Eigenvector Continuation: General Concepts

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Eigenvector continuation and related techniques
in nuclear structure and reaction theory
CEA Paris-Saclay
May 30 – June 2, 2023

Outline

Motivation and three questions

Perturbation theory

Analytic continuation

Eigenvector continuation

Early papers

Projection-based emulators

Trimmed sampling algorithm

Matrix eigenvalue emulators

Summary

Motivation and three questions

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.

Question 1

Eur. Phys. J. A (2015) **51**: 92
DOI 10.1140/epja/i2015-15092-1

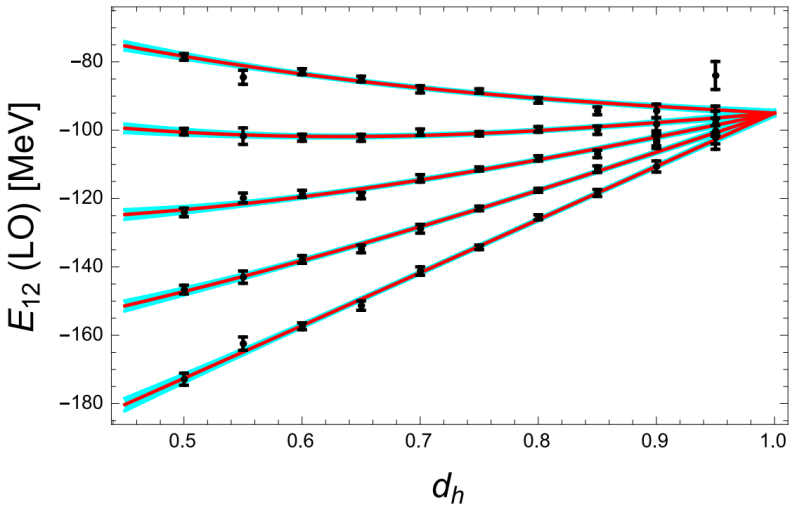
THE EUROPEAN PHYSICAL JOURNAL A

Regular Article – Theoretical Physics

Nuclear lattice simulations using symmetry-sign extrapolation

Timo A. Lähde[1,a], Thomas Luu[1], Dean Lee[2], Ulf-G. Meißner[3,1,4], Evgeny Epelbaum[5], Hermann Krebs[5], and Gautam Rupak[6]

$$H = d_h H_{\mathrm{LO}} + (1 - d_h) H_{\mathrm{symmetric}}$$



How can this extrapolation be done more accurately?

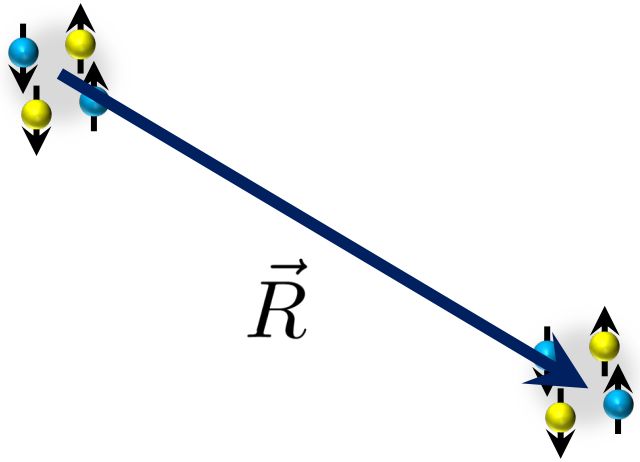
Is there a general systematic framework?

Question 2

Adiabatic Projection Method

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

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



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

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

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

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

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

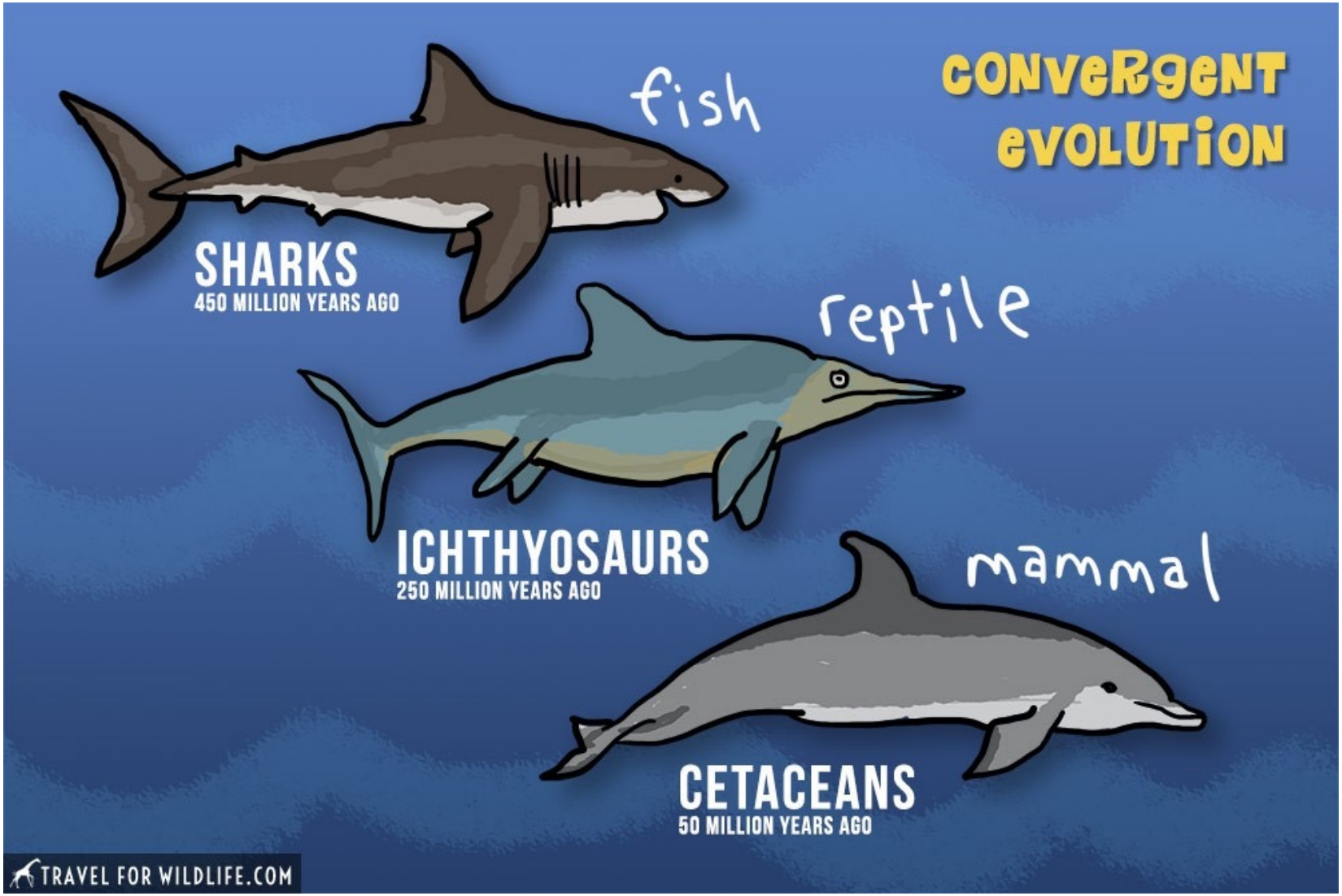
How can we use perturbation theory beyond first order in this framework?

Question 3

In order to find the extremal eigenvectors of H, the Lanczos method diagonalizes a small Krylov subspace starting from an initial vector

$$|v_I\rangle\,,\ H\,|v_I\rangle\,,\ H^2\,|v_I\rangle\,,\ \cdots,\ H^n\,|v_I\rangle$$

Are there other subspaces that might converge even faster, while allowing for the treatment of linear spaces that are too large to store in memory?


CONVERGENT EVOLUTION
fish
SHARKS
450 MILLION YEARS AGO
reptile
ICHTHYOSAURS
250 MILLION YEARS AGO
mammal
CETACEANS
50 MILLION YEARS AGO
TRAVEL FOR WILDLIFE.COM

Perturbation theory

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

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

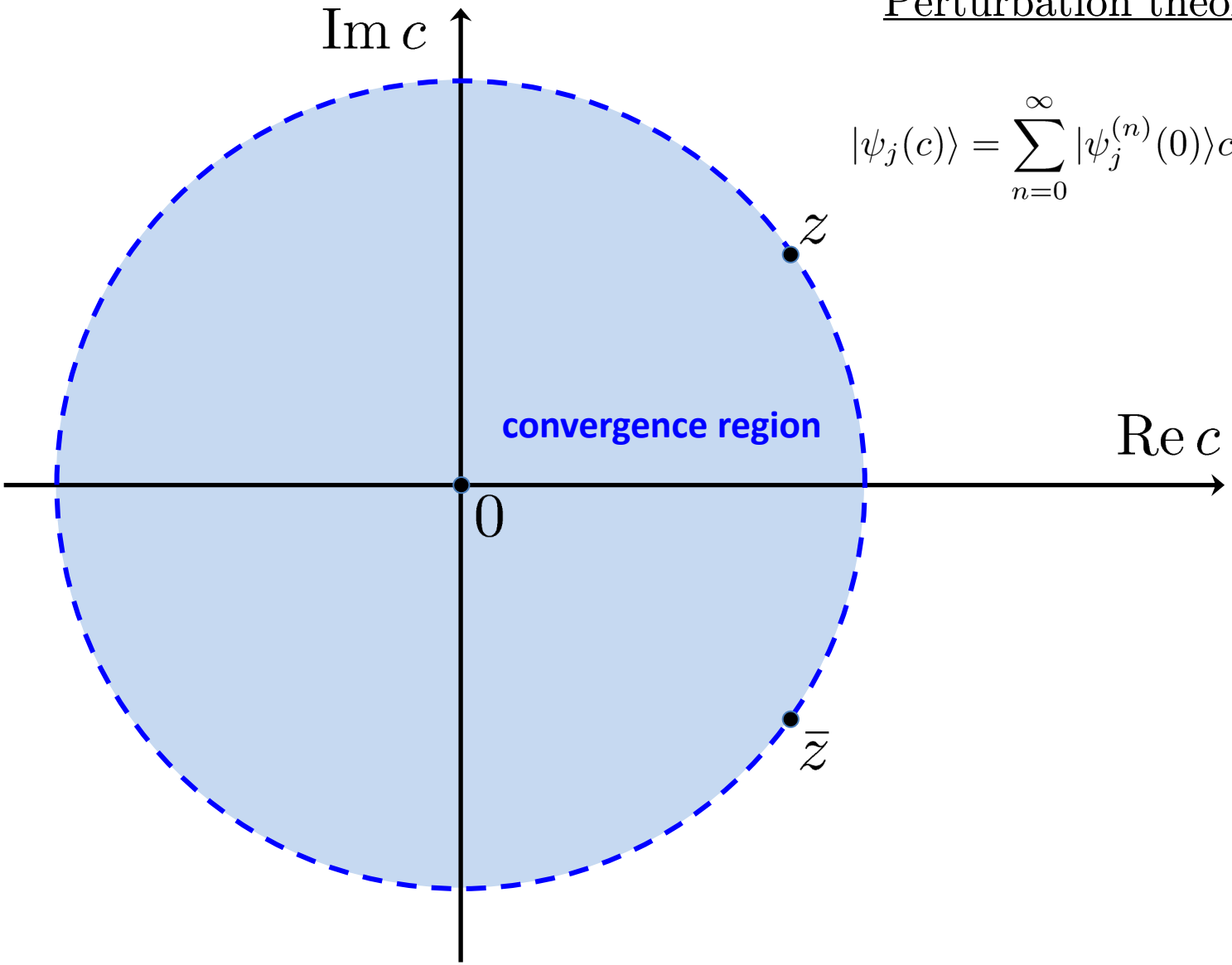
We can perform series expansions around the point $c = 0$.

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

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.

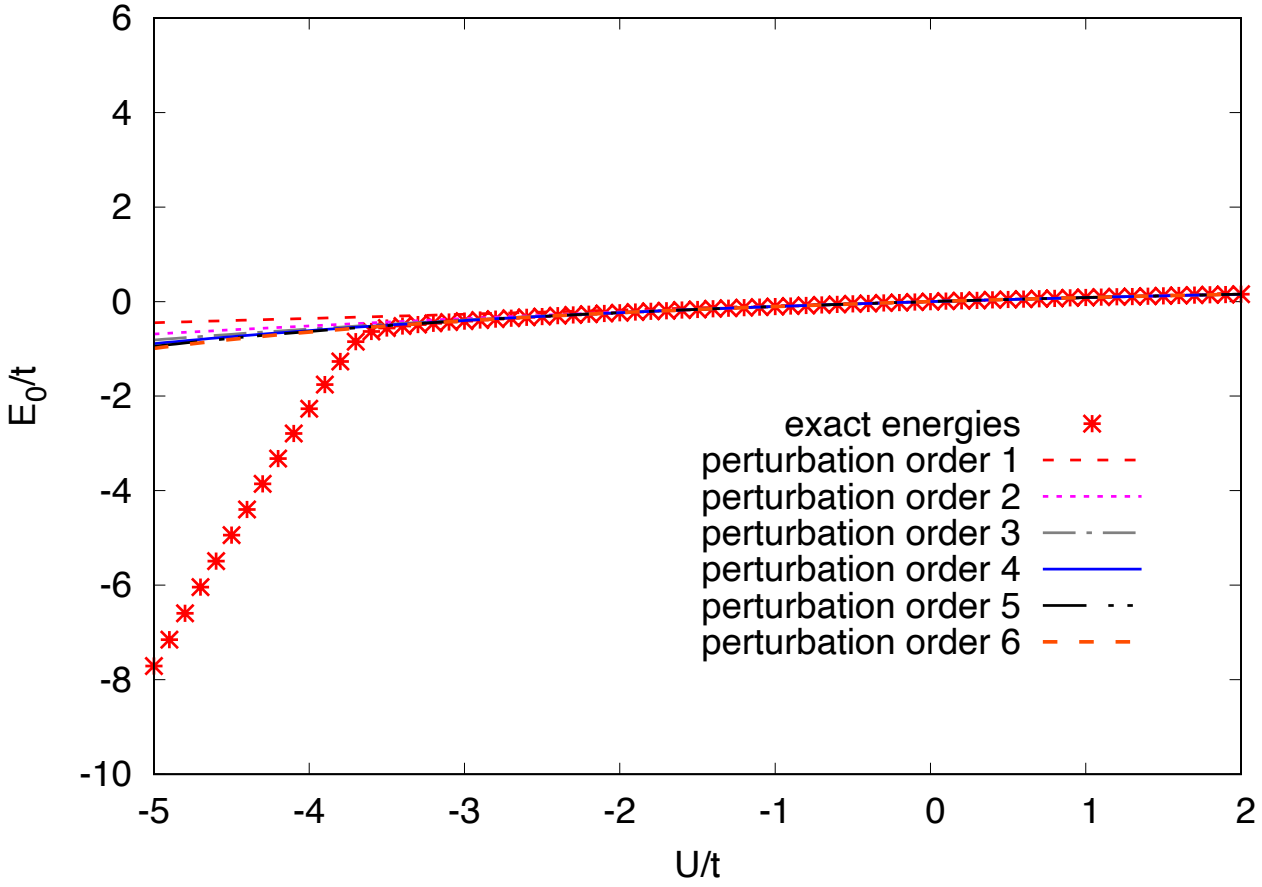
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

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

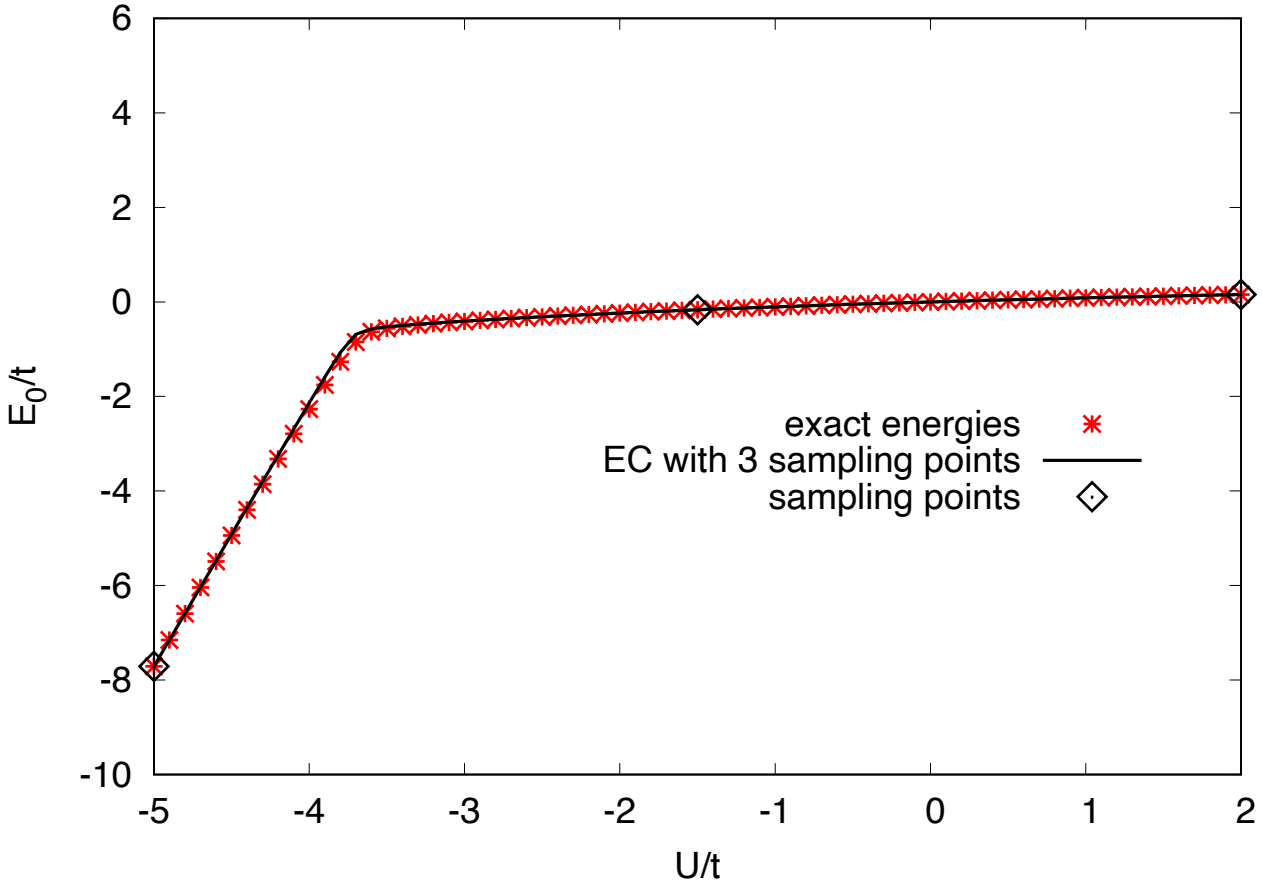
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

Perturbation theory fails at strong attractive coupling

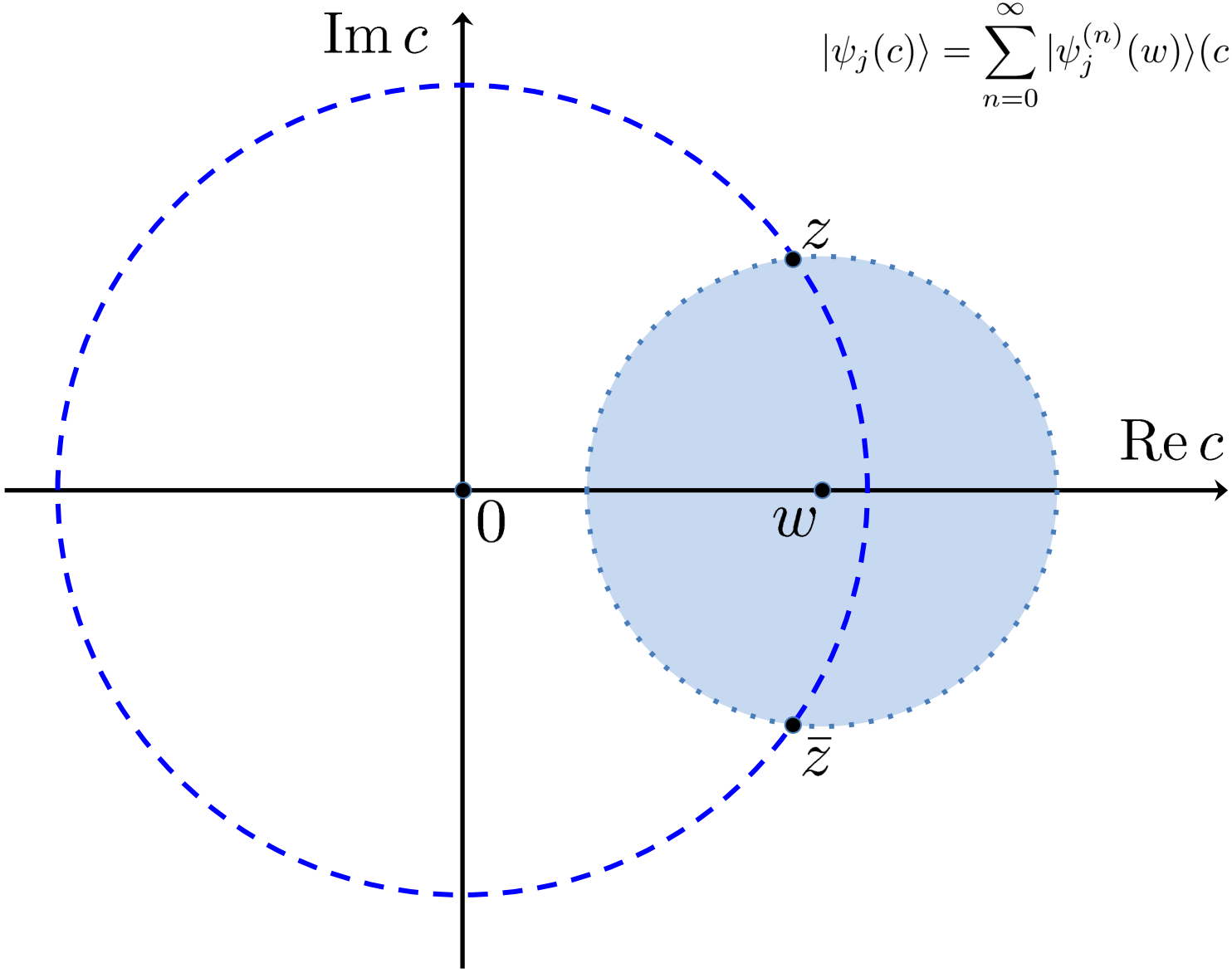


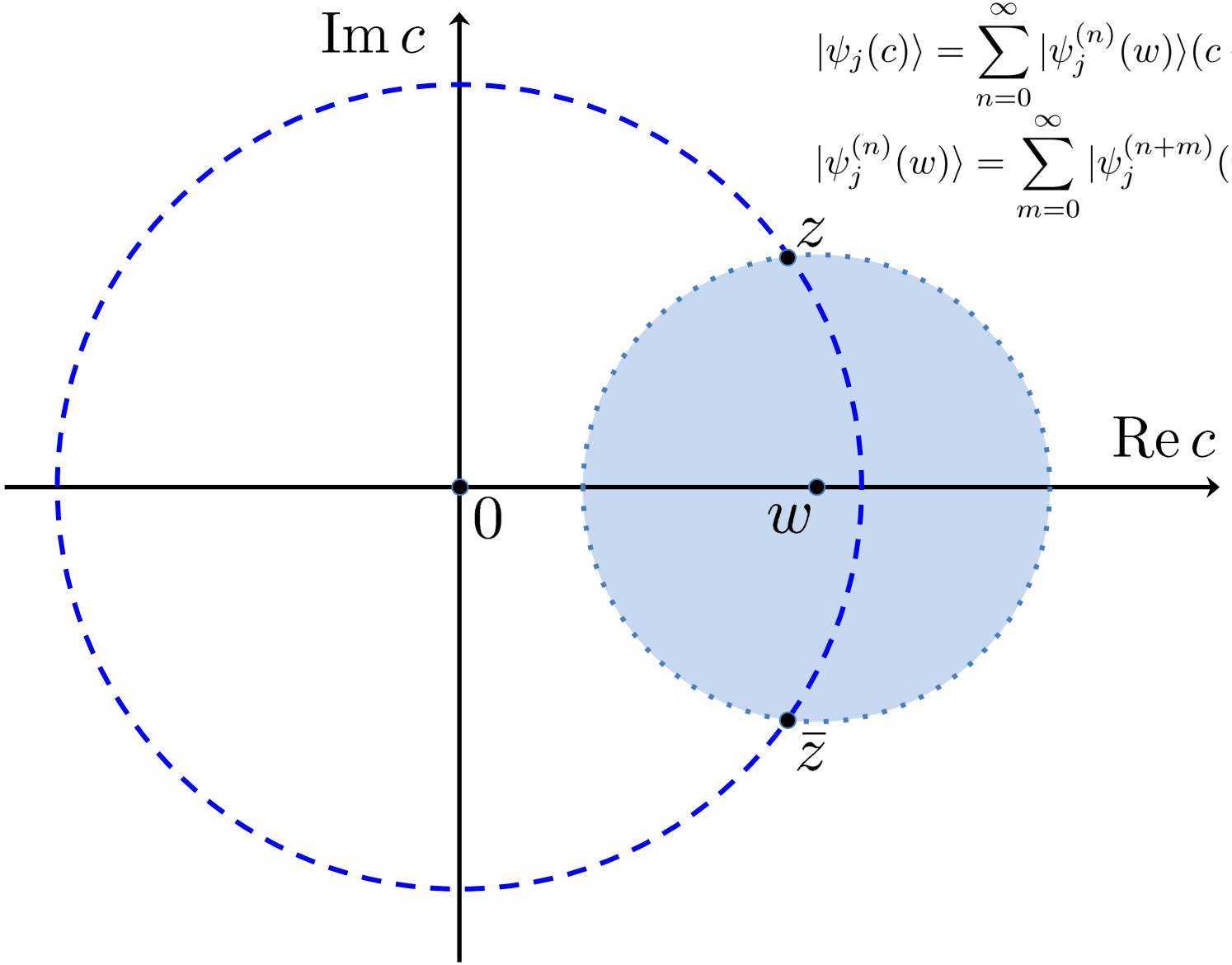
Restrict the linear space to the span of three vectors



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

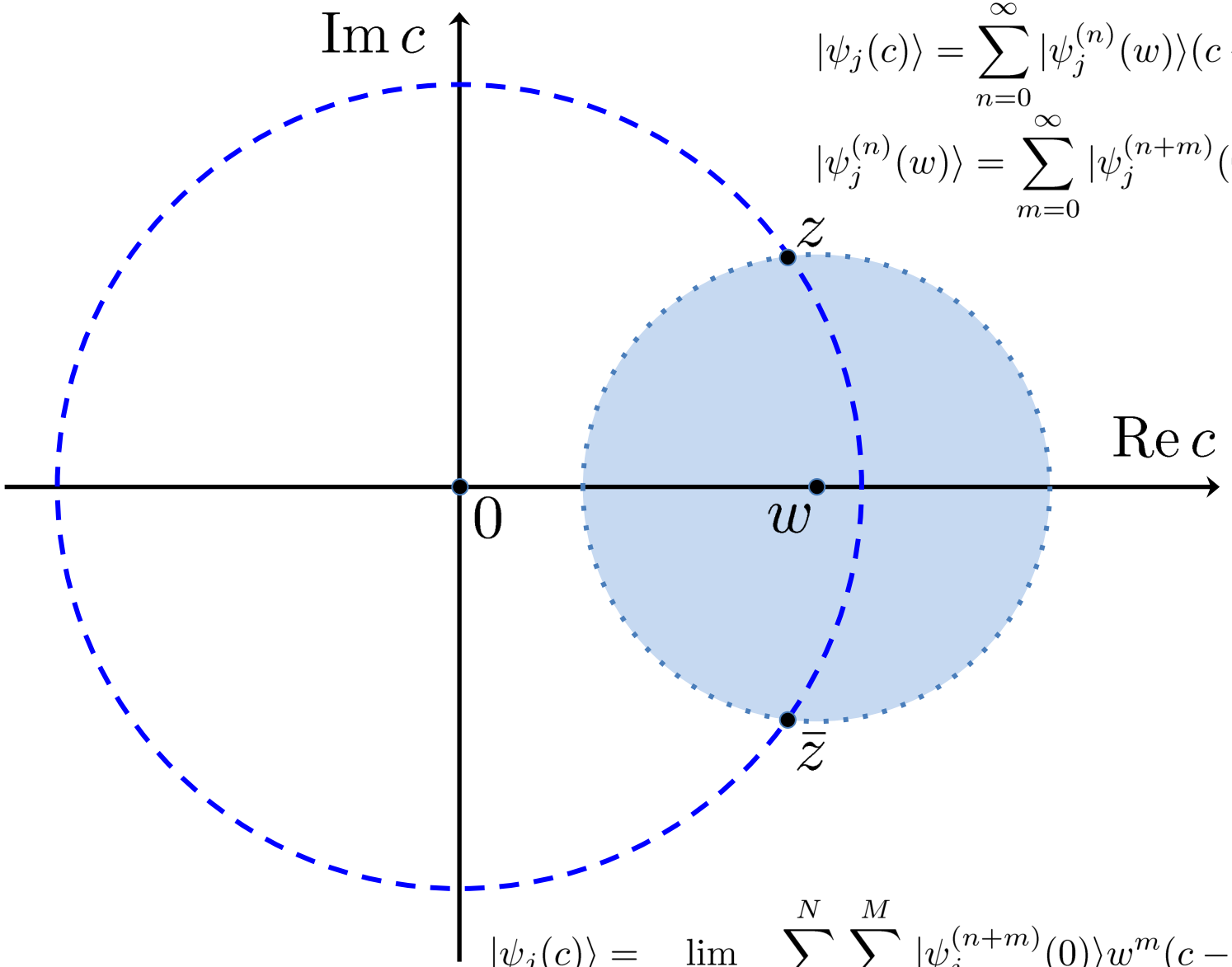
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





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

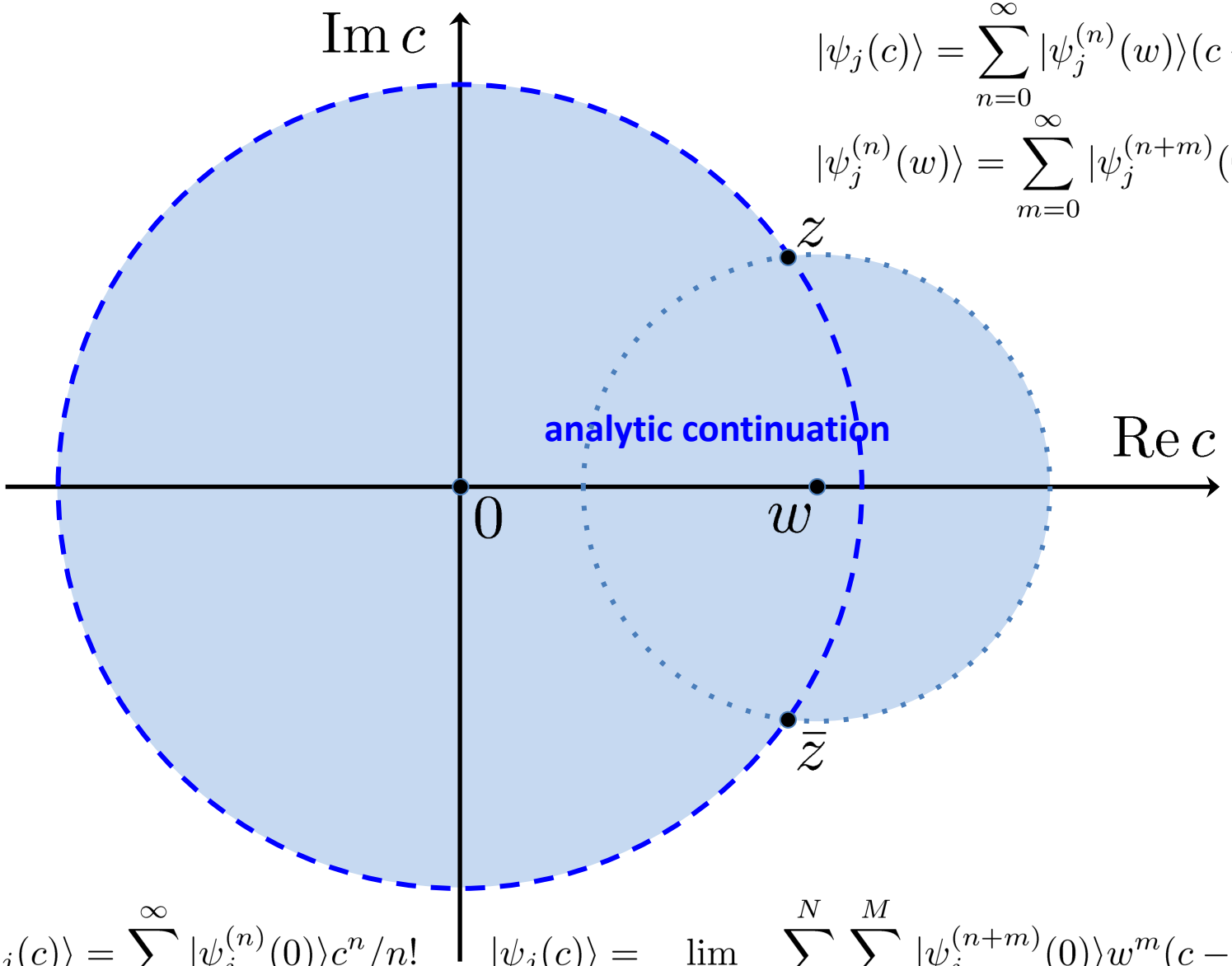
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



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

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

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



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

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

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

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

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

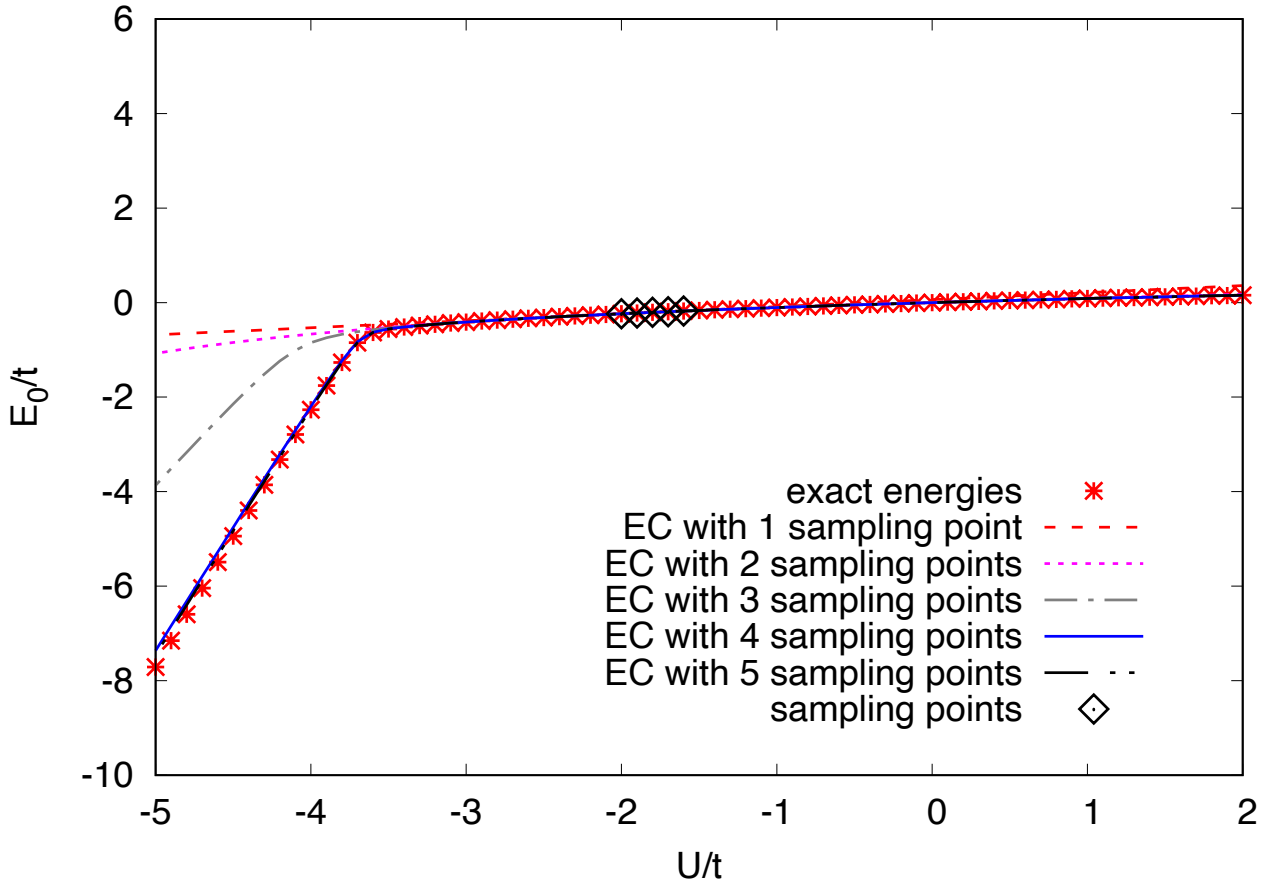
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

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

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

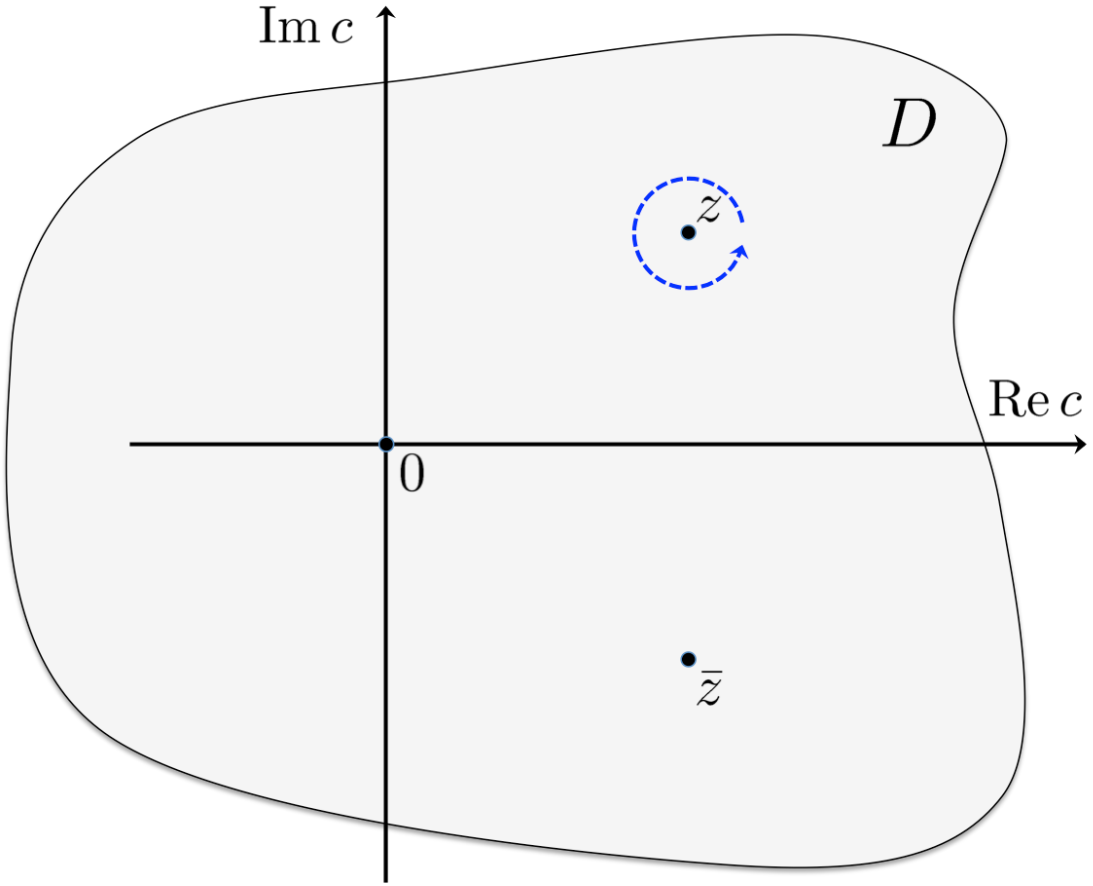
As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

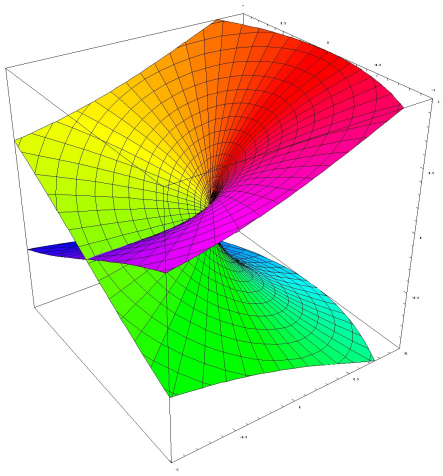
We can "learn" the eigenvector trajectory in one region and perform eigenvector continuation to another region



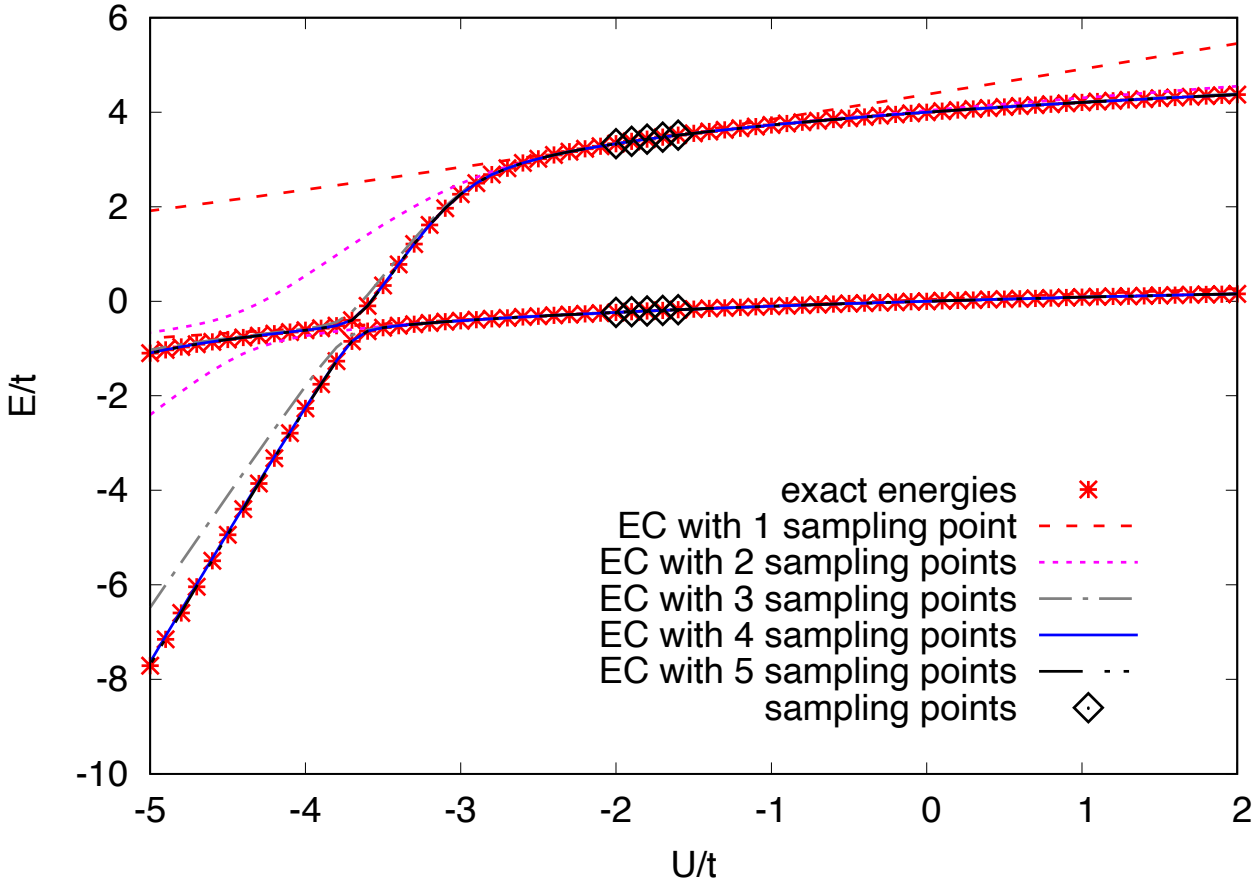
D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121 (2018) 032501

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.



Improved many-body expansions from eigenvector continuation

P. Demol, T. Duguet, A. Ekström, M. Frosini, K. Hebeler, S. König, D. Lee, A. Schwenk, V. Somà, and A. Tichai
Phys. Rev. C **101**, 041302(R) – Published 9 April 2020

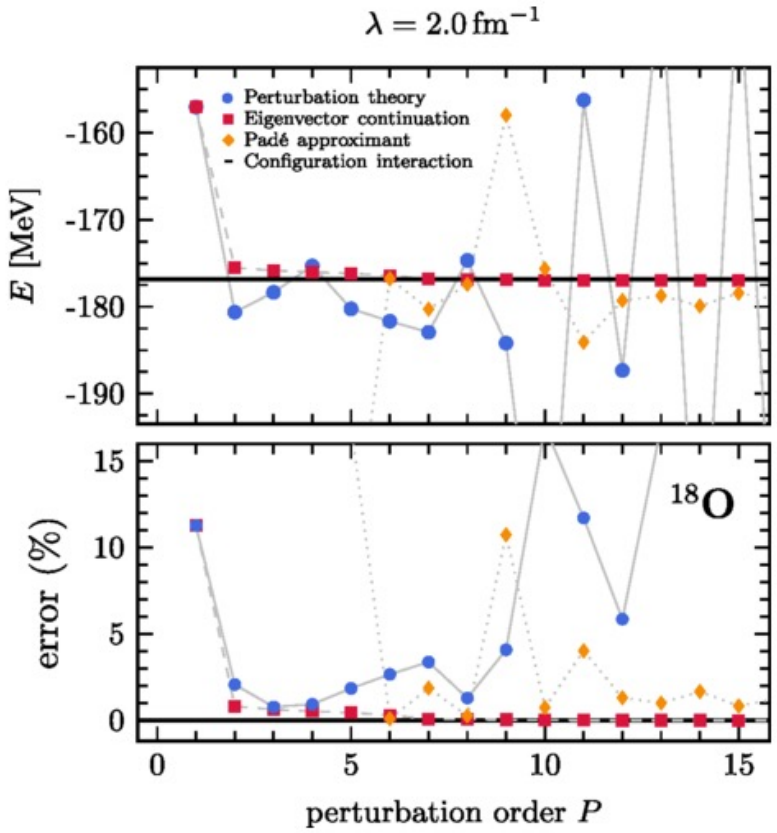


Figure 2

Ground-state energy of ^{18}O for BMBPT (blue circles), BMBPT-based EC (red squares), and BMBPT-based Padé (yellow diamonds) as a function of the perturbative order P against exact CI diagonalization (full line) for $\lambda = 2.0\ \mathrm{fm}^{-1}$. Top panel: absolute energies. Bottom panel: relative error to the CI result.

See talk by Pepjin Demol on Thursday

Physics Letters B
Volume 810, 10 November 2020, 135814

Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification

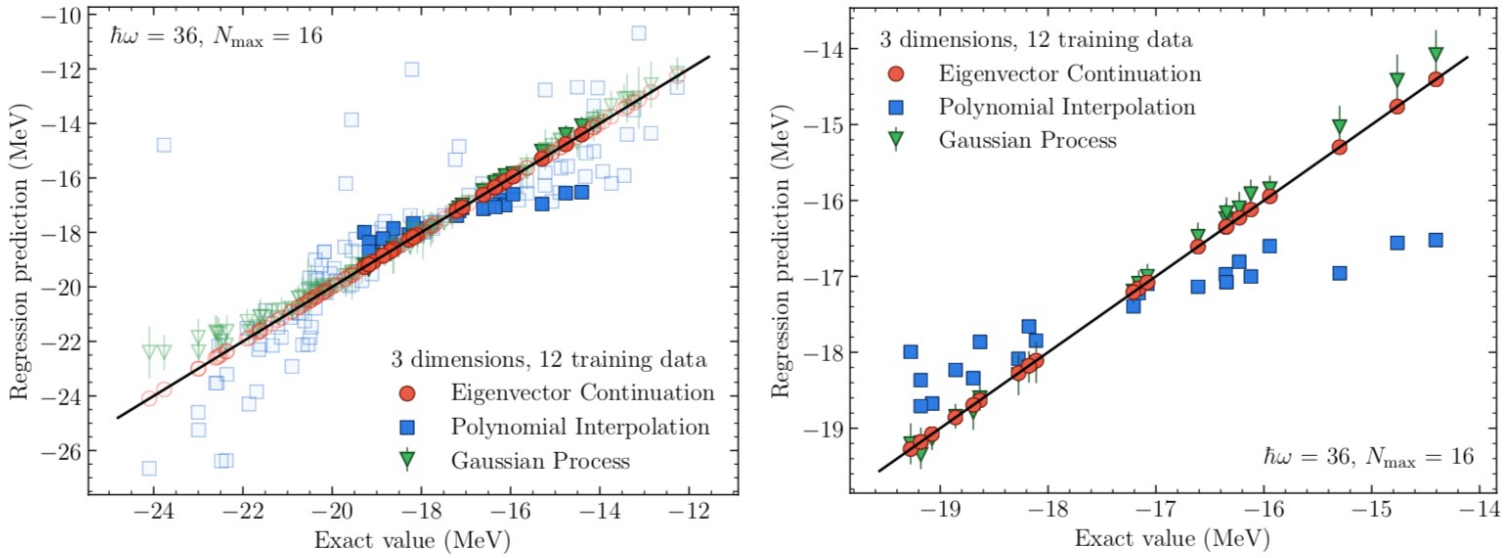
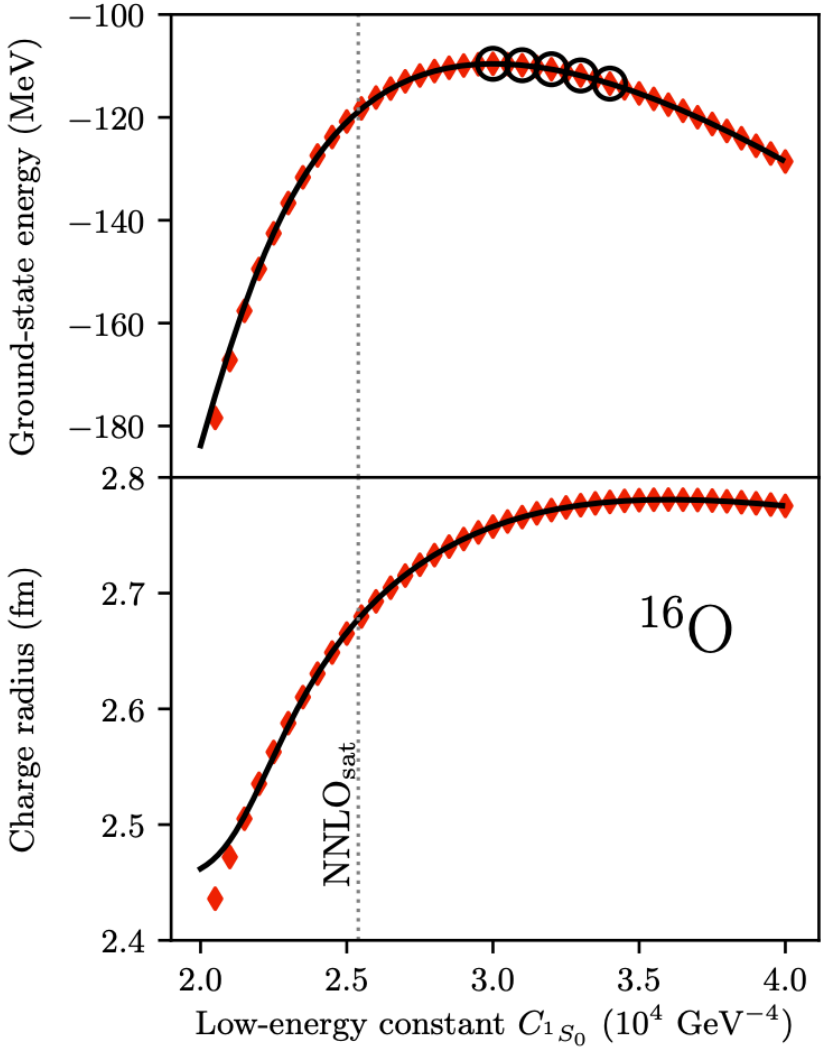


Figure 1. Comparison of different emulators for the ^{4}He ground-state energy using 12 training data points to explore a space where three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols). See main text on how these are defined. The right panel shows the same data restricted to interpolation samples (note the smaller axis range).

See talk by Sebastian König today

Sub-space projected coupled-cluster

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



- Generalization of the eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018)]
- Write the Hamiltonian in a linearized form

$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\rm LECs}=16} \alpha_i h_i$$

- Select "training points" where we solve exact CCSD
- Project the target Hamiltonian onto sub-space of training vectors and diagonalize the generalized eigen value problem

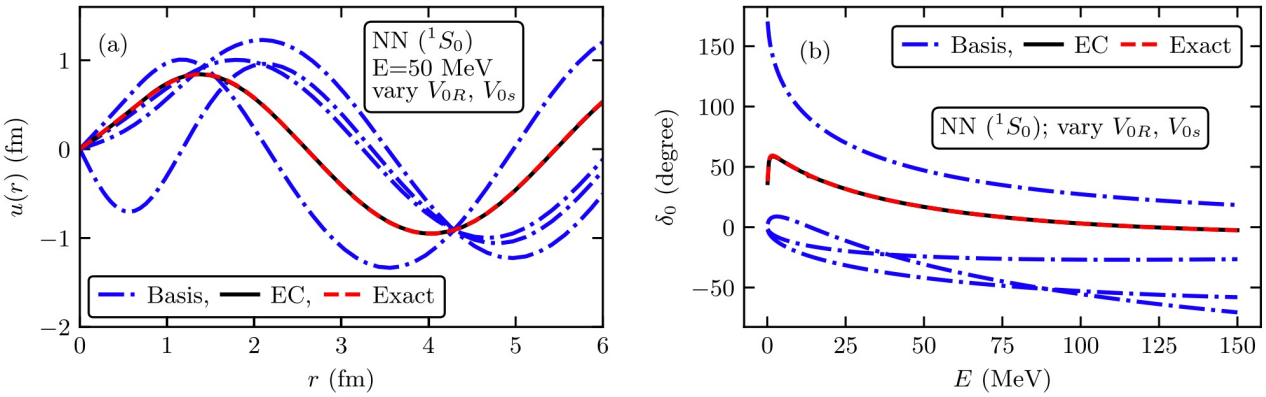
$$\mathbf{H}(\vec{\alpha}_\odot)\,\vec{c} = E(\vec{\alpha}_\odot)\,\mathbf{N}\,\vec{c}$$

See talk by Gaute Hagen on Wednesday

Physics Letters B
Volume 809, 10 October 2020, 135719

Efficient emulators for scattering using eigenvector continuation

R.J. Furnstahl, A.J. Garcia, P.J. Millican, Xilin Zhang



See talks by Christian Drischler on Wednesday and Xilin Zhang on Thursday

Kohn variational principle

Consider the differential operator for partial wave scattering

$$D \equiv -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r) - p^2.$$

Consider the functional

$$\beta[u_{\rm t}] = \tau_{\rm trial} - \int_0^\infty dr\; u_{\rm t}(r) D u_{\rm t}(r),$$

$$u_{\rm t}(r) \xrightarrow[r\to\infty]{} \tfrac{1}{p}\sin(pr - \tfrac{1}{2}\ell\pi) + \tau_{\rm trial}\cos(pr - \tfrac{1}{2}\ell\pi).$$

For trial states close to the exact scattering wave function,

$$u_{\rm t}(r) = u_{\rm exact}(r) + \delta u(r),$$

the linear variation of the functional vanishes,

$$\delta\beta = 0 + \mathcal{O}(\delta u^2).$$

Convergence of Eigenvector Continuation

Avik Sarkar* and Dean Lee†
Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

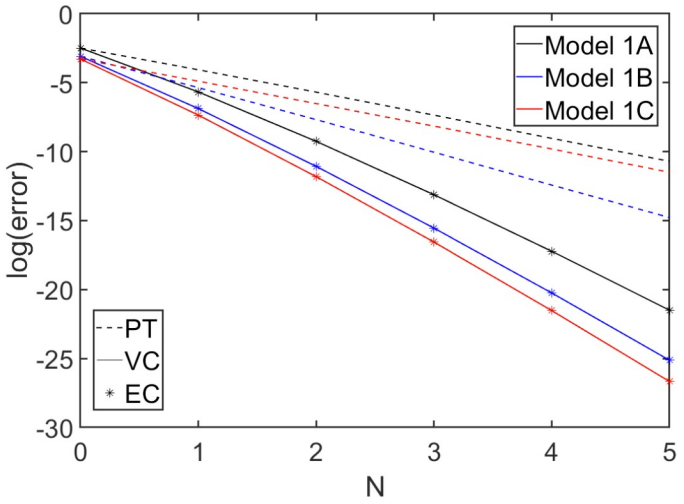
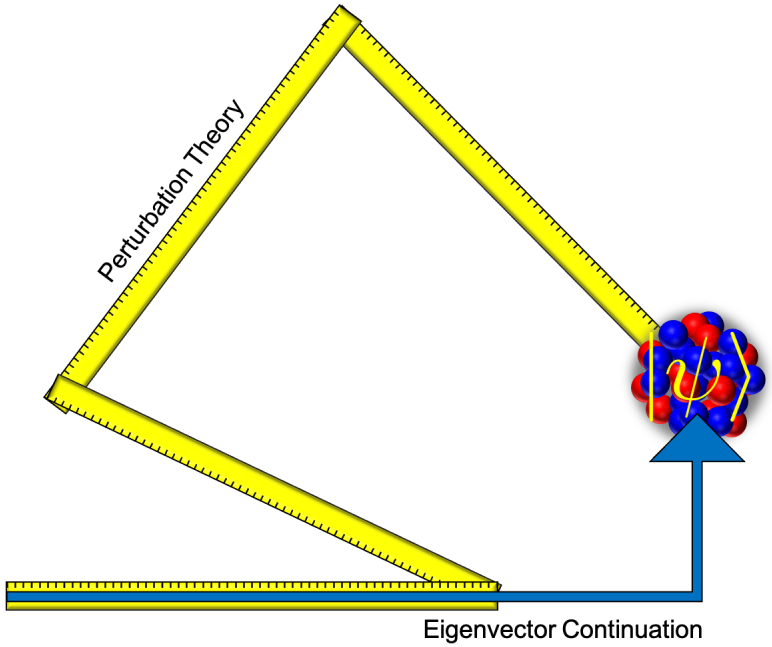
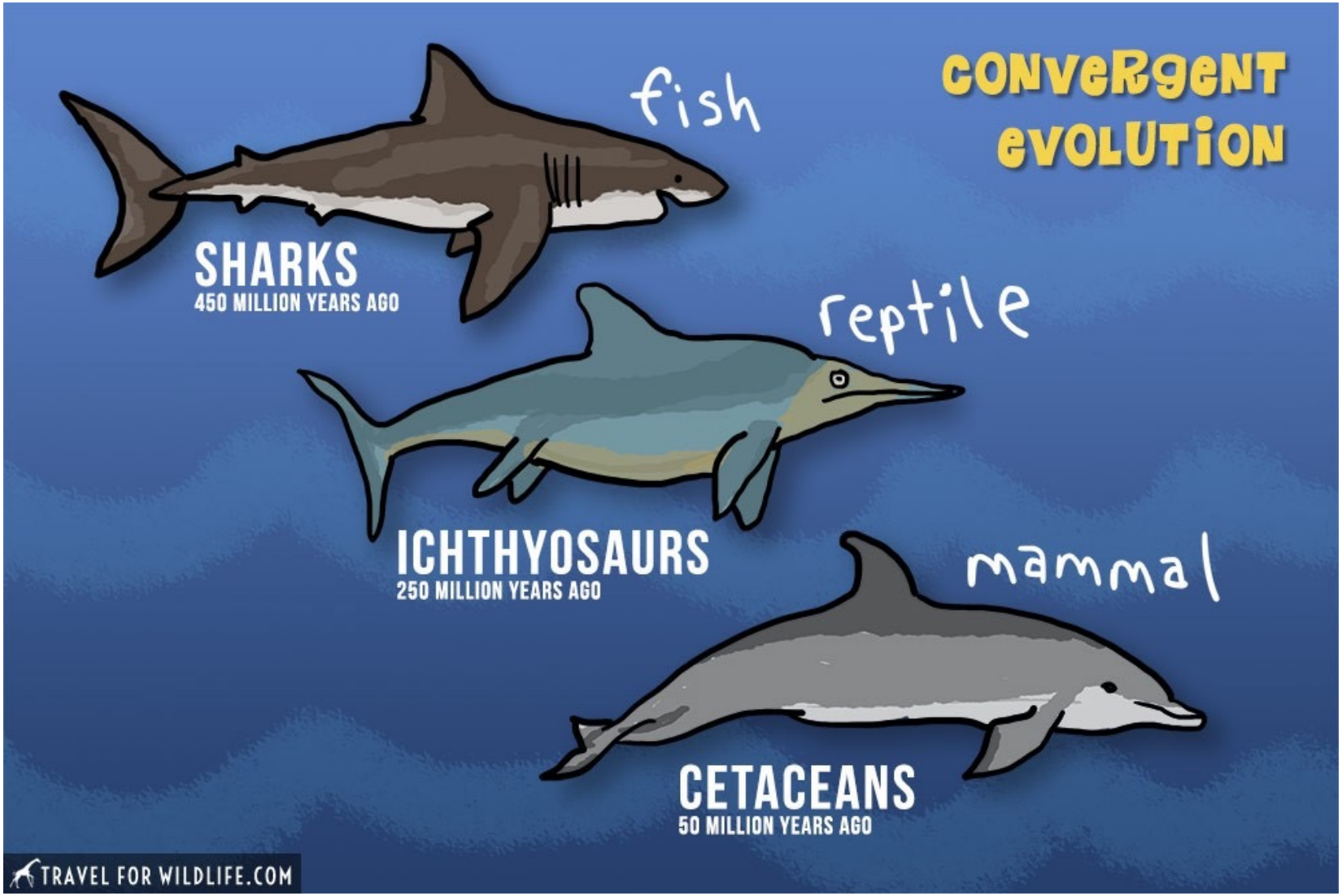


FIG. 1: (Color online) Logarithm of the error versus order N for eigenvector continuation (asterisks), vector continuation (solid lines), and perturbation theory (dashed lines). The three different colors (black, blue and red) correspond with Models 1A, 1B, and 1C respectively.



See talk by Avik Sarkar on Wednesday


CONVERGENT EVOLUTION
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Projection-based emulators

Model reduction methods for nuclear emulators

J A Melendez[1], C Drischler[2], R J Furnstahl[3,1], A J Garcia[1] and Xilin Zhang[2]

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Journal of Physics G: Nuclear and Particle Physics, Volume 49, Number 10

Citation J A Melendez *et al* 2022 *J. Phys. G: Nucl. Part. Phys.* **49** 102001

DOI 10.1088/1361-6471/ac83dd

Training and projecting: A reduced basis method emulator for many-body physics

Edgard Bonilla, Pablo Giuliani, Kyle Godbey, and Dean Lee

Phys. Rev. C **106**, 054322 – Published 17 November 2022

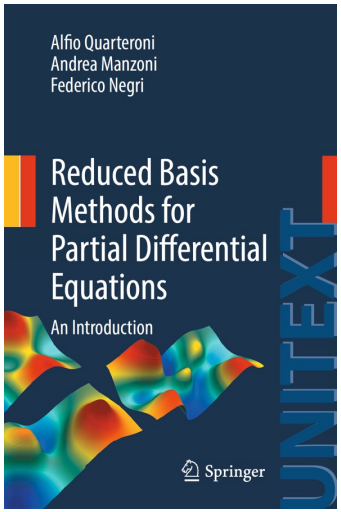
Reduced basis methods have been well-studied in the field of partial differential equations for several decades. Part of a larger class of methods called model order reduction. Use of Galerkin methods, extensions to nonlinear systems, etc.

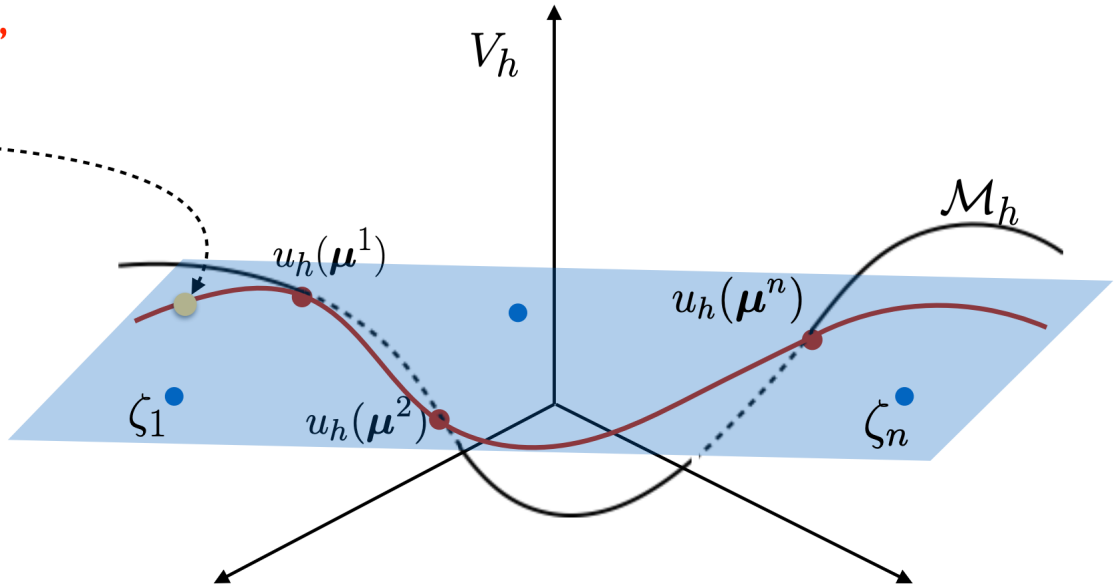
See talks by Pablo Giuliani on Thursday
and Kyle Godbey on Friday

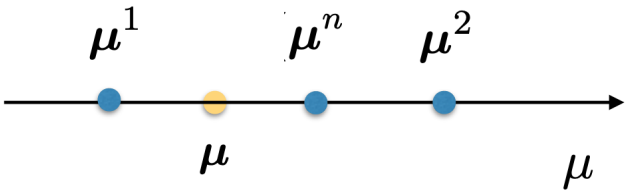
RB Approximation

RB Approximation
(new parameter value, PROJECTION)

$$\{u_n(\boldsymbol{\mu}) \ : \boldsymbol{\mu} \in \mathcal{P}\}$$







- **Snapshots computed offline** (properly selected parameters)
- **RB space**: $V_n = \text{span}\{u_h(\boldsymbol{\mu}^1), \ldots, u_h(\boldsymbol{\mu}^n)\} = \text{span}\{\zeta_1, \ldots, \zeta_n\}$
- **RB problem** $P_n(\mu)$ solved **online**

Trimmed sampling algorithm

Projection-based emulator such as eigenvector continuation require solving the generalized eigenvalue problem. This can be very difficult if there are errors in the calculations of the matrix elements.

$$H\,|\psi\rangle = EN\,|\psi\rangle$$

PHYSICAL REVIEW RESEARCH **5**, L022001 (2023)

Letter

Trimmed sampling algorithm for the noisy generalized eigenvalue problem

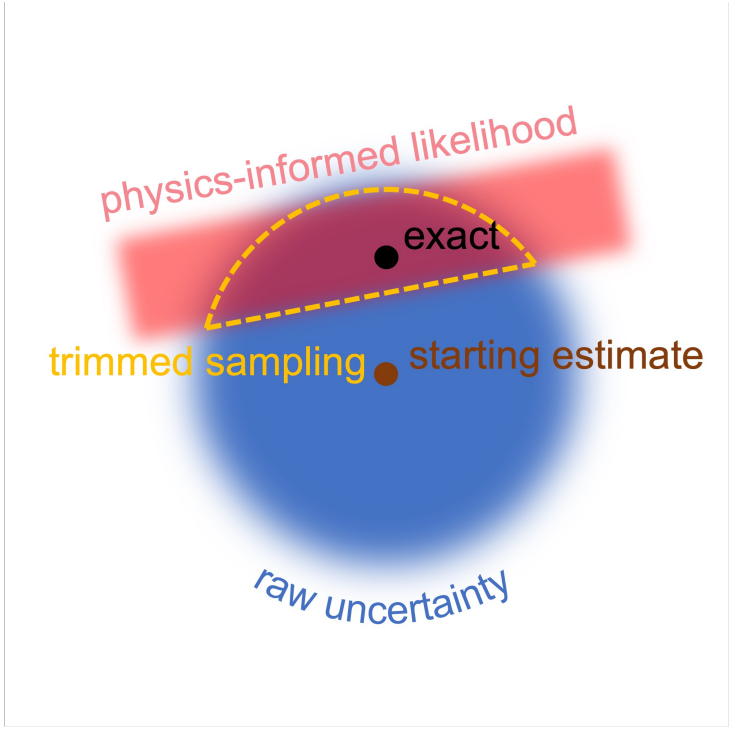
Caleb Hicks and Dean Lee

Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

Trimmed sampling uses the mean values and error estimates for the elements of N and H to produce a large ensemble of random samples. These correspond to the Bayesian prior distribution. The Bayesian likelihood functions are composed of physics-informed constraints.

$$N_{\text{trial}} = N + \Delta N$$

$$H_{\text{trial}} = H + \Delta H$$



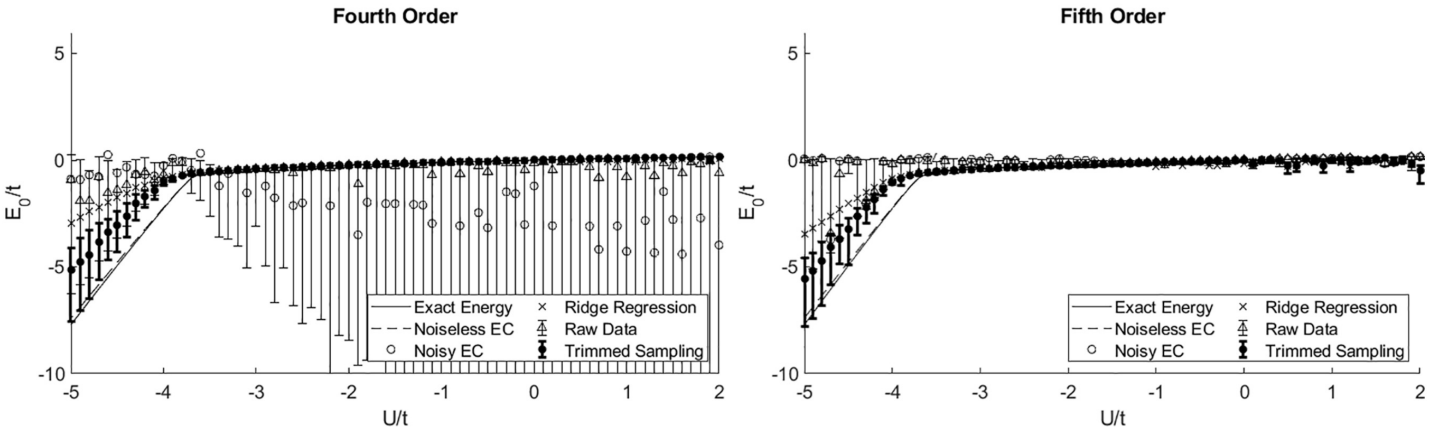


FIG. 1. Ground-state energy of the Bose-Hubbard model as a function of coupling strength U/t. The "exact" ground-state energies are plotted as solid lines. The "noiseless EC" data are presented with dashed lines. The "noisy EC" results corresponding to matrix elements $\tilde{H}$ and $\tilde{N}$ are plotted with open circles. The results using "ridge regression" are shown with times symbols. The "raw data" obtained by sampling the prior probability distribution are displayed with open triangles and error bars. The "trimmed sampling" results are plotted as filled circles with error bars.

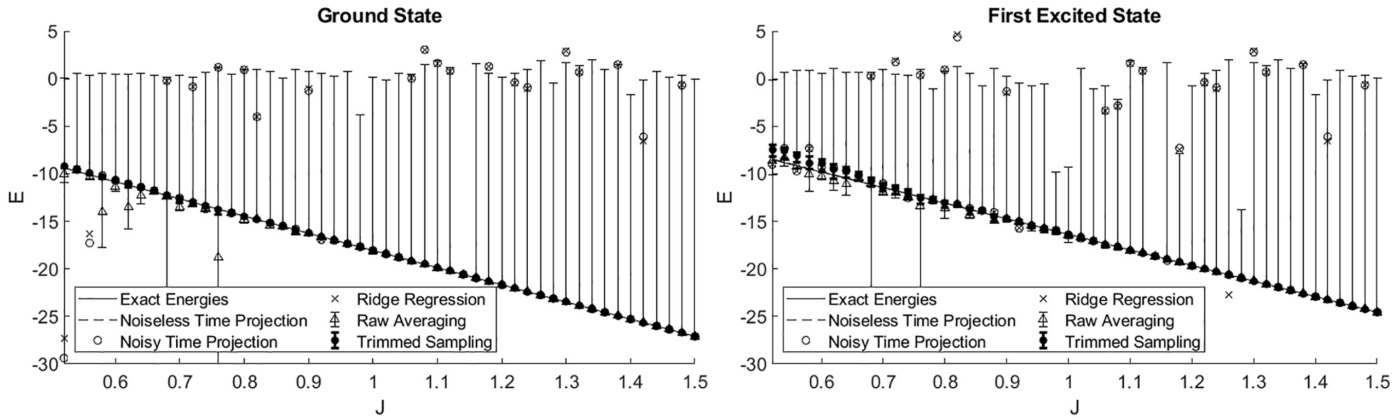


FIG. 2. Ground-state and first excited state energies of the one-dimensional Heisenberg chain as a function of coupling strength J. The "exact" energies are plotted as solid lines. The "noiseless time projection" data are dashed lines. The "noisy time projection" results corresponding to the matrix elements $\tilde{H}$ and $\tilde{N}$ are plotted with open circles. The data obtained using "ridge regression" are shown with times symbols. The "raw data" obtained by sampling the prior probability distribution are drawn with open triangles and error bars. The "trimmed sampling" results are plotted as filled circles with error bars.

Matrix eigenvalue emulators

Consider the one-parameter affine problem

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

We now do eigenvector continuation with A training vectors. This corresponds to solving the eigenvalue problem for the new one-parameter affine system,

$$M(c) = M_0 + cM_1$$

where the matrices are A by A.

Note that the eigenvalues will be roots of the characteristic polynomial

$$P[E(c)] = \det\left[E(c)I - M(c)\right] = \det\left[E(c)I - M_0 - cM_1\right]$$

The polynomial P will be degree A in with respect to $E(c)$ and degree A with respect to c.

$$P[E(c)] = [E(c)]^A + b_{A-1,1}[E(c)]^{A-1}c^1 + b_{A-1,0}[E(c)]^{A-1}c^0 + \cdots + b_{0,A}[E(c)]^0 c^A$$

In contrast with polynomial interpolation or rational interpolation (Pade approximants), we see that eigenvector continuation is performing algebraic interpolation using roots of polynomials.

Suppose that we don't have access to the training vectors. We then still make the matrix model

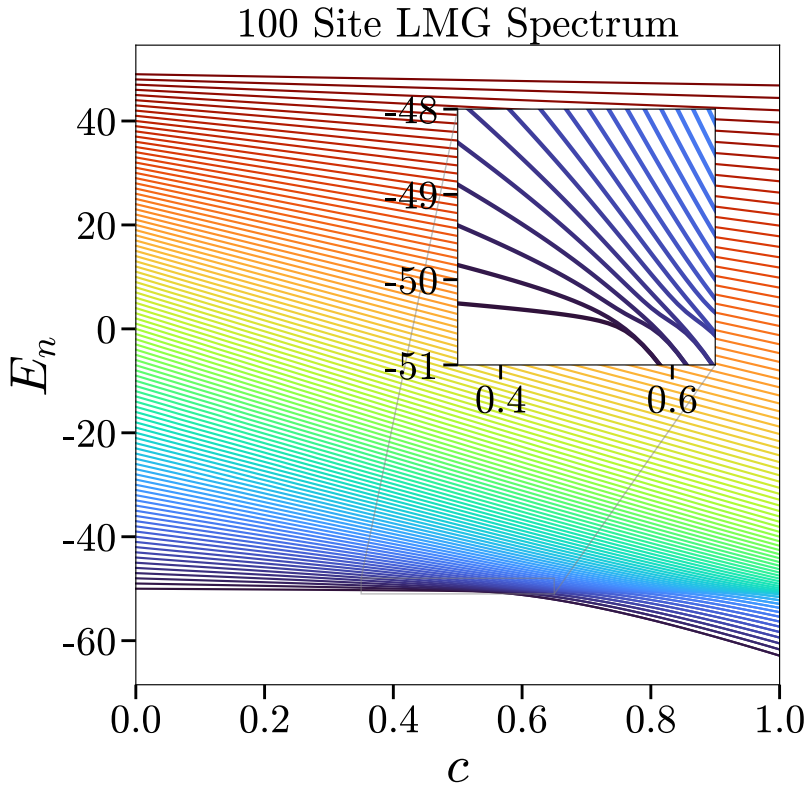
$$M(c) = M_0 + cM_1$$

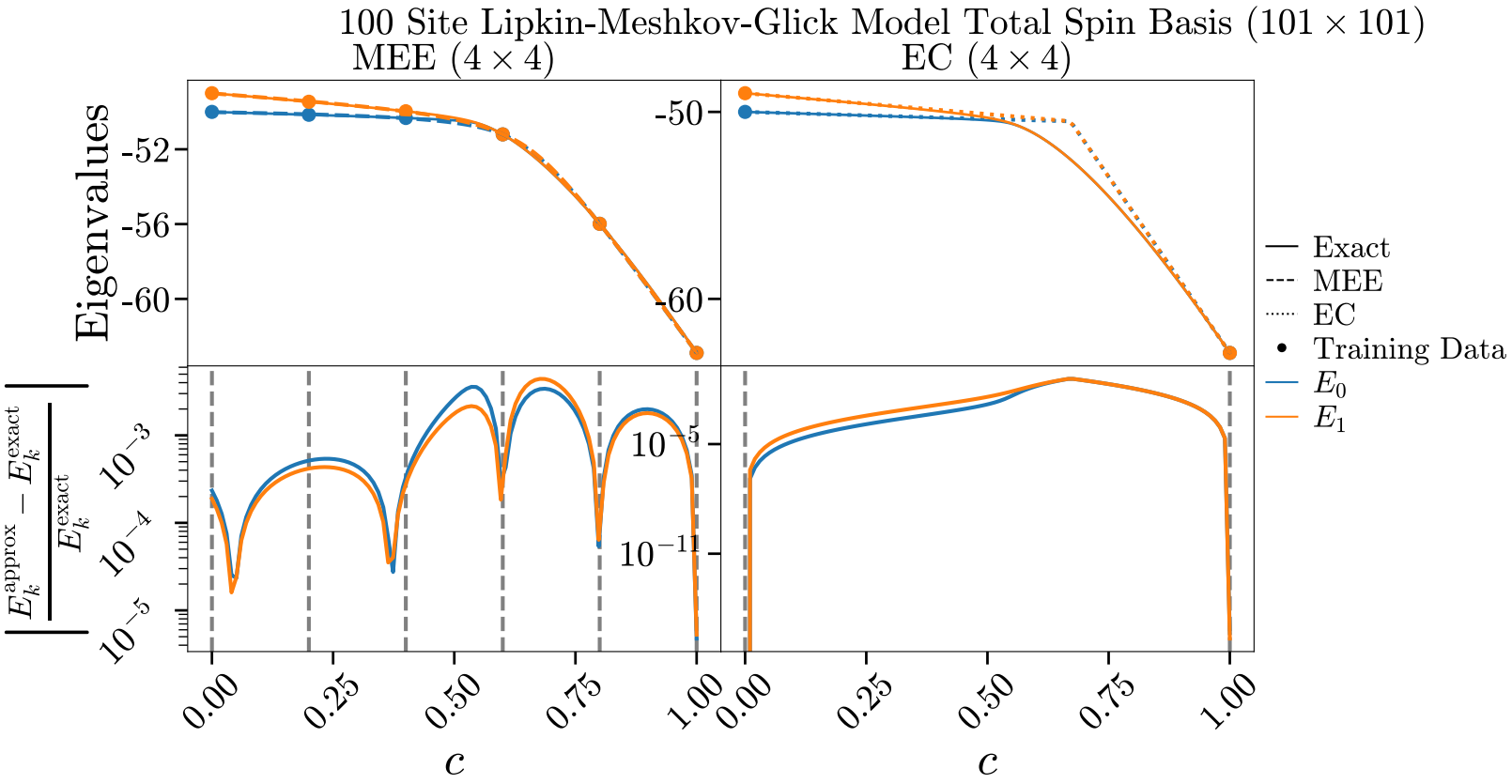
The unknown elements of these matrices are learned using the training data for the eigenvalues $E(c)$. This is an example of physics-informed implicit deep learning.

Cook, Jammooa, Hjorth-Jensen, D.L., et al., work in progress

Lipkin-Meshkov-Glick Model

$$H(c) = -S_z - \frac{2c}{N}\left(S_x^2 + \frac{1}{2}S_y^2\right) = -\sum_{i=1}^{N}\sigma_i^z - \frac{2c}{N}\sum_{i<j}^{N}\left(\sigma_i^x\sigma_j^x + \frac{1}{2}\sigma_i^y\sigma_j^y\right)$$





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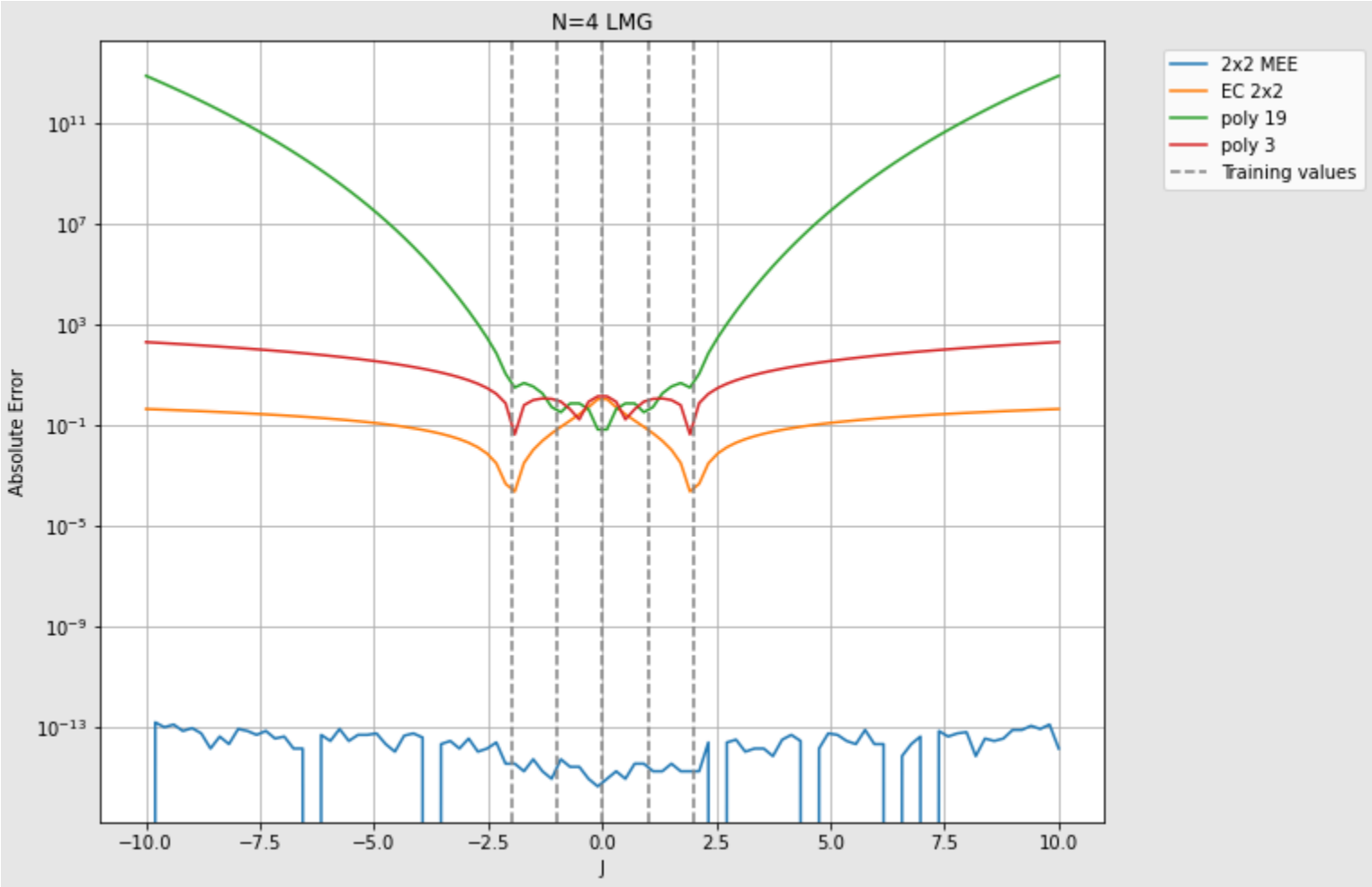
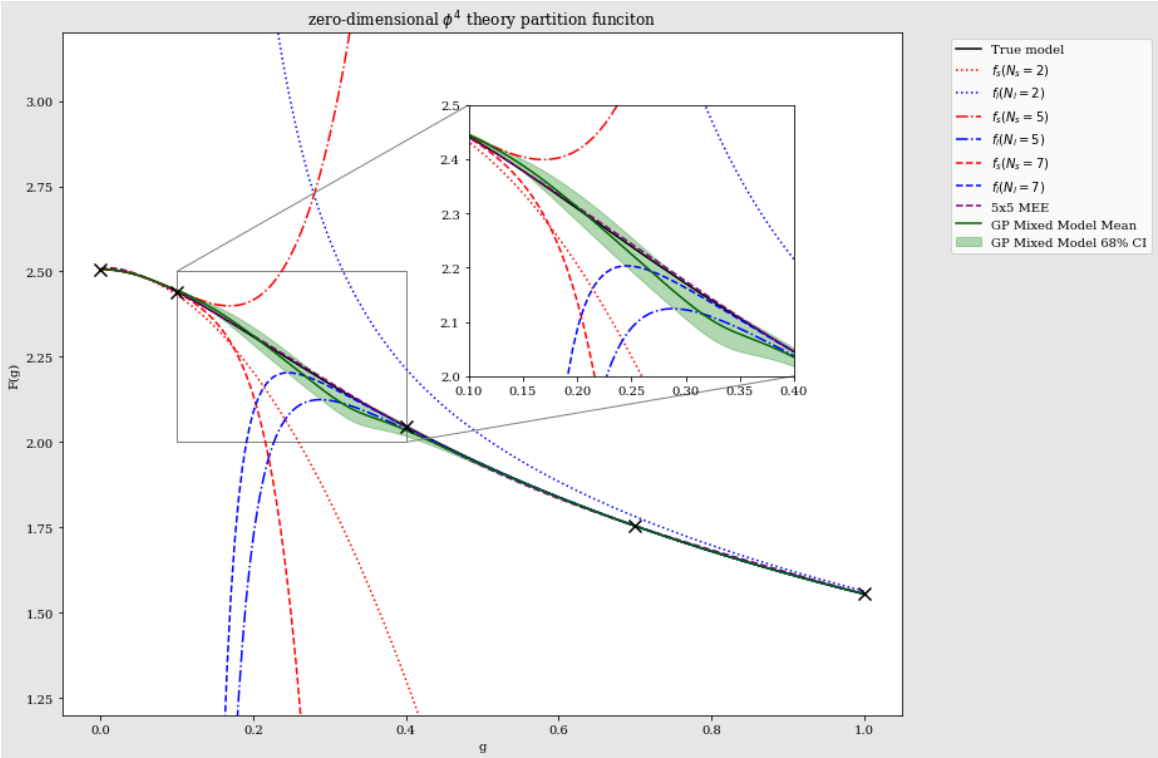


Cook, Jammooa, Hjorth-Jensen, D.L., et al., work in progress

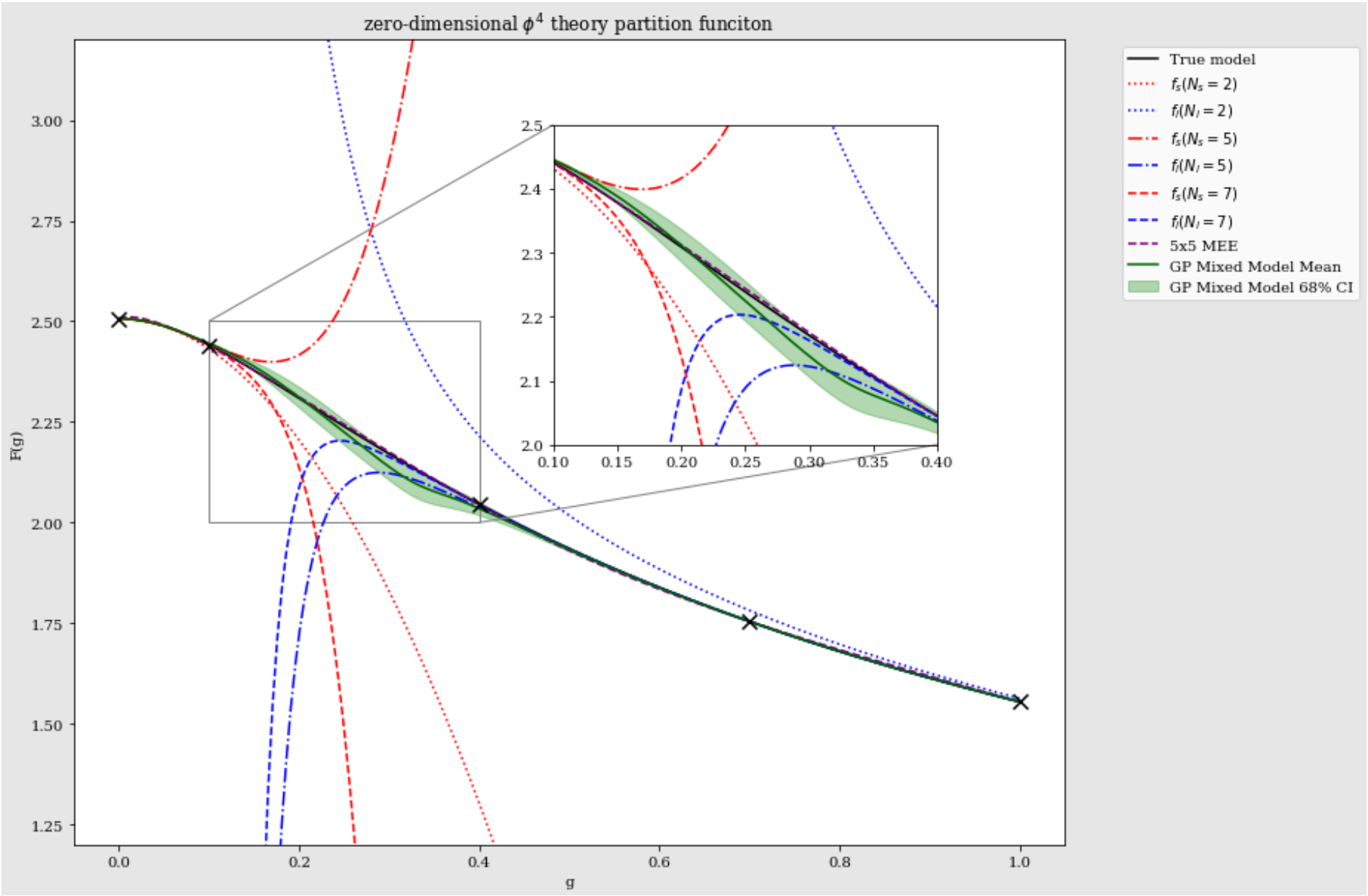
Interpolating between small- and large-g expansions using Bayesian model mixing

A. C. Semposki, R. J. Furnstahl, and D. R. Phillips
Phys. Rev. C **106**, 044002 – Published 20 October 2022

$$F(g) = \int_{-\infty}^{\infty} dx\; e^{-\frac{x^2}{2} - g^2 x^4} = \frac{e^{\frac{1}{32g^2}}}{2\sqrt{2}g} K_{\frac{1}{4}}\left(\frac{1}{32g^2}\right), \quad (3)$$



Cook, Jammooa, Hjorth-Jensen, D.L., et al., work in progress


zero-dimensional ϕ^4 theory partition funciton
True model
$f_s(N_s = 2)$
$f_l(N_l = 2)$
$f_s(N_s = 5)$
$f_l(N_l = 5)$
$f_s(N_s = 7)$
$f_l(N_l = 7)$
5x5 MEE
GP Mixed Model Mean
GP Mixed Model 68% CI
F(g)
g
3.00
2.75
2.50
2.25
2.00
1.75
1.50
1.25
0.0
0.2
0.4
0.6
0.8
1.0
2.5
2.4
2.3
2.2
2.1
2.0
0.10
0.15
0.20
0.25
0.30
0.35
0.40

Summary

This talk discussed several general concepts related to eigenvector continuation. The list included motivation from problems in quantum many-body theory, connections to perturbation theory and analytic continuation. We also discussed some early work in the field and the connection to other work on projection-based emulators. The last part of the talk covered some new material on the trimmed sampling algorithm and matrix eigenvalue emulators. The hope is that this discussion of general concepts will lead to fruitful discussion!