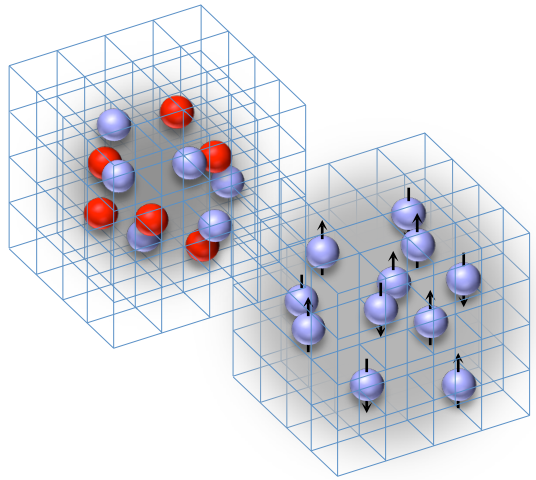
Monte Carlo algorithms for nuclear lattice simulations

Dean Lee
Facility for Rare Isotope Beams
Department of Physics and Astronomy
Michigan State University
Nuclear Lattice EFT Collaboration

INT Workshop
Advances in Monte Carlo Techniques
for Many-Body Systems
August 15, 2018



FRIB

MICHIGAN STATE UNIVERSITY

National Nuclear Security Administration

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project

JÜLICH
FORSCHUNGSZENTRUM

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

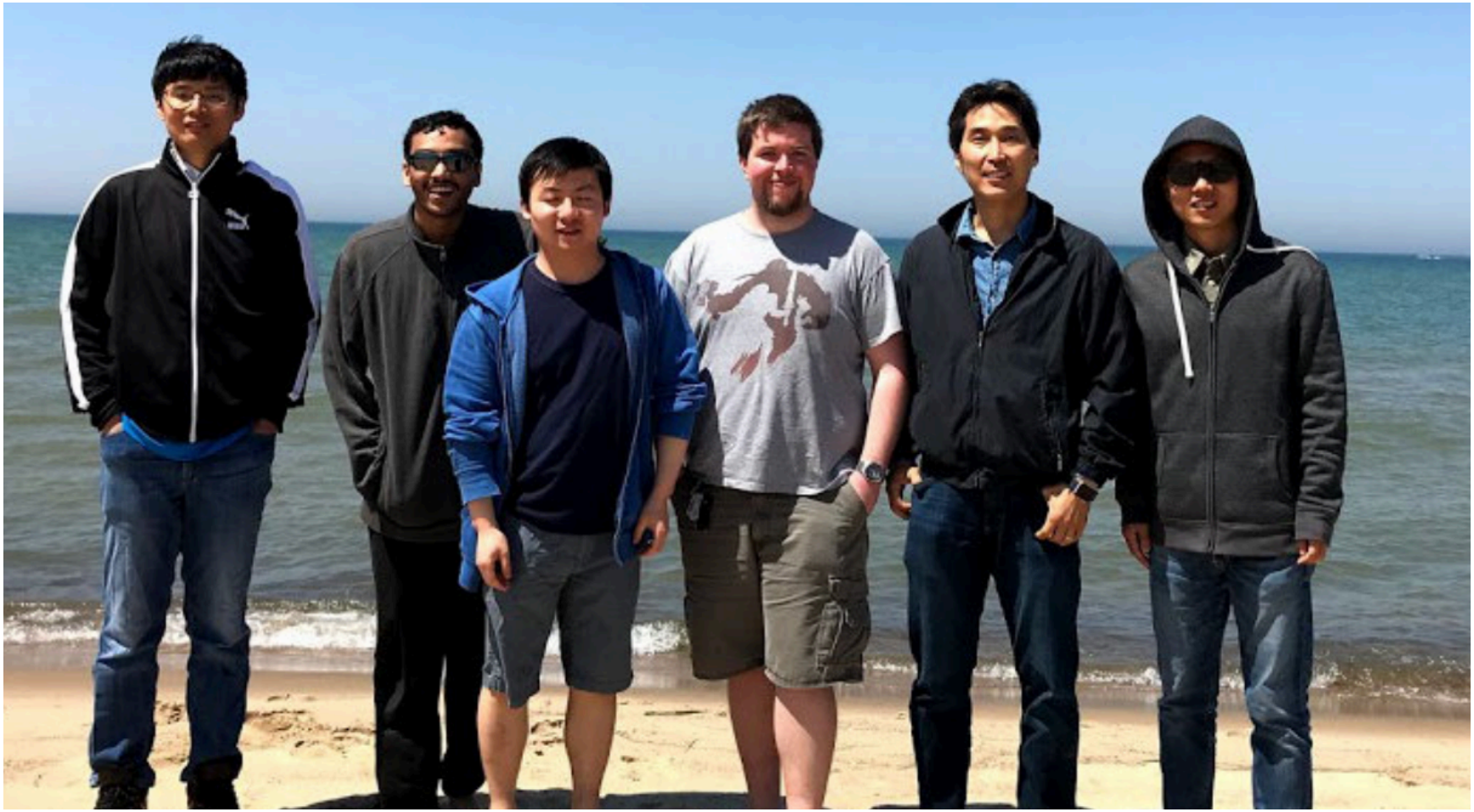
Dr. Bing-Nan Lu

Avik Sarkar

Rongzheng He

Dillon Frame

Dr. Ning Li



Not shown: Joseph Bonitati, Caleb Hicks

Outline

Lattice effective field theory

Pinhole algorithm

Applications to nuclear structure

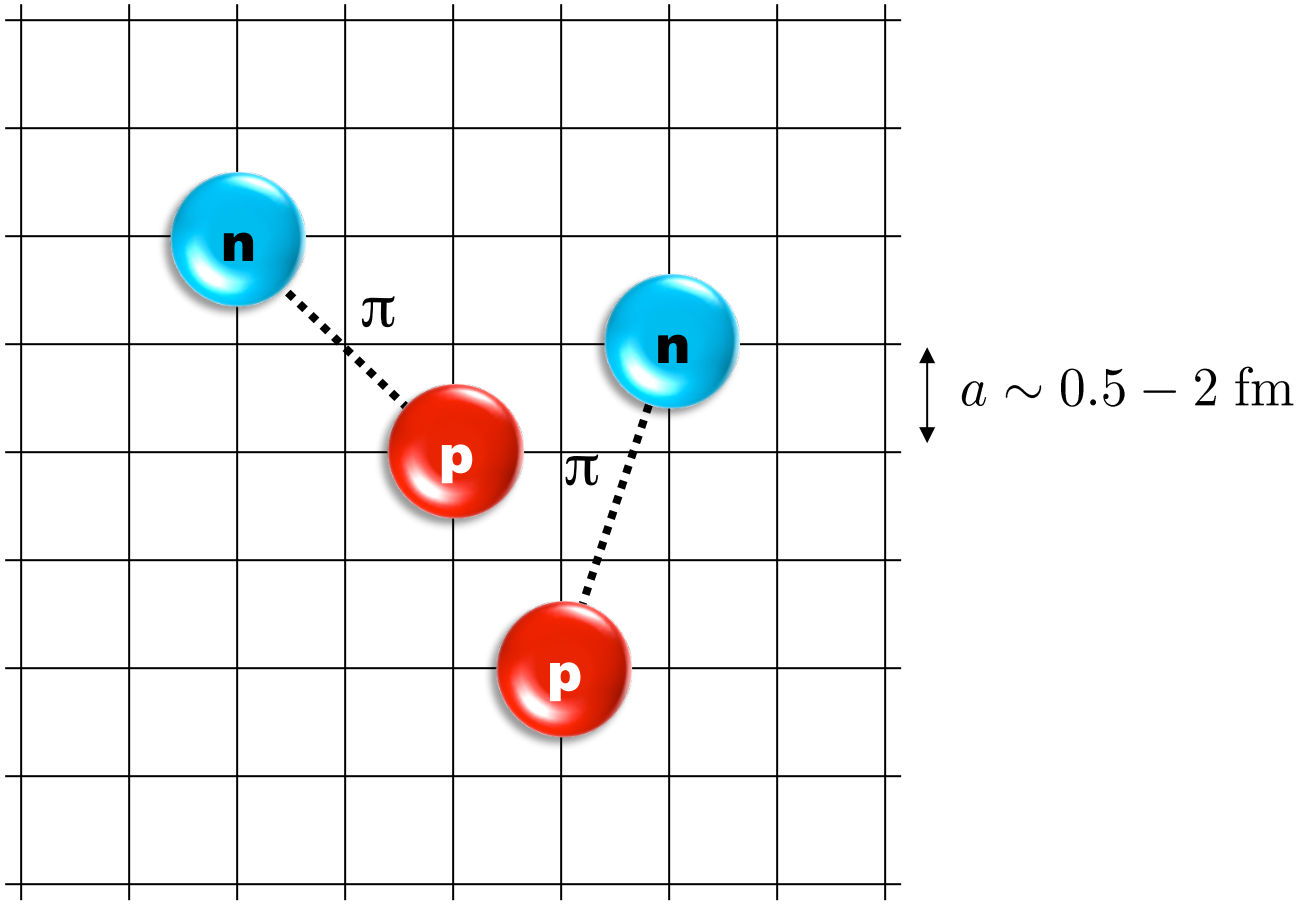
Applications to thermodynamics

Eigenvector continuation

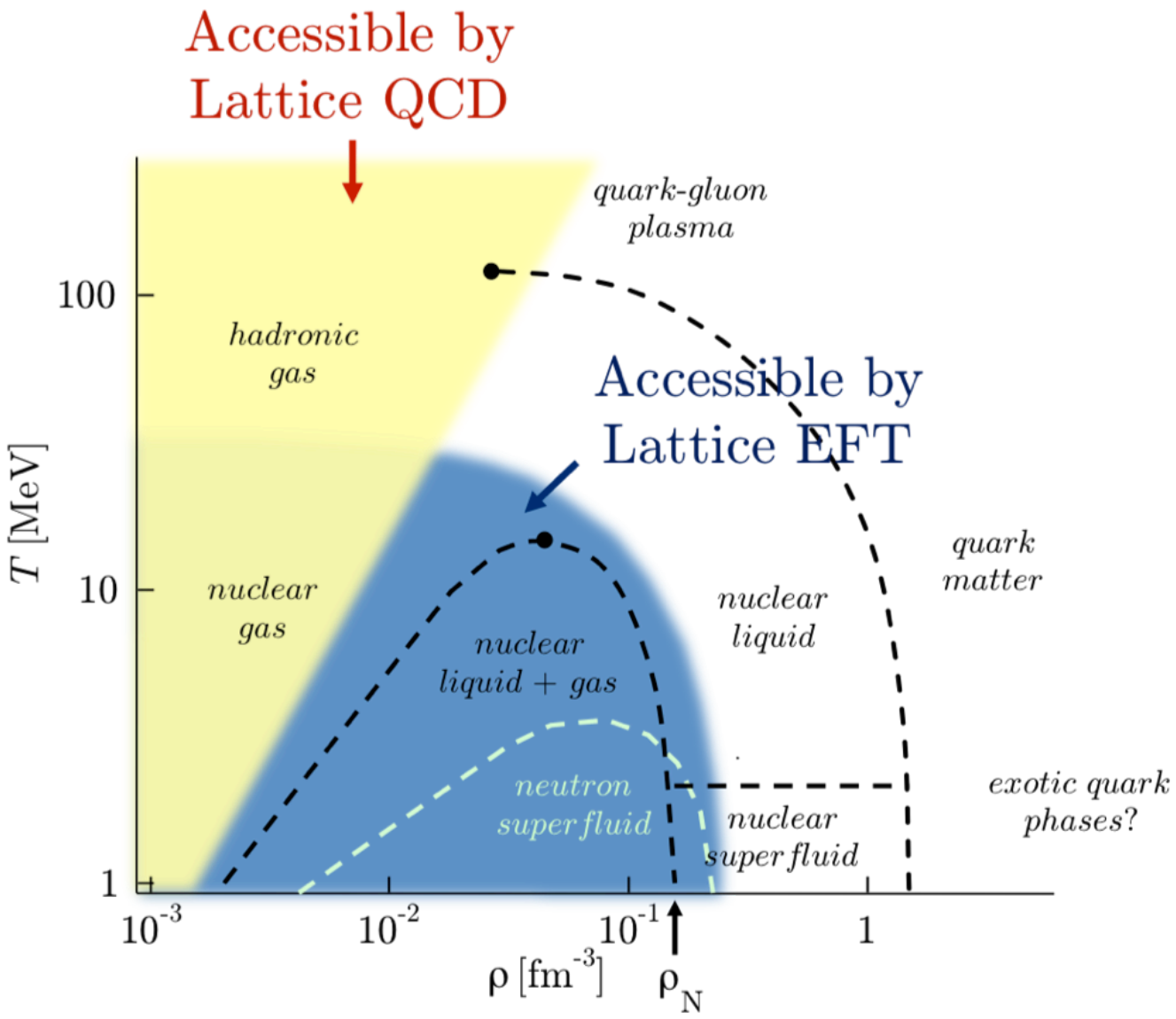
Applications of eigenvector continuation

Summary and outlook

Lattice effective field theory

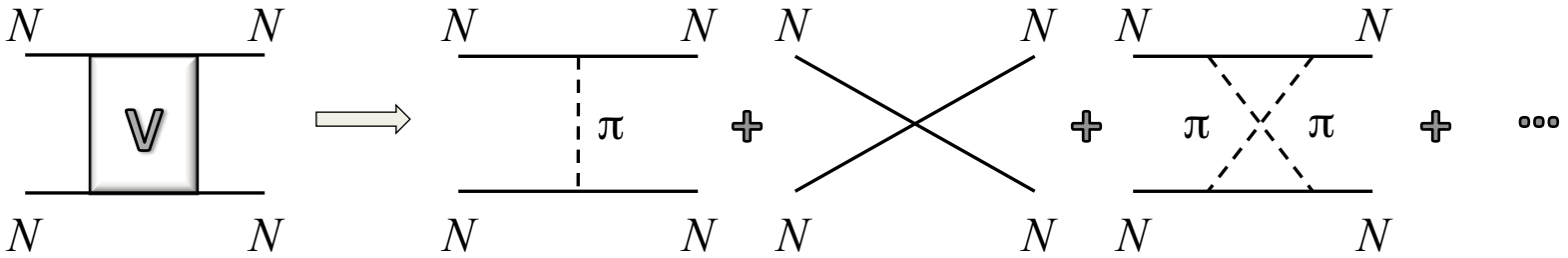


Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
TALENT summer school lectures: qmc2016.wordpress.ncsu.edu


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

Chiral effective field theory

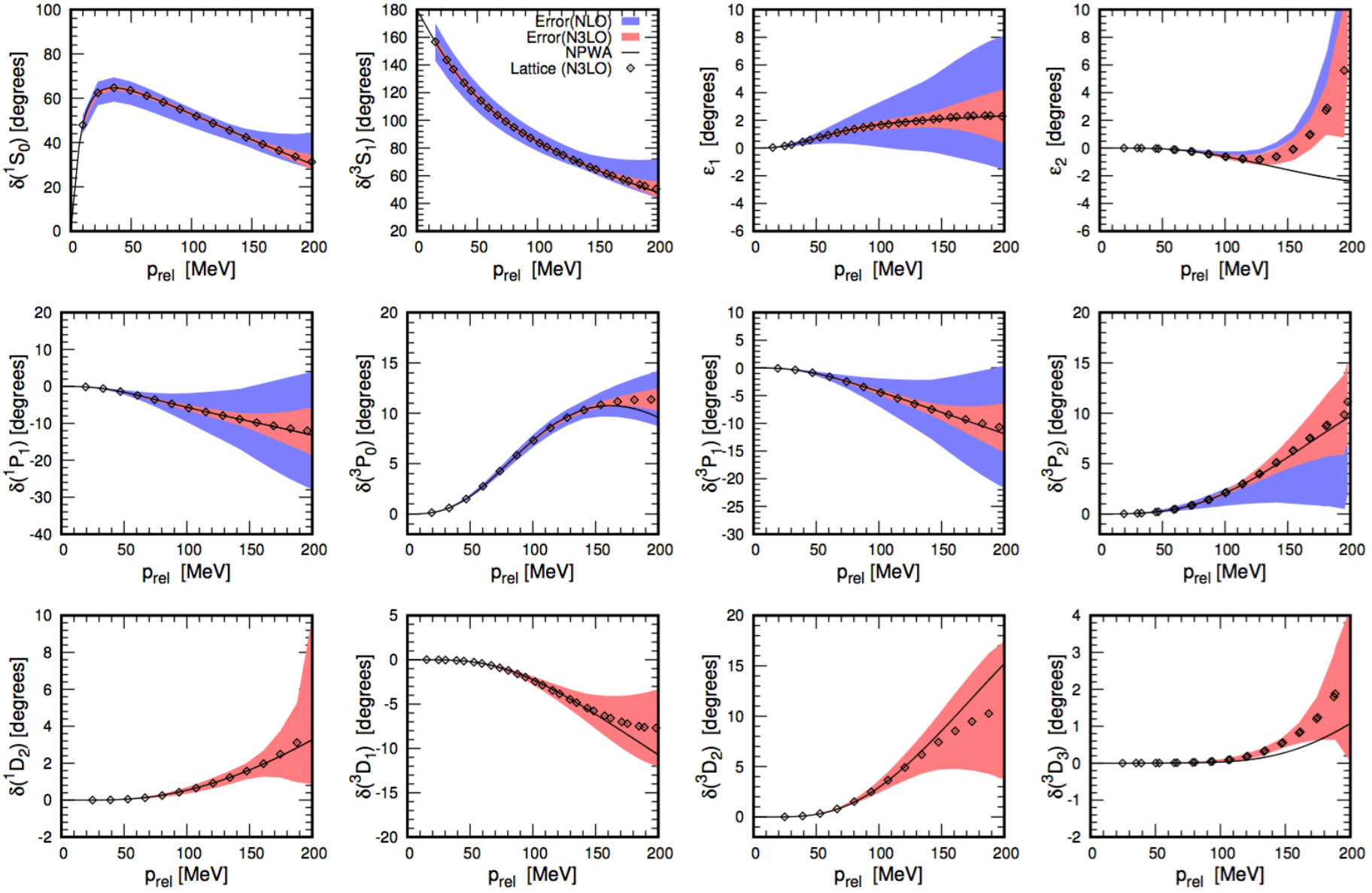
Construct the effective potential order by order



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

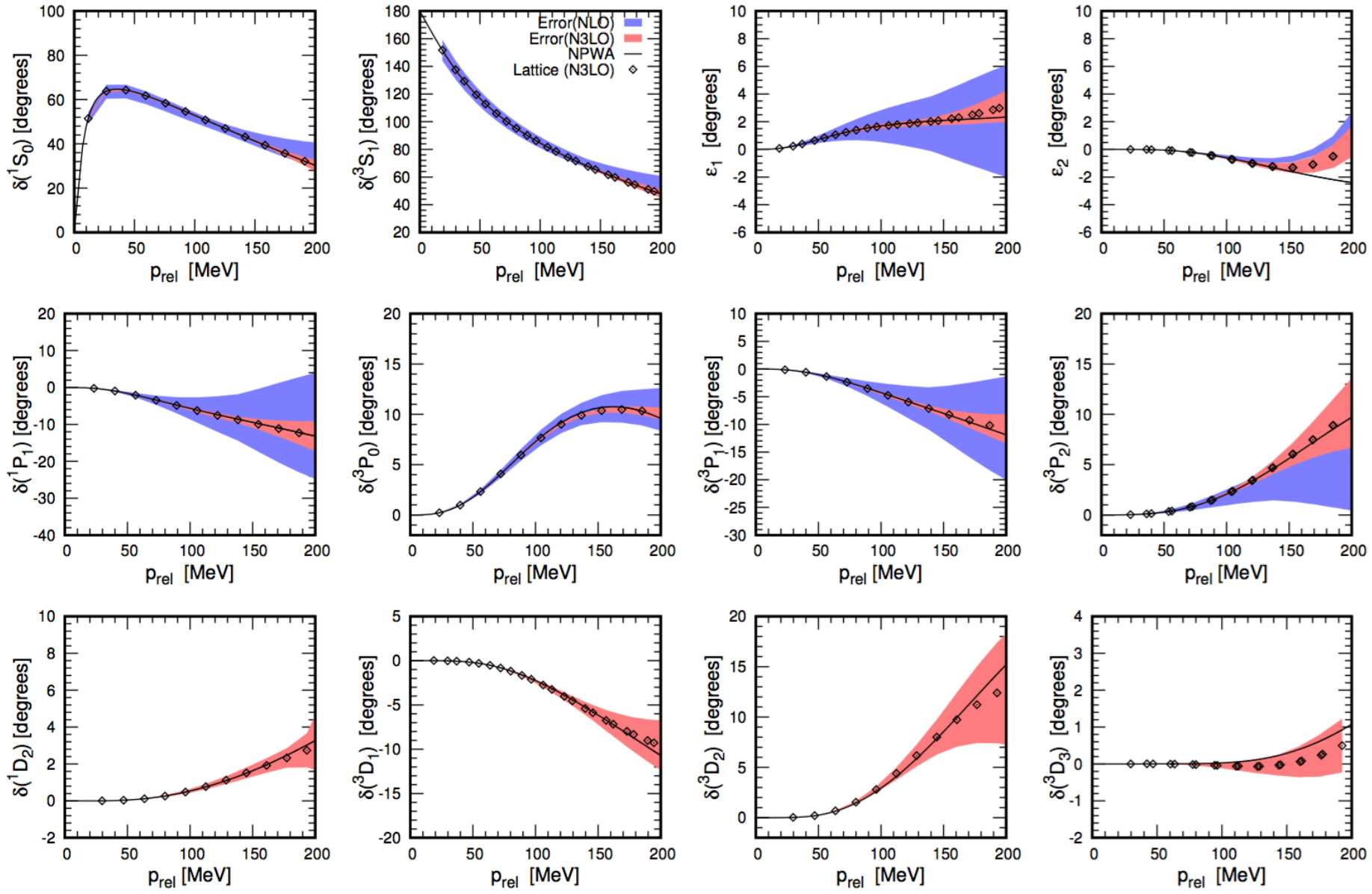
Leading order (LO) Next-to-leading order (NLO)

$a = 1.973\,\mathrm{fm}$



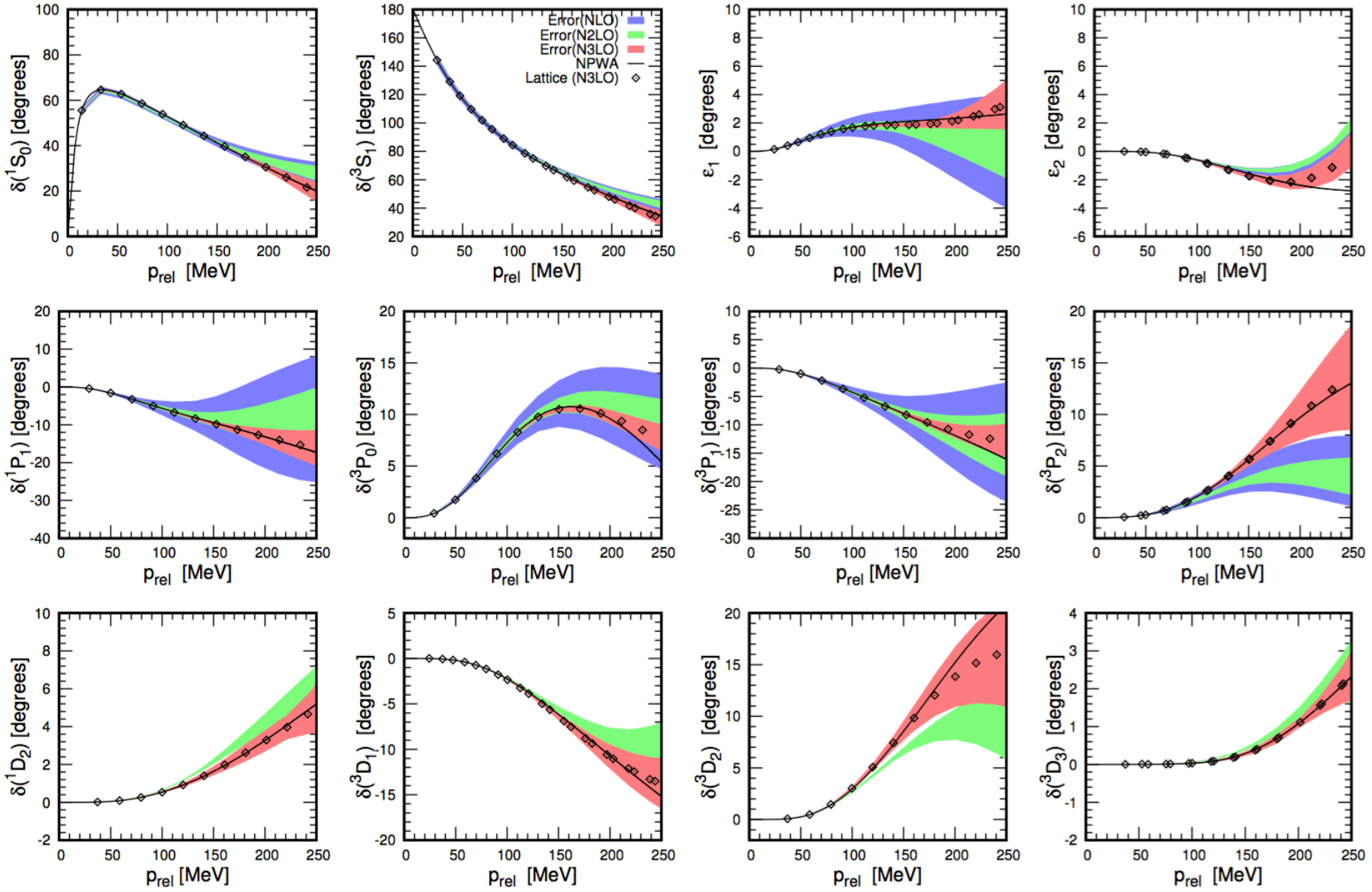
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, 1806.07994

$a = 1.644\,\mathrm{fm}$



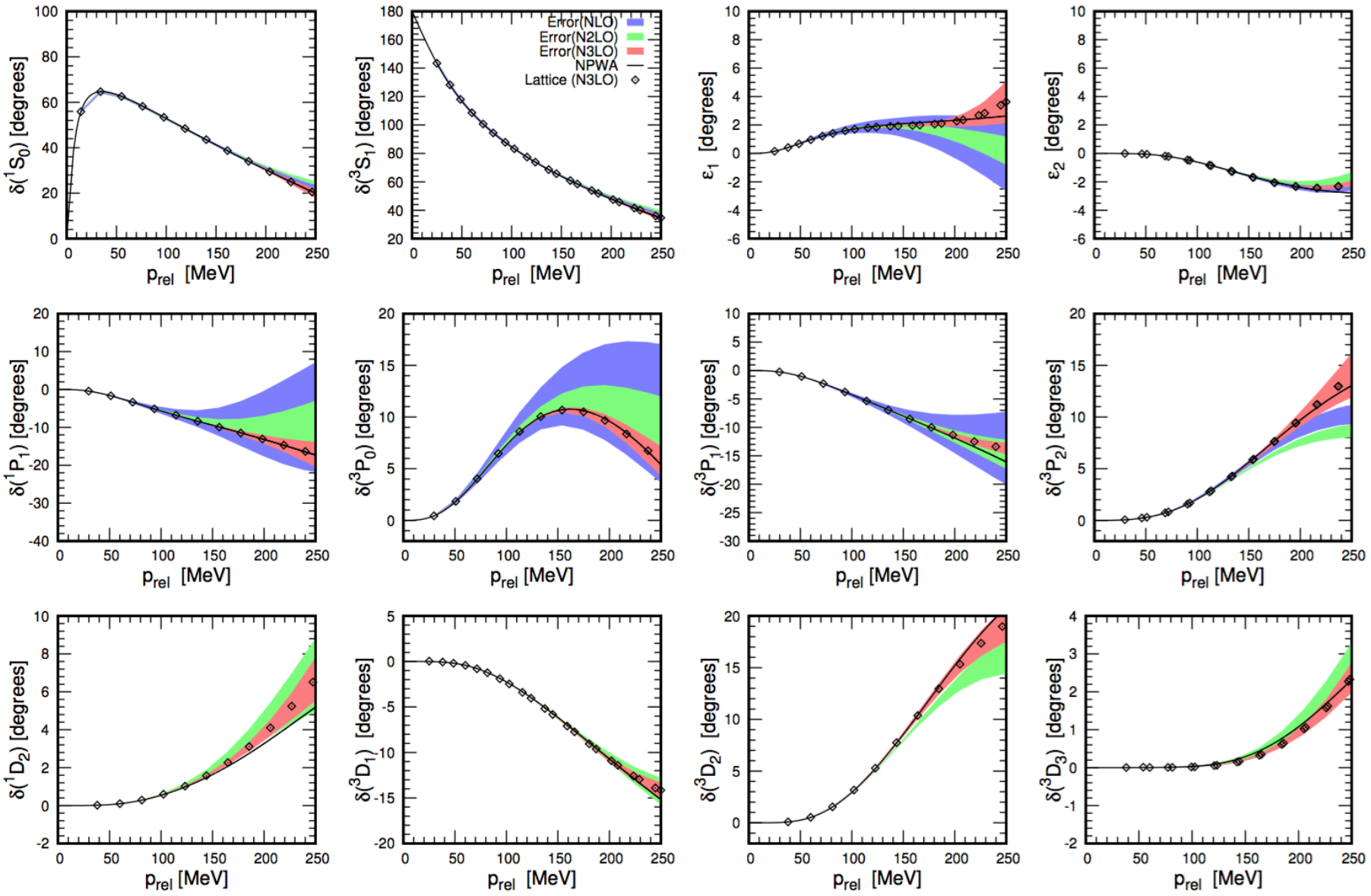
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, 1806.07994

$a = 1.315\,\mathrm{fm}$



Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, 1806.07994

$a = 0.987\,\mathrm{fm}$



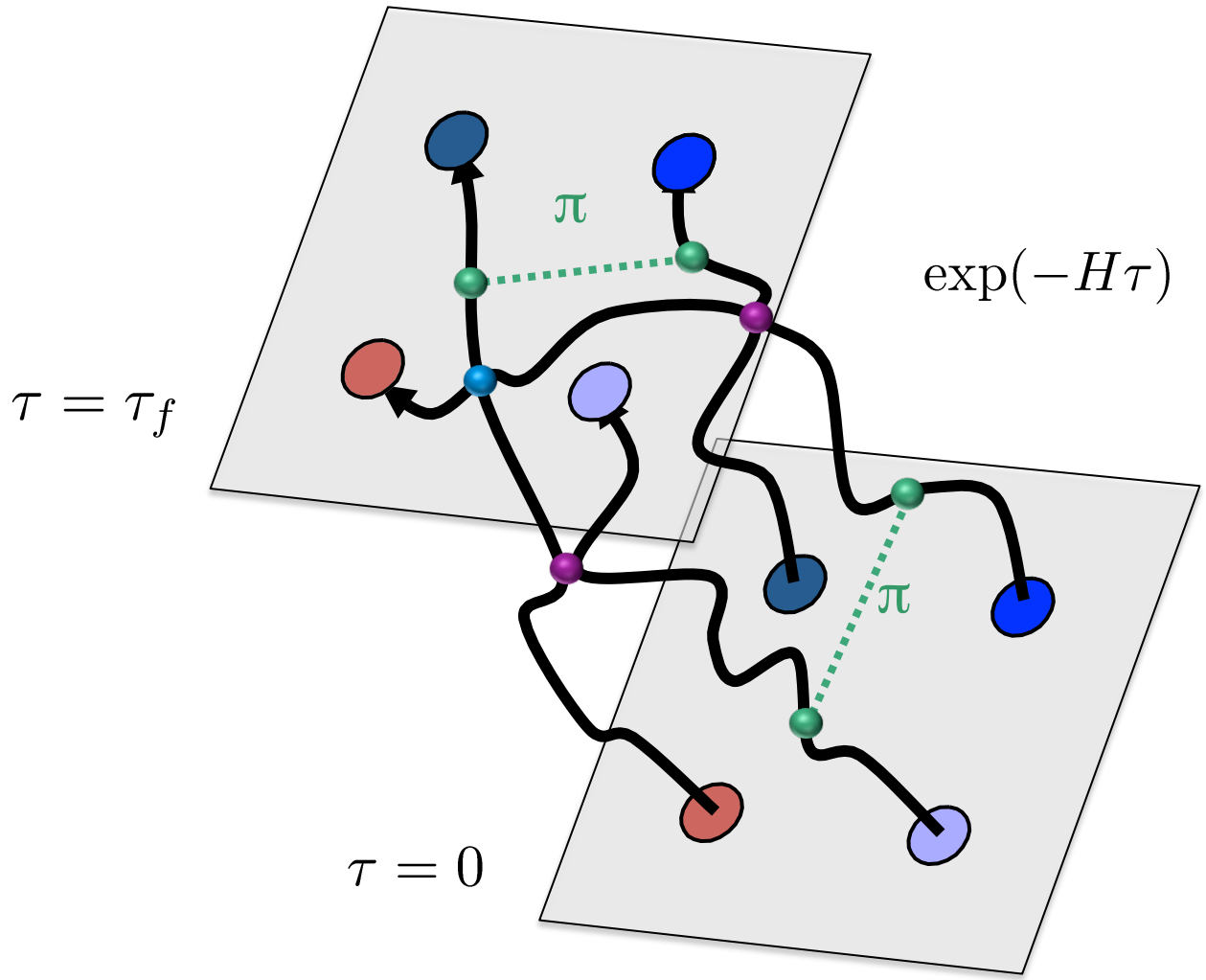
Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, 1806.07994

TABLE II. The deuteron properties and S-wave parameters calculated with the full NN interaction up to chiral order $O(Q^4)$ using $a = 0.99$ fm. The error bars we quote in this table indicate uncertainties from the fitting procedure only.

	LO	NLO	N^{2}LO	N^{3}LO	Empirical
E_d (MeV)	2.2246 ± 0.0002	2.224575 ± 0.000016	2.224575 ± 0.000025	2.224575 ± 0.000011	2.224575(9)[24]
$A_s(\mathrm{fm}^{-1/2})$	0.8662 ± 0.0007	0.8772 ± 0.0003	0.8777 ± 0.0004	0.8785 ± 0.0004	0.8846(9)[25]
η	0.0212 ± 0.0000	0.0258 ± 0.0001	0.0257 ± 0.0002	0.0254 ± 0.0001	0.0256(4) [26]
$Q_d(\mathrm{fm}^2)$	0.2134 ± 0.00000	0.2641 ± 0.0016	0.2623 ± 0.0023	0.2597 ± 0.0013	0.2859(3) [27]
r_d (fm)	1.9660 ± 0.0001	1.9548 ± 0.0005	1.9555 ± 0.0008	1.9545 ± 0.0005	1.97535(85) [28]
$a_{^3S_1}$	5.461 ± 0.000	5.415 ± 0.001	5.421 ± 0.002	5.417 ± 0.001	5.424(4) [29]
$r_{^3S_1}$	1.831 ± 0.0003	1.759 ± 0.002	1.760 ± 0.003	1.758 ± 0.002	1.759(5)[29]
$a_{^1S_0}$	-23.8 ± 0.1	-23.69 ± 0.05	-23.8 ± 0.2	-23.678 ± 0.038	−23.748(10)[29]
$r_{^1S_0}$	2.666 ± 0.001	2.647 ± 0.003	2.69 ± 0.02	2.647 ± 0.004	2.75(5) [29]

Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, 1806.07994

Euclidean time projection



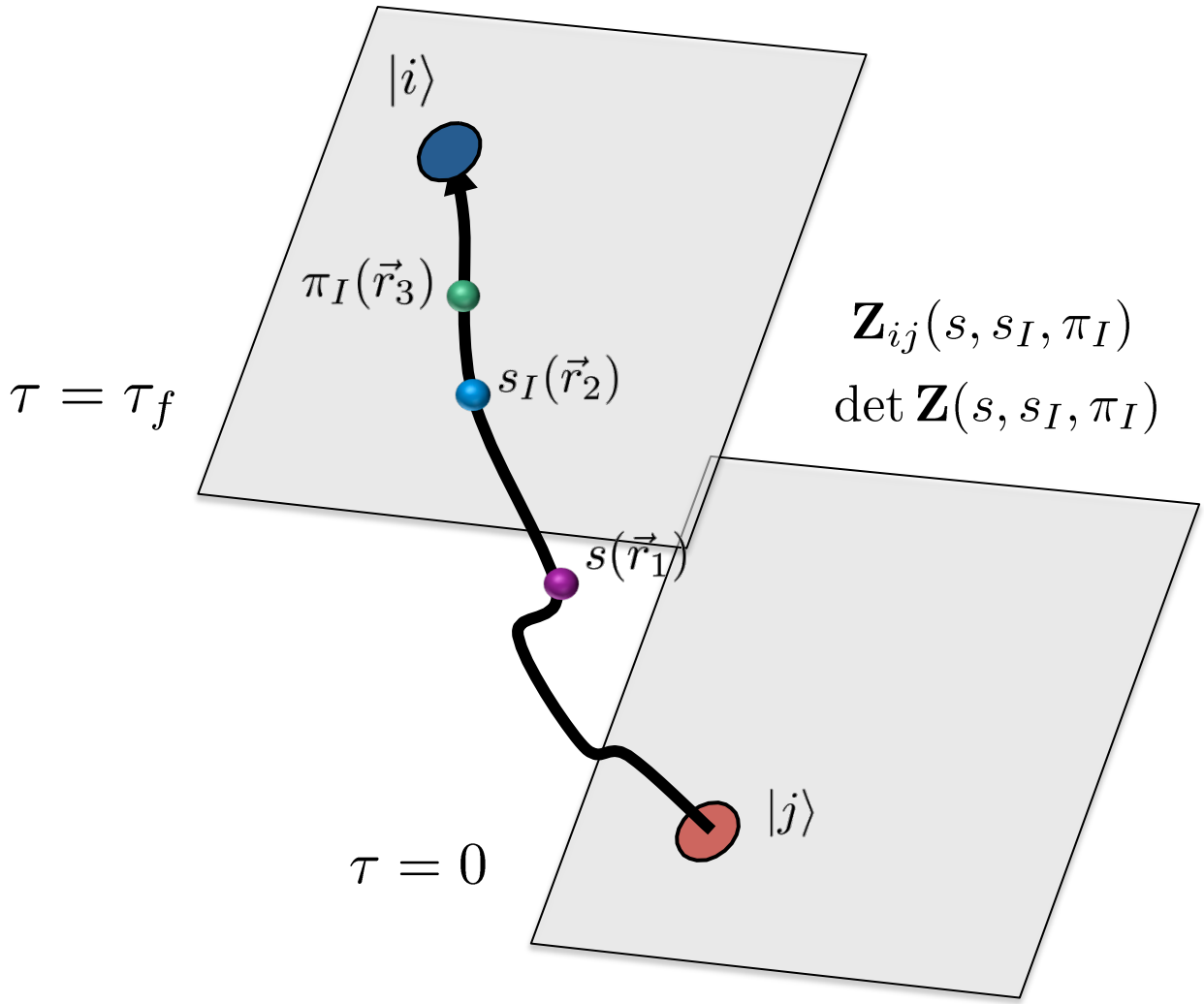
Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] \qquad \times \quad (N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle\!\bullet \quad sN^\dagger N$$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.


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

Challenge

There has been no efficient algorithm available for 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

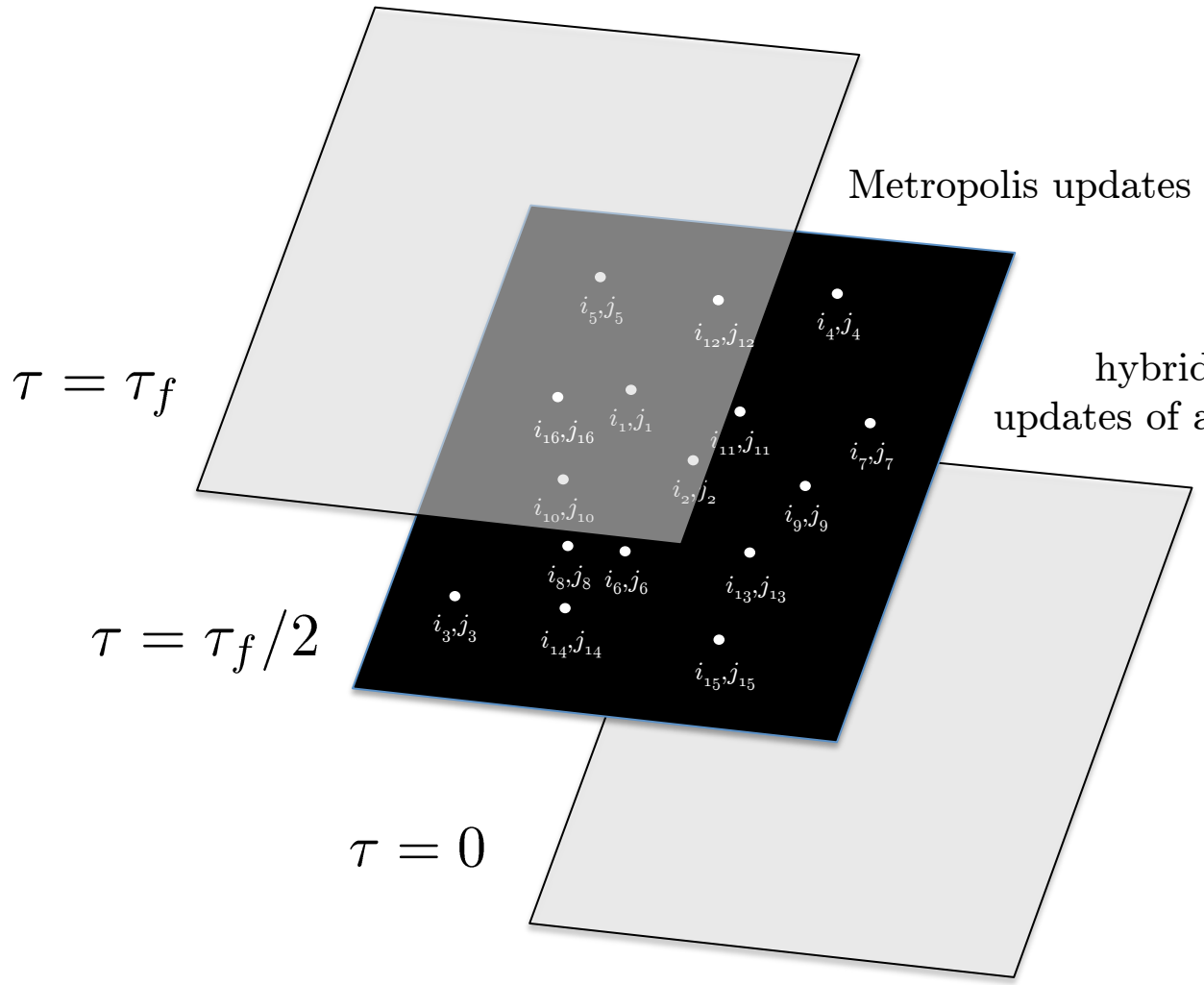
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

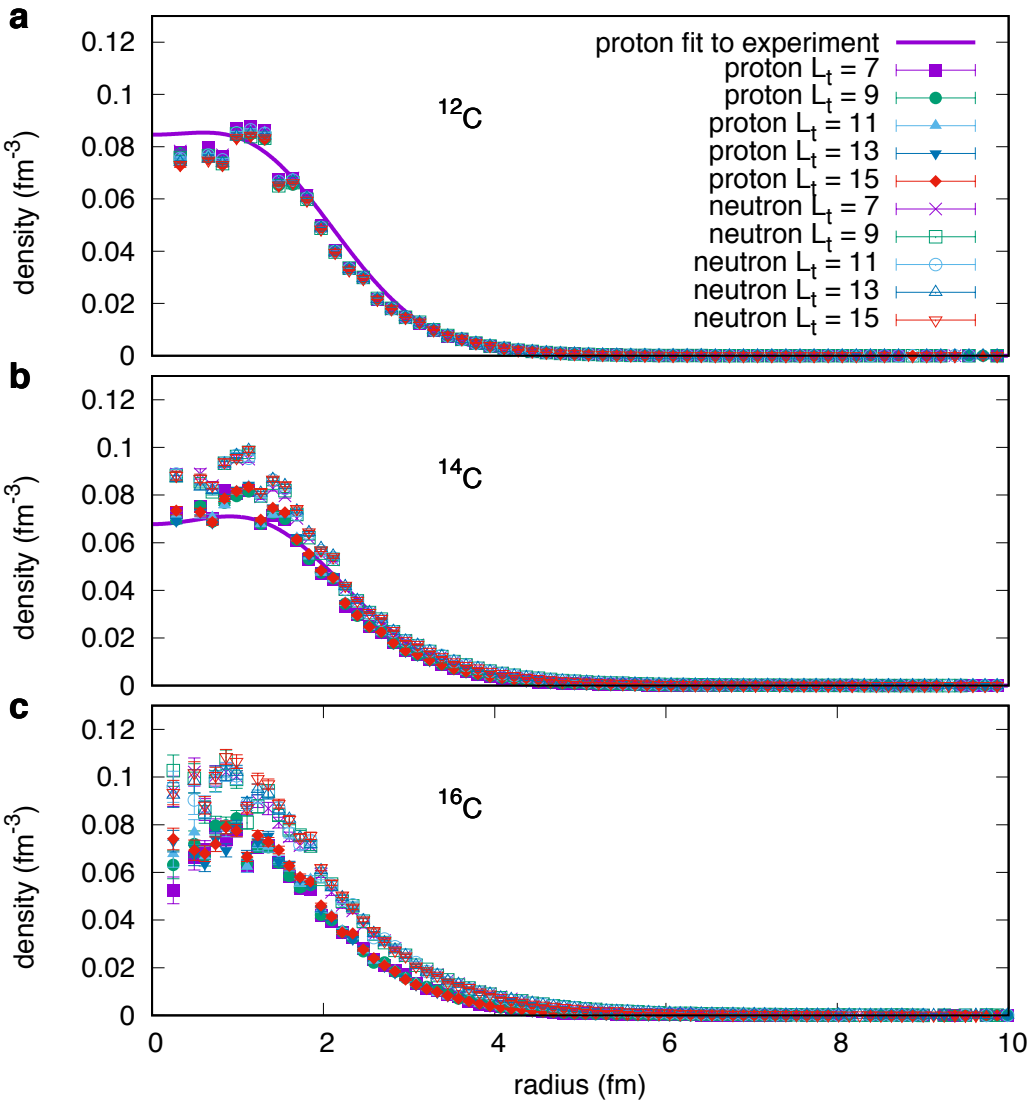
We construct the normal-ordered A-body density operator

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

In the simulations we do Monte Carlo sampling of the amplitude

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

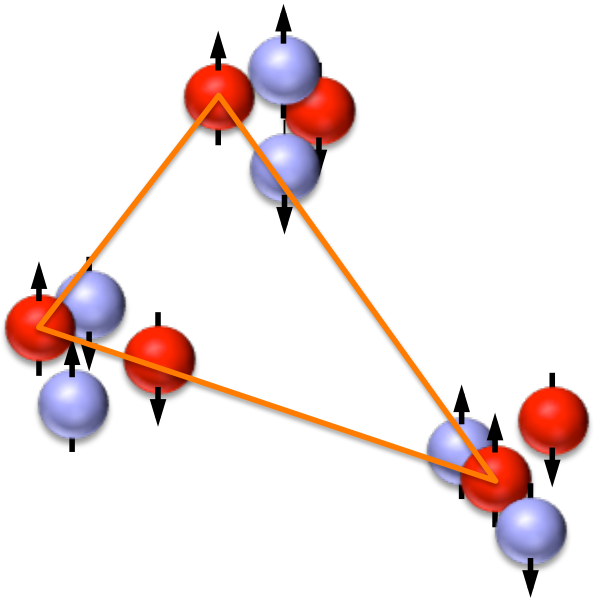

Metropolis updates of pinholes
hybrid Monte Carlo
updates of auxiliary/pion fields
$\tau = \tau_f$
$\tau = \tau_f/2$
$\tau = 0$
i_5,j_5
i_{12},j_{12}
i_4,j_4
i_{16},j_{16}
i_1,j_1
i_{11},j_{11}
i_7,j_7
i_2,j_2
i_{10},j_{10}
i_9,j_9
i_8,j_8
i_6,j_6
i_{13},j_{13}
i_3,j_3
i_{14},j_{14}
i_{15},j_{15}



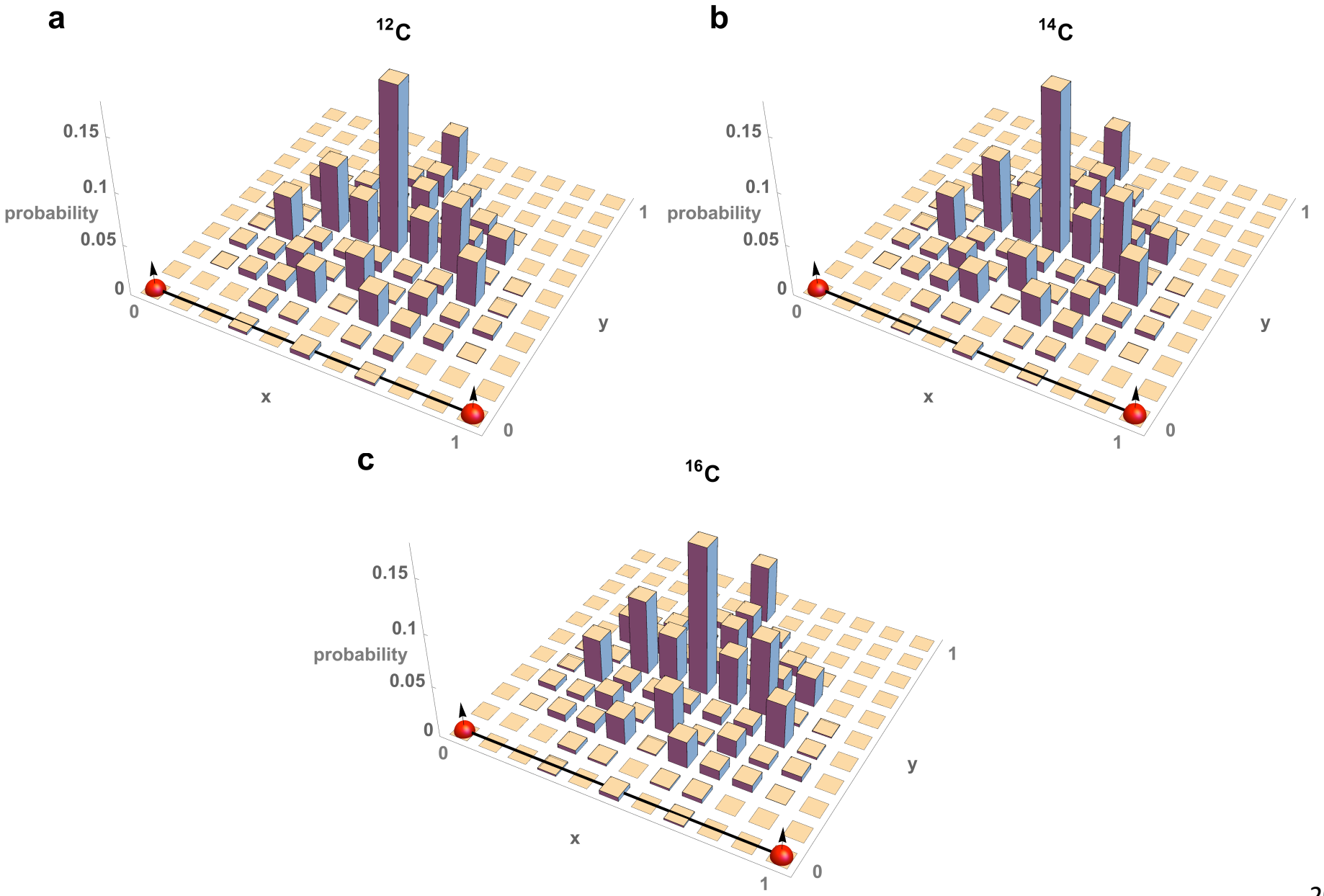
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

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.



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


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

Challenge

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

$$\mathrm{Tr}\exp(-\beta H)$$

The standard method for computing the partition function involves calculating determinants of matrices of size $4V \times 4V$, where V is the number of lattice points filling the spatial volume. Since V is usually several hundred or several thousand, these calculations are very expensive.

Pinhole trace algorithm

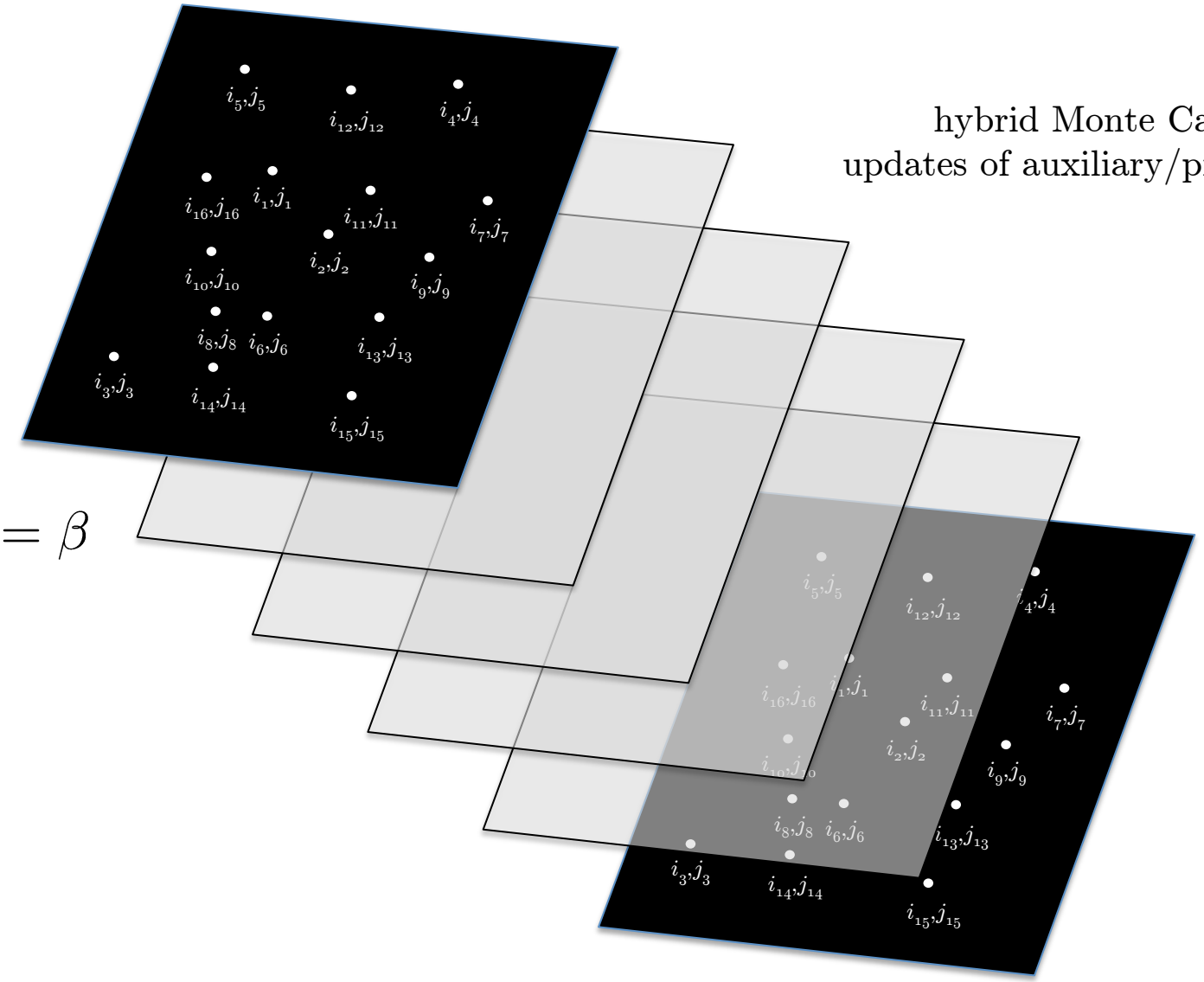
We have developed an alternative method using pinholes that calculates determinants of matrices of size $A \times A$, where A is the number of nucleons. The method does not suffer from severe sign oscillations.

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

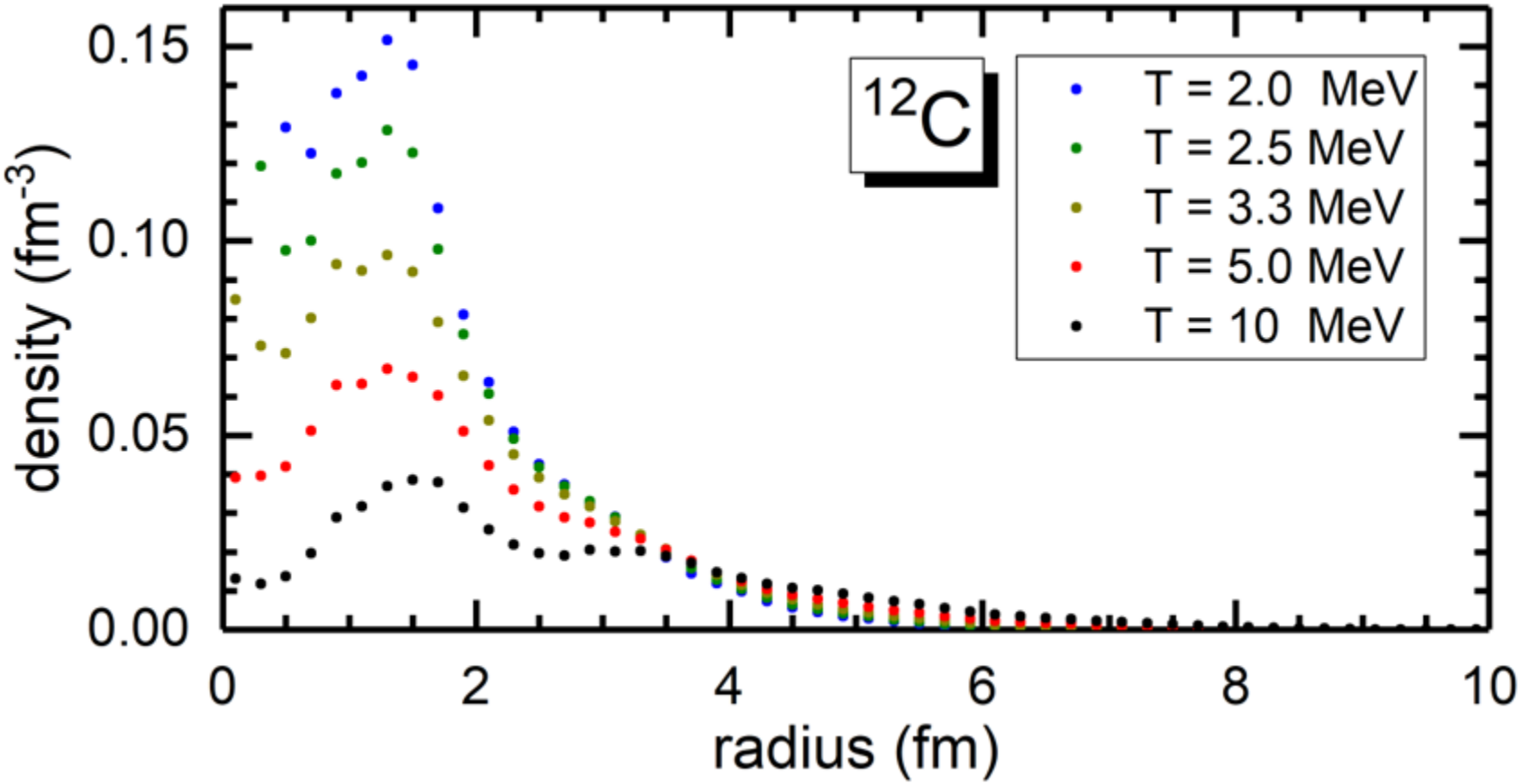


Figure courtesy of Bingnan Lu

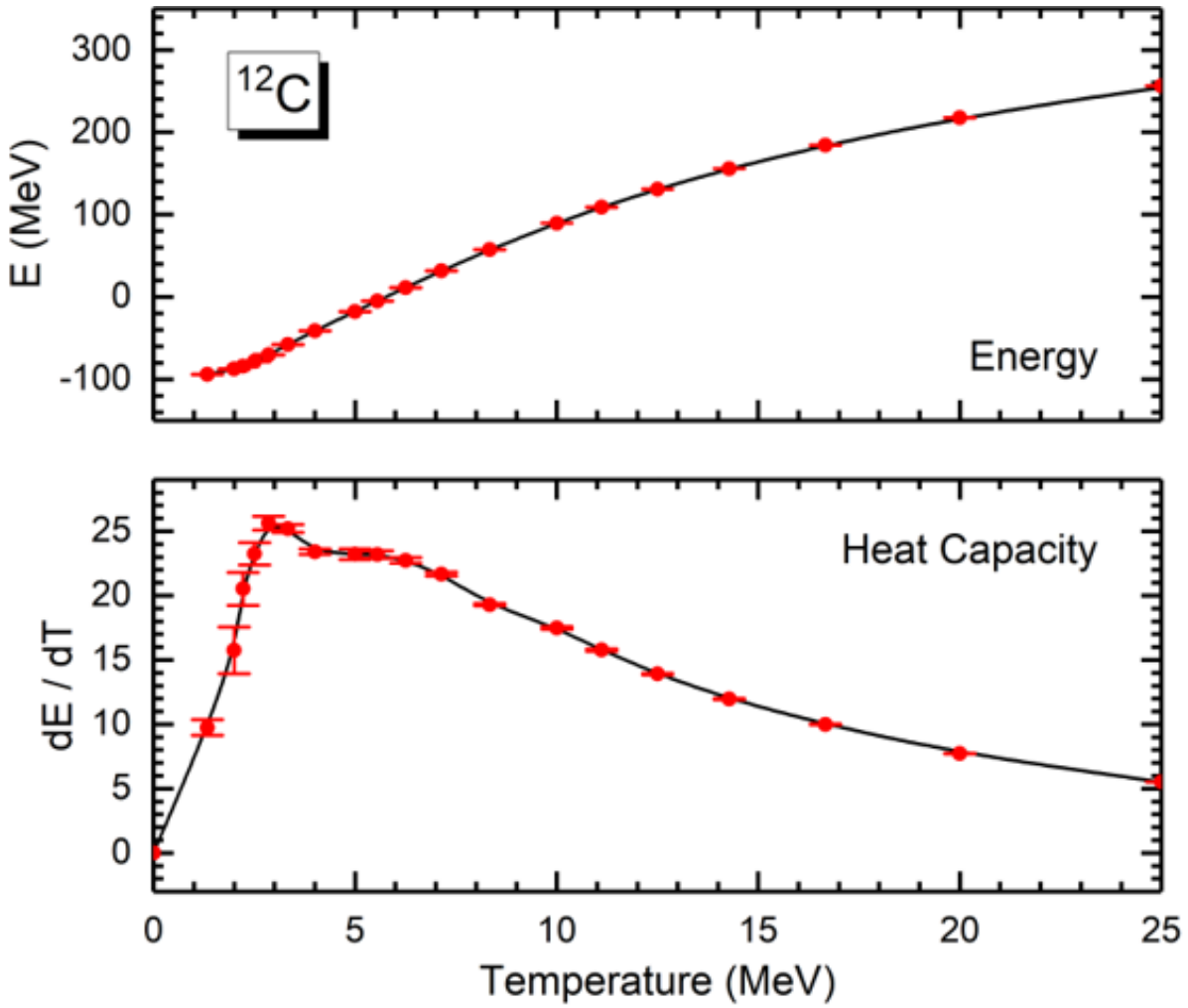


Figure courtesy of Bingnan Lu

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, PRL 121, 032501 (2018)

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

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

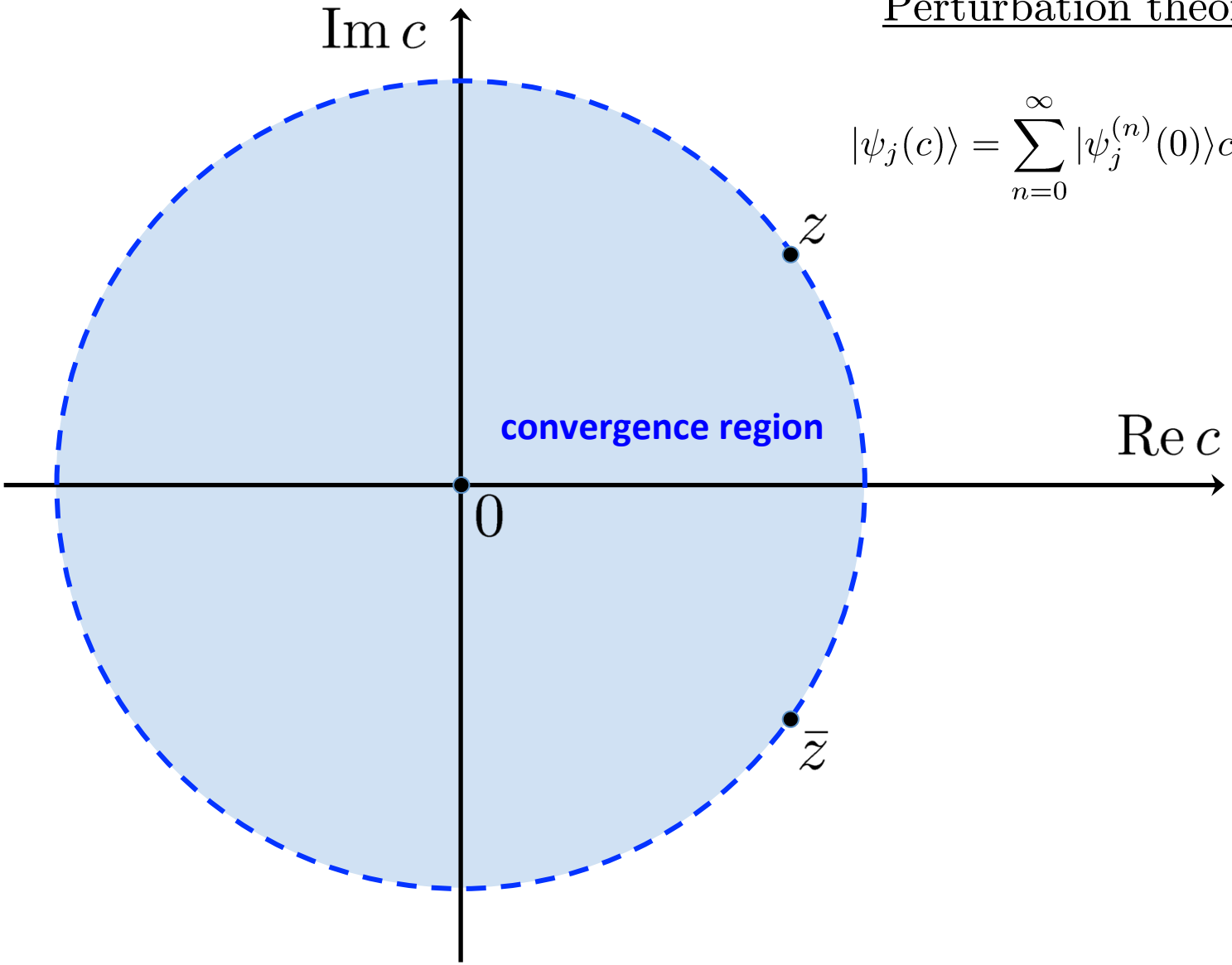
We can perform series expansions around the point $c = 0$.

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

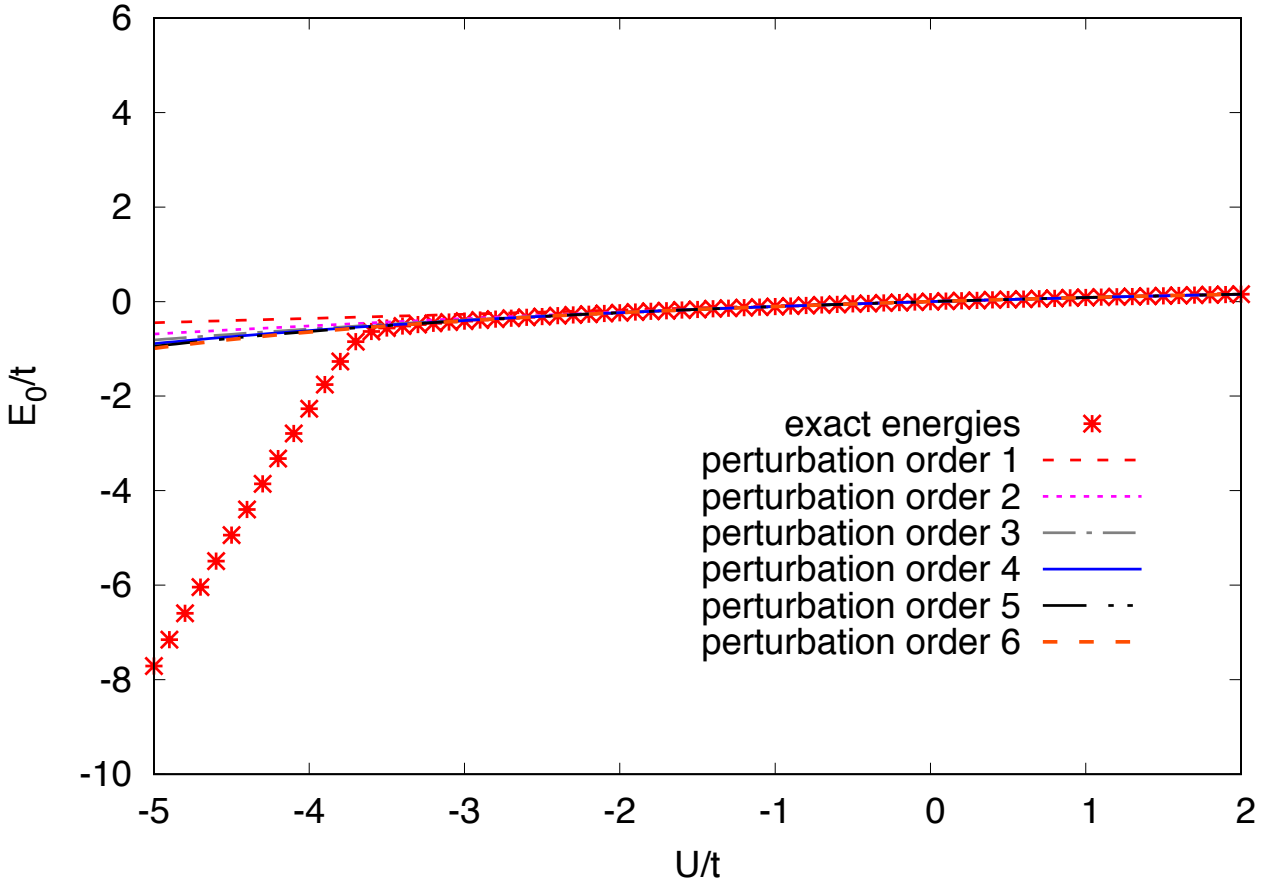
This is the strategy of perturbation theory. We can compute each term in the series when the eigenvalues and eigenvectors of H_0 are known or computable.

Perturbation theory

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

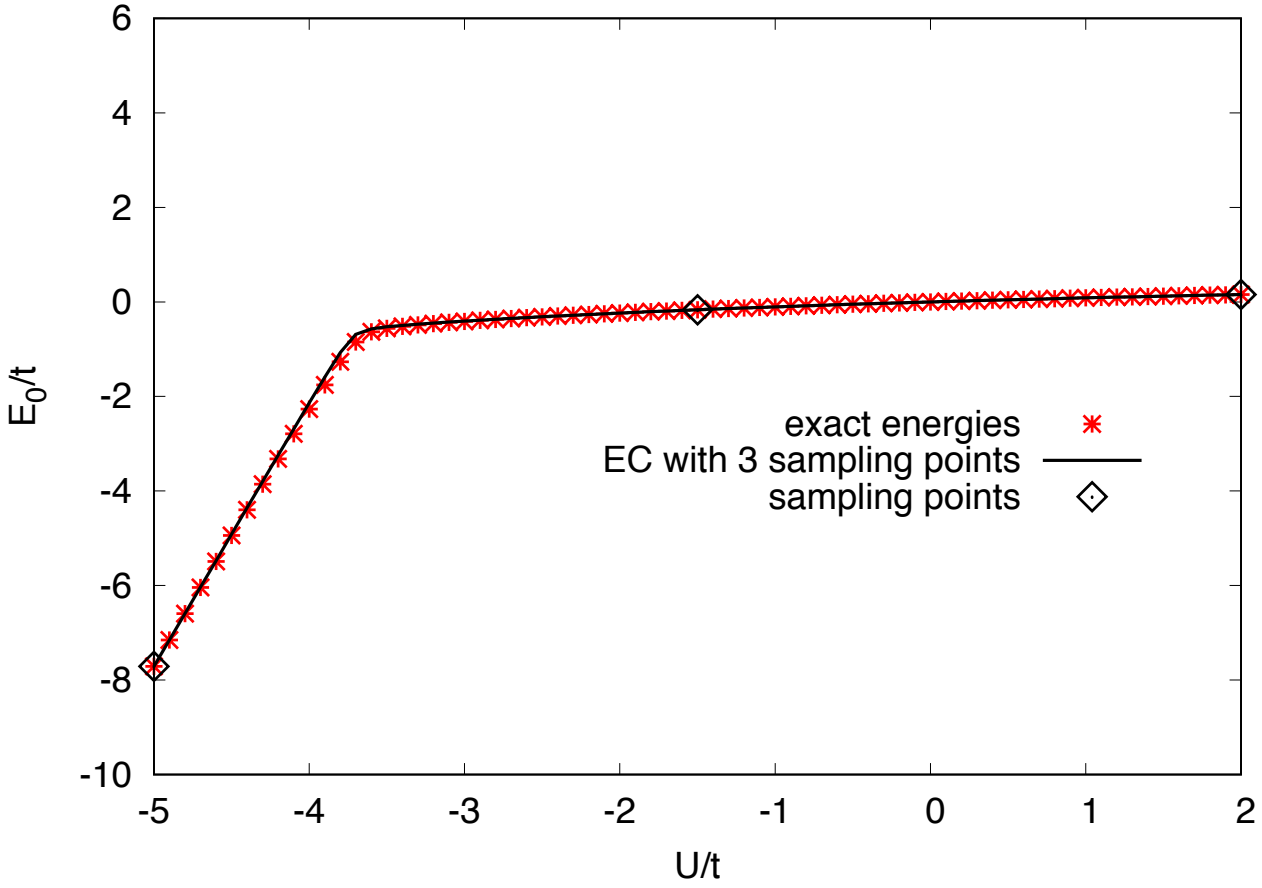


Bose-Hubbard model

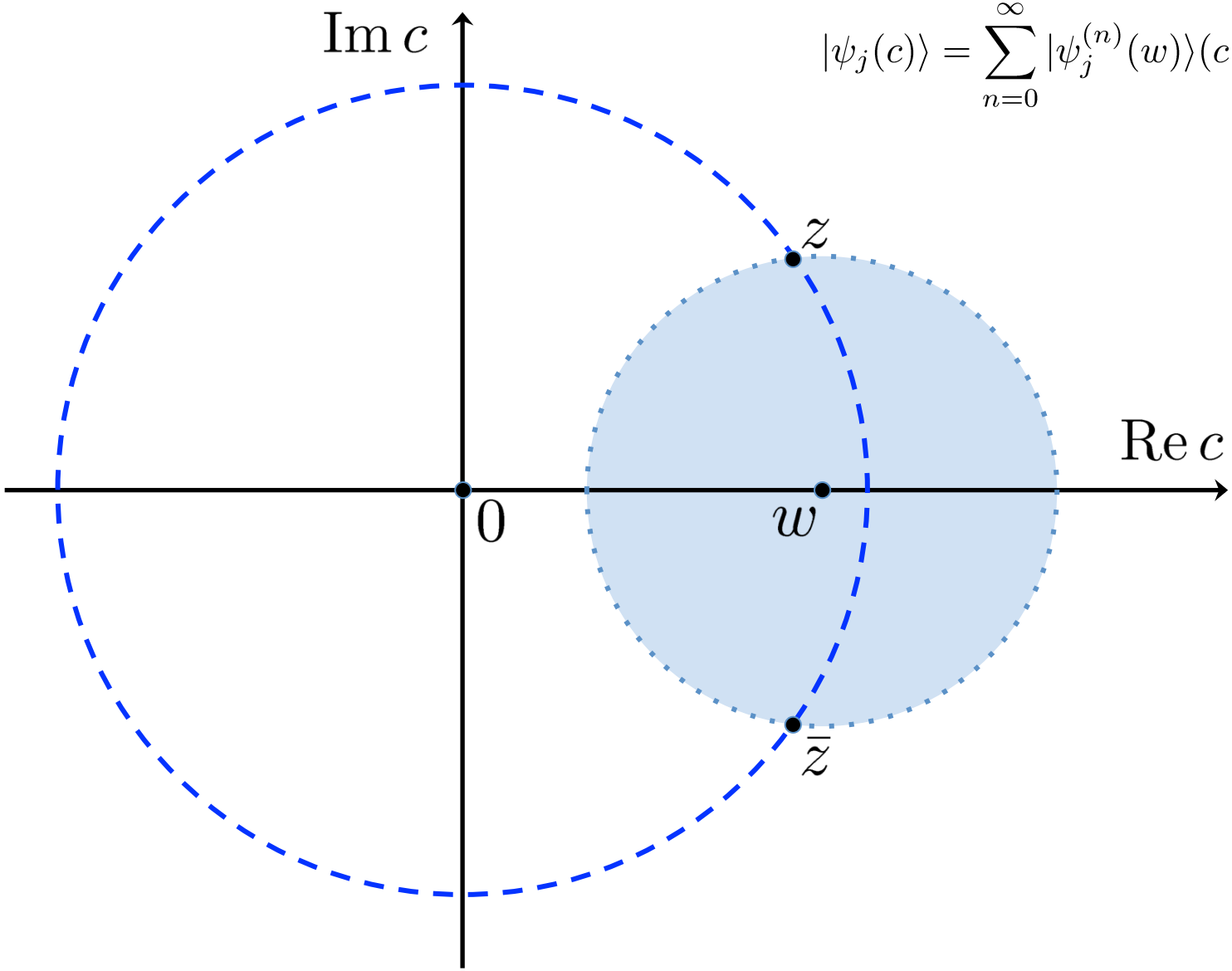


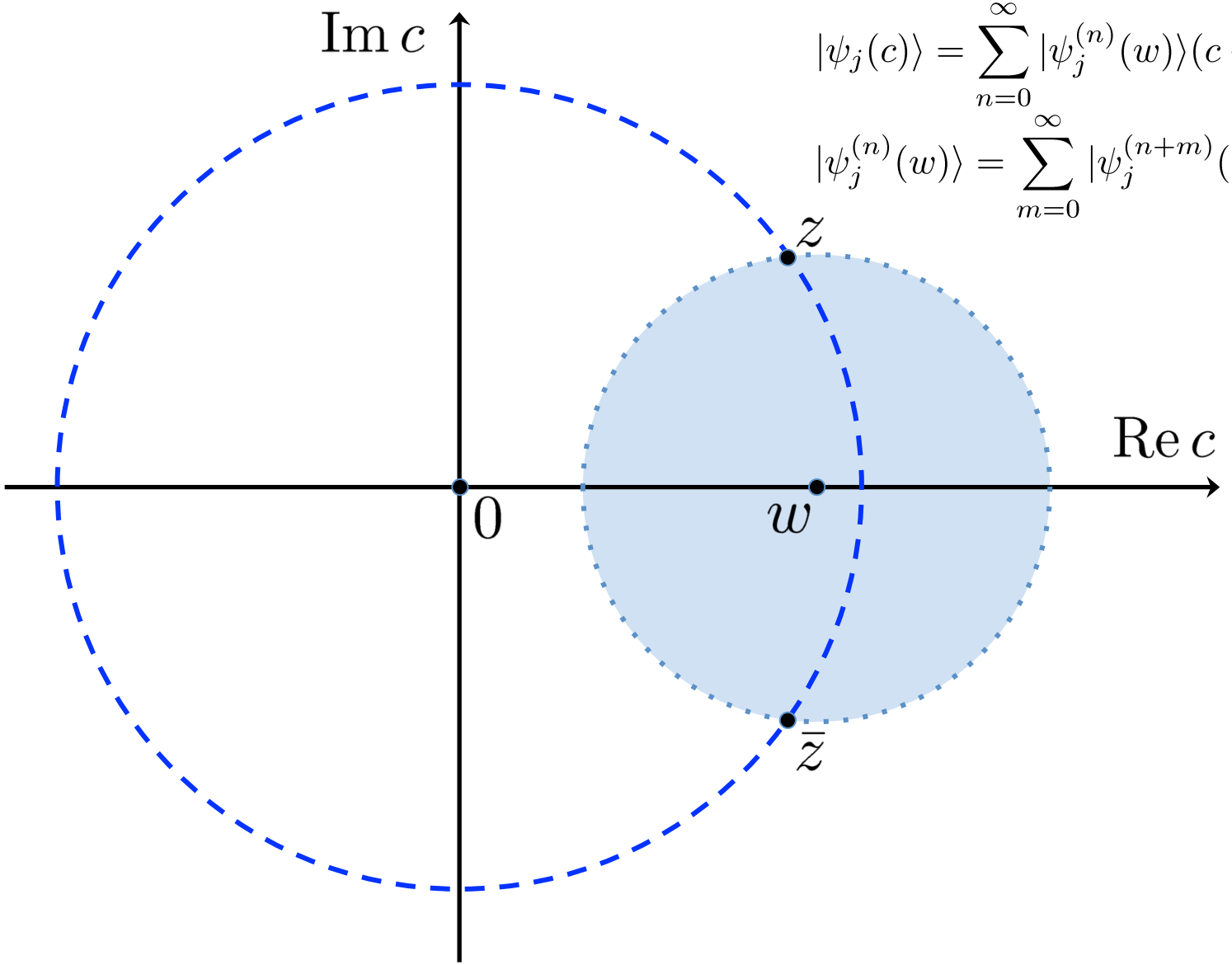
Perturbation theory fails at strong attractive coupling

Restrict the linear space to the span of three vectors



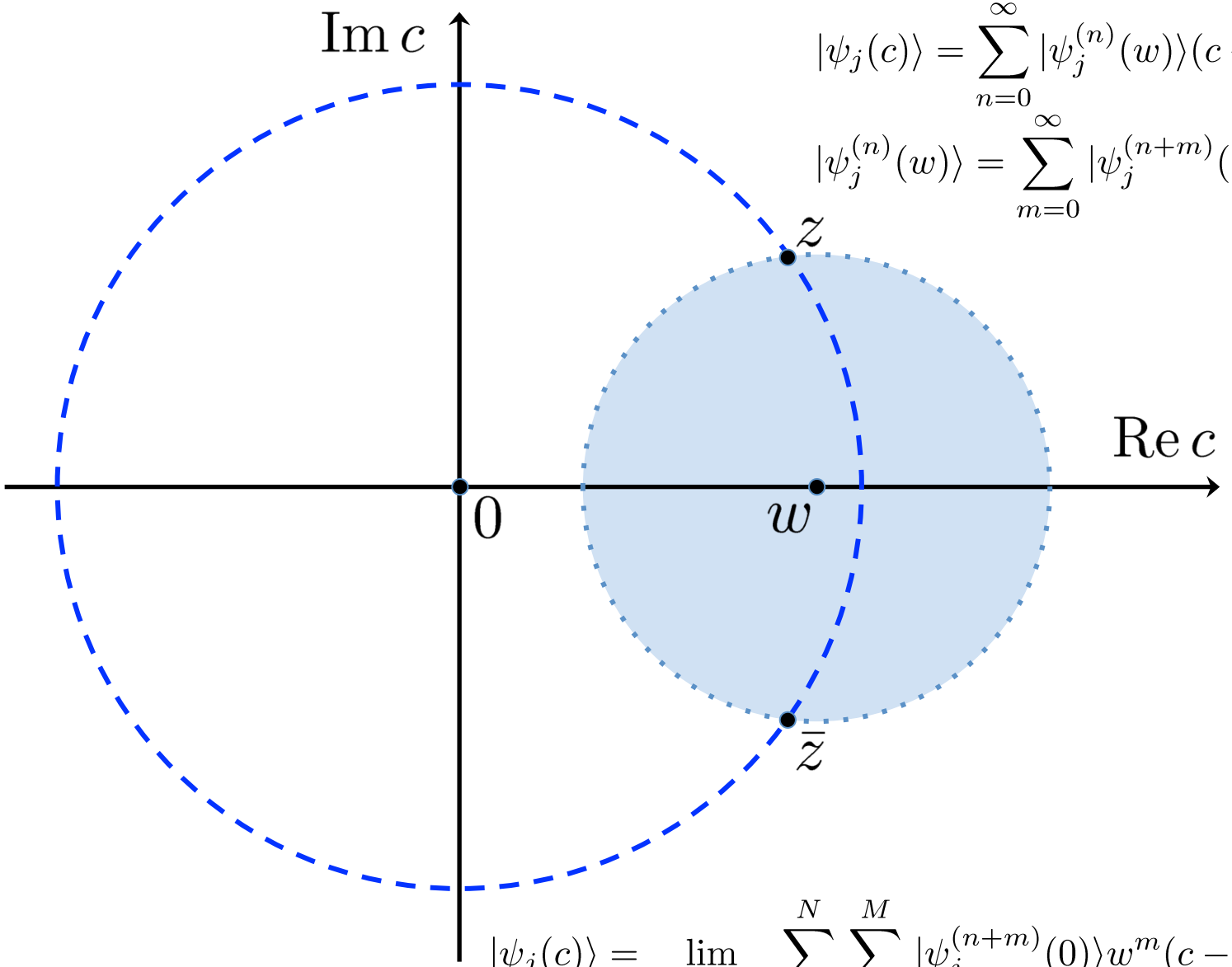
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





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

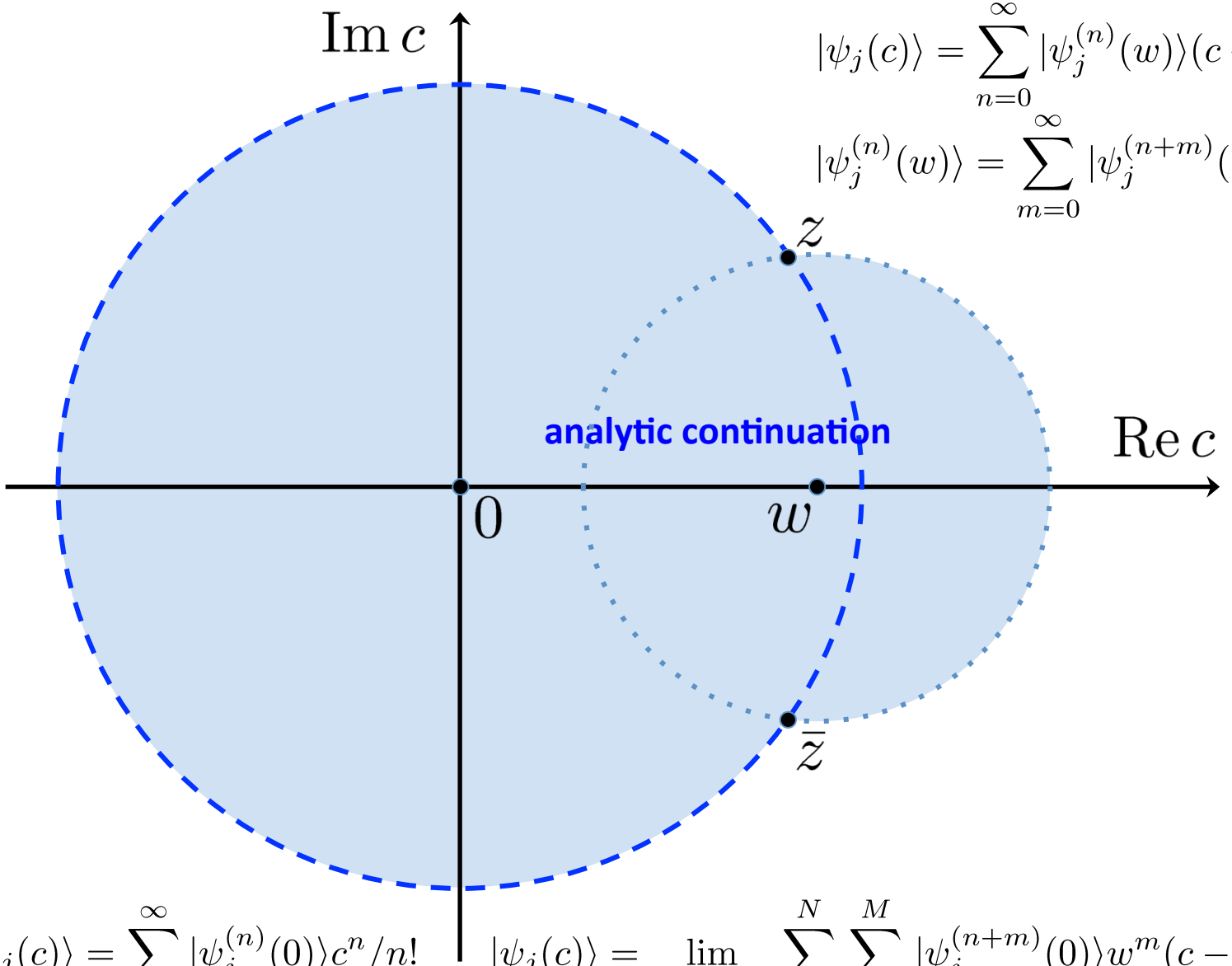
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



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

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

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



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

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

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

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

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

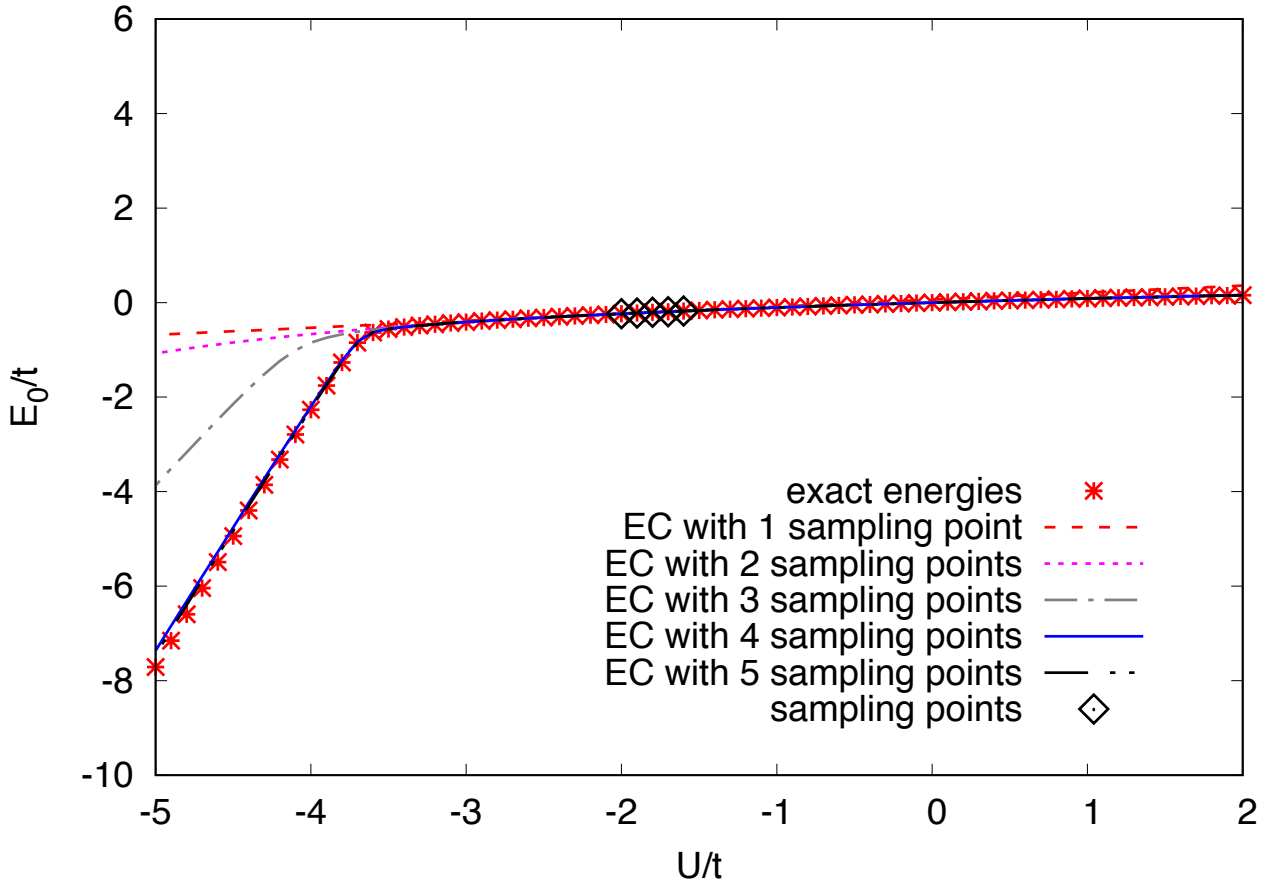
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

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

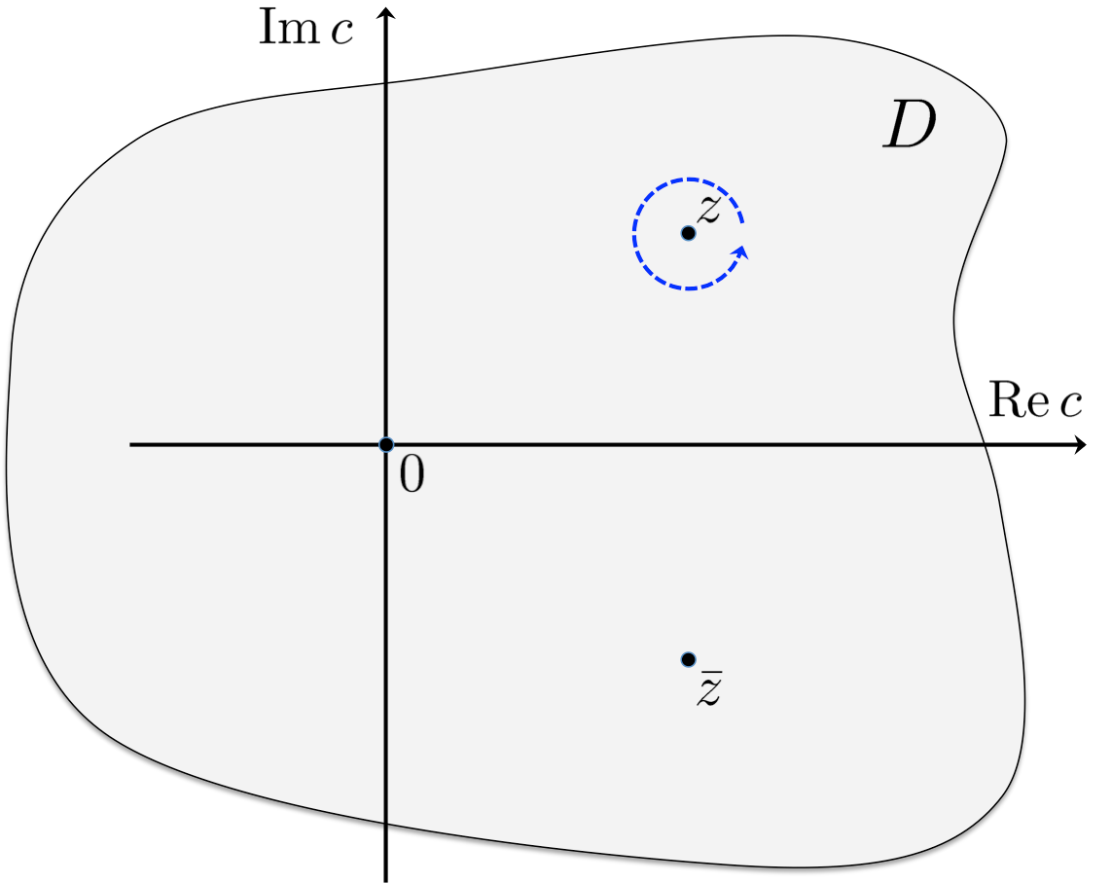
As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

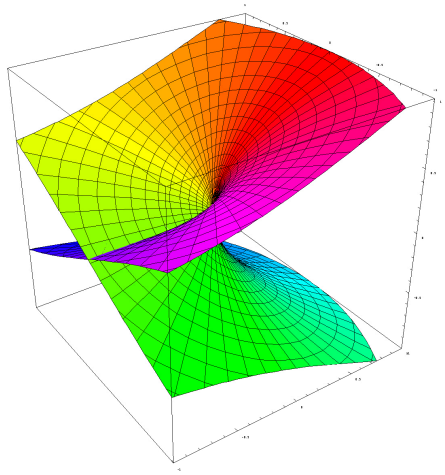
We can "learn" the eigenvector trajectory in one region and perform eigenvector continuation to another region



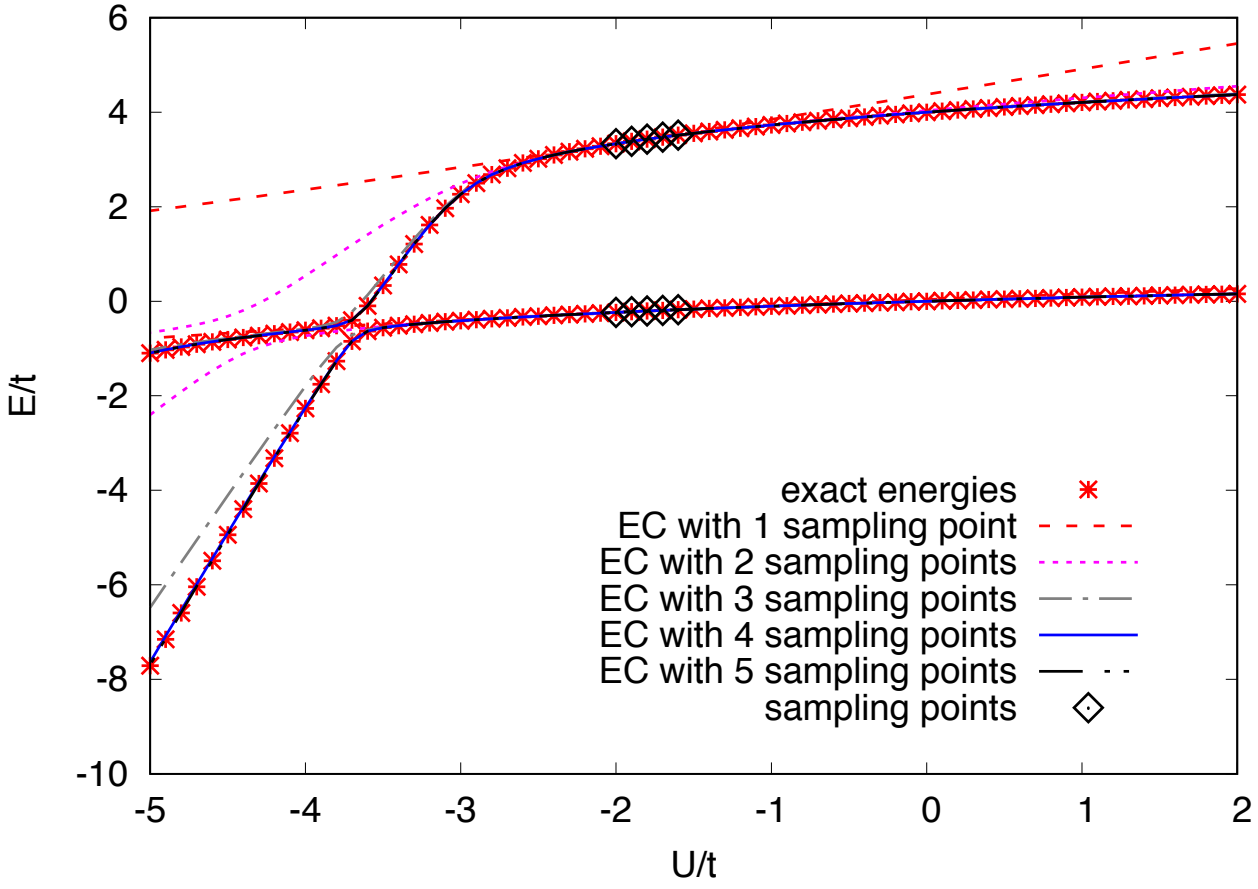
D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121, 032501 (2018)

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.



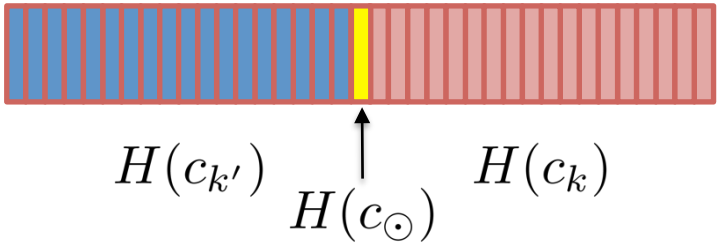
Eigenvector continuation with quantum Monte Carlo

Use Monte Carlo simulations to compute projection amplitudes

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

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

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



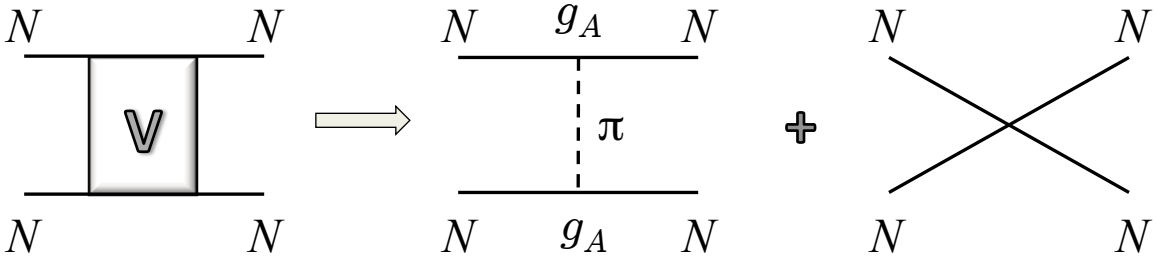
$$|\psi_{\text{init}}\rangle$$

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

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

Application: Neutron matter simulations

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

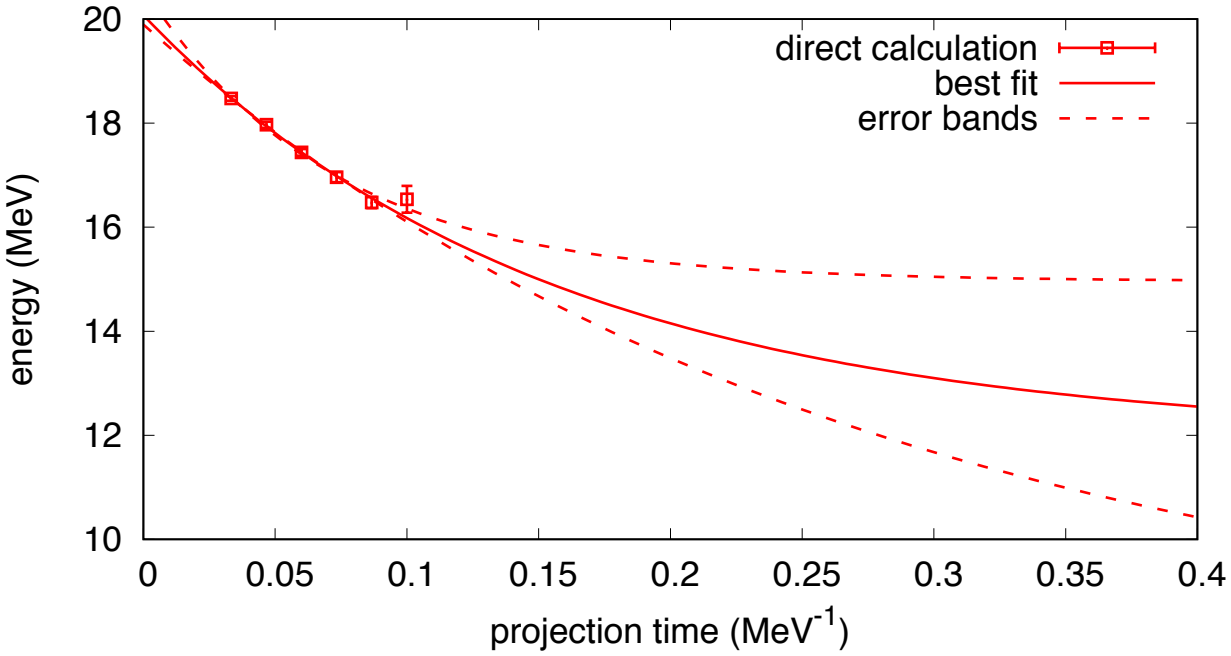


V^{OPEP} Contact interactions

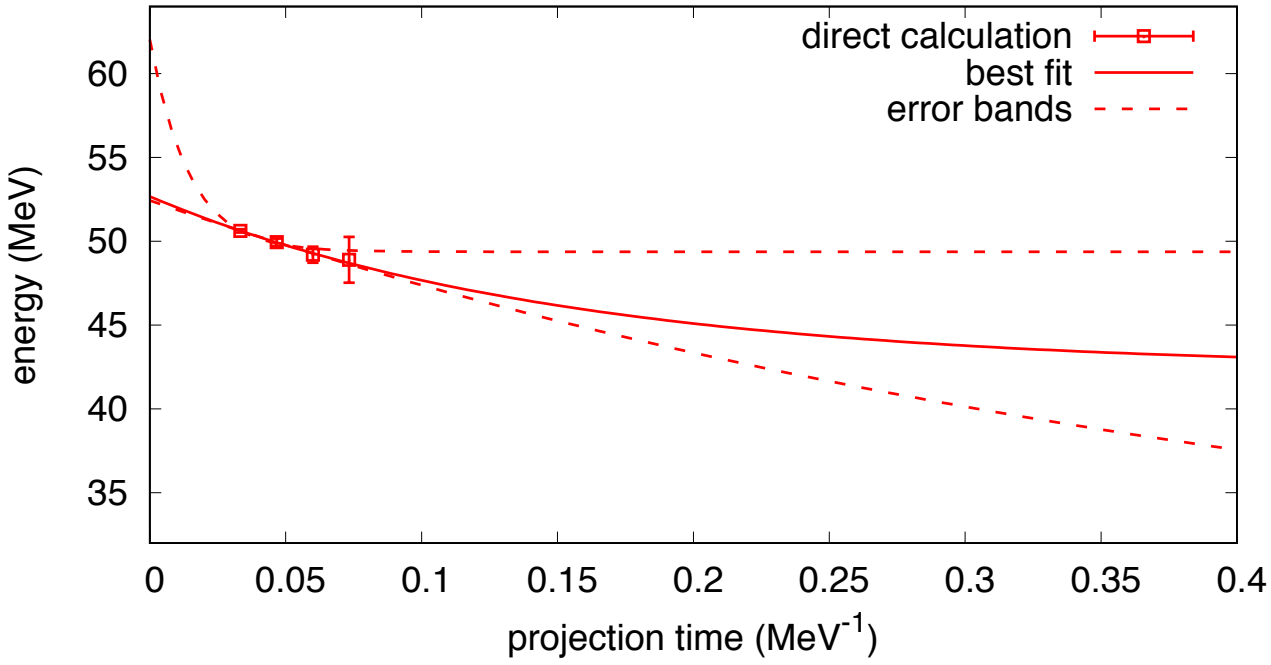
As a challenge to the eigenvector continuation technique, we use a lattice action for one-pion exchange that causes severe Monte Carlo sign oscillations.

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]

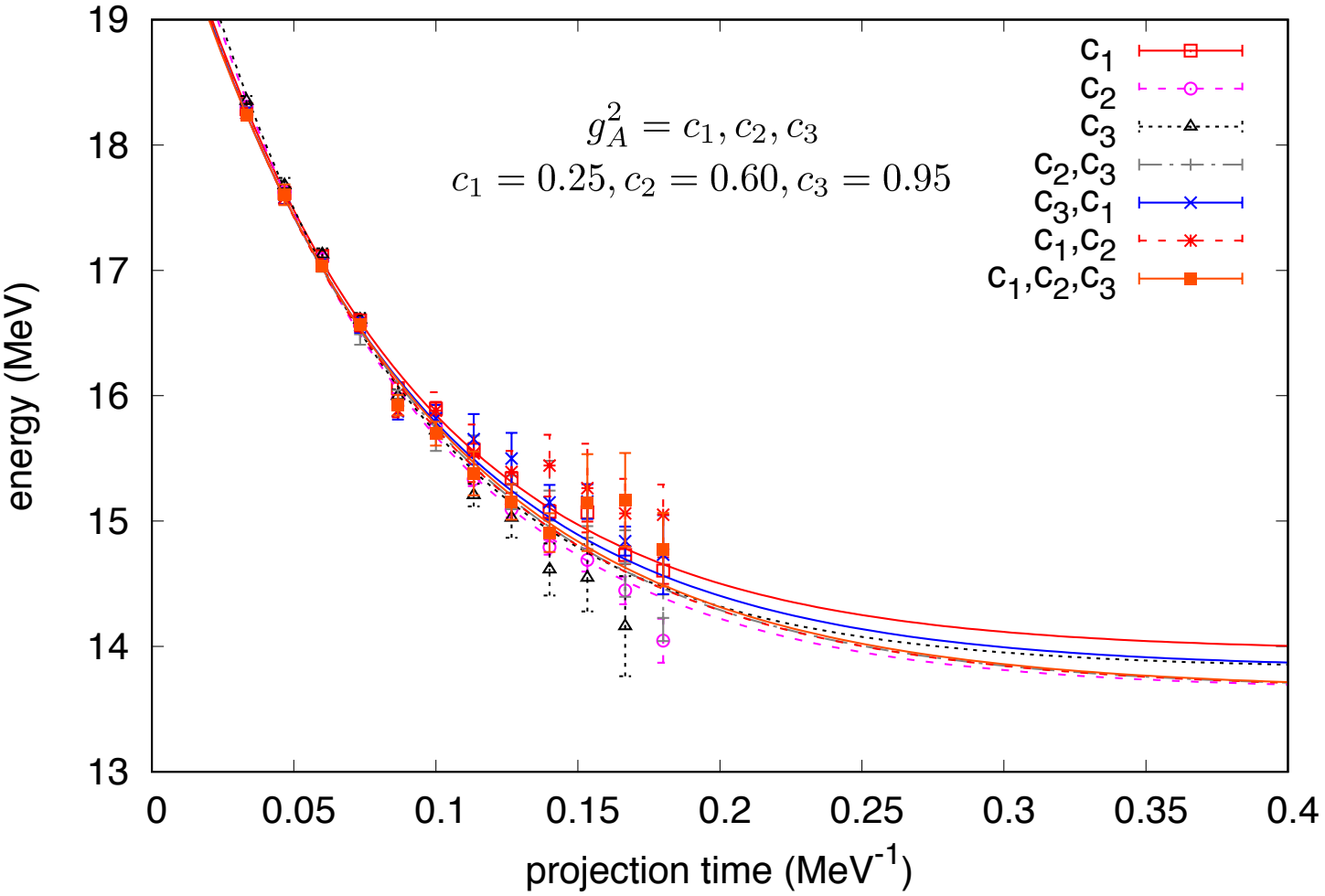
Direct calculation of six neutrons ($L = 8$ fm)



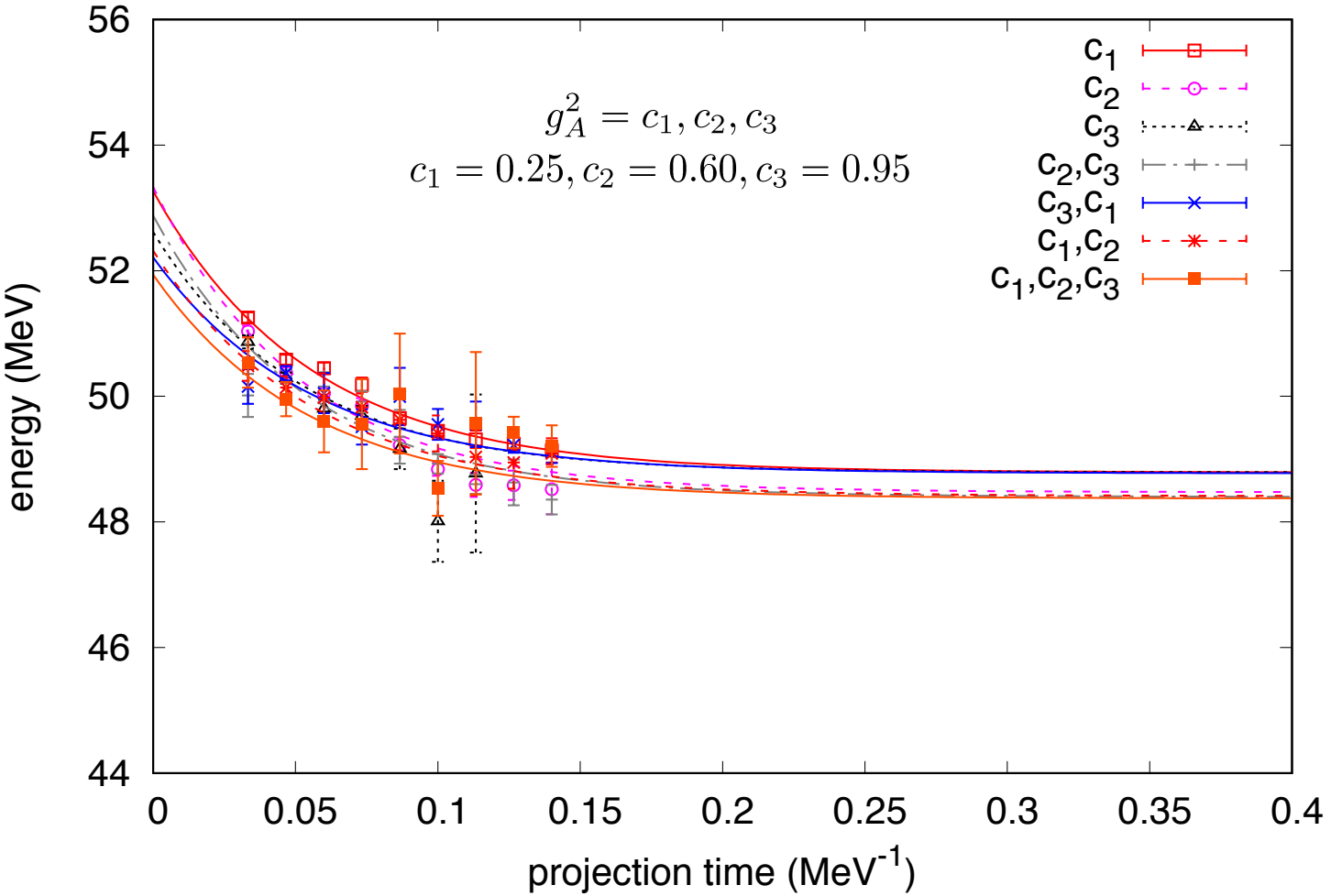
Direct calculation of fourteen neutrons ($L = 8$ fm)



Eigenvector continuation 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	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, 032501 (2018)

Anharmonic oscillator

As a test of eigenvector continuation, we use it to improve perturbation theory for the anharmonic oscillator with a quartic interaction.

$$H(c) = \frac{p^2}{2} + \frac{x^2}{2} + cx^4$$

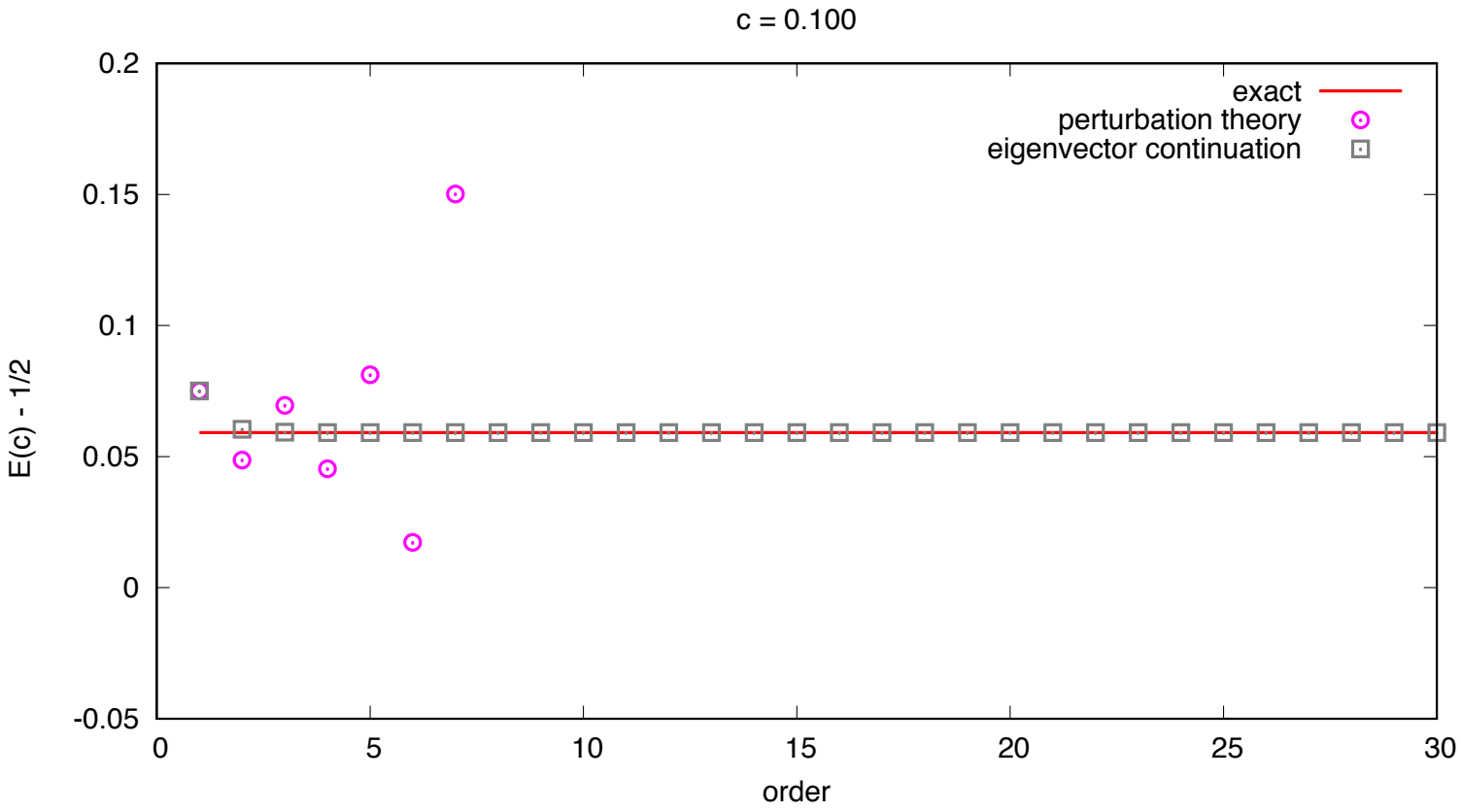
In this case perturbation theory has a zero radius of convergence. This fact can deduced from the observation that $H(c)$ is unbounded below for any negative c. Mathematically what happens is that we have branch points that accumulate near $c = 0$.

Bender, Wu, Phys. Rev. 184, 1231 (1969)

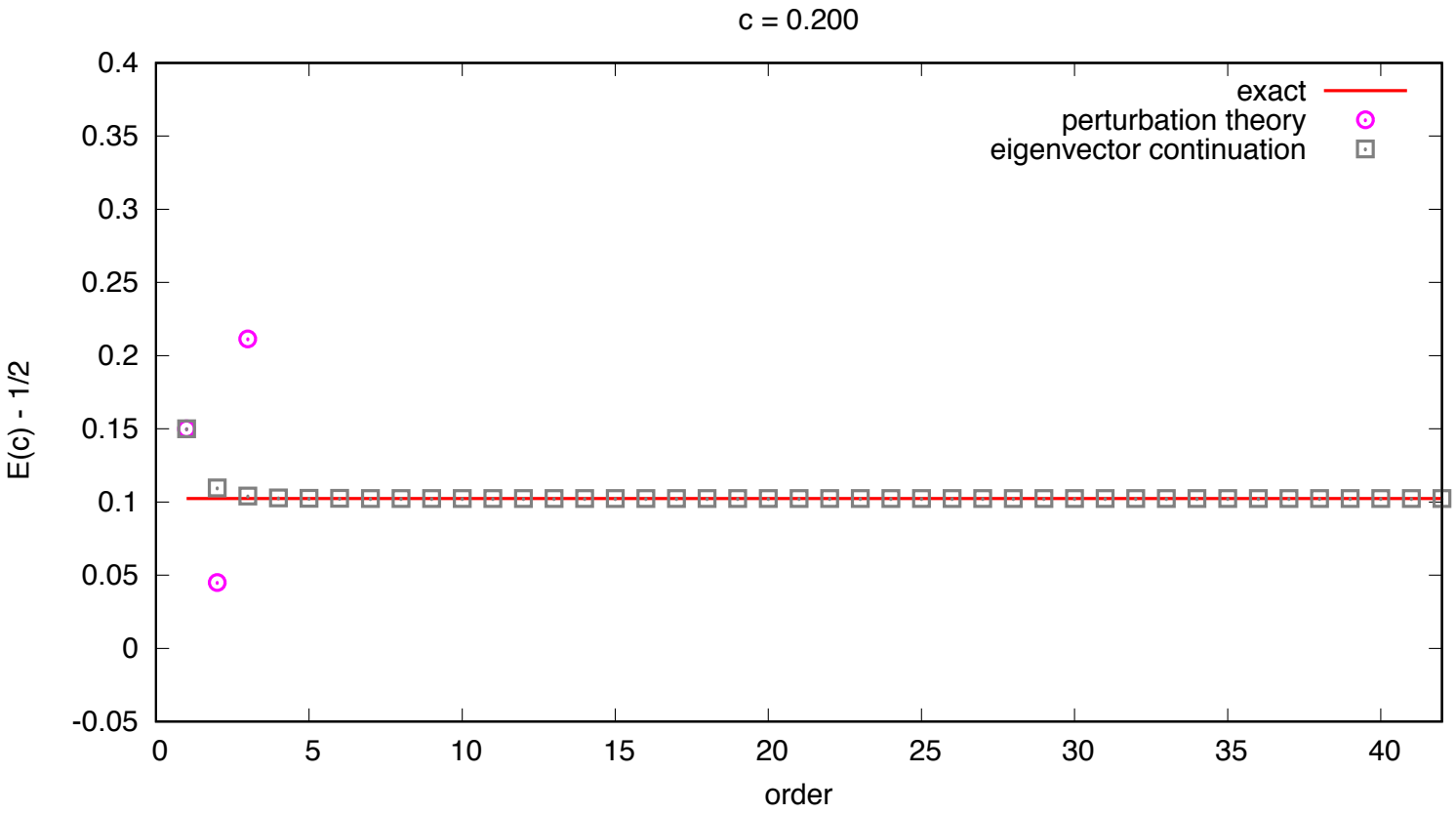
For the eigenvector continuation calculations we project onto the subspace

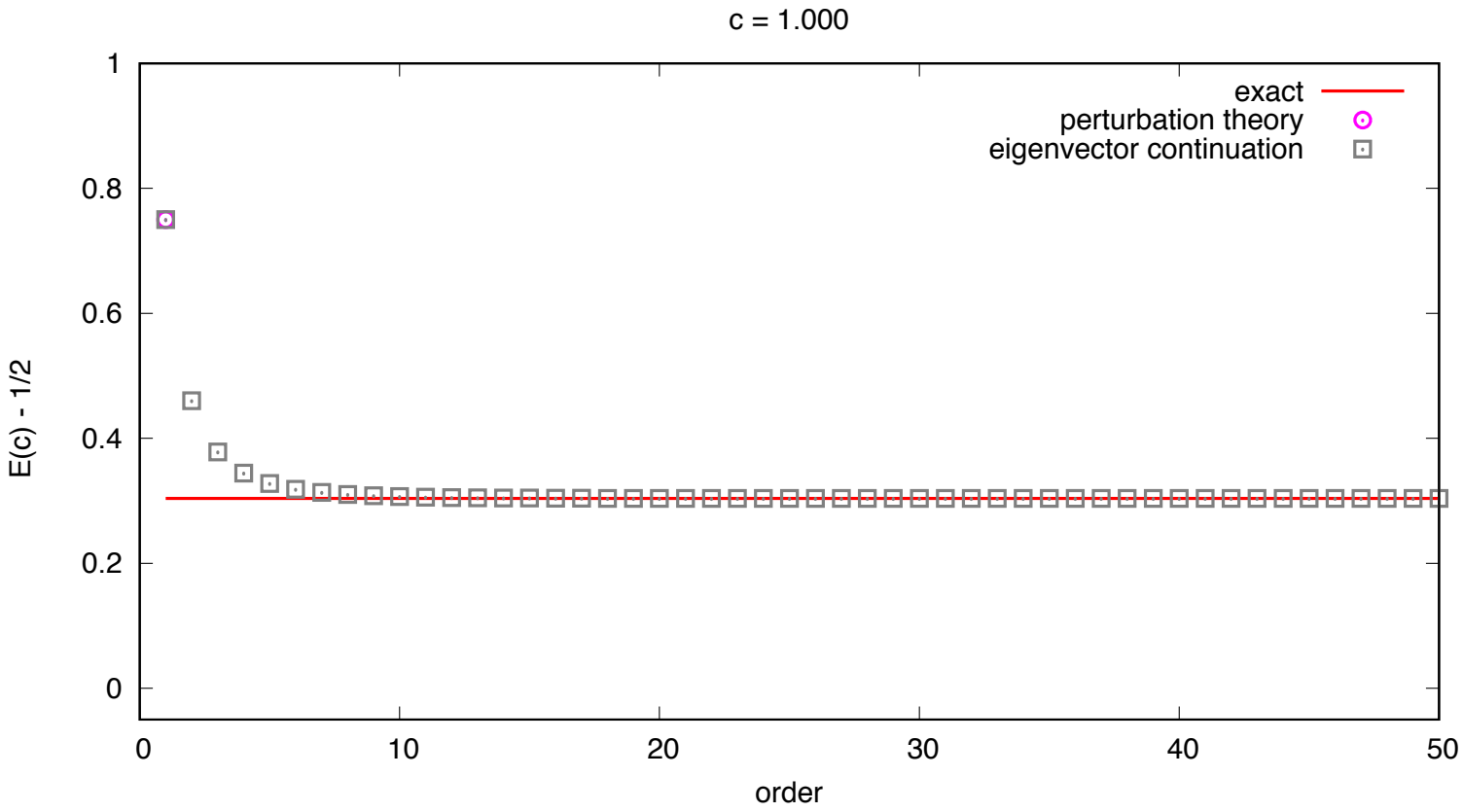
$$\left\{|\psi^{(0)}(0)\rangle, |\psi^{(1)}(0)\rangle, |\psi^{(2)}(0)\rangle, \cdots\right\}$$

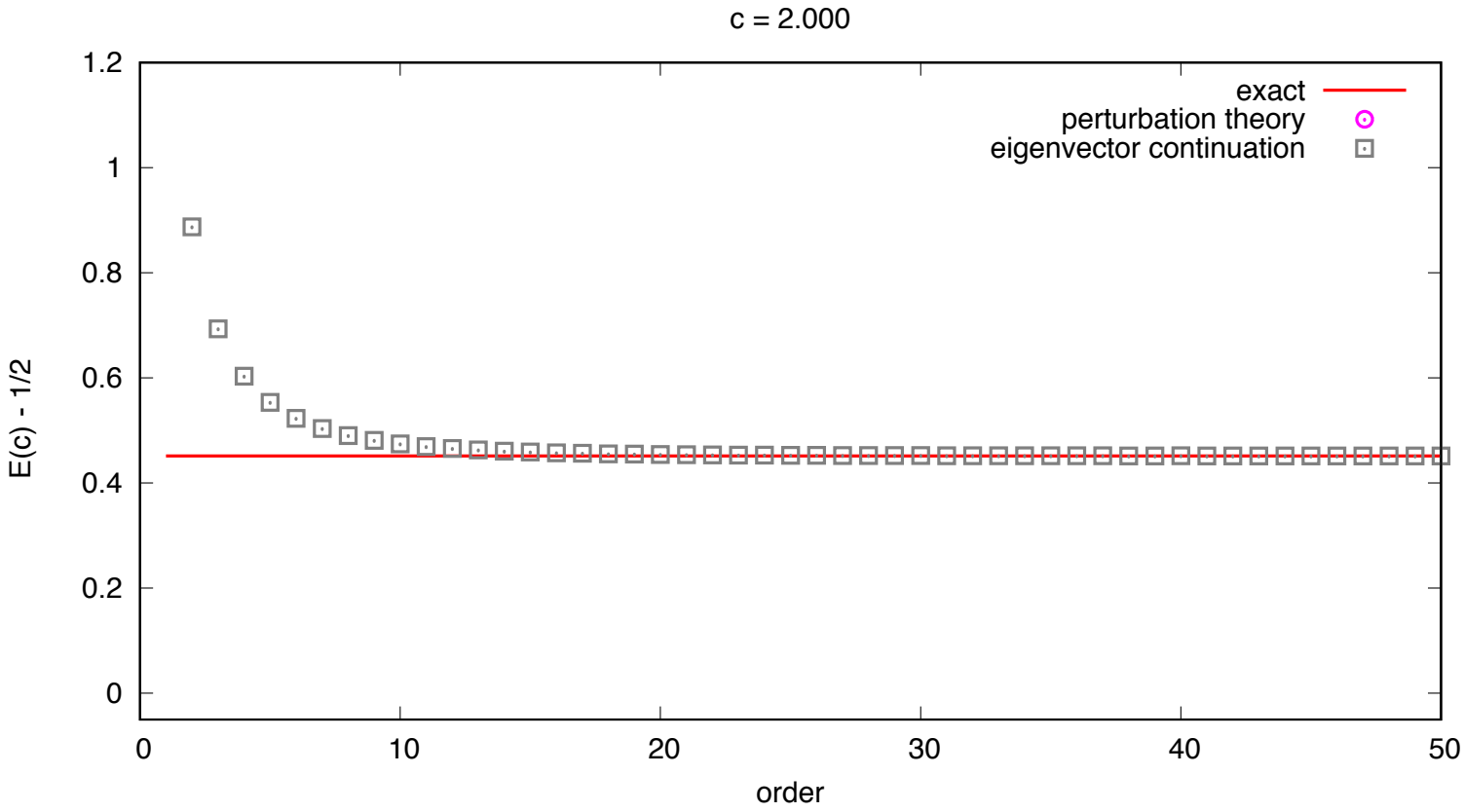
The order of the eigenvector continuation calculation is the dimensionality of the subspace.

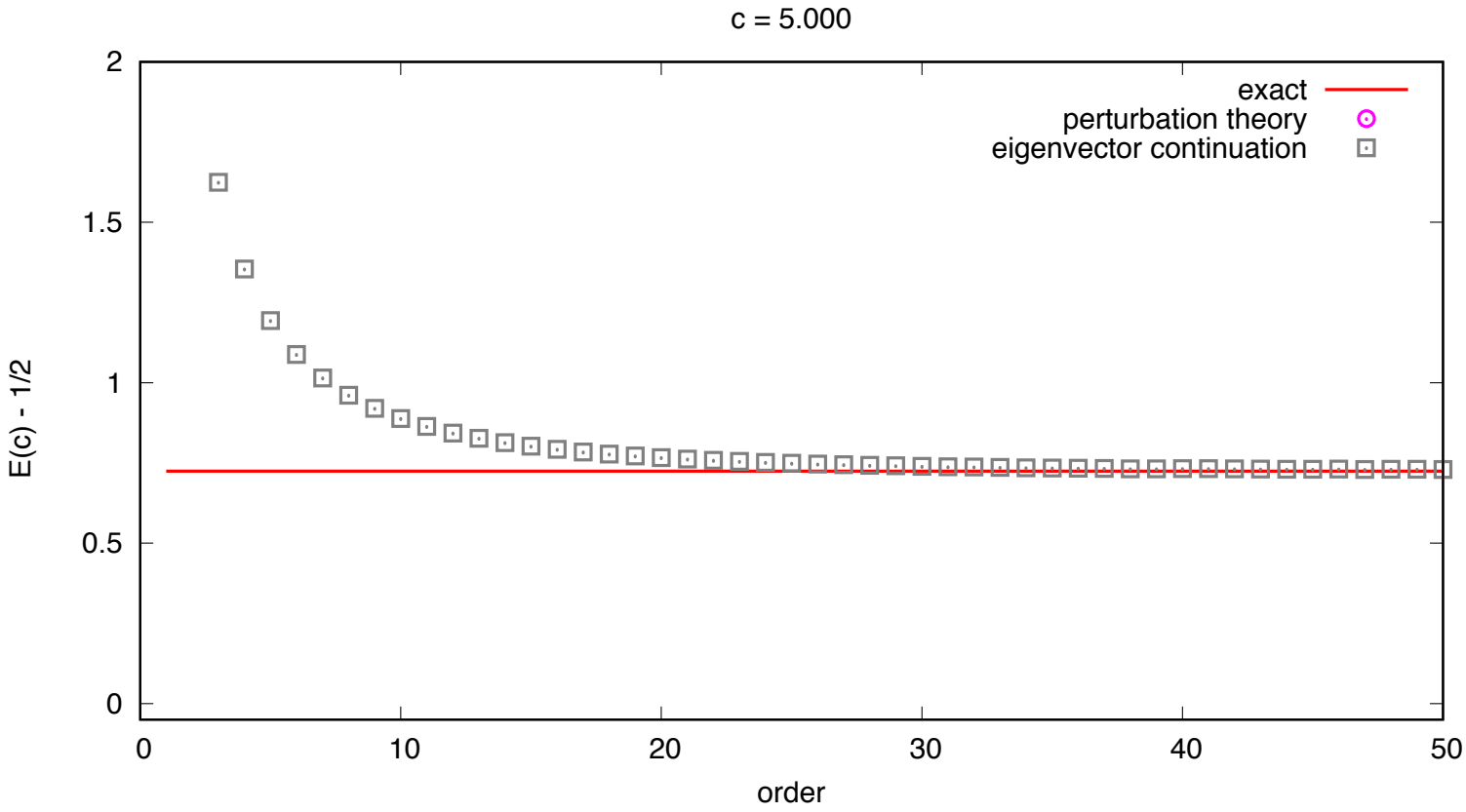


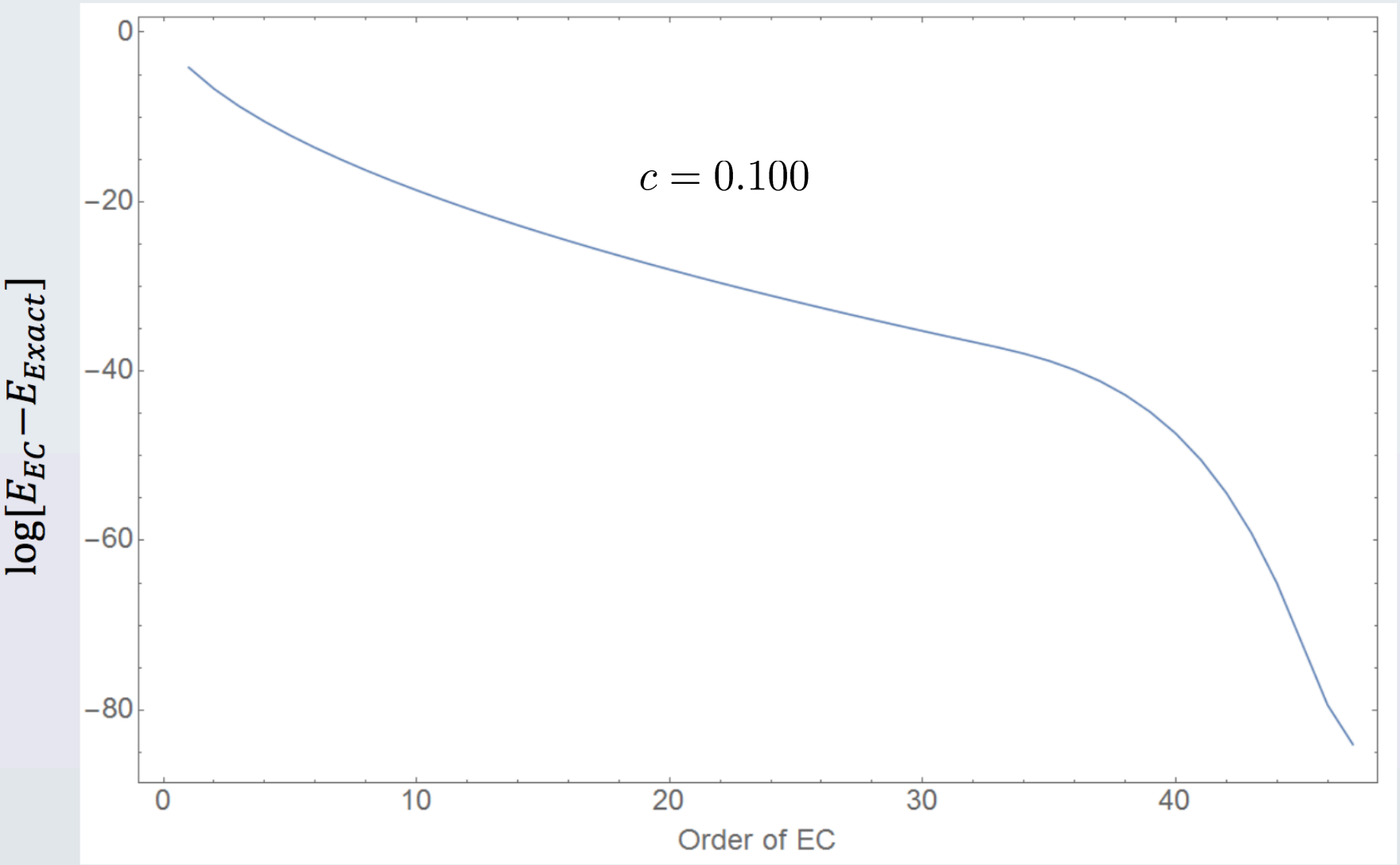
Codes and results courtesy of Avik Sarkar


c = 0.200
exact
perturbation theory
eigenvector continuation
E(c) - 1/2
order
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
5
10
15
20
25
30
35
40

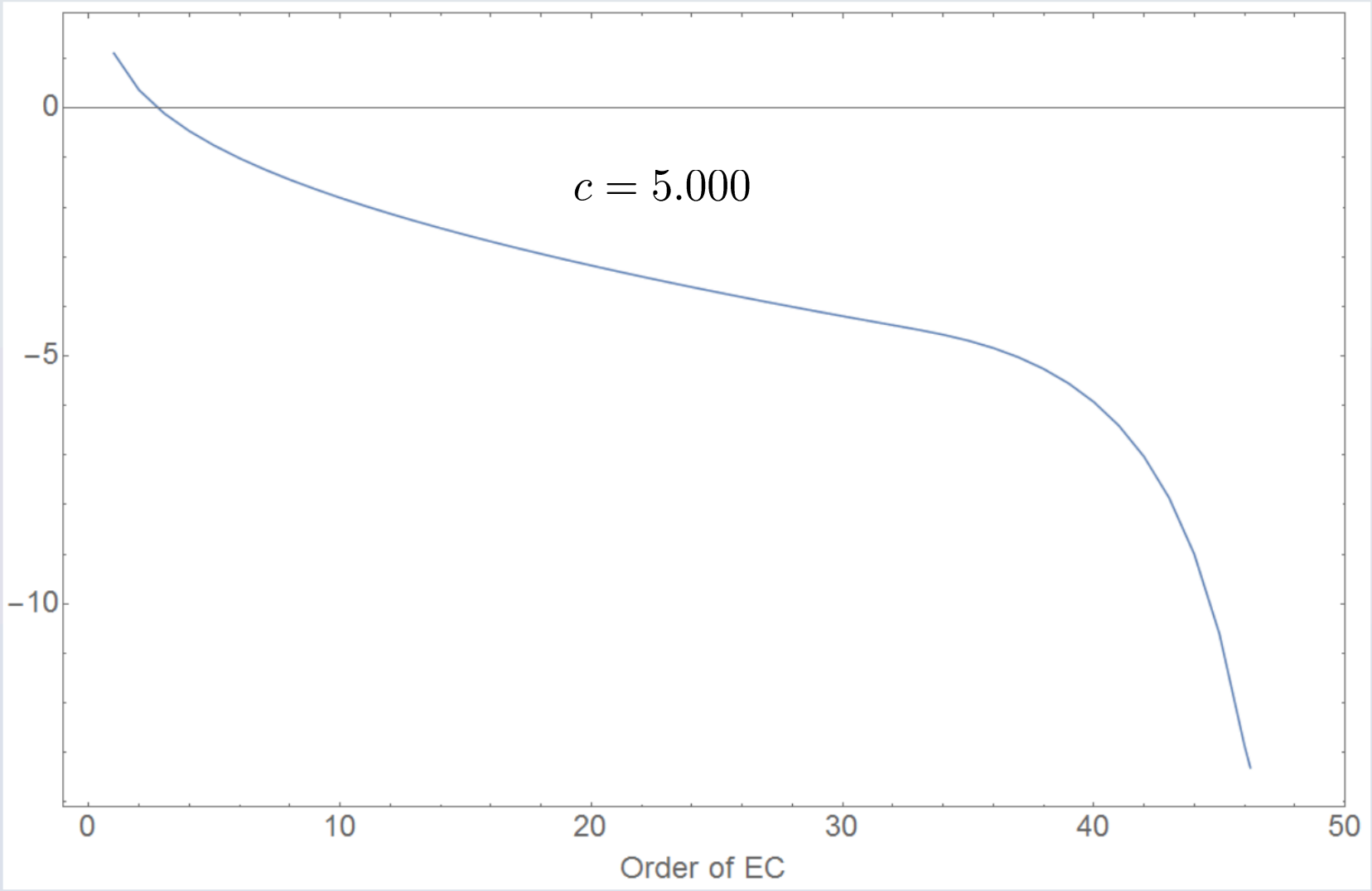

c = 1.000
exact
perturbation theory
eigenvector continuation
E(c) - 1/2
order
0
0.2
0.4
0.6
0.8
1
0
10
20
30
40
50


c = 2.000
E(c) - 1/2
order
exact
perturbation theory
eigenvector continuation
1.2
1
0.8
0.6
0.4
0.2
0
0
10
20
30
40
50


c = 5.000
exact
perturbation theory
eigenvector continuation
E(c) - 1/2
order
0
0.5
1
1.5
2
0
10
20
30
40
50



Note the acceleration in the rate of convergence



Note the acceleration in the rate of convergence

Summary and Outlook

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

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 and other applications.

Improving 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.

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