Lecture 29: Eigenvector Continuation, Unitary Limit, and Superfluidity

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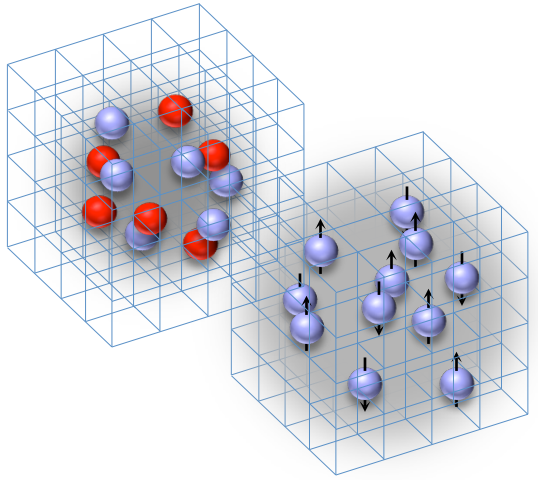


From Quarks and Gluons to Nuclear Forces and Structure

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.

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, PRL 121 (2018) 032501

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

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

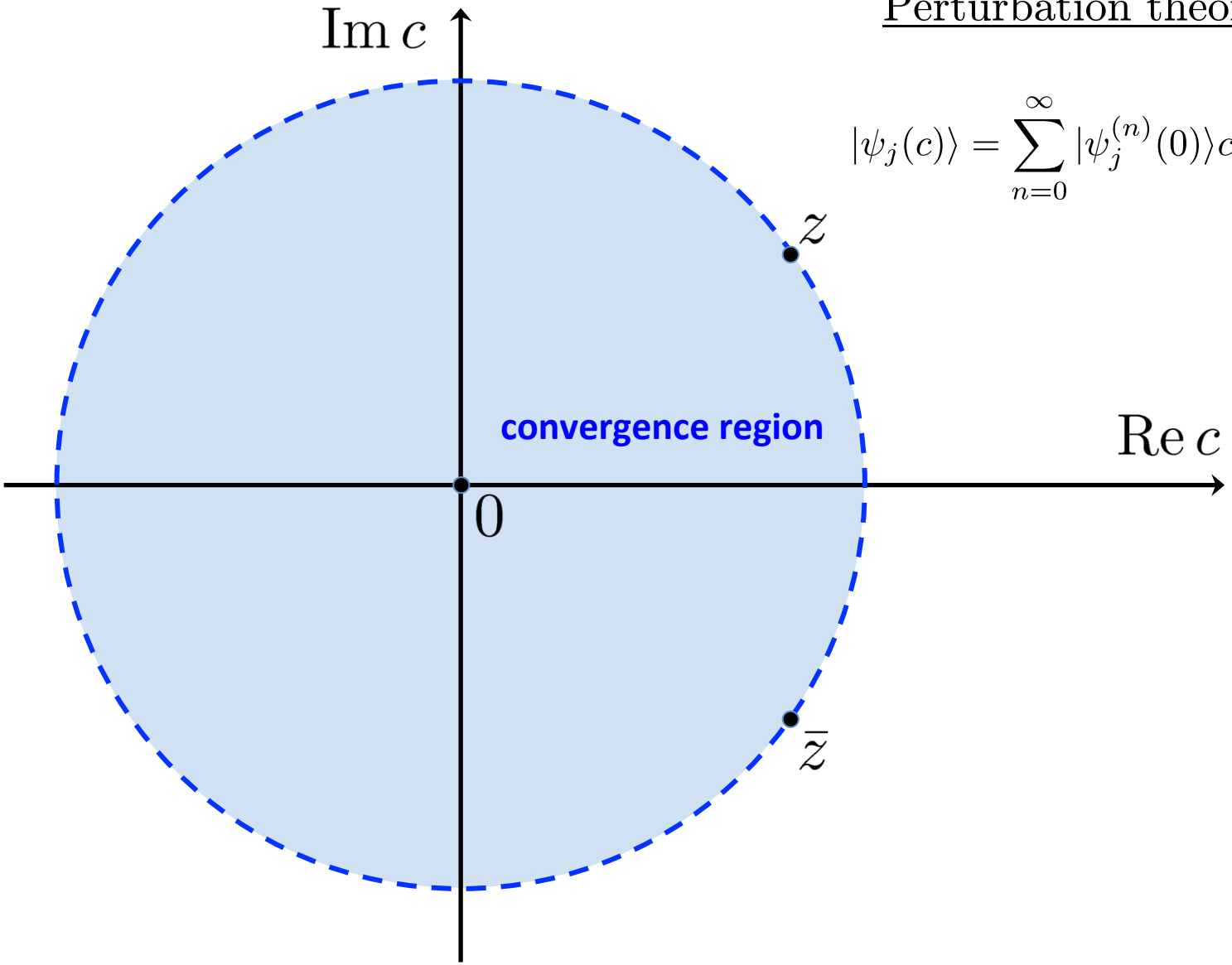
We can perform series expansions around the point $c = 0$.

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

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.

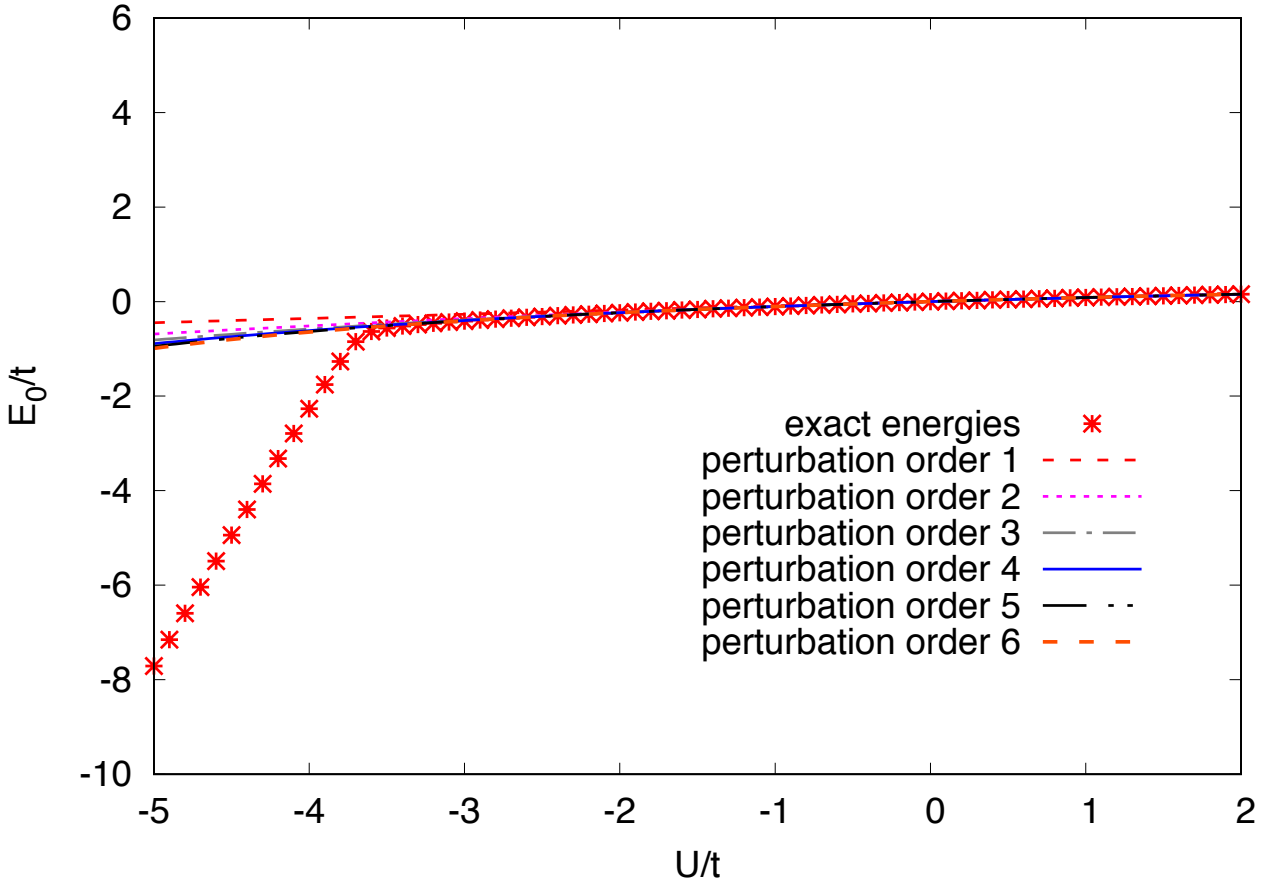
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

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

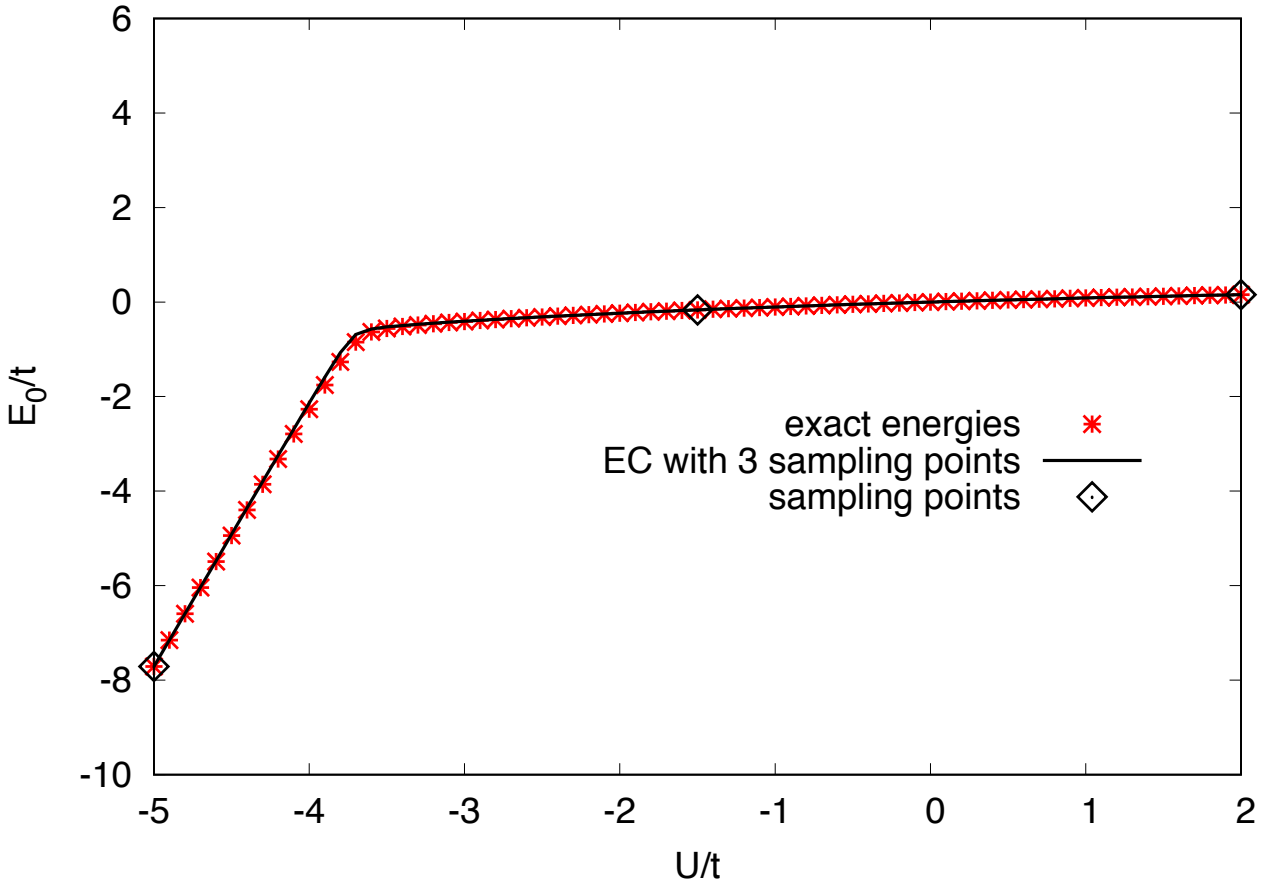
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

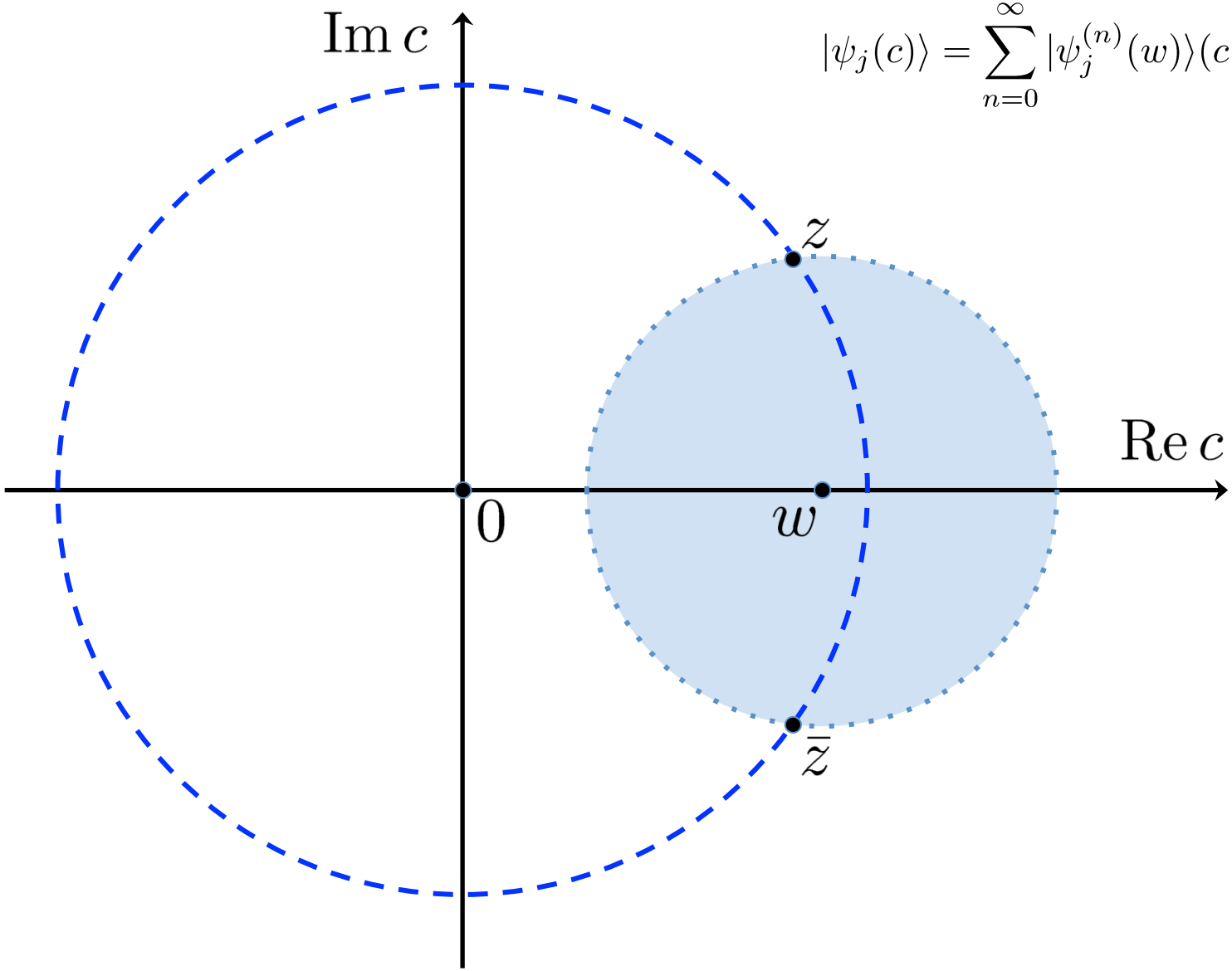
Perturbation theory fails at strong attractive coupling

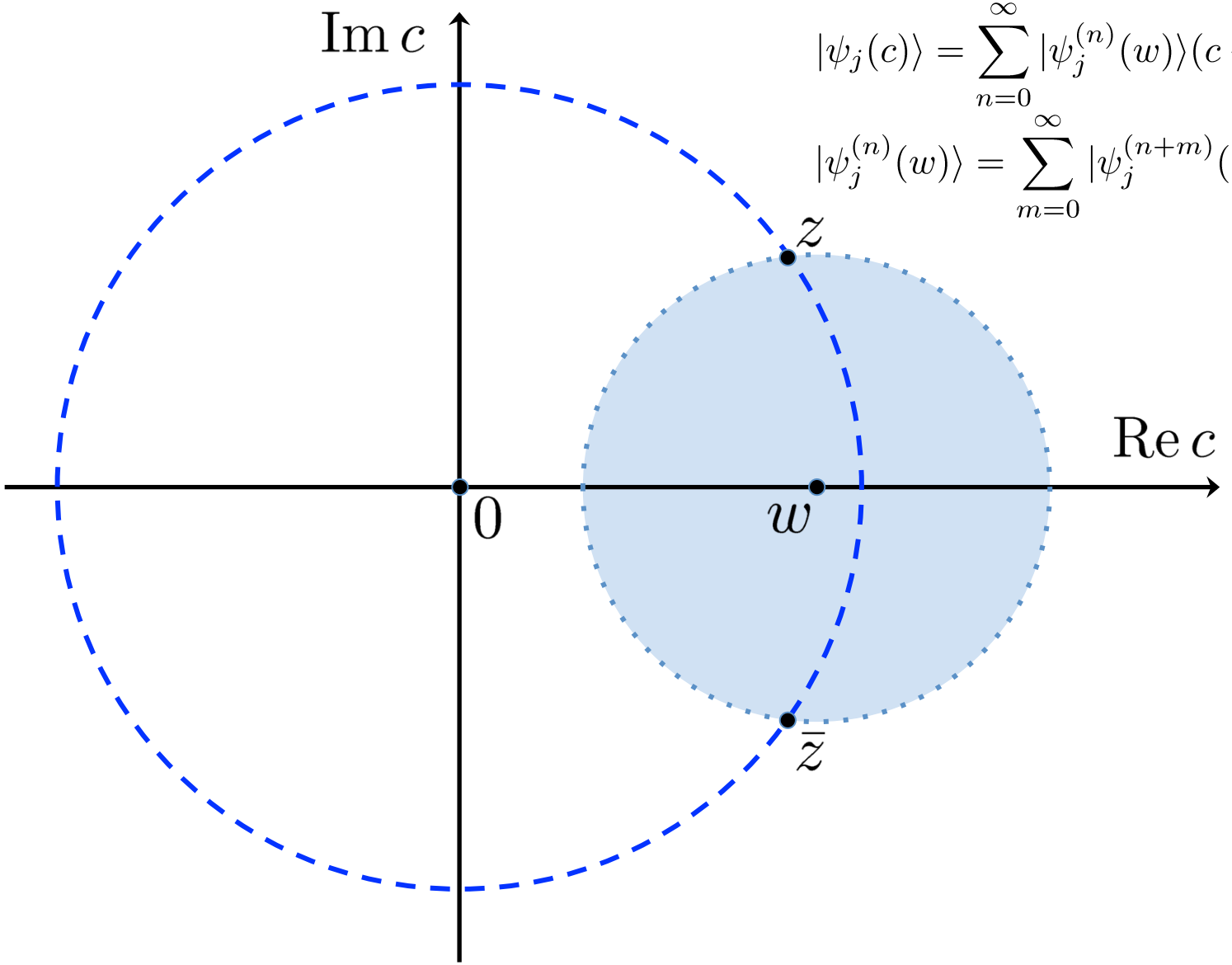


Restrict the linear space to the span of three vectors



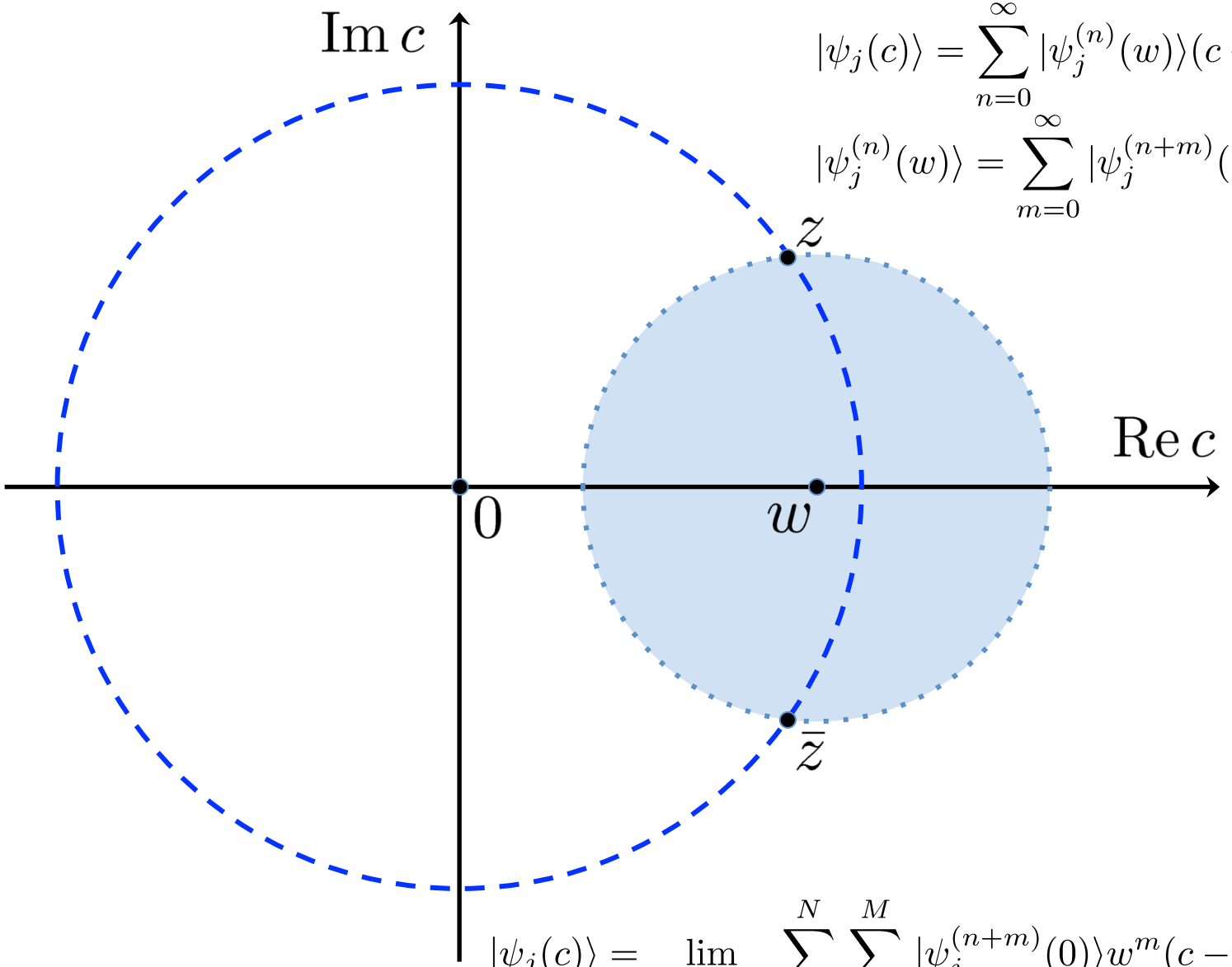
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





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

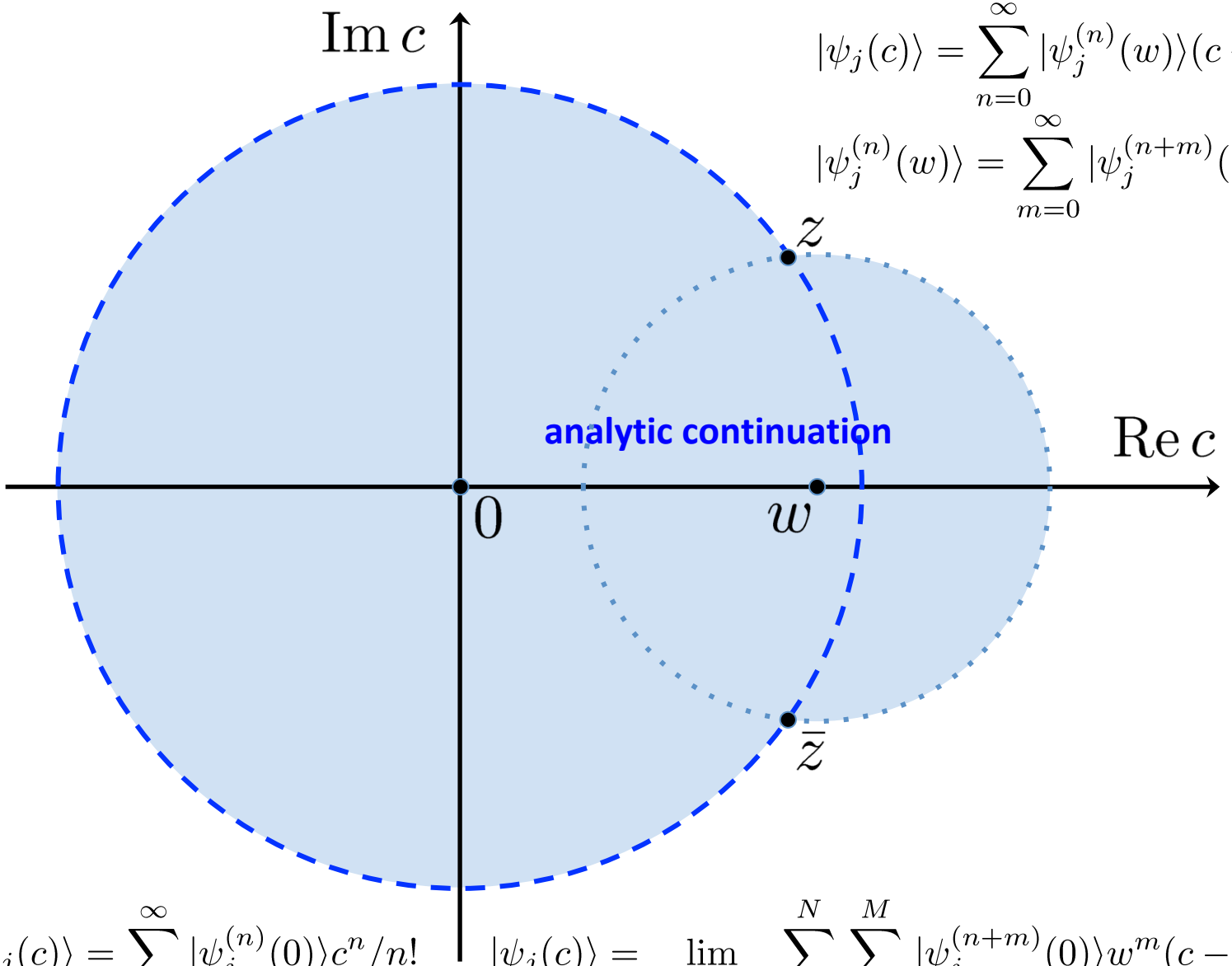
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



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

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

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



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

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

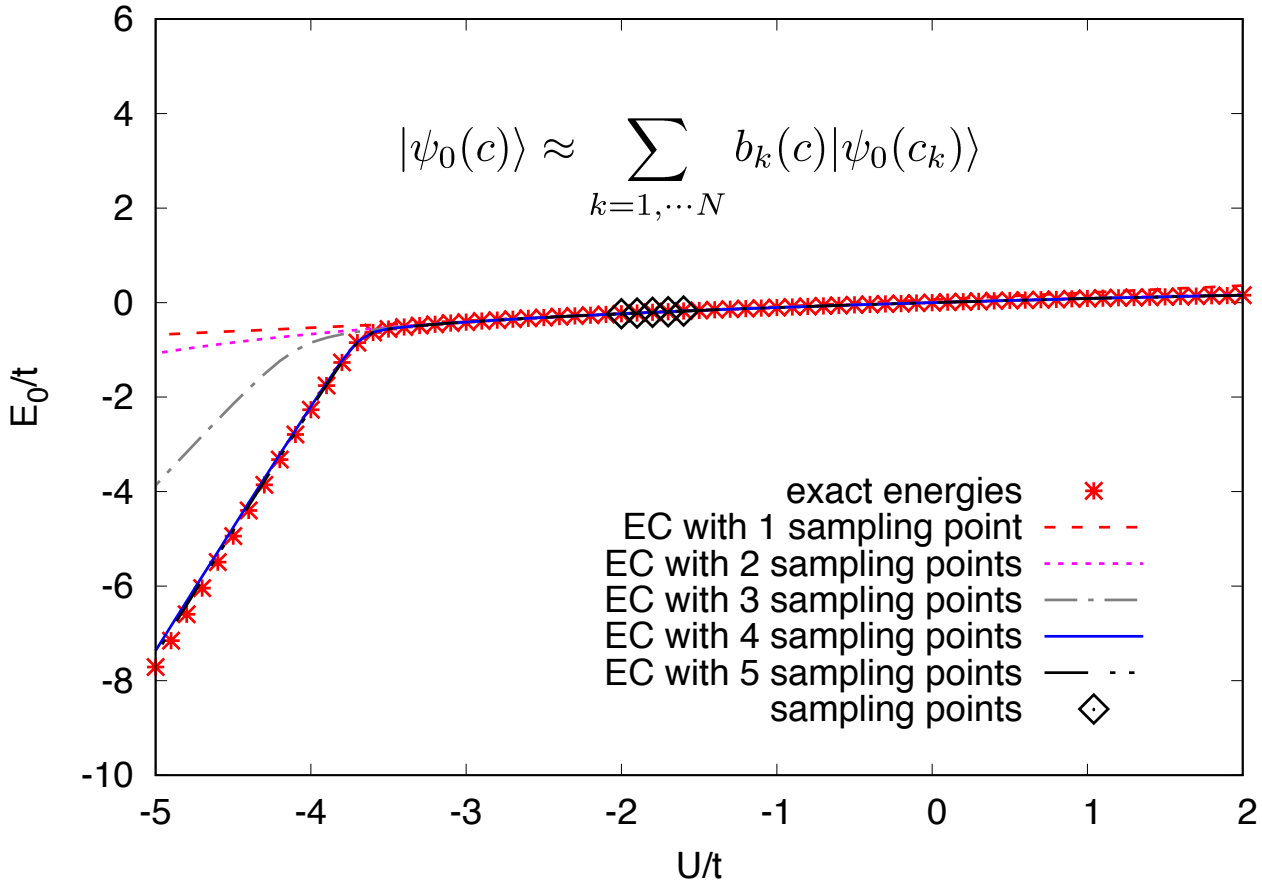
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

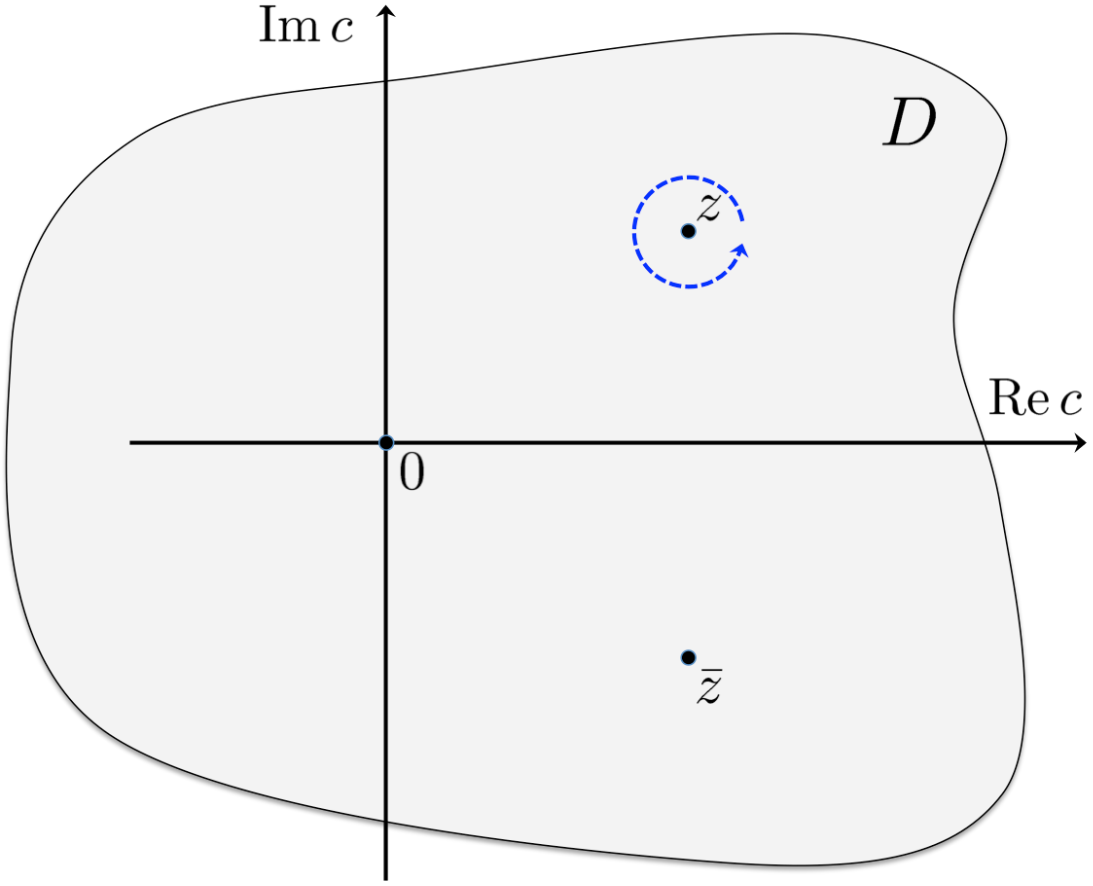
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

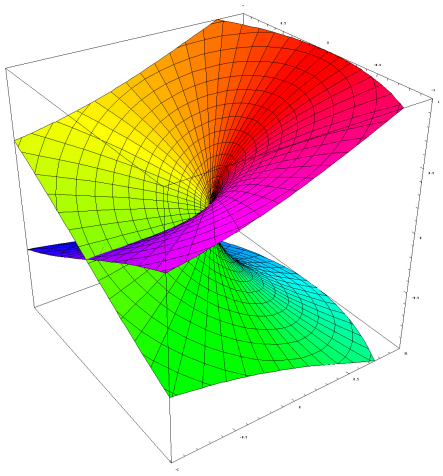
As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

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

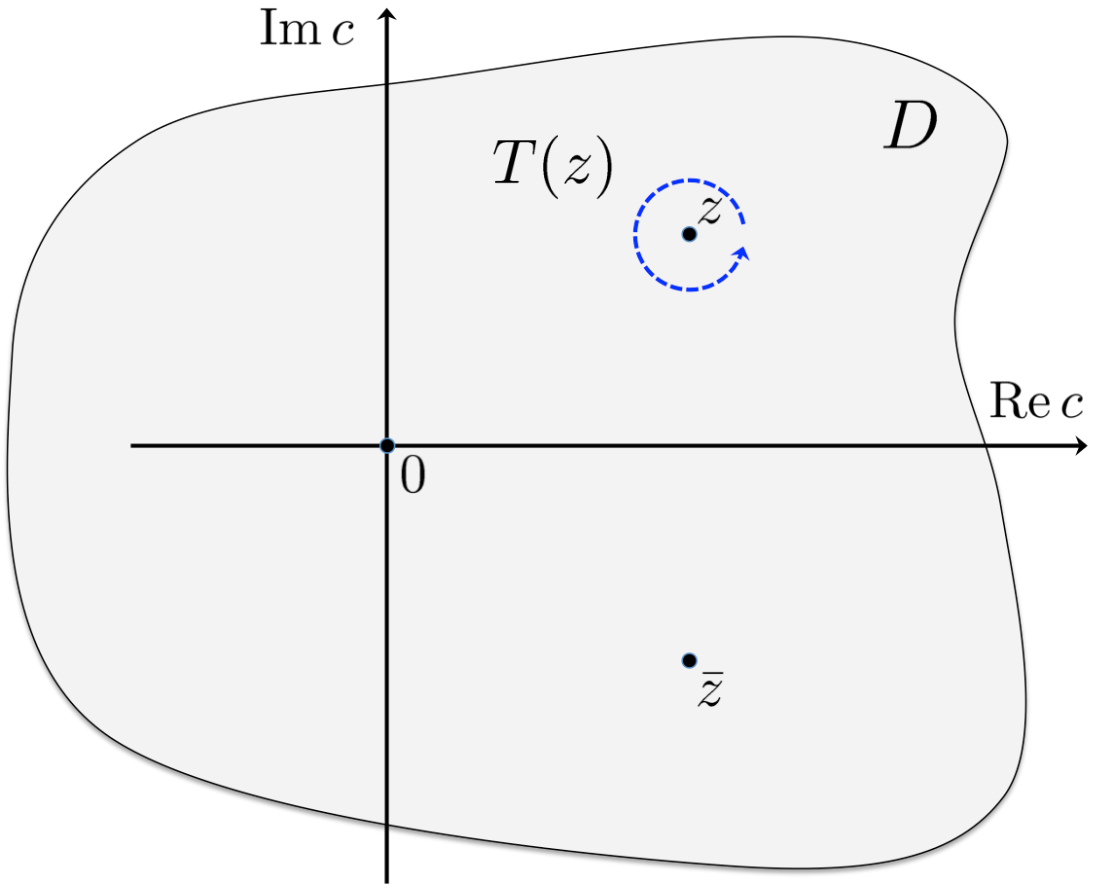


The Riemann surfaces of the degenerate eigenvectors are entwined at branch point singularities.





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

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

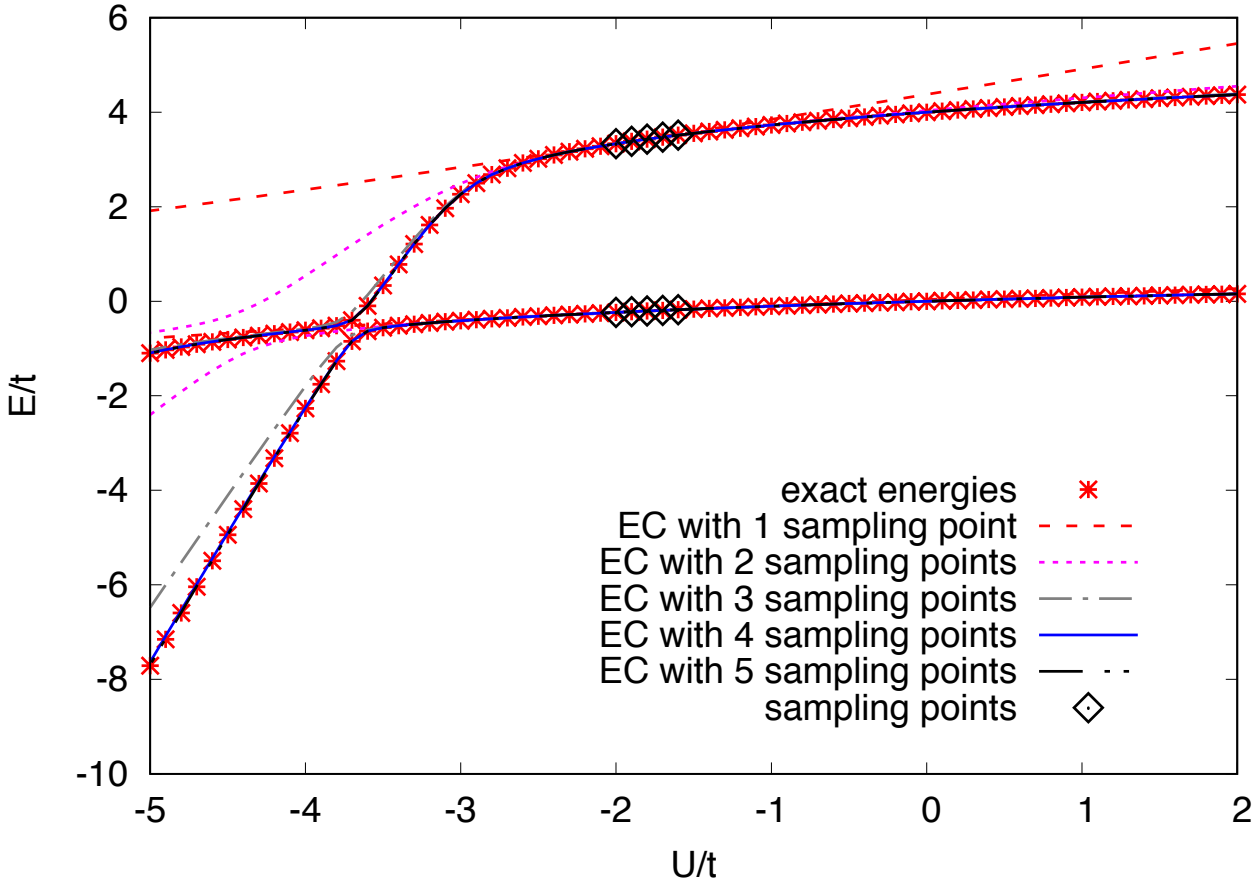
We now diagonalize the monodromy transformation and obtain a new basis where each basis state is analytic at z

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

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

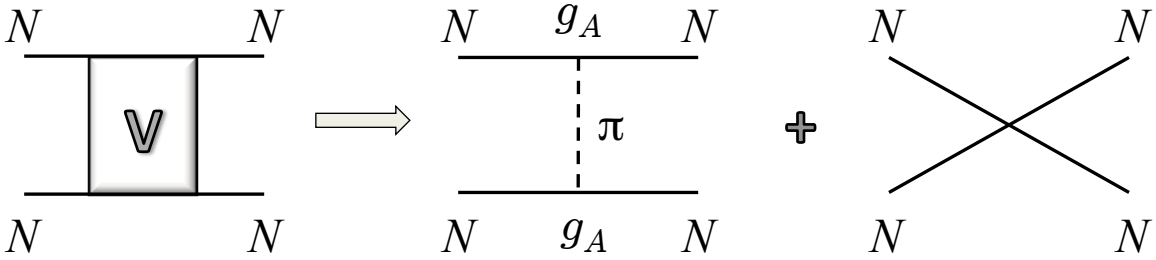
Of course, we don't know *a priori* how to construct this new basis. But if we perform eigenvector continuation for all k degenerate eigenvectors together, we remove convergence problems due to the branch point at z.

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



Application: Neutron matter simulations

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

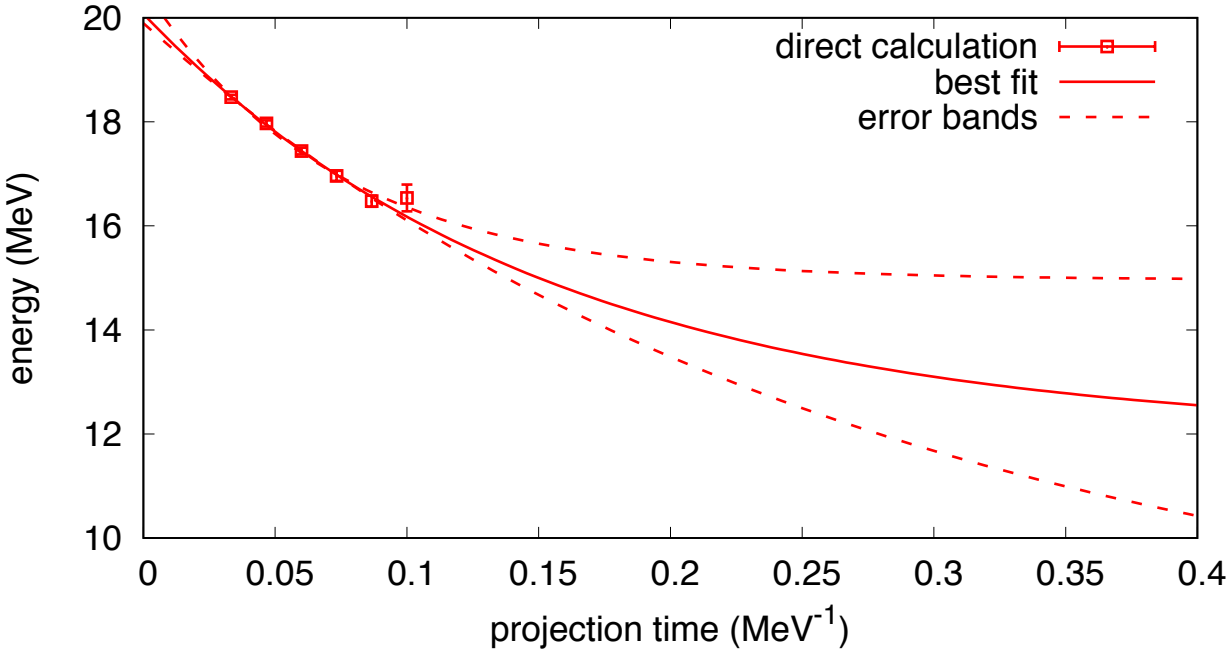


V^{OPEP} Contact interactions

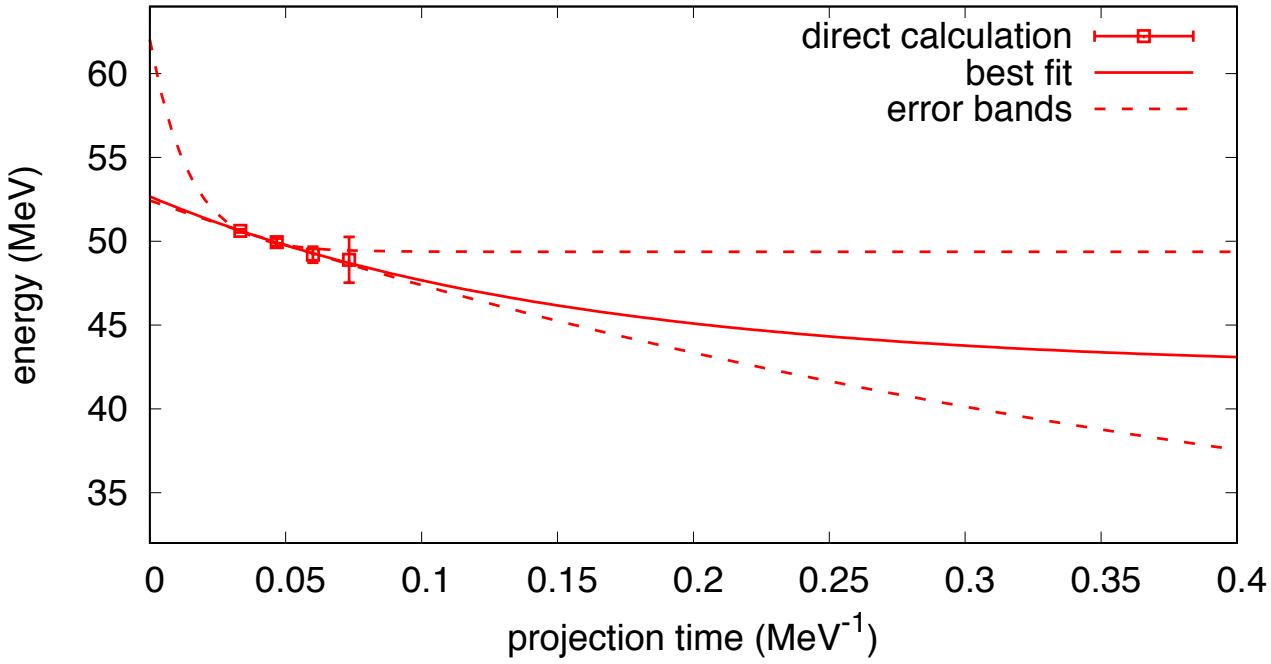
As a challenge to the eigenvector continuation technique, we use a lattice action for one-pion exchange that causes severe Monte Carlo sign oscillations.

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

Use Monte Carlo simulations to compute projection amplitudes

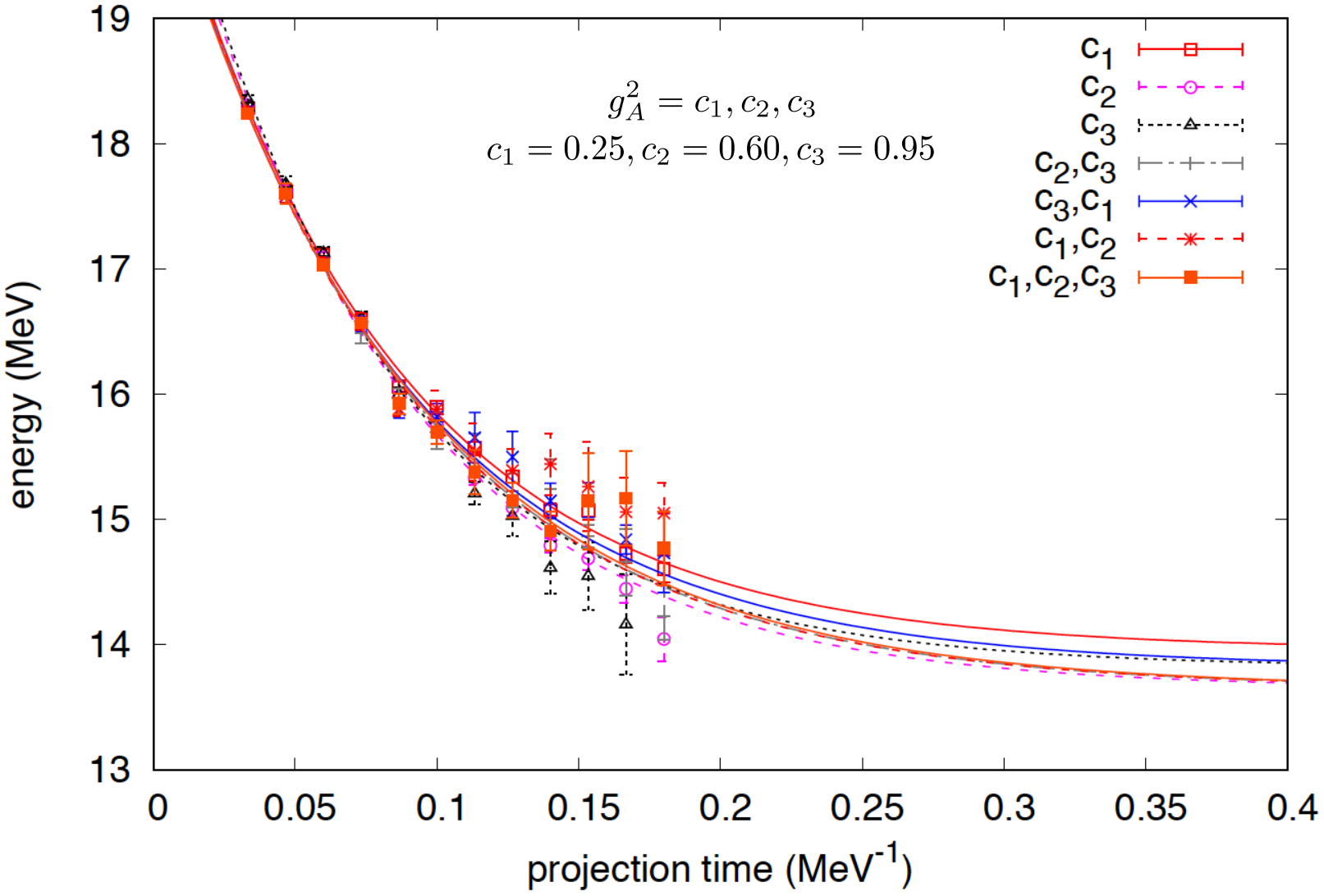
$$N_{k',k} = \langle \psi_{\text{init}} | \; H(c_{k'}) \quad H(c_k) \; | \psi_{\text{init}} \rangle$$

$$H_{k',k} = \langle \psi_{\text{init}} | \; H(c_{k'}) \quad H(c_\odot) \quad H(c_k) \; | \psi_{\text{init}} \rangle$$

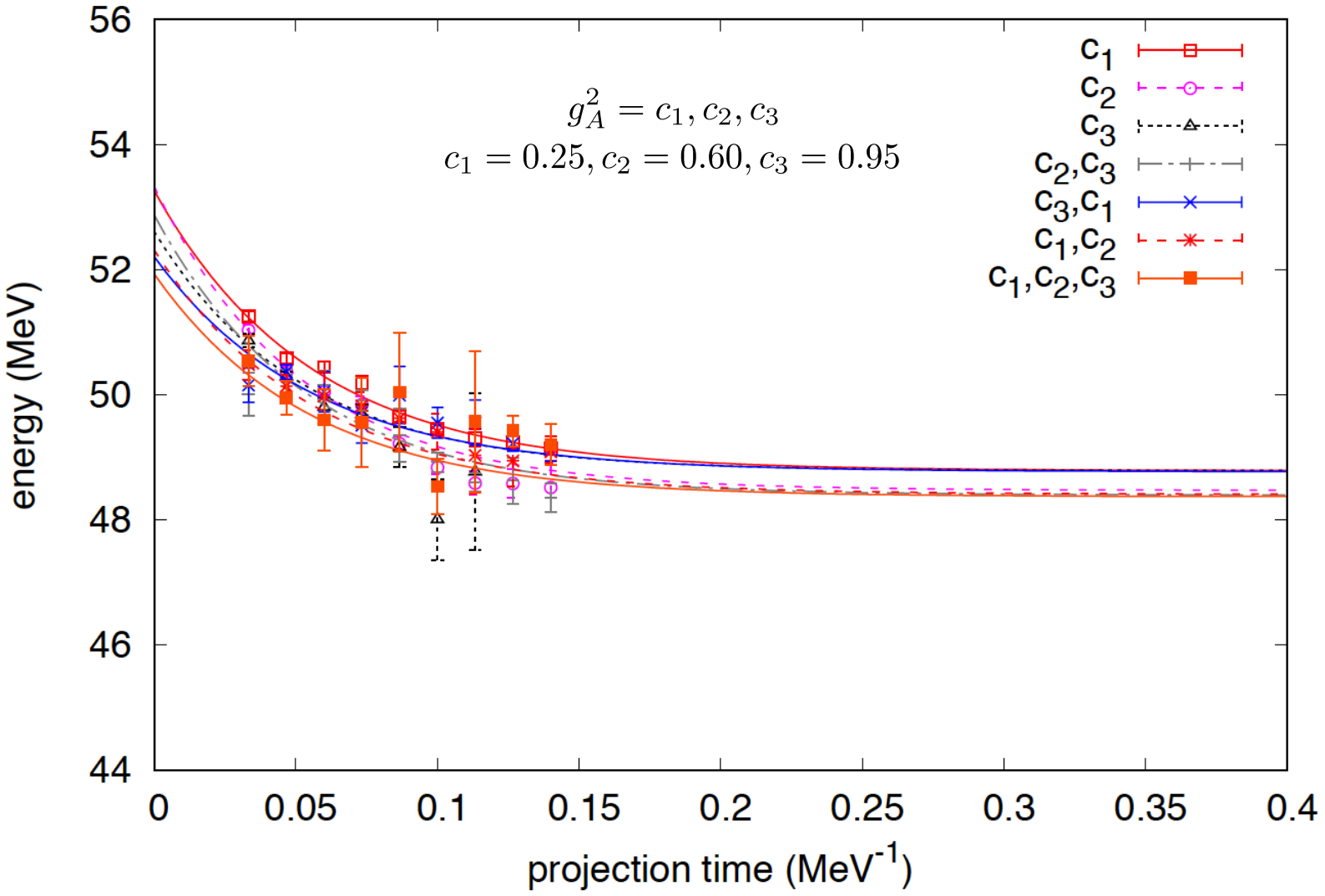
Solve the generalized eigenvalue problem by finding the eigenvalues and eigenvectors of

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

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



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



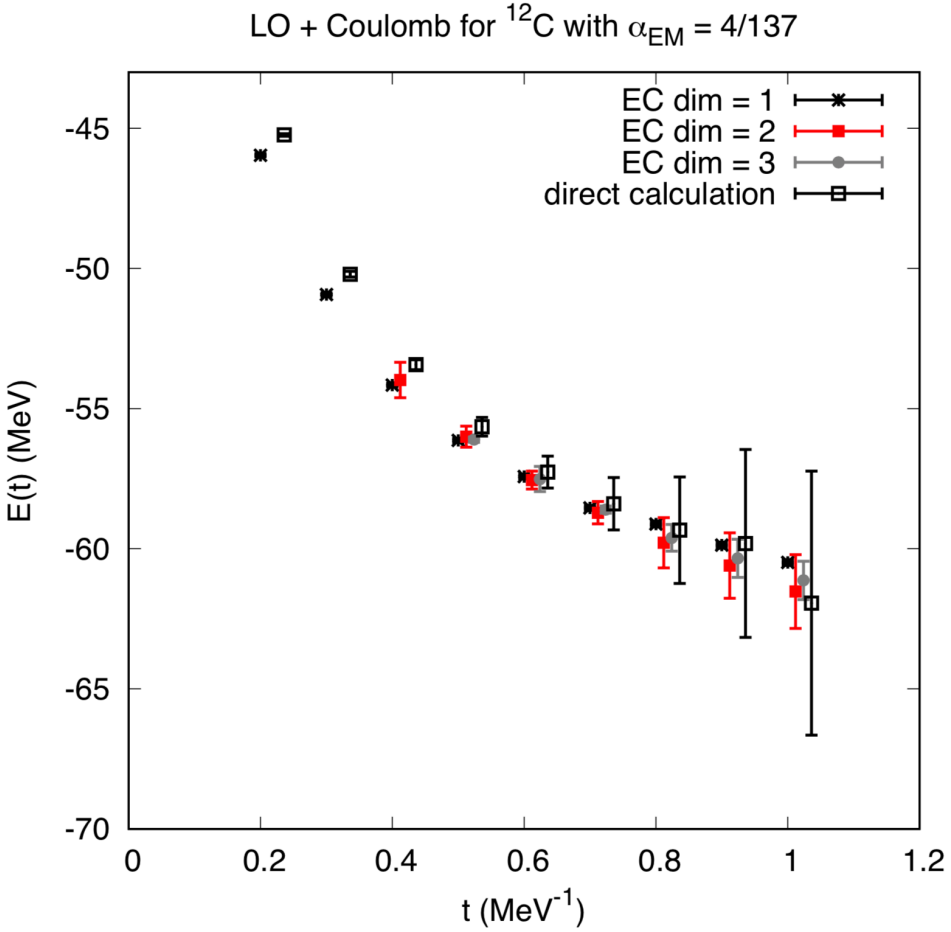
g_A^2 values	$E_0(N=6)$ [MeV]	$E_0(N=14)$ [MeV]
c_1	14.0(4)	48.8(6)
c_2	13.7(4)	48.5(7)
c_3	13.8(6)	48.8(8)
c_2, c_3	13.7(4)	48.4(7)
c_3, c_1	13.8(4)	48.8(6)
c_1, c_2	13.7(4)	48.4(7)
c_1, c_2, c_3	13.7(4)	48.4(7)
direct calculation	$12(^{+3}_{-4})$	$42(^{+7}_{-15})$

D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121 (2018) 032501

Eigenvector continuation with error stabilization

D. Frame, N. Li, B.-N. Lu, D.L.

Work in progress



Eigenvector Continuation as a Fast and Accurate Emulator for Uncertainty Quantification in Nuclear Systems

A. Ekström,[1,*] K. Hebeler,[2,3,†] S. König,[2,3,‡] D. Lee,[4,§] and A. Schwenk[2,3,5,¶]

Work in progress

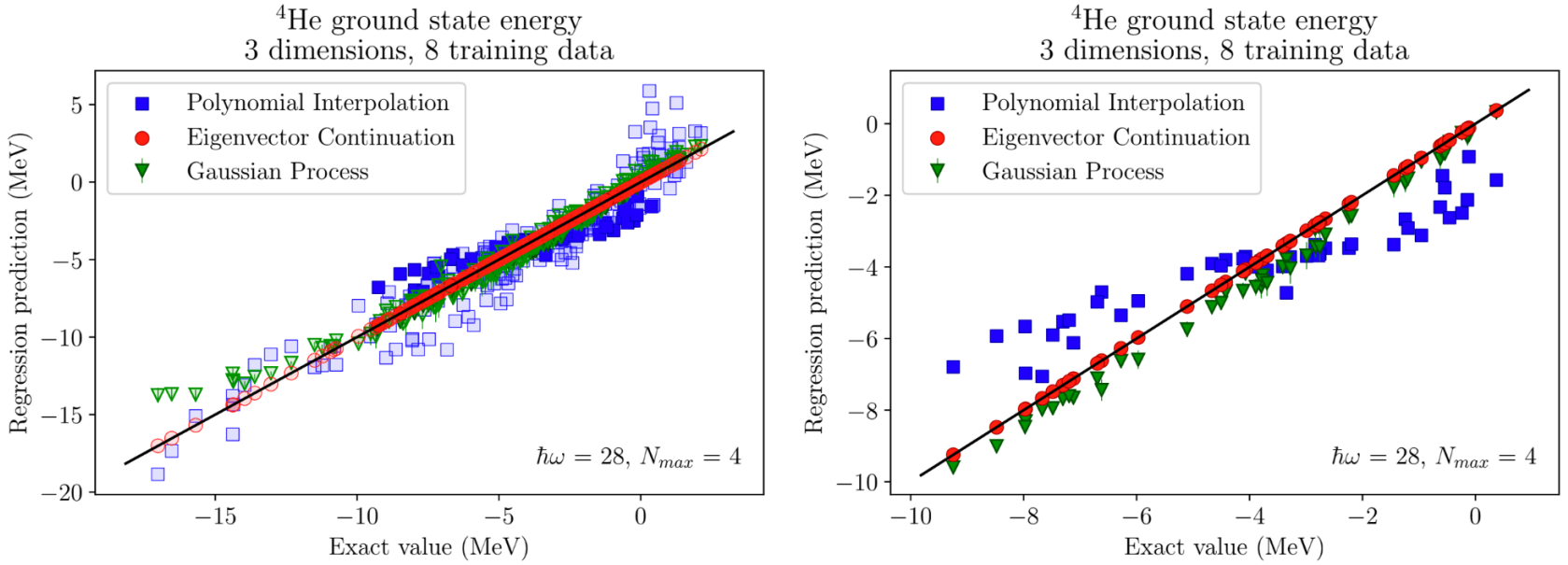
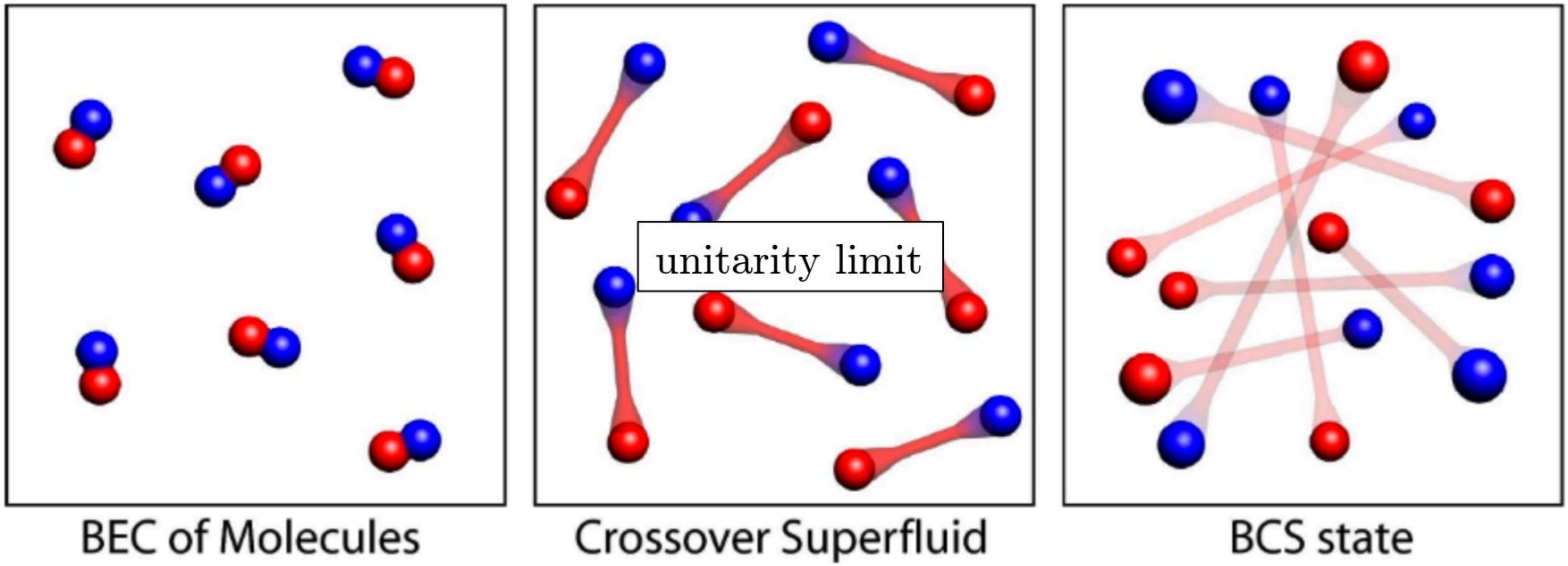


Figure 1. Cross validation for the ^{4}He ground-state energy using 8 training data points to explore a space where the first three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols); see text for how these are defined. The right panel shows the same data restricted to interpolation samples.

Superfluidity and pairing in the unitarity limit

R. He, N. Li, B.-N. Lu, D. L.

Work in progress



Ketterle, Zwierlein

Fermi gas in the unitarity limit

The Fermi gas in unitary limit describes non-relativistic two-component fermions with mass m in the limit that the range of the interactions is zero, and interactions are attractive, with the scattering length tuned to infinity. Therefore we are sitting at the threshold where the bound state has zero energy.

Since the unitary limit has no intrinsic length scales, all many-body observables must equal some dimensionless number times the appropriate power of the Fermi momentum, k_F. For energies and temperatures, there will also be a factor of the inverse particle mass, m^{-1}.

For example, the energy per particle must be proportional the Fermi energy, E_F. This similar to the case for a free non-interacting Fermi gas. For the free Fermi gas, the ground state energy per particle in the thermodynamic limit is

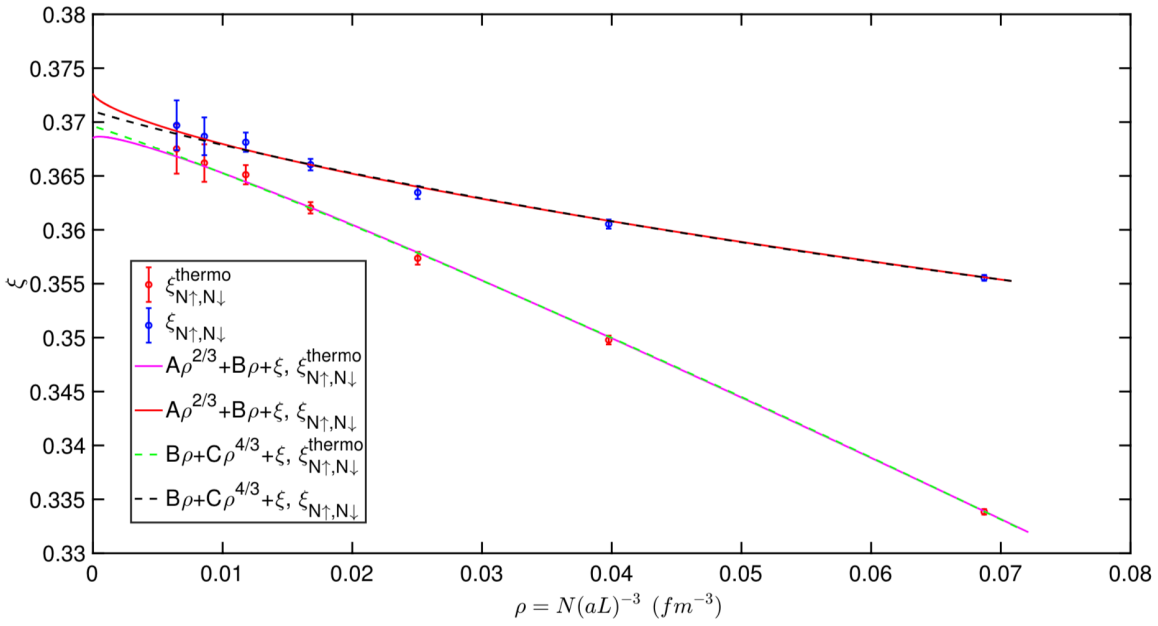
$$\frac{E_0^{\text{free}}}{A} = \frac{3}{5} E_F$$

It is conventional to define the parameter ξ for the ratio between the ground state energy per particle in the unitary limit and the ground state energy per particle for the free gas.

$$\frac{E_0}{A} = \xi \frac{E_0^{\text{free}}}{A} = \frac{3}{5} \xi E_F$$

Table 4.2: Bertsch parameter extrapolation to infinite volume for fixed particle number $N = 66$ with different fitting functions.

Function	A	B	C	ξ	err	χ^2/DOF
$A\rho^{2/3} + B\rho + \xi$	0.0824	-0.7046		0.3685	0.0016	1.2
	-0.0100	-0.0040		0.3726	0.0016	1.2
$B\rho + C\rho^{4/3} + \xi$		-0.3447	-0.4283	0.3696	0.0010	1.1
		-0.4130	0.4604	0.3710	0.0010	1.3



Theory: 0.372(5) Carlson, Gandolfi, Schmidt, Zhang, PRA 84 (2011) 061602(R)
Experiment: 0.376(4) Ku, Sommer, Cheuk, Zwierlein, Science 335 (2012) 563

Superfluidity and pairing correlations

The two-body density matrix is defined as

$$\rho_2(\vec{r}\,'_1, \vec{r}\,'_2, \vec{r}_1, \vec{r}_2) = \left\langle \psi^\dagger_\downarrow(\vec{r}\,'_2)\psi^\dagger_\uparrow(\vec{r}\,'_1)\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2) \right\rangle$$

Long-range correlations in the two-body density matrix is a signature for pair superfluidity:

$$\rho_2(\vec{r}\,'_1, \vec{r}\,'_2, \vec{r}_1, \vec{r}_2) \to \alpha N/2 \cdot \phi^*(|\vec{r}\,'_1 - \vec{r}\,'_2|)\phi(|\vec{r}_1 - \vec{r}_2|)$$
$$|\vec{r}_1 - \vec{r}\,'_1|, |\vec{r}_2 - \vec{r}\,'_2| \to \infty$$

Yang, RMP 34, 694 (1962)

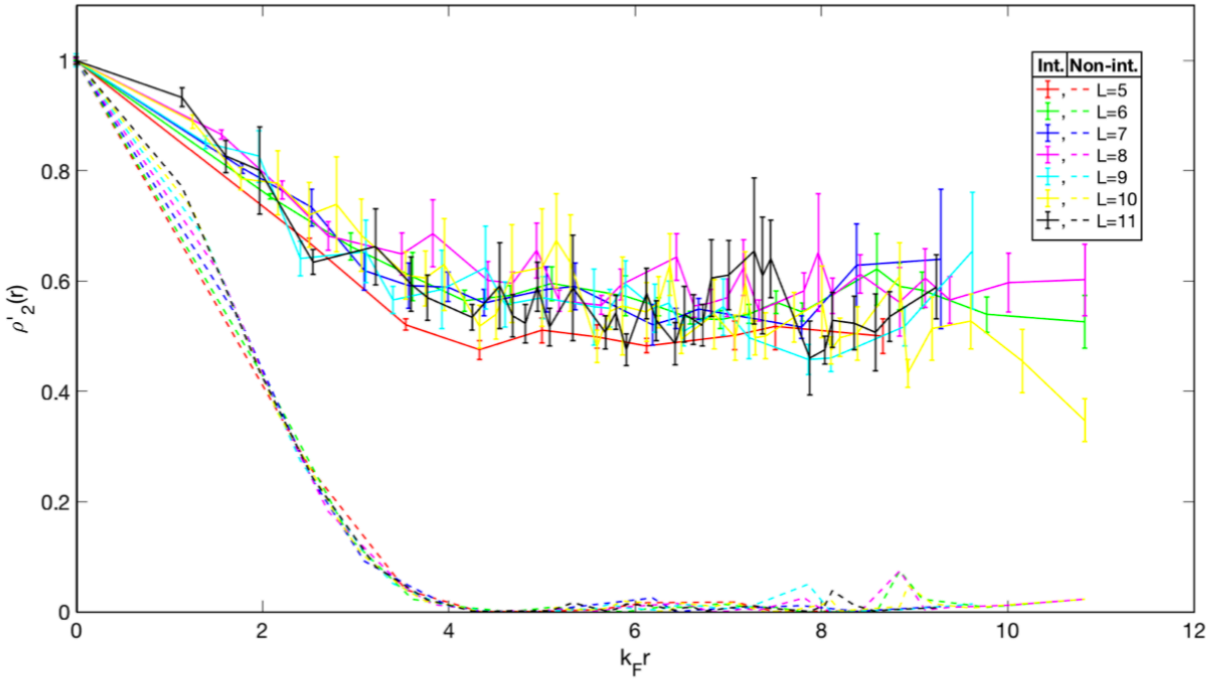
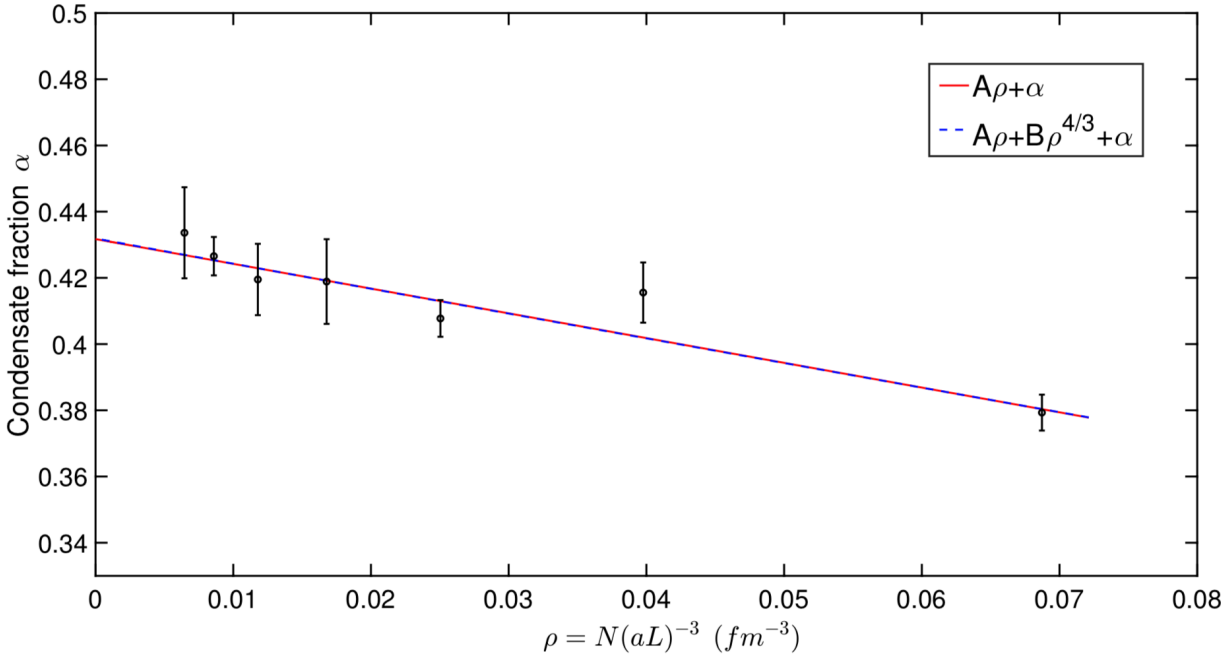


Figure 4.8: Renormalized pair correlation function of interacting (solid curves) and non-interacting (dashed curves) systems. Systems in same lattice, with or without interaction, are plotted with same color.

Table 4.4: Condensate fraction at unitary limit extrapolated to infinite volume for fixed particle number $N = 66$ with different fitting functions.

Function	A	B	α	err	χ^2/DOF
$A\rho + B\rho^{4/3} + \alpha$	-0.7750	0.0623	0.4319	0.0109	0.9
$A\rho + \alpha$	-0.7474		0.4317	0.0047	0.7



Experiment: 0.46(7) Zwierlein, Stan, Schunck, Raupach, Kerman, Ketterle, PRL 92 (2004) 120403

$$\Phi(r) \propto \frac{e^{-r/\zeta_p}}{r}$$

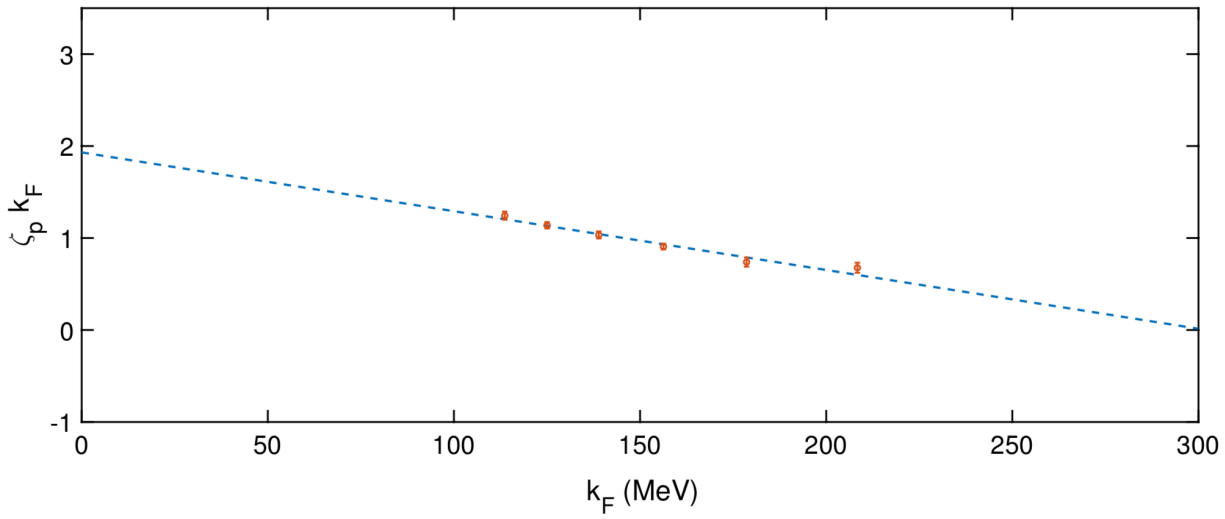


Figure 4.18: Values of $\zeta_p k_F$ as a function of k_F. Measurements are made at large projection time t.

$$\zeta_p = 1.93(9) k_F^{-1}$$

Homework for August 2

Consider a lattice Hamiltonian for one non-relativistic particle interacting with a delta potential at the origin with coupling c,

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

$$H_0 = -\frac{1}{2m}\sum_{\vec{n}}\sum_{l=1,2,3} a^\dagger(\vec{n})\left[a(\vec{n}+\hat{l}) - 2a(\vec{n}) + a(\vec{n}-\hat{l})\right]$$

$$H_1 = a^\dagger(\vec{0})a(\vec{0})$$

Find the ground state energy of this system in a cubic periodic lattice of length 20, mass m equal to 1 (in lattice units), and coupling c ranging from 0 to -10 (in lattice units).

Now use eigenvector continuation with training values
c = 0.0, -0.2, -0.4, -0.6, -0.8 to find a variational approximation to the ground state energy for coupling c ranging from 0 to -10 (in lattice units) using the first one, two, three, four, and five training eigenvectors.

Results should look like this: