Uses of eigenvector continuation in nuclear structure and reaction theory

Sebastian König
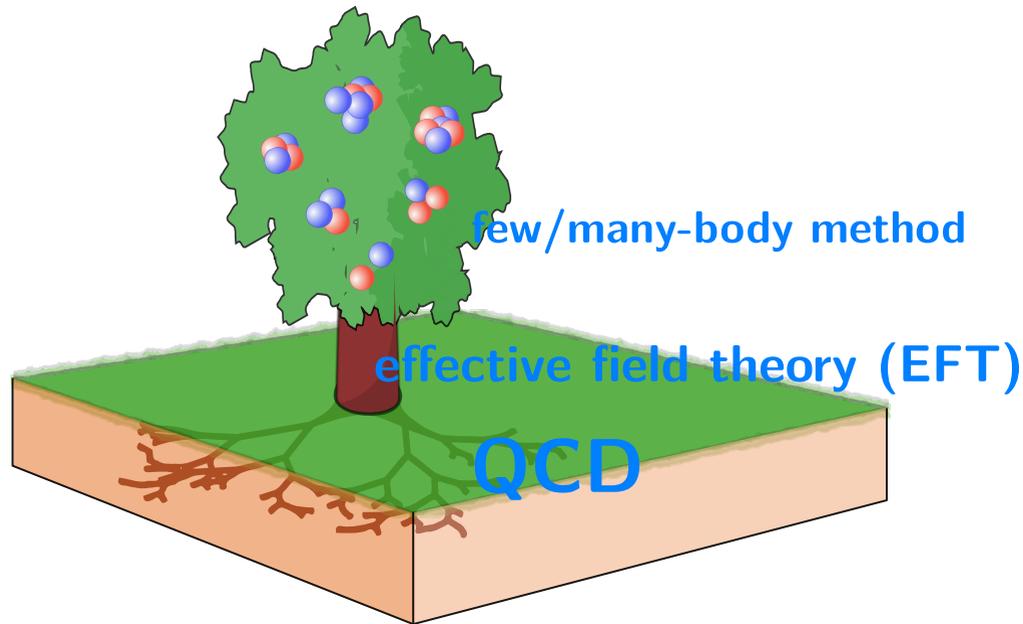
ESNT Workshop: Eigenvector continuation and related techniques in nuclear structure and reaction theory

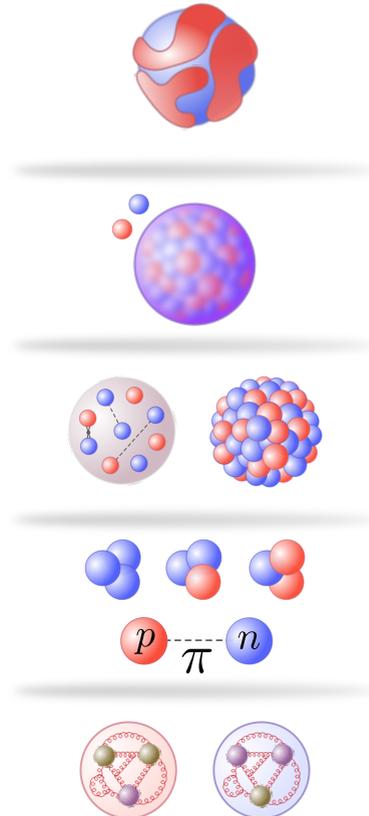**CEA Saclay, France, May 30, 2023**

Nuclear theory tower


few/many-body method

effective field theory (EFT)

QCD

- **QCD** = underlying theory of strong interaction
- **EFT** = effective description in terms of hadrons
- **degrees of freedom depend on resolution scale**

Nuclear effective field theories

- choose **degrees of freedom** approriate to energy scale
- only restricted by **symmetry**, ordered by **power counting**

- $\rightsquigarrow$ **ab initio predictions with fully quantified uncertainties**
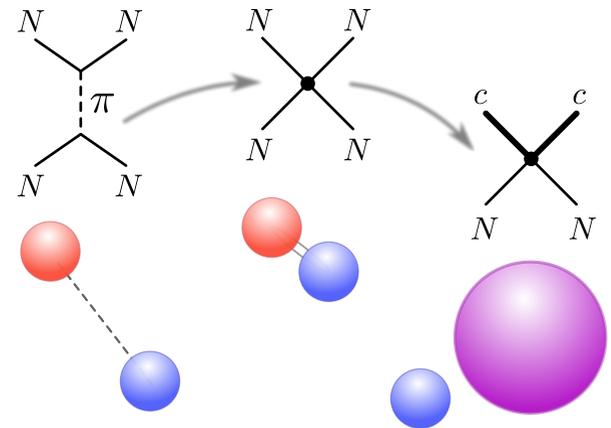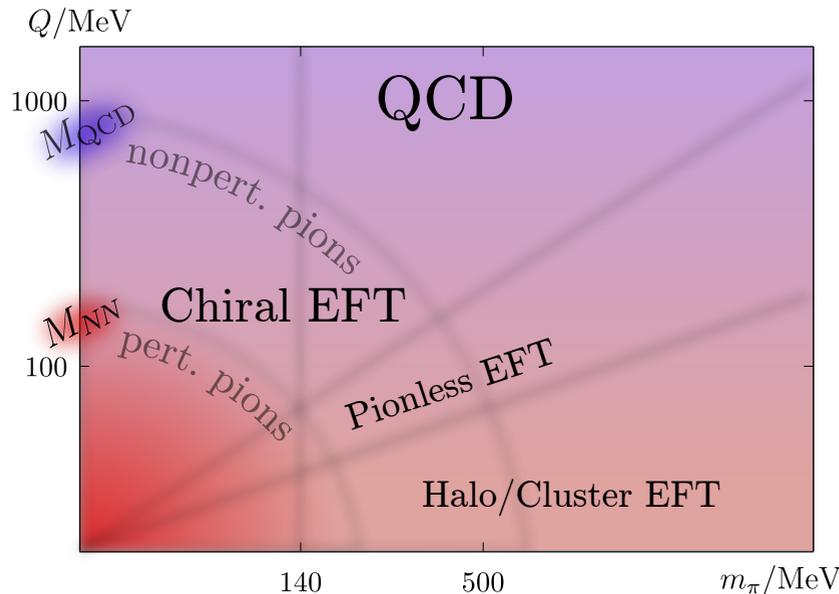
- degrees of freedom here: nucleons (and clusters thereof)
- even more effective d.o.f.: rotations, vibrations

Outline

Introduction ✔
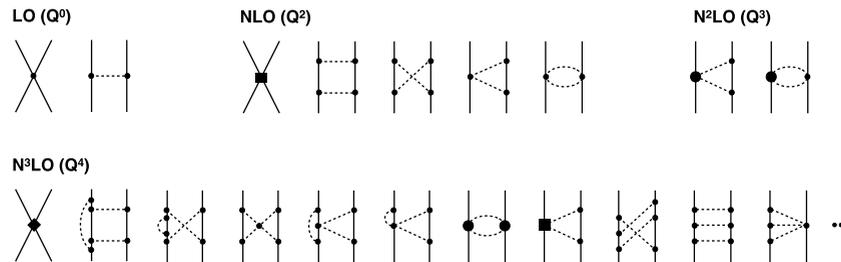
Emulators

Resummation

Outlook

Part I

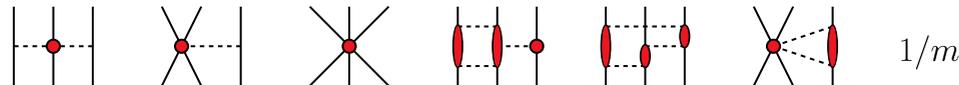**Efficient Emulators via Eigenvector Continuation**

Chiral interactions

Many remarkable results based on chiral potentials

- Chiral EFT: expand in $(Q \sim M_\pi)/M_{\mathrm{QCD}}$, derive potential (2N, 3N, ...)

  Weinberg (90); Rho (91); Ordoñez + van Kolck (92); van Kolck (93); Epelbaum et al. (98); Entem + Machleidt (03); ...

LO (Q^0) NLO (Q^2) N²LO (Q^3)

N³LO (Q^4)

Epelbaum et al., EPJA **51** 53 (2015)

$1/m$

Hebeler et al., PRC **91** 044001 (2015)

However...

- potential expansion not necessarily consistent with EFT paradigm
- **typically needs high orders $\rightsquigarrow$ rather large number of parameters**
  - ‣ e.g. 14 (two-body) + 2 (three-body) at third order

Recap

Recall the general EC idea as presented earlier today... talk by Dean

Scenario Frame et al., PRL **121** 032501 (2018)

- consider physical state (eigenvector) in a large space
- **parametric dependence of Hamiltonian $H(c)$ traces only small subspace**

Prerequisite
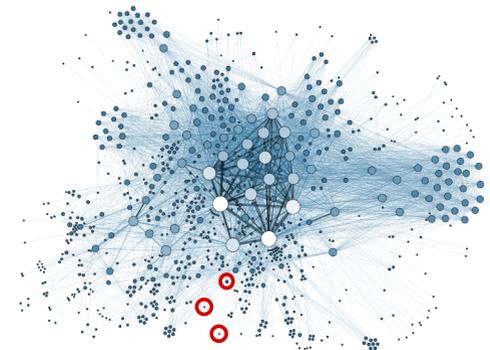
- smooth dependence of $H(c)$ on c
- enables analytic continuation of $|\psi(c)\rangle$ from c_{easy} to c_{target}

Procedure

- calculate $|\psi(c_i)\rangle$, $i = 1, \ldots N_{\text{EC}}$ in "easy" regime
- solve generalized eigenvalue problem $H|\psi\rangle = \lambda N|\psi\rangle$
  - $H_{ij} = \langle \psi_i | H(c_{\text{target}}) | \psi_j \rangle$
  - $N_{ij} = \langle \psi_i | \psi_j \rangle$
- particular case of a **reduced basis method**

Bonilla et al., PRC **106** 054322; Melendez et al., JPG **49** 102001
talk by Pablo on Thursday, talk by Kyle on Friday

Martin Grandjean, via Wikimedia Commons (CC-AS 3.0)

Need for emulators

1. Fitting of LECs to few- and many-body observables

- common practice now to use $A > 3$ to constrain nuclear forces, e.g.:
  - ‣ JISP16, NNLO$_{\text{sat}}$, α-α scattering
    Shirokov et al., PLB **644** 33 (2007); Ekström et al., PRC **91** 051301 (2015); Elhatisari et al., PRL **117** 132501 (2016)

- **fitting needs many calculations with different parameters**

2. Propagation of uncertainties

- statistical fitting gives posteriors for LECs
- LEC posteriors propagate to observables
  - ‣ typically achieved via Bayesian statistics
    Wesolowski et al., JPG **46** 045102 (2019)

- **need to sample a large number of calculations**
  - ‣ expensive already in few-body sector
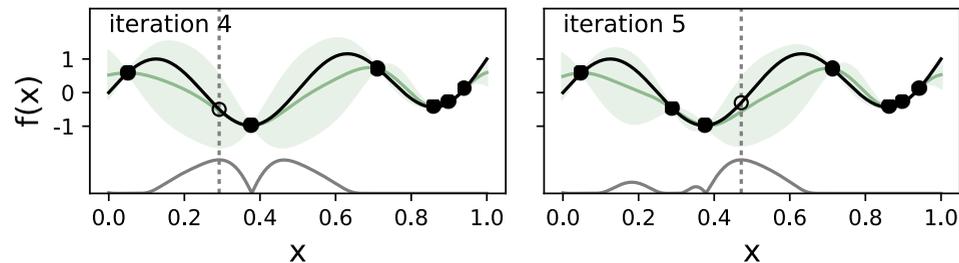 - ‣ typically not doable for many-body problems!
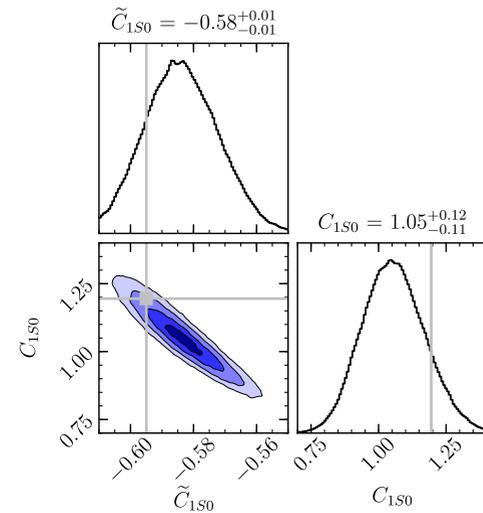
Exact calculations can be prohibitively expensive!

Emulators

- an **emulator** (also called **surrogate model**) can help overcome this problem!

Options for emulator construction

- **Multi-dimensional Polynomial Interpolation**
  - ‣ simplest possible choice
  - ‣ generally **too** simple, no way to assess uncertainty
- **Gaussian Process (GP)**

Ekström et al., JPG **46** 095101 (2019)

  - ‣ statistical modeling, iteratively improvable
  - ‣ interpolation with inherent uncertainty estimate
- **Eigenvector Continuation**
  - ‣ typically fast, efficient, and accurate!

Hamiltonian parameter spaces

- original EC: single parameter, $H = H(c)$
- **consider a Hamiltonian depending on several parameters:**

$$H = H_0 + V = H_0 + \sum_{k=1}^{d} c_k V_k \tag{1}$$
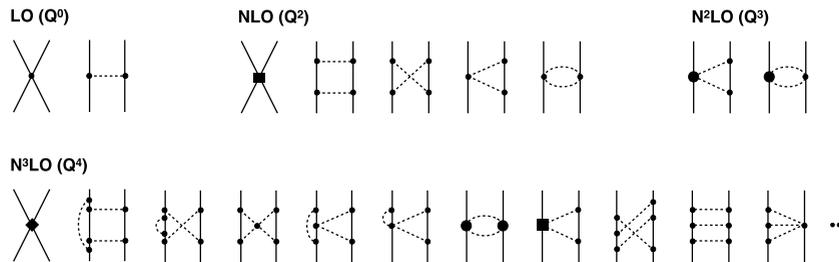
  ‣ in particular, V can be a chiral potential with LECs c_k
  ‣ Hamiltonian is element of d-dimensional parameter space
  ‣ convenient notation: $\vec{c} = \{c_k\}_{k=1}^{d}$
  ‣ typical for $\mathcal{O}(Q^3)$ calculation: 14 two-body LECs + 2 three-body LECs
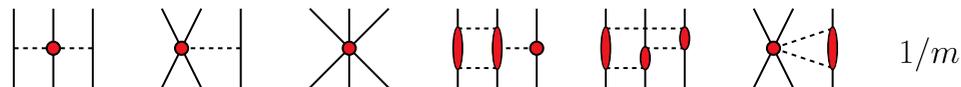
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Generalized EC

- **EC construction is straightforward to generalize to this case:**
- simply replace $c_i \to \vec{c}_i$ in construction
  ‣ $|\psi_i\rangle = |\psi(\vec{c}_i)\rangle$ for $i = 1, \cdots N_{\mathrm{EC}}$
  ‣ $H_{ij} = \langle \psi_i | H(\vec{c}_{\mathrm{target}}) | \psi_j \rangle$, $N_{ij} = \langle \psi_i | \psi_j \rangle$
- the sum in Eq. (1) can be carried out in small (dimension $= N_{\mathrm{EC}}$) space!
  ‣ this permits an **offline/online decomposition** of the problem

Interpolation and extrapolation

Hypercubic sampling

- **want to cover parameter space efficiently with training set $S = \{\vec{c}_i\}$**
- Latin Hypercube Sampling can generate near random sample
- for examples that follow:
  - ▸ sample each component $c_k \in [-2, 2]$
  - ▸ vary d LECs, fix the rest at NNLO$_{\text{sat}}$ point   Ekström et al., PRC **91** 051301 (2015)

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Convex combinations

- **distinguish interpolation and extrapolation target points**
- interpolation region is convex hull of the $\{\vec{c}_i\}$
  - ‣ $\mathrm{conv}(S) = \sum_i \alpha_i \vec{c}_i$ with $\alpha_i \geq 0$ and $\sum_i \alpha_i = 1$
- extrapolation for $\vec{c}_{\mathrm{target}} \notin \mathrm{conv}(S)$
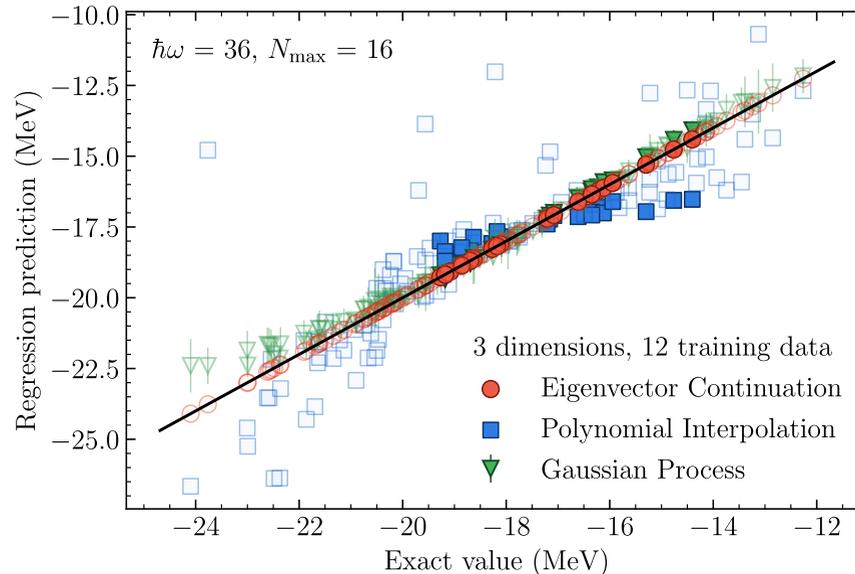- **EC emulators can handle both!**
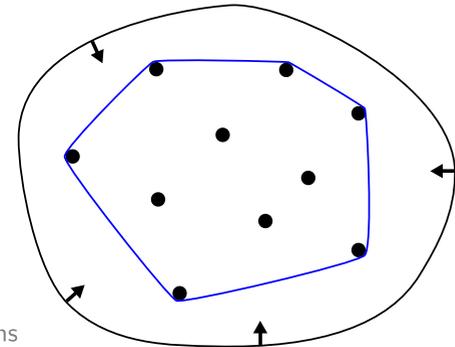
Pbroks13, Wikimedia Commons

Performance comparison: energy

Cross validation

- **compare emulation prediction agains exact result for set $\{\vec{c}_{\text{target},j}\}_{j=1}^{N}$**
- underlying calculation: Jacobi NCSM
- observable: ^{4}He ground-state energy
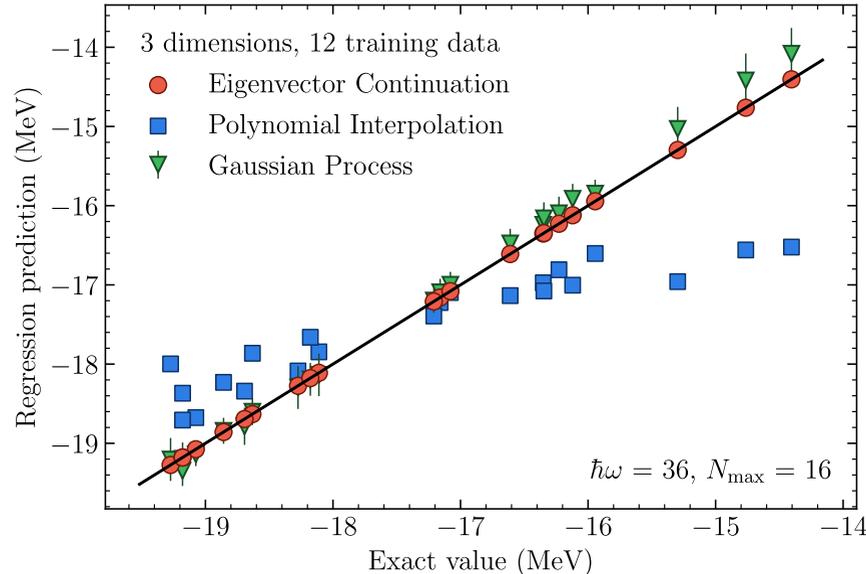- transparent symbols indicate extrapolation targets

Performance comparison: energy

Cross validation SK, A. Ekström, K. Hebeler, D. Lee, A. Schwenk, PLB **810** 135814 (2020)

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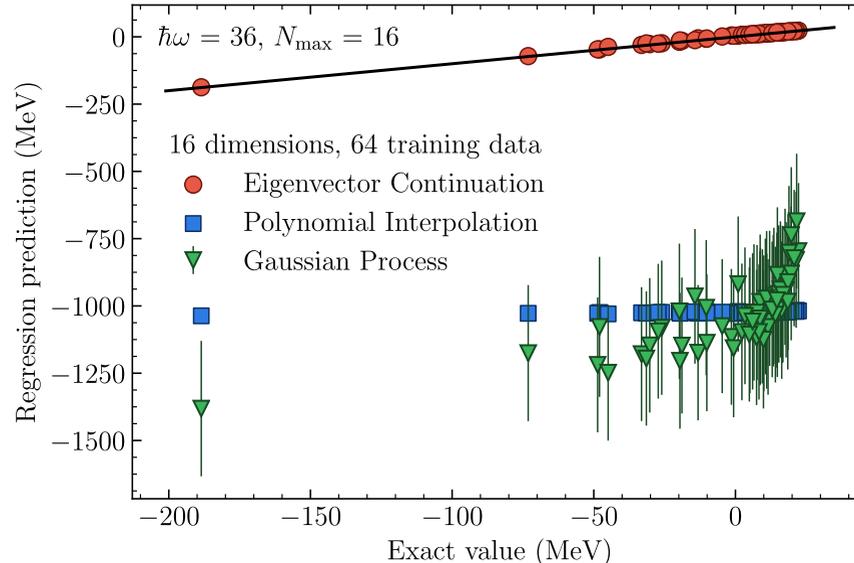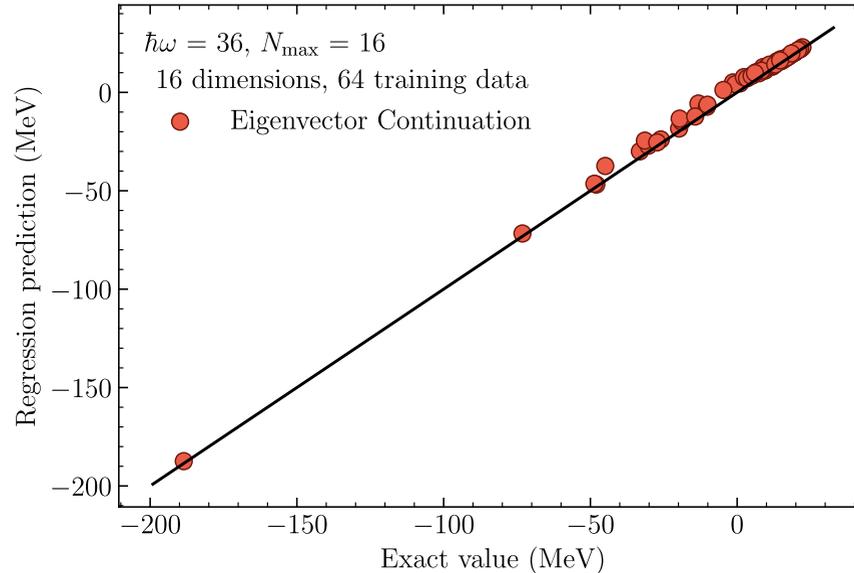- transparent symbols indicate extrapolation targets

Performance comparison: radius

Operator evaluation

- generalized eigenvalue problem
- EC gives not only energy, but also a continued wavefunction
- **straightforward (and inexpensive) to evaluate arbitrary operators**

^{4}He ground state radius squared

$\hbar\omega = 36$, $N_{max} = 16$

Regression prediction (fm^2)

Exact value (fm^2)

6 dimensions, 40 training data
- Polynomial Interpolation
- Eigenvector Continuation
- Gaussian Process
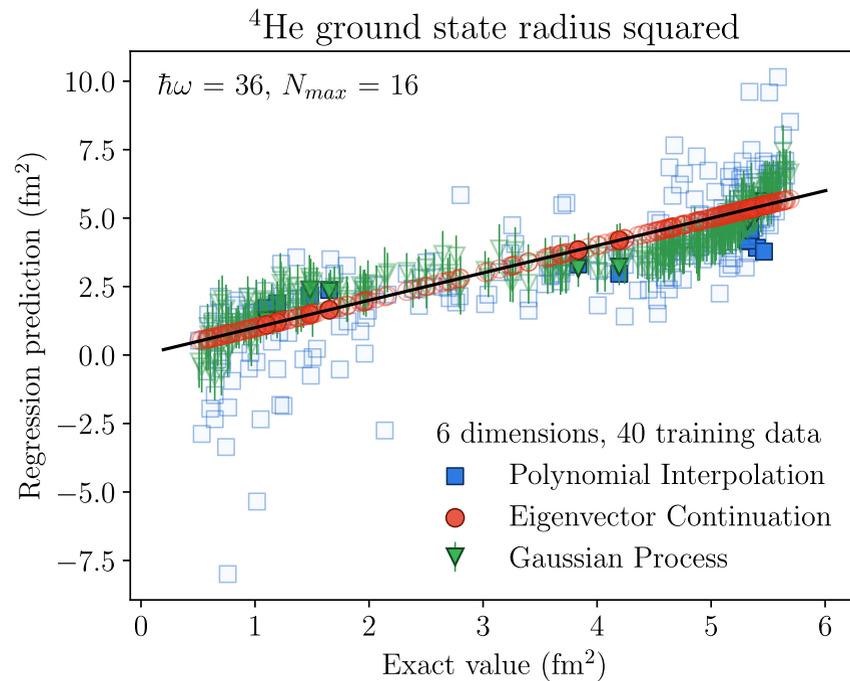
EC uncertainty estimate

- **EC is a variational method**
  - ‣ projection of Hamiltonian onto a subspace
  - ‣ dimension of this subspace determines the accuracy
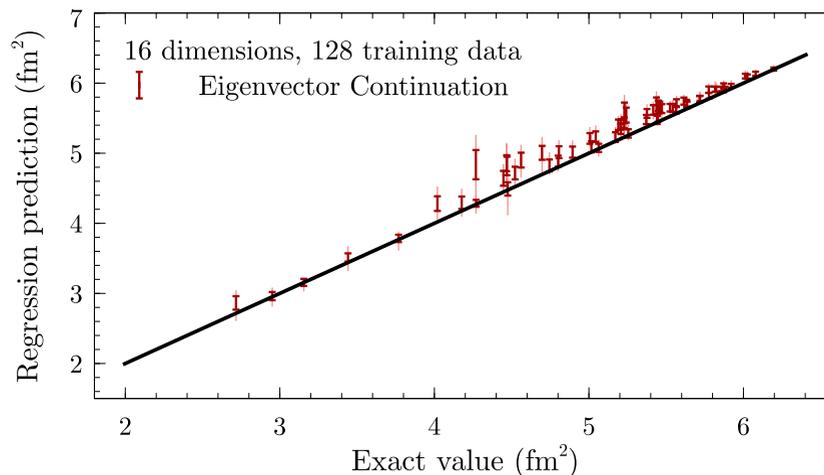 - ‣ excellent convergence properties

  Sarkar+Lee, PRL **126** 032501 (2021)

Bootstrap approach

SK, A. Ekström, K. Hebeler, D. Lee, A. Schwenk, PLB **810** 135814 (2020)

- construct a training data set larger than necessary
- **sample different training data sets, take mean and standard deviation**

Application: correlation analysis

- take 10^4 LEC samples 10% around NNLO_{sat} point, correlate different observables
  - known energy-radius correlation well reflected
  - ^{2}H radius only gives lower bound for ^{4}He radius
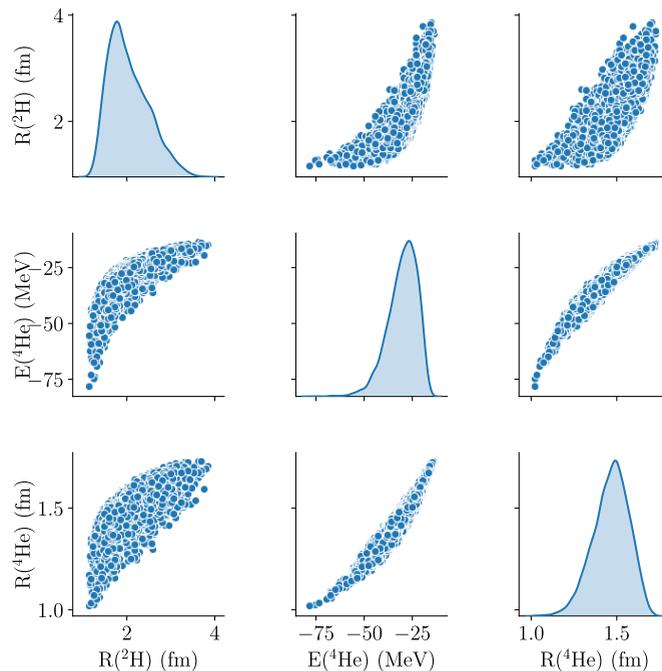
- **already this kind of analysis would be very expensive without EC!**

EC emulators have since been extended in various ways

Let's look at a few!

Subspace-projected coupled cluster method

- coupled cluster (CC) is a well established and powerful many-body technique
  - ▸ based on non-unitary similarity transformation of the Hamiltonian

$$\bar{H}(\vec{\alpha}) = \mathrm{e}^{-T(\vec{\alpha})} H(\vec{\alpha}) \mathrm{e}^{T(\vec{\alpha})}$$

  - ▸ the **cluster operator** $T(\vec{\alpha})$ is truncated in the space of particle-whole excitations
  - ▸ eigenvector continuation was developed for this non-Hermitian scenario

    talk by Gaute tomorrow   Ekström+Hagen, PRL **123** 252501 (2019)

Application: Global Sensitivity Analysis
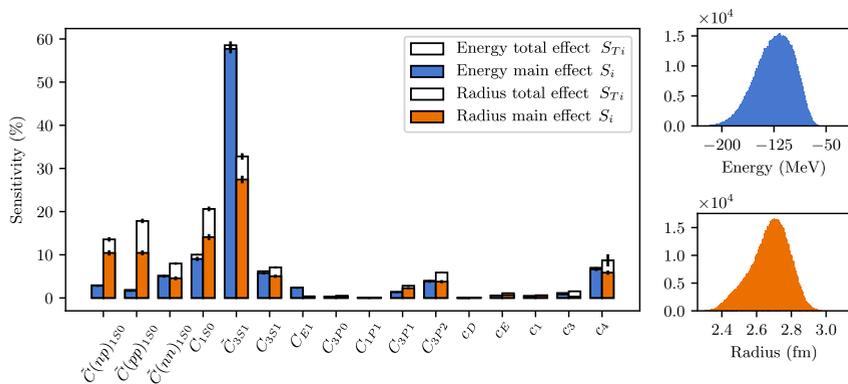
- study sensitivity of ^{16}O ground state to individual LECs
- **plot based on >1 million emulator evaluations!**
- recent extension to nuclear matter calculations Jiang et al., arXiv:2212.13216
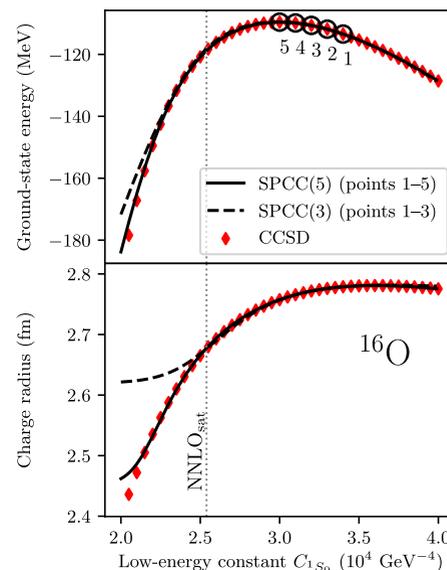
Scattering observables

- different methods have been developed to apply EC to scattering calculations
- this is particularly relevant for LEC fitting, that is primarily based on scattering data

EC via Kohn variational principle

- consider Hamiltonian $H = H(\boldsymbol{\theta})$, training points $\boldsymbol{\theta}_i$
- trial wave function $|\psi_{\text{trial}}\rangle = \sum_i c_i \psi_E(\boldsymbol{\theta}_i)\rangle$ for energy $E > 0$
- the condition that

$$\beta\left[|\psi_{\text{trial}}\rangle\right] \equiv \tau_{\text{trial}} - 2\mu\langle|\psi_{\text{trial}}|H(\boldsymbol{\theta}) - E|\psi_{\text{trial}}\rangle$$

should be stationary yields solutions for the c_i

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Furnstahl et al., PLB **809** 135719 (2020)

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Extensions and generalizations

- Newton's variational principle makes it possible to use trial scattering matrices instead of trial wave functions

  Melendez et al., PLB **821** 136608 (2021)

- the approach has been extended to three-body scattering

  talk by Xilin on Thursday

  Zhang+Furnstahl, PRC **105** 064004 (2022)

- a momentum-space formulation makes it possible to mitigate problems due to so-called Kohn anomalies

  Garcia et al., PRC **107** 054001 (2023)

- alternative strategy: simultaneous evaluation of multiple boundary conditions

  talk by Christian tomorrow Drischler et al., PLB **821** 13677 (2021)

Resonances

- **many states in nuclear physics are resonances**
  - ▸ i.e., metastable states with a finite lifetime to decay
- in stationary scattering theory, resonances are described as generalized eigenstates
  - ▸ S-matrix poles at comples energies $E = E_R - \mathrm{i}\Gamma/2$ (lifetime $\sim 1/\Gamma$)
  - ▸ wave functions are not normalizable (exponentially growing in r-space)
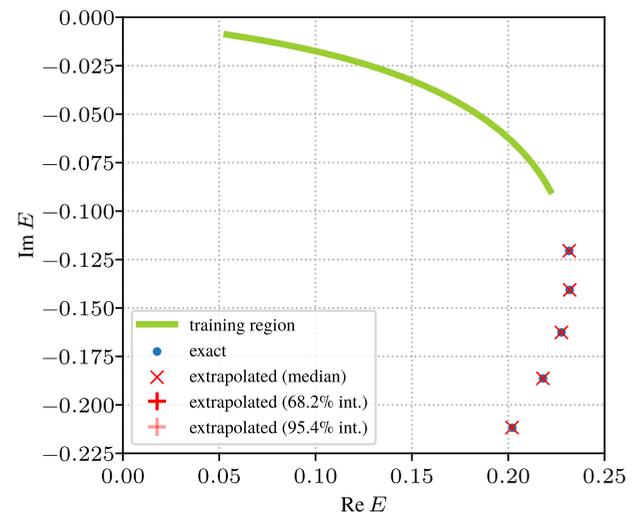
Resonance continuation

- one way to circumvent this problem is the complex scaling method:

$$r \to \mathrm{e}^{\mathrm{i}\phi} r \quad , \quad p \to \mathrm{e}^{-\mathrm{i}\phi} p$$

- along the rotated contour, resonance wave functions become normalizable
- formalism changes the inner product!
- **eigenvector continuation has been extended to this scenario**

  Yapa, SK, Fossez, 2303.06139 [nucl-th]

  talk by Nuwan on Friday

p. 25

More applications and extensions

R-matrix formalism for fusion observables

- use of calculable R-matrix formalism with boundary condition to simulate absorption

  Bai+Ren, PRC **103** 014612 (2021); Bai, PRC **106** 024611 (2022)

- EC applied based on solutions of the Bloch-Schrödinger equation
  - ▸ based on previously mentioned EC scattering developments

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Single-neutron spectra of heavy nuclei   Anderson et al., PRC **106** L031302 (2022)

- spherical mean-field Hamiltonian tuned to reproduce an energy density functional
- prescription to train an emulator that discribes simultaneously all spherical nuclei

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More structure emulators

- use EC as emulator and Lanczos preprocessor for shell-model calculations

  talk by Yoshida-san tomorrow   Yoshida+Shimizu, PTEP **2022** 053D02

- collectivity and clustering via symmetry-adapted NCSM   Becker et al., FP **11** 1064601

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  Becker et al., FP **11** 1064601

Pairing Hamiltonian   Companys Franzke et al., arXiv:2302.08373

- exactly solvable model for nuclear supefluidity   talk by Margarida on Friday
- **also uses EC as a resummation tool $\rightarrow$ next part of this talk**

Part II

Accurate Resummation via Eigenvector Continuation
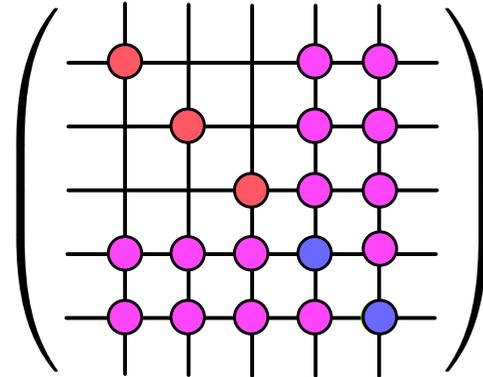
Model-space perturbation theory

- consider a Hamiltonian diagonalized in a (small) subspace

$$H = \begin{pmatrix} H_{\phi\phi} & H_{\phi\psi} \\ H_{\psi\phi} & H_{\psi\psi} \end{pmatrix}$$

$$N_0 = \dim H_{\phi\phi} \ll \dim H = N_1$$

$$H_{\phi\phi} = \mathrm{diag}(\{\lambda_i\}_{i=1,\cdot\cdot N_0})$$

- factor out large number X from diagonal entries of $H_{\psi\psi}$
- perturbative expansion for lowest eigenvalue and vector

$$|\psi\rangle = \sum_{n=0}^{\infty} X^{-n} \left(\sum_{i=1}^{N_0} \alpha_i^{(n)} |\phi_i\rangle + \sum_{j=N_0+1}^{N_1} \alpha_j^{(n)} |\psi_j\rangle \right) \ , \ E = \sum_{n=0}^{\infty} X^{-n} E^{(n)}$$

▸ **matching powers gives coupled recursive expressions for $\alpha_j^{(n)}$ and $E^{(n)}$**

Model-space perturbation theory

Diagonalizing a small space can still be too expensive...

Model-space perturbation theory

Diagonalizing a small space can still be too expensive...

- actually, a partial diagonalization *per se* is still doable ($\rightarrow$ Lanczos)
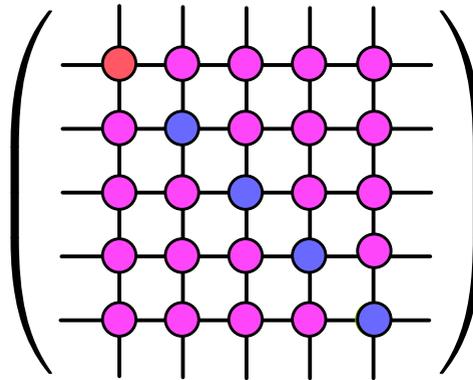- but transforming the Hamiltonian is problematic...
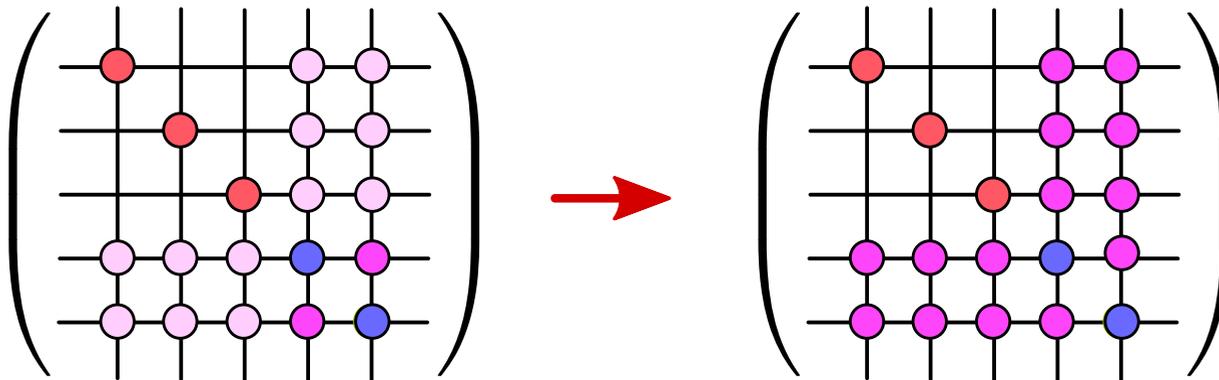
- **cost for adjusting off-diagonal elements is significant**
  - ‣ scales with size of the full (large) space

Model-space perturbation theory

Simplest case

- start from one-dimensional space $(N_{\mathrm{max}} = 0)$
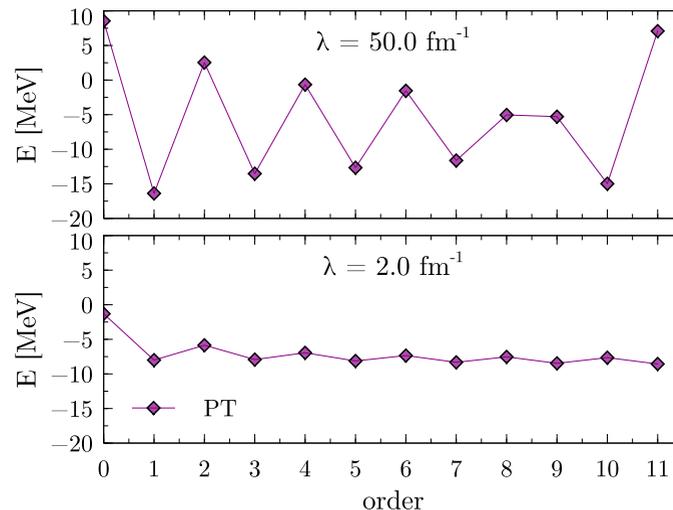 - ▸ i.e., directly use the given Hamiltonian

- **this is equivalent to a simple (many-body) perturbation theory expansion**
  - ▸ $H_0|\Phi^{(0)}\rangle = E^{(0)}|\Phi^{(0)}\rangle$: orthonormal basis, $H(c) = H_0 + c\,H_1$
  - ▸ $|\Psi_P(c)\rangle = \displaystyle\sum_{p=0}^{P} c^p|\Phi^{(p)}\rangle$, want $c = 1, P \to \infty \;\; \rightsquigarrow \;\; E = E^{(0)} + E^{(1)} + \cdots$

Failure of perturbation theory

^{3}H NCSM calculation, $N_{\mathrm{max}} = 12$ model space

- EMN N3LO 500 interaction, plus SRG evolution

- **perturbation theory does not converge!**
  - ▸ however, interaction clearly "more perturbative" for small SRG λ
  - ▸ convergence perhaps for very small λ
- **note:** the situation can be somewhat improved with better reference states

Resummation via eigenvector continuation

- span space by the wavefunction corrections $|\Phi^{(p)}\rangle$
- evaluate Hamiltonian between these states
- **i.e., use energy and wavefunction information**
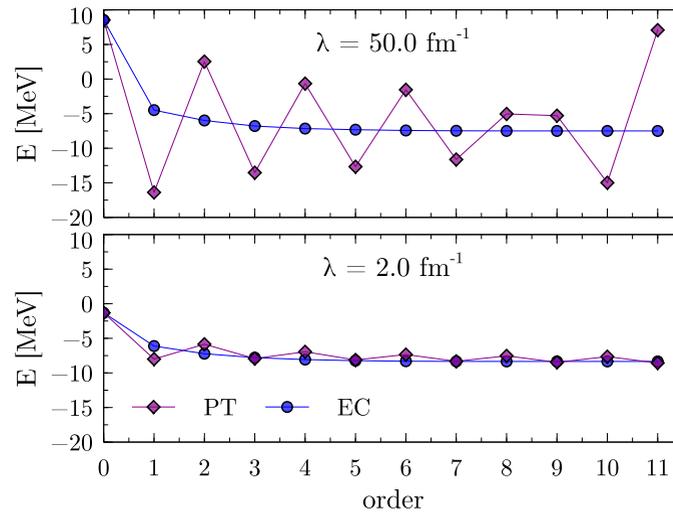
- **this uses the same input as PT, but now the series converges!**
  - ‣ rapid convergence to the correct result!
  - ‣ smooth behavior, significant oscillations are gone

Continued perturbation theory

- let's recap what exactly we have done:

General setup

- $H = H_0 + c\,H_1$, EC-extrapolate to $c = 1$
- perturbation theory converges for sufficiently small c

$$
\begin{pmatrix} |\Psi_P(c_1)\rangle \\ |\Psi_P(c_2)\rangle \\ \vdots \\ |\Psi_P(c_{N_{\mathrm{EC}}})\rangle \end{pmatrix} = \begin{pmatrix} 1 & c_1 & c_1^2 & \cdots & c_1^P \\ 1 & c_2 & c_2^2 & \cdots & c_2^P \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c_{N_{\mathrm{EC}}} & c_{N_{\mathrm{EC}}}^2 & \cdots & c_{N_{\mathrm{EC}}}^P \end{pmatrix} \begin{pmatrix} |\Phi^{(0)}\rangle \\ |\Phi^{(1)}\rangle \\ \vdots \\ |\Phi^{(P)}\rangle \end{pmatrix}
$$

Eigenvector continuation

- assume we have eigenvetors for some set $\{c_i\}_{i=1}^{N_{\mathrm{EC}}}$ of such c
- linear combinations of perturbative corrections up to order P
- **we can instead use the perturbative corrections directly as EC basis!**

Application to larger systems
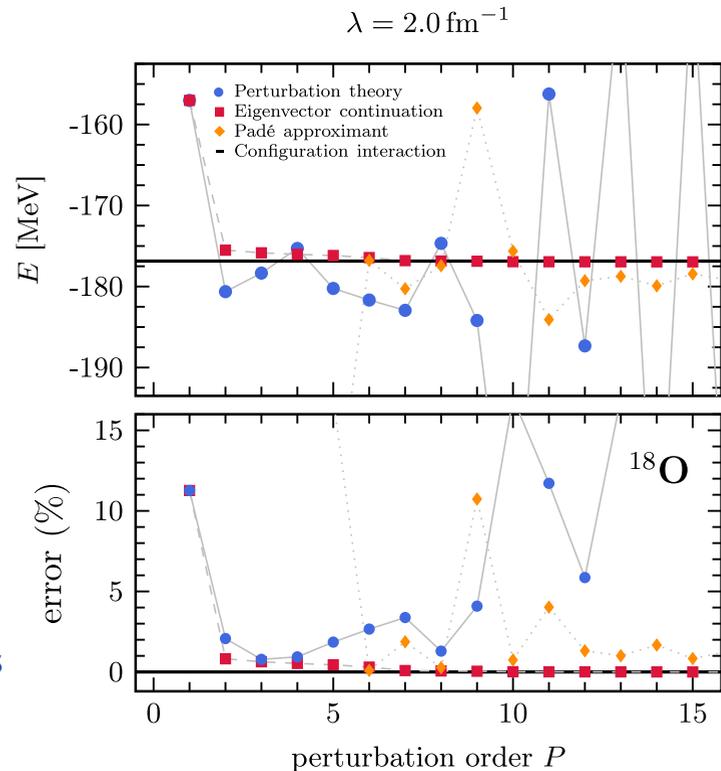
Consider ^{18}O in Bogoliubov MBPT as example

- break particle number conservation in reference state
- restore average particle number to target value at each order
- perturbation theory under constraint   Demol et al., Annals Phys. **424** 168358 (2021)

  talk by Pepijn on Thursday

- **for proof of principle study, consider a very limited model space**

  ‣ one-body cutoff at $e_{\max} = 2n + l = 4$

  ‣ symmetry-broken Hartree-Fock-Bogoliubov reference state

  ‣ two-, four-, and selected six-quasiparticle excitations on top

- recursive theme makes it possible to go high orders P

  ‣ realistic in practice with larger model spaces: $P \leq 3$

Application to larger systems

Results

- EM500 interaction
- SRG evolved to $\lambda = 2.0\mathrm{fm}^{-1}$
- full CI calculation as reference
- **compare various methods**
  - ‣ simple perturbation theory
  - ‣ eigenvector continuation
  - ‣ Padé resummation

- direct perturbation theory clearly diverges
- **EC is accurate and reliable**
- Padé becomes erratic at high orders

$\lambda = 2.0\,\mathrm{fm}^{-1}$

Perturbation theory
Eigenvector continuation
Padé approximant
Configuration interaction

^{18}O

perturbation order P

Demol, SK, et al., PRC **101** 041302(R) (2020)

- **recent further application:** EC resummation for pairing Hamiltonian

talk by Margarida on Friday   Companys Franzke et al., arXiv:2302.08373

Outlook

Finite-volume eigenvector continuation

- finite-volume spectra encode infinite-volume properties Lüscher, CMP **104** 177 (1986); …

- resonances can be identified from avoided crossings in finite-volume spectra
  Wiese, NPB (Proc. Suppl.) **9** 609 (1989), Klos, SK et al., PRC **98** 034004 (2018)

- to find/exclude low-energy resonances, one needs many calculations in large boxes

- this comes with a substantial numerical cost

- **finite-volume eigenvector continuation** can be used to mitigate this
  - ▸ extrapolation/interpolation across substantial volume ranges
  - ▸ parametric dependence directly in basis

  talk by Nuwan on Friday
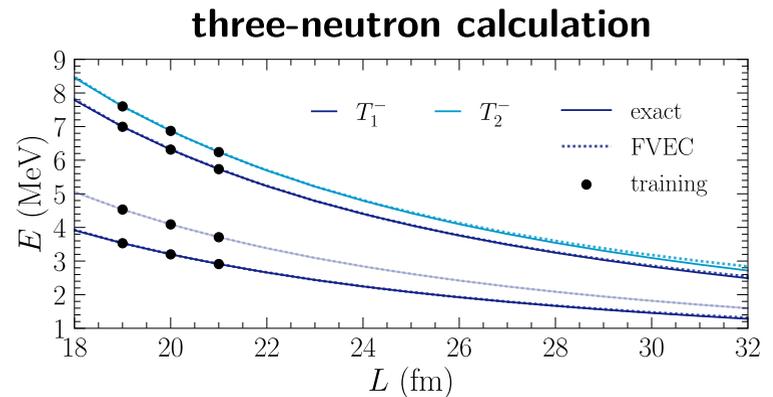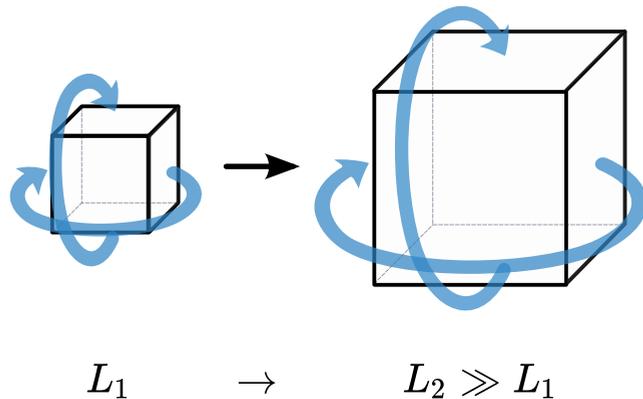
$$L_1 \quad \rightarrow \quad L_2 \gg L_1$$
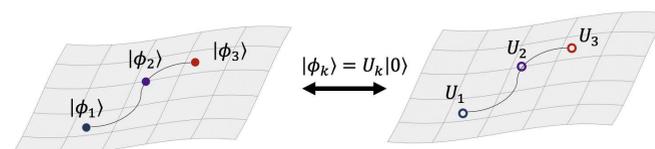
three-neutron calculation

Quantum computing and chemistry

- **EC has found new exciting applications outside nuclear physics**

Subspace diagonalization

Francis et al., arXiv:2209.10571

- quantum-classical hybrid method
- Hamiltonian projected to a smaller subspace
- **ideal scenario to apply EC!**
  - ‣ extension to space of unitary matrices that
  generate states

Quantum computing and chemistry
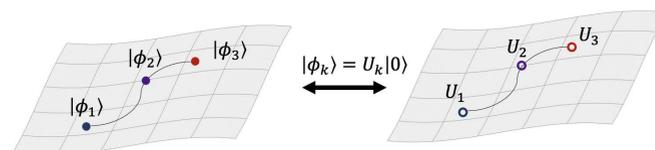
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Potential energy surfaces

Mejuto-Zaera+Kemper, arXiv:2305.00060

- application to full configuration interaction of molecular orbitals
- involves inner products between separate sets of atomic orbitals
  - ▸ **similar to basis matching in FVEC!**
- accurate results for pot. energy surfaces with moderate number of training points
  - ▸ demonstrates access to excited states   cf. also Companys Franzke et al., arXiv:2108.02824

Summary and outlook

Eigenvector continuation as efficient emulator

- highly competitive, accurate and efficient
- can both interpolate and extrapolate from training sets
- possible to provide extrapolation uncertainty estimates
- broadly applied to nuclear structure and reactions

Eigenvector continuation as resummation tool

- possible to effectively tame divergent expansion coefficients
- interesting as computational method
- applications to finite nuclei and nuclear matter models

More exciting applications and surely more to come!

Summary and outlook

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***

Thanks very much for your attention!

Backup slides

NCSM EC emulator: computational cost

- **setup of EC subspace basis**
  - ‣ combination of Hamiltonian for given $\vec{c}_i$, Lanczos diagonalization
  - ‣ total cost $= M^2 \times (2n + N_{\mathrm{mv}})$ flops
- **calculation of norm matrix:** $2n^2 M$ flops
- **reduction of Hamiltonian parts:** $(d+1) \times (2nM^2 + 2n^2 M)$ flops
- **cost per emulated sample point**
  - ‣ combination of Hamiltonian parts in small space: $2dn^2$ flops
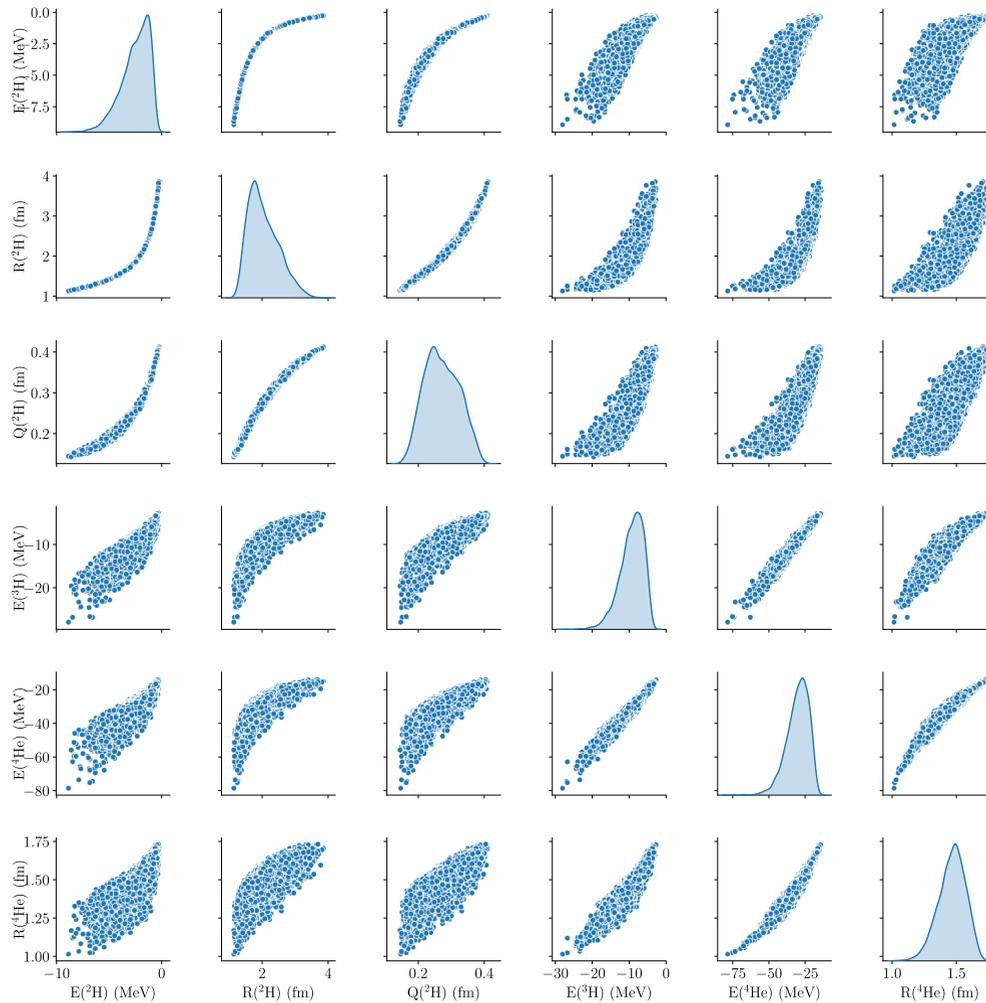 - ‣ orthogonalization $+$ diagonalization: $26n^3/3 + \mathcal{O}(n^2)$ flops

$M = M(N_{\mathrm{max}})$: model-space dim., n: training data, N: samples, N_{mv}: matrix-vector prod. (Lanczos)

Example

- $N_{\mathrm{max}} = 16$
- $d = 16$, $N_{\mathrm{EC}} = 64$
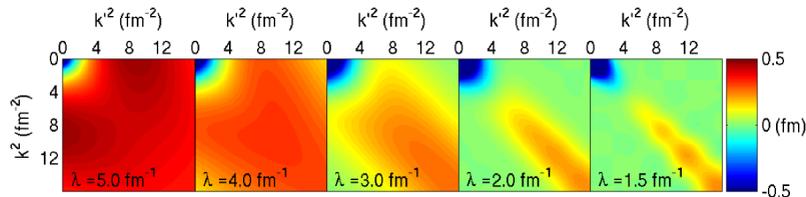- max. speed-up factor ~ 600
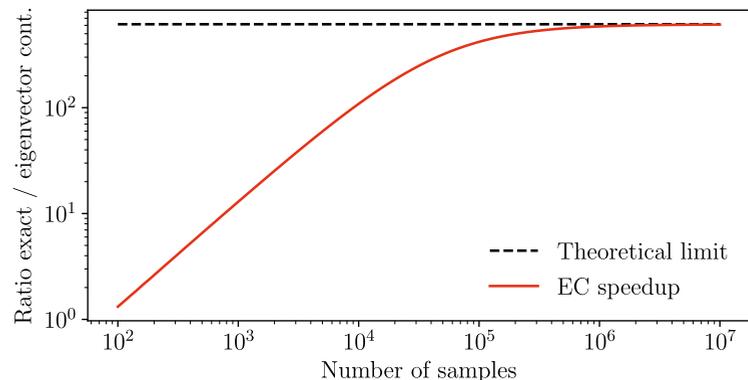
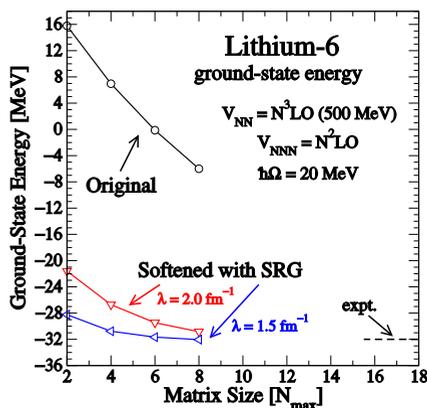# Complete correlation analysis

Reverse SRG Evolution

Similarity Renormalization Group (SRG)

- nuclear potentials (from EFT or otherwise) can be difficult to handle numerically
- unitary transformation of Hamiltonian: $H \rightarrow H_\lambda = U_\lambda H U_\lambda^\dagger \rightsquigarrow V_\lambda$ -decouple low and high momenta at scale λ
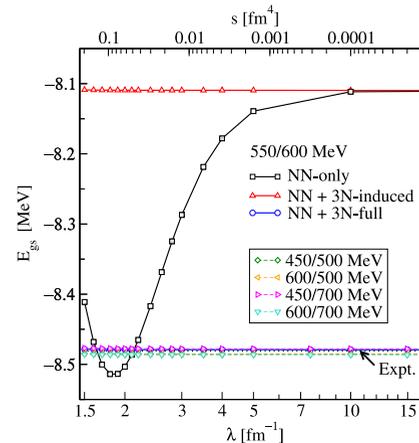
- **interaction becomes more amenable to numerical methods...**
- **...at the cost of induced many-body forces!**

SRG evolution = ODE solving

$$\frac{\mathrm{d}H_s}{\mathrm{d}s} = \frac{\mathrm{d}V_s}{\mathrm{d}s} = [[G, H_s], H_s], \; \lambda = 1/s^{1/4}$$

ordinary differential equation ensures smooth parametric dependence

$\hookrightarrow$ **SRG evolution satisfies EC prerequisites!**

Reverse SRG

Consider A = 3,4 test cases
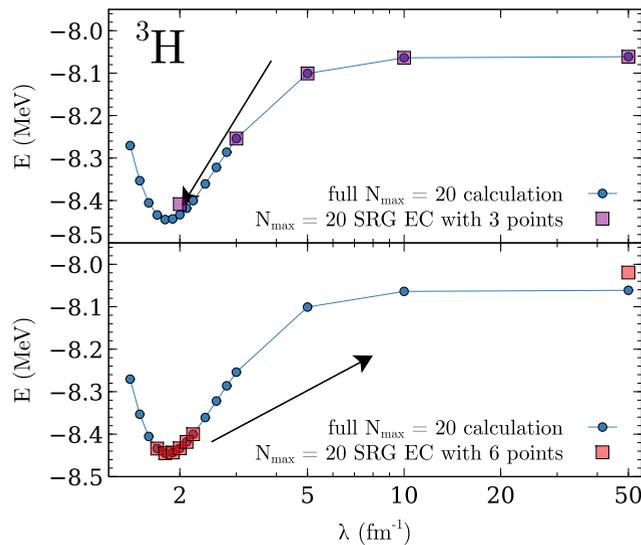
- EMN N3LO(500) interaction, Jacobi NCSM calculation

  Entem et al., PRC **96** 024004 (2017); A. Ekström implementation of Navratil et al., PRC **61** 044001 (2000)
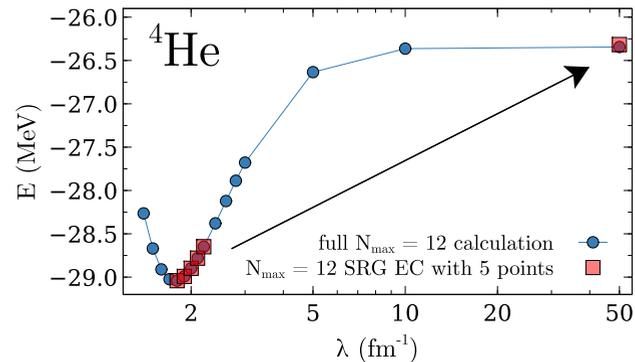
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Not even induced 3N forces kept here!

- possible to extrapolate back from small λ to bare interaction
- **information about missing many-body forces in wavefunctions**
  - ▸ not in any single wavefunction, but in how they change

Mind the gap

Still no free lunch, however...

- EC is a variational method
- **cannot go beyond what bare interaction gives in same model space!**