

Antisymmetrization, Eigenvector Continuation, and Parametric Matrix Models

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Antisymmetrization

In the occupation basis, each 0 or 1 represents whether we have a particle occupying that orbital.

$$|f_0 f_1 \cdots f_{n-1}\rangle = (a_0^\dagger)^{f_0} (a_1^\dagger)^{f_1} \cdots (a_{n-1}^\dagger)^{f_{n-1}} |00 \cdots 0\rangle$$

The creation and annihilation operators acting on orbital j needs to hop over

$$\sum_{s=0}^{j-1} f_s$$

fermionic particles. Each hop over a particle gives a minus sign. So then

$$a_j^\dagger |f_0 \cdots f_{j-1} 0 f_{j+1} \cdots f_{n-1}\rangle = (-1)^{\sum_{s=0}^{j-1} f_s} |f_0 \cdots f_{j-1} 1 f_{j+1} \cdots f_{n-1}\rangle$$

$$a_j |f_0 \cdots f_{j-1} 1 f_{j+1} \cdots f_{n-1}\rangle = (-1)^{\sum_{s=0}^{j-1} f_s} |f_0 \cdots f_{j-1} 0 f_{j+1} \cdots f_{n-1}\rangle$$

Tranter et al., Int. J. Quantum Chem. 115, 1431 (2015)

Bravyi, Kitaev, Ann. Phys. 298, 210 (2002)

We define the qubit operators

$$Q_j^+ = {}_j|1\rangle\langle 0|_j = \frac{1}{2}(X_j - iY_j)$$
$$Q_j^- = {}_j|0\rangle\langle 1|_j = \frac{1}{2}(X_j + iY_j)$$

In the occupation basis, the annihilation and creation operators are given by the Jordan-Wigner transformation

$$a_i^\dagger = Q_i^+ \otimes \prod_{j=1}^{i-1} Z_j$$
$$a_i = Q_i^- \otimes \prod_{j=1}^{i-1} Z_j$$

Unfortunately, this can produce long strings of Pauli Z_j operators. So, it is worthwhile to consider transformations of the occupation basis that might yield less computational overhead.

Let us define the following qubit sets:

The update set, $U(i)$. This is the set of qubits other than i that must be flipped when the occupancy f_i changes.

The parity set, $P(i)$. This is the set of qubits whose sum gives the parity p_i , which is defined as

$$p_i = \sum_{j=0}^{i-1} f_j$$

All sums are computed using modulo 2 arithmetic.

The flip set, $F(i)$. This is the set of qubits whose sum, when added to qubit i , equals the occupancy f_i .

The remainder set, $R(i)$. We will work with bases where the flip set is always a subset of the parity set. It is convenient to define the remainder set as the complement of the flip set within the parity set

$$R(i) = P(i) \setminus F(i)$$

For the occupation basis, these qubit sets are

$$U(i) = \emptyset$$

$$P(i) = \{0, 1, \dots, i-1\}$$

$$F(i) = \emptyset$$

$$R(i) = \{0, 1, \dots, i-1\}$$

Let us now consider the case with $n = 2^k$ qubits. The Bravyi-Kitaev basis is defined by the following Bravyi-Kitaev transformation on the occupation basis

$$\beta_n \vec{f}_n = \vec{b}_n$$

For $n = 8$ qubits we have

$$\beta_8 \vec{f}_8 = \vec{b}_8$$

$$\begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 + f_0 \\ f_2 \\ f_3 + f_2 + f_1 + f_0 \\ f_4 \\ f_5 + f_4 \\ f_6 \\ f_7 + f_6 + f_5 + f_4 + f_3 + f_2 + f_1 + f_0 \end{pmatrix}$$

The recursion formula for any $n = 2^k$ qubits is

$$\beta_n = \begin{pmatrix} \beta_{n/2} & 0_{(n/2) \times (n/2)} \\ 0_{(n/2-1) \times (n/2)} & \beta_{n/2} \end{pmatrix} \quad \beta_1 = 1$$

The Bravyi-Kitaev update set for can be generated recursively using

$$U_n(j) = \begin{cases} \{ U_{n/2}(j), (n-1) \}, & \text{for } j < \frac{n}{2}, \\ \{ U_{n/2}(j - \frac{n}{2}) + \frac{n}{2} \}, & \text{for } j \geq \frac{n}{2} \end{cases}$$

$$U_1(0) = \emptyset$$

We are using the shorthand notation

$$\{S + m\} = \{x + m | x \in S\}$$

The Bravyi-Kitaev parity set can be generated recursively as

$$P_n(j) = \begin{cases} \{ P_{n/2}(j) \}, & \text{for } j < \frac{n}{2}, \\ \{ P_{n/2}(j - \frac{n}{2}) + \frac{n}{2}, (\frac{n}{2} - 1) \}, & \text{for } j \geq \frac{n}{2} \end{cases}$$

$$P_1(0) = \emptyset$$

The Bravyi-Kitaev flip set can be generated recursively as

$$F_n(j) = \begin{cases} \{ F_{n/2}(j) \}, & \text{for } j < \frac{n}{2}, \\ \{ F_{n/2}\left(j - \frac{n}{2}\right) + \frac{n}{2} \}, & \text{for } \frac{n}{2} \leq j < (n-1), \\ \{ F_{n/2}\left(j - \frac{n}{2}\right) + \frac{n}{2}, \frac{n}{2} - 1 \}, & \text{for } j = n-1 \end{cases}$$

$$F_1(0) = \emptyset$$

For any $n = 2^k$ and any even j , we observe that

$$F_n(j) = \emptyset$$

The Bravyi-Kitaev remainder set is obtained directly by removing elements of the flip set from the parity set

$$R_n(j) = P_n(j) \setminus F_n(j)$$

We note from the recursion formulas that the number of set elements increases by at most one as we go from $n/2$ to n . This proves that the asymptotic scaling for each set is $O(\log n)$.

The Bravyi-Kitaev creation and annihilation operators take the form

$$a_j^\dagger = \frac{1}{2} \left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} - i X_{U(j)} \otimes Y_j \otimes Z_{\rho(j)} \right)$$

$$a_j = \frac{1}{2} \left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} + i X_{U(j)} \otimes Y_j \otimes Z_{\rho(j)} \right)$$

where

$$\rho(j) = \begin{cases} P(j), & j \text{ even} \\ R(j), & j \text{ odd} \end{cases}$$

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 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 find the desired eigenvector using a variational subspace approximation.

Frame, He, Ipsen, Da. Lee, D.L., Rrapaj, Phys. Rev. Lett. 121, 032501 (2018)

Duguet, Ekström, Furnstahl, König, Lee, Rev. Mod. Phys. 96, 031002 (2024)

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

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

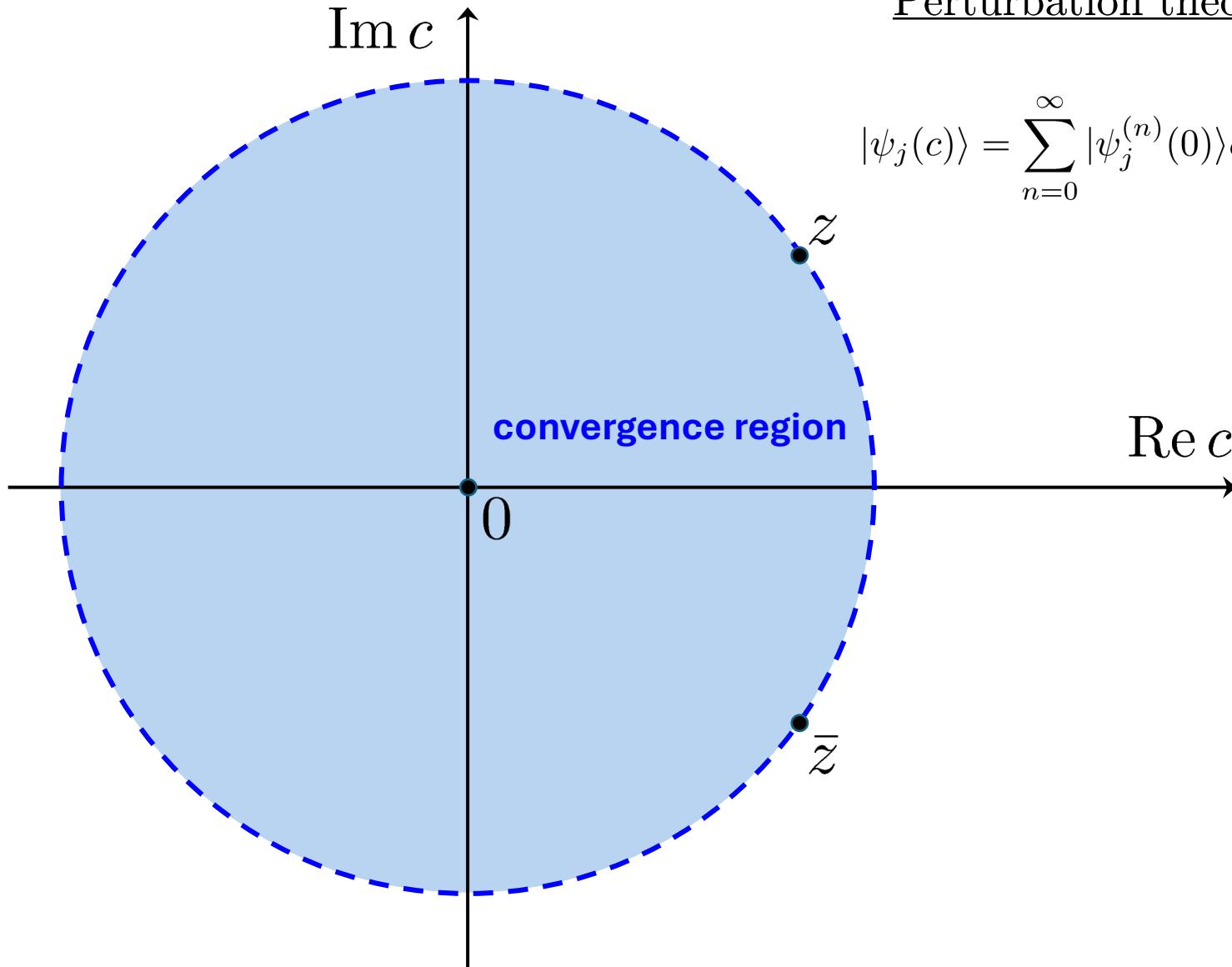
We can perform series expansions around the point $c = 0$.

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

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

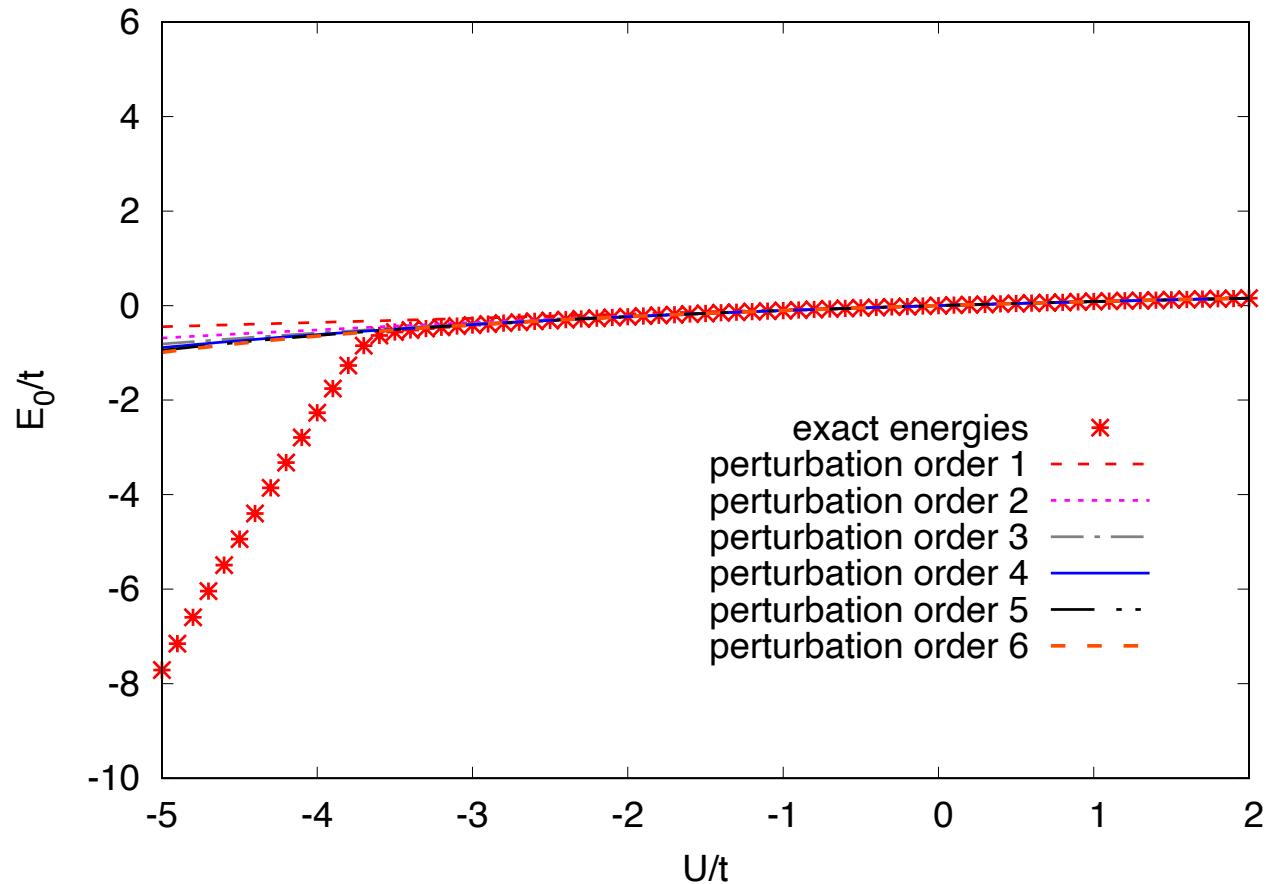
In order to illuminate our discussion with a concrete example, we consider a quantum Hamiltonian known as the Bose-Hubbard model in three dimensions. It describes a system of identical bosons on a three-dimensional cubic lattice.

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

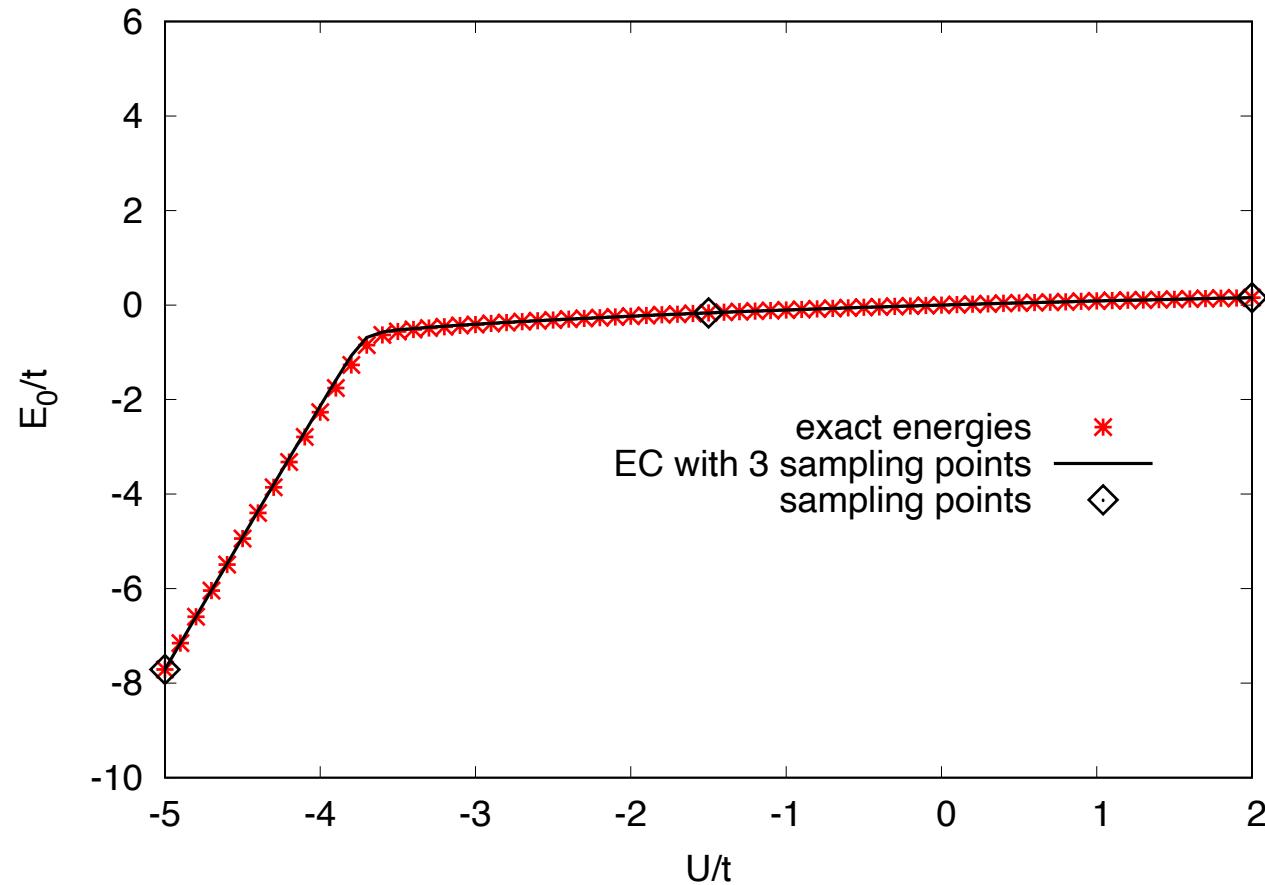
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

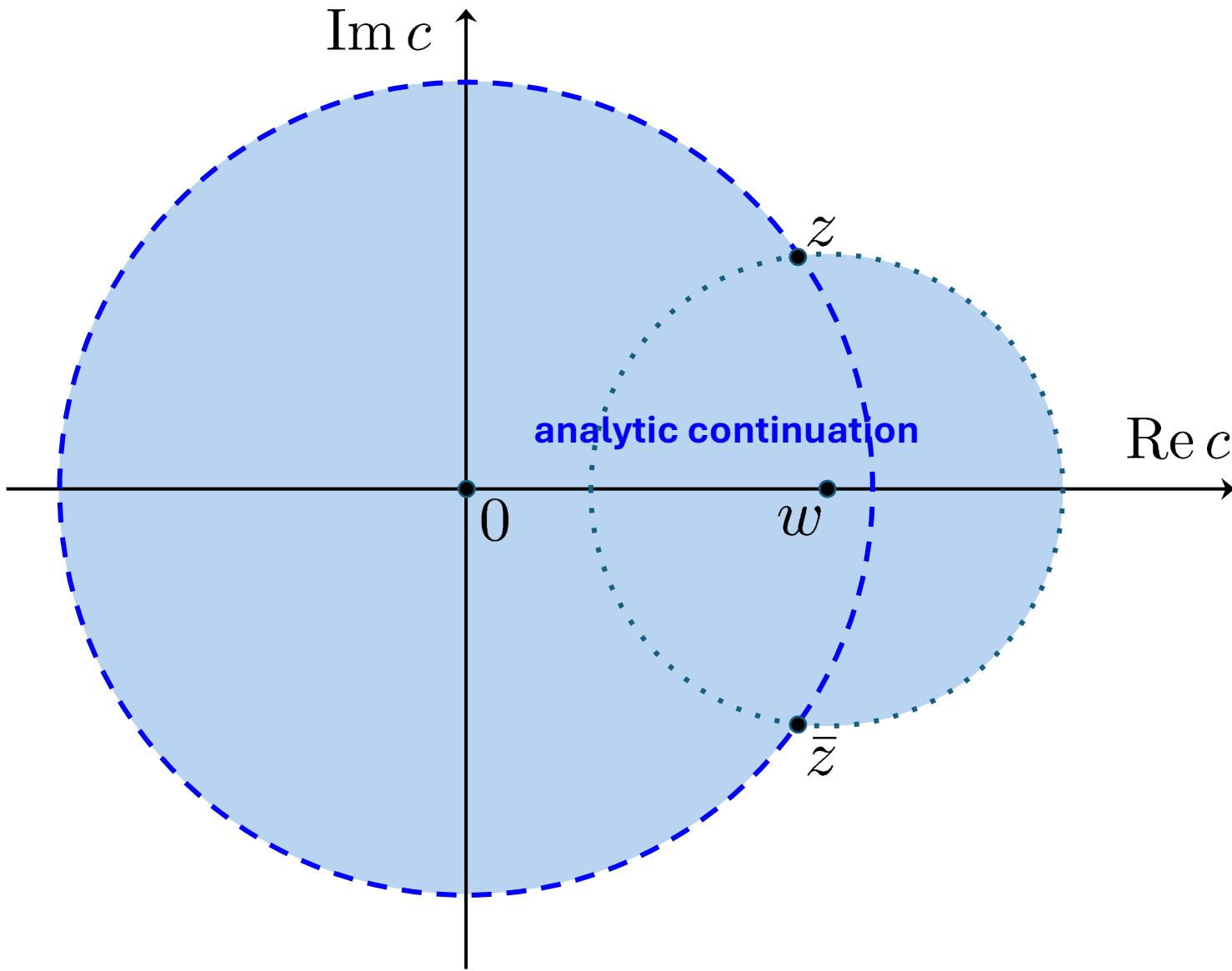
$$\mu = -6t$$

Perturbation theory fails at strong attractive coupling



Restrict the linear space to the span of three vectors





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

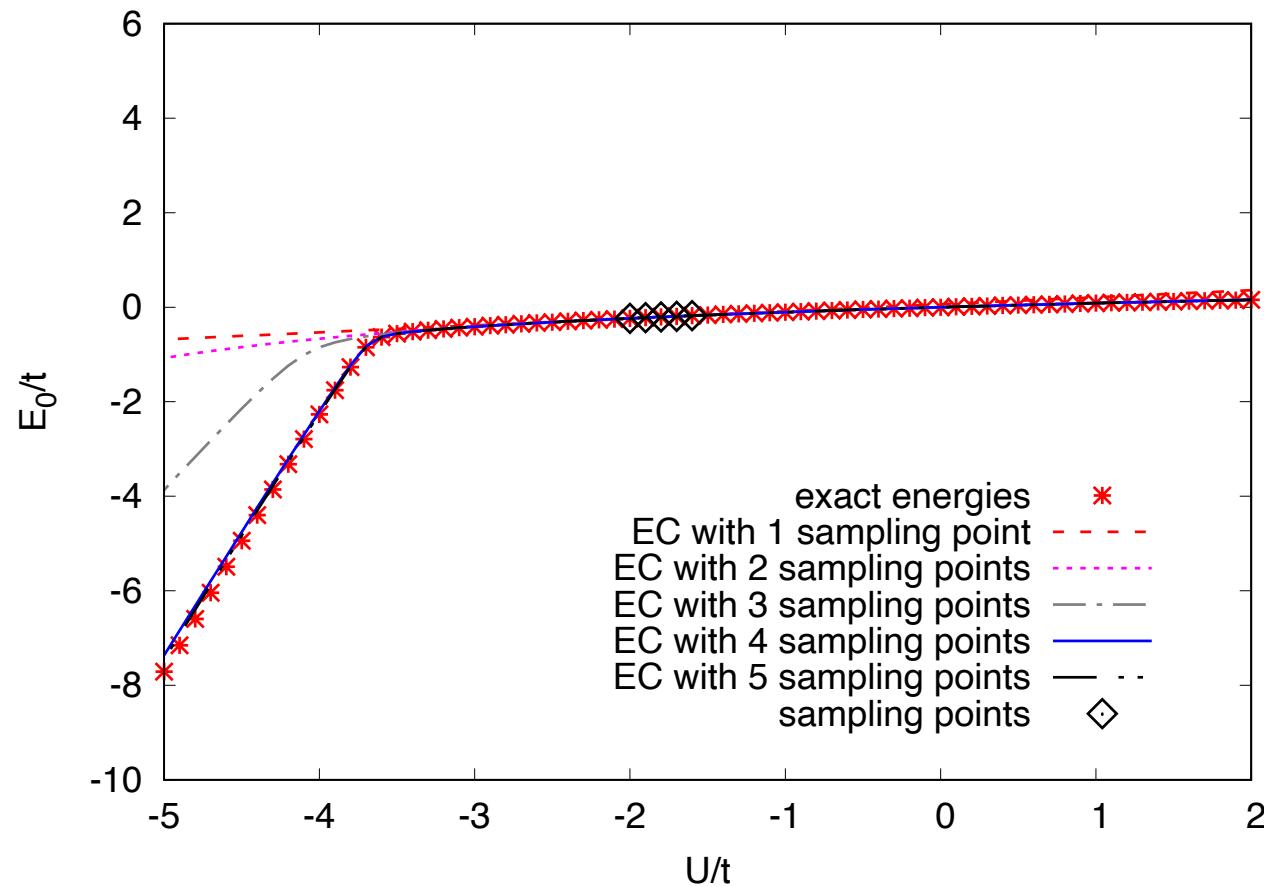
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n / n!$$

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

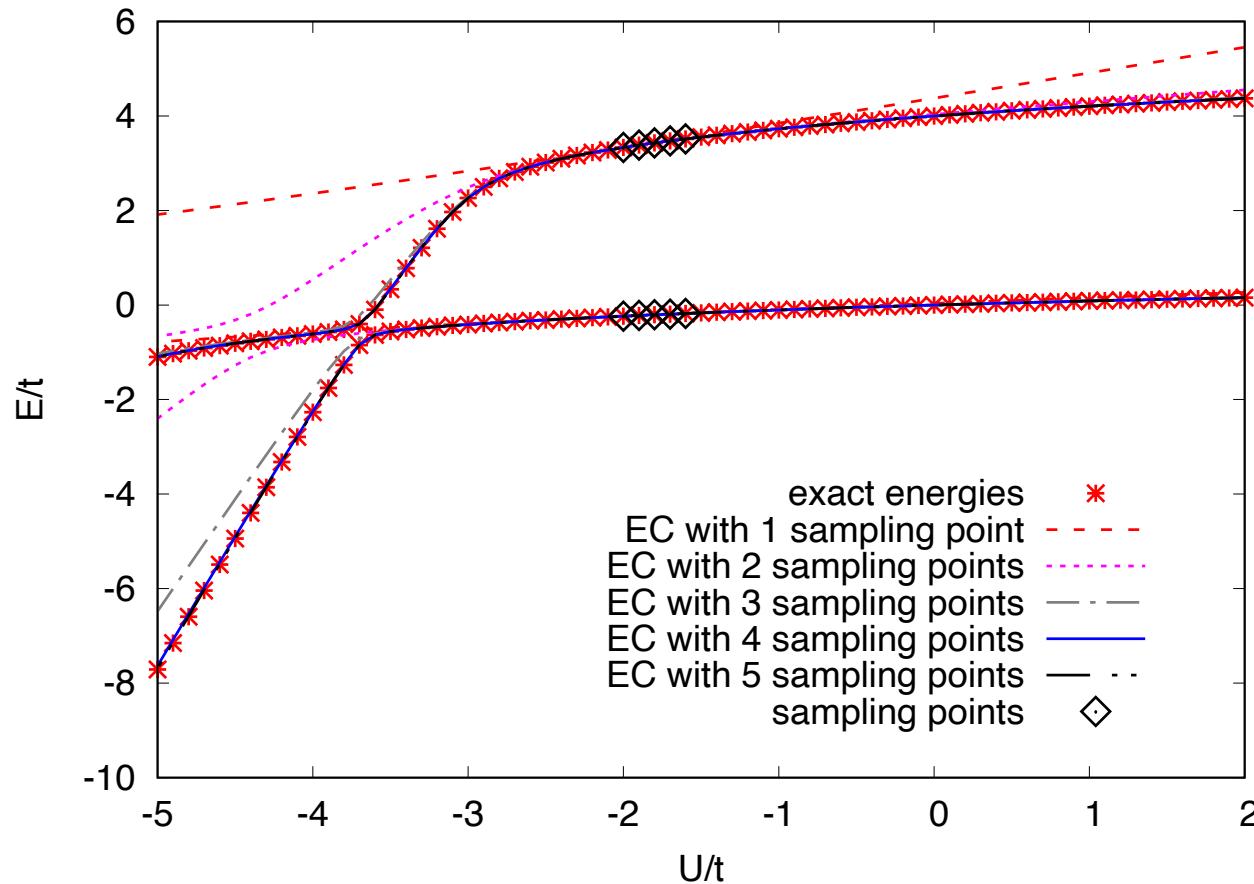
$$|\psi_j(c)\rangle = \lim_{N,M \rightarrow \infty} \sum_{n=0}^N \sum_{m=0}^M |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n / (m! n!)$$

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



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





Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification

S. König ^{a, b, c} , A. Ekström ^d , K. Hebeler ^{a, b} , D. Lee ^e , A. Schwenk ^{a, b, f} 

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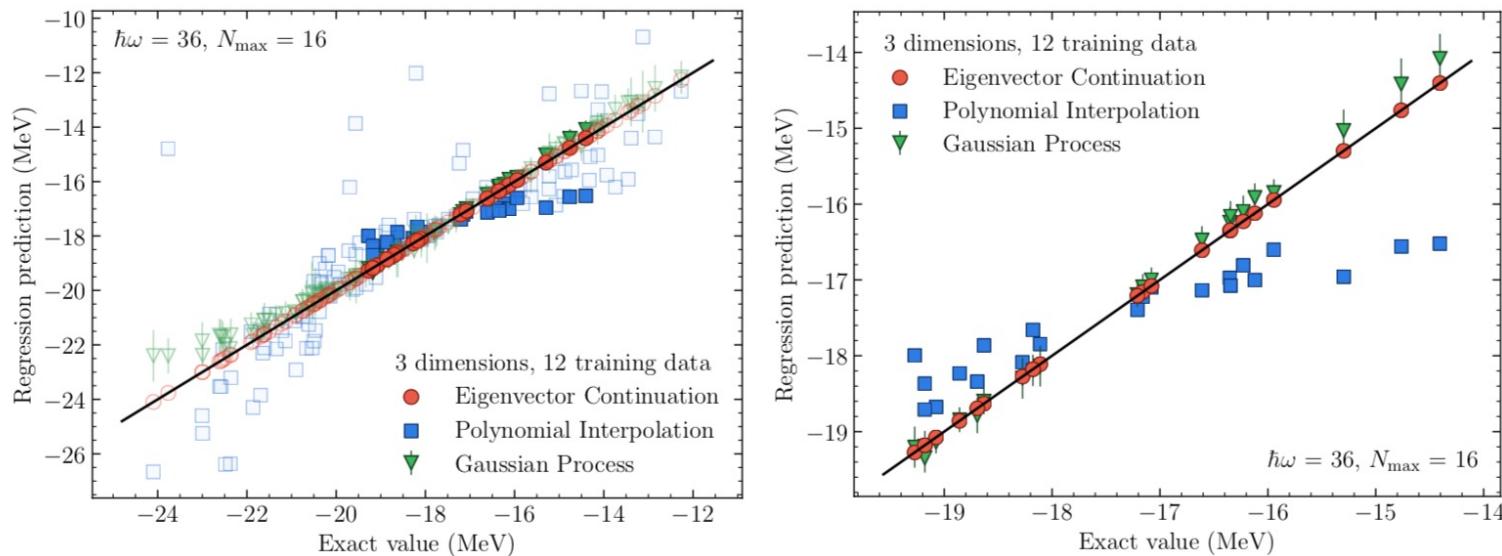


Figure 1. Comparison of different emulators for the ${}^4\text{He}$ ground-state energy using 12 training data points to explore a space where three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols). See main text on how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

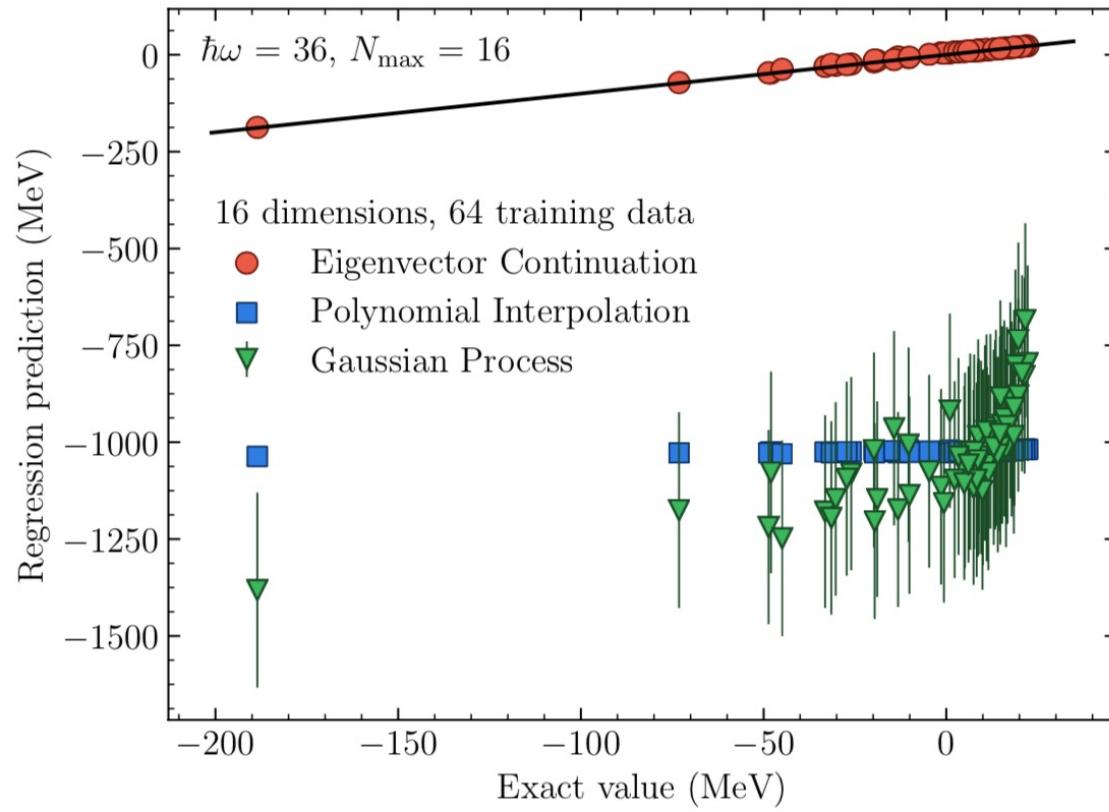
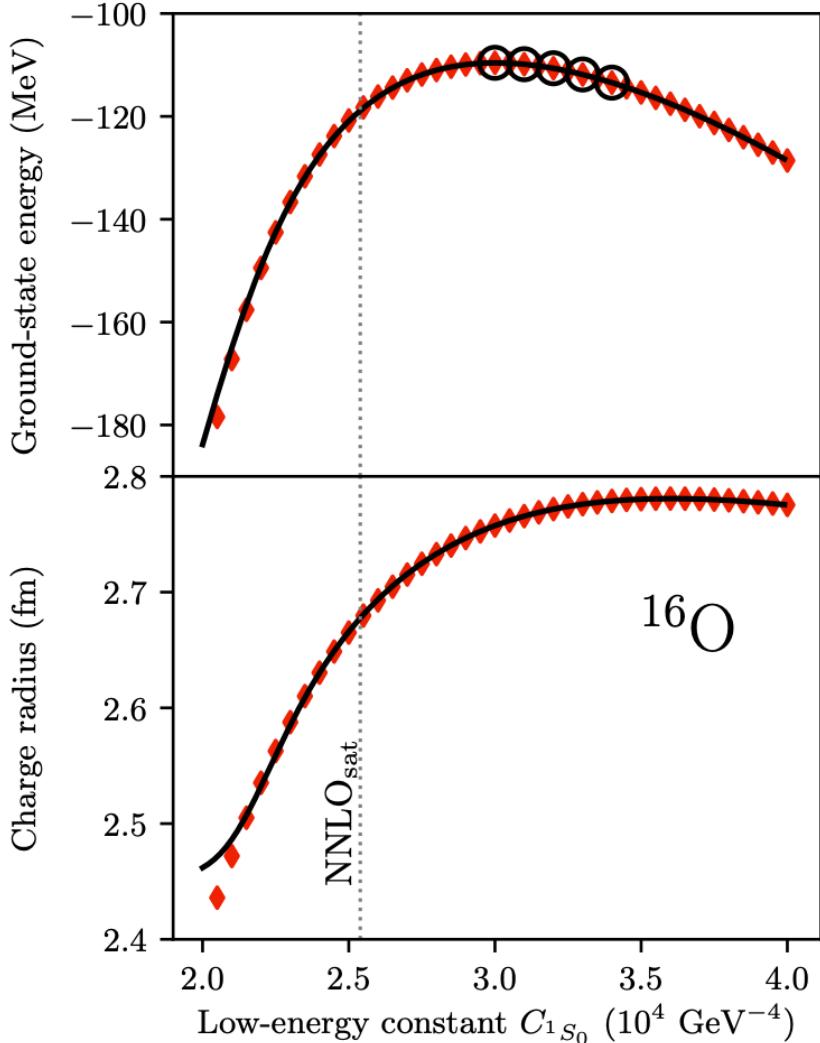


Figure 2. Comparison of different emulators for the ${}^4\text{He}$ ground-state energy using 64 training data points to explore a space where all 16 LECs are varied.

Sub-space projected coupled-cluster

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



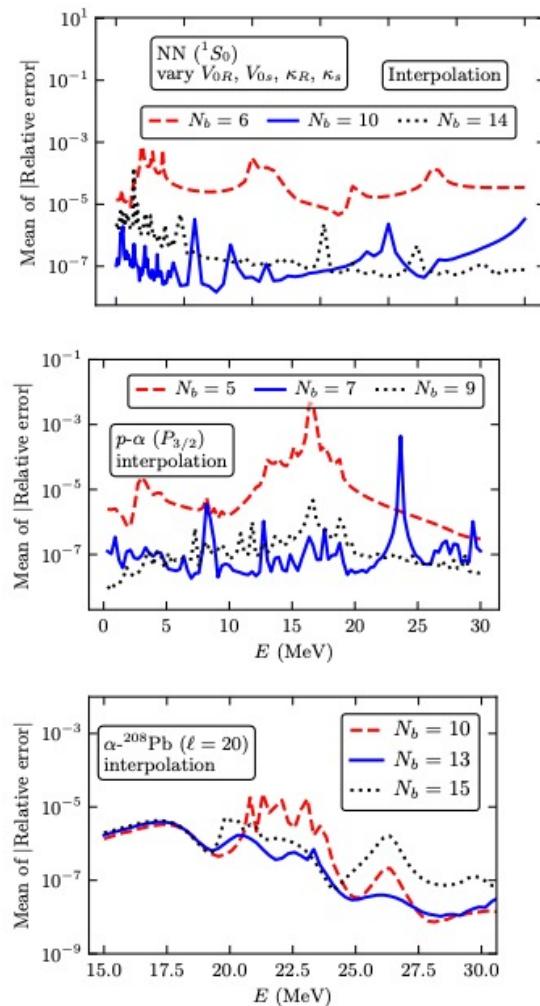
- Generalization of the eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018)]
- Write the Hamiltonian in a linearized form

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

- 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

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

Efficient emulators for scattering using eigenvector continuation



Objectives

- Bayesian inference for parameter estimation requires very many expensive calculations of scattering with different parameter sets.
Solution: model ("emulate") the calculations.
- Extend the eigenvector continuation (EC) approach for efficient emulators to scattering processes and test on model problems.

Impact

- EC emulators successfully tested for model nucleon-nucleon scattering (top figure); charged-particle scattering (middle); complex, non-local optical potentials (bottom). These figures show small mean errors with moderate basis sizes.
- Success of EC enables development of efficient emulators for realistic optical potentials and three-body scattering.

Accomplishments

R.J. Furnstahl et al., Phys. Lett. B **809**, 135719 (2020).

Convergence of Eigenvector Continuation

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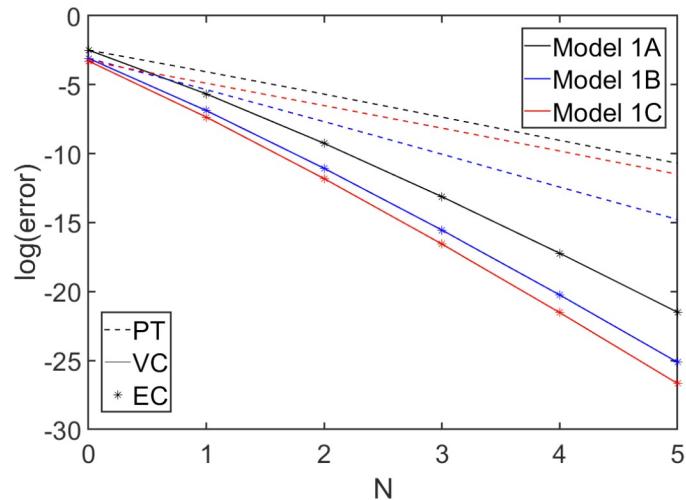
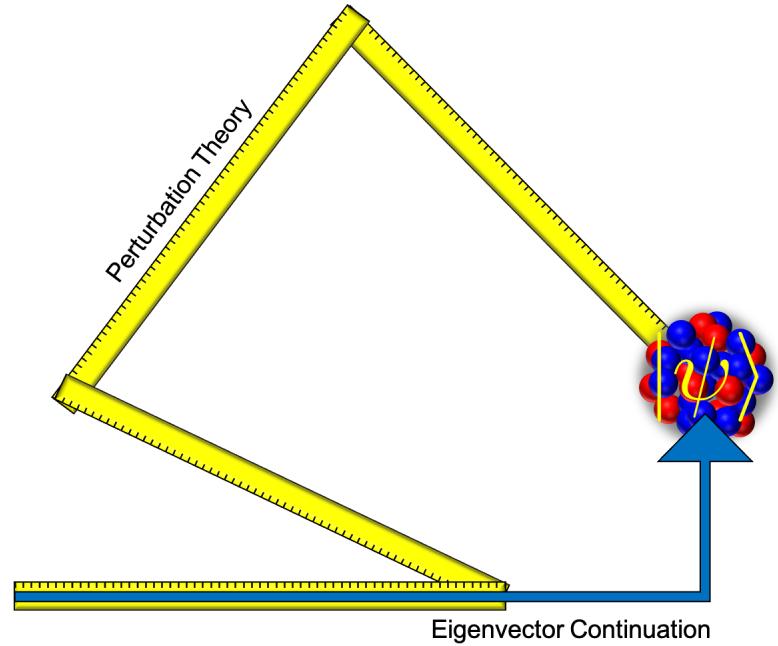


FIG. 1: (Color online) Logarithm of the error versus order N for eigenvector continuation (asterisks), vector continuation (solid lines), and perturbation theory (dashed lines). The three different colors (black, blue and red) correspond with Models 1A, 1B, and 1C respectively.



Quantum eigenvector continuation for chemistry applications

Carlos Mejuto-Zaera^{1,*}  and Alexander F Kemper² 

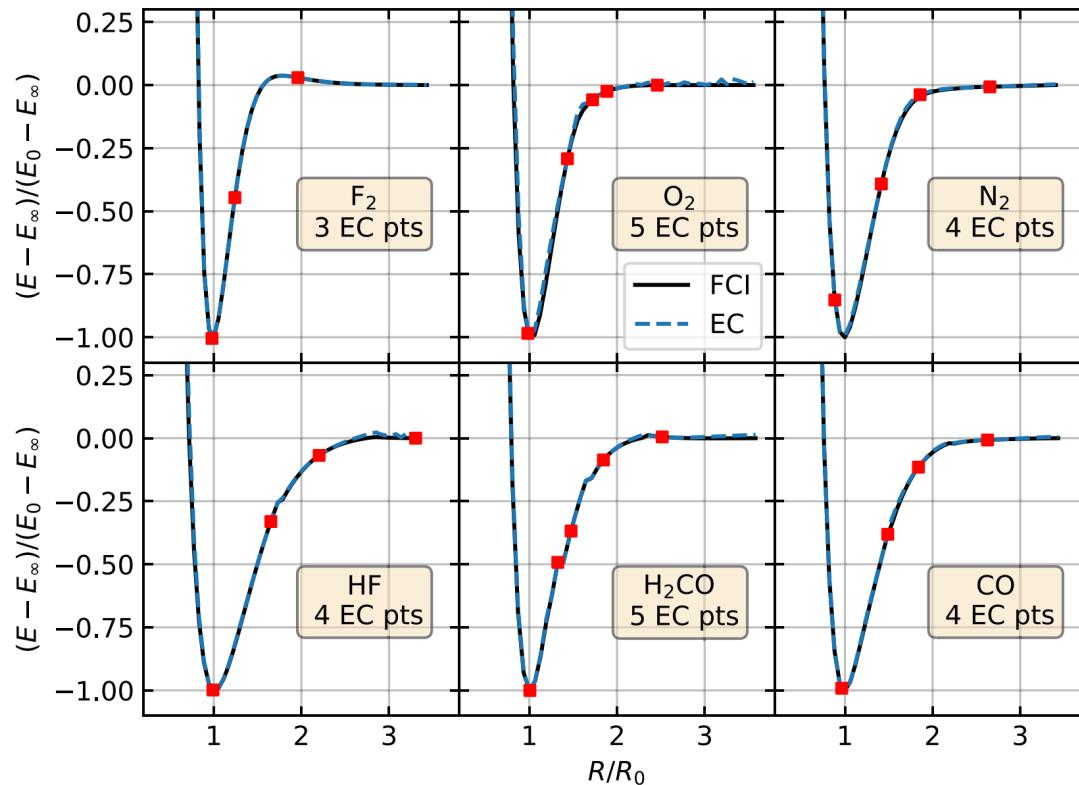


Figure 4. Bond stretching potential energy surfaces (PES) for small molecules, comparing FCI and eigenvector continuation (EC). The x-axis is the bond length rescaled with the equilibrium value for the given molecule, and the y-axis is the ground state energy rescaled by the minimum value and shifted by the large distance asymptotic (i.e. the bond energy). Symmetric bonds are shown in the upper row, while asymmetric bonds are found in the lower row.

Projection-based emulators

Model reduction methods for nuclear emulators

J A Melendez¹ , C Drischler² , R J Furnstahl^{3,1} , A J Garcia¹  and Xilin Zhang² 

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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](https://doi.org/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.

Parametric matrix models

Consider the one-parameter affine problem

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

We now do eigenvector continuation with d 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 d by d .

Note that the eigenvalues will be roots of the characteristic polynomial

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

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

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

Suppose that we don't have access to the training vectors. We can still make a 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 a very simple example of a general technique that we call parametric matrix models (PMM).

Instead trying to directly fit some output functions, we try to learn the set of matrix equations whose solutions produce the output functions. This is similar to how we usually solve physics problems. We start from the equations.

Basic form for parametric matrix models

Input features

$$\{c_1, c_2, \dots, c_{N_c}\}$$

Hermitian or unitary primary matrices that are analytic functions of the input features

$$\{P_1, P_2, \dots, P_{N_P}\}$$

Normalized eigenvectors of primary matrices

$$\{v_1^{(1)}, v_1^{(2)}, \dots, v_2^{(1)}, \dots, v_{N_P}^{(1)}, \dots\}$$

Secondary matrices that are analytic functions of the input features

$$\{S_1, S_2, \dots, S_{N_P}\}$$

Scalar outputs

$$\{v_j^{(i)\dagger} S_k v_{j'}^{(i')}, \dots\}$$

Affine eigenvalue parametric matrix models

Input features

$$\{c_1, c_2, \dots, c_{N_c}\}$$

Only one primary matrix P which is an affine function (degree 1 polynomial) of the input features

$$\{P_1, P_2, \dots, P_{N_P}\} \rightarrow P$$

Only one eigenvector of the primary matrix P

$$\{v_1^{(1)}, v_1^{(2)}, \dots, v_2^{(1)}, \dots, v_{N_P}^{(1)}, \dots\} \rightarrow v^{(i)}$$

Only one secondary matrix S that equals P

$$\{S_1, S_2, \dots, S_{N_P}\} \rightarrow S = P$$

The scalar output is the eigenvalue

$$v^{(i)\dagger} S v^{(i)} = v^{(i)\dagger} P v^{(i)} = \lambda_P^{(i)}$$

Universal approximation theorem

Any continuous function of the input features

$$\{c_1, c_2, \dots, c_{N_c}\}$$

over any compact domain can be uniformly approximated to arbitrary accuracy using an affine eigenvalue PMM.

$$[P]_{i,i'} = a_{i,i',0} + a_{i,i',1}c_1 + a_{i,i',2}c_2 + \dots + a_{i,i',m}c_m$$

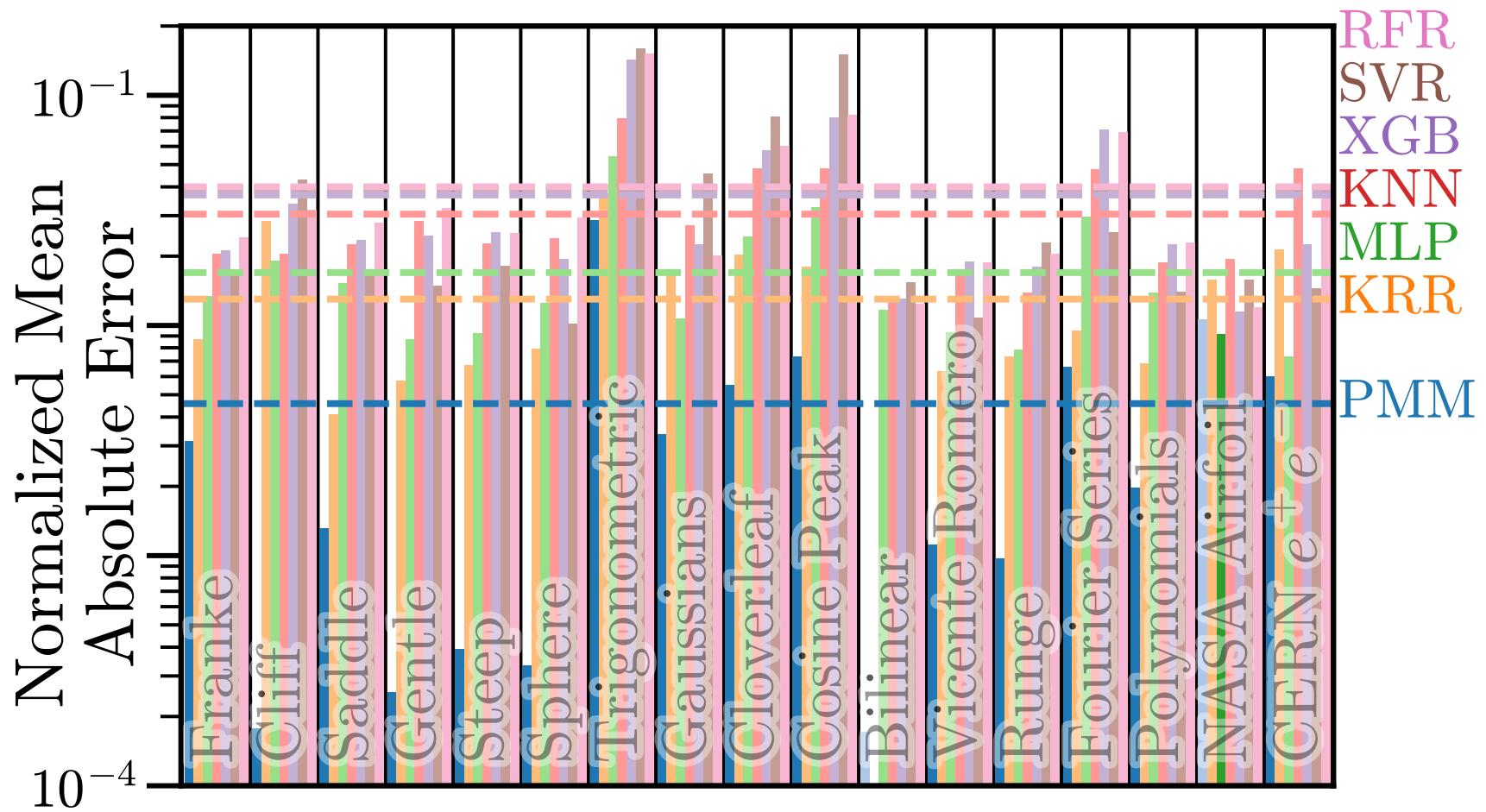
$$\lambda_P^{(i)} \rightarrow f(\{c_1, c_2, \dots, c_{N_c}\})$$

Application to multivariate function interpolation

Name	Equation
Franke ^{†36, 38}	$\frac{3}{4} \exp\left\{-\frac{(9x-2)^2 + (9y-2)^2}{4}\right\} + \frac{3}{4} \exp\left\{-\frac{(9x+1)^2 - 9y+1}{49}\right\} \\ + \frac{1}{2} \exp\left\{-\frac{(9x-7)^2 + (9y-3)^2}{4}\right\} - \frac{1}{5} \exp\left\{-(9x-4)^2 - (9y-7)^2\right\}$
Cliff ^{†38}	$\frac{1}{9} \tanh[9(y-x)] + \frac{1}{9}$
Saddle ^{†38}	$\frac{5/4 + \cos(27y/5)}{6 + 6(3x-1)^2}$
Gentle ^{†38}	$\frac{1}{3} \exp\left\{-\alpha \left[(x-\frac{1}{2})^2 + (y-\frac{1}{2})^2\right]\right\}, \quad \alpha = 81/16$
Steep ^{†38}	$\frac{1}{3} \exp\left\{-\alpha \left[(x-\frac{1}{2})^2 + (y-\frac{1}{2})^2\right]\right\}, \quad \alpha = 81/4$
Sphere ^{†38}	$-\frac{1}{2} + \sqrt{\left(\frac{8}{9}\right)^2 - (x-\frac{1}{2})^2 - (y-\frac{1}{2})^2}$
Trigonometric ^{†38}	$2 \cos(10x) \sin(10y) + \sin(10xy)$
Gaussians ^{†38}	$\exp\left\{-u^2/2\right\} + \frac{3}{4} \exp\left\{-v^2/2\right\} [1 + \exp\left\{-u^2/2\right\}], \quad \begin{cases} u = 5 - 10x \\ v = 5 - 10y \end{cases}$
Cloverleaf ^{†38}	$\left[\left(\frac{20}{3}\right)^3 uv\right]^2 \left[\left(\frac{1}{1+u}\right) \left(\frac{1}{1+v}\right)\right]^5 \left[u - \frac{2}{1+u}\right] \left[v - \frac{2}{1+v}\right], \quad \begin{cases} u = \exp\left\{\frac{10-20x}{3}\right\} \\ v = \exp\left\{\frac{10-20y}{3}\right\} \end{cases}$
Cosine Peak ^{†38}	$\exp\left\{-\frac{2}{5}r\right\} \cos\left(\frac{3}{2}r\right), \quad r = \sqrt{(8x-4)^2 + (9y-\frac{9}{2})^2}$
Bilinear ^{†38}	$xy + x$
Vicente Romero ^{†37, 38}	$\frac{6}{5}r + \frac{21}{40} \sin\left(\frac{12\pi}{5\sqrt{2}}r\right) \sin\left[\frac{13}{10} \text{atan2}(y,x)\right], \quad r = \sqrt{x^2 + y^2}$
Runge ^{†35, 38}	$[(10x-5)^2 + (10y-5)^2 + 1]^{-1}$
Fourier series [‡]	$\sum_{n=1}^N \sum_{m=1}^M \left[a_{nm} \sin\left(\frac{n\pi x}{3}\right) \sin\left(\frac{m\pi y}{3}\right) + b_{nm} \cos\left(\frac{n\pi x}{3}\right) \cos\left(\frac{m\pi y}{3}\right) \right], \quad a_{nm}, b_{nm} \sim \mathcal{N}(0, 1)$
Polynomials [‡]	$\sum_{n=0}^N \sum_{m=0}^M a_{nm} x^n y^m, \quad a_{nm} \sim \mathcal{N}(0, 1)$

† $(x,y) \in [0,1] \times [0,1]$

‡ $(x,y) \in [-1,1] \times [-1,1]$



Parametric Matrix Model (PMM), Kernel Ridge Regression (KRR), Multilayer Perceptron (MLP), k-Nearest Neighbors (KNN), Extreme Gradient Boosting (XGB), Support Vector Regression (SVR), and Random Forest Regression (RFR)

Application to quantum computing

Trotter product formula

$$[H_i, H_j] \neq 0 \quad e^{-iHt} \neq \Pi_k e^{-iH_k t}$$

- Trotter formula

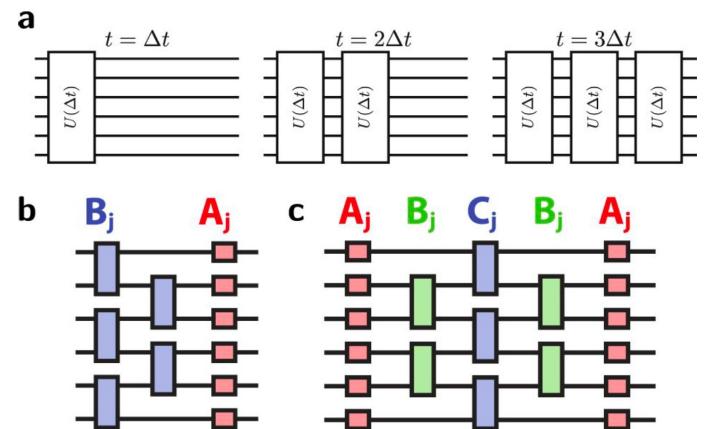
$$\lim_{r \rightarrow \infty} (e^{iAt/r} e^{iBt/r})^r = e^{i(A+B)t}$$

- Lie-Trotter

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} + \mathcal{O}(\Delta t^2)$$

- Suzuki-Trotter

$$e^{i(A+B)\Delta t} = e^{iA\Delta t/2} e^{iB\Delta t} e^{iA\Delta t/2} + \mathcal{O}(\Delta t^3)$$



Smith, A., Kim, M.S., Pollmann, F. et al. Simulating quantum many-body dynamics on a current digital quantum computer. *npj Quantum Inf* 5, 106 (2019). <https://doi.org/10.1038/s41534-019-0217-0>

1D Heisenberg spin chain

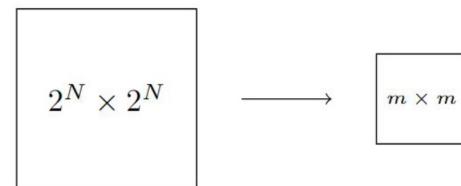
$$H = B \sum_i^N r_i \sigma_i^z + J_1 \sum_i^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) \\ + J_2 \sum_i^N (\sigma_i^x \sigma_{i+2}^x + \sigma_i^y \sigma_{i+2}^y + \sigma_i^z \sigma_{i+2}^z)$$

$$H_B = B \sum_i^N r_i \sigma_i^z$$

$$H_{J_1}^{0|1} = J_1 \sum_{i \text{ even}| \text{ odd}}^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z)$$

$$H_{J_2}^{0|1} = J_2 \sum_{i \text{ even}| \text{ odd}}^N (\sigma_i^x \sigma_{i+2}^x + \sigma_i^y \sigma_{i+2}^y + \sigma_i^z \sigma_{i+2}^z)$$

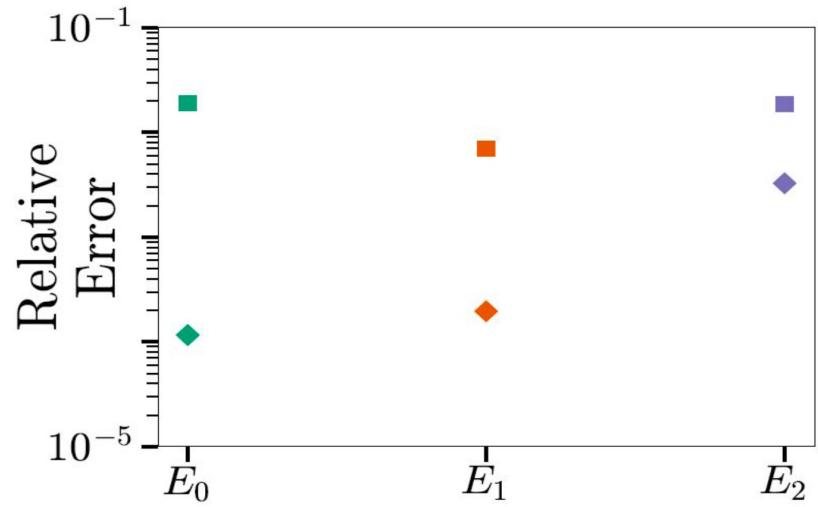
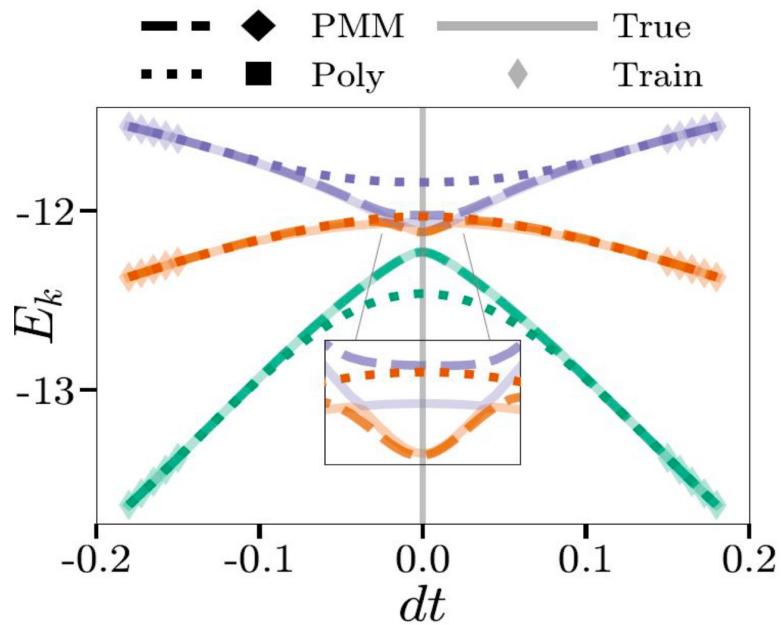
$$U(dt) = \exp \{-iH_B dt\} \exp \{-iH_{J_1}^0 dt\} \\ \times \exp \{-iH_{J_1}^1 dt\} \exp \{-iH_{J_2}^0 dt\} \\ \times \exp \{-iH_{J_2}^1 dt\}.$$



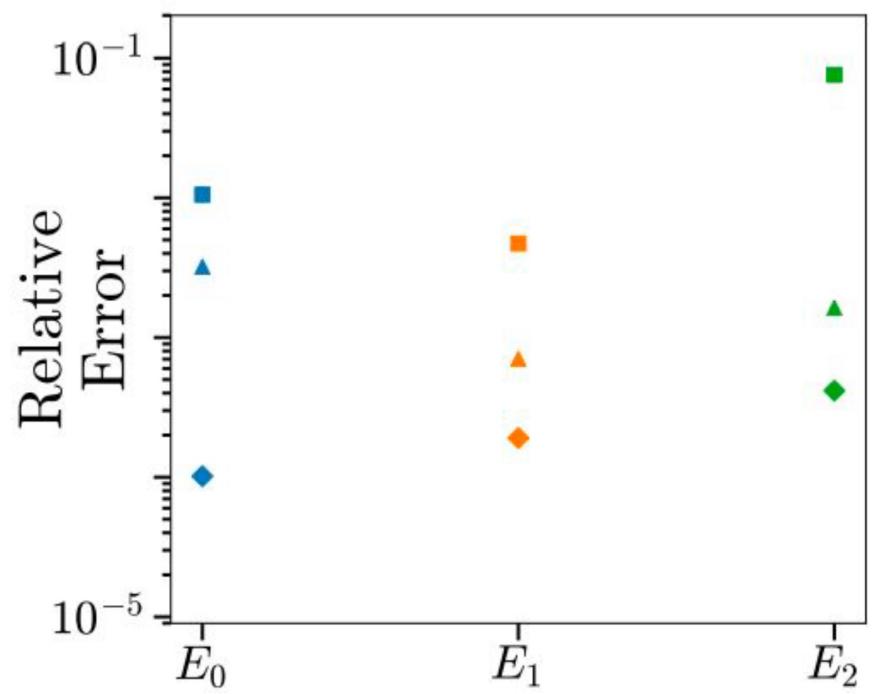
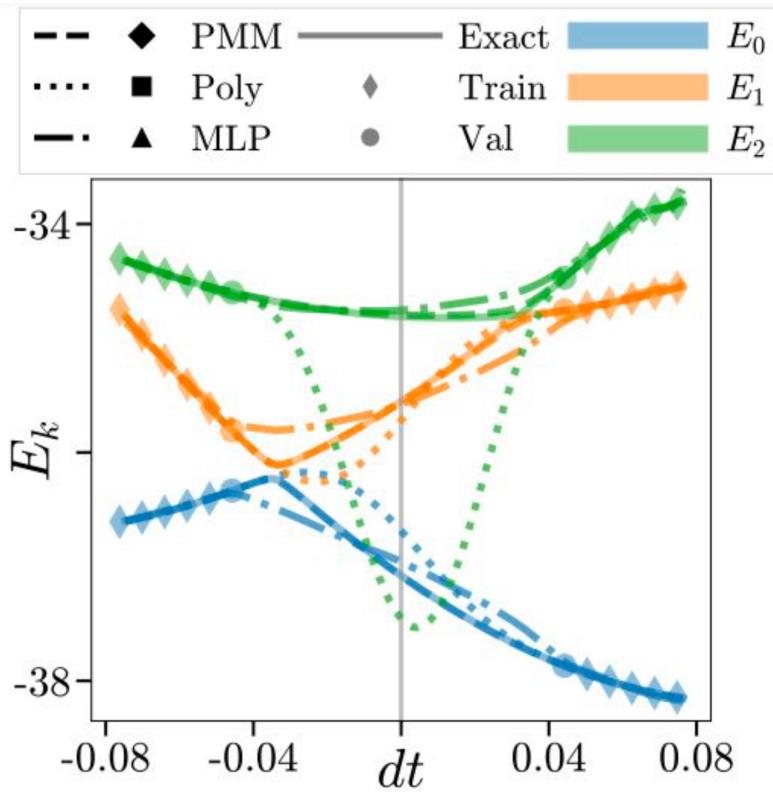
$$M = M_1 + M_2 + M_3 + M_4 + M_5$$

$$U_M(dt) = \exp \{-iM_1 dt\} \exp \{-iM_2 dt\} \\ \times \exp \{-iM_3 dt\} \exp \{-iM_4 dt\} \\ \times \exp \{-iM_5 dt\}$$

1D Heisenberg spin chain



Dzyaloshinskii-Moriya (DM) interaction

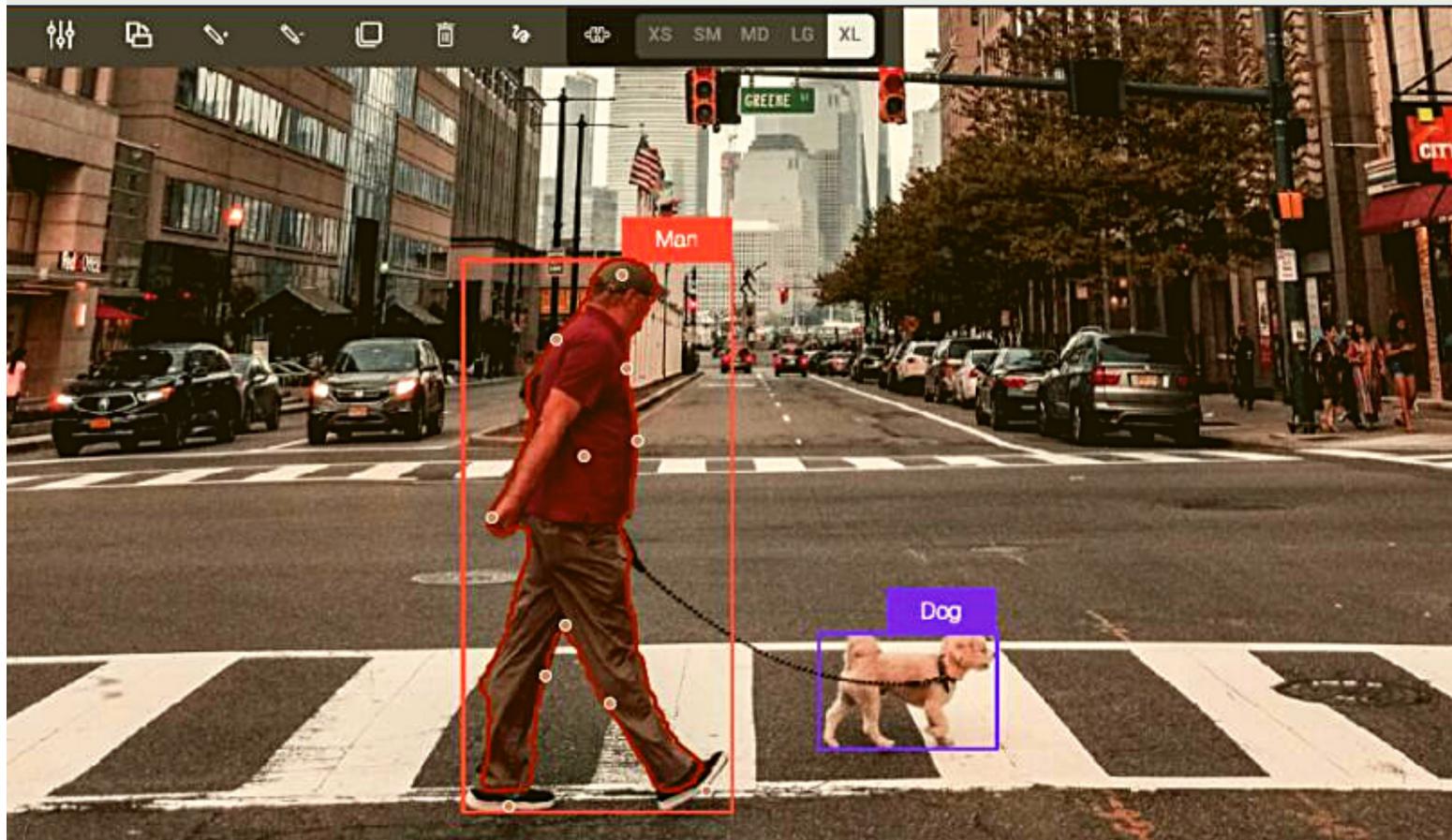


$$H_B = B \sum_i r_i \sigma_i^z,$$

$$H_J^{0|1} = J \sum_{i \text{ even}| \text{ odd}} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z),$$

$$H_D^{0|1} = D \sum_{i \text{ even}| \text{ odd}} (\sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x),$$

Applications to image recognition



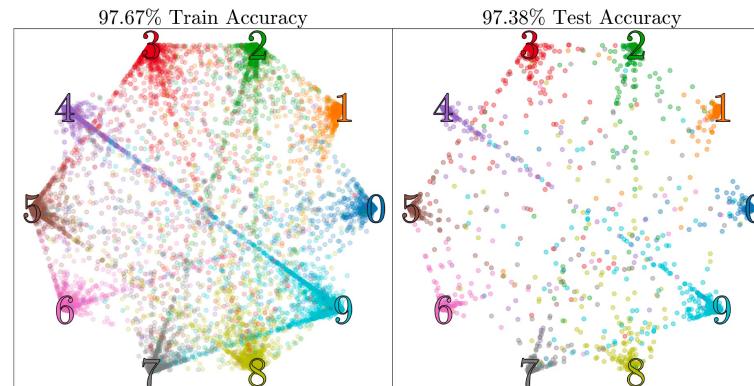
Kili Technology

MNIST Digits

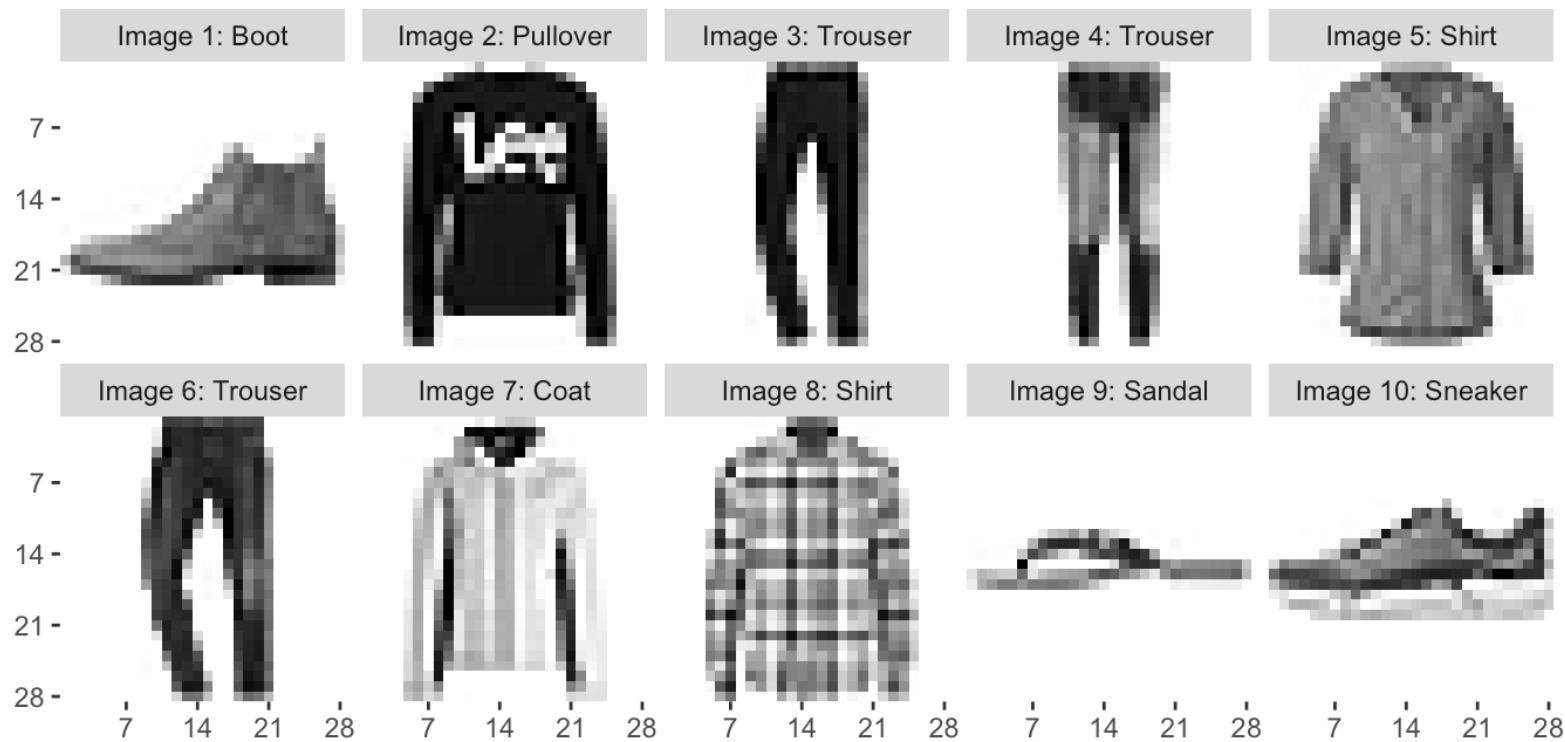


DNN-2 96.4% with 5500 parameters

PMM 97.4% with 4990 parameters



Fashion MNIST



Extended MNIST



Dataset	Model	Accuracy	Trainable float
MNIST Digits ⁵³	PMM [†]	97.38	4990
	DNN-2 ⁵⁴	96.5	5500
	DNN-3 ⁵⁴	97.0	80 598
	DNN-5 ⁵⁴	97.2	175 180
	GECCO ⁵⁵	98.04	19 000
	CTM-250 ⁵⁶	98.82	31 750
	CTM-8000 ⁵⁶	99.33	527 250
Fashion MNIST ⁵⁸	Efficient-CapsNet ⁵⁷	99.84	161 824
	PMM [†]	88.58	16 744
	GECCO ⁵⁵	88.09	19 000
	CTM-250 ⁵⁶	88.25	31 750
	CTM-8000 ⁵⁶	91.18	527 250
	MLP [†] ⁵⁹	91.63	2.9×10^6
	VGG8B(2x) ⁵⁹	95.45	28×10^6
EMNIST Balanced ⁶¹	Fine-Tuning DARTS ⁶⁰	96.91	3.2×10^6
	PMM [†]	81.57	13 792
	OPIUM [†] ⁶¹	78.02	8.32×10^6
	HM2-BP ⁶²	85.57	6.7×10^5
	CNN ⁶³	79.61	21 840
	CNN (Spinal FC) ⁶³	82.77	13 820
	CNN (Spinal FC) ⁶³	83.21	16 050

All-order summation of perturbation theory

$$\boxed{} = M_{\text{LO}} =: e^{-H_{\text{LO}} d\tau} : \quad \boxed{} = O$$

$$Z_{n_t,i,j} = \langle \psi_{\text{init},i} | \boxed{} | \psi_{\text{init},j} \rangle$$

$$Z_{n_t,i,j}^O = \langle \psi_{\text{init},i} | \boxed{} | \boxed{} | \psi_{\text{init},j} \rangle$$

$$O = H_{\text{NLO}}, H_{\text{N}^2\text{LO}}, H_{\text{N}^3\text{LO}}, \dots, F[\rho(\vec{r})], \dots$$

Make a low-dimensional parametric matrix model to represent vectors and matrices in the subspace of low-energy states of H_{LO} . Then diagonalize to get nonperturbative eigenvectors. Extrapolate in the dimensions of the parametric model to eliminate systematic errors.

