Eigenvector continuation in nuclear physics

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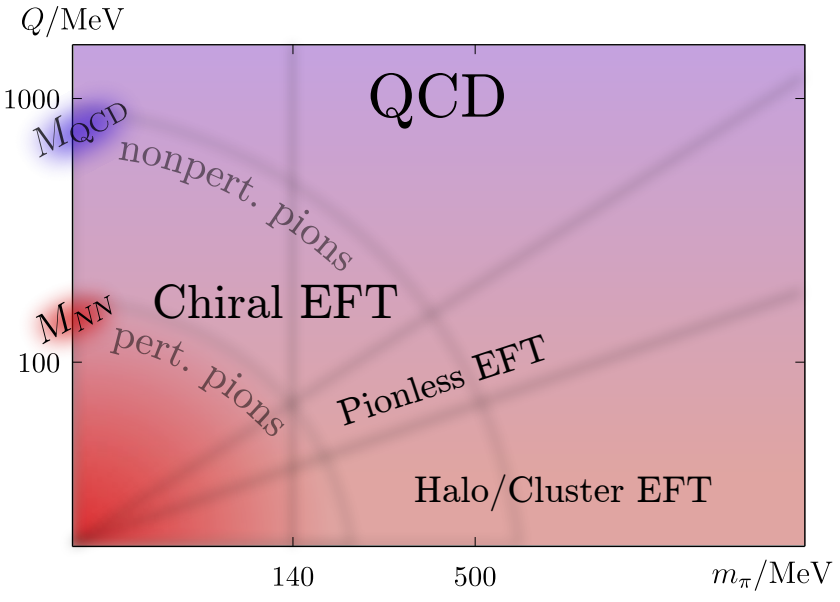
SK, Ekström, Hebeler, Lee, Schwenk, PLB **810** 135814 (2020)
Yapa, SK, arXiv:2201.08313 (2022)

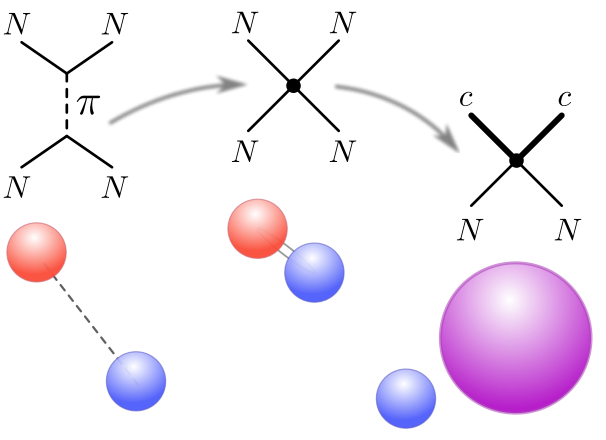
Nuclear effective field theories

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

Hammer, SK, van Kolck, RMP **92** 025004 (2020)

- $\rightsquigarrow$ **ab initio predictions with fully quantified uncertainties**





- degrees of freedom here: nucleons (and clusters thereof)
- even more effective d.o.f.: rotations, vibrations

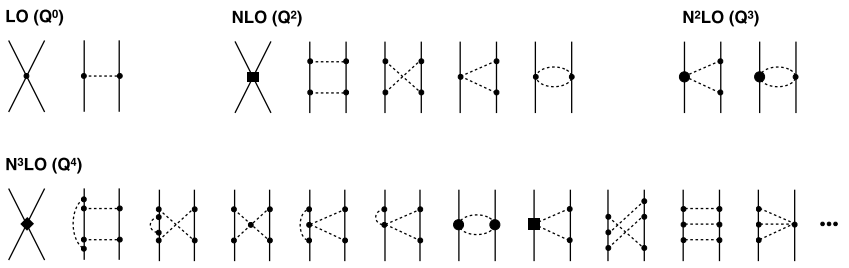
Papenbrock, NPA **852** 36 (2011); ...

Chiral interactions

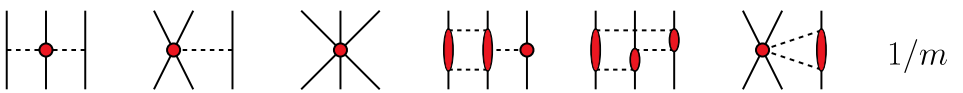
Many remarkable results based on chiral potentials

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

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



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



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

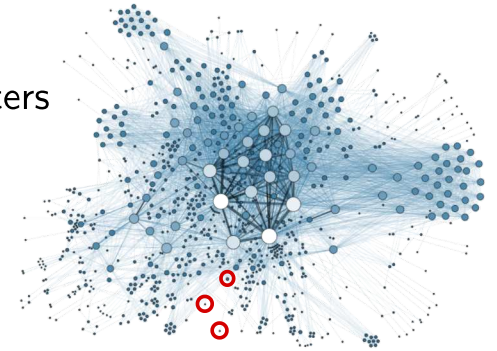
However...

- **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

Eigenvector continuation

Many physics problems are tremendously difficult...

- huge matrices, possibly too large to store
  - ever more so given the evolution of typical HPC clusters
- most exact methods suffer from exponential scaling
- **interest only in a few (lowest) eigenvalues**



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

Introducing eigenvector continuation

D. Lee, TRIUMF Ab Initio Workshop 2018; Frame et al., PRL **121** 032501 (2018)

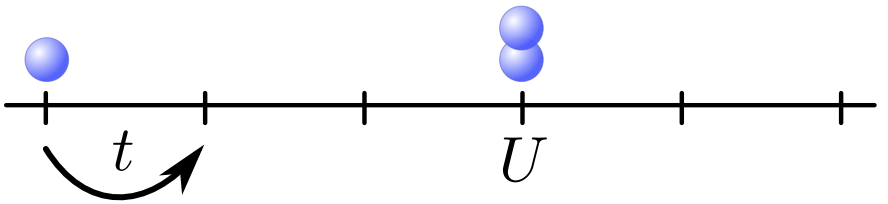
KDE Oxygen Theme

- novel numerical technique
- can solve otherwise untractable problems
- amazingly simple in practice
- broadly applicable
- **pretty big hammer, nails everywhere**

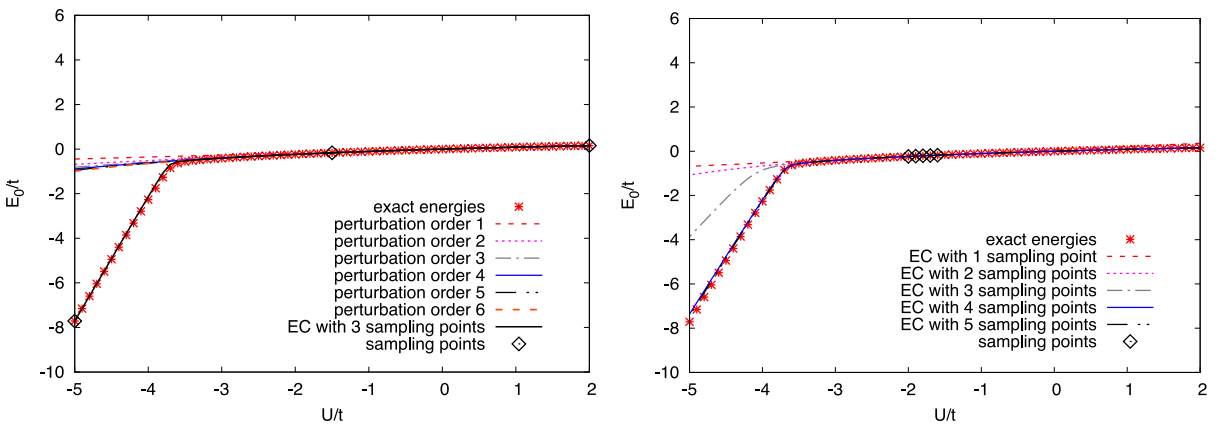
Hubbard model

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

- three-dimensional Bose-Hubbard model (4 bosons on $4 \times 4 \times 4$ lattice)
- hopping parameter t, on-site interaction $U \rightsquigarrow H = H(c = U/t)$



- Bose gas for $c > 0$, weak binding for $-3.8 < c < 0$, tight cluster for $c < -3.8$
- **eigenvector continuation can extrapolate across regimes**



General idea

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**

Procedure

- calculate $|\psi(c_i)\rangle$, $i = 1, \dots N_{\mathrm{EC}}$ in "easy" regime
- solve generalized eigenvalue problem $H|\psi\rangle = \lambda N|\psi\rangle$ with
  - $H_{ij} = \langle\psi_i|H(c_{\mathrm{target}})|\psi_j\rangle$
  - $N_{ij} = \langle\psi_i|\psi_j\rangle$

Prerequisite

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

Outline

Introduction ✔

Reverse SRG Evolution

Efficient Emulators

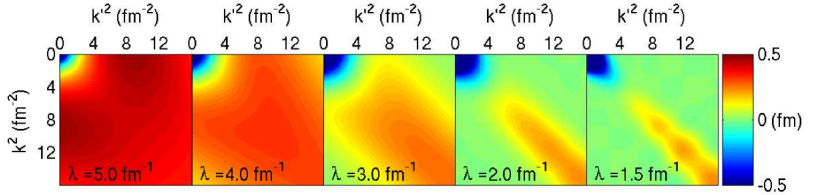
Volume Extrapolation

Part I

Reverse SRG Evolution

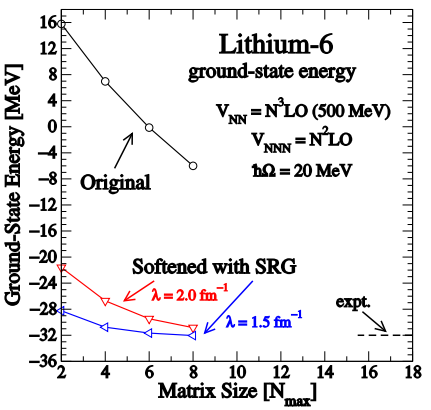
Similarity Renormalization Group (SRG)

- nuclear potentials (from EFT or otherwise) can be difficult to handle numerically
- unitary transformation of Hamiltonian: $H \to H_\lambda = U_\lambda H U_\lambda^\dagger \rightsquigarrow V_\lambda$ -decouple low and high momenta at scale λ

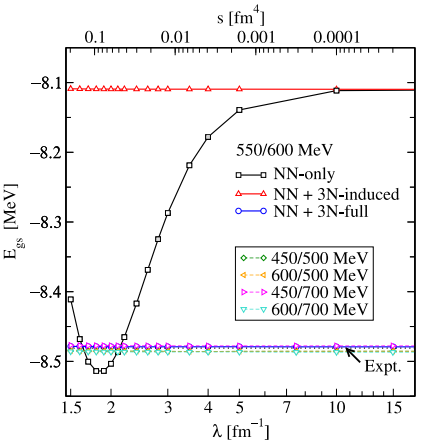


R. Furnstahl, HUGS 2014 lecture slides

- **interaction becomes more amenable to numerical methods...**
- **...at the cost of induced many-body forces!**



Bogner et al., PPNP 65 94 (2010)



Hebeler+Furnstahl, RPP **76** 126301 (2013)

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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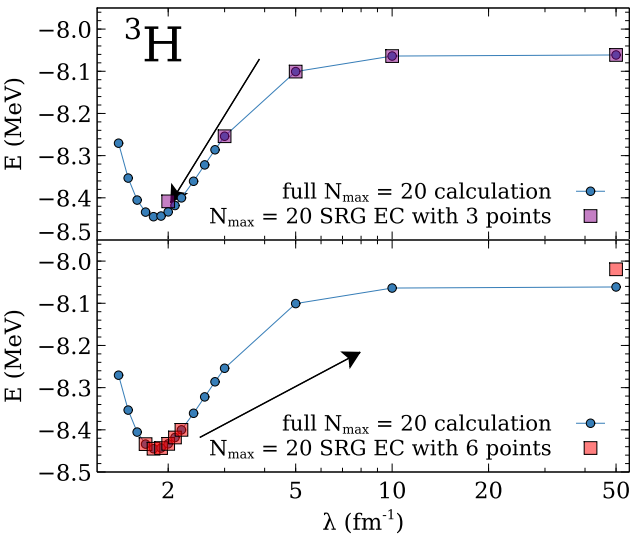
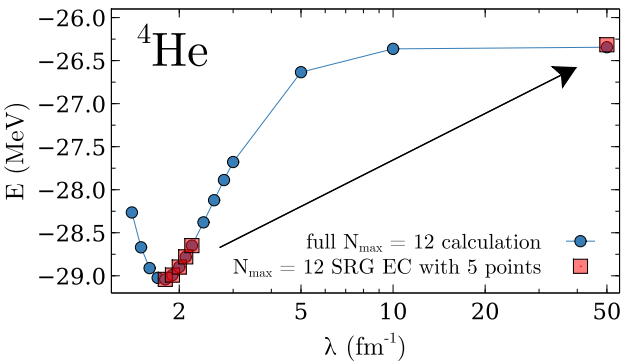


Not even induced 3N forces kept here!

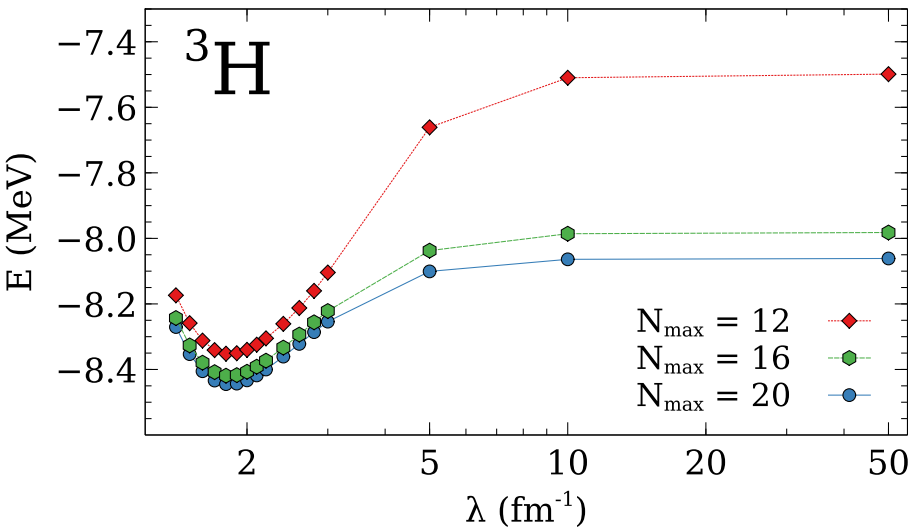


- possible to extrapolate back from small λ to bare interaction
- **information about missing many-body forces in wavefunctions**
  - not in any single wavefunction, but in how they change

Mind the gap

Still no free lunch, however...

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



Part II

Efficient Emulators via Eigenvector Continuation

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

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)

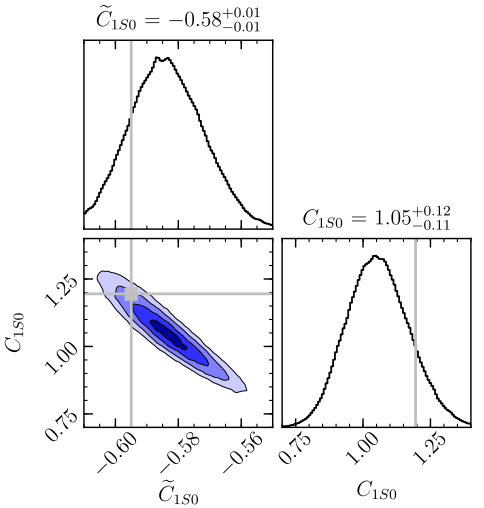
- **fitting needs many calculations with different parameters**

2. Propagation of uncertainties

- statistical fitting gives posteriors for LECs
- LEC posteriors propagate to observables

  Wesolowski et al., JPG **46** 045102 (2019)

- **need to sample a large number of calculations**
  - expensive already in few-body sector!

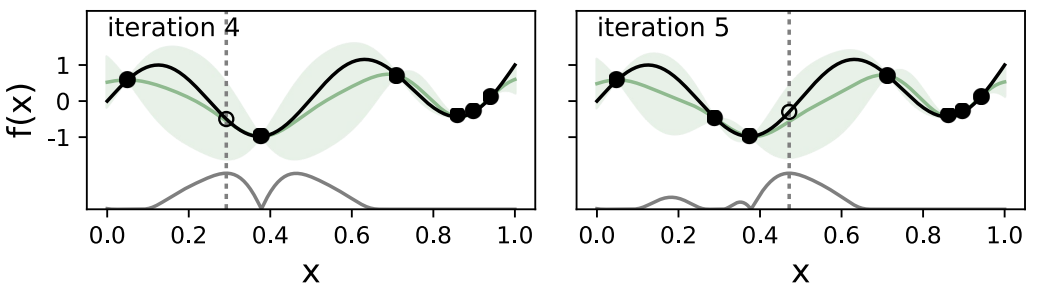


Emulators

Exact calculations can be prohibitively expensive!

Options

- **multi-dimensional polynomial interpolation**
  - simplest possible choice
  - typically too simple, no way to assess uncertainty
- **Gaussian Process (GP)**



  - statistical modeling, iteratively improvable
  - interpolation with inherent uncertainty estimate

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

Recall

Eigenvector continuation can interpolate and extrapolate!

Hamiltonian parameter spaces

- original EC: single parameter, $H = H(c)$ Frame et al., PRL **121** 032501 (2018)
- **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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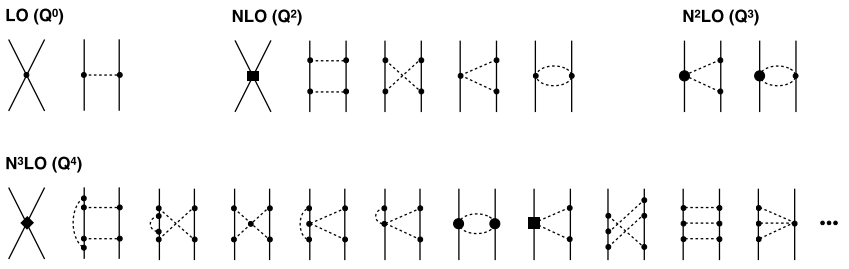

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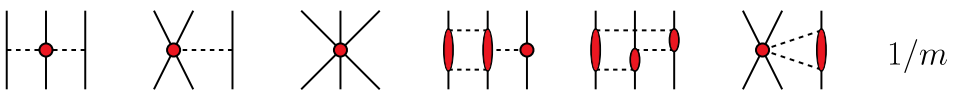

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Generalized EC

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

- **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 $i = 1, \cdot\cdot N_{\rm EC}$
  - $H_{ij} = \langle\psi_i|H(\vec{c}_{\rm target})|\psi_j\rangle$, $N_{ij} = \langle\psi_i|\psi_j\rangle$

Note: sum in Eq. (1) can be carried out in small (dimension = $N_{\rm EC}$) space!

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_{sat} point

Ekström et al., PRC **91** 051301 (2015)

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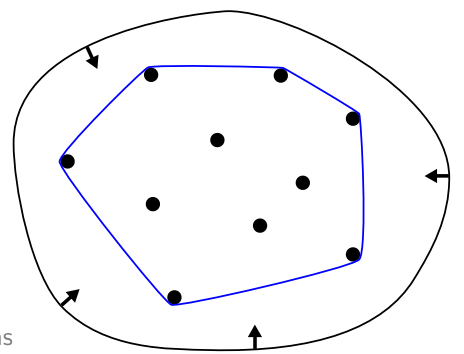
Ekström et al., PRC **91** 051301 (2015)

Convex combinations

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

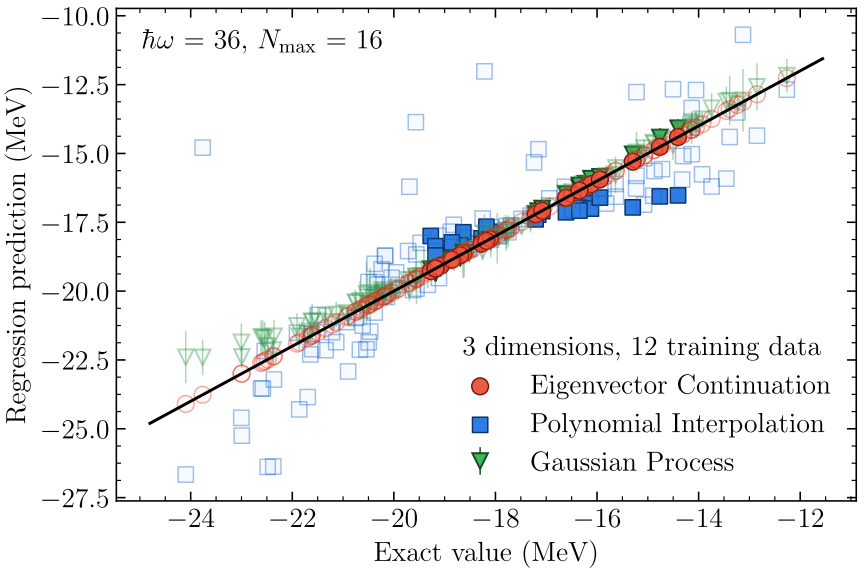


Pbroks13, Wikimedia Commons

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 Ekström implementation of Navratil et al., PRC **61** 044001 (2000)
- observable: ^{4}He ground-state energy
- transparent symbols indicate extrapolation targets



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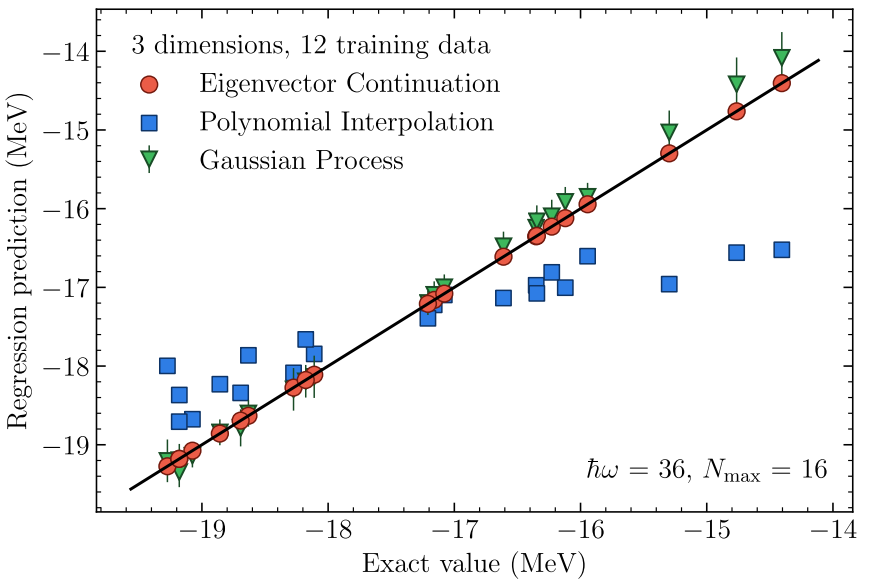

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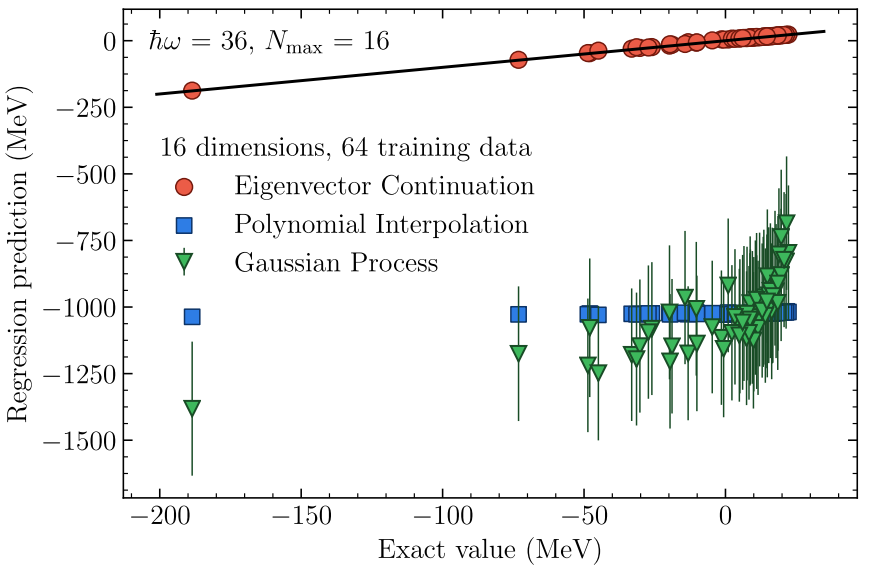

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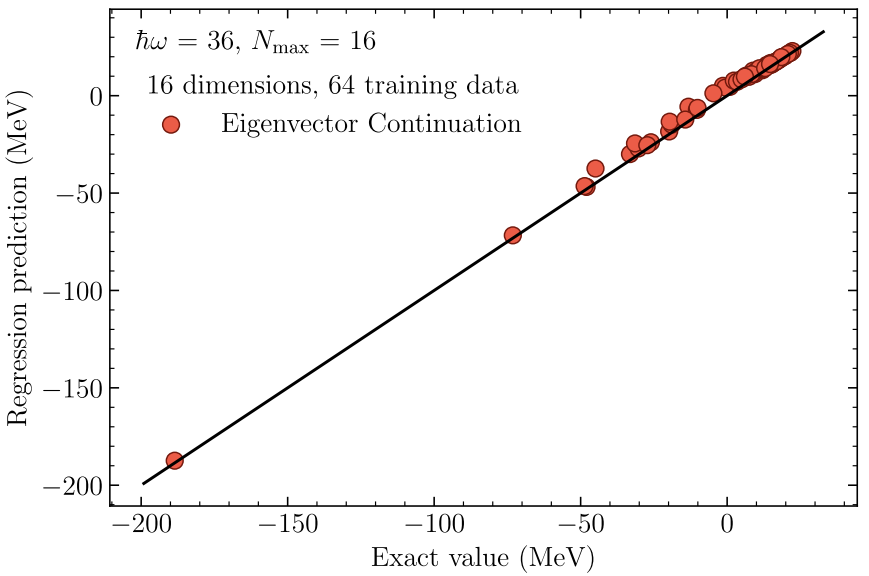
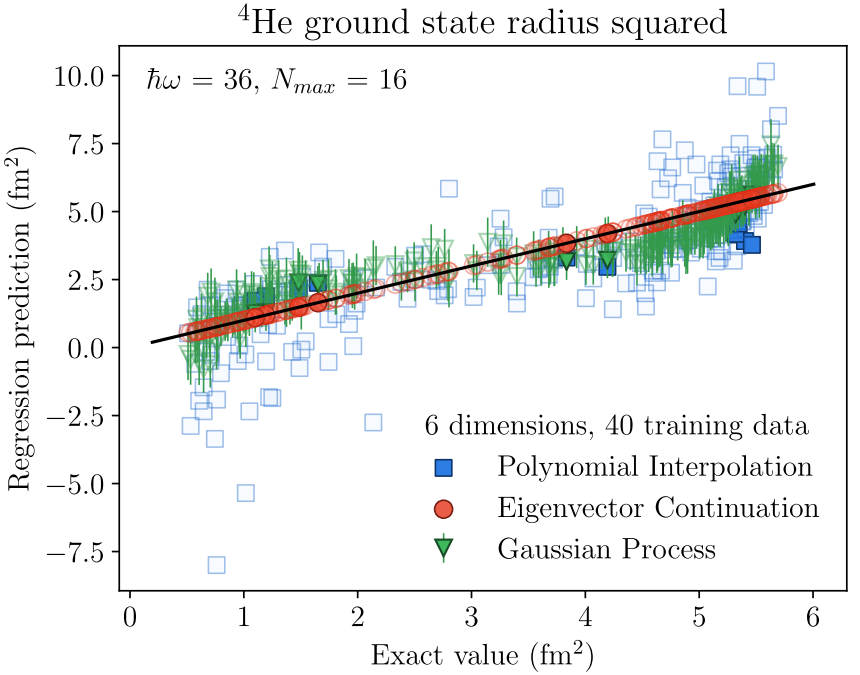


Performance comparison: radius

Operator evaluation

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



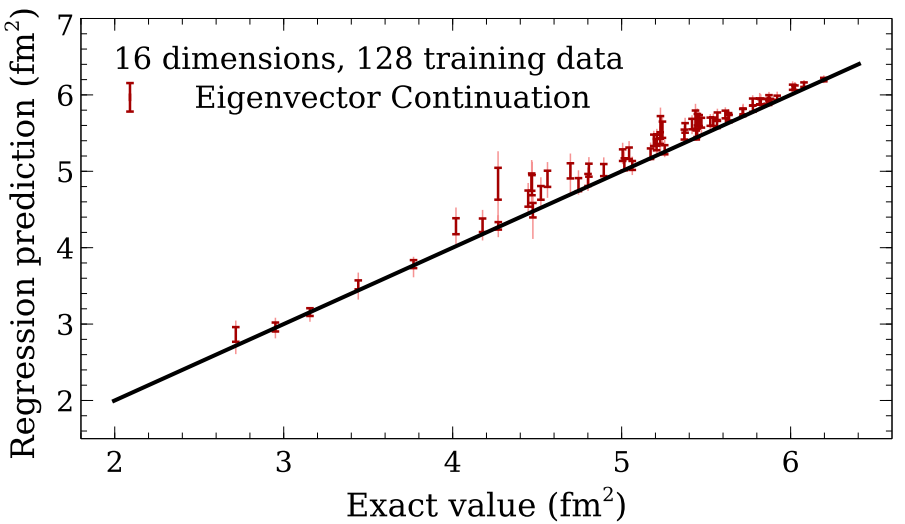
EC uncertainty estimate

- **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

- **leave out sets of basis vectors, take mean and standard deviation**



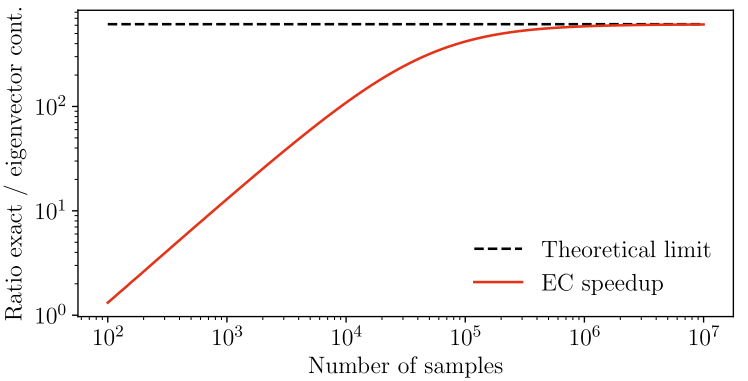
Computational cost

- **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

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

Example

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

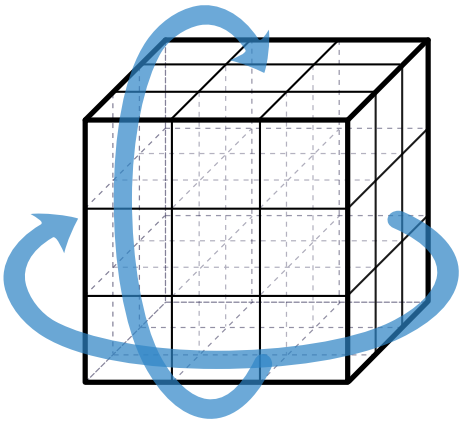


Part III

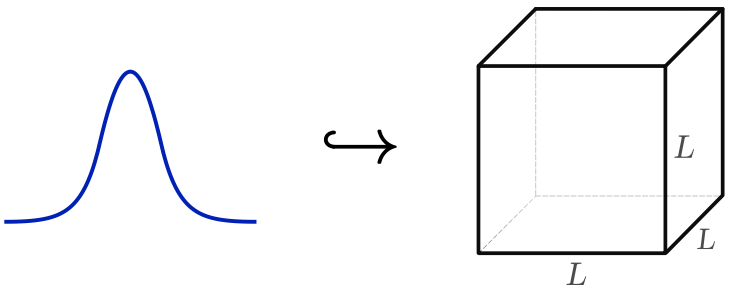
Volume Extrapolation via Eigenvector Continuation

N. Yapa, SK, arXiv:2201.08313 (2022)

Finite periodic boxes



- physical system enclosed in finite volume (box)
- typically used: periodic boundary conditions
- **leads to volume-dependent energies**

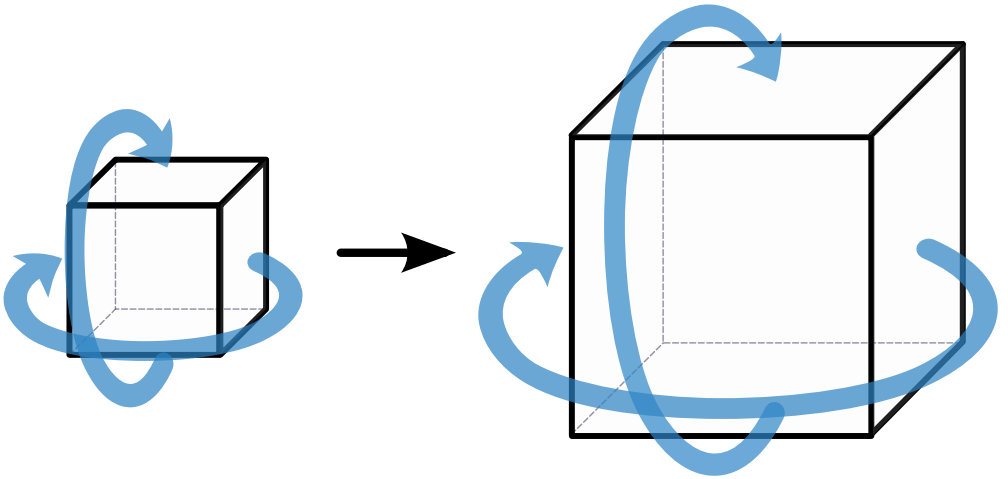


Lüscher formalism

- physical properties encoded in the volume-dependent energy levels
- infinite-volume S-matrix governs discrete finite-volume spectrum
- **finite volume used as theoretical tool**

Lüscher, Commun. Math. Phys. **104** 177 (1986); ...

Volume extrapolation



$$L_1 \qquad \rightarrow \qquad L_2 \gg L_1$$

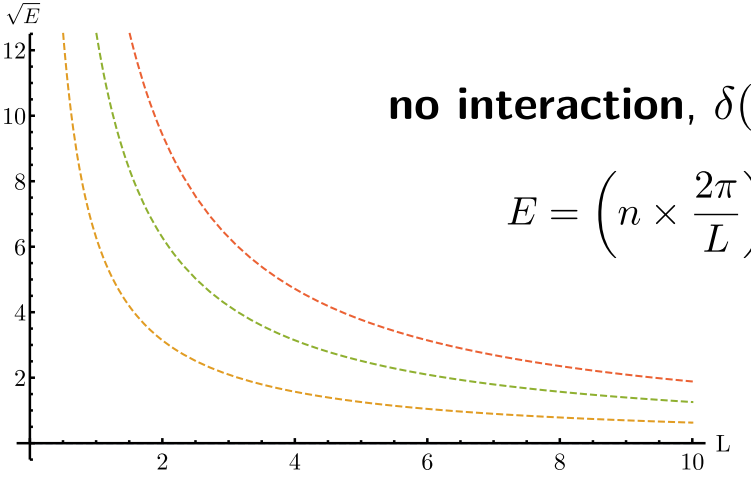
Why?

Finite-volume resonance signatures

Lüscher formalism

- finite volume $\rightarrow$ discrete energy levels $\rightarrow p \cot \delta_0(p) = \frac{1}{\pi L} S(E(L)) \rightarrow$ phase shift
- **resonance contribution $\leftrightarrow$ avoided level crossing**

Lüscher, NPB **354** 531 (1991); ...
Wiese, NPB (Proc. Suppl.) **9** 609 (1989); ...



no interaction, $\delta(p) = 0$

$$E = \left(n \times \frac{2\pi}{L} \right)^2$$

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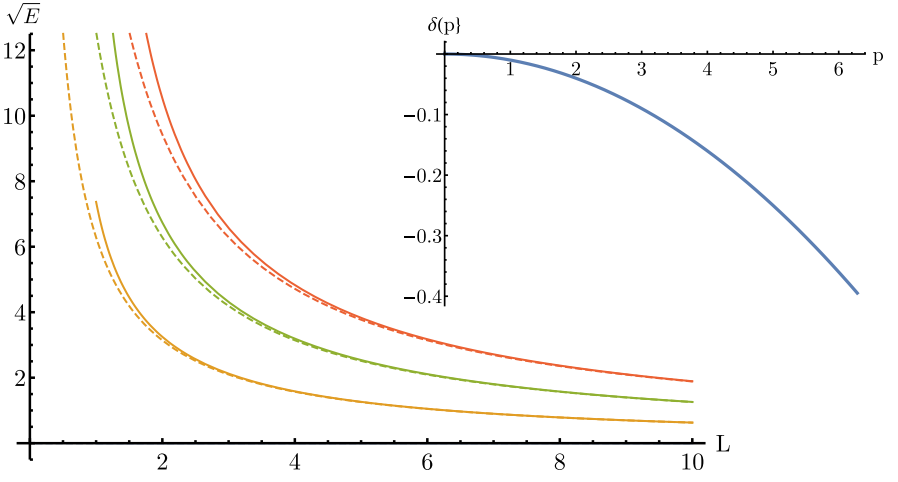

Finite-volume resonance signatures

Lüscher formalism

- finite volume $\rightarrow$ discrete energy levels $\rightarrow p \cot \delta_0(p) = \frac{1}{\pi L} S(E(L)) \rightarrow$ phase shift
- **resonance contribution $\leftrightarrow$ avoided level crossing**

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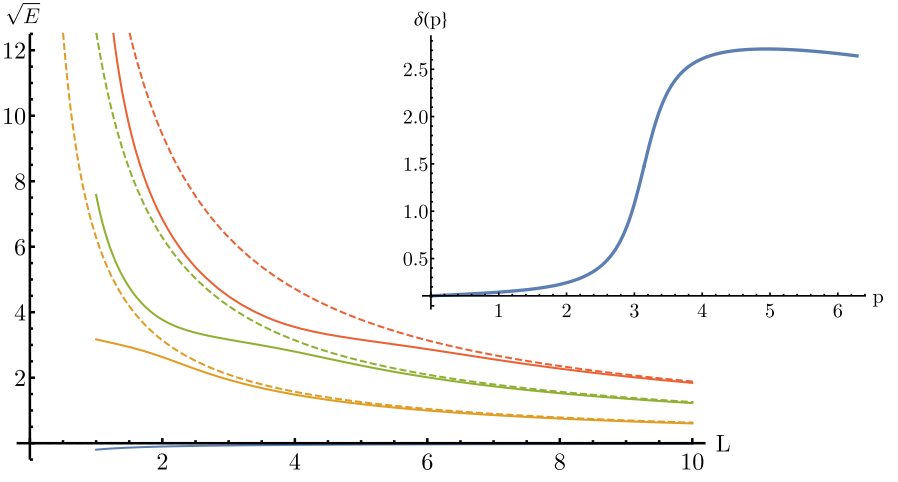

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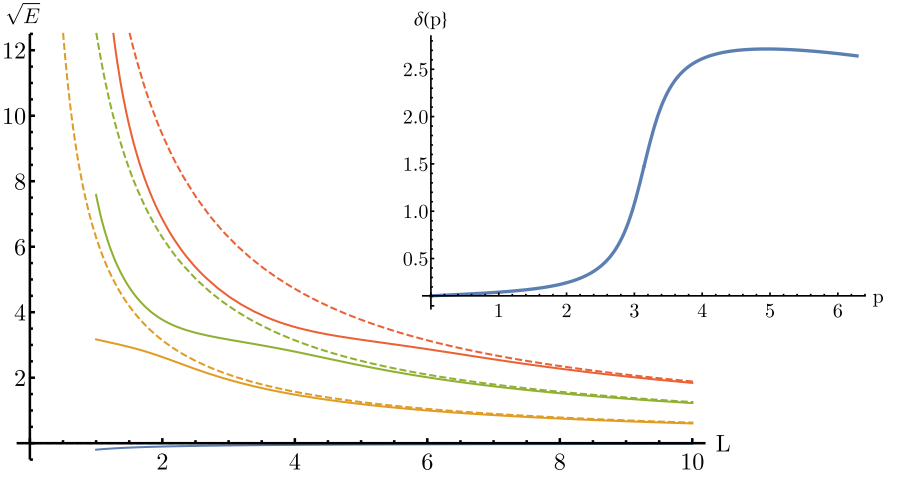

- direct correspondence between phase-shift jump and avoided crossing only for two-body systems, but the spectrum signature **carries over to few-body systems**

Klos, SK et al., PRC **98** 034004 (2018)

Finite-volume eigenvector continuation

Naive setup

- consider states $|\psi_{L_i}\rangle$ at volume L_i
- want to use these to extrapolate via EC to target volume L_*
- to that end, we'd consider Hamiltonian and norm matrices like this:

$$H_{ij} = \langle \psi_{L_i} | H_{L_*} | \psi_{L_j} \rangle$$
$$N_{ij} = \langle \psi_{L_i} | \psi_{L_j} \rangle$$

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However...

All the $|\psi_{L_i}\rangle$ are defined in different Hilbert spaces!

- parametric dependence now not only in the Hamiltonian...
- ...but inherent in the basis
- **need to generalize EC to deal with this scenario**

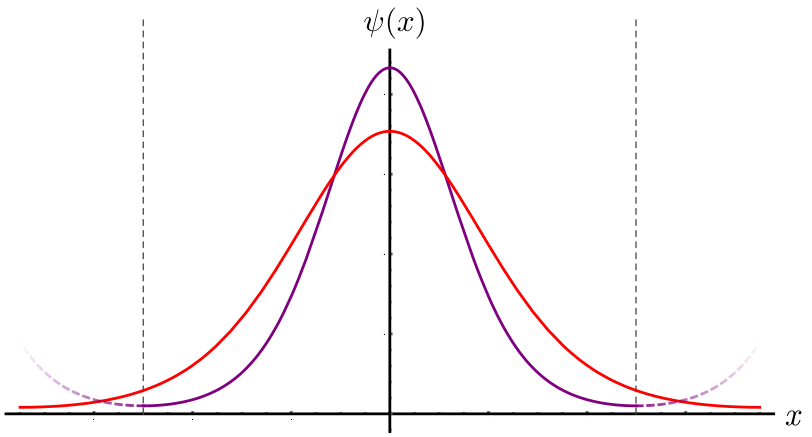
Dilatations

- consider a function f with period L, $f \in \mathcal{H}_L$
- this can be mapped onto a function with period L' by means of a dilatation:

$$(D_{L,L'} f)(x) = \sqrt{\frac{L}{L'}}\, f\left(\frac{L}{L'} x\right)$$

- this provides a bijection between the Hilbert spaces $\mathcal{H}_L$ and $\mathcal{H}'_L$

Example: periodic bound-state wavefunction



Periodic matching

- consider the union of all periodic Hilbert spaces: $\mathcal{H} = \bigcup_{L>0} \mathcal{H}_L$
  - not a Hilbert space with normal pointwise addition
- define a new operation for $f \in \mathcal{H}_L$, $g \in \mathcal{H}_{L'}$, $L' > L$:

$$(f \overset{\max}{+} g)(x) = (D_{L,L'} f)(x) + g(x)$$

- similarly, define inner products between different periodicities:

$$\langle f, g \rangle_{\max} = \langle D_{L,L'} f, g \rangle_{\mathcal{H}_{L'}} = \int_{-L'/2}^{L'/2} (D_{L,L'} f)(x)^* g(x) \, \mathrm{d}x$$

- **together, these make $\mathcal{H}$ a vector space with inner product**

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Truncated periodic bases

- let $S_{L,N}$ be a truncated basis of plane-wave states
- then for $\psi \in S_{L,N}$ and $\psi' \in S_{L',N}$, the $\mathbb{R}^N$ inner product of coefficient vectors is the same as $\langle \cdot, \cdot \rangle_{\max}$

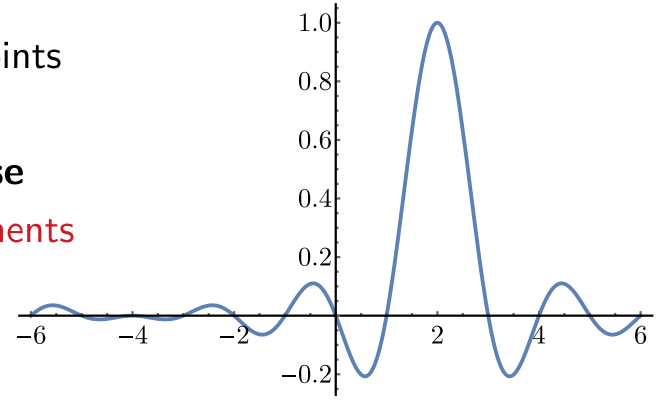
Discrete variable representation

Efficient calculation of several few-body energy levels

- **use a Discrete Variable Representation (DVR)**

  well established in quantum chemistry, suggested for nuclear physics by Bulgac+Forbes, PRC **87** 051301 (2013)

- basis functions localized at grid points
- potential energy matrix diagonal
- **kinetic energy matrix very sparse**
  - precalculate only 1D matrix elements

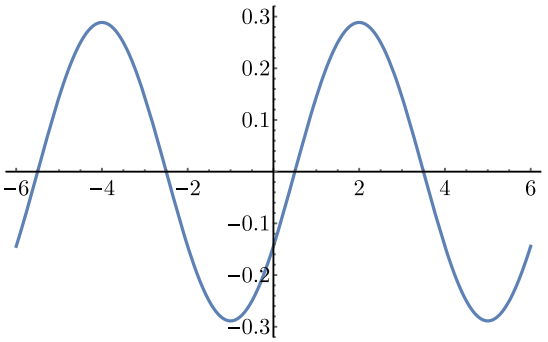


- periodic boundary condistions $\leftrightarrow$ plane waves as starting point
- **efficient implementation for large-scale calculations**
  - handle arbitrary number of particles (and spatial dimensions)
  - numerical framework scales from laptop to HPC clusters — SK et al., PRC **98** 034004 (2018)
  - recent extensions: GPU acceleration, separable interactions — Dietz, SK et al. arXiv:2109.11356

DVR construction

Basic idea

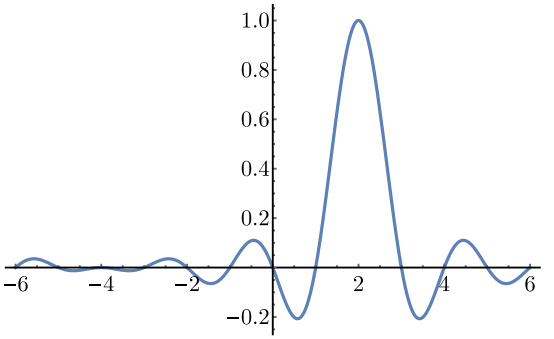
- start with some initial basis; here: plane waves $\phi_i(x) = \dfrac{1}{\sqrt{L}} \exp\left(\mathrm{i}\dfrac{2\pi i}{L} x\right)$
- consider (x_k, w_k) such that $\sum_{k=-N/2}^{N/2-1} w_k\, \phi_i^*(x_k)\phi_j(x_k) = \delta_{ij}$



unitary trans.

$\longrightarrow$

$\mathcal{U}_{ki} = \sqrt{w_k}\phi_i(x_k)$

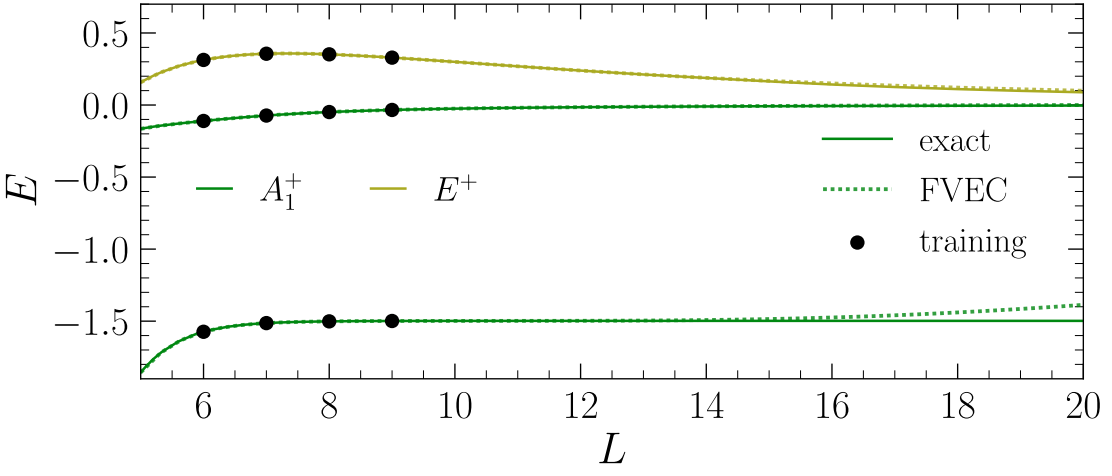


DVR states

- $\psi_k(x)$ localized at x_k, $\psi_k(x_j) = \delta_{kj}/\sqrt{w_k}$
- **note duality:** momentum mode ϕ_i $\leftrightarrow$ spatial mode ψ_k

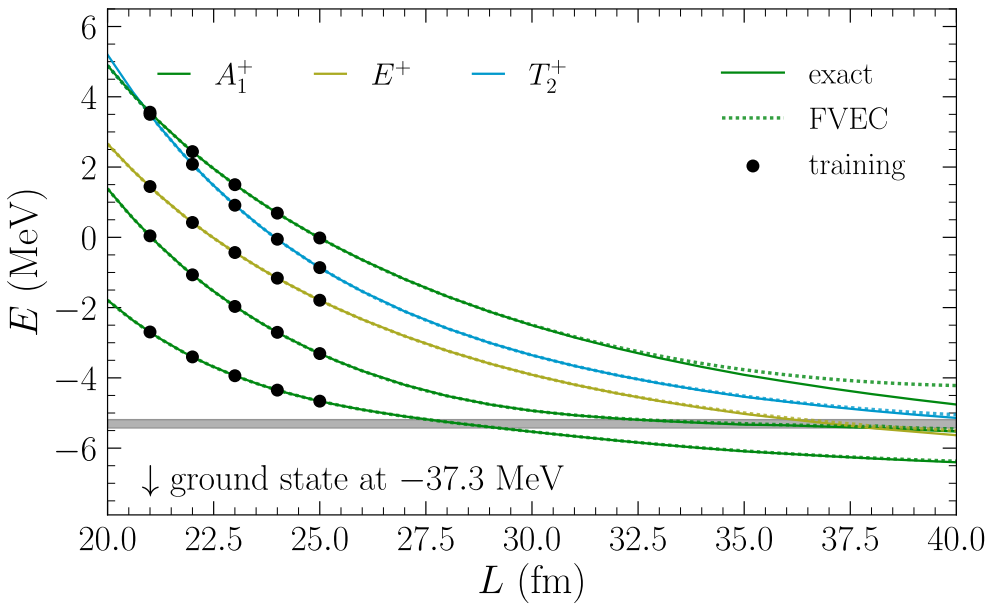
Two-body proof of concept

- consider a simple two-body system as first example
  - attractive Gaussian interaction: $V(r) = V_0 \exp\left(-\left(\frac{r}{R}\right)^2\right)$, $R = 2$, $V_0 = -4$
- **note: cubic finite volume breaks spherical symmetry**
  - angular momentum no longer good quantum number
  - instead: cubic irreducible representations $\Gamma \in A_1, A_2, E, T_1, T_2$
  - to good approximation, S-wave states $\sim A_1^+$ irrep. (positive parity)



Three-boson resonance

- three bosons with mass $m = 939.0$ MeV, potential = sum of two Gaussians
- **three-body resonance at**
  - $-5.31 - i0.12$ MeV (Blandon et al., PRA **75** 042508 (2007))
  - $-5.96 - i0.40$ MeV (Fedorov et al., FB Syst. **33** 153 (2003)) (potential S-wave projected!)



- **avoided crossing well reproduced by FVEC calculation**

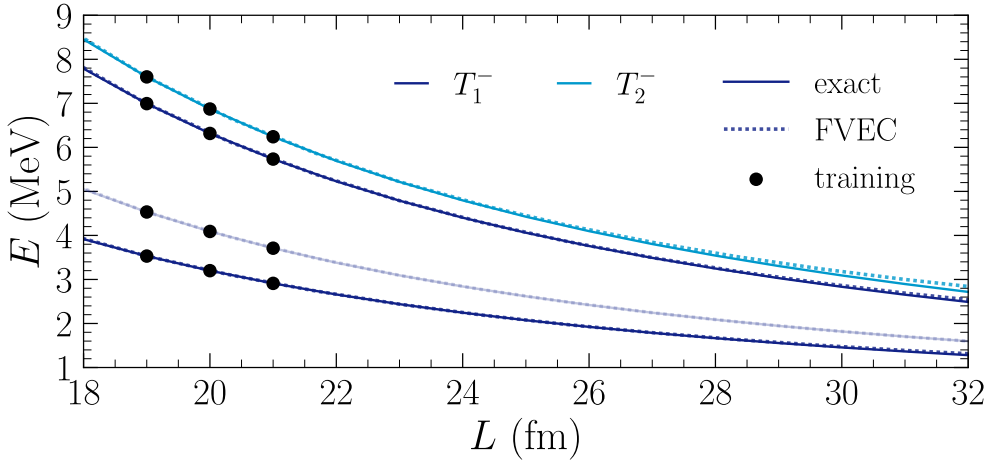
Three neutrons

- now consider three neutrons with Pionless EFT leading-order interaction

$$V(q,q') = C\, g(q) g(q') \quad , \quad g(q) = \exp(-q^{2n}/\Lambda^{2n})$$

- separable super-Gaussian form with $n = 2$ and $\Lambda = 250$ MeV
- efficiently implemented within DVR framework

Dietz, SK et al. arXiv:2109.11356

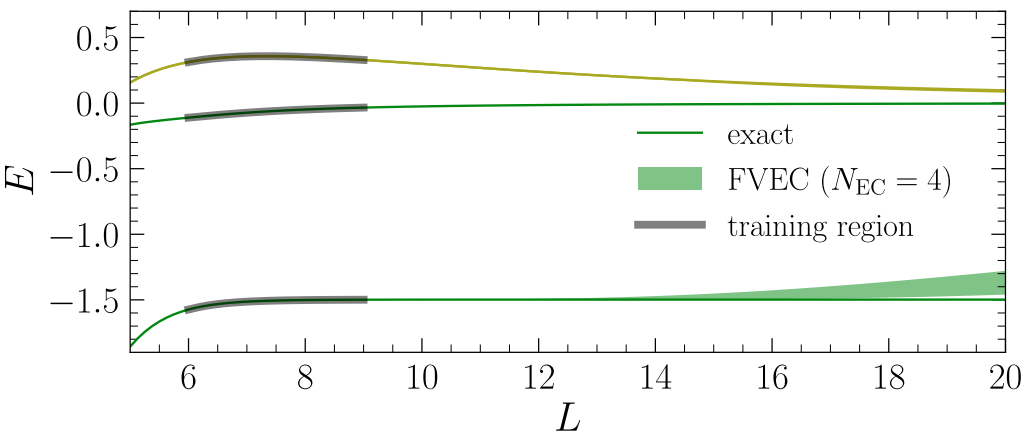


- total number of training data: $3 \times 8 = 24$ (partly covering cubic group multiplets)

Uncertainty quantification

- **FVEC uncertainty depends on choice of training data**
  - domain to choose from (note also: extrapolation vs. interpolation)
  - number N_{EC} of training space (controls dimension of FVEC subspace)
- use this dependence to estimate uncertainty
  - calculate initial pool of training data
  - from that pool, consider combinations with fixed N_{EC}

Application to two-body system



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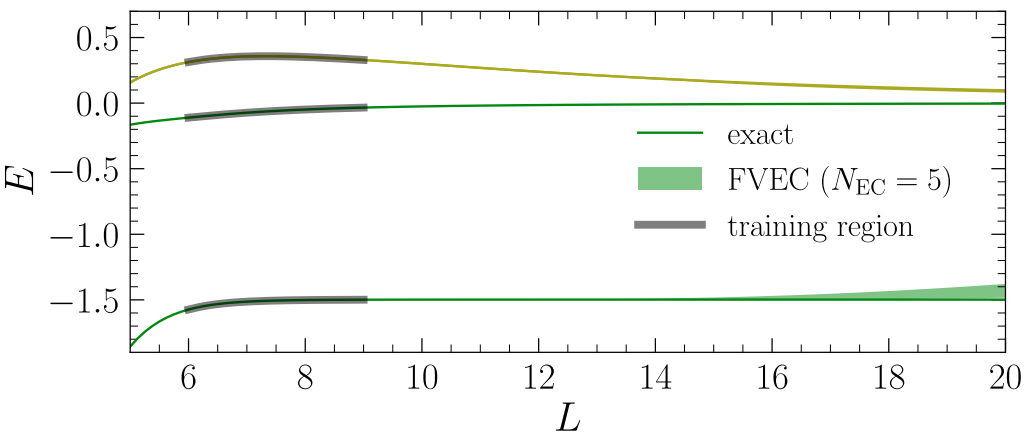

Summary and outlook

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  - possible to undo unitary transformation of potential
  - recover unevolved result without including induced many-body force

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  - can both interpolate and extrapolate from training set
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Other applications and future directions

- **large-scale uncertainty quantification** — Ekström + Hagen, PRL **123** 252501 (2019)
- **scattering calculations** — Furnstahl et al., PLB **809** 135719 (2020)
- **resonances** — Yapa, Fossez, SK, work in progress

Thanks...

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