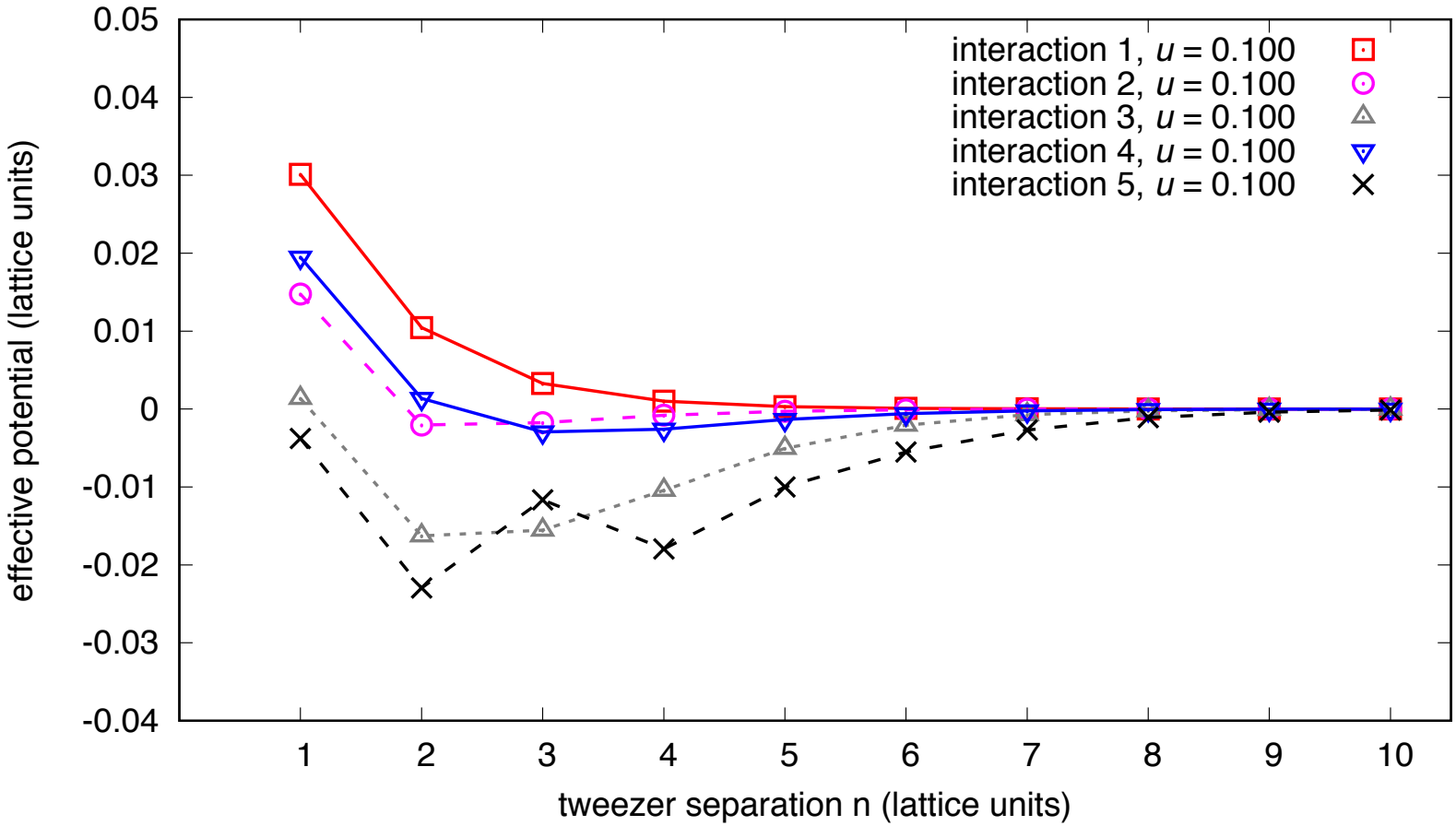
Effective forces between bound states

Numerical tweezers used to probe the relation connecting particle-particle interactions and the effective forces between bound states



Rokash, Epelbaum, Krebs, D.L., Rupak, PRL 118, 232502 (2017)

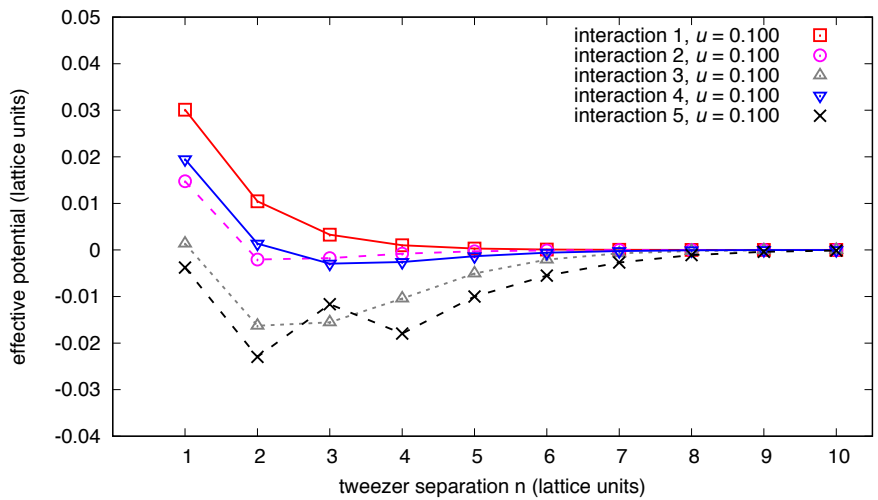
Effective dimer-dimer potential



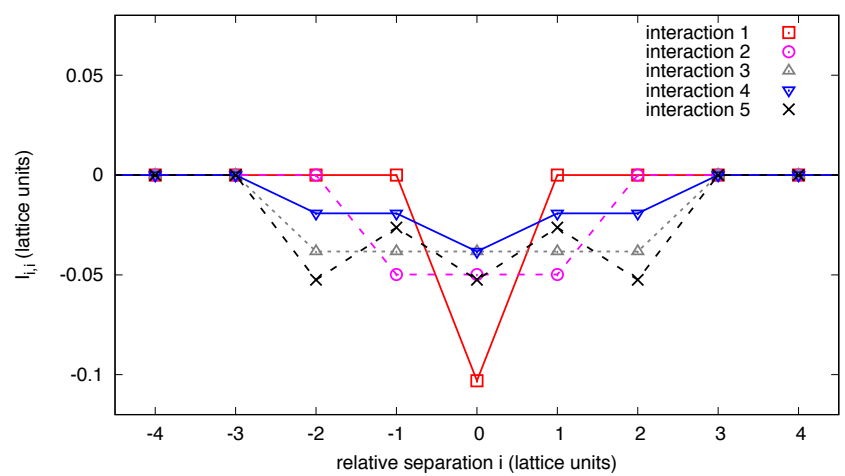
All five interactions produce the same dimer binding energy

Control parameters: Sensitivity to interaction range and locality

Effective dimer-dimer potential



Local part of particle-particle interaction



Pinhole algorithm

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

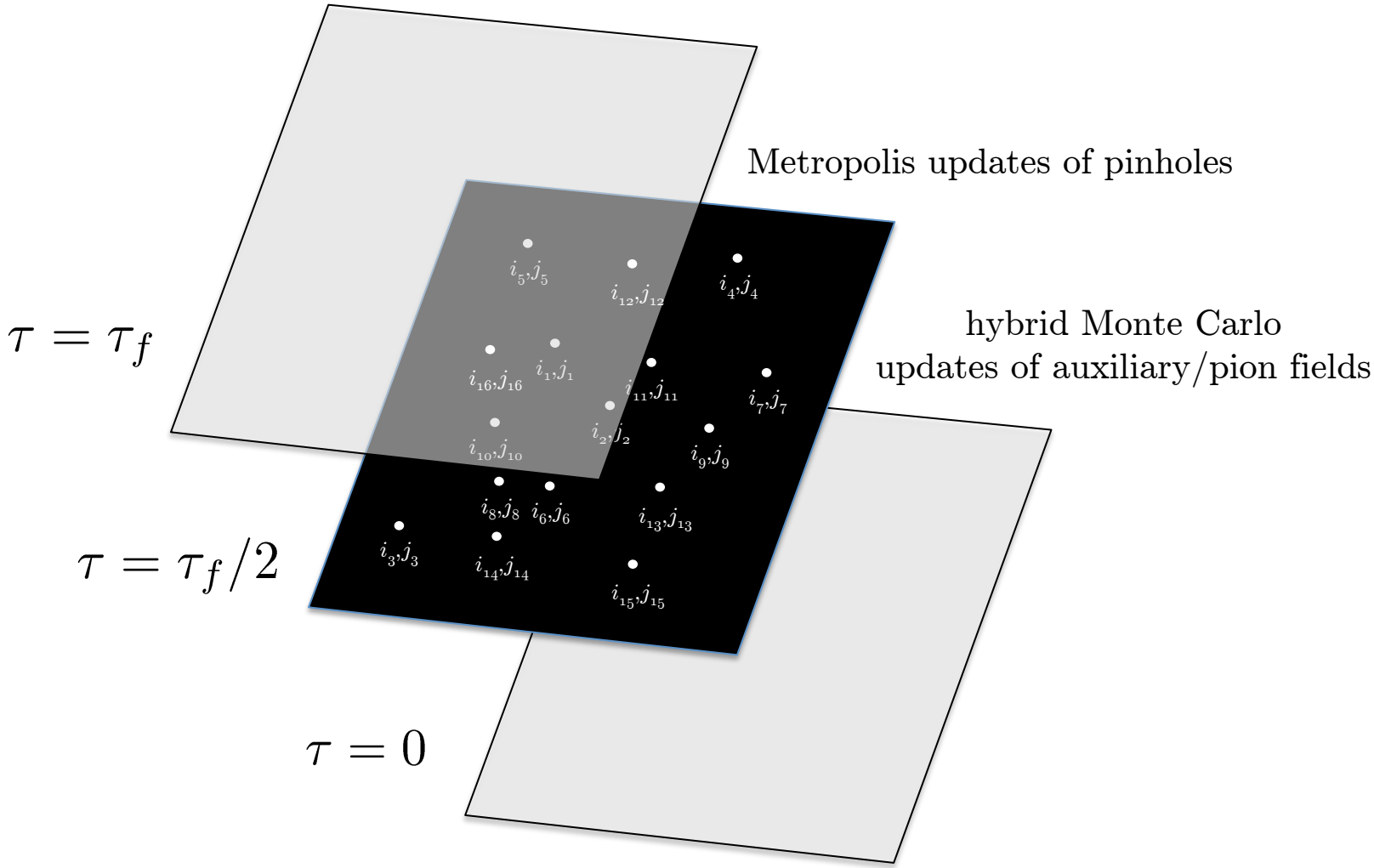
$$\rho_{i,j}(\mathbf{n}) = a^\dagger_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

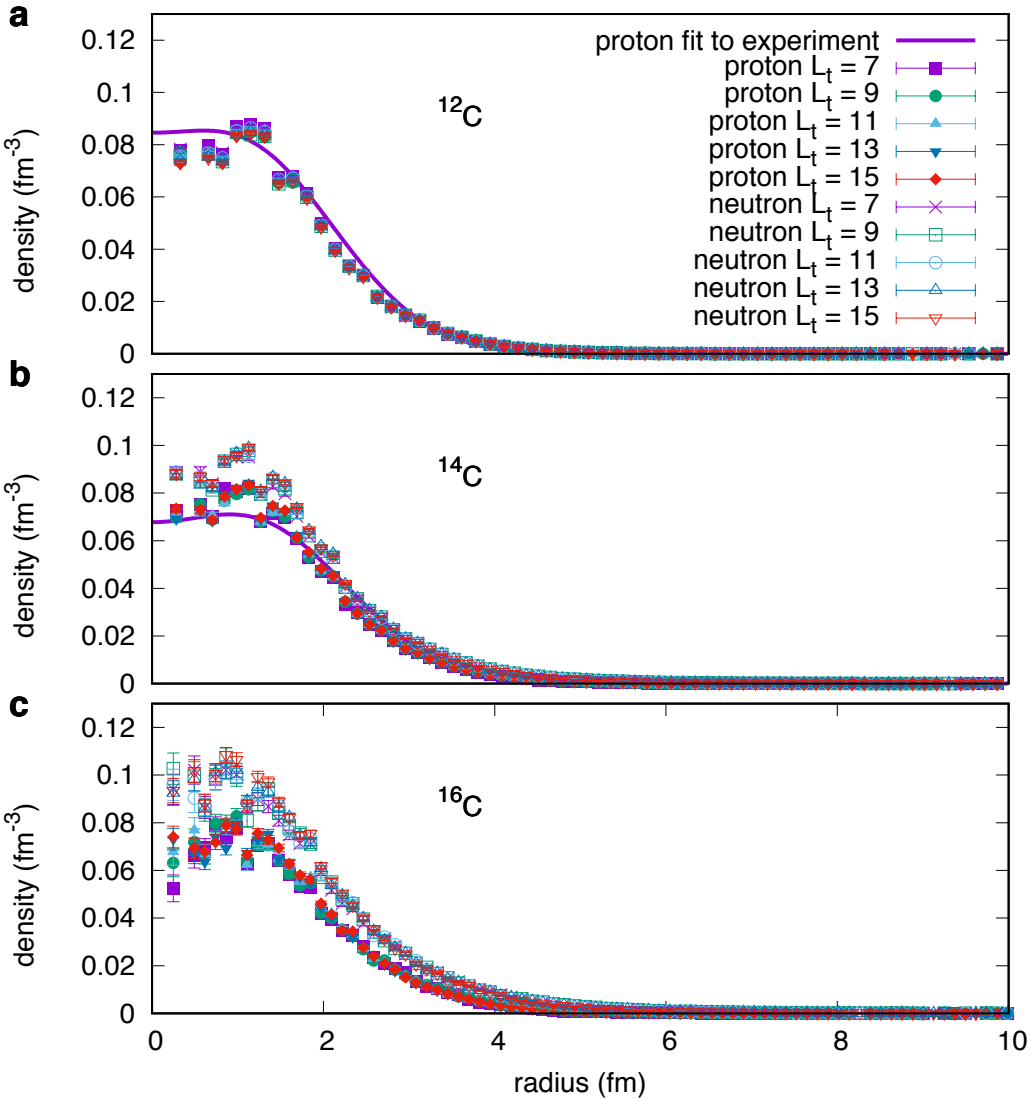
We construct the normal-ordered A-body density operator

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

In the simulations we do Monte Carlo sampling of the amplitude

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


Metropolis updates of pinholes
hybrid Monte Carlo
updates of auxiliary/pion fields
$\tau = \tau_f$
$\tau = \tau_f/2$
$\tau = 0$
i_5,j_5
i_{12},j_{12}
i_4,j_4
i_{16},j_{16}
i_1,j_1
i_{11},j_{11}
i_7,j_7
i_2,j_2
i_{10},j_{10}
i_9,j_9
i_8,j_8
i_6,j_6
i_{13},j_{13}
i_3,j_3
i_{14},j_{14}
i_{15},j_{15}



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

Pinhole trace algorithm

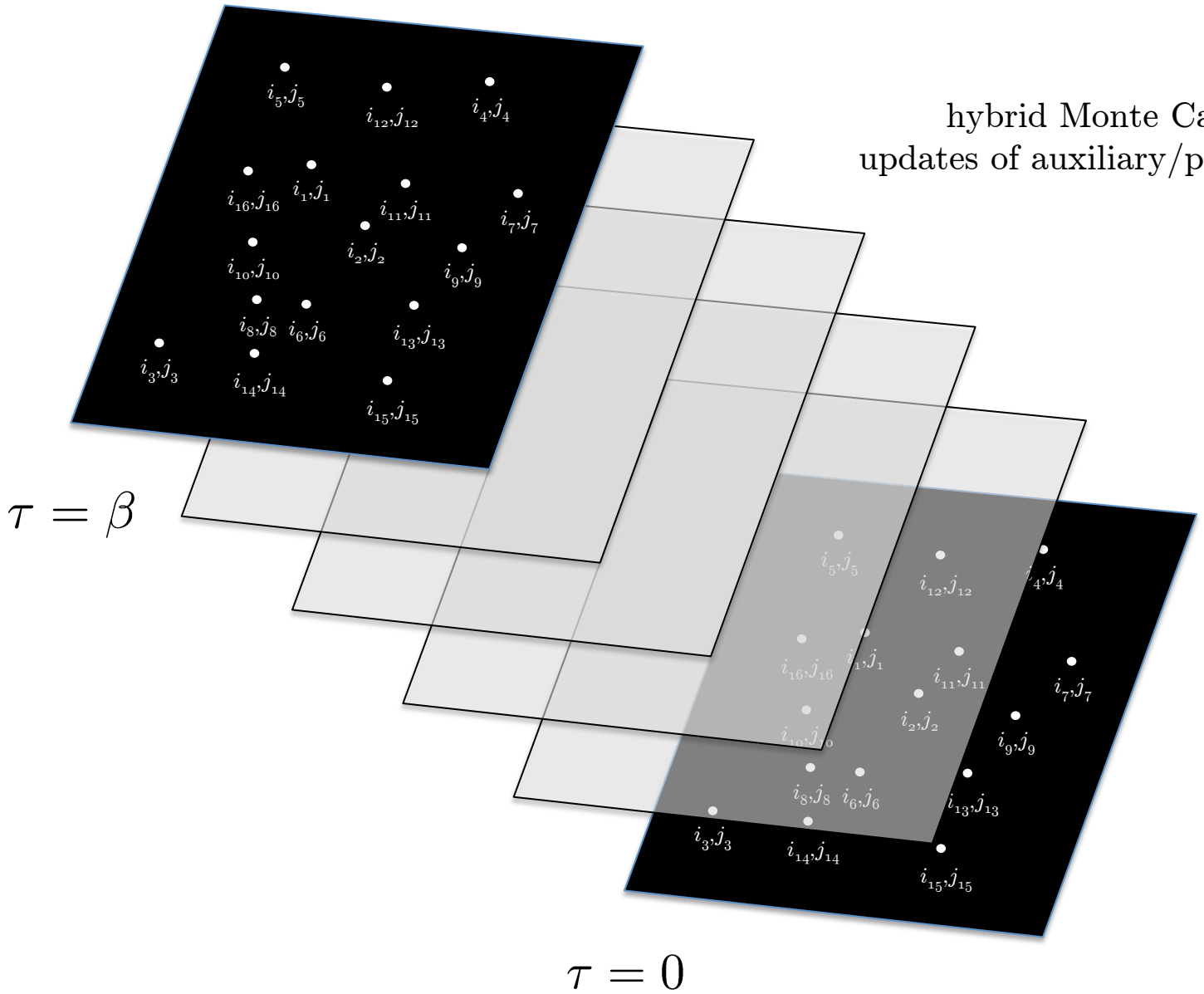
We have developed a new method to calculate the trace over quantum states using determinants of matrices of size $A \times A$, where A is the number of nucleons. The algorithm between 10^3 to 10^6 times faster than existing methods.

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

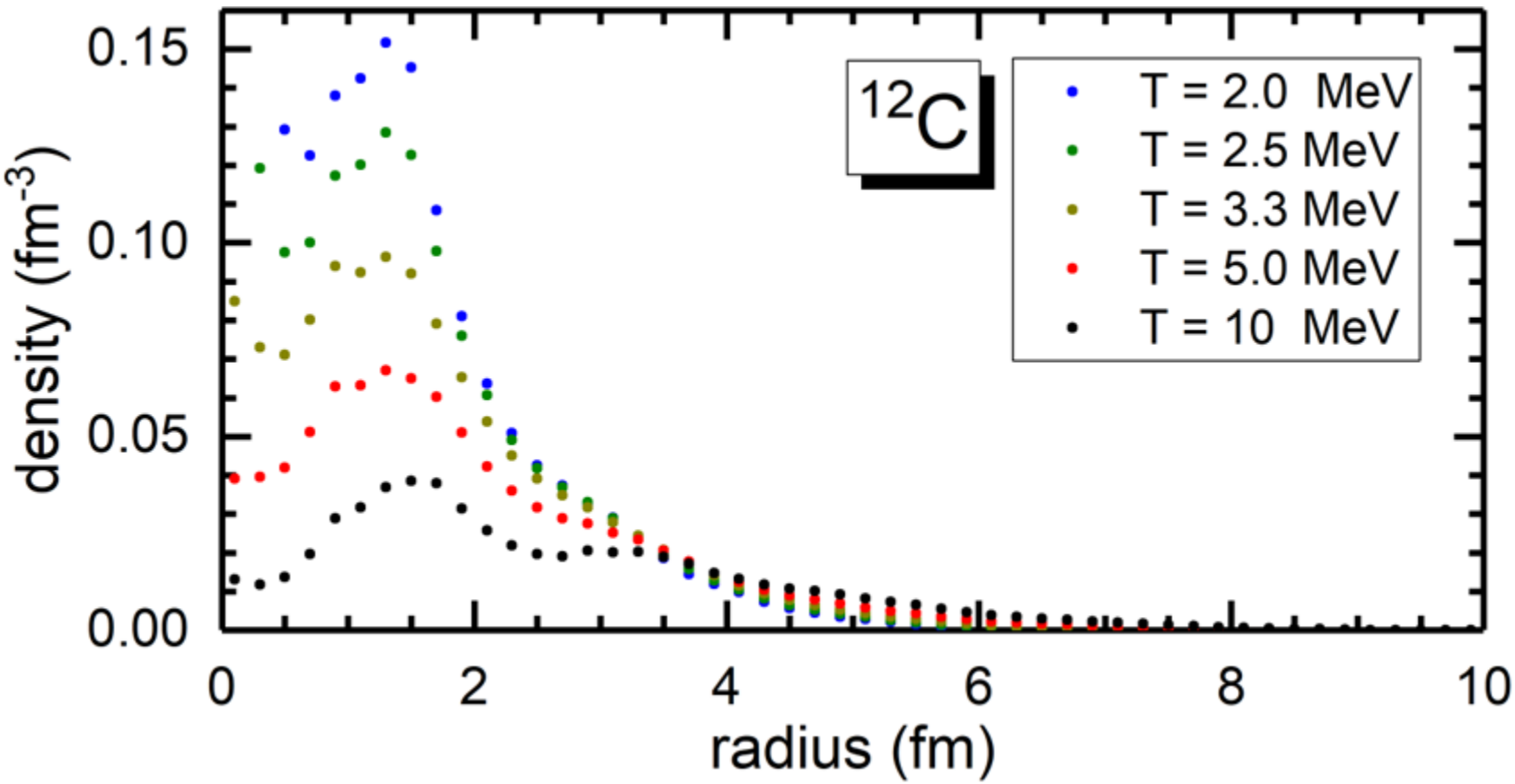


Figure courtesy of Bingnan Lu

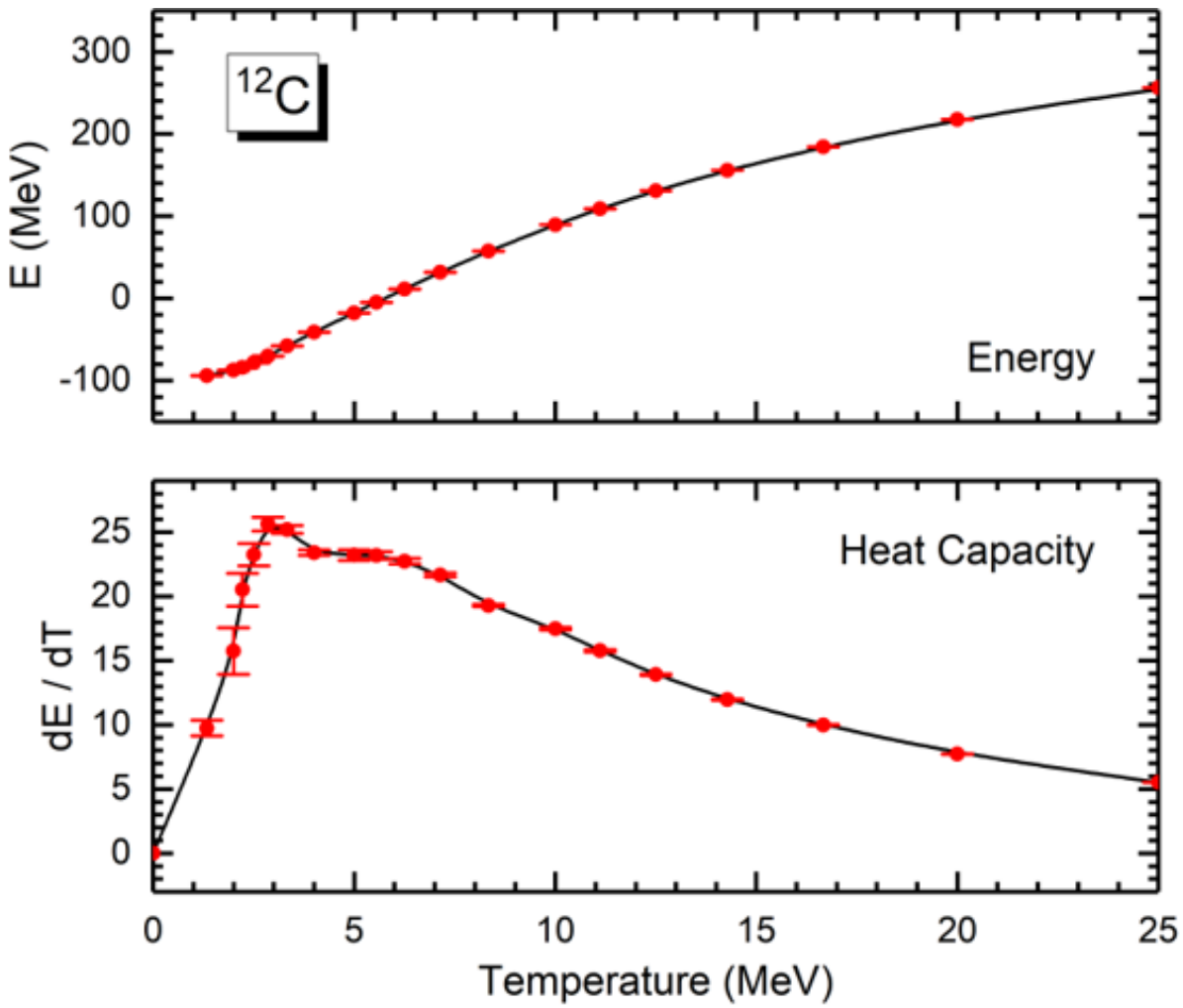
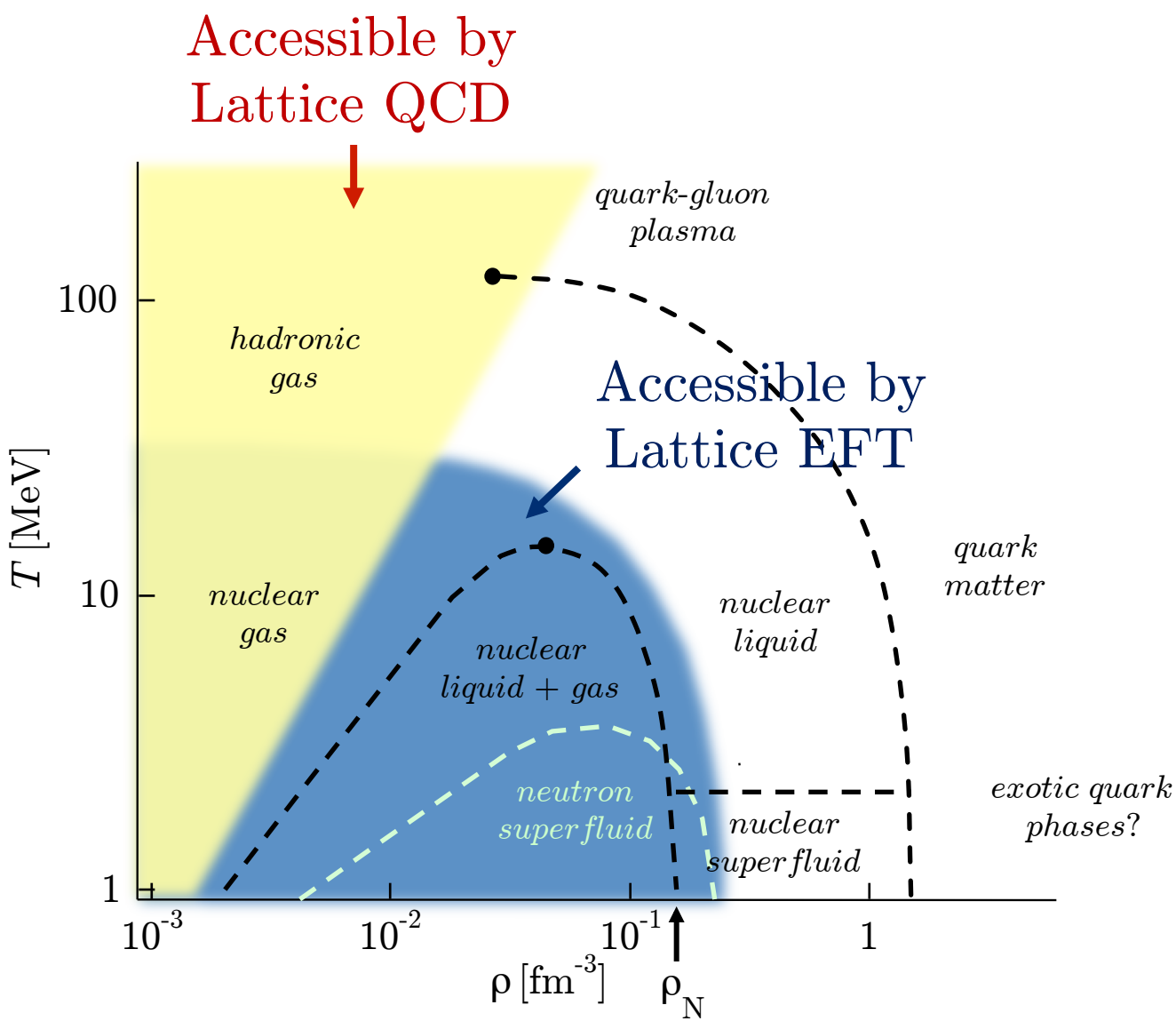


Figure courtesy of Bingnan Lu


Accessible by
Lattice QCD
quark-gluon
plasma
hadronic
gas
Accessible by
Lattice EFT
quark
matter
nuclear
gas
nuclear
liquid
nuclear
liquid + gas
neutron
super fluid
nuclear
super fluid
exotic quark
phases?
T [MeV]
100
10
1
10^-3
10^-2
10^-1
1
ρ [fm^-3]
ρ_N

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 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 methods similar to image recognition in machine learning.

D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, arXiv:1711.07090

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

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

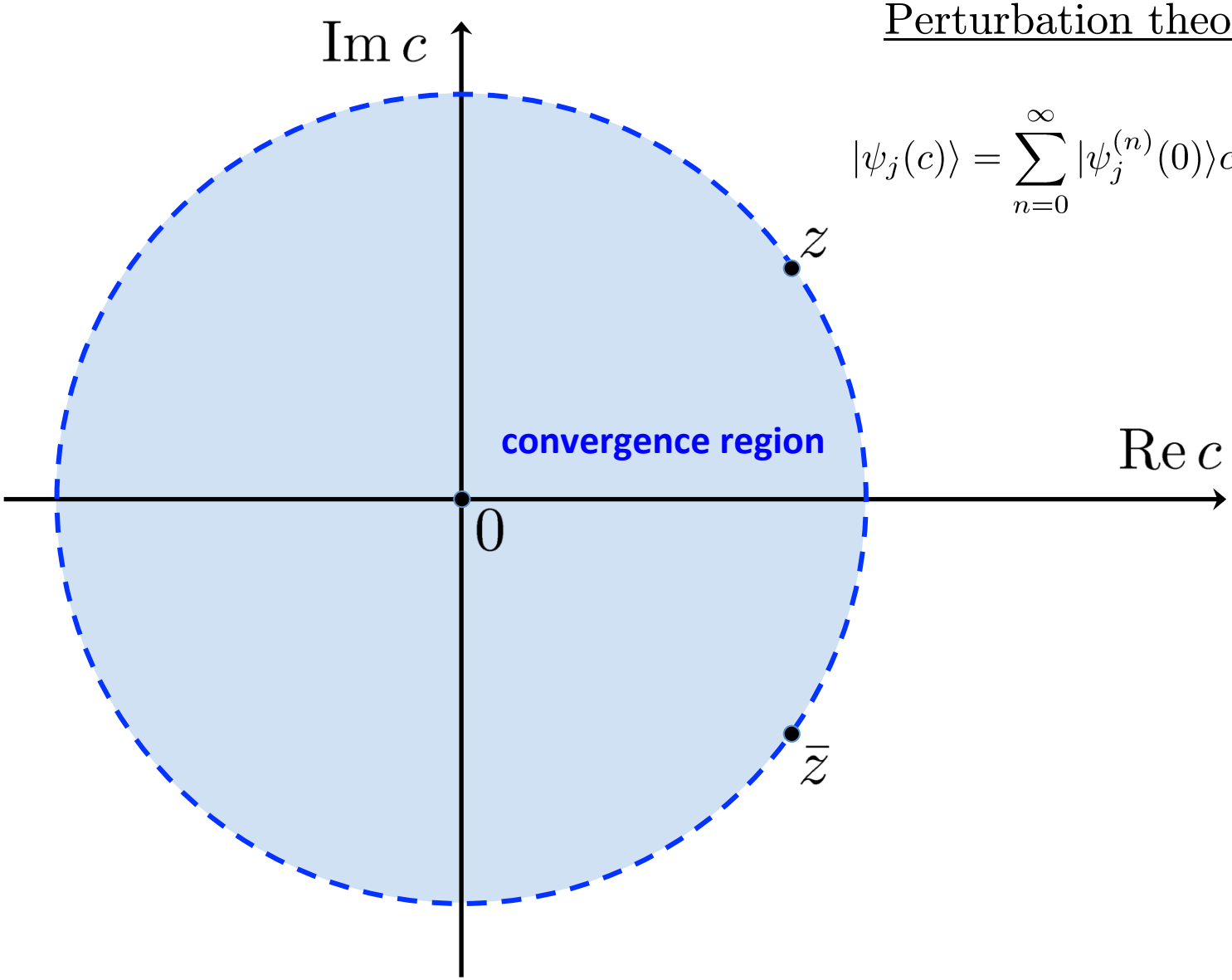
where H_0 and H_1 are Hermitian. Let the eigenvalues and eigenvectors be

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

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

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

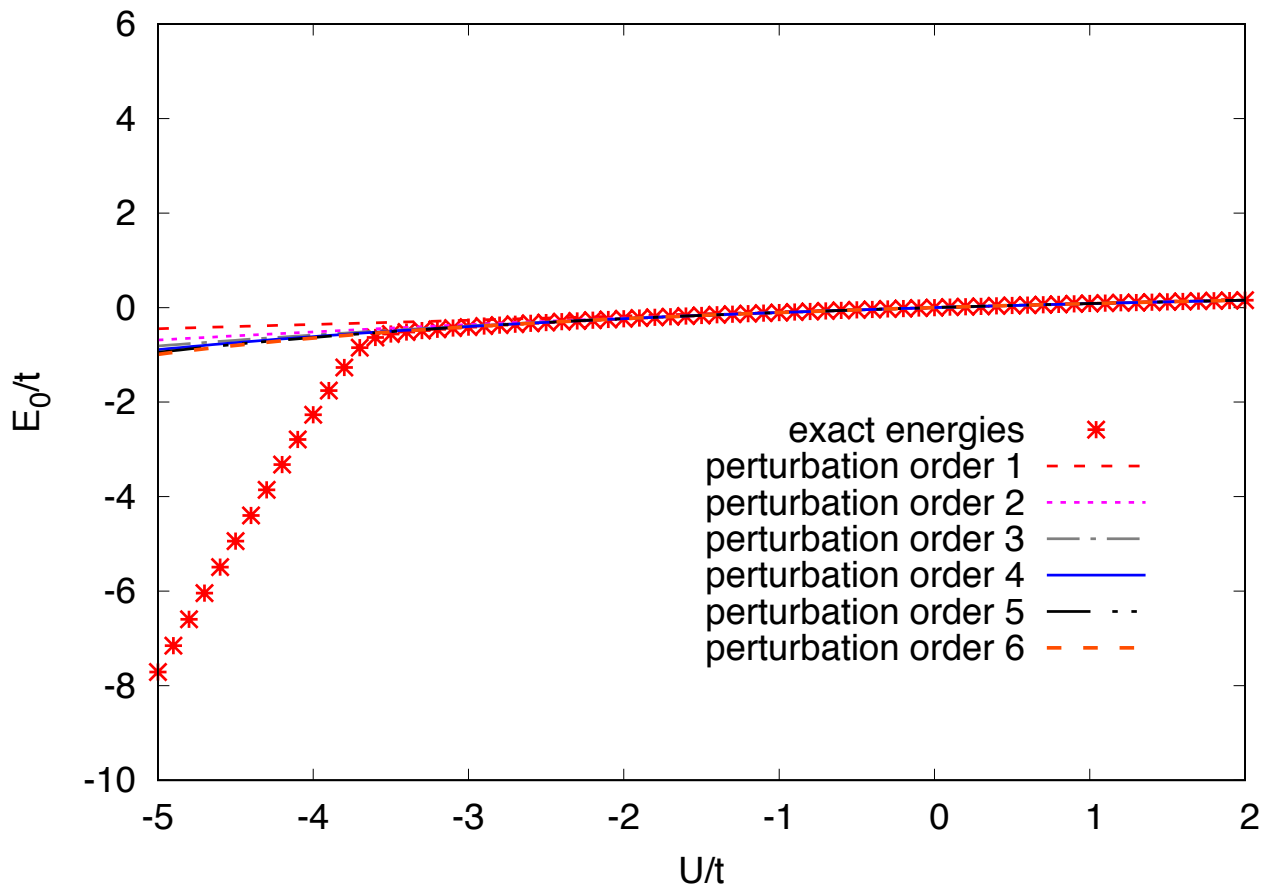
This is the strategy of perturbation theory. We can compute each term in the series when the eigenvalues and eigenvectors of H_0 are known or computable.



Perturbation theory

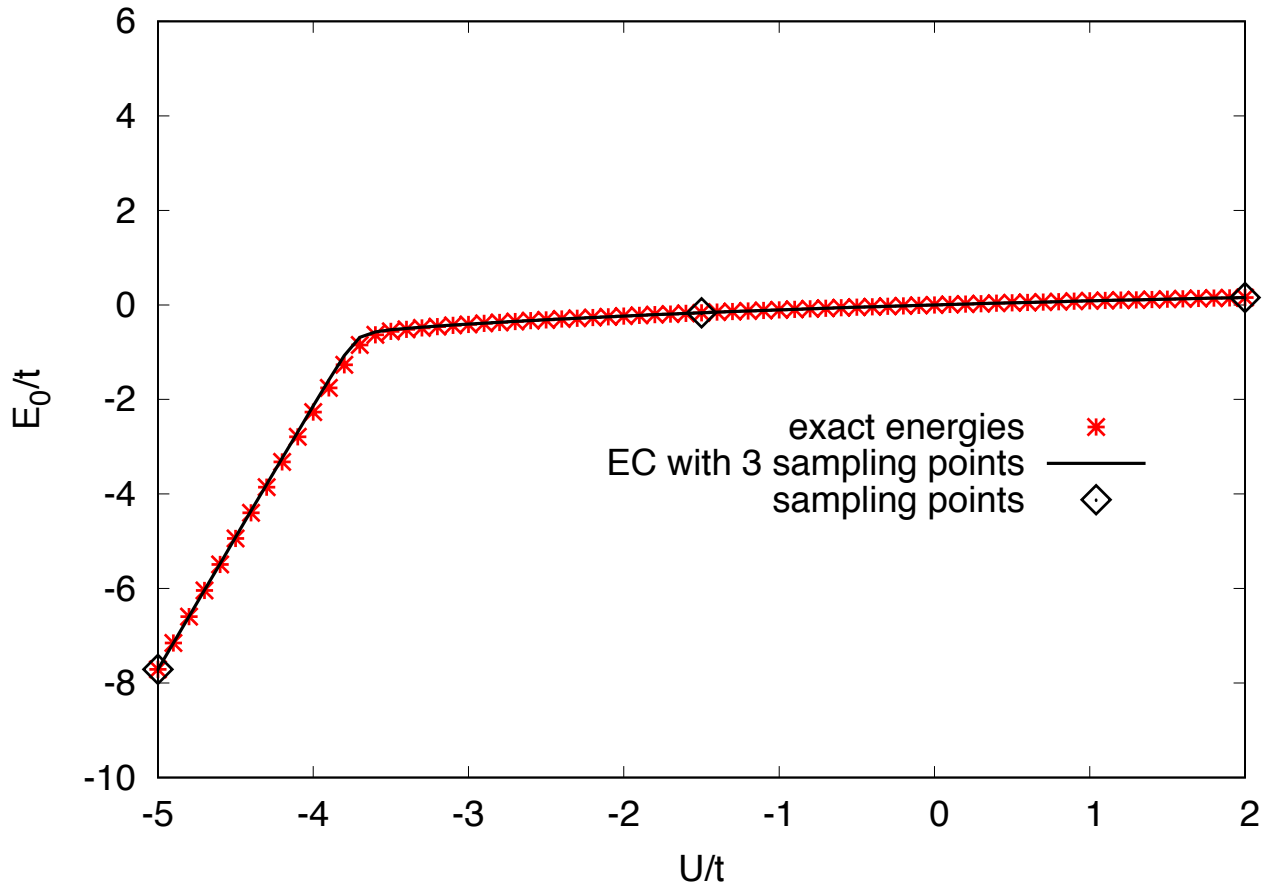
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

Bose-Hubbard model

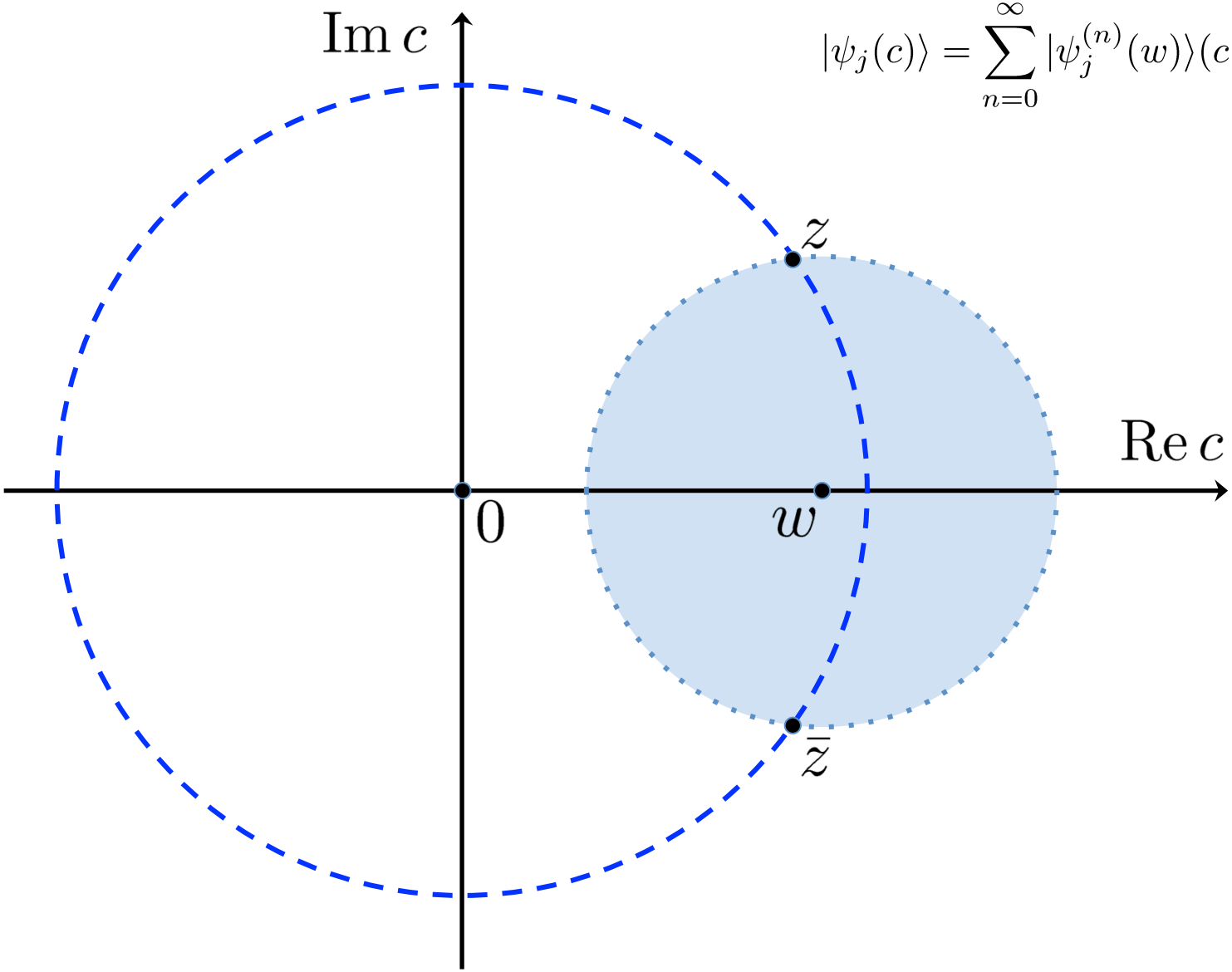


Perturbation theory fails at strong attractive coupling

Restrict the linear space to the span of three vectors

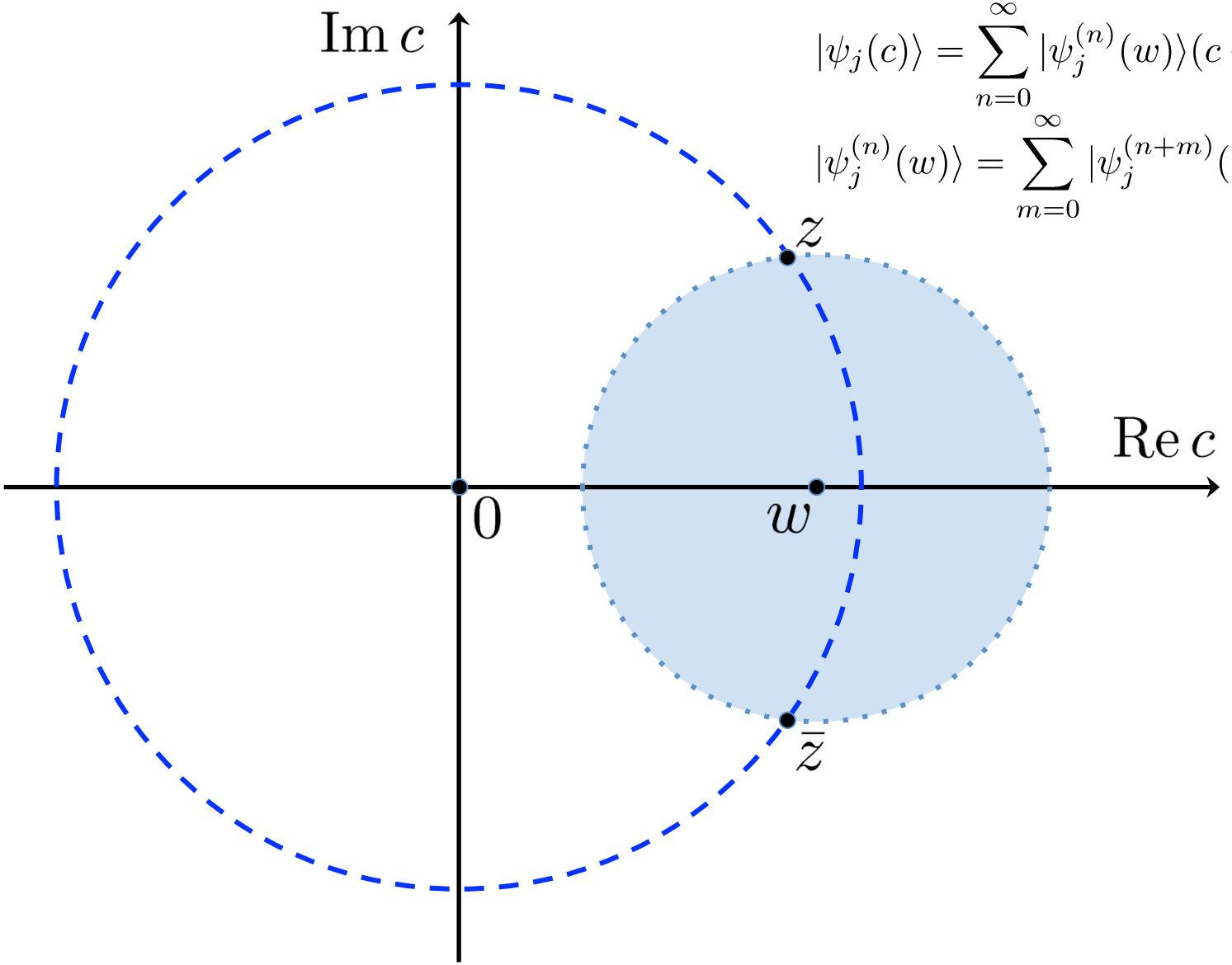


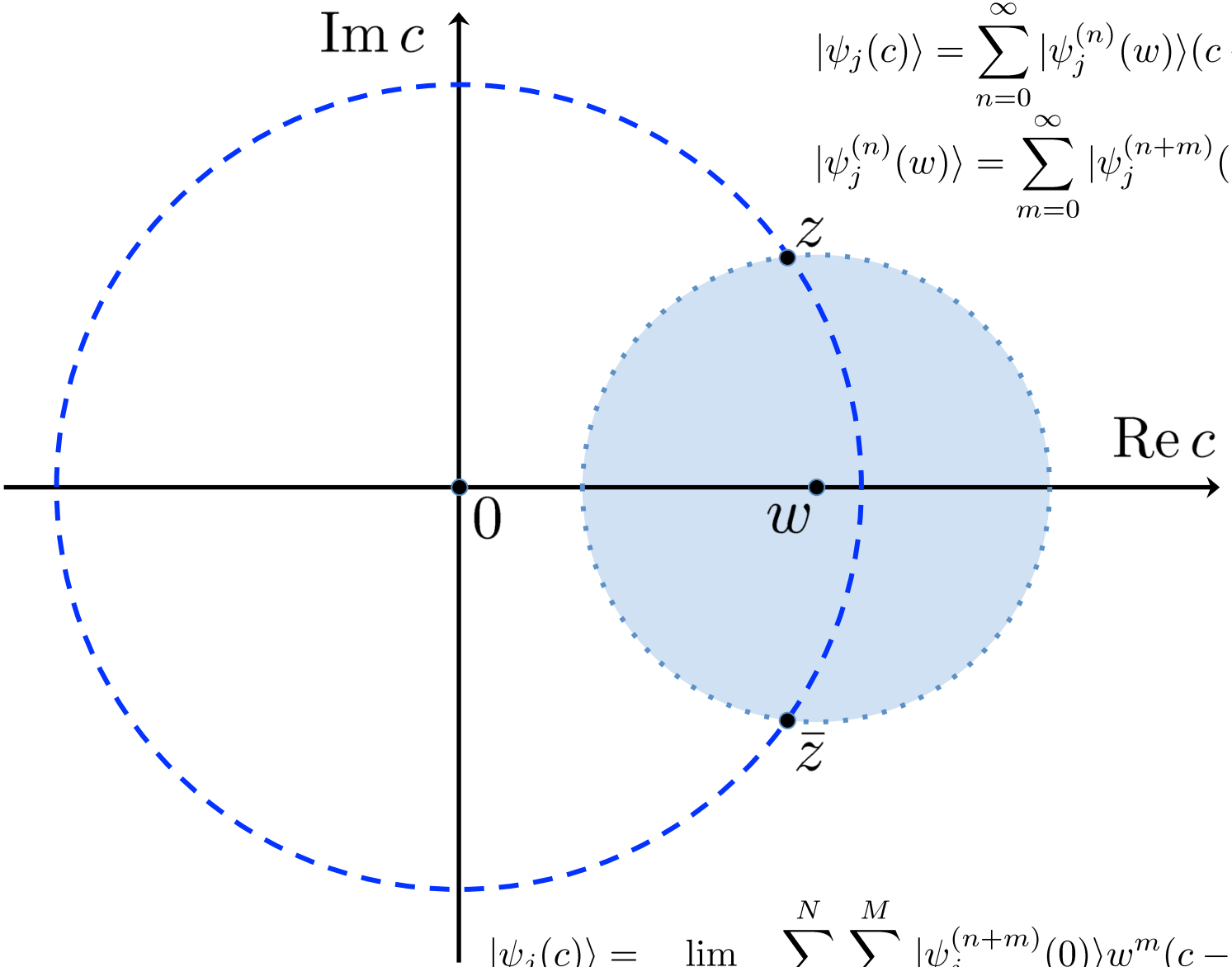
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$



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

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





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

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

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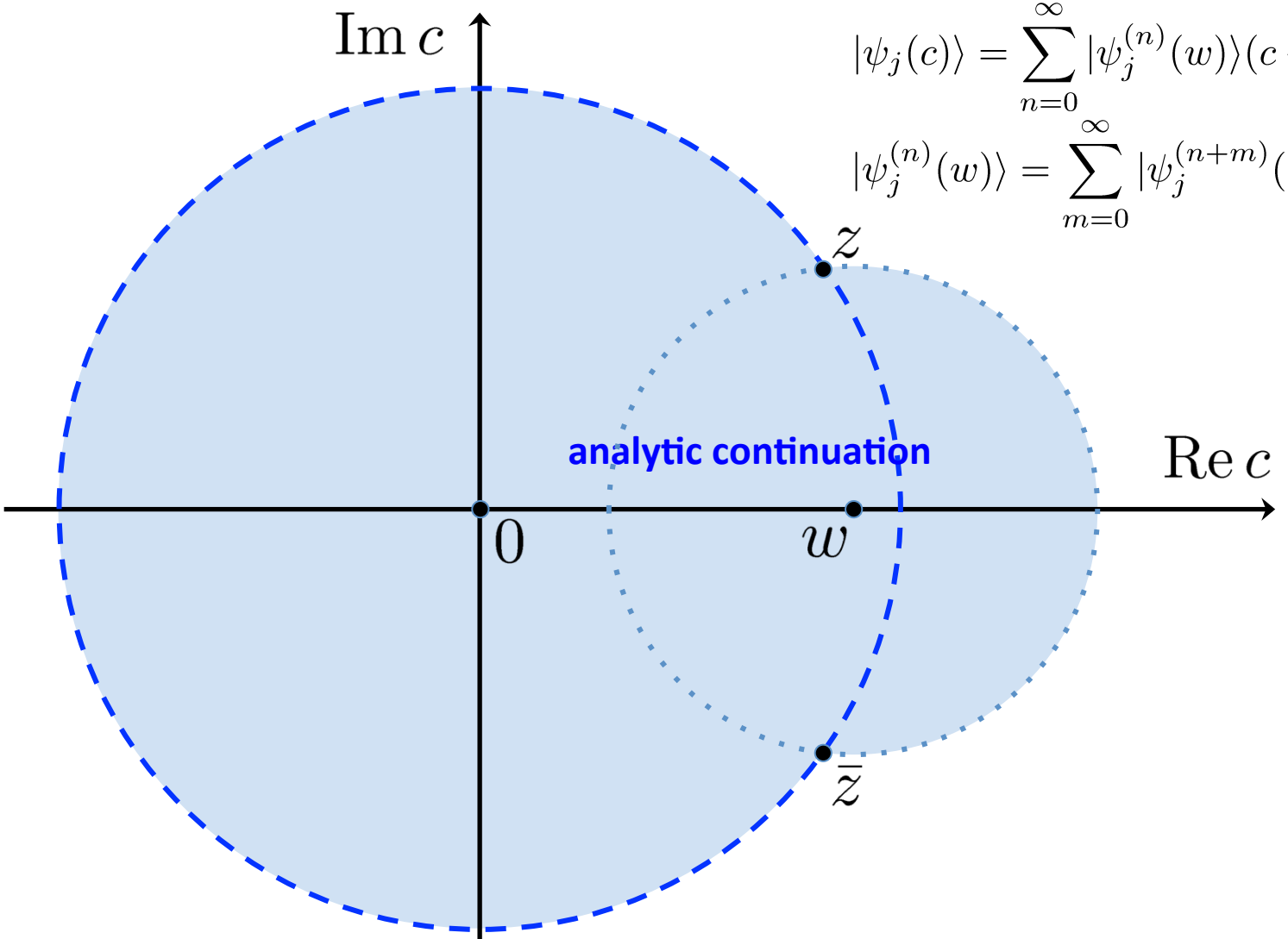

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The eigenvector can be well approximated as a linear combination of a few vectors, using either the original series expansion

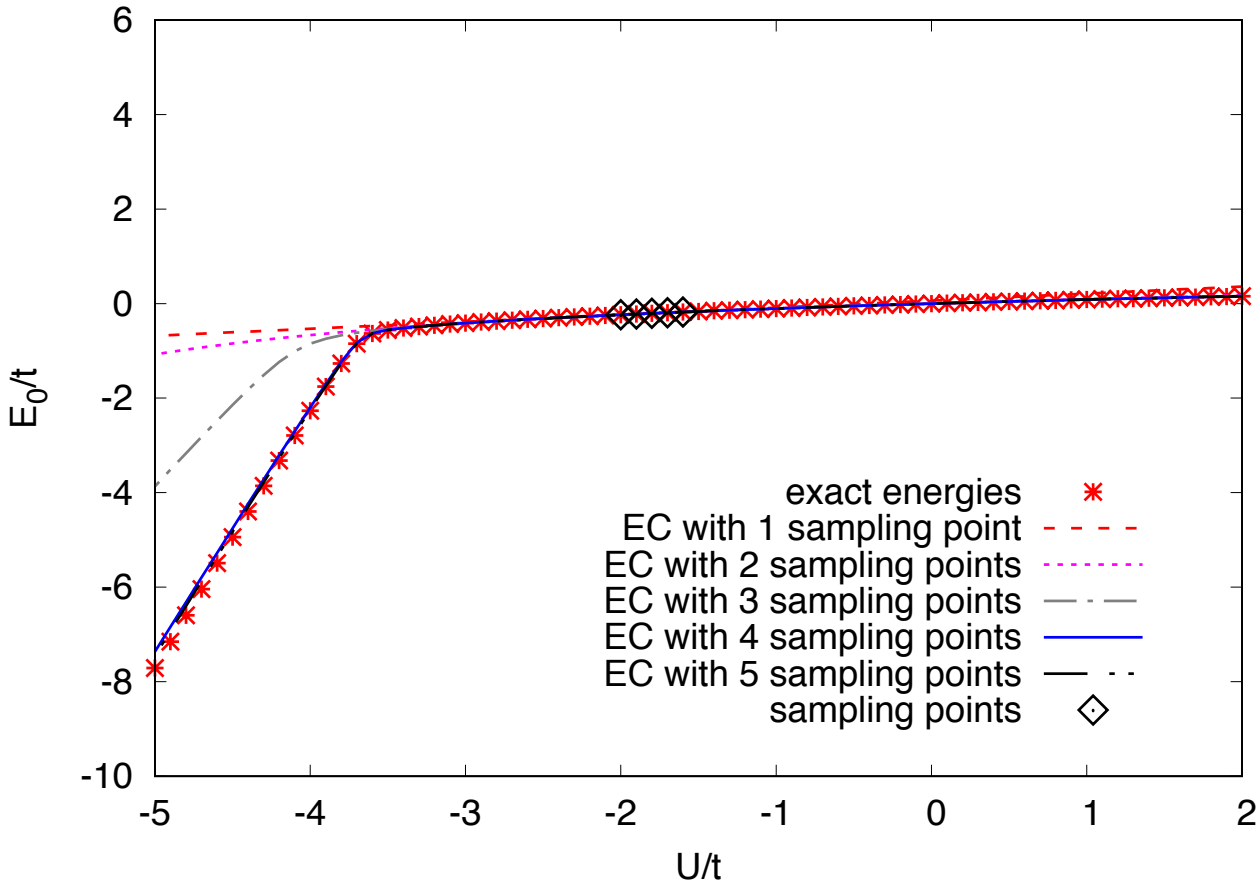
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

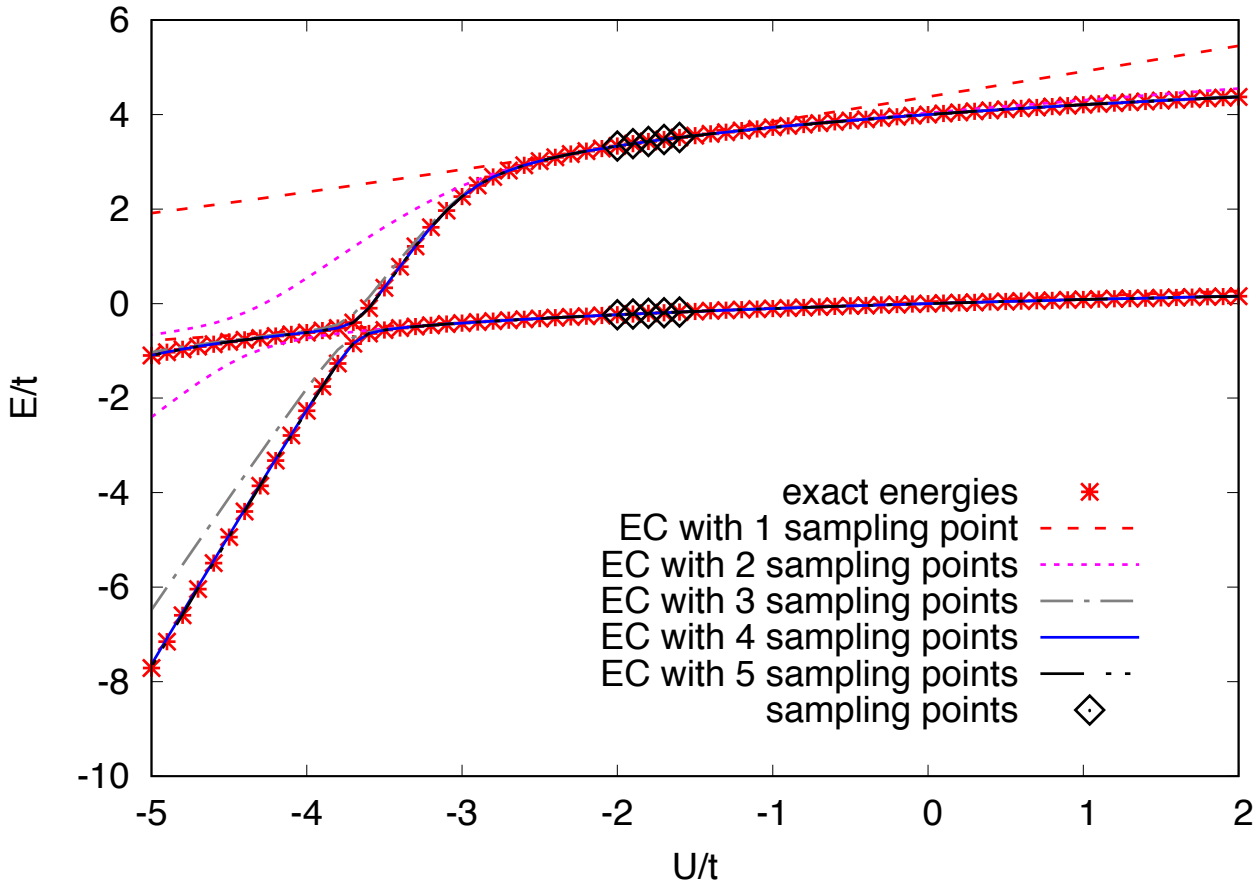
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

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.



Discussion questions

Why causes the sensitivity to interaction range and locality in larger A systems?

How can we systemically accelerate the convergence of chiral effective field theory for larger A systems?

Can we use cluster effective field theory and light nucleus scattering to accelerate the convergence of chiral effective field theory?

Can we use external potentials to constrain nuclear forces?

Can we use thermodynamics and lattice QCD matching to constrain nuclear forces?

Summary and Outlook

These are exciting times for the *ab initio* nuclear theory community. In lattice EFT, we have new projects in motion which are pushing the current frontiers.

Currently working to improve our understanding of the detailed connection between bare nuclear forces and nuclear structure for light and medium-mass nuclei.

Applying the adiabatic projection method to low-energy nucleon-nucleus and alpha-nucleus scattering and reactions.

Using the pinhole algorithm to study the detailed structure of nuclei and thermodynamics of finite nuclei, nuclear matter, and neutron matter.

Implementing eigenvector continuation to treat all higher-order interactions in chiral effective field theory.

Calculating the two-body density matrix to measure pairing correlations in neutron matter and finite nuclei.