Review of lattice EFT methods and connections to lattice QCD

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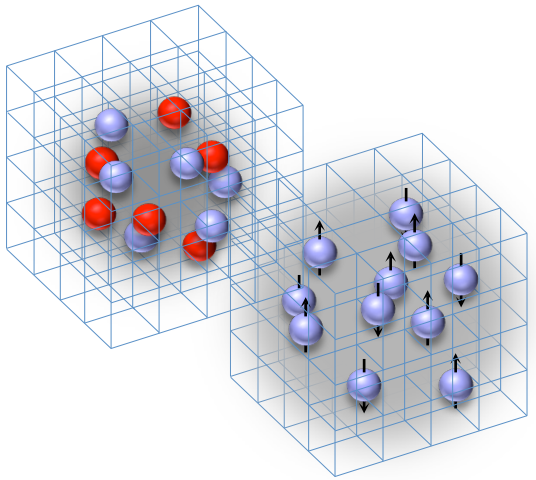
Nuclear Lattice EFT Collaboration

Multi-Hadron Systems from Lattice QCD
Institute for Nuclear Theory
Feburary 7, 2018



Outline

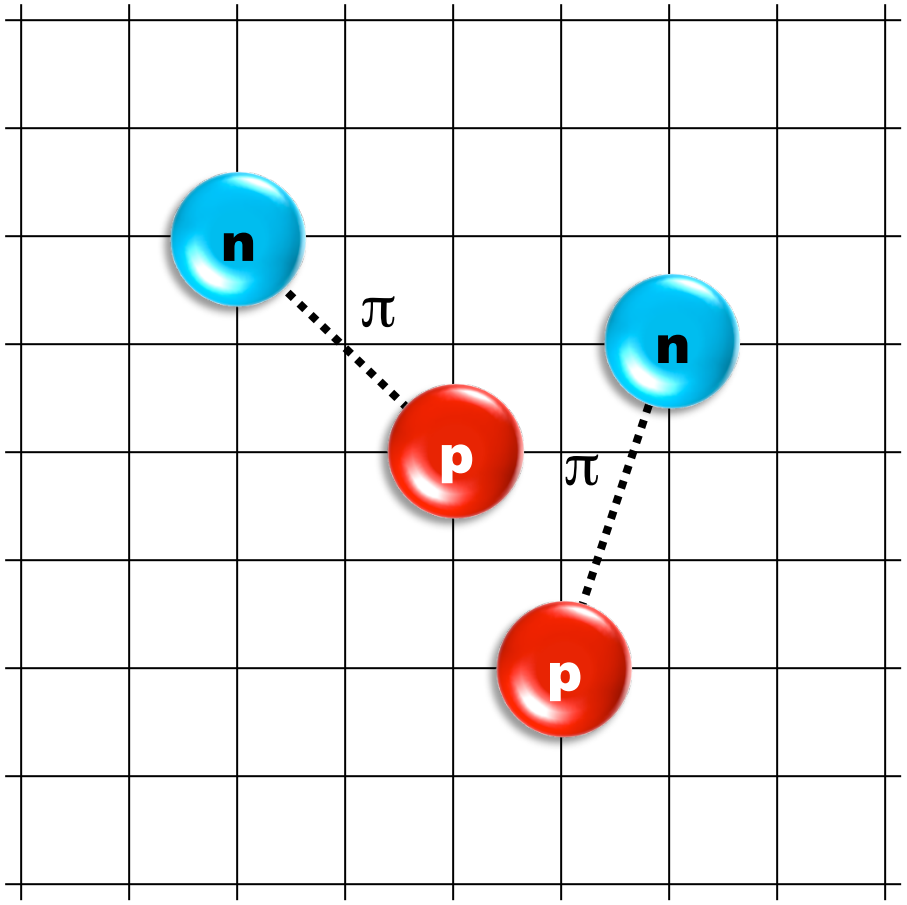
Lattice effective field theory

Adiabatic projection method

Eigenvector continuation

Summary and outlook

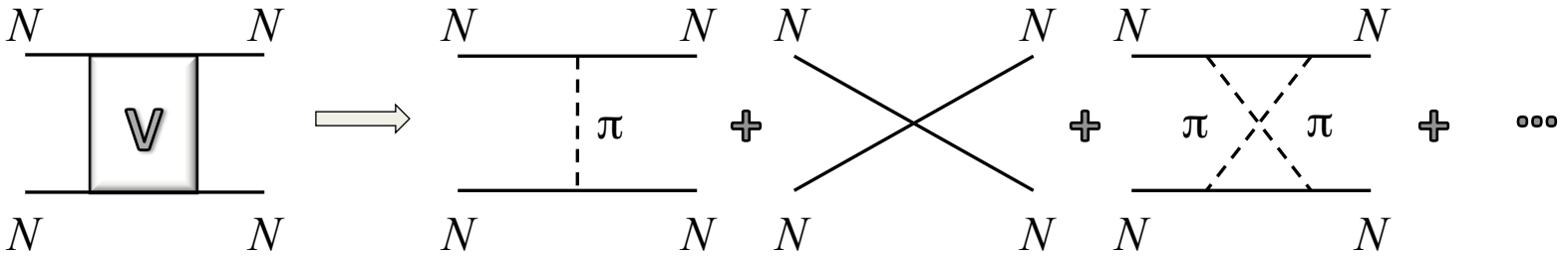
Lattice chiral effective field theory



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

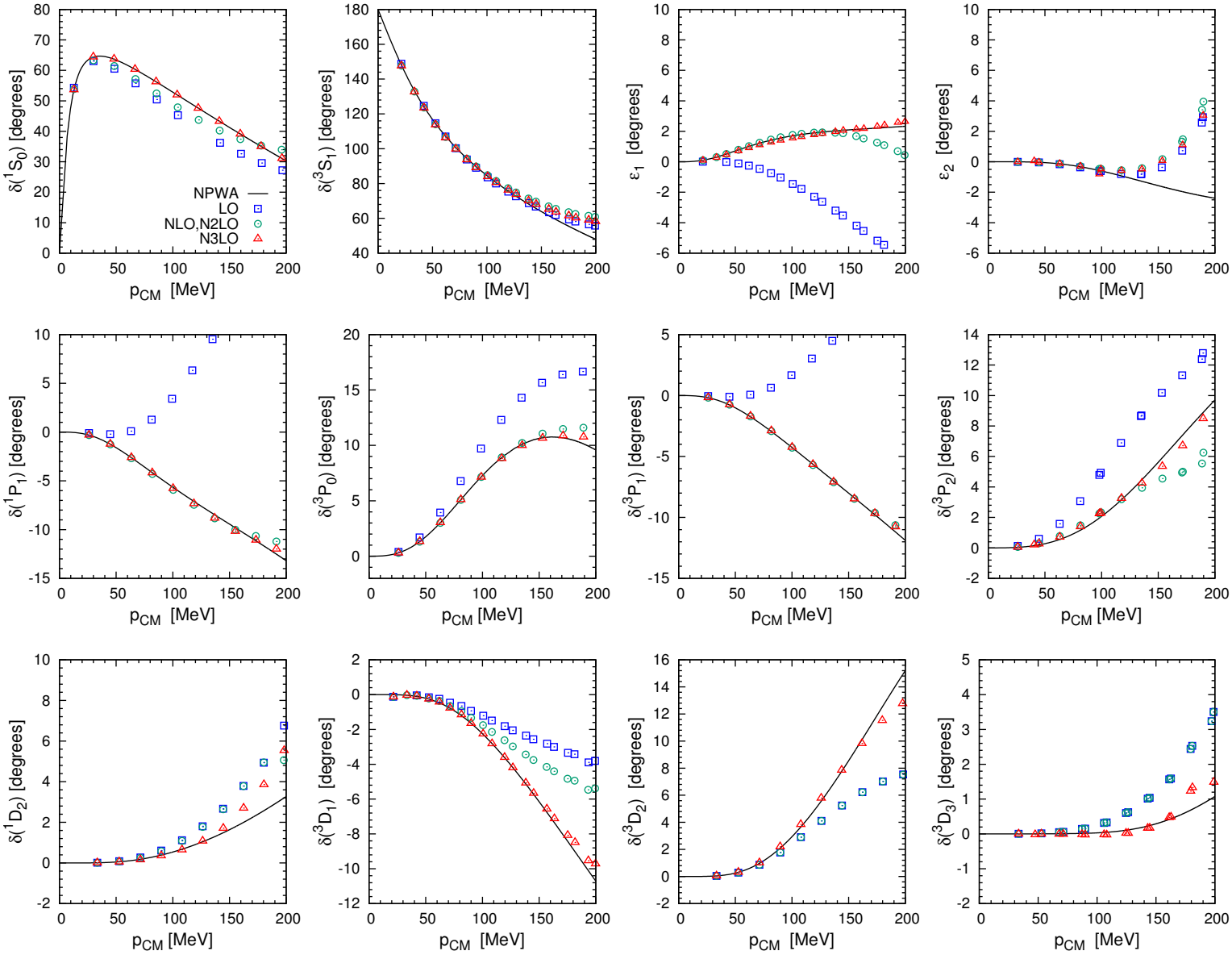
Chiral effective field theory

Construct the effective potential order by order

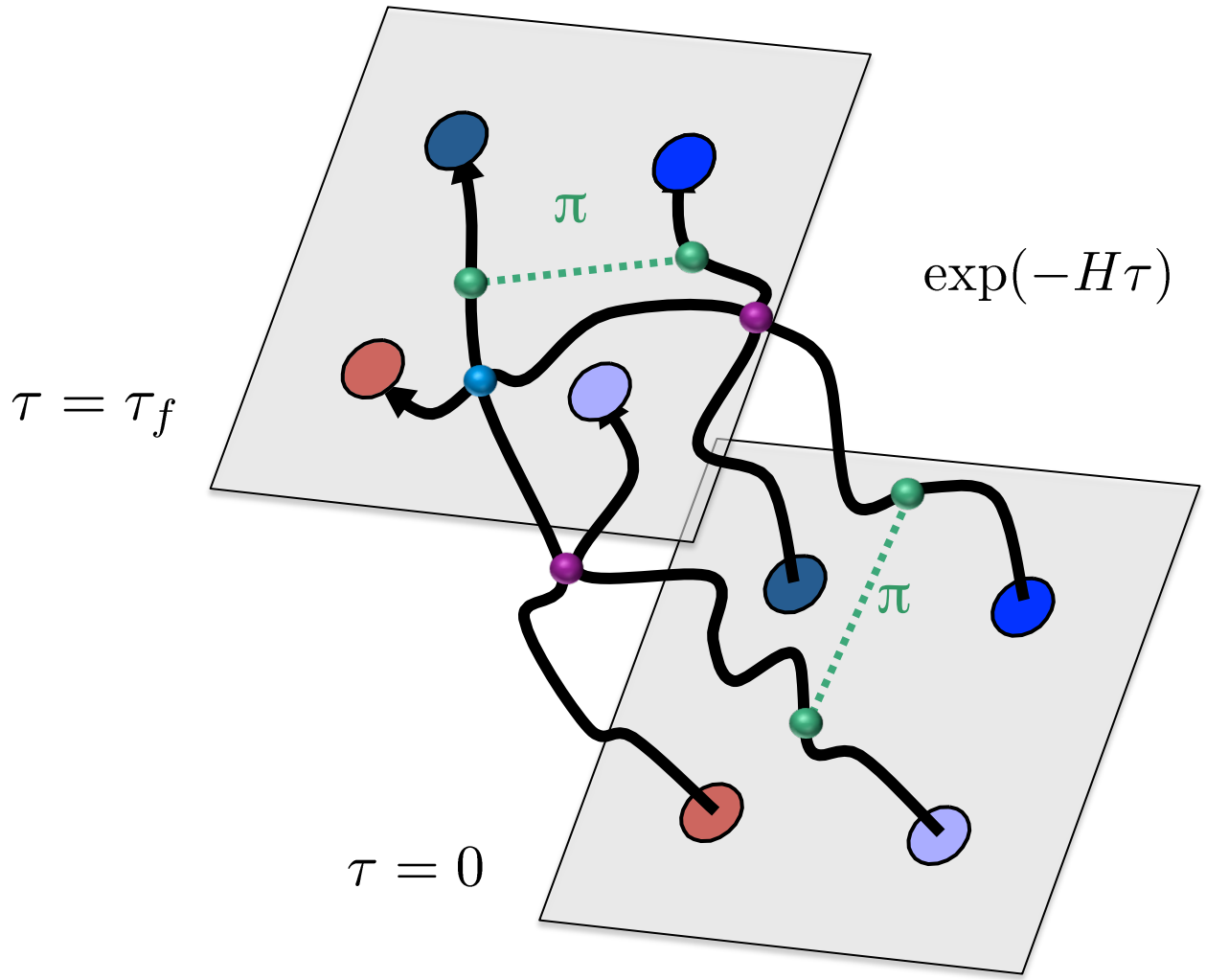


V^{OPEP} Contact interactions V^{TPEP}

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


δ(1S0) [degrees]
δ(3S1) [degrees]
ε1 [degrees]
ε2 [degrees]
δ(1P1) [degrees]
δ(3P0) [degrees]
δ(3P1) [degrees]
δ(3P2) [degrees]
δ(1D2) [degrees]
δ(3D1) [degrees]
δ(3D2) [degrees]
δ(3D3) [degrees]
pCM [MeV]
NPWA
LO
NLO,N2LO
N3LO

Euclidean time projection



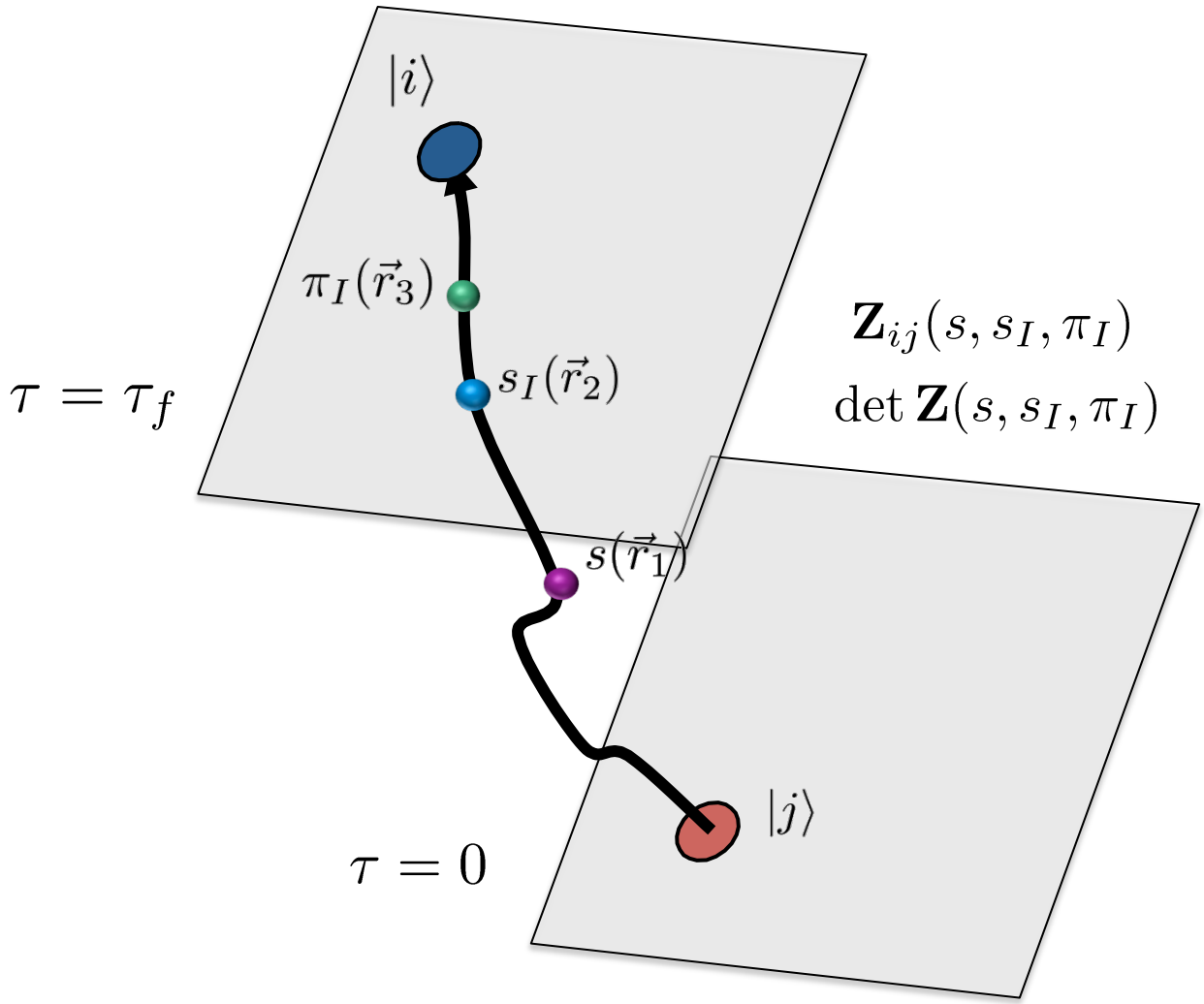
Auxiliary field method

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.


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

Science objectives

Want *ab initio* calculations of scattering and reactions relevant to alpha processes in stellar evolution and Type Ia supernovae

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$

$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma$

$^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma$

$^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma$

$^{20}\mathrm{Ne} + {}^4\mathrm{He} \rightarrow {}^{24}\mathrm{Mg} + \gamma$

$^{24}\mathrm{Mg} + {}^4\mathrm{He} \rightarrow {}^{28}\mathrm{Si} + \gamma$

$^{12}\mathrm{C} + {}^{12}\mathrm{C} \rightarrow {}^{20}\mathrm{Ne} + {}^4\mathrm{He}$

$^{16}\mathrm{O} + {}^{16}\mathrm{O} \rightarrow {}^{28}\mathrm{Si} + {}^4\mathrm{He}$

Challenge

How to reduce the computational scaling of the calculations with number of nucleons?

Adiabatic projection method

The adiabatic projection method is a first principles method for scattering and reactions. It computes enough scattering information from Monte Carlo simulations to construct an effective Hamiltonian.

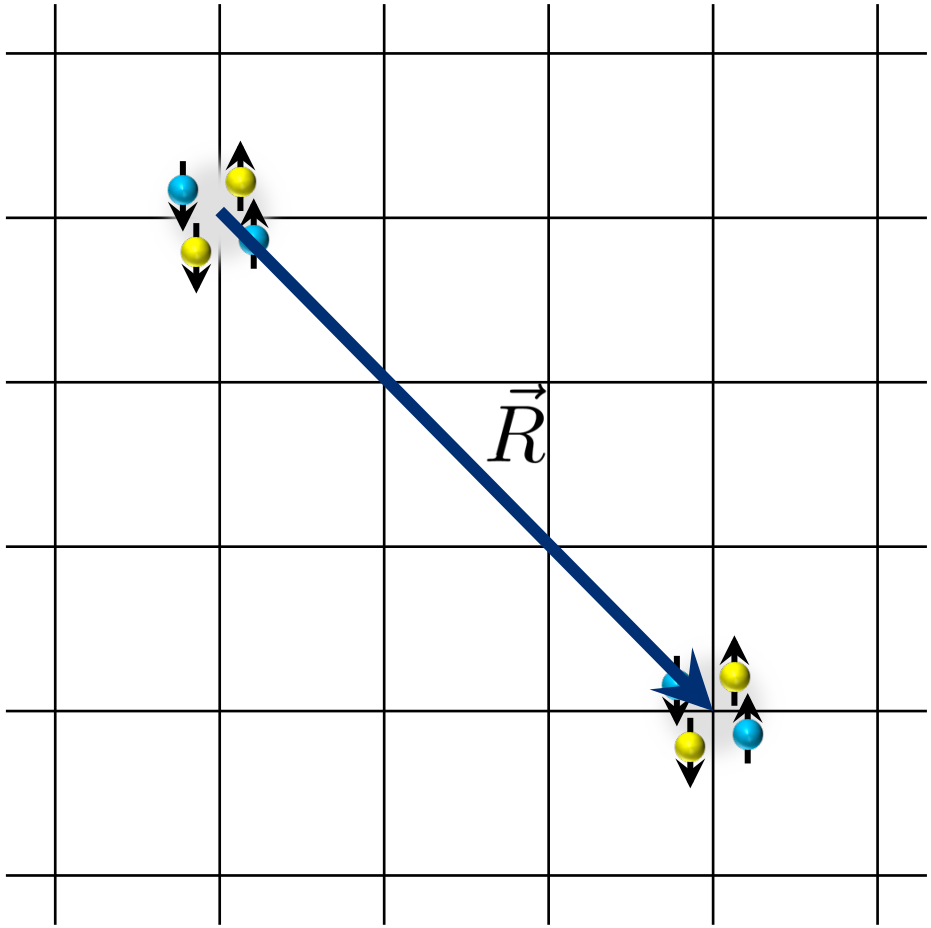
Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian.

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

Computational scaling is roughly quadratic in the number of nucleons.

Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Use projection Monte Carlo to propagate cluster wave functions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

We then evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

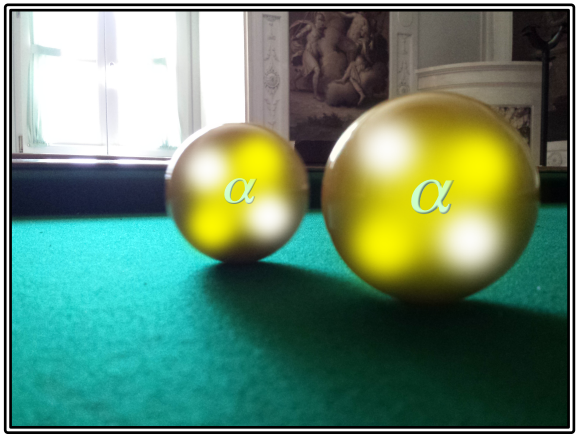
$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

We now treat the adiabatic Hamiltonian as an effective two-particle Hamiltonian for scattering and reaction calculations.

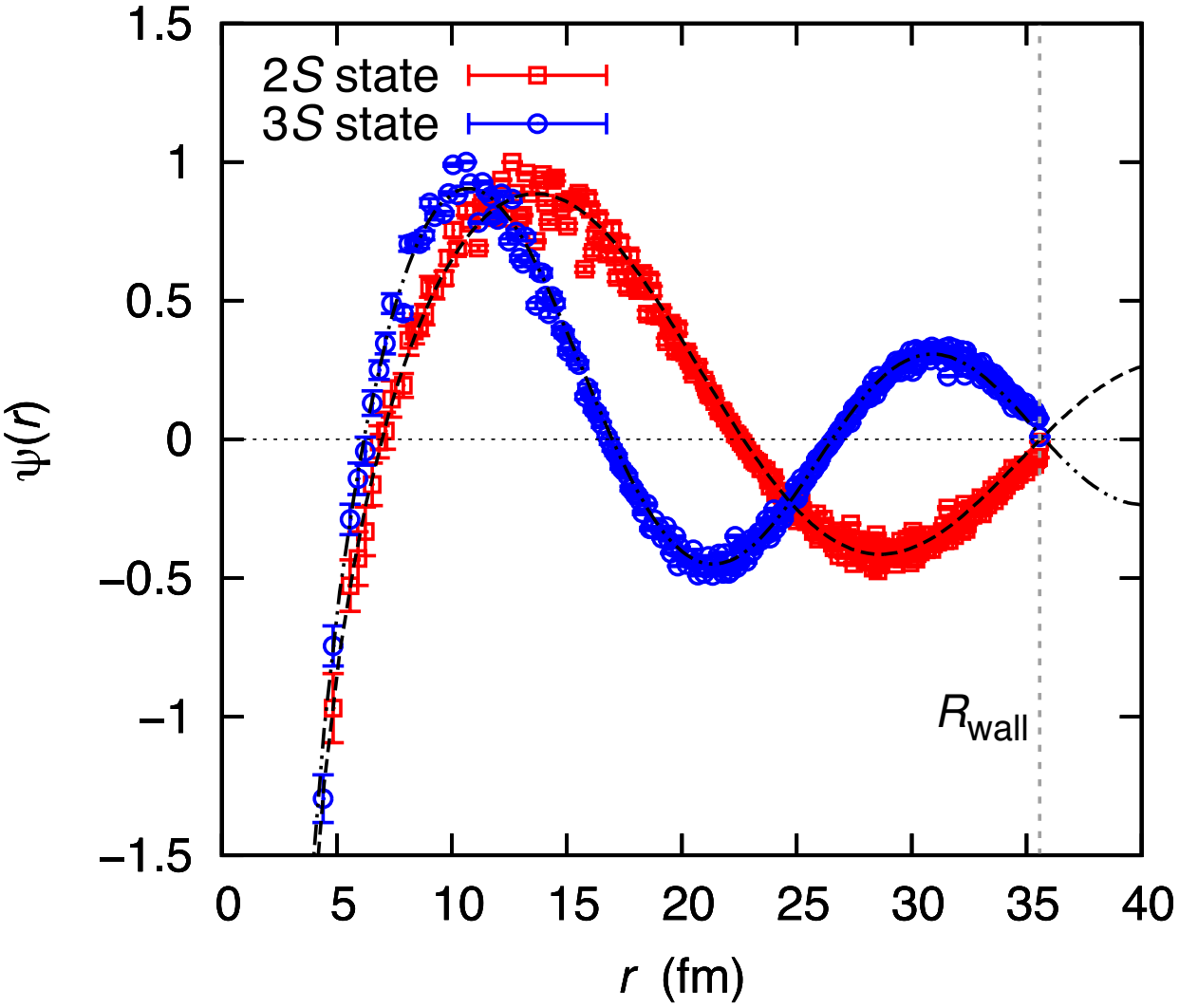
$$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$$



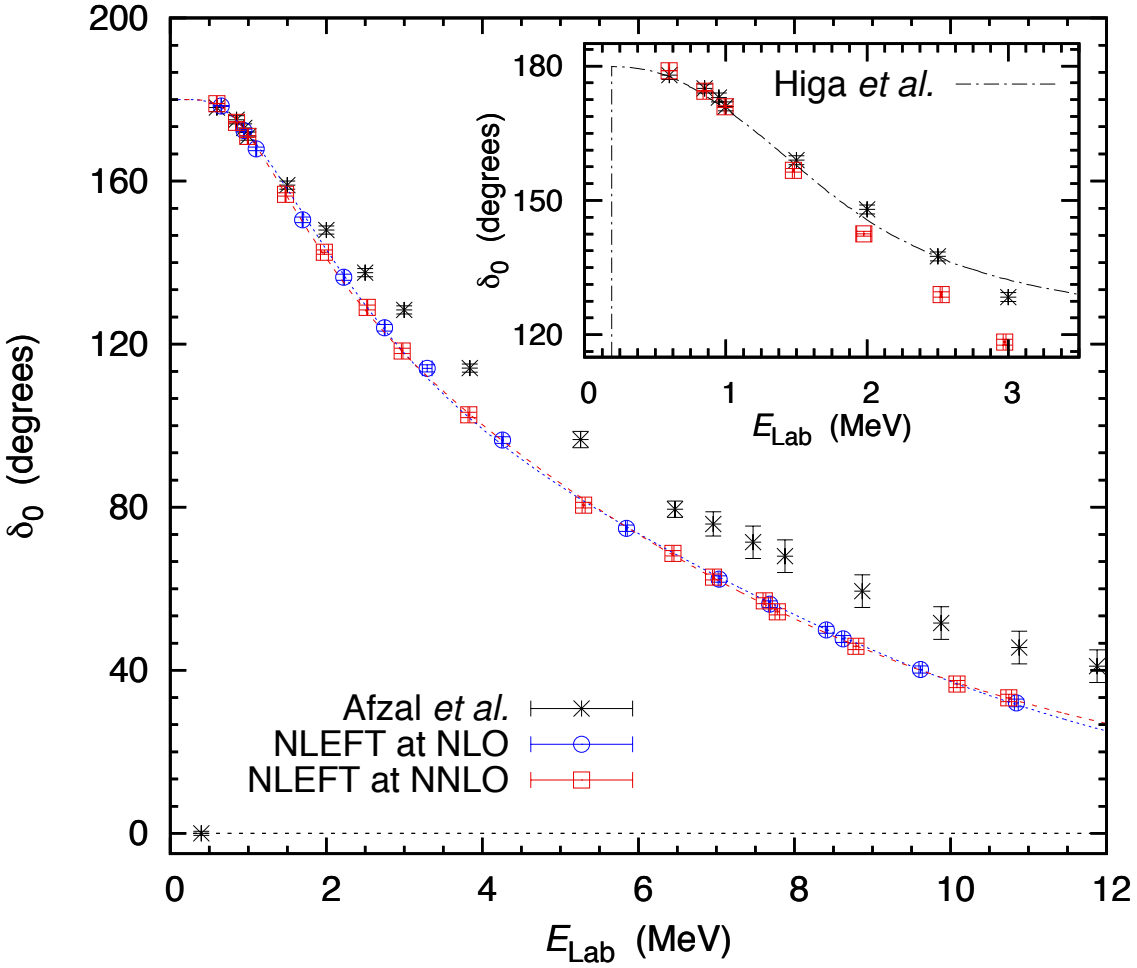
Ab initio results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the *S*-wave and *D*-wave channels.

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

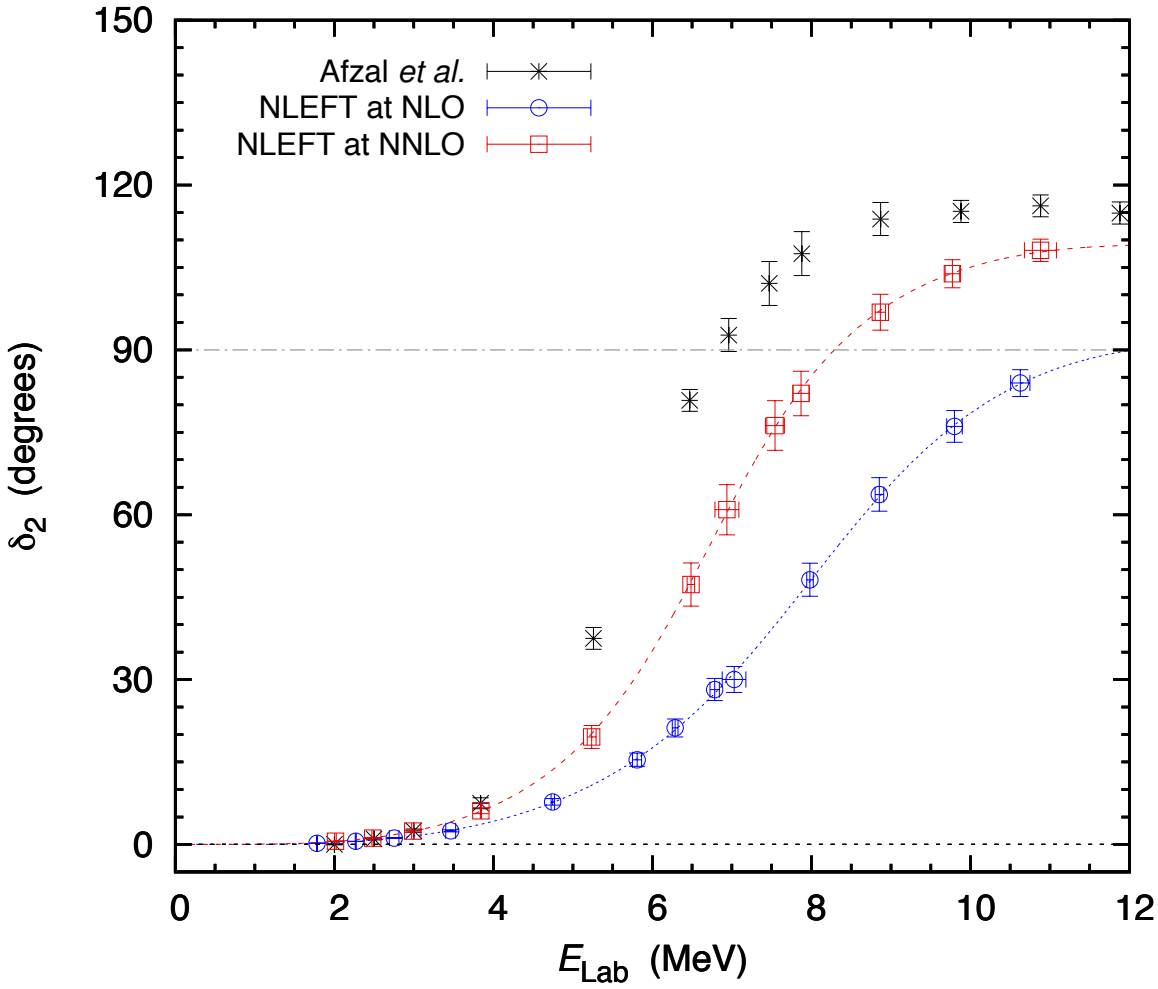
$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$



Challenge

A common challenge faced in many fields of quantum physics is finding the extremal eigenvalues and eigenvectors of a Hamiltonian matrix too large to store in computer memory.

There are numerous efficient methods developed for this task. All existing methods either use Monte Carlo simulations, diagrammatic expansions, variational methods, or some combination.

The problem is that they generally fail when some control parameter in the Hamiltonian matrix exceeds some threshold value.

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

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

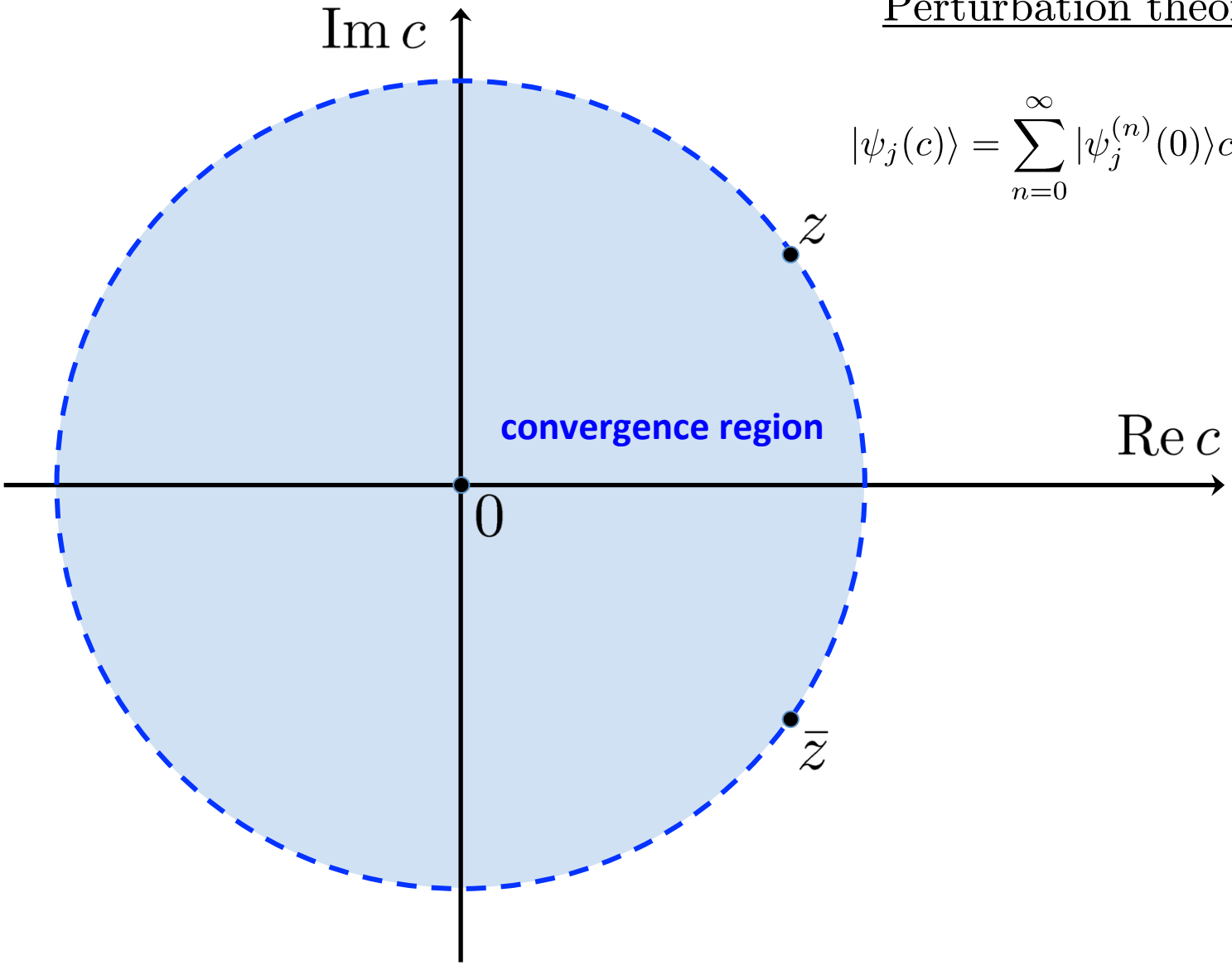
We can perform series expansions around the point $c = 0$.

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

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

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.

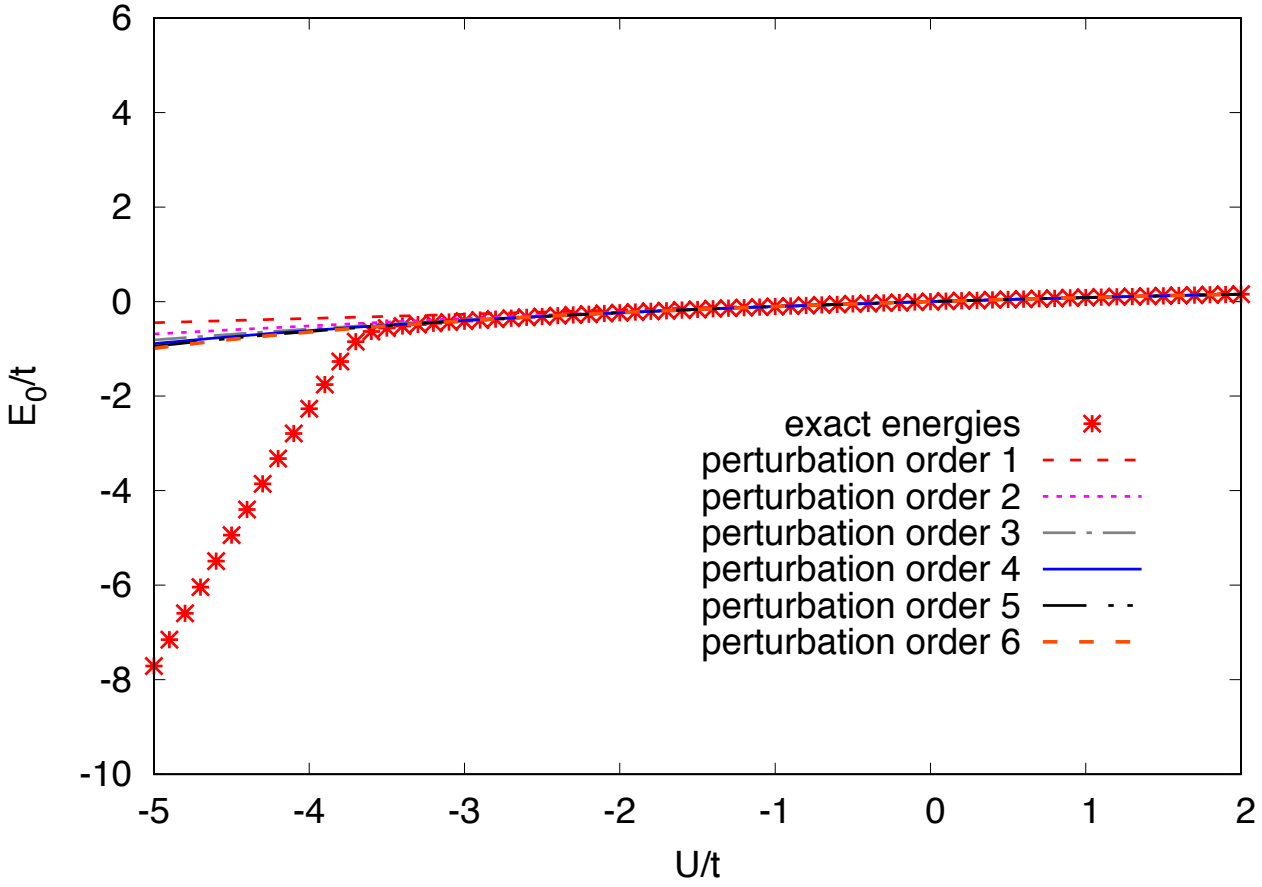
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

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

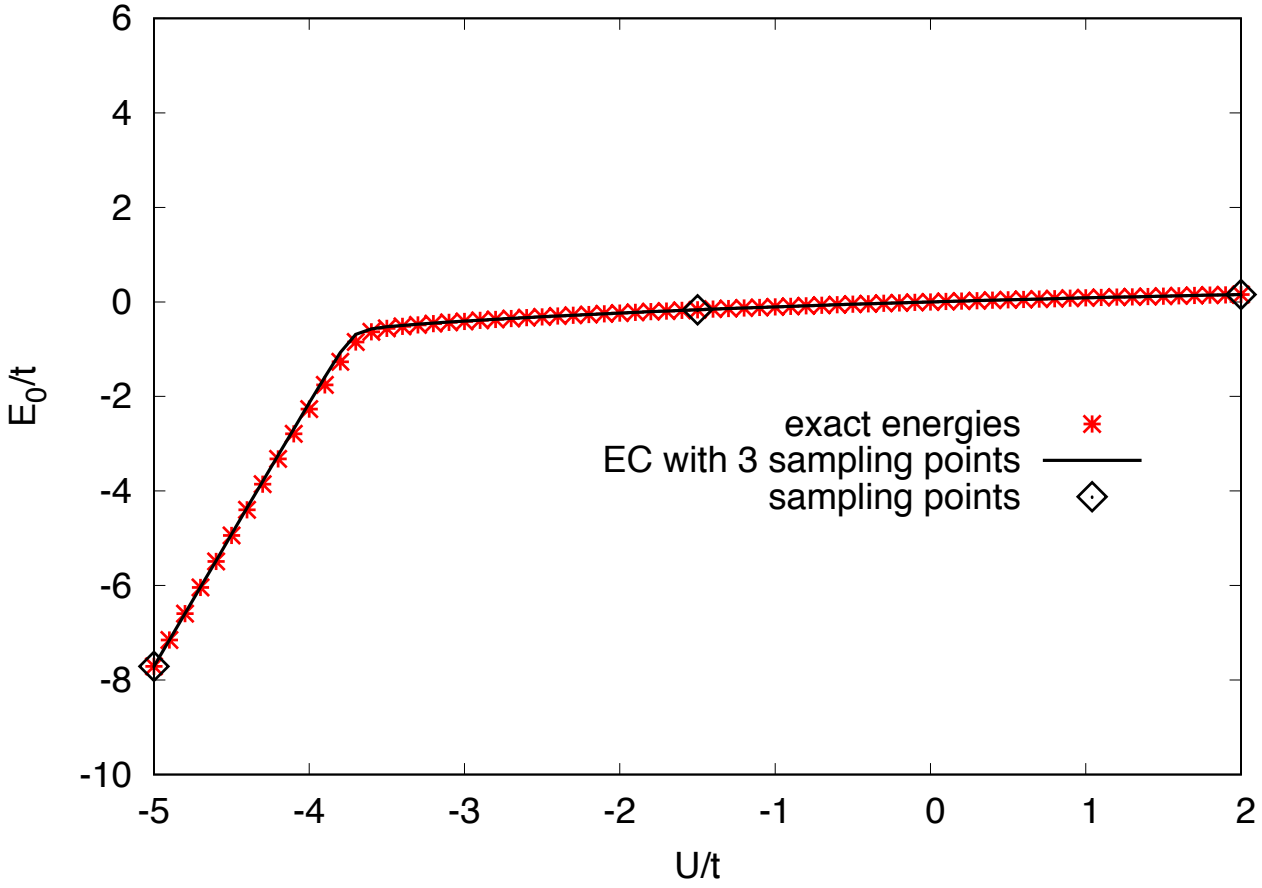
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

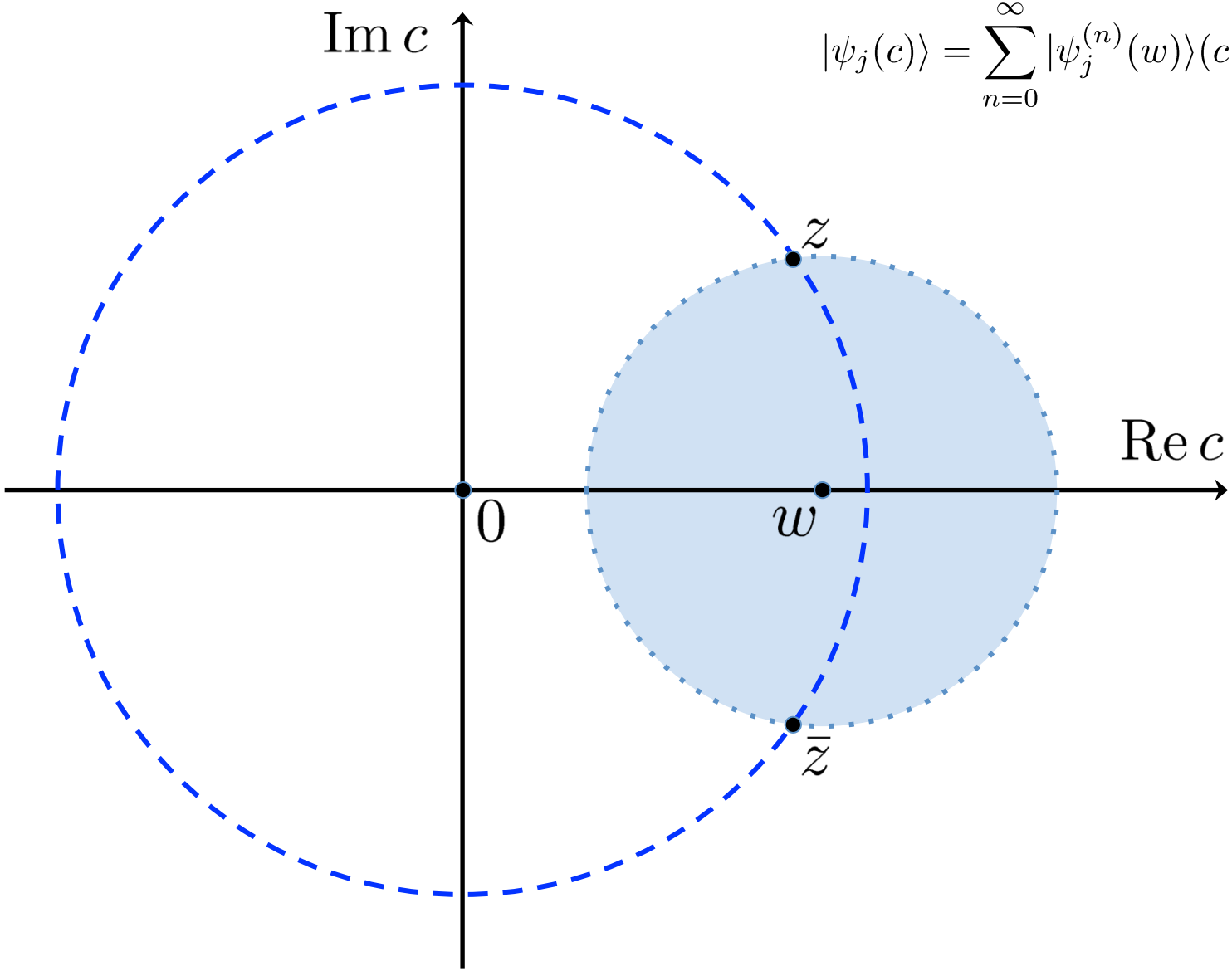
Perturbation theory fails at strong attractive coupling

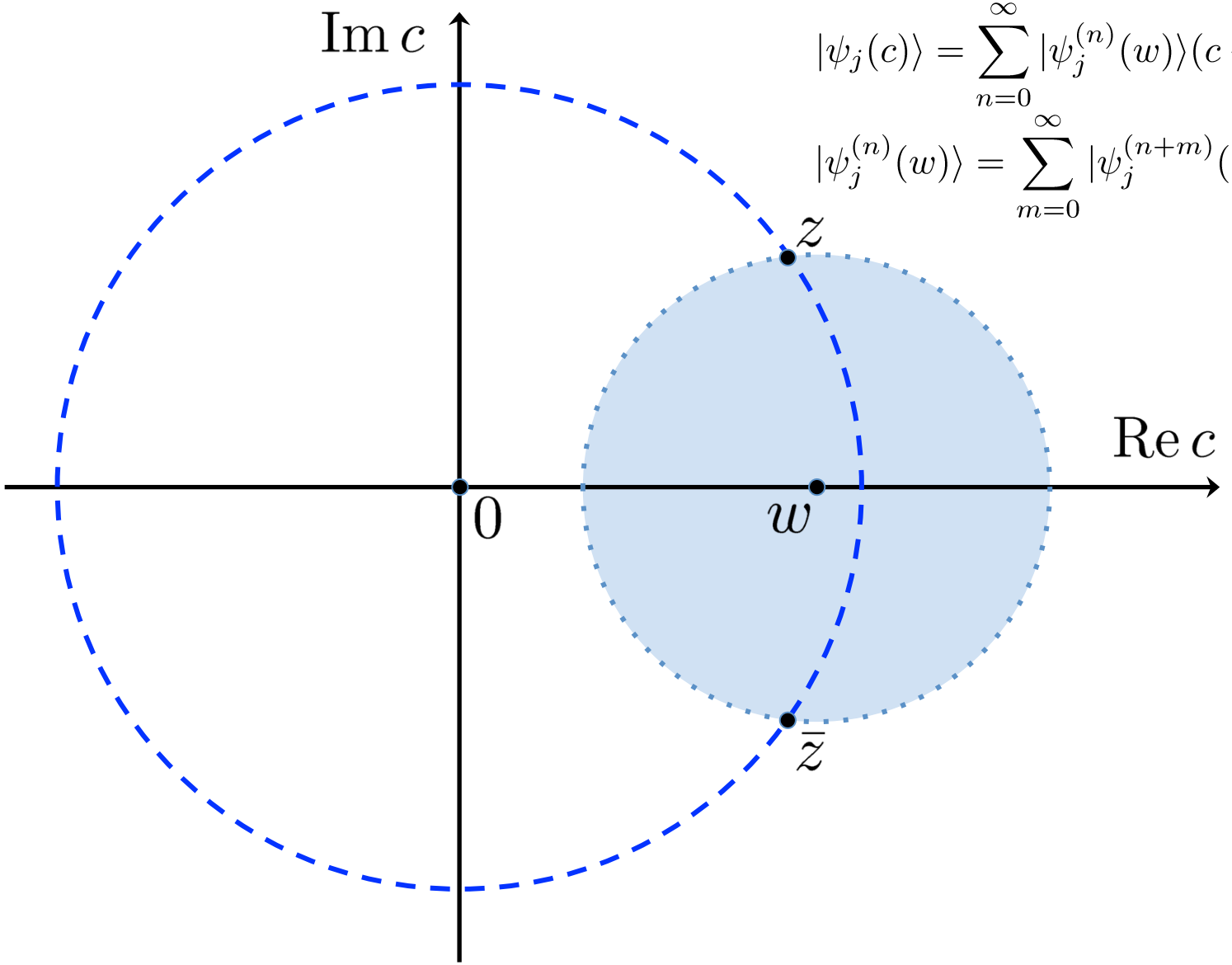


Restrict the linear space to the span of three vectors



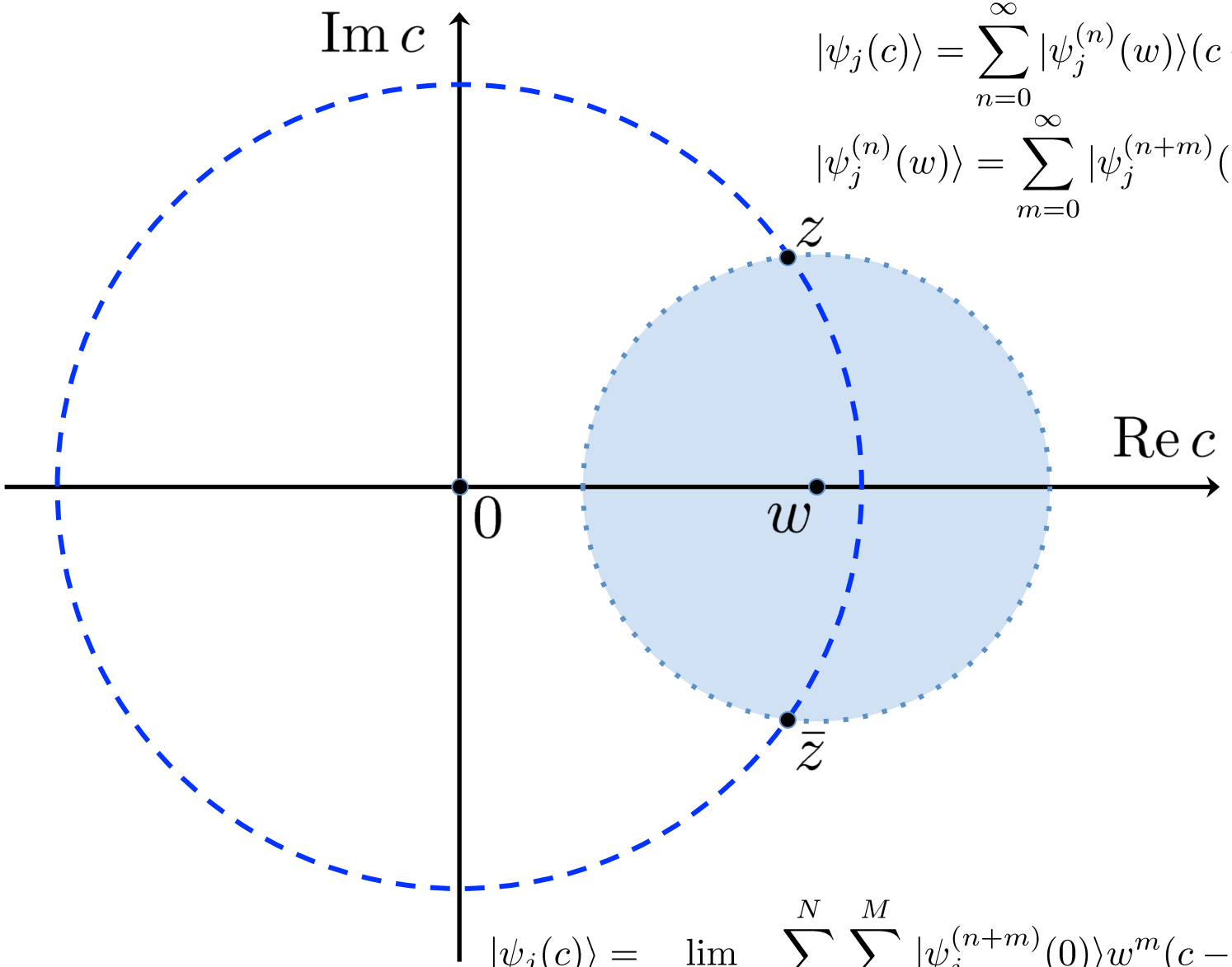
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





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

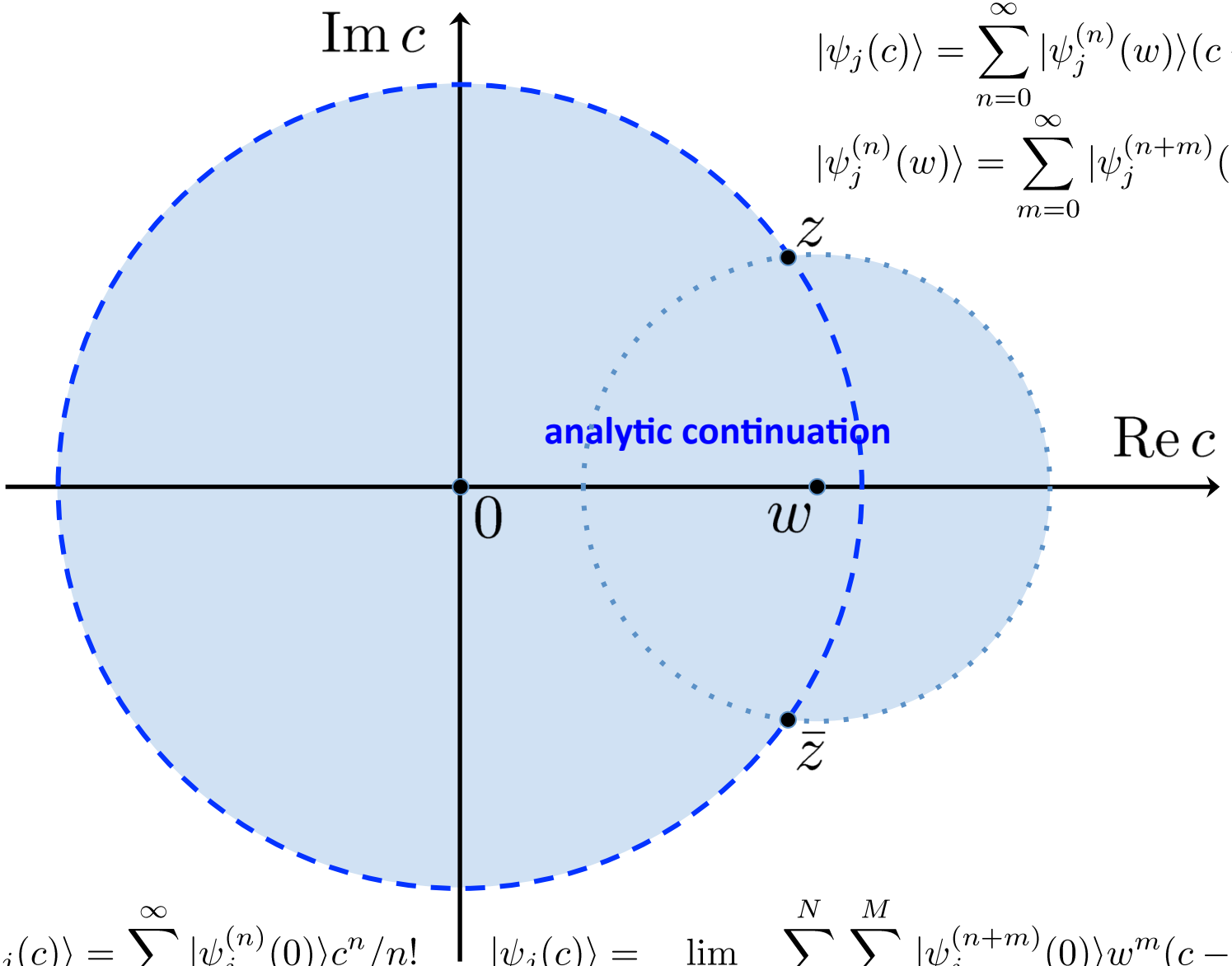
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



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

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

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



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

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

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

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

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

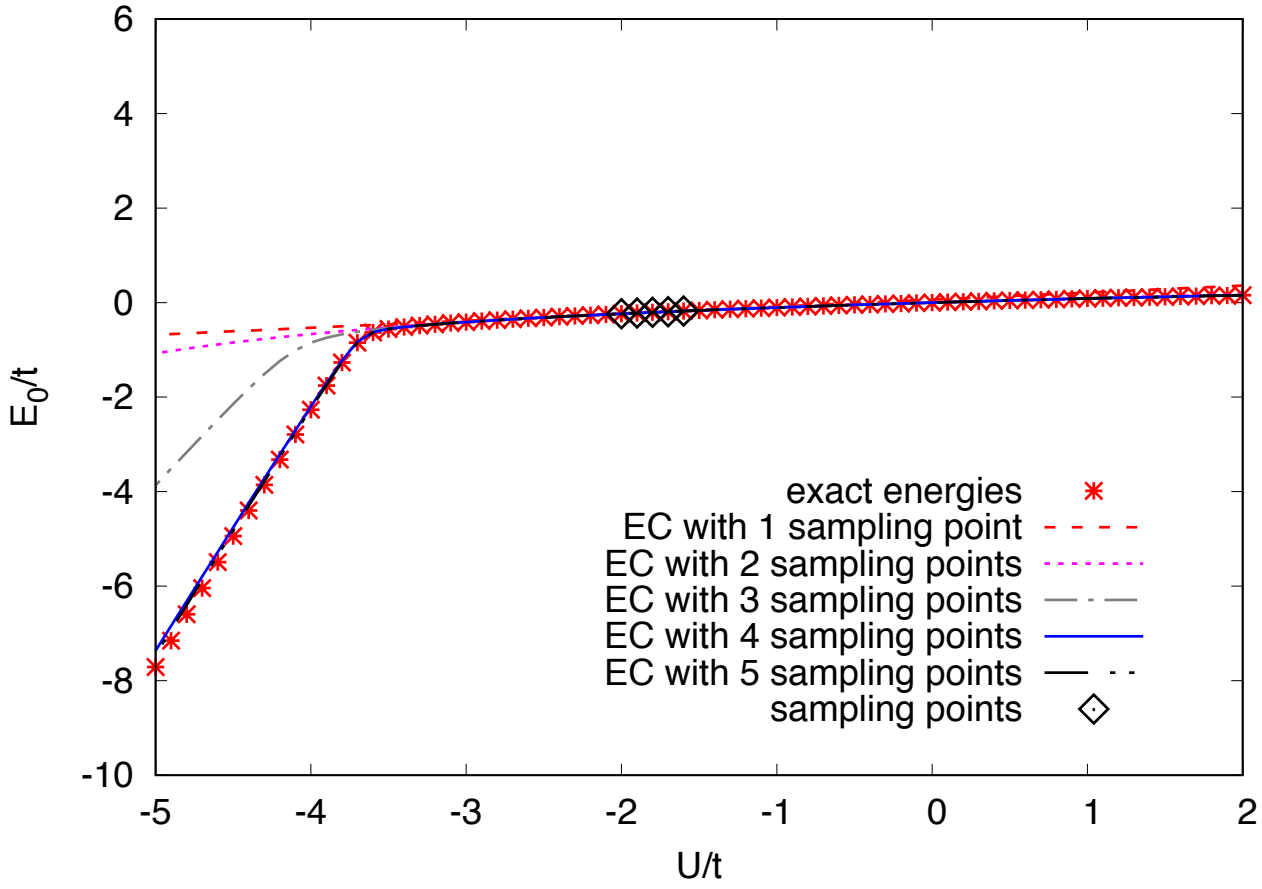
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

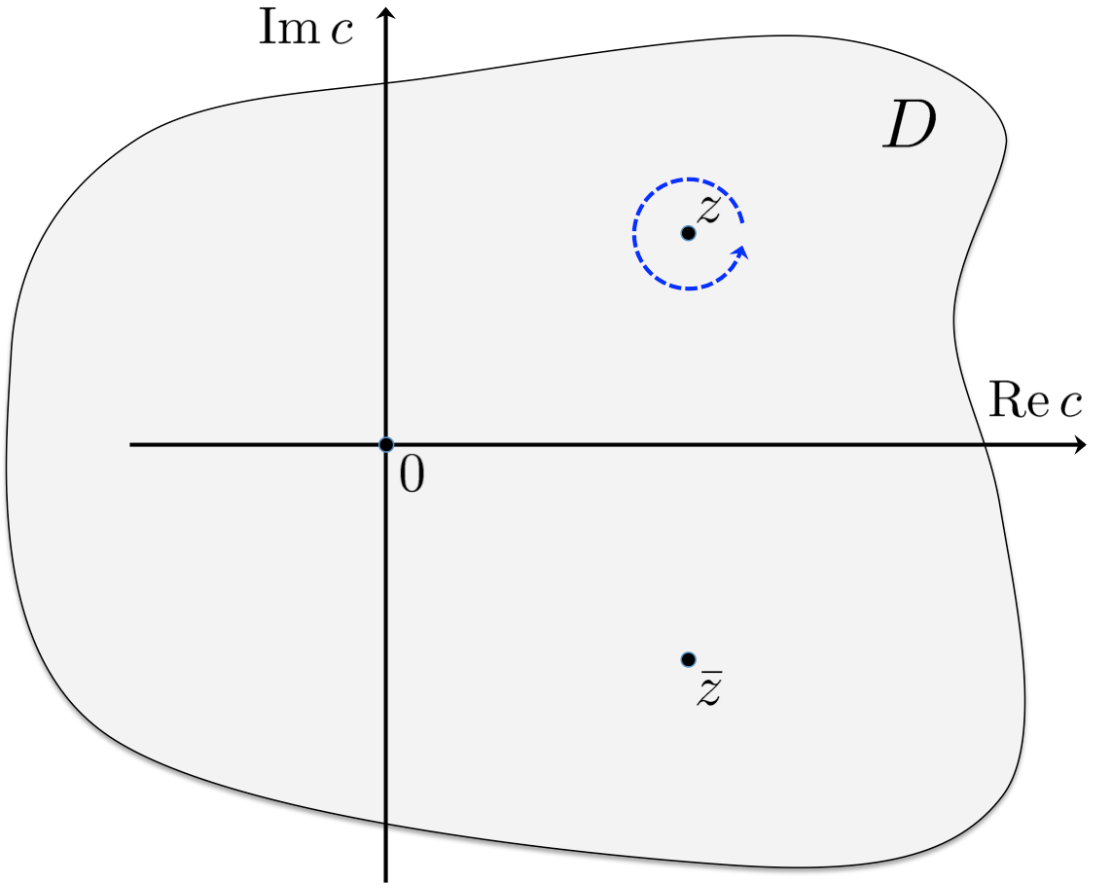
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

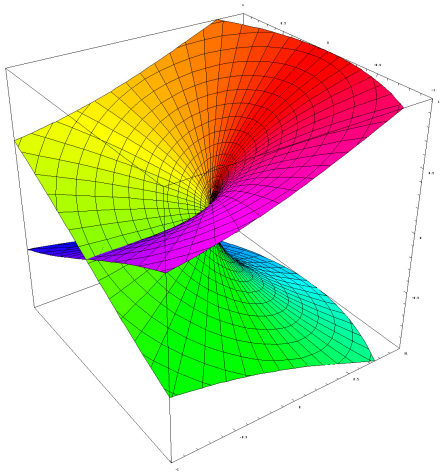
As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

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

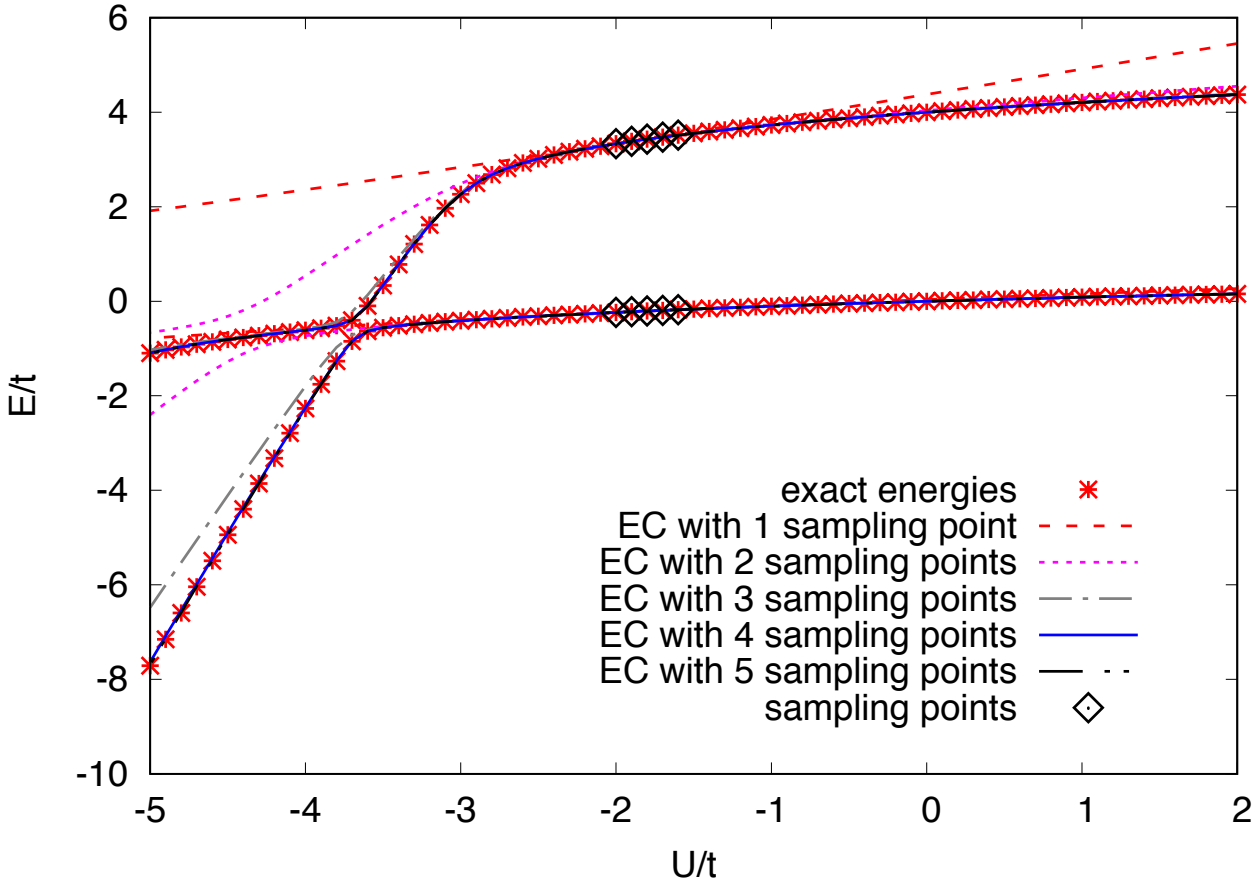


The Riemann surfaces of the degenerate eigenvectors are entwined at branch point singularities.



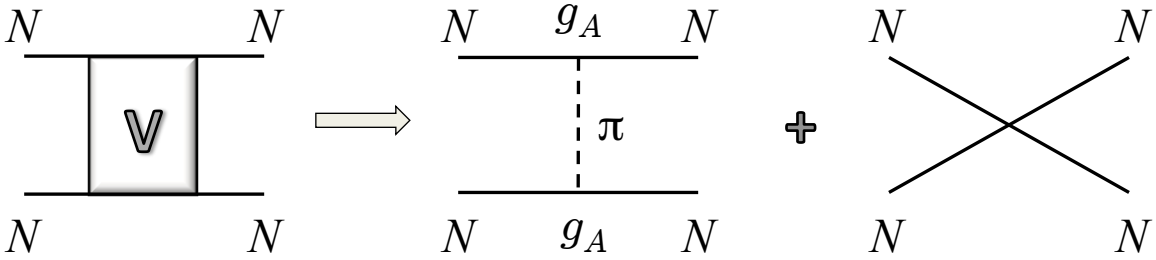


Applying eigenvector continuation to more than one eigenvector at a time accelerates convergence near avoided level crossings.



Application: Neutron matter simulations

We consider lattice effective field theory simulations of the neutron matter at the leading order.

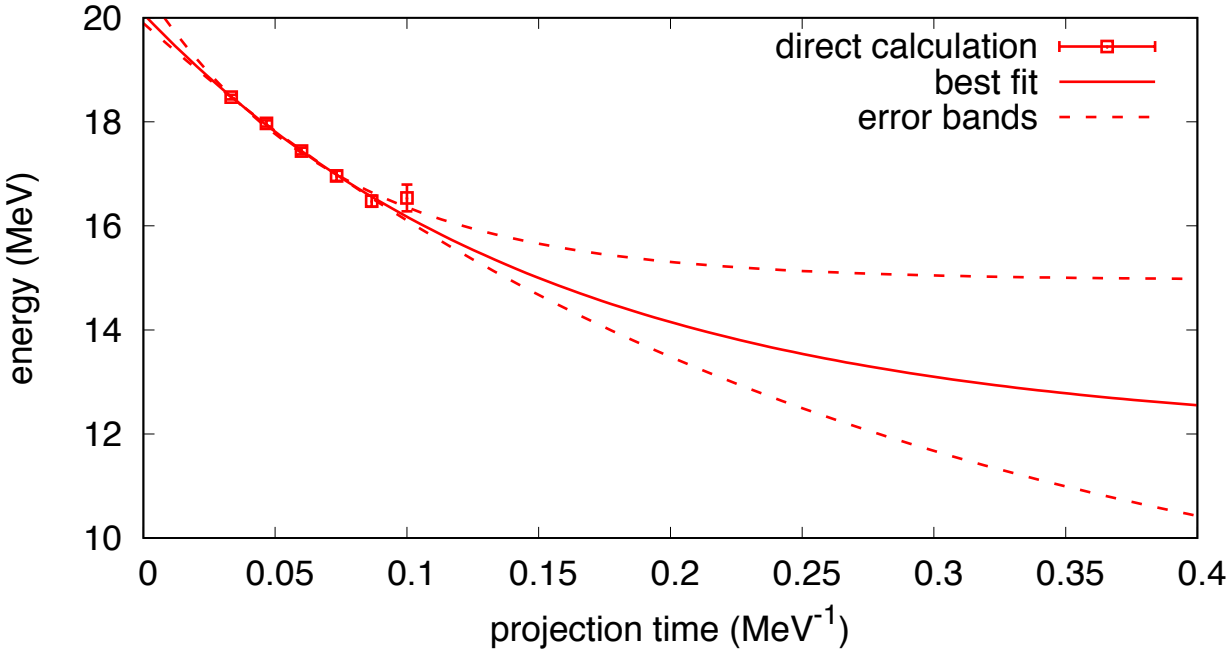


V^{OPEP} Contact interactions

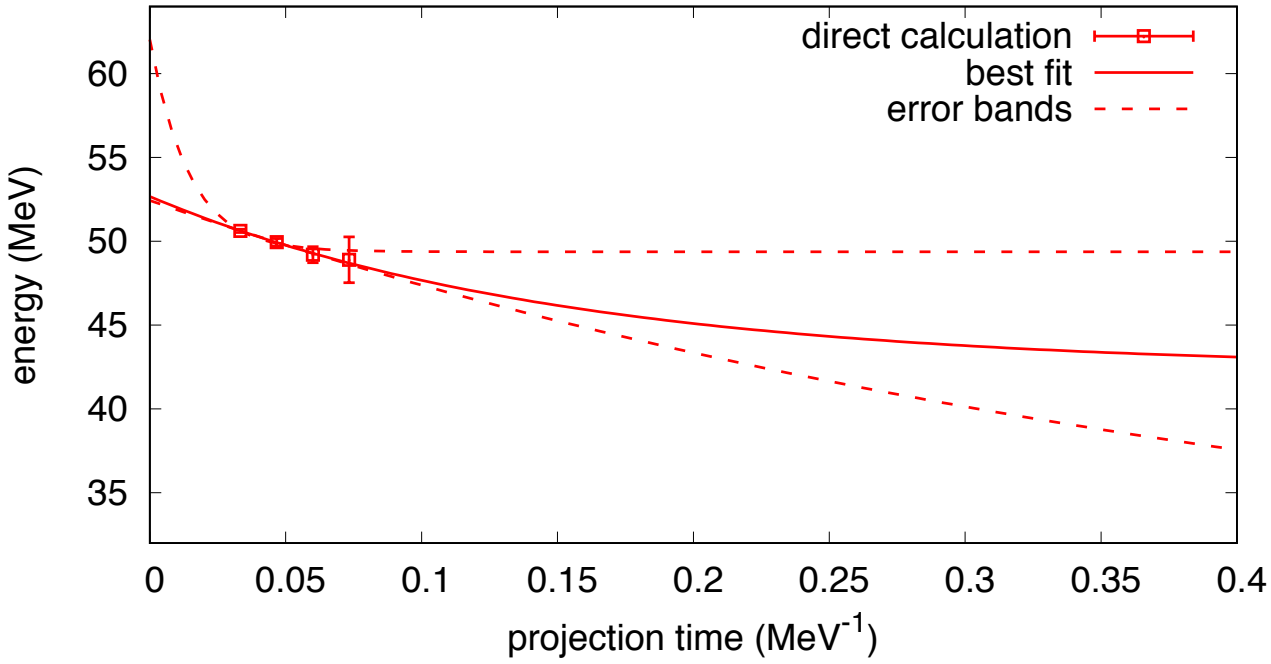
As a challenge to the eigenvector continuation technique, we use a lattice action for one-pion exchange that causes severe Monte Carlo sign oscillations.

D.L., in "An Advanced Course in Computational Nuclear Physics", Hjorth-Jensen, Lombardo, van Kolck, Eds., Lecture Notes in Physics, Volume 936 [arXiv:1609.00421]

Direct calculation of six neutrons ($L = 8$ fm)



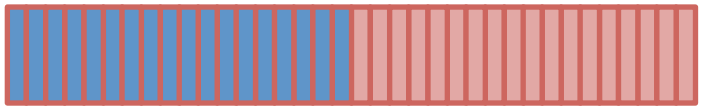
Direct calculation of fourteen neutrons ($L = 8$ fm)



Eigenvector continuation with quantum Monte Carlo

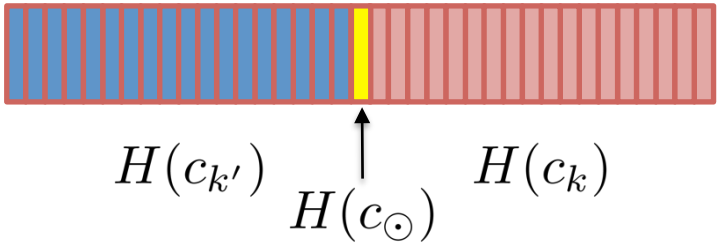
Use Monte Carlo simulations to compute projection amplitudes

$$N_{k',k} = \langle \psi_{\text{init}} |$$



$$|\psi_{\text{init}}\rangle$$

$$H_{k',k} = \langle \psi_{\text{init}} |$$

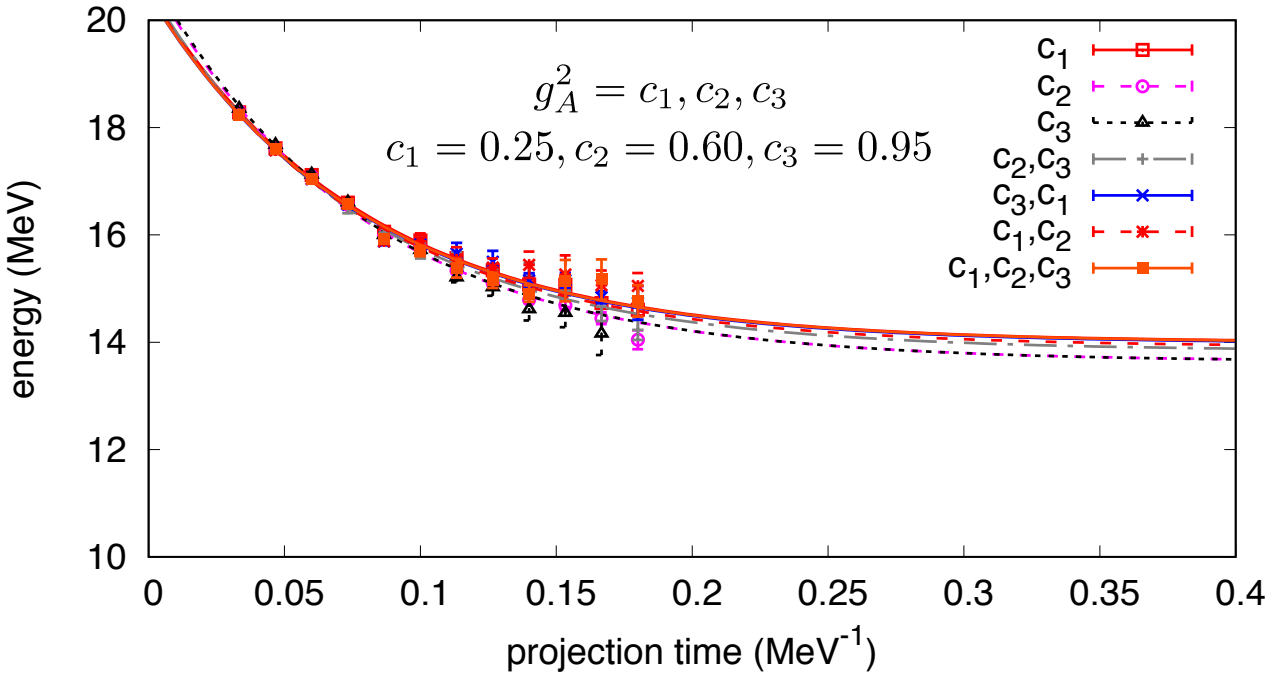


$$|\psi_{\text{init}}\rangle$$

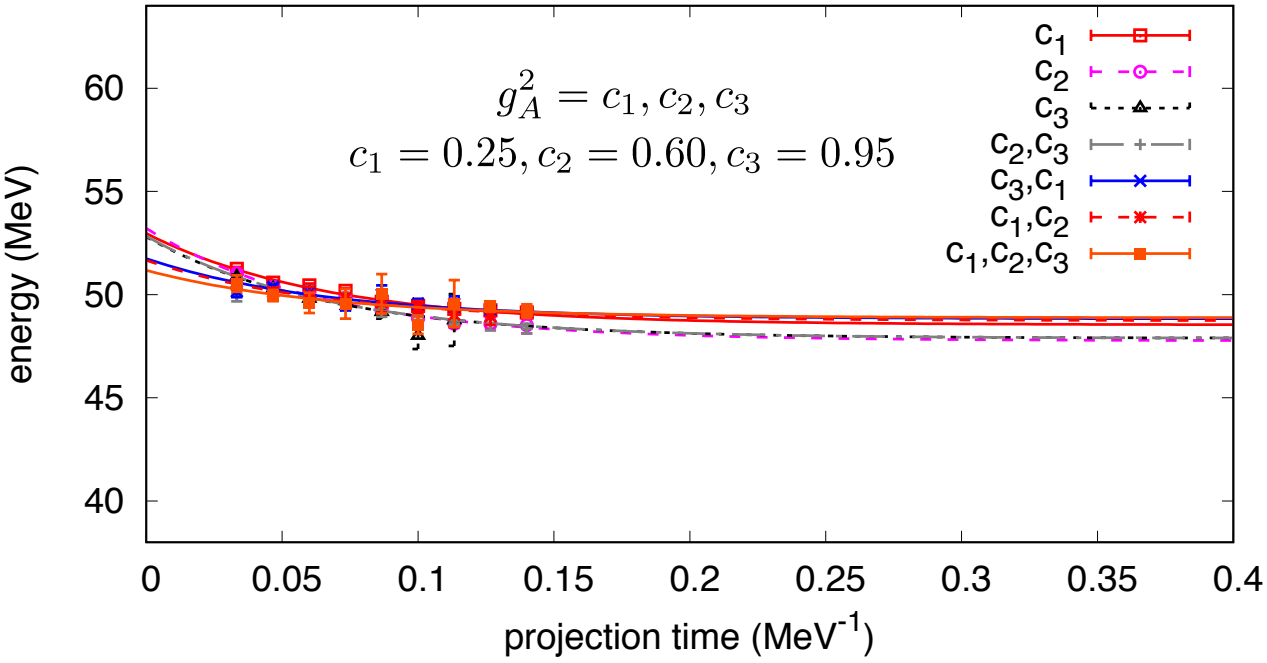
Solve the generalized eigenvalue problem by finding the eigenvalues and eigenvectors of

$$N^{-1/2} H N^{-1/2}$$

Eigenvector continuation for six neutrons ($L = 8$ fm)



Eigenvector continuation for fourteen neutrons ($L = 8$ fm)



g_A^2 values	E_0 for six neutrons (MeV)	E_0 for fourteen neutrons (MeV)
c_1	13.8(1)	48.9(4)
c_2	13.6(2)	48.4(5)
c_3	13.6(2)	48.9(6)
c_2, c_3	13.6(2)	48.1(6)
c_3, c_1	13.6(2)	48.9(6)
c_1, c_2	13.6(2)	48.0(6)
c_1, c_2, c_3	13.6(2)	48.0(6)
direct calculation	$12(^{+3}_{-4})$	$42(^{+7}_{-15})$

If we combine the adiabatic projection method with eigenvector continuation, then the dressed cluster states have the form

$$|\vec{R}, c\rangle_\tau = \exp[-H(c)\tau]|\vec{R}\rangle$$

We evaluate matrix elements of the full microscopic Hamiltonian at the target coupling using the dressed cluster states,

$$[H_\tau]_{\vec{R},c;\vec{R}',c'} = {}_\tau\langle \vec{R}, c|H(c_\odot)|\vec{R}', c'\rangle_\tau$$

The norm matrix is given by the inner product

$$[N_\tau]_{\vec{R},c;\vec{R}',c'} = {}_\tau\langle \vec{R}, c|\vec{R}', c'\rangle_\tau$$

The adiabatic Hamiltonian is given by the matrix product

$$[H^a_\tau]_{\vec{R},c;\vec{R}',c'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},c;\vec{R}',c'}$$

We had already been using this formalism in its simplest form for the Coulomb interaction. We were setting the electromagnetic coupling for the dressed cluster states to zero and setting the target electromagnetic coupling to the physical value.

But now the eigenvector continuation formalism provides a complete theoretical framework that can be systematically improved.

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.

Implementing eigenvector continuation to treat all higher-order interactions in chiral effective field theory. Also starting to implement eigenvector continuation in lattice QCD for quark mass extrapolations.

Extra Slides

Asymptotic cluster scattering wave functions

In the far asymptotic region where our dressed clusters are widely separated, they interact only through infinite-range forces such as the Coulomb interaction.

Therefore we can describe everything with an effective cluster Hamiltonian $H^{\rm eff}$ that is nothing more than a free lattice Hamiltonian for two point particles plus any infinite-range interactions inherited from the full microscopic Hamiltonian. So in the asymptotic region we have

$$[N_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-2H^{\rm eff}\tau} \right]_{\vec{R},\vec{R}'} ,$$

$$[H_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-H^{\rm eff}\tau} H^{\rm eff} e^{-H^{\rm eff}\tau} \right]_{\vec{R},\vec{R}'} ,$$

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 92, 054612 (2015)

Extra Slides

Since

$$\left[N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'} = c^{-1/2} \cdot \left[e^{H^{\text{eff}}\tau}\right]_{\vec{R},\vec{R}'}$$

we conclude that the adiabatic Hamiltonian coincides with the effective cluster Hamiltonian in the asymptotic region

$$[H_\tau^a]_{\vec{R},\vec{R}'} = \left[H^{\text{eff}}\right]_{\vec{R},\vec{R}'}$$

In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.