New results in lattice effective field theory: Eigenvector continuation

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

Outline

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Perturbation theory

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Motivation

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.

A new strategy

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.

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

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

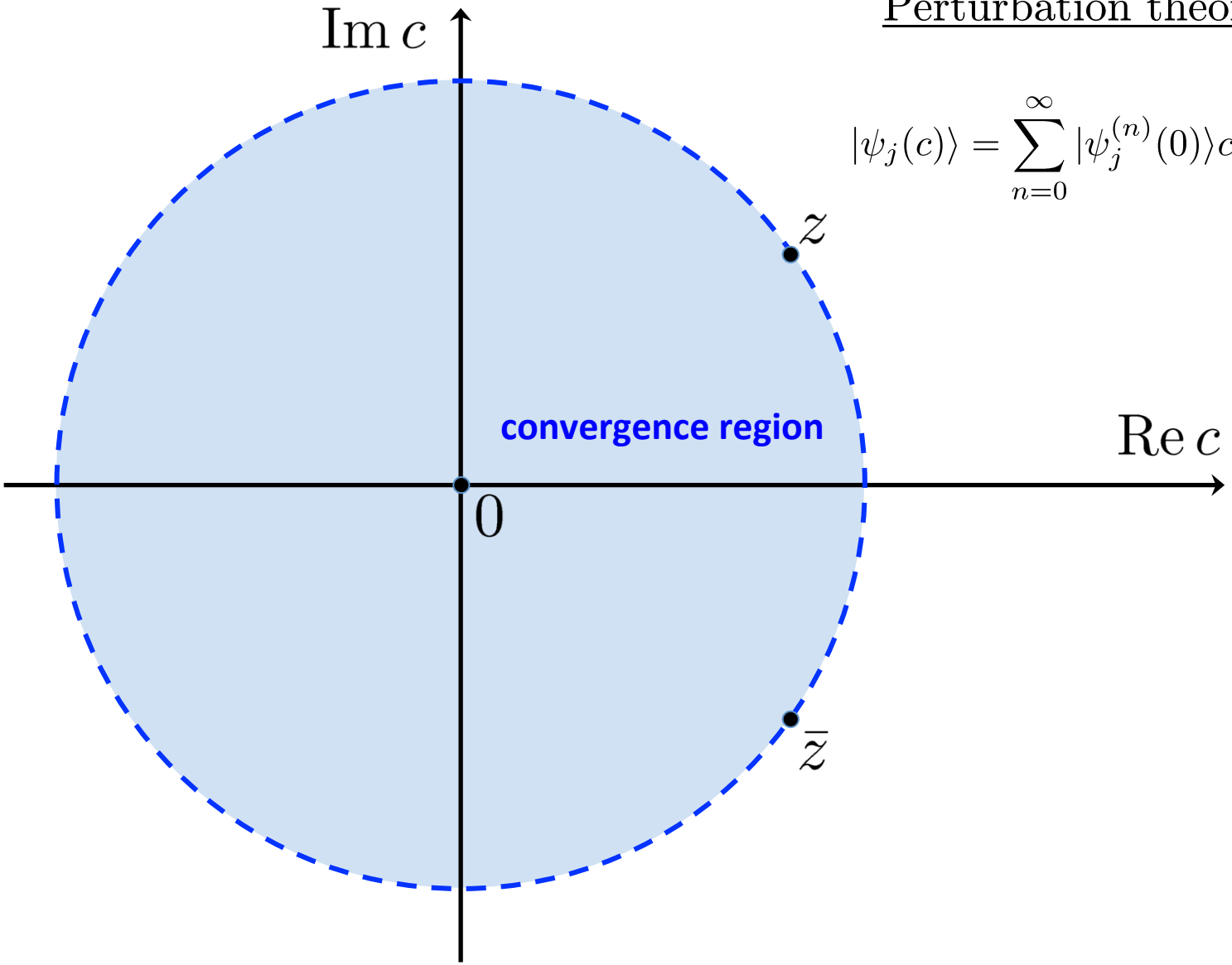
We can perform series expansions around the point $c = 0$.

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

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.

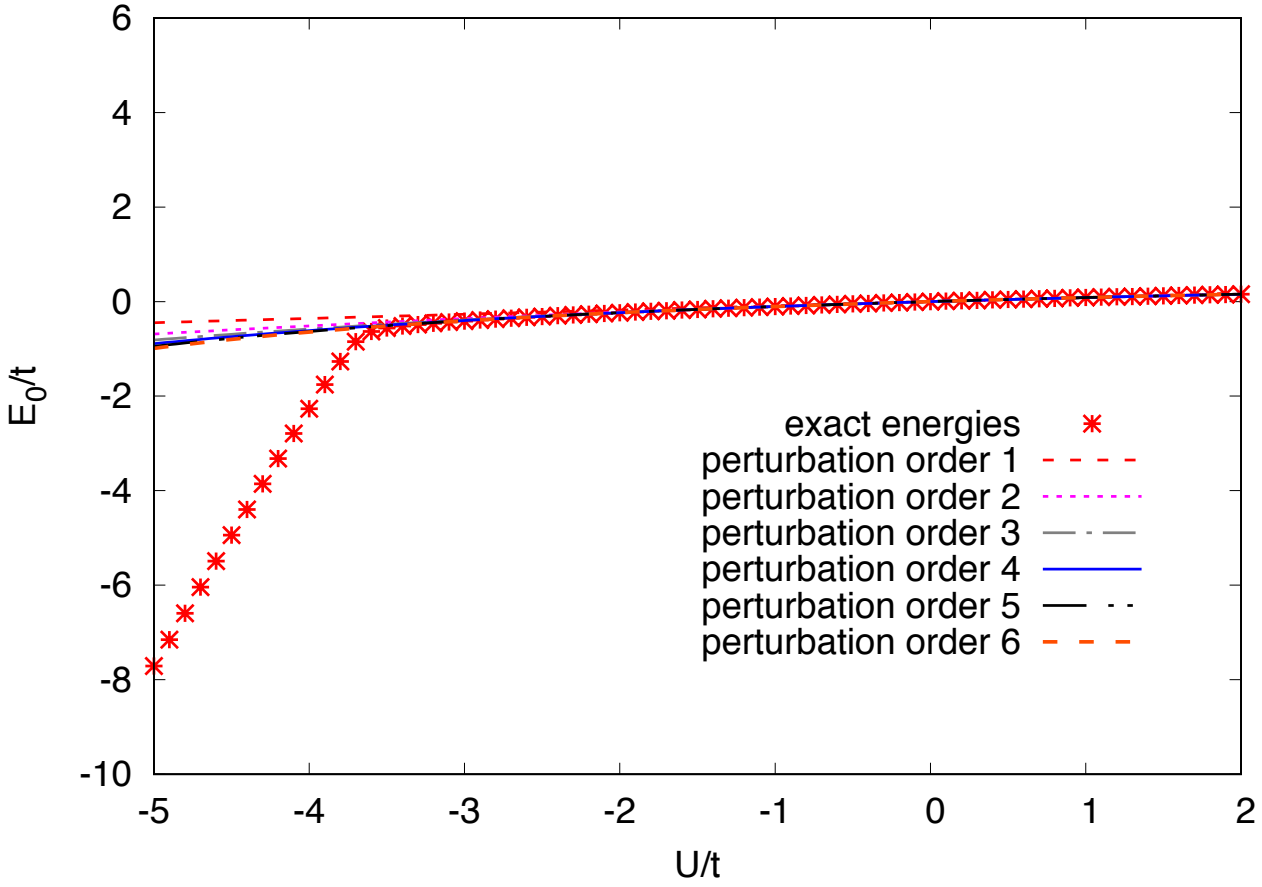
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

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

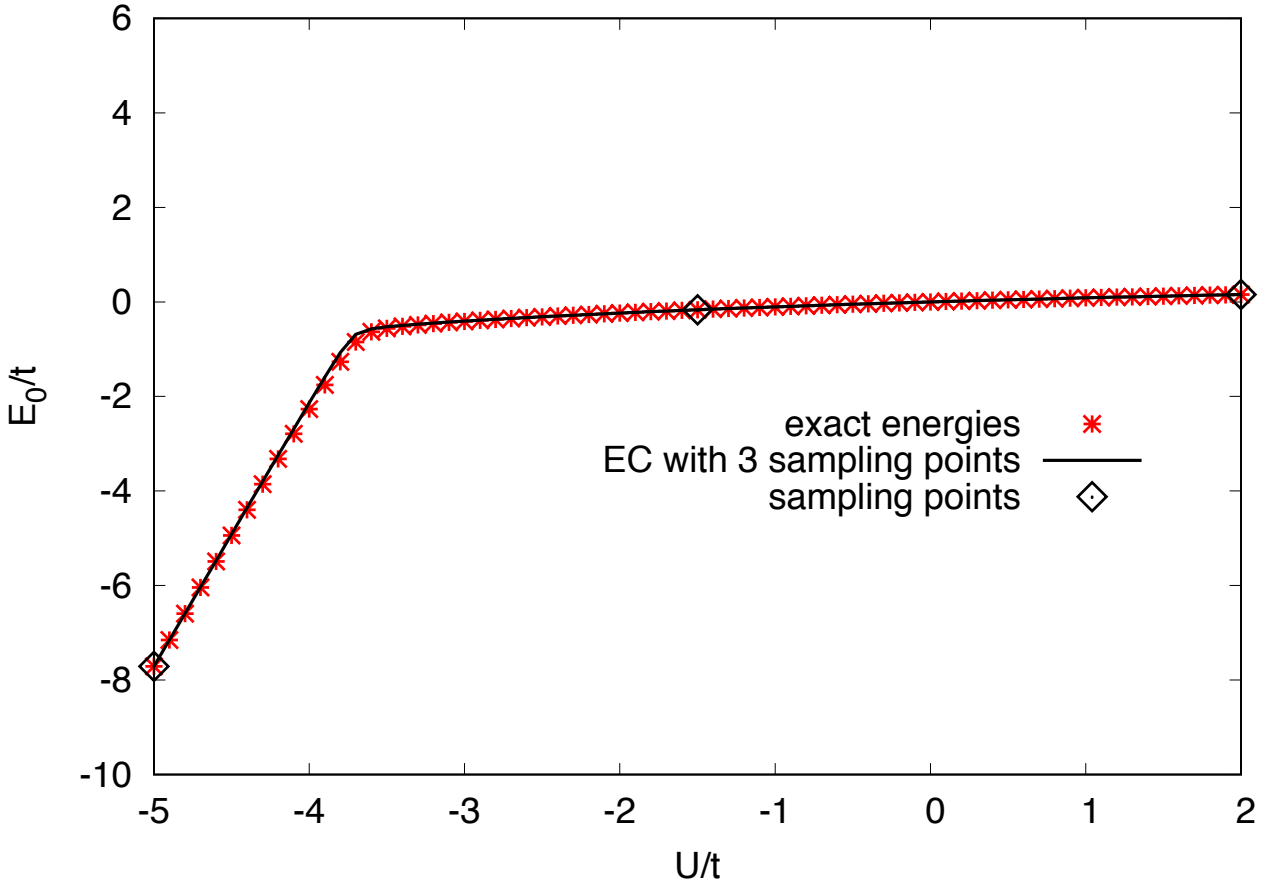
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

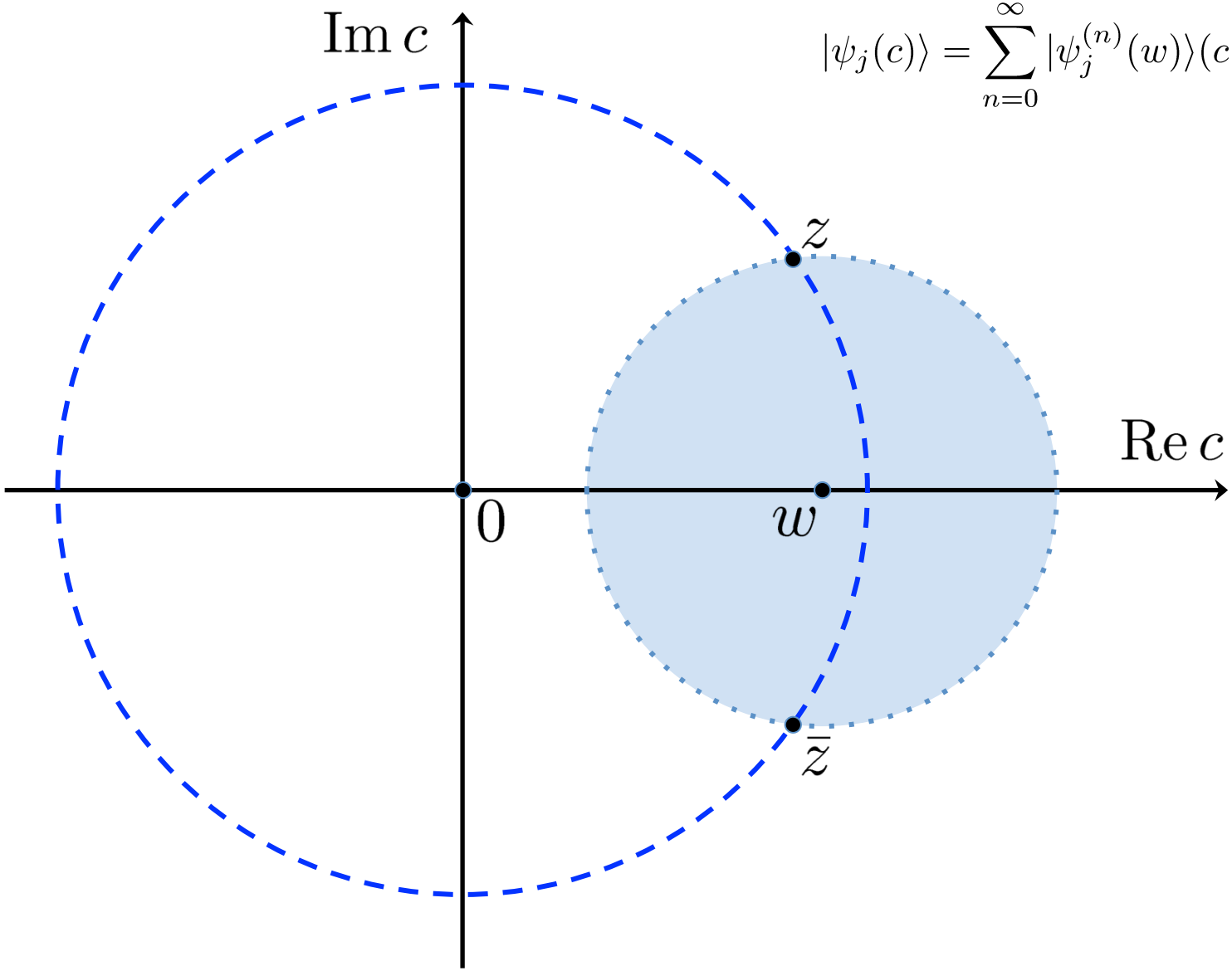
Perturbation theory fails at strong attractive coupling

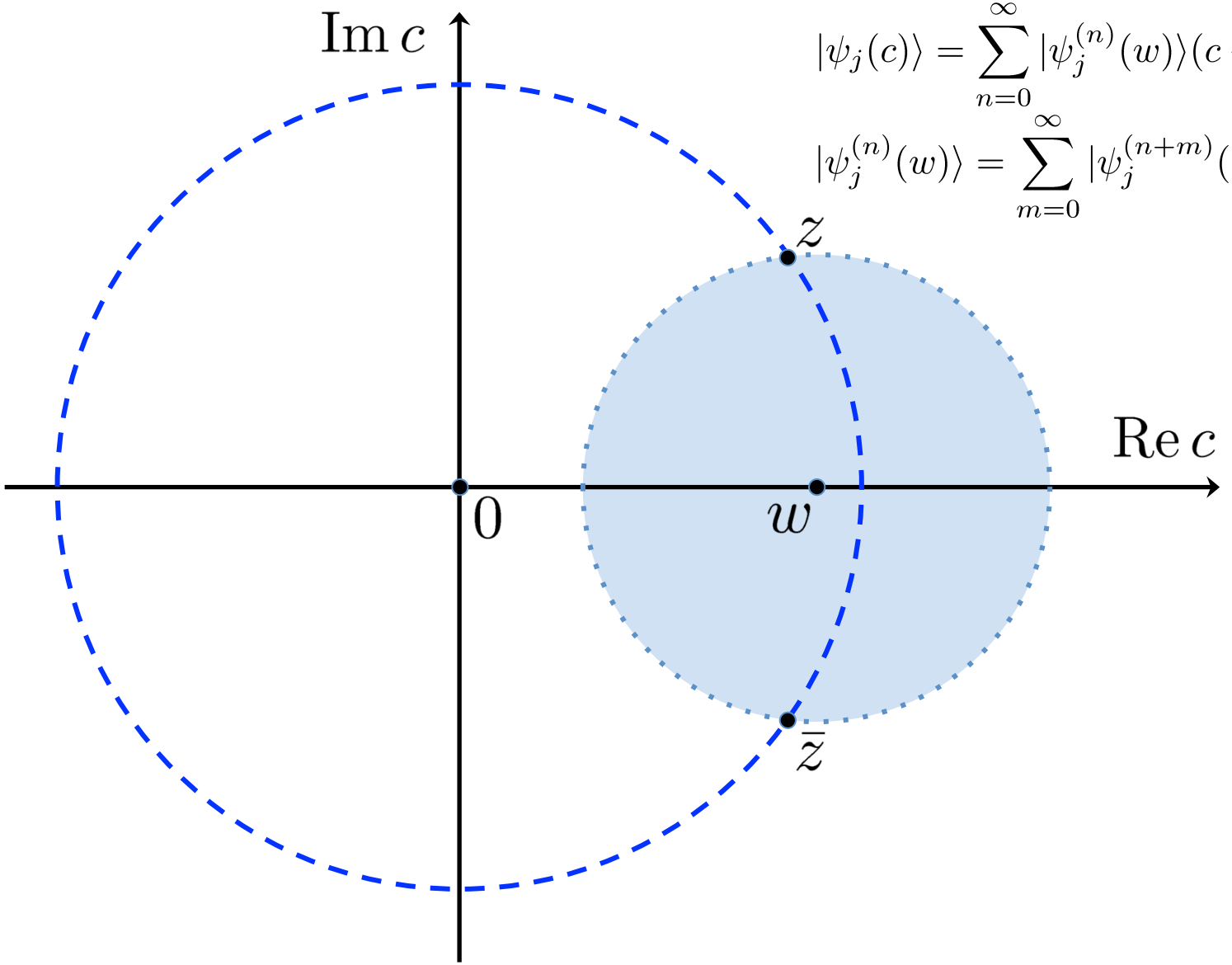


Restrict the linear space to the span of three vectors



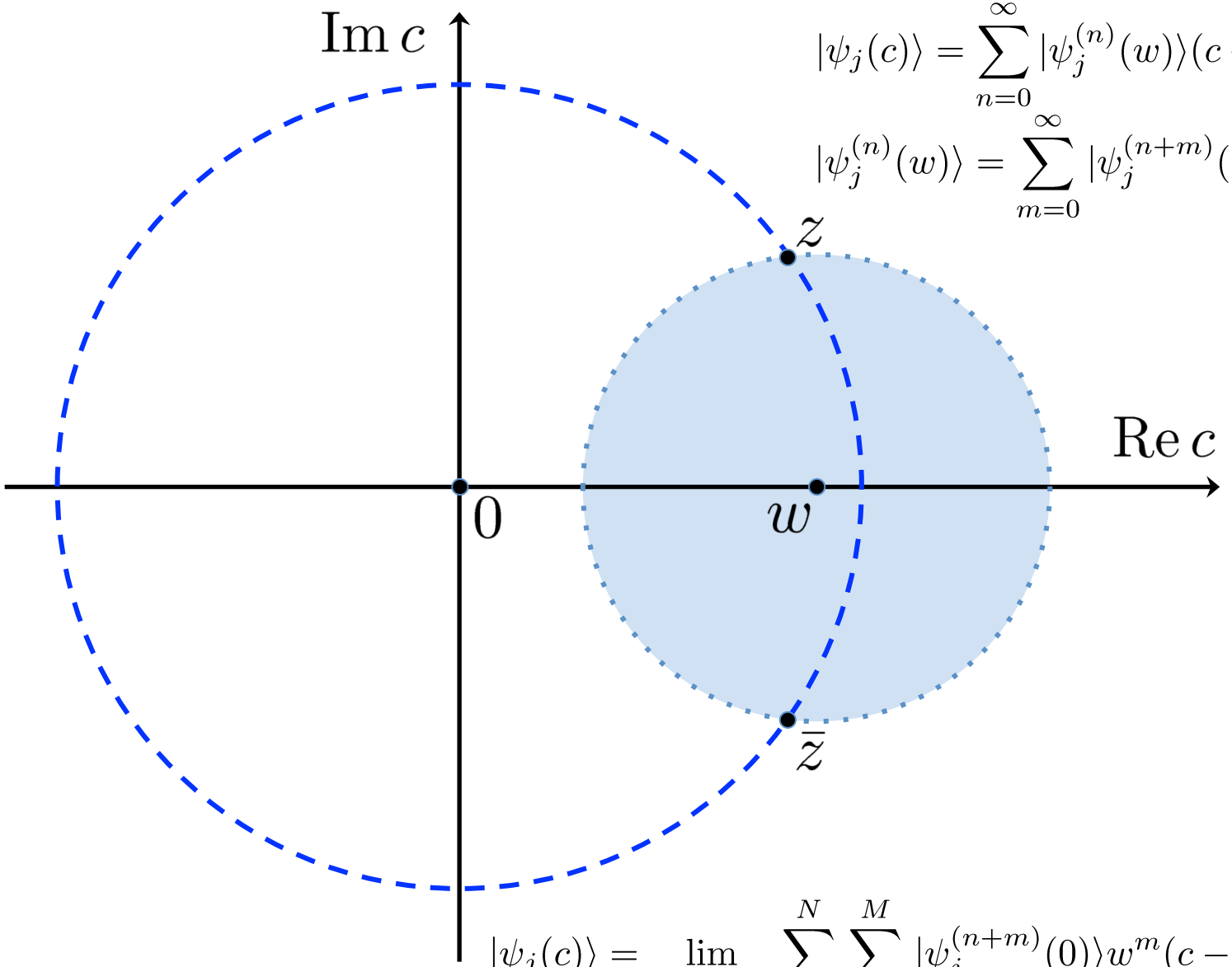
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





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

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



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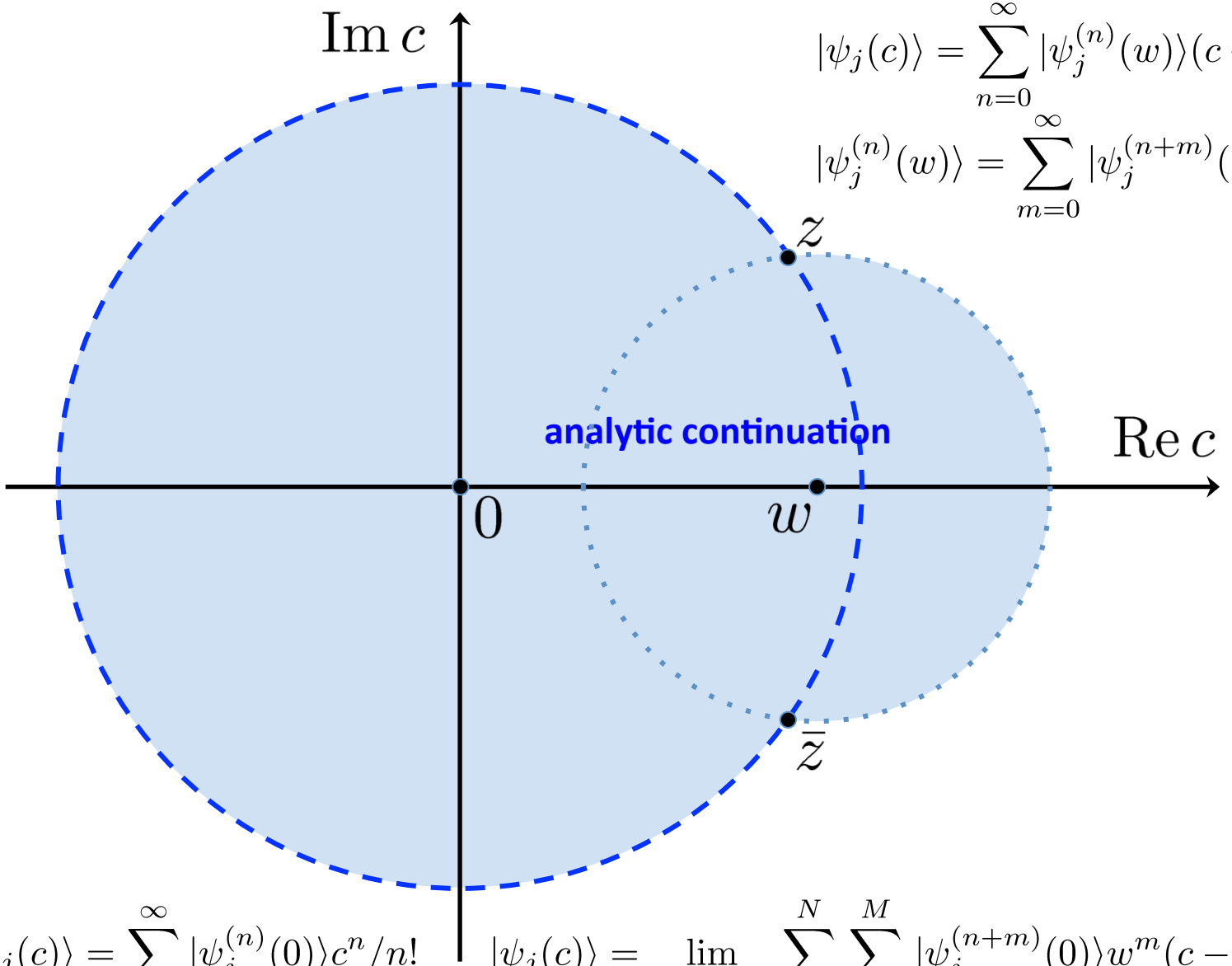
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$



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

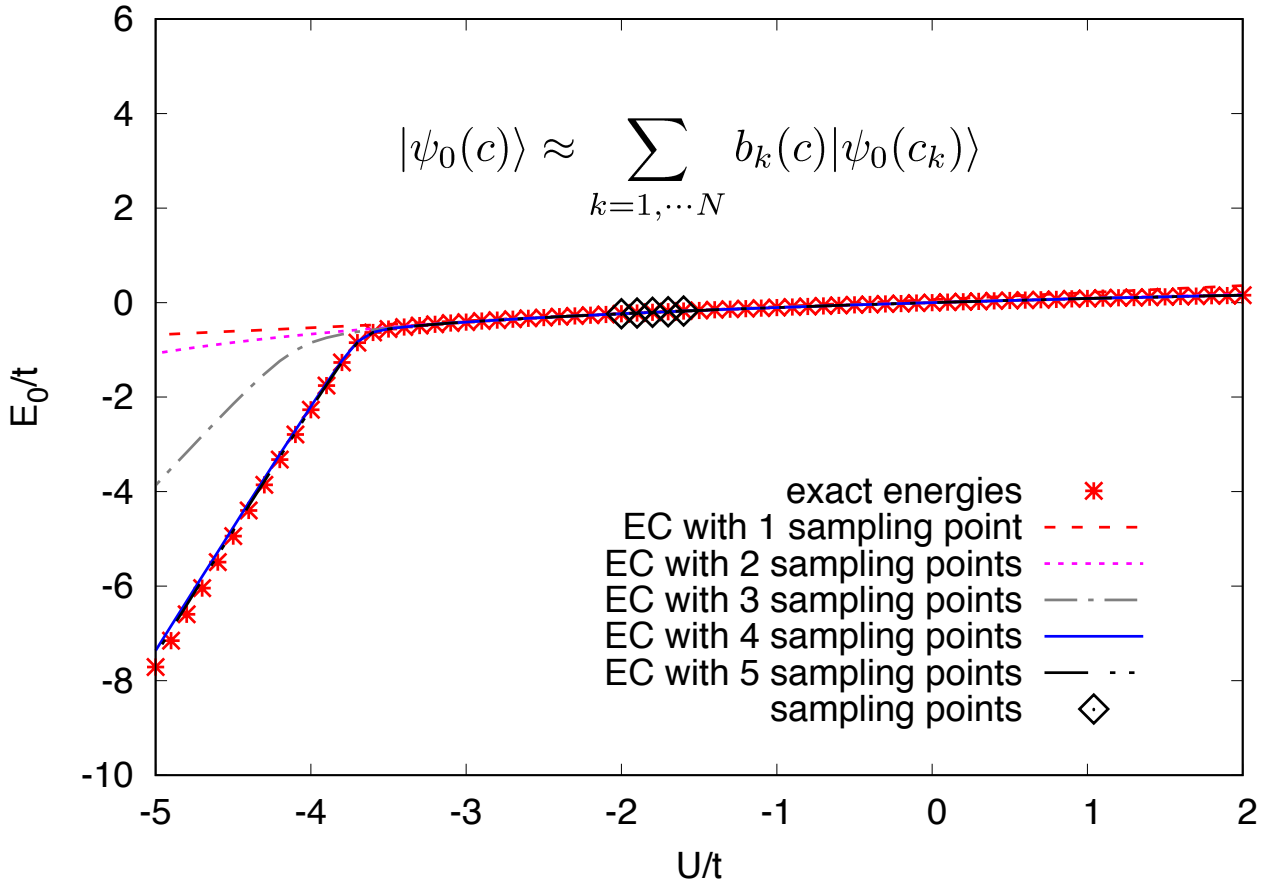
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

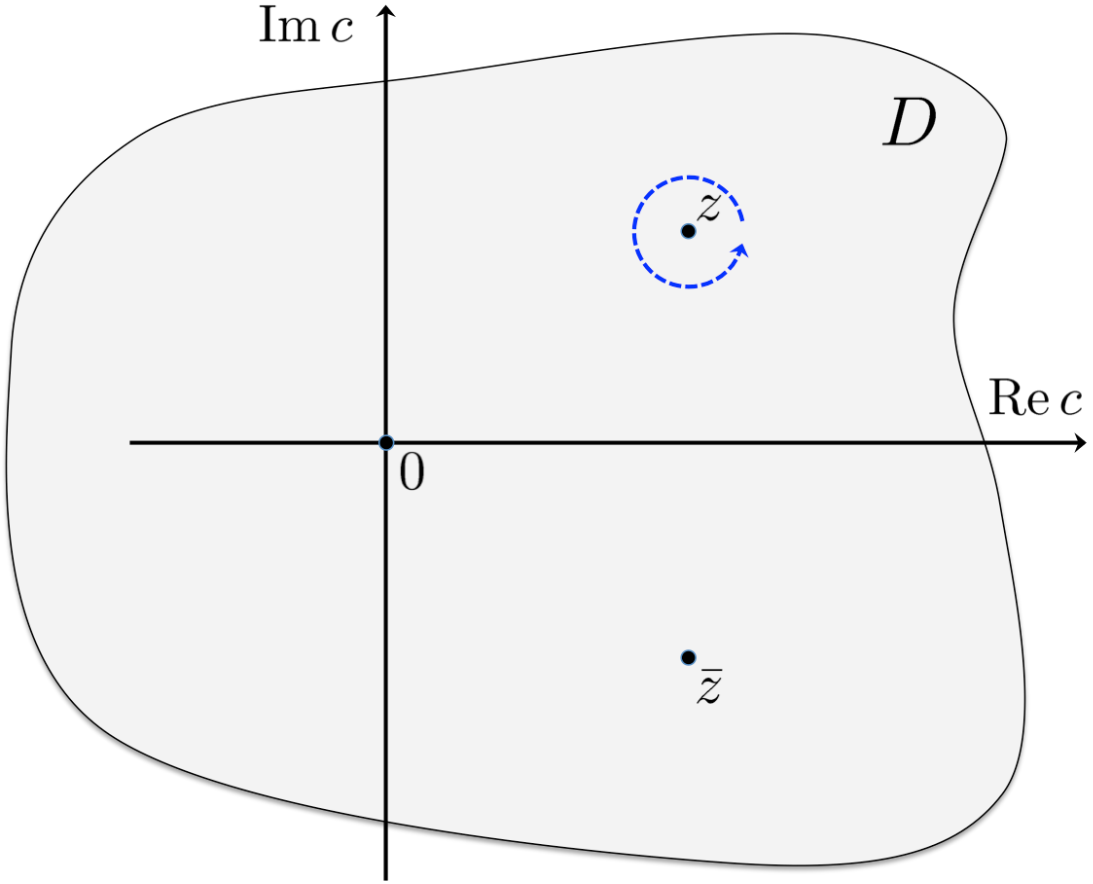
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

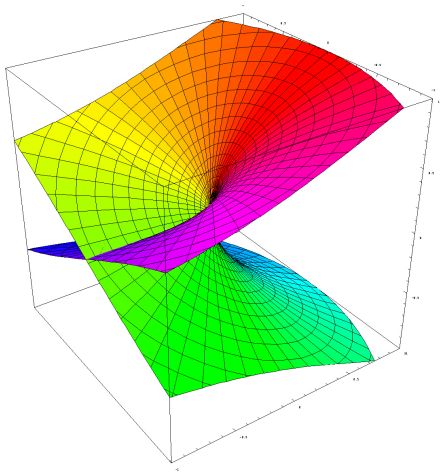
As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

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

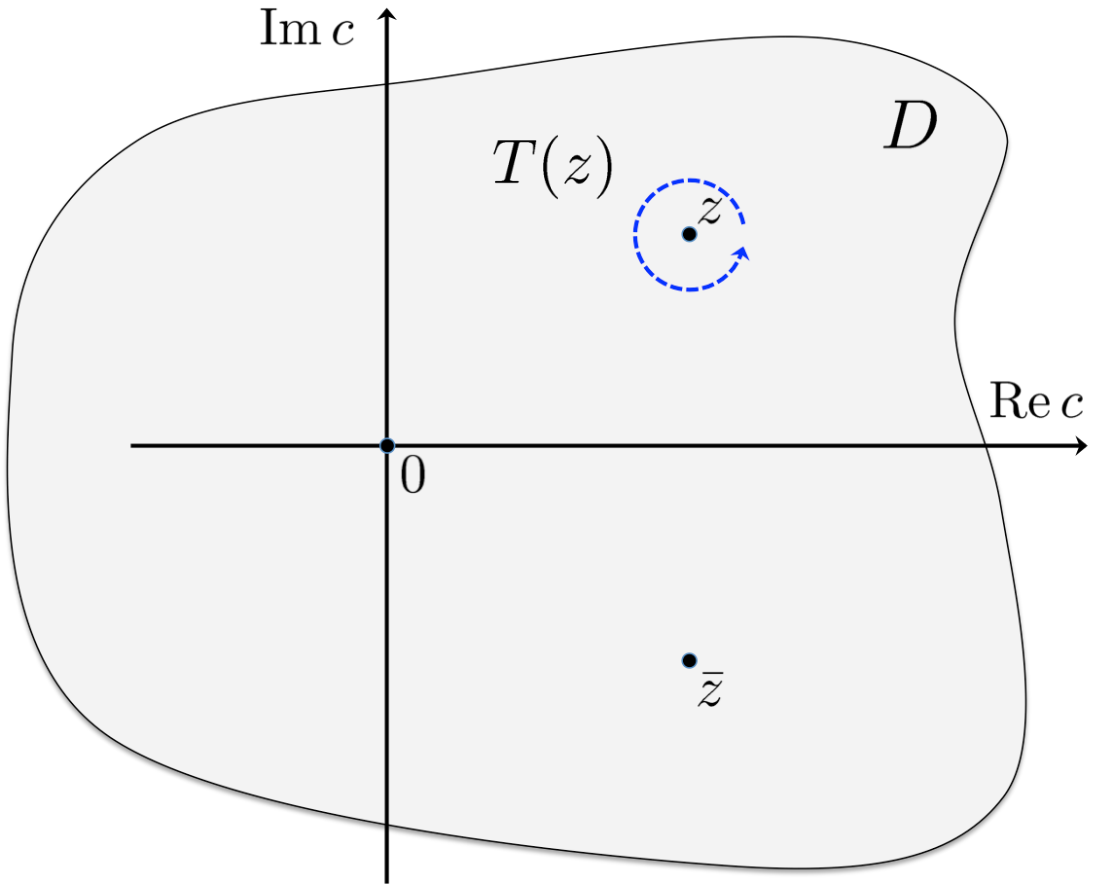


The Riemann surfaces of the degenerate eigenvectors are entwined at branch point singularities.





Let us define a monodromy transformation $T(z)$ which corresponds to traversing a counterclockwise loop in c around the branch point z.



Suppose there are k eigenvectors of $H(c)$ which comprise an irreducible representation of the monodromy transformation $T(z)$. Let us label these eigenvectors as

$$|\psi_1(c)\rangle, \cdots, |\psi_k(c)\rangle$$

with corresponding eigenvalues

$$E_1(c), \cdots, E_k(c)$$

These eigenvalues will be degenerate at $c = z$. The characteristic polynomial for $H(c)$ is analytic everywhere. Hence the monodromy transformation generates a cyclic permutation of the eigenvalues. Without loss of generality,

$$T(z) : E_1(c) \to E_2(c) \to \cdots \to E_k(c) \to E_1(c)$$

We can now define a new basis for the k eigenvectors

$$|\phi_1(c)\rangle, \cdots, |\phi_k(c)\rangle$$

such that the action of the monodromy transformation is a cyclic permutation on the eigenvectors

$$T(z) : |\phi_1(c)\rangle \to |\phi_2(c)\rangle \to \cdots \to |\phi_k(c)\rangle \to |\phi_1(c)\rangle$$

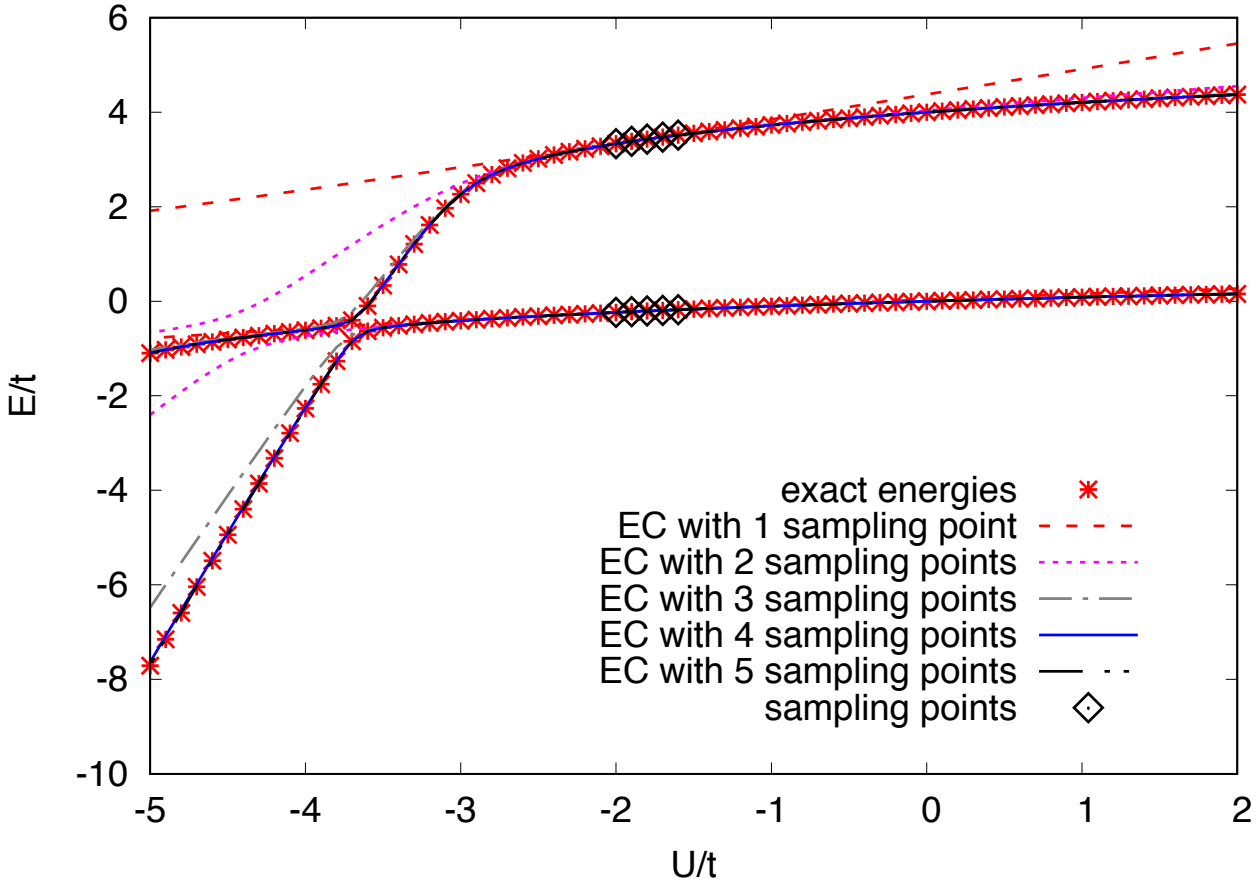
We now diagonalize the monodromy transformation and obtain a new basis where each basis state is analytic at z

$$|\gamma_n(c)\rangle = (c-z)^{n/k} \sum_{j=0}^{k-1} e^{i2\pi nj/k} |\phi_j(c)\rangle \qquad n = 0, \cdots k-1$$

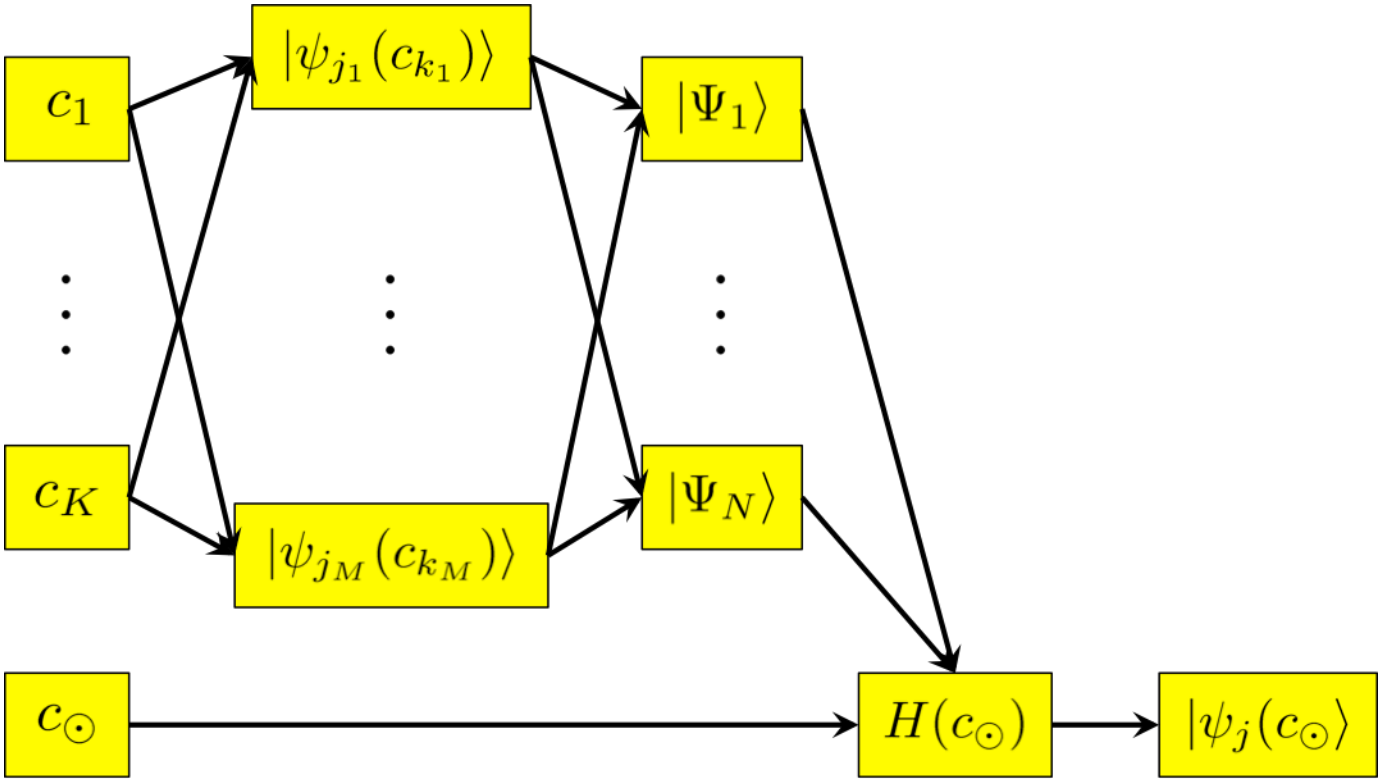
If we perform eigenvector continuation using these basis states there are no convergence problems due to the branch point at z.

Of course, we don't know *a priori* how to construct this new basis. But if we perform eigenvector continuation for all k degenerate eigenvectors together, we remove convergence problems due to the branch point at z.

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

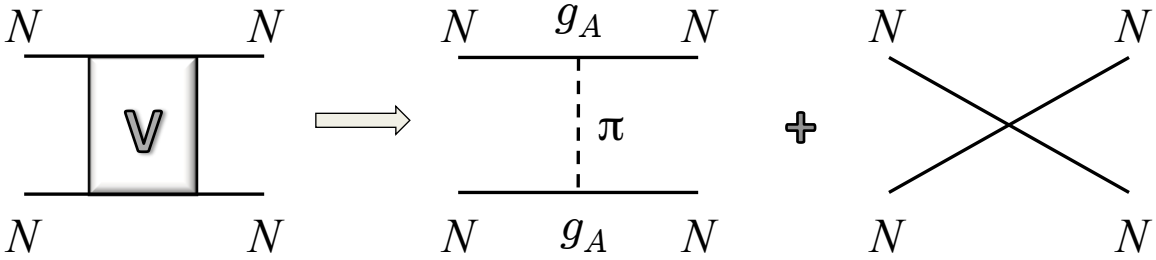


Network diagram for eigenvector continuation



Application: Neutron matter simulations

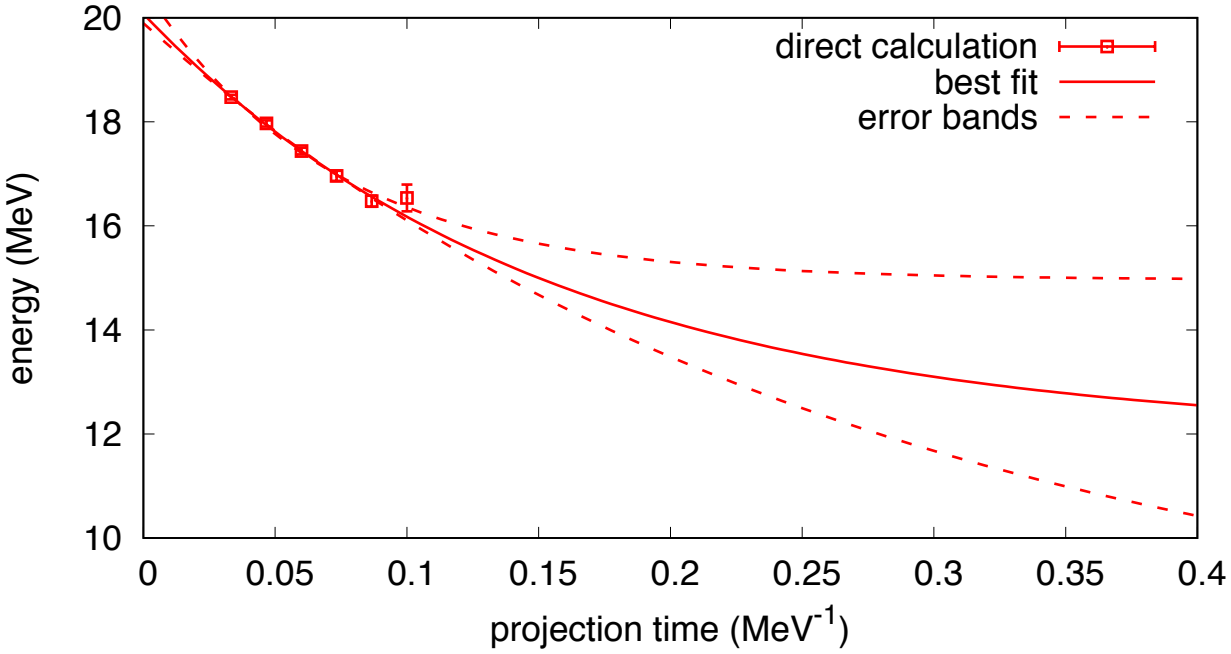
We consider lattice effective field theory simulations of the neutron matter at the leading order.



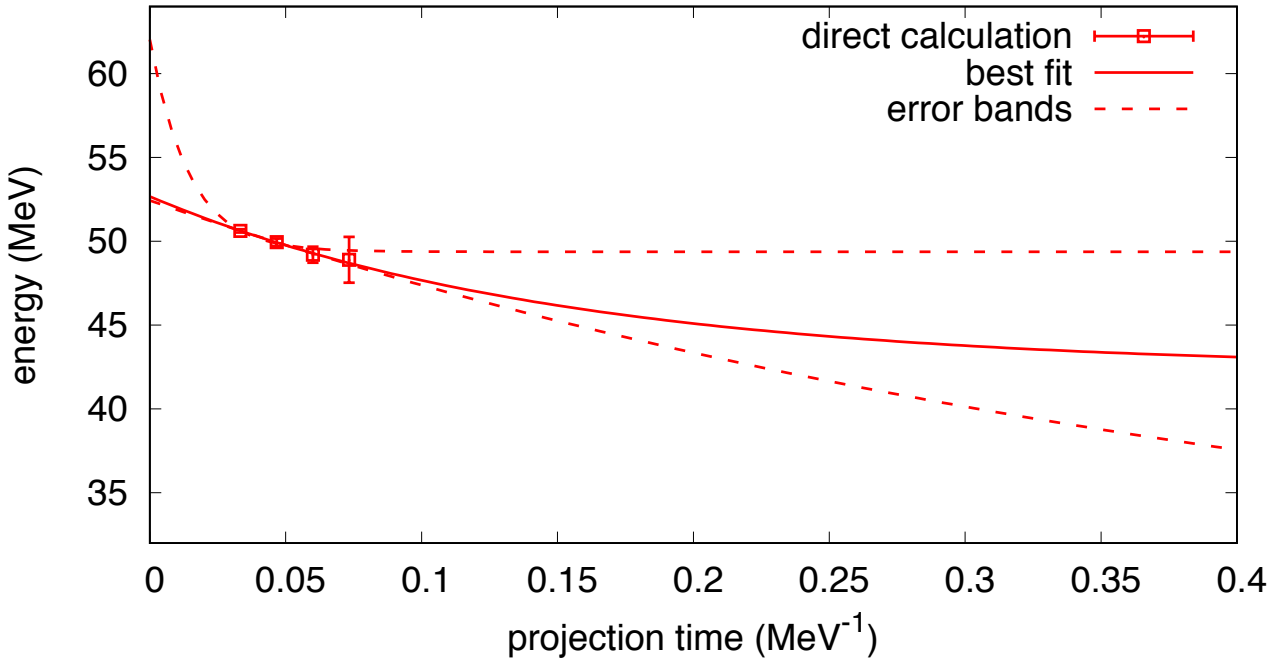
As a challenge to the eigenvector continuation technique, we use a lattice action for one-pion exchange that causes severe Monte Carlo sign oscillations.

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)



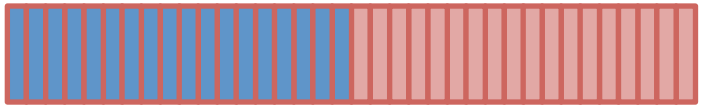
Direct calculation of fourteen neutrons ($L = 8$ fm)



Eigenvector continuation

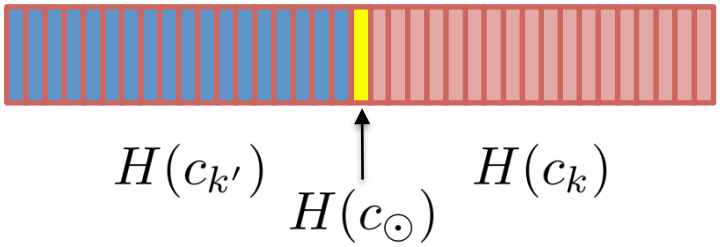
Use Monte Carlo simulations to compute projection amplitudes

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



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

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

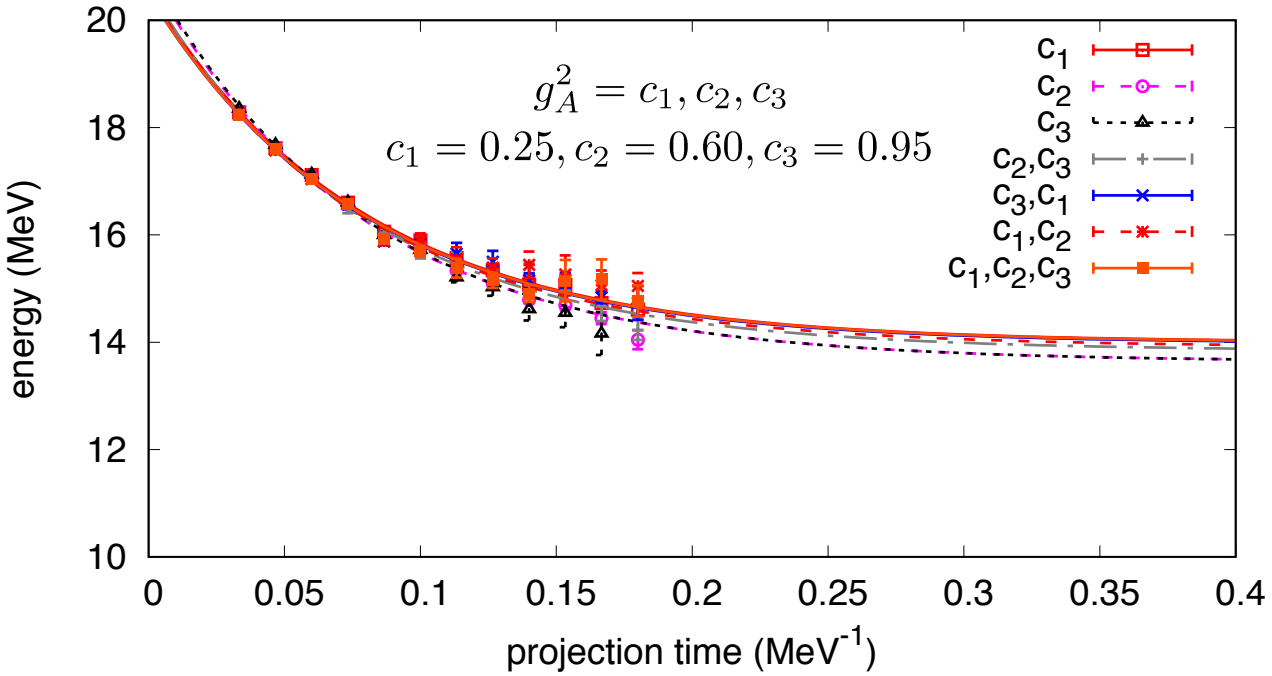


$$|\psi_{\text{init}}\rangle$$

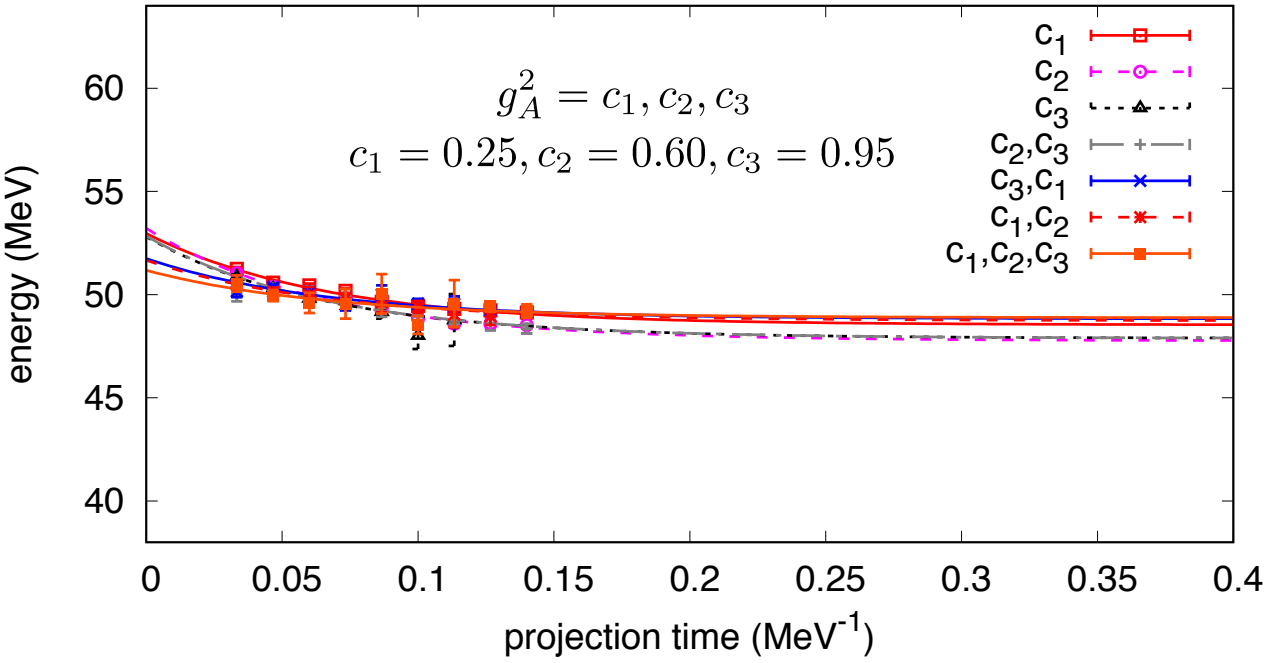
Solve the generalized eigenvalue problem by finding the eigenvalues and eigenvectors of

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

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	$12(^{+3}_{-4})$	$42(^{+7}_{-15})$

Adiabatic projection method

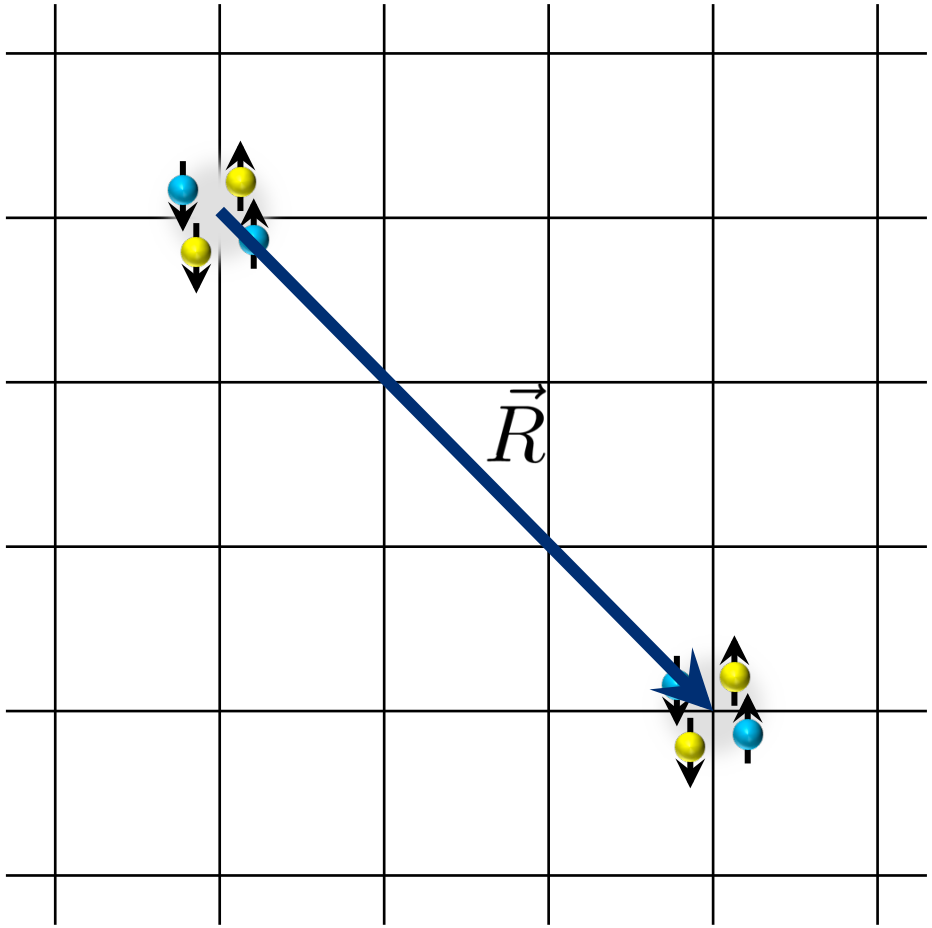
When working with states in the continuum, we can also combine eigenvector continuation with the adiabatic projection method.

The adiabatic projection method consists of two parts. In the first part, we use Euclidean time projection 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.

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,

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

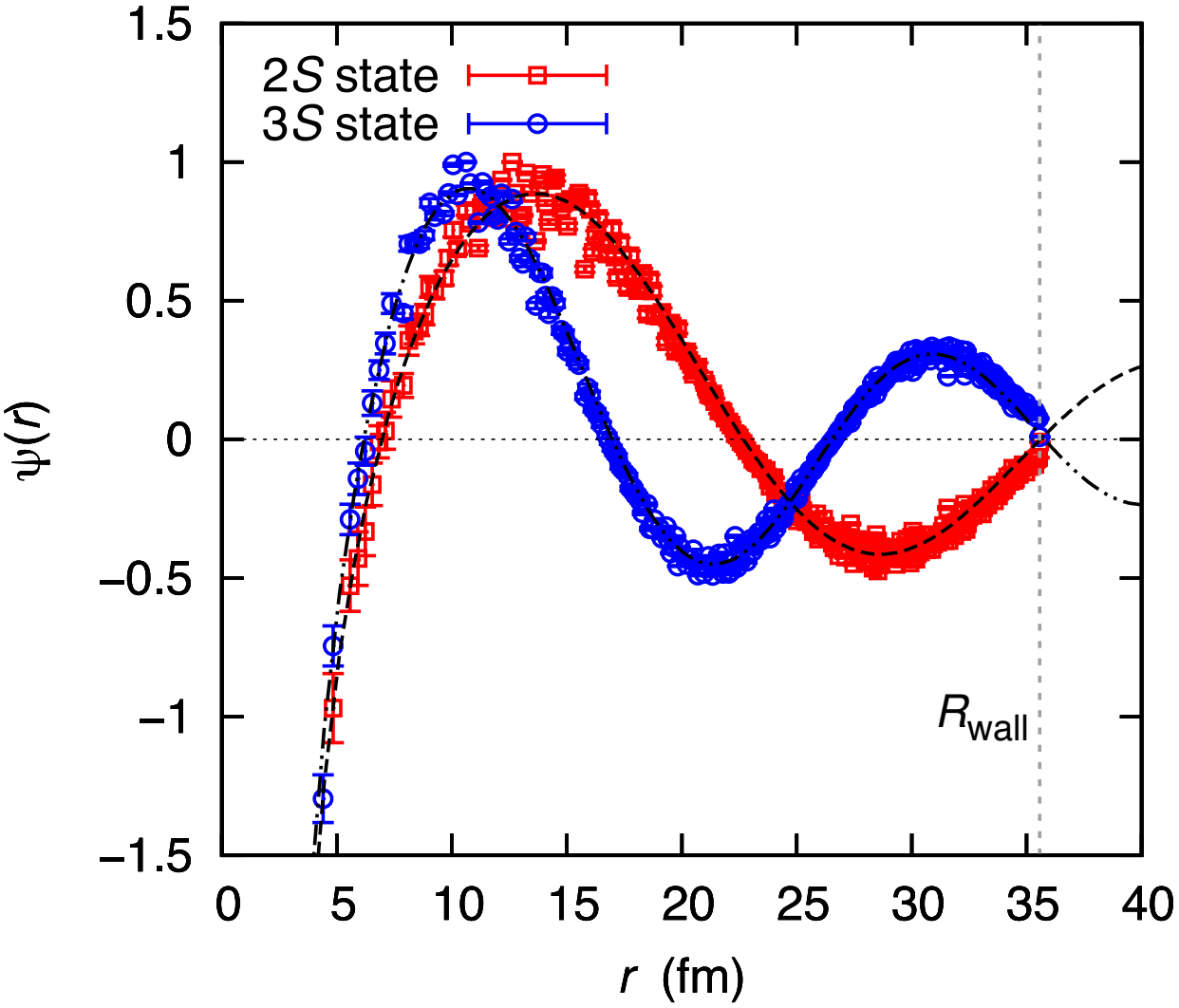
Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

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

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.



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

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

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

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

When a control parameter in the Hamiltonian matrix is varied smoothly, the extremal eigenvectors do not explore the large dimensionality of the linear space.

The eigenvector trajectory lives on a low-dimensional manifold and we can determine the desired eigenvector by "learning" a set of basis vectors for the manifold.

Outlook

Numerous applications to quantum Monte Carlo simulations for systems with sign oscillations. Now being implemented in nuclear lattice effective field theory simulations of nuclear structure and reactions.

Possible applications to generate non-perturbative correlations in many-body perturbation theory. Possible applications to physical quark mass extrapolations in lattice quantum chromodynamics.