Eigenvector continuation and machine learning

Dean Lee
Facility for Rare Isotope Beams
Michigan State University

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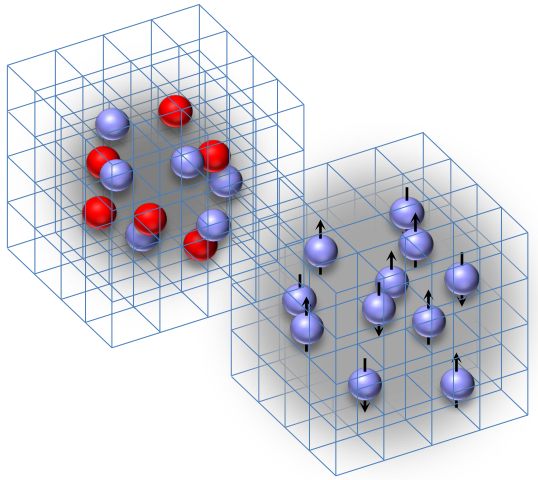

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Eigenvector continuation

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 can 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 learn the shape of this eigenvector manifold using variational subspace approximation.

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

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

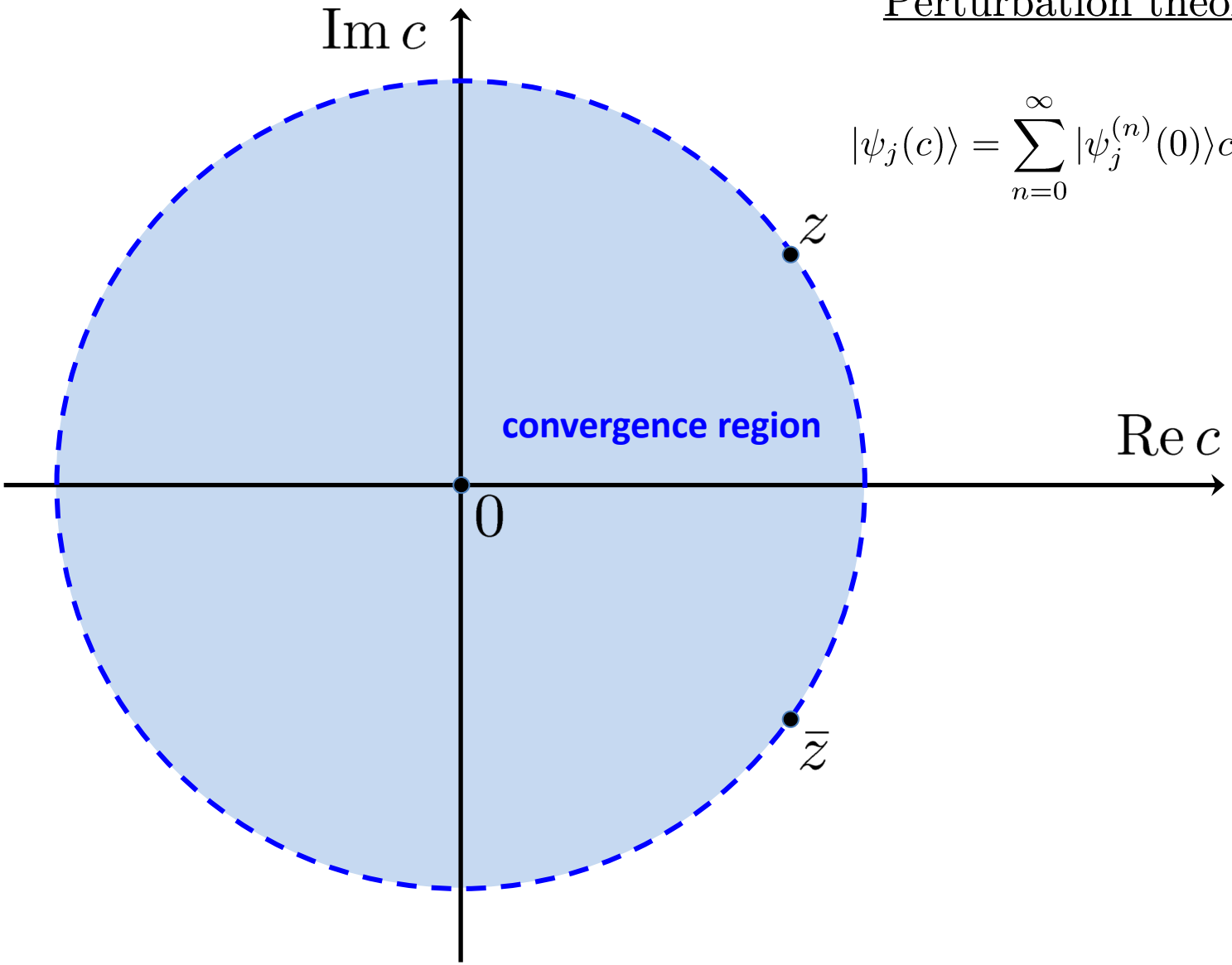
We can perform series expansions around the point $c = 0$.

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

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.

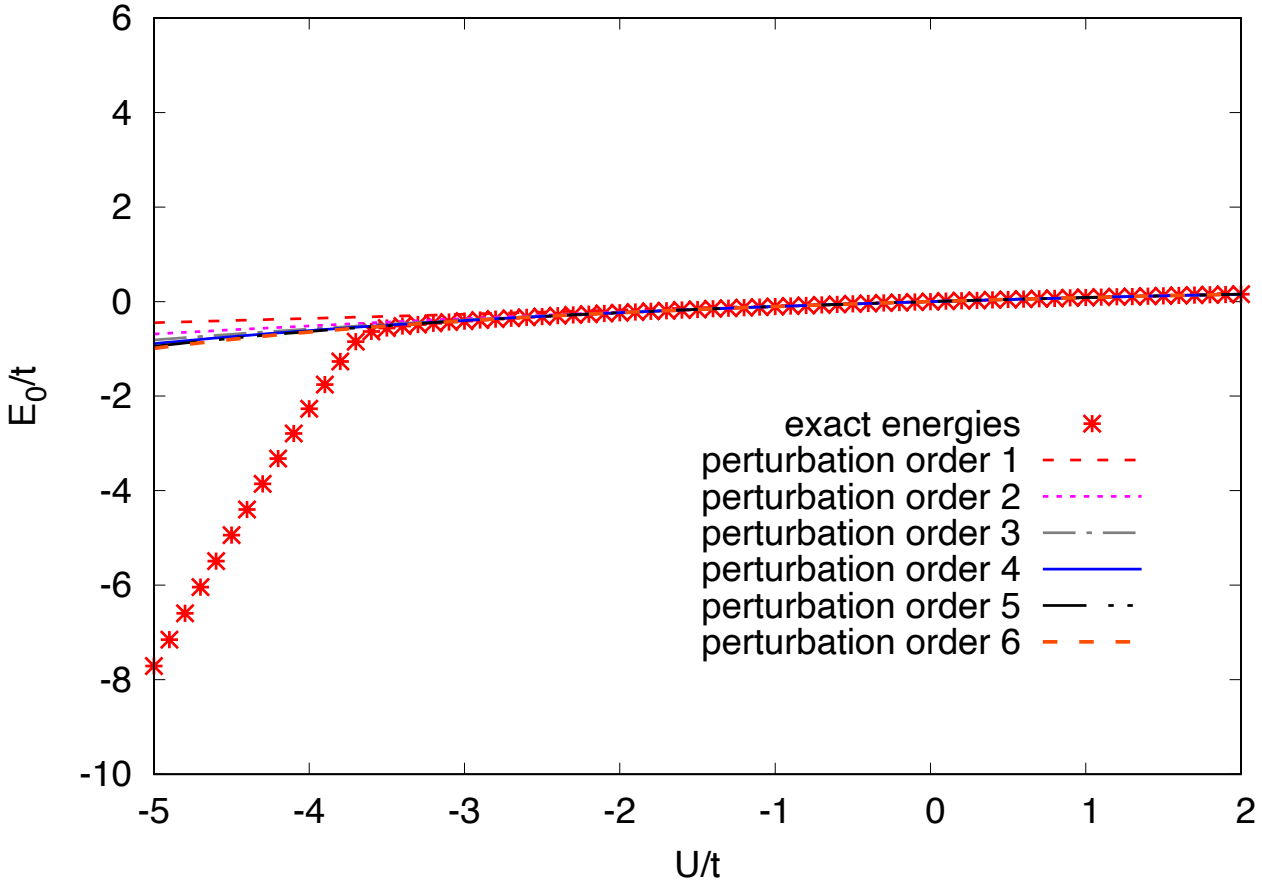
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

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

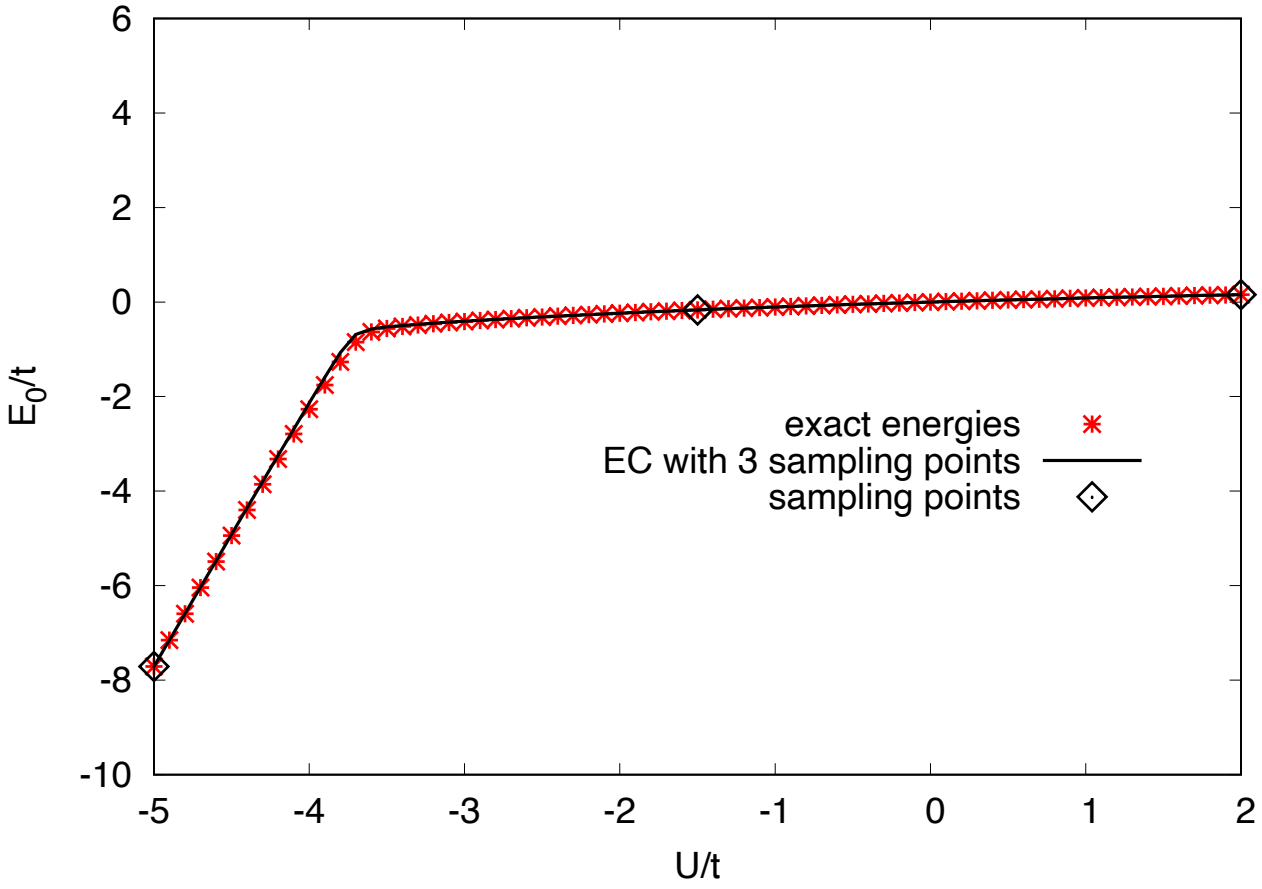
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

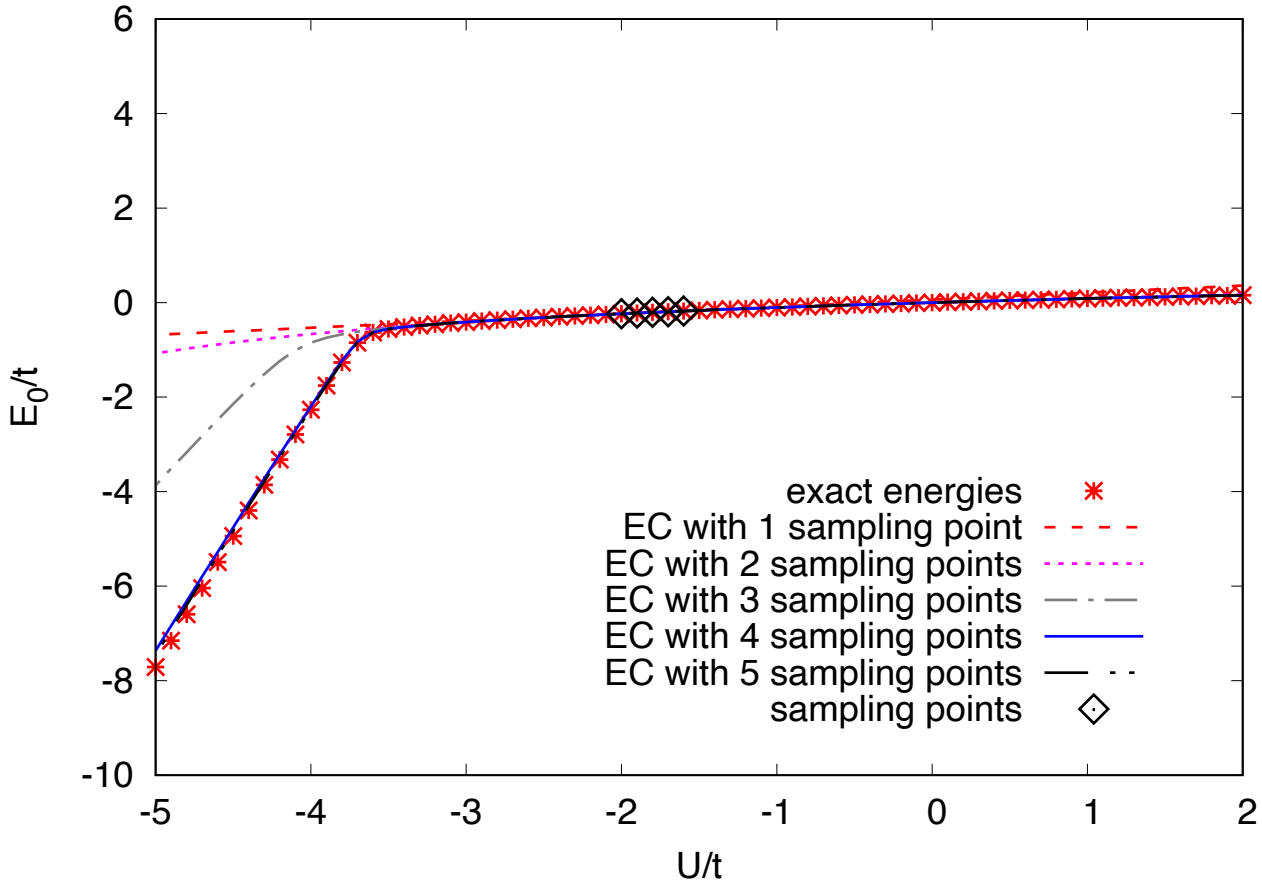
Perturbation theory fails at strong attractive coupling



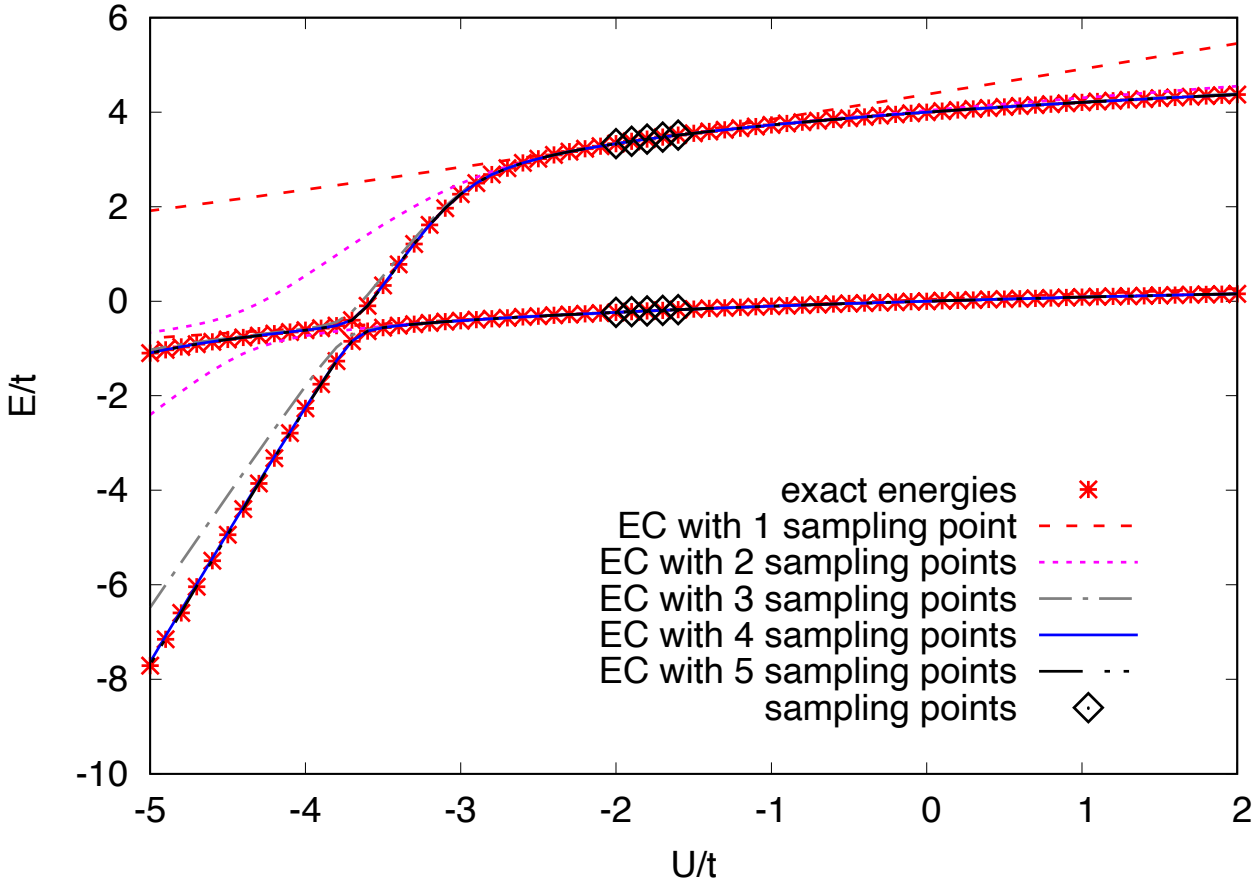
Restrict the linear space to the span of three vectors

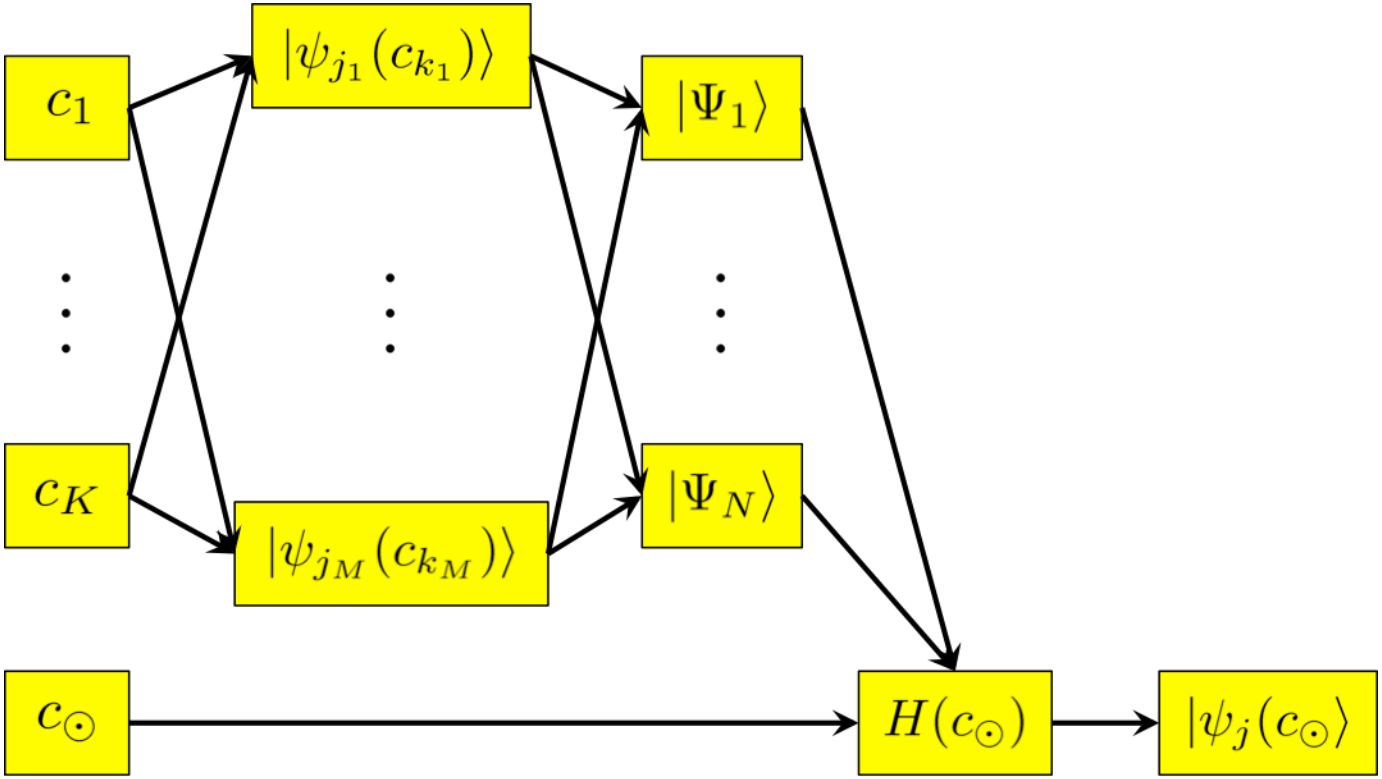


We can learn the eigenvector trajectory in one region and use eigenvector continuation to extrapolate to another region.



Applying eigenvector continuation to more than one eigenvector at a time accelerates convergence near avoided level crossings. We can learn the properties of the system near branch points.





$$\sum_{m=0}^{N}\sum_{n=0}^{N} a_{mn}[E_j(c_\odot)]^m c_\odot^n = 0$$

Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification

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

arXiv:1909.08446

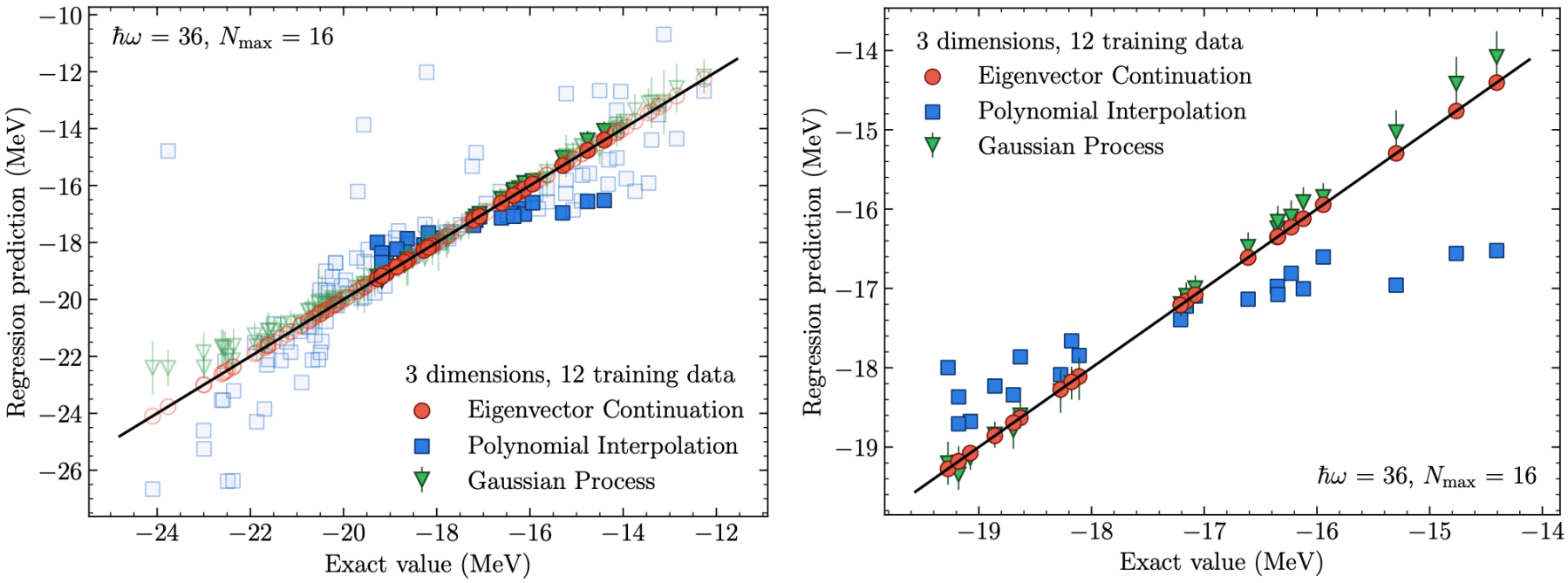


Figure 1. Comparison of different emulators for the ^{4}He ground-state energy using 12 training data points to explore a space where three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols). See main text on how these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

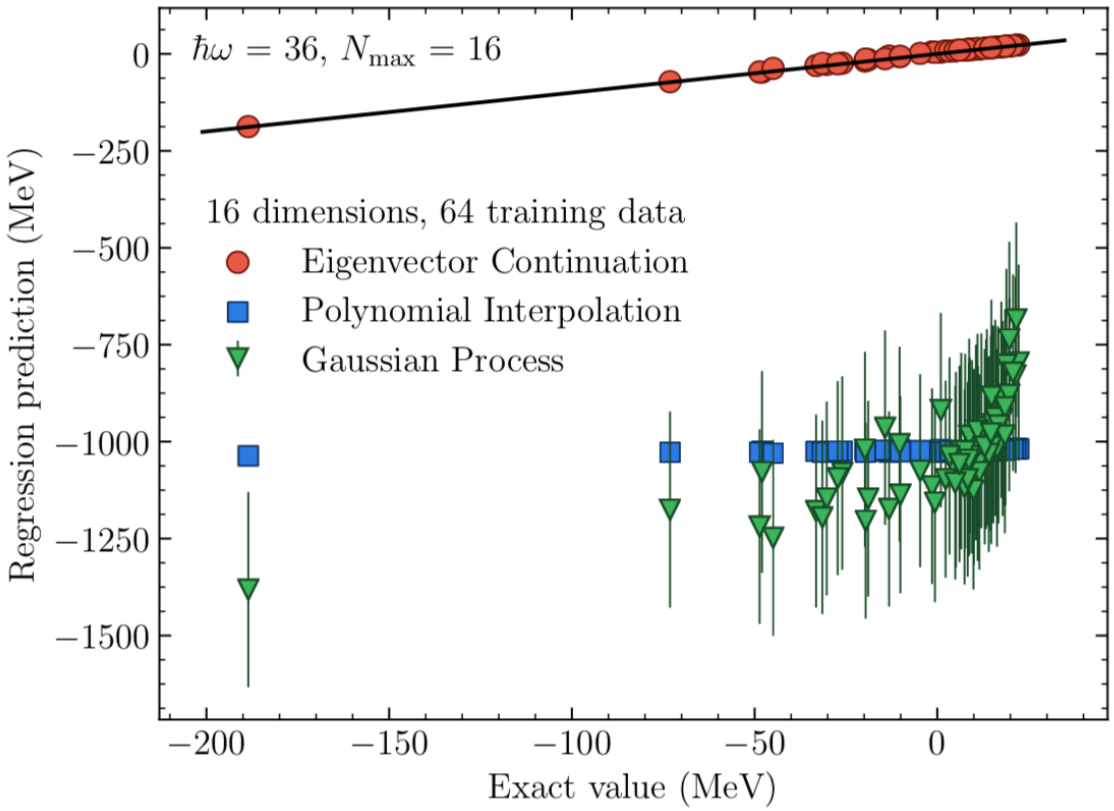
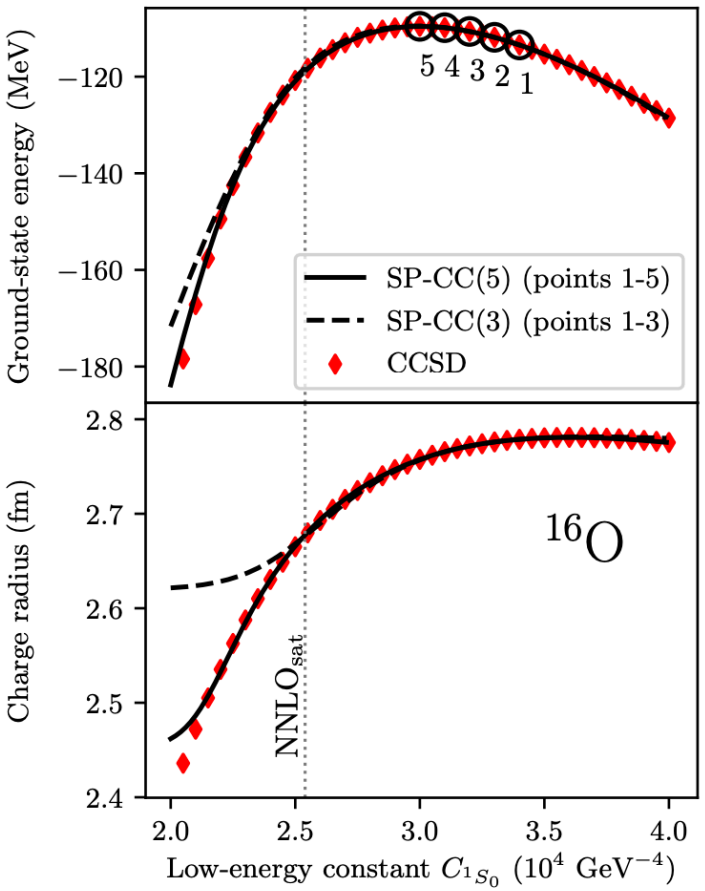
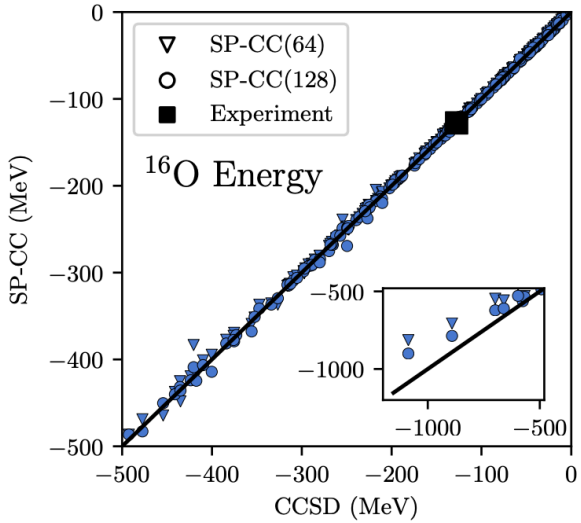


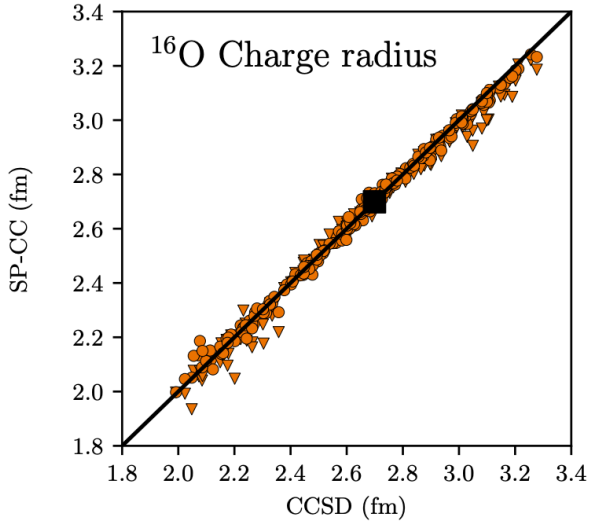
Figure 2. Comparison of different emulators for the ^{4}He ground-state energy using 64 training data points to explore a space where all 16 LECs are varied.

Global Sensitivity Analysis of Bulk Properties of an Atomic Nucleus

Andreas Ekström[1] and Gaute Hagen[2,3]







"With SP-CC(64) this took about 1 hour on a standard laptop, while an equivalent set of exact CCSD computations would require 20 years."

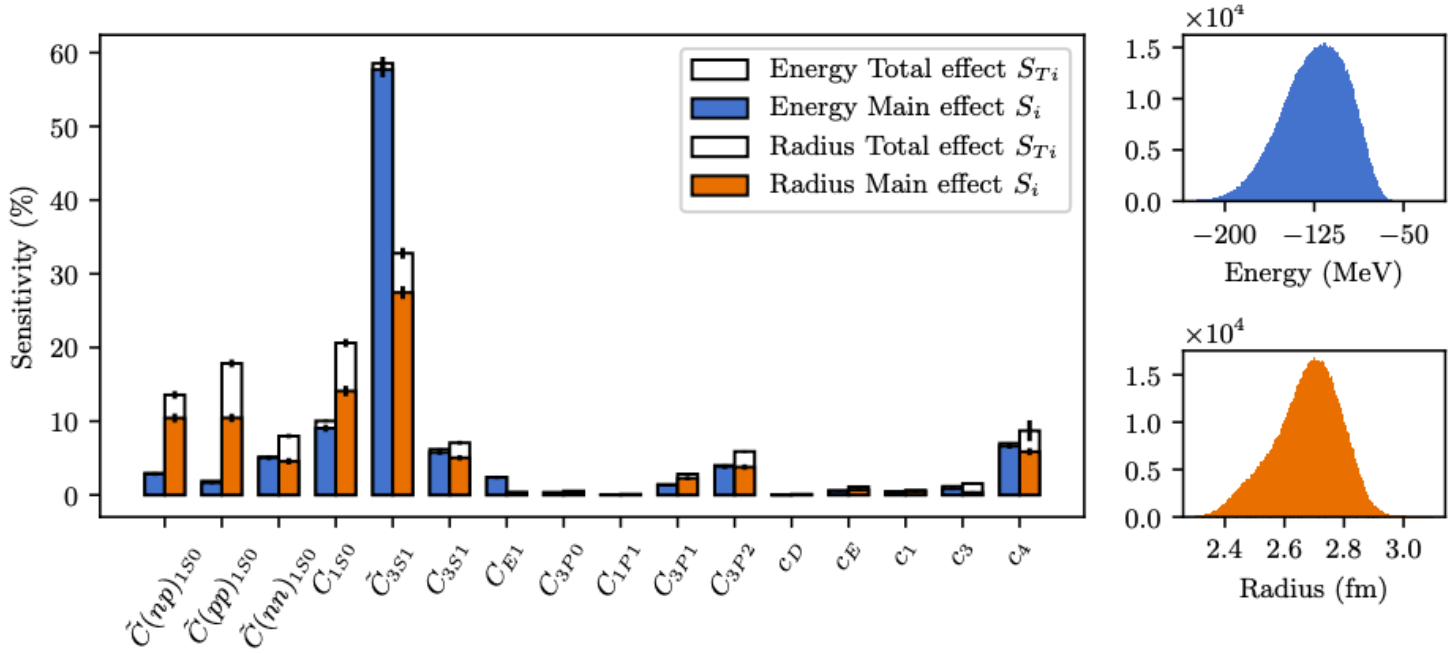


FIG. 3. (Color Online) (Left panel) Main and total effects (in %) for the ground-state energy (left bar) and charge radius (right bar) in ^{16}O, grouped per LEC. The main and total effects were computed from $(16+1)\cdot 2^{16} = 1,114,112$ quasi MC evaluations of the SP-CC(64) Hamiltonian. The vertical lines on each bar indicate bootstrapped 95% confidence intervals. A larger sensitivity value implies that the corresponding LEC is more critical for explaining the variance in the model output. (Right panels) Histograms of the ground-state energy (top) and charge radius (bottom) from which total variances are decomposed.

Summary

Eigenvector continuation is a method that learns eigenvector trajectories by using variational subspace approximation. Eigenvector continuation itself can be regarded as machine learning where the training consists of finding optimized subspace bases. It also can be used with no explicit training as an accurate and fast emulator for applications such as uncertainty quantification and mapping out quantum phase diagrams.