Nuclear structure and reactions from lattice simulations

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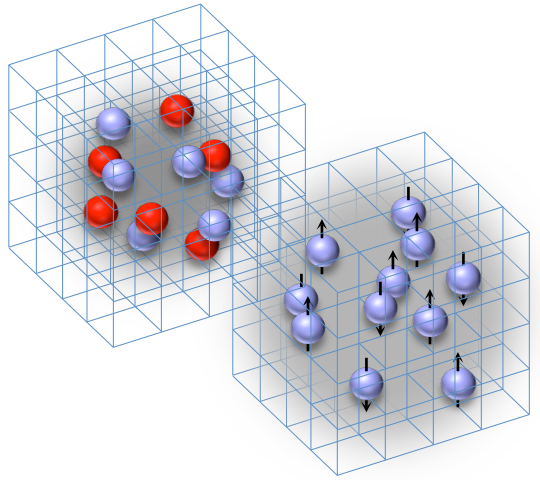
Nuclear Lattice EFT Collaboration

Shapes and Symmetries in Nuclei:
from Experiment to Theory

CNRS, Gif-sur-Yvette, November 9, 2017



Outline

Introduction and motivation

Lattice effective field theory

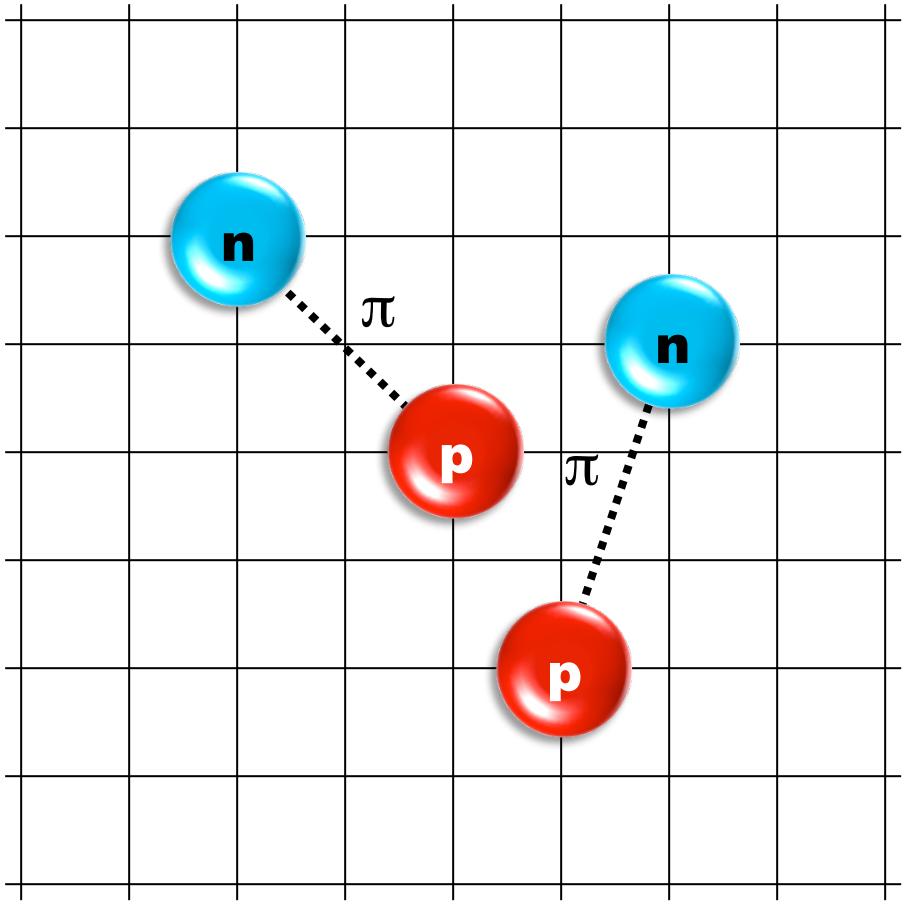
Proton- and neutron-rich systems

Nuclear clustering

Eigenvector subspace continuation

Summary and outlook

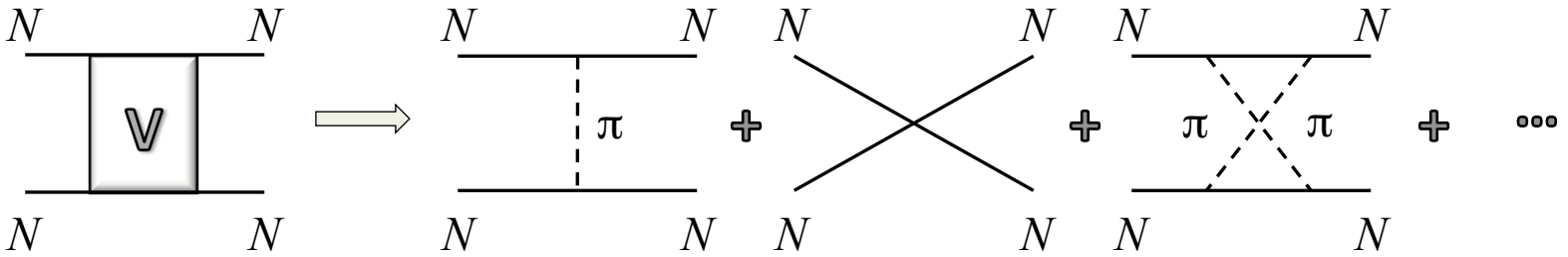
Lattice effective field theory



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

Chiral effective field theory

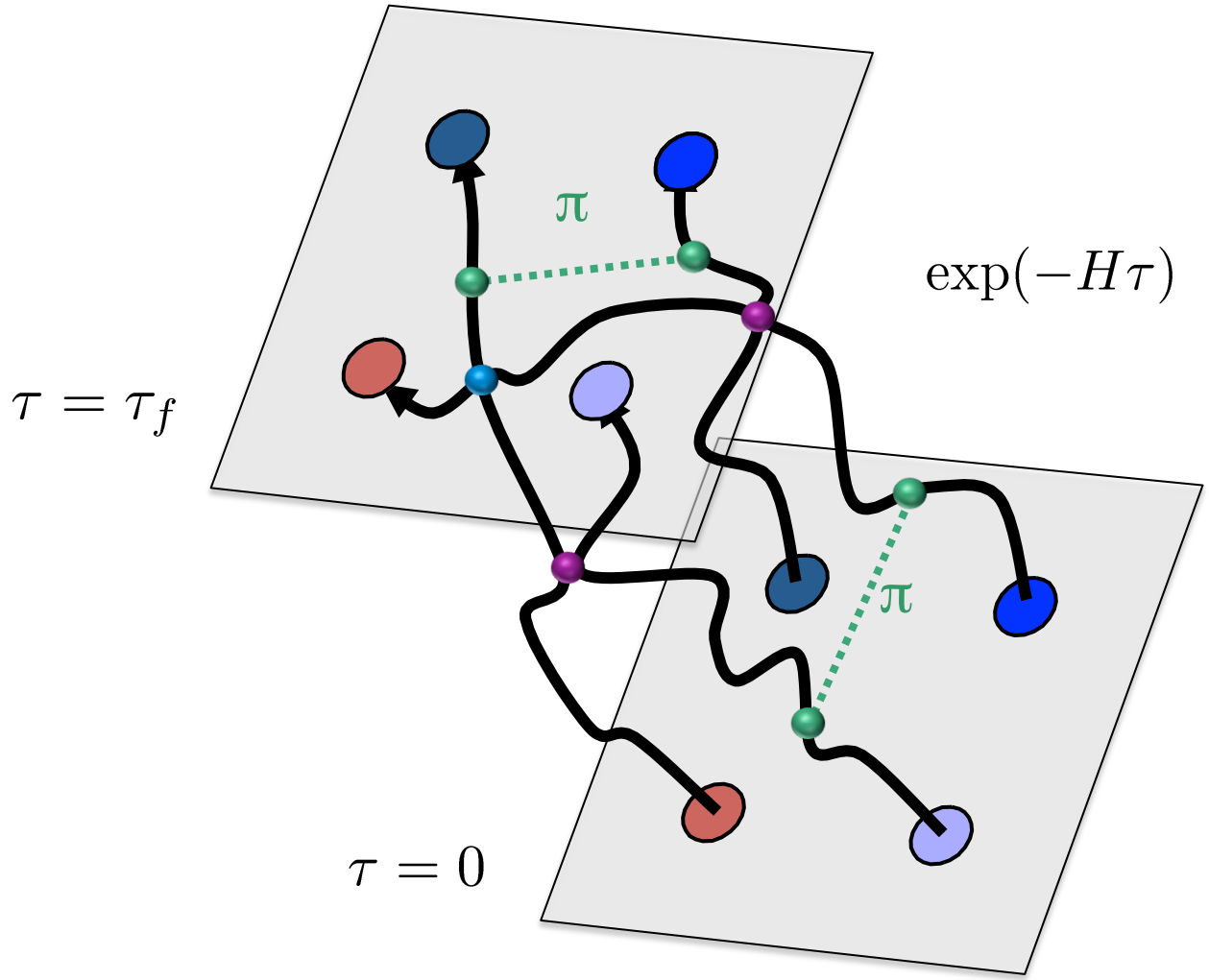
Construct the effective potential order by order



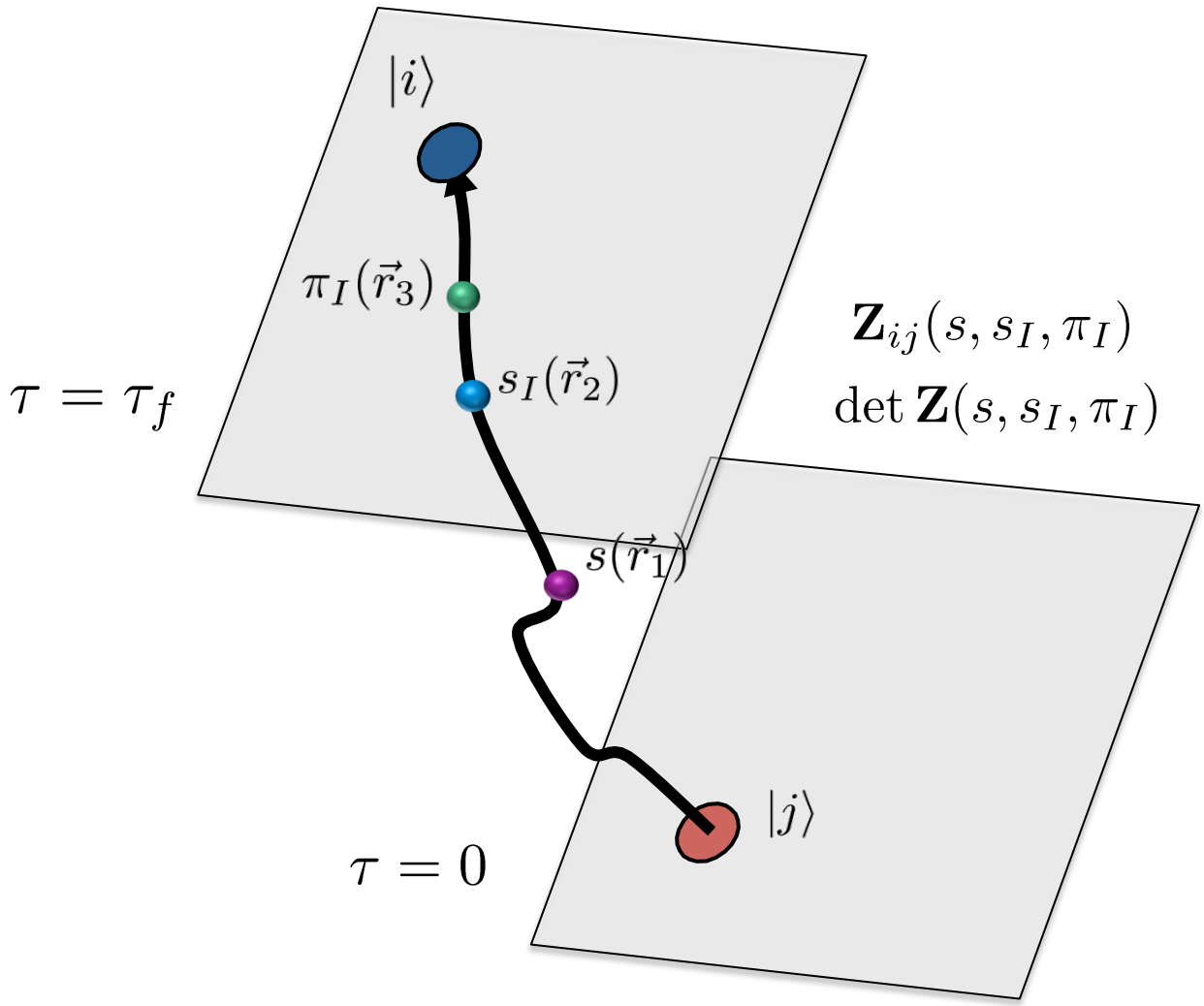
V^{OPEP} Contact interactions V^{TPEP}

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

Euclidean time projection



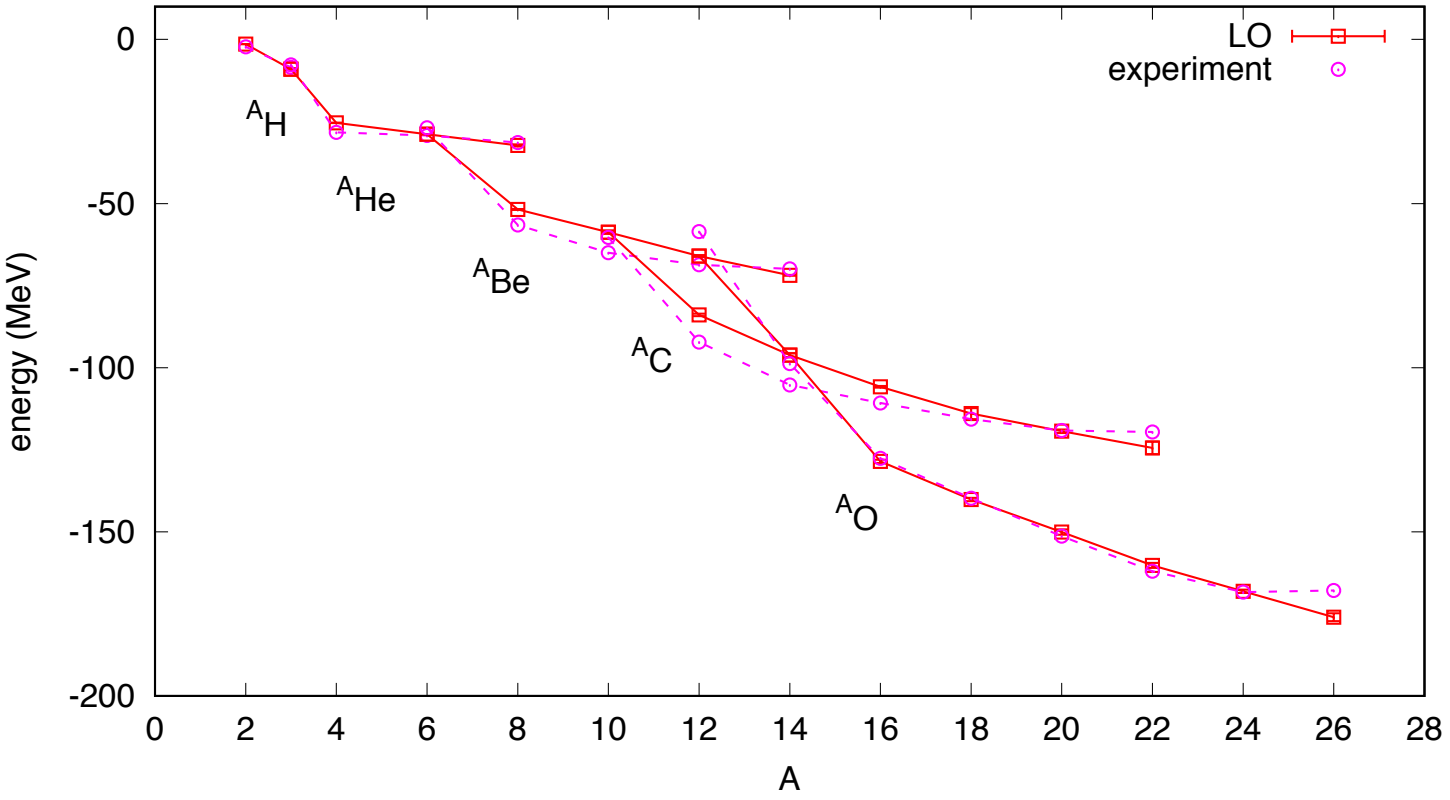
Auxiliary field method



Proton- and neutron-rich systems

Lattice simulations had been restricted to nuclei with $N = Z$ due to Monte Carlo sign oscillations. This problem has now been resolved using a different choice of leading-order action.

Ground state energies



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL in press, arXiv:1702.05177

Model-independent measure of clustering

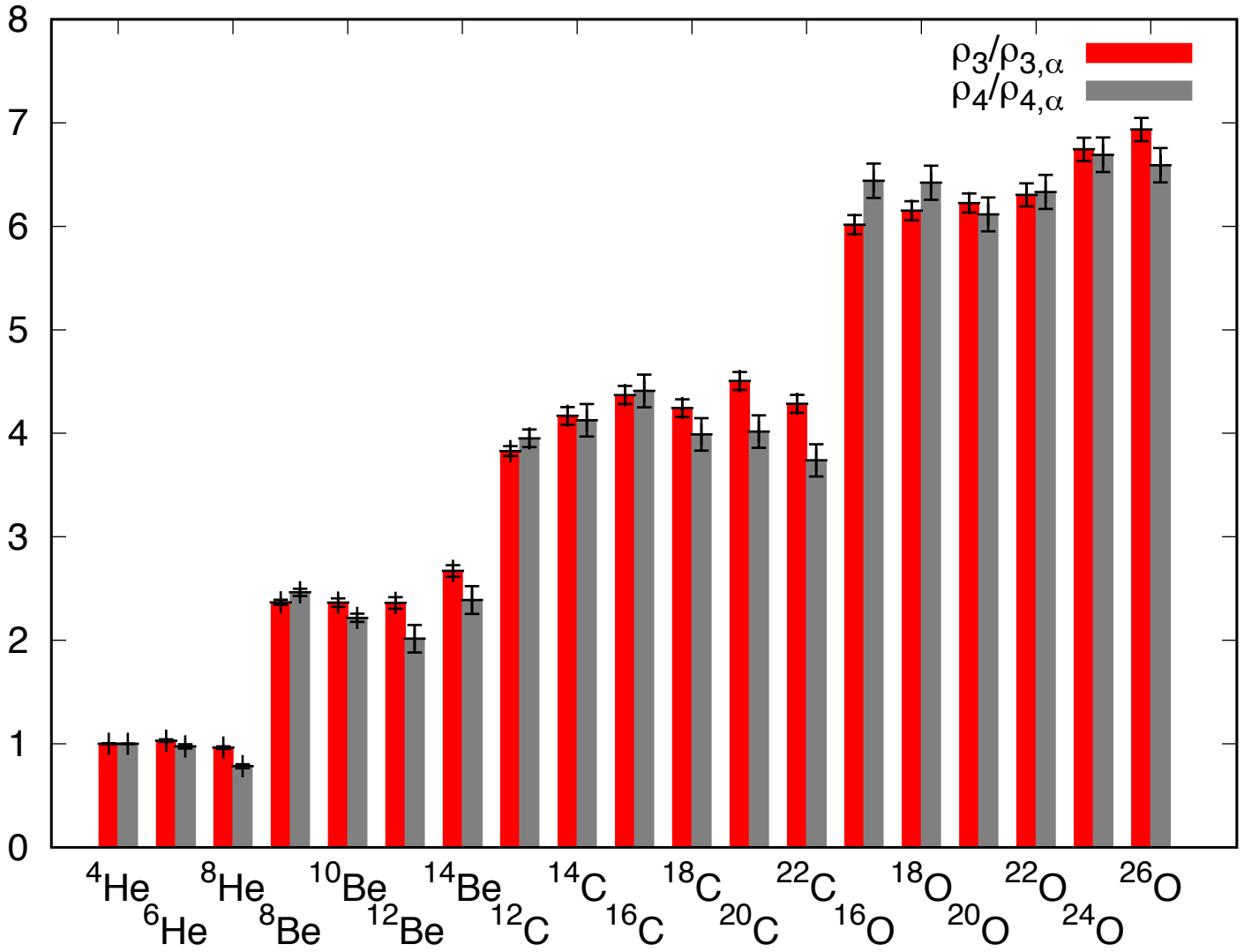
Let $\rho(\mathbf{n})$ be the total nucleon density operator on lattice site $\mathbf{n}$. To construct a probe for alpha clusters, we measure the strength of four-nucleon short-range correlations. We define ρ_4 as the expectation value of $:\rho^4(\mathbf{n})/4!:$ summed over $\mathbf{n}$.

Due to divergences at short distances, ρ_4 will depend on the short-distance regularization scale, which in our case is the lattice spacing. However, at leading order in an operator product expansion the regularization-scale dependence will drop out in ratios of ρ_4 for different nuclei.

We let $\rho_{4,\alpha}$ be the value of ρ_4 for the alpha particle. We consider then the ratio $\rho_4/\rho_{4,\alpha}$, which is free from short-distance divergences and is model independent at leading order in an operator product expansion.

For nuclei with even Z and even N, there are likely no well-defined ^{3}H or ^{3}He clusters since their formation is not energetically favorable.

Therefore we can use short-distance three-nucleon correlations as a another probe of alpha clusters. We define ρ_3 as the expectation value of $:\rho^3(\mathbf{n})/3!:$ summed over $\mathbf{n}$. We can also consider the analogous ratio $\rho_3/\rho_{3,\alpha}$, where $\rho_{3,\alpha}$ is the value of ρ_3 for the alpha particle.



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL in press, arXiv:1702.05177

Unfortunately there is no algorithm available for *ab initio* auxiliary field Monte Carlo simulations to determine the density distribution of particles relative to the center of mass. The problem is that the particle wave functions in the auxiliary field simulation are a superposition of many values for the center of mass.

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

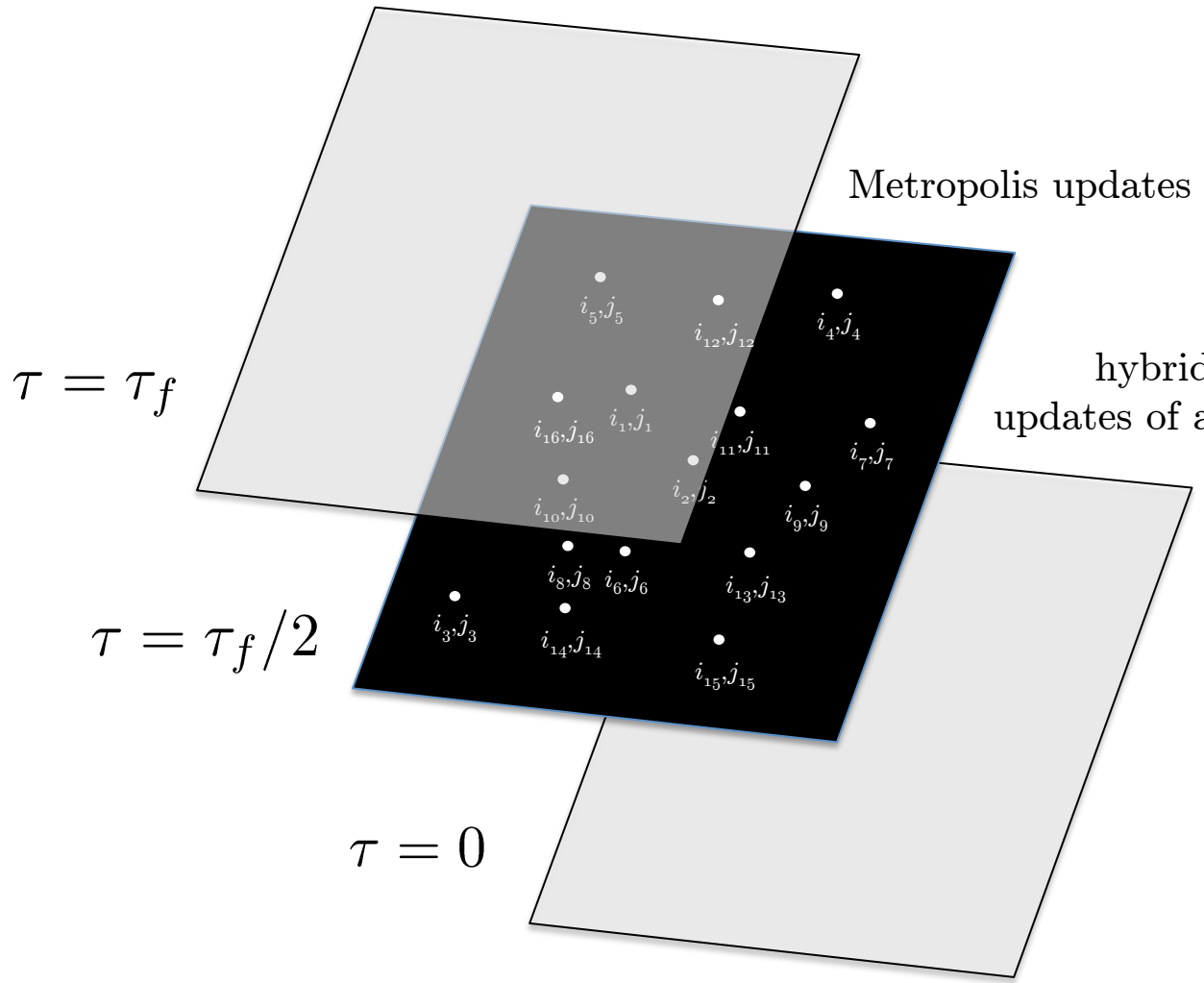
$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

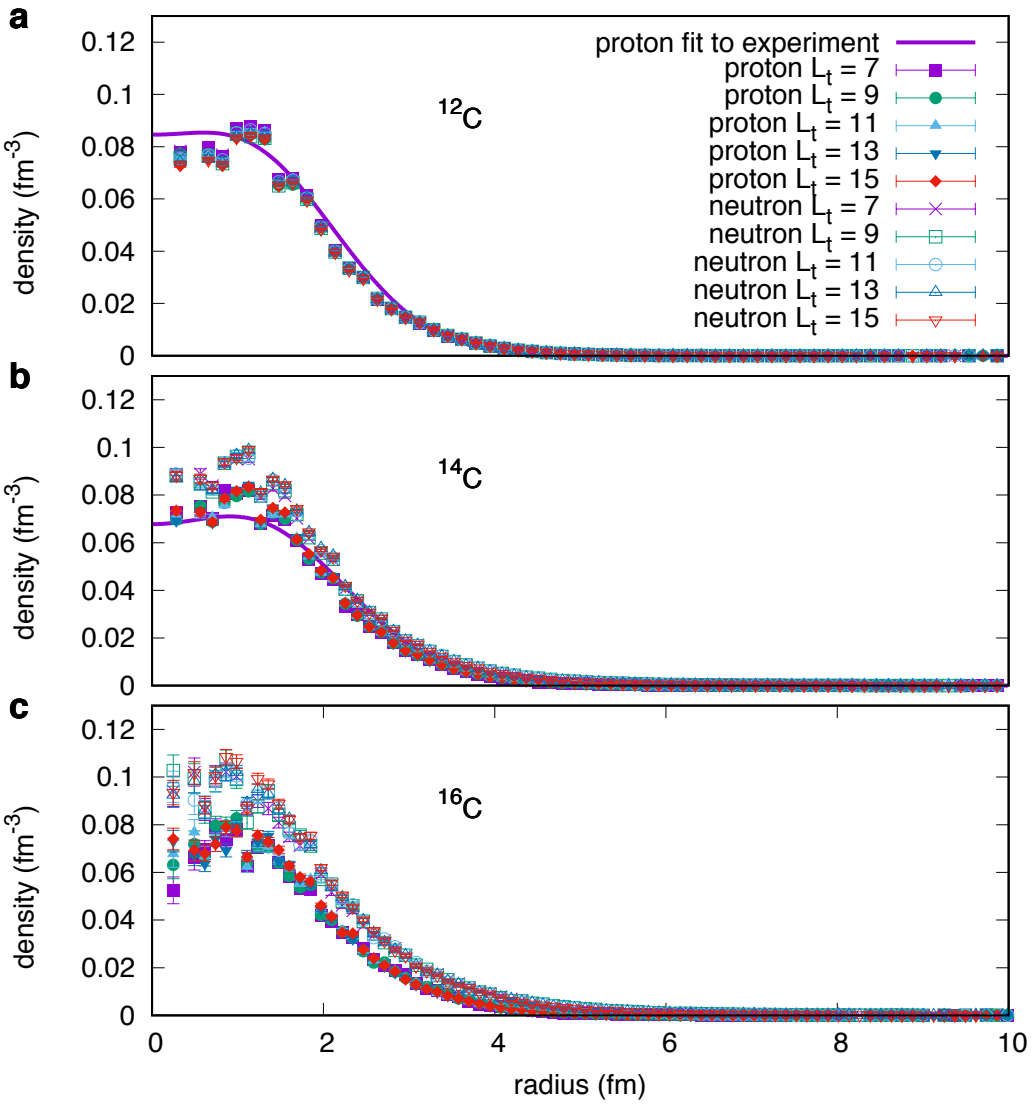
In the A-particle subspace, we have the identity

$$\sum_{i_1,j_1,\cdots i_A,j_A} \sum_{\mathbf{n}_1,\cdots \mathbf{n}_A} \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) \;= A!$$

In the simulations we do Monte Carlo sampling of the amplitude

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

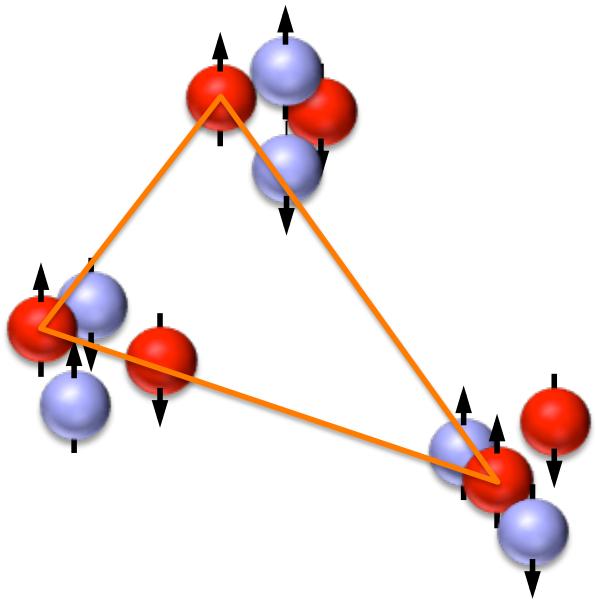

Metropolis updates of pinholes
hybrid Monte Carlo
updates of auxiliary/pion fields
$\tau = \tau_f$
$\tau = \tau_f/2$
$\tau = 0$
i_5,j_5
i_{12},j_{12}
i_4,j_4
i_{16},j_{16}
i_1,j_1
i_{11},j_{11}
i_7,j_7
i_2,j_2
i_{10},j_{10}
i_9,j_9
i_8,j_8
i_6,j_6
i_{13},j_{13}
i_3,j_3
i_{14},j_{14}
i_{15},j_{15}



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL in press, arXiv:1702.05177

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.



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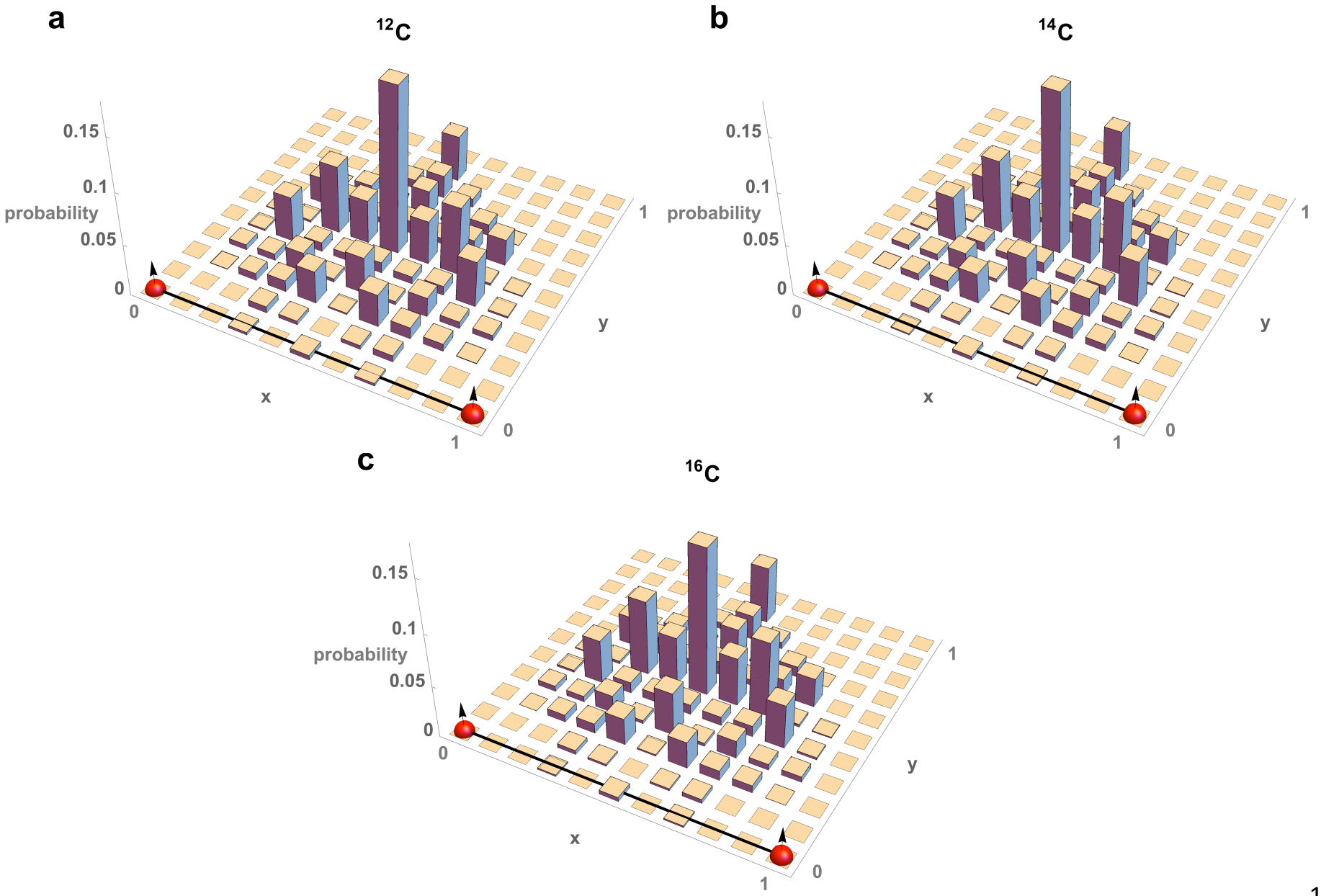

a
^{12}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
b
^{14}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
c
^{16}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1

Given the rich cluster structure of the excited states of ^{12}C, this raises the interesting possibility of similar cluster states appearing in ^{14}C and ^{16}C.

In particular, the bound 0_2^+ state at 6.59 MeV above the ground state of ^{14}C may be a bound-state analog to the Hoyle state resonance in ^{12}C at 7.65 MeV. It may also have a clean experimental signature since low-lying neutron excitations are suppressed by the shell closure at eight neutrons.

There is also a bound 0_2^+ in ^{16}C, however in this case one expects low-lying two-neutron excitations to be important, thereby making the analysis more complicated.

Eigenvector continuation

Consider the case with strong quantum correlations are but the required linear space is so immense that only Monte Carlo methods can be used. But it may be that the parameters are such that the sign problem renders the Monte Carlo simulation impractical.

Eigenvector continuation might be able to help. It is a method for the calculation of extremal eigenvectors of a quantum Hamiltonian by applying some basic concepts from machine learning.

While a eigenvector resides in a linear space with enormous dimensions, the effective dimensionality of the subspace spanned by the eigenvector over a range of interaction couplings can be quite small. But instead of using a restricted Boltzmann machine to find this subspace, we use the variational principle.

Frame, He, Ipsen, Lee, D.L., Rrapaj, in progress

Consider the ground state of a Hamiltonian that depends on the real parameter c.

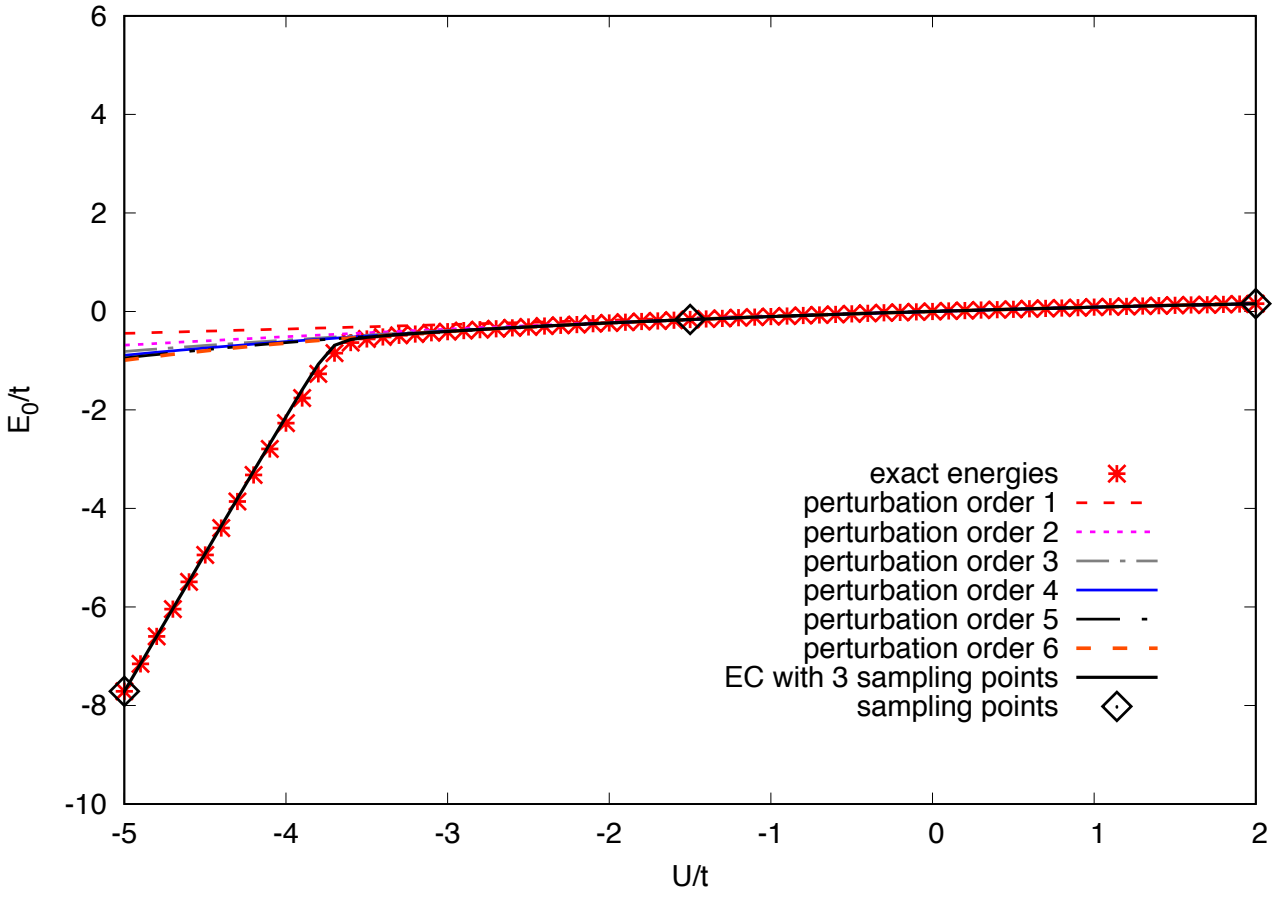
$$H(c)|\psi_0(c)\rangle = E_0(c)|\psi_0(c)\rangle$$

The "training" coupling values c_k are chosen within some interval where Monte Carlo simulations can be done. The target value c may be inaccessible due to sign oscillations.

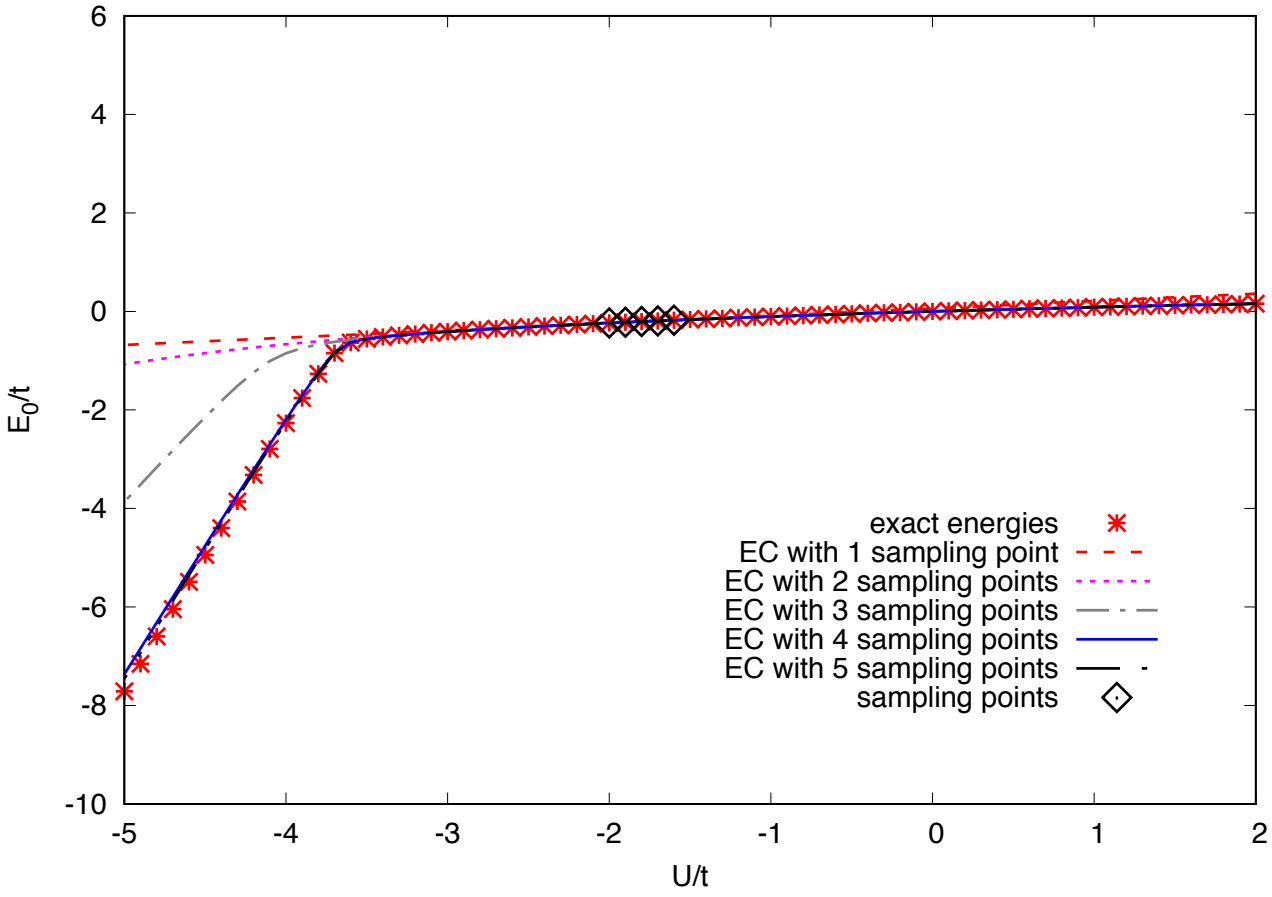
$$|\psi_0(c)\rangle \approx \sum_{k=1,\cdots N} b_k(c)|\psi_0(c_k)\rangle$$

We consider four bosons on a three-dimensional lattice with equal masses and zero-range attractive interactions with kinetic energy coefficient t and coupling U.

Perturbation theory



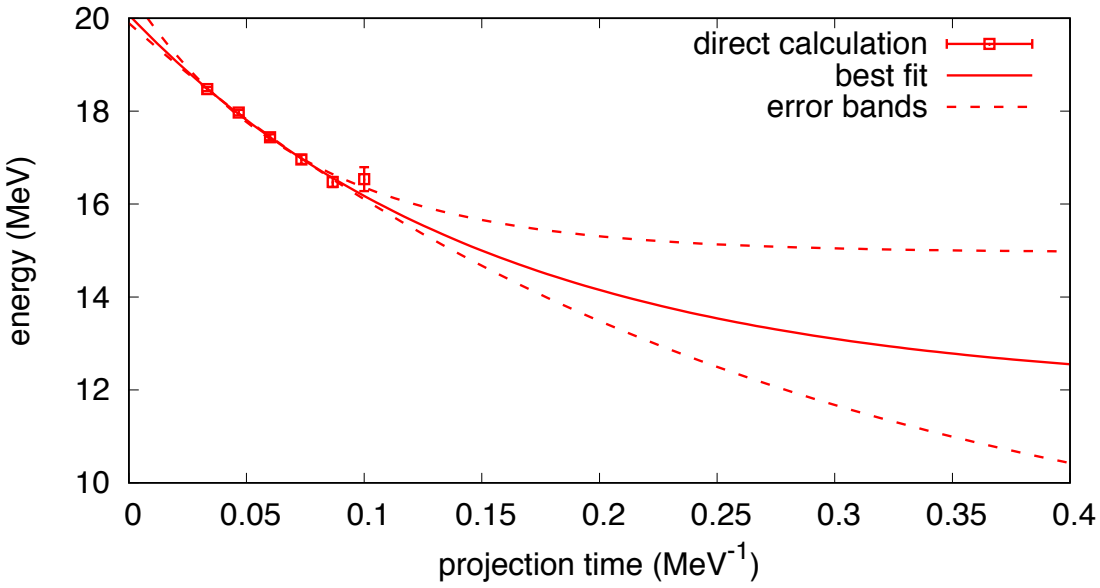
Eigenvector continuation



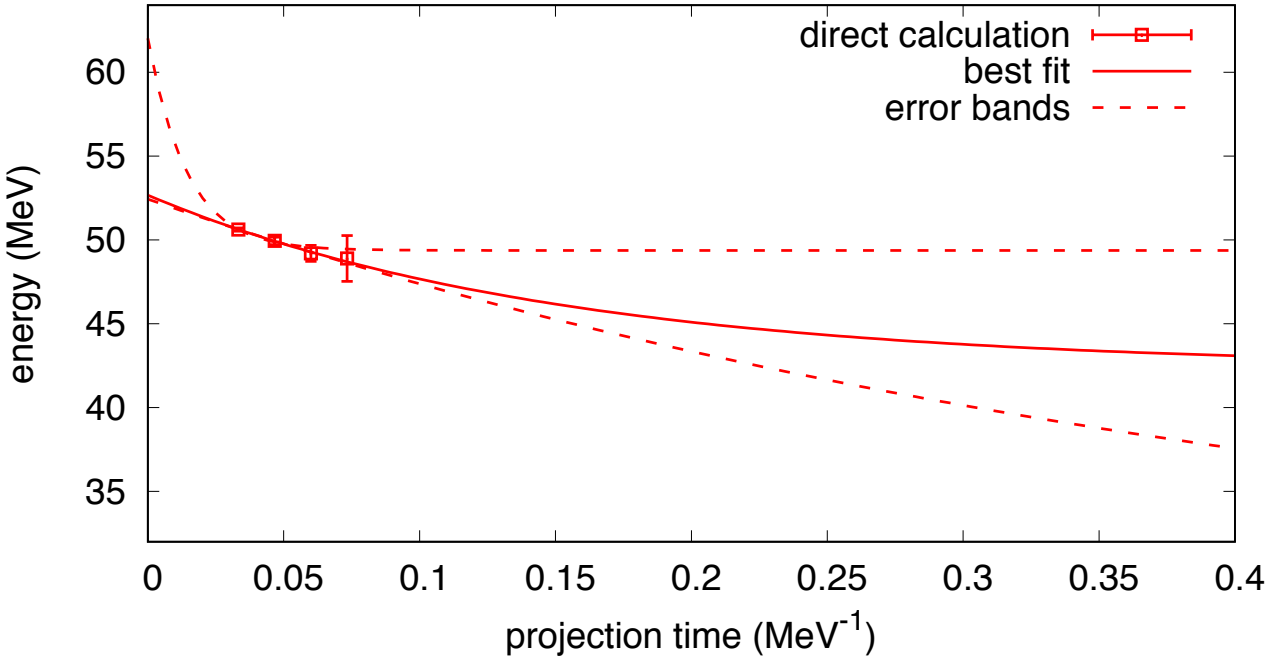
Neutron matter using a difficult lattice action*

*D.L., in "An Advanced Course in Computational Nuclear Physics", Lecture Notes in Physics, Volume 936, arXiv:1609.00421

Six neutrons ($L = 8$ fm)

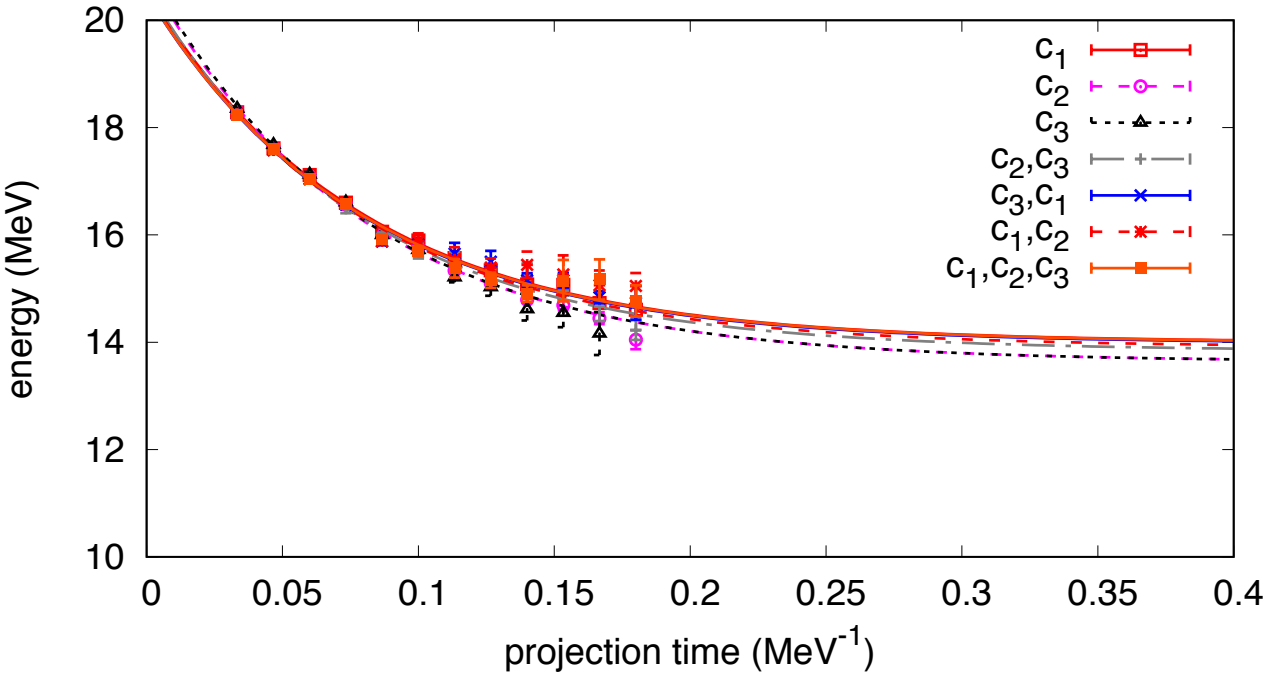


Fourteen neutrons ($L = 8$ fm)



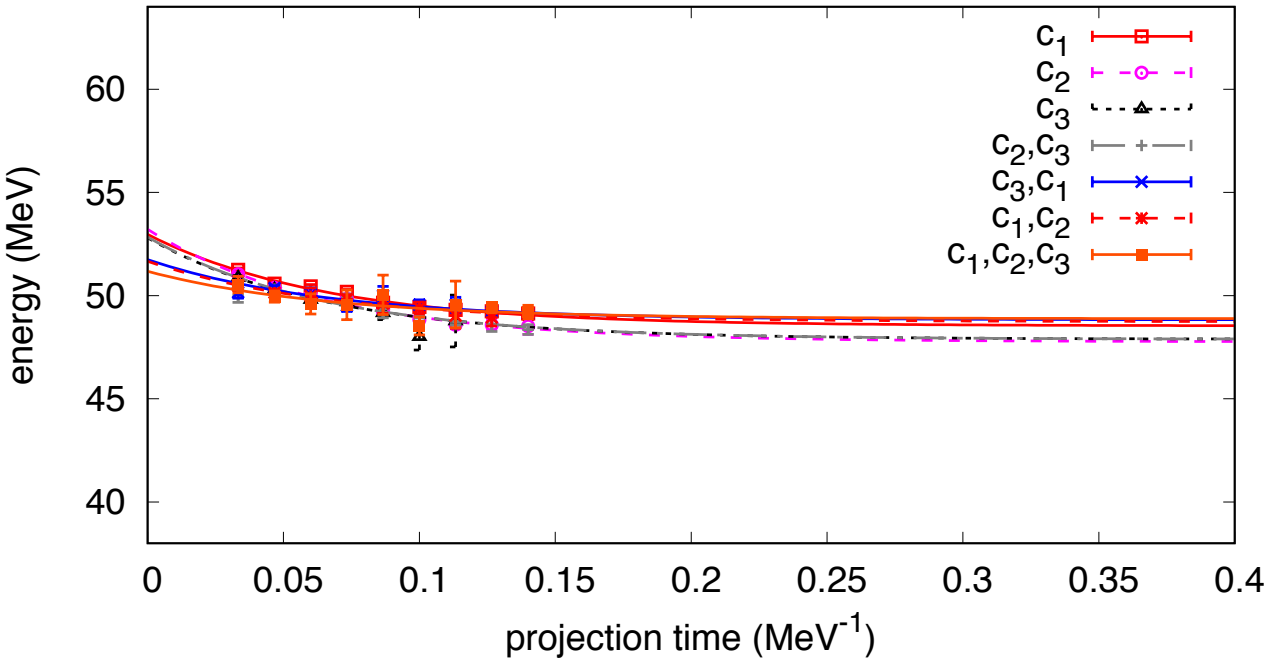
Eigenvector continuation results

Six neutrons ($L = 8$ fm)



Eigenvector continuation results

Fourteen neutrons ($L = 8$ fm)



g_A^2 values	E_0 for six neutrons (MeV)	E_0 for fourteen neutrons (MeV)
c_1	14.0(2)	48.5(5)
c_2	13.6(2)	47.8(5)
c_3	13.6(2)	47.9(5)
c_2, c_3	13.8(2)	47.9(5)
c_3, c_1	14.0(2)	48.9(5)
c_1, c_2	13.9(2)	48.7(5)
c_1, c_2, c_3	14.0(2)	48.9(5)
direct calculation	$12(^{+3}_{-4})$	$42(^{+7}_{-15})$

Frame, He, Ipsen, Lee, D.L., Rrapaj, in progress

Summary and Outlook

These are exciting times for *ab initio* nuclear theory with progress by many groups using many different methods. With nuclear lattice simulations, we now have several projects in motion that are pushing the frontiers of first-principles nuclear structure and reaction theory.