# Extrapolation and emulation techniques for few-body resonances

**Sebastian König**

**Next-Generation Ab Initio Nuclear**

**ECT*, Trento, July 15, 2025**

Yapa, Fossez, SK, PRC **107** 064316 (2023); PRC **111** 064318 (2025)

NC STATE UNIVERSITY

FRIB Theory Alliance

STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

NSF

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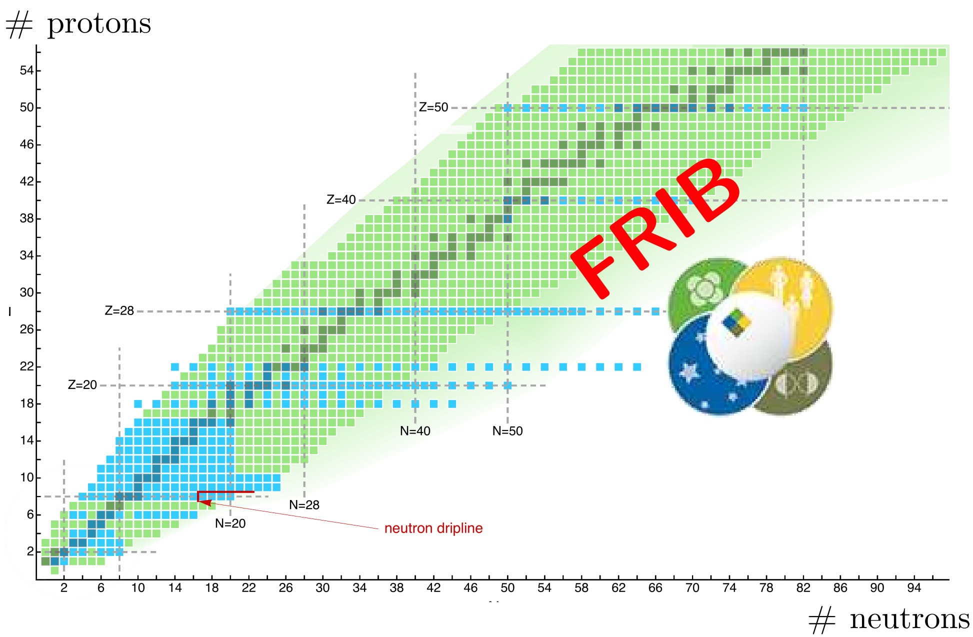
# Motivation




original chart: Hergert et al., Phys. Rep. **621** 165 (2016)

- **rare isotope facilities will discover unknown nuclei near the edge of stability**
  - among those there are likely exotic states
  - halos, clusters ⇝ **few-body resonances**

# Agenda

**Resonances**

**Eigenvector Continuation**

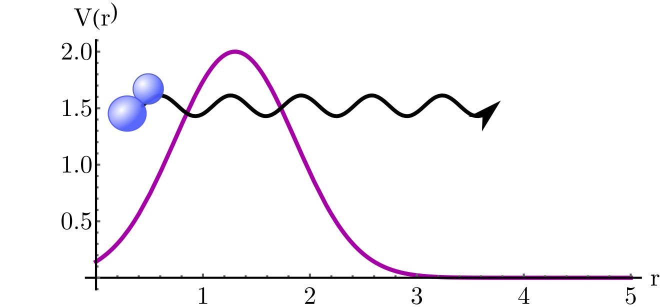
**Complex Scaling Method**

**All above combined**

# Resonances

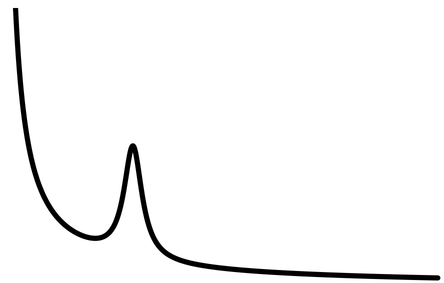
## Intuitive

- **metastable state (finite lifetime)**
- tunneling through potential barrier



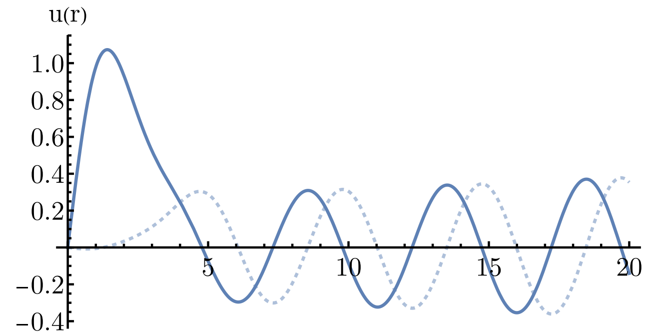

## Experimentally

- **peak in cross section**
- related to sharp jump in scattering phase shift
- $\sigma \sim \dfrac{\Gamma^2}{(E - E_R)^2 + \Gamma^2/4}$



## Formally

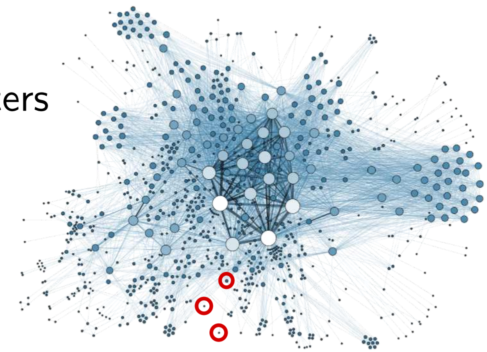
- **S-matrix pole at complex energy**
- wave function similar to bound state...
- ...but not quite normalizable



# 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, broadly applicable**
  - emulators, perturbation theory, ...

Duguet, Ekström, Furnstahl, SK, Lee, RMP **96** 031002 (2024)

- **amazingly simple in practice**
- special case of "reduced basis method" (RBM)

Bonilla et al., PRC **106** 054322 (2022); Melendez et al., JPG **49** 102001 (2022)

# Eigenvector continuation 101

## Scenario

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

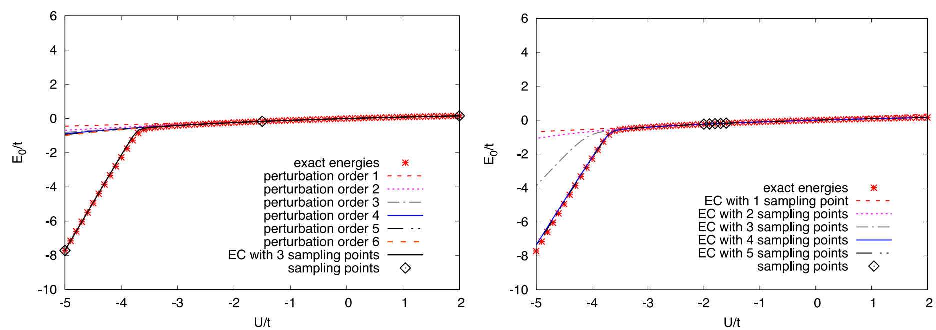
- consider physical state (eigenvector) in a large space
- **parametric dependence of Hamiltonian $H(c)$ traces only small subspace**
- prerequisite: smooth dependence of $H(c)$ on $c$ (or $\vec{c}$)
- enables analytic continuation of $|\psi(c)\rangle$ from $c_{\mathrm{train}}$ to $c_{\mathrm{target}}$

## Procedure

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

## Example

- Hubbard model
- $c = U/t$




- **large number of applications/extensions in recent years!**

Duguet, Ekström, Furnstahl, SK, Lee, RMP **96** 031002 (2024)

# 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, $\mathrm{NNLO_{sat}}$, $\alpha$-$\alpha$ scattering

    Shirokov et al., PLB **644** 33 (2007); Ekström et al., PRC **91** 051301 (2015); Elhatisari et al., PRL **117** 132501 (2016)

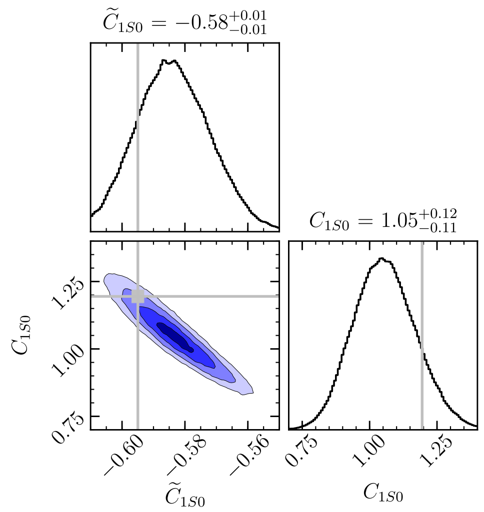
- **fitting needs many calculations with different parameters**

## 2. Propagation of uncertainties

- statistical fitting gives posteriors for LECs
- LEC uncertainties **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!



# Hamiltonian parameter spaces

- **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 $\mathcal{O}(Q^3)$ potential: 14 two-body LECs + 2 three-body LECs

## EC emulation

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

- **EC can accomodate multi-dimensional parameter spaces** $(c_i \to \vec{c}_i)$
  - $|\psi_i\rangle = |\psi(\vec{c}_i)\rangle$ for $i = 1, \cdot\cdot N_{\mathrm{EC}}$
  - $H_{ij} = \langle\psi_i|H(\vec{c}_{\mathrm{target}})|\psi_j\rangle$, $N_{ij} = \langle\psi_i|\psi_j\rangle$
- 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
- generally highly efficient and accurate

# Many more EC applications, e.g.:

- **Many-body perturbation theory** Demol, SK, et al., PRC **101** 041302(R) (2020)
- **Two- and three-body scattering**
  Melendez et al. PLB (2021); Drischler et al. PLB (2021); Zhang + Furnstahl (2022)
- **Volume extrapolation** Yapa + SK, PRC **106** 014309 (2022)
- **Shell-model emulators** Yoshida+Shimizu, PTEP **2022** 053D02 (2022)
- **...**

Duguet, Ekström, Furnstahl, SK, Lee, RMP **96** 031002 (2024)

# Now back to resonances...

# Formal look at resonances

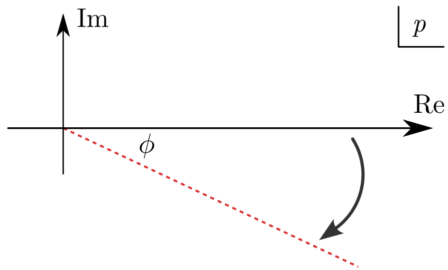
- in stationary scattering theory, resonances are described as generalized eigenstates
  - S-matrix poles at comples energies $E = E_R - \mathrm{i}\Gamma/2$ (lifetime $\sim 1/\Gamma$)
  - wave functions are not normalizable (exponentially growing in $r$-space)

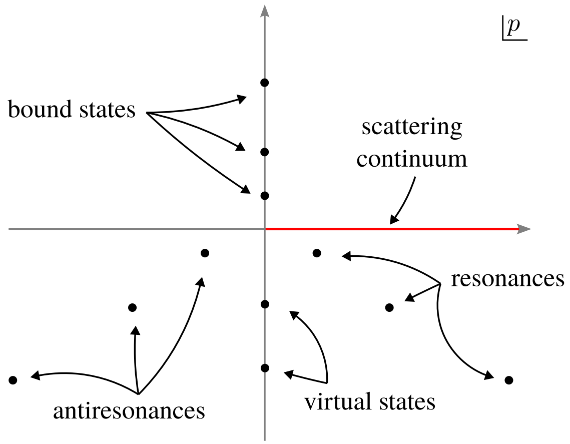
## Complex scaling method

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

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

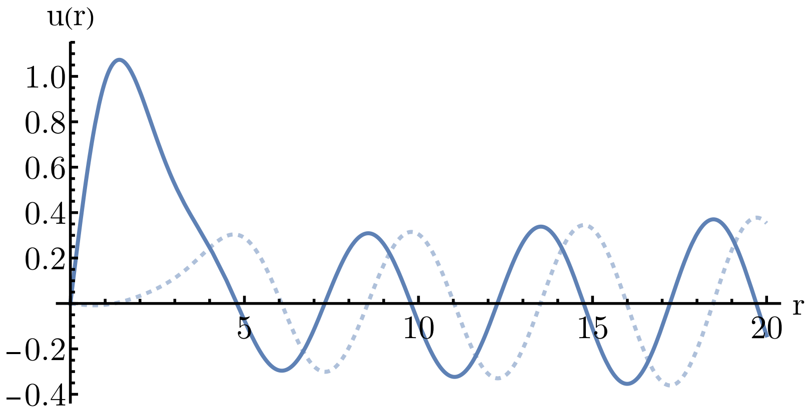
$\rightsquigarrow$ **"reveals" the resonance regime**

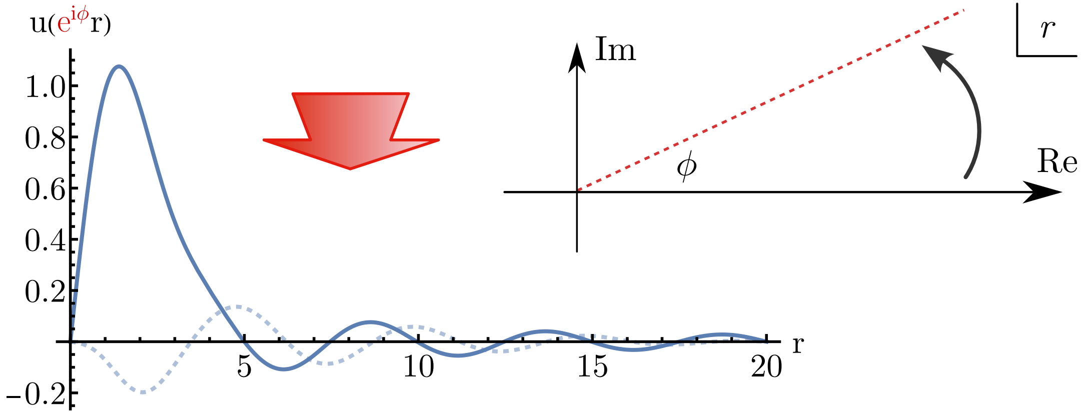


# Complex-scaled resonance wave functions

- complex scaling suppresses the exponentially growing tail of the wave function




calculations by Nuwan Yapa

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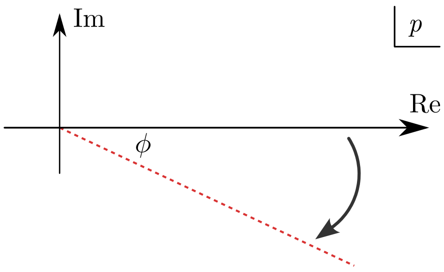


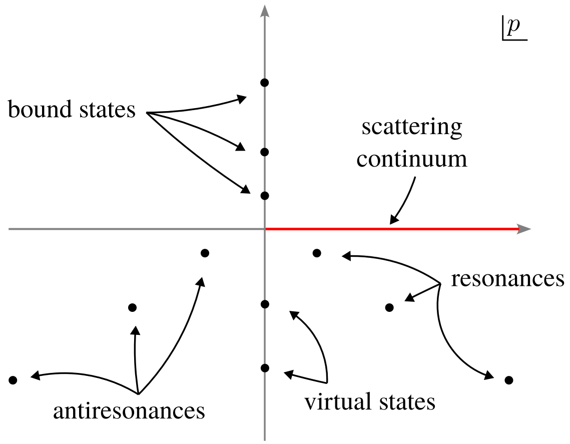

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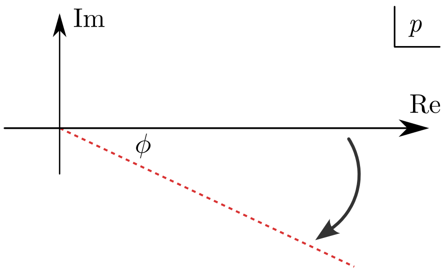


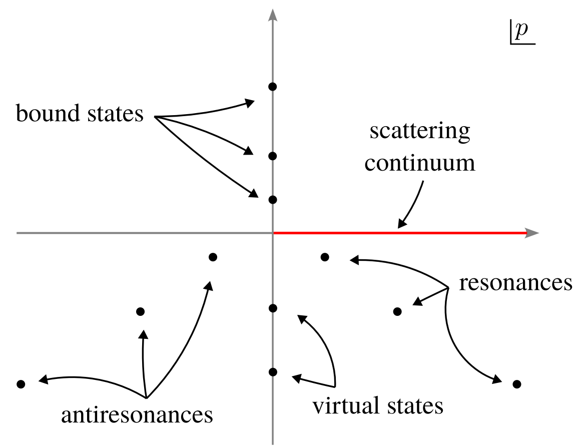


## Notes

- this particular method is also called "uniform" complex scaling
- essentially, one uses a basis of complex momentum modes

# EC for resonances

## Why?

- **LEC fitting and/or observable predictions may include unstable states**
  - accurate and efficient resonance emulators are needed for this
  - especially in the few-body sector, where calculations rapidly become expensive
- **but there is also an important technical reason:**
  - basis expansion methods are typically good for targeting extremal eigenvalues
  - Lanczos/Arnoldi iteration and related techniques
  - complex physical resonance eigenvalues can be difficult to identify
  - bound states, on the other hand, are easy to find
  - tracking a state from being bound to becoming unbound can help!

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## How?

- combine EC with complex scaling, work with complex eigenvalues
- **formalism needs to be developed/adapted for this task**

  Yapa, Fossez, SK, PRC **107** 064316 (2023); PRC **111** 064318 (2025)
- related work discusses other extension of EC to non-Hermitian systems

  see e.g. Zhang, 2408.03309 [nucl-th], 2411.06712 [nucl-th]; Cheng et al., 2411.15492 [nucl-th]

# One important detail

- **under complex scaling, the Hamiltonian becomes non-Hermitian**

$$r \rightarrow \mathrm{e}^{\mathrm{i}\phi} r \quad , \quad p \rightarrow \mathrm{e}^{-\mathrm{i}\phi} p \quad \rightsquigarrow H \neq H^*$$

  - instead, it becomes complex symmetric
  - as such, it can have complex eigenvalues ✔

- **this changes the inner product between states**

$$\langle \phi | \psi \rangle = \int \mathrm{d}r \, \phi(r) \psi(r)$$

  - no complex conjugation for bra-side states
  - this is called the "c-product"
  - physical states with different energies are orthogonal w.r.t. c-product

Moiseyev, Certain, Weinhold, Mol. Phys. **36** 1613 (1978)

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## Note

- bound-state energies remain invariant under complex scaling
- but the c-product is still needed in the non-Hermitian framework

# Resonance-to-resonance continuation

- **for resonance to-resonance continuation, EC works directly...**
- **...if one simply uses the c-product for all matrix elements**

Yapa, Fossez, SK, PRC **107** 064316 (2023)

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

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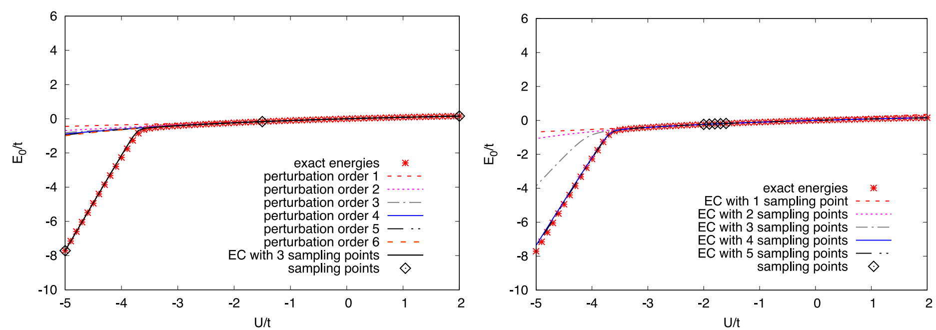


- **large number of applications/extensions in recent years!**

Duguet, Ekström, Furnstahl, SK, Lee, RMP **96** 031002 (2024)

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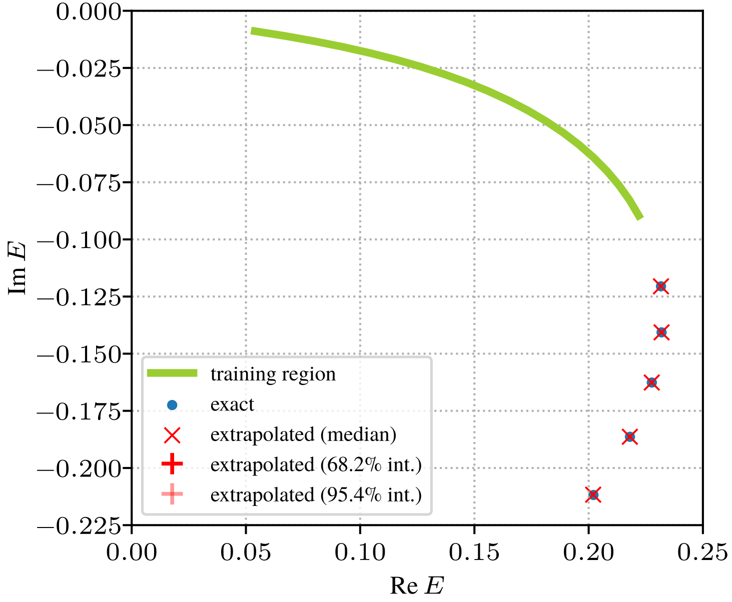
Yapa, Fossez, SK, PRC **107** 064316 (2023)




- momentum-space two-body calculation

$$V(c;r) = c\left[-5\mathrm{e}^{-r^2/3} + 2\mathrm{e}^{-r^2/10}\right]$$

- sampled points within training regime
- repeated EC evaluation with 5 points
- benchmark against exact result
- **excellent agreement**

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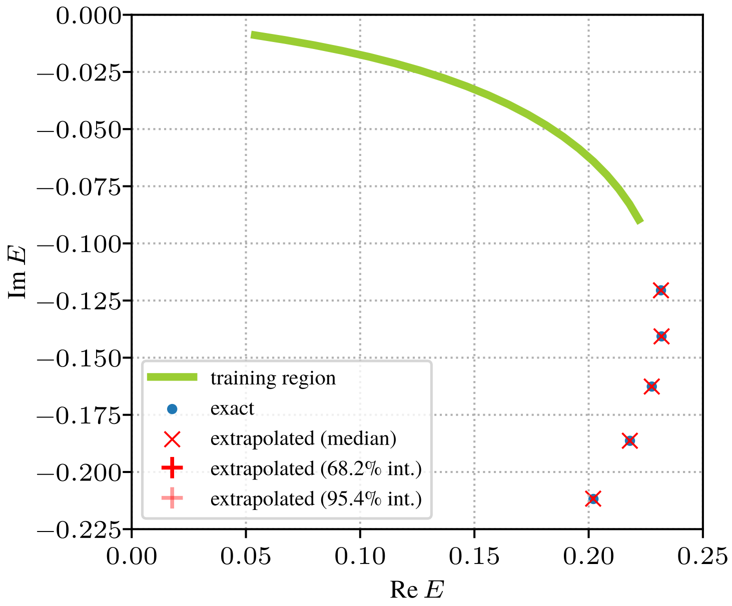
Yapa, Fossez, SK, PRC **107** 064316 (2023)

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- sampled points within training regime
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- benchmark against exact result
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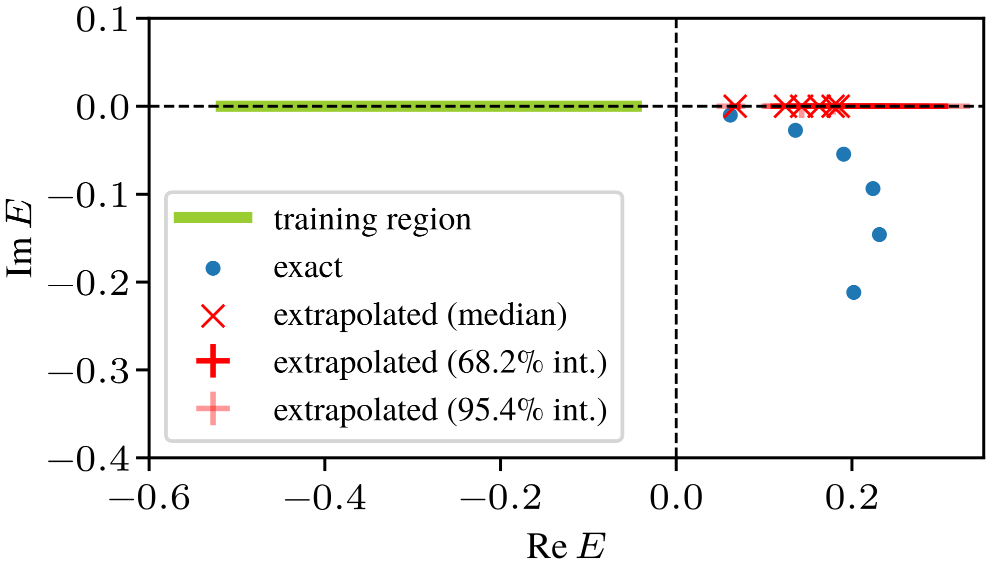
- **Note:** in the plot, we only show benchmarks for EC extrapolation
  - that is because interpolation is generally much easier
  - for resonance emulators, both are relevant and needed

# Bound-state-to-resonance continuation

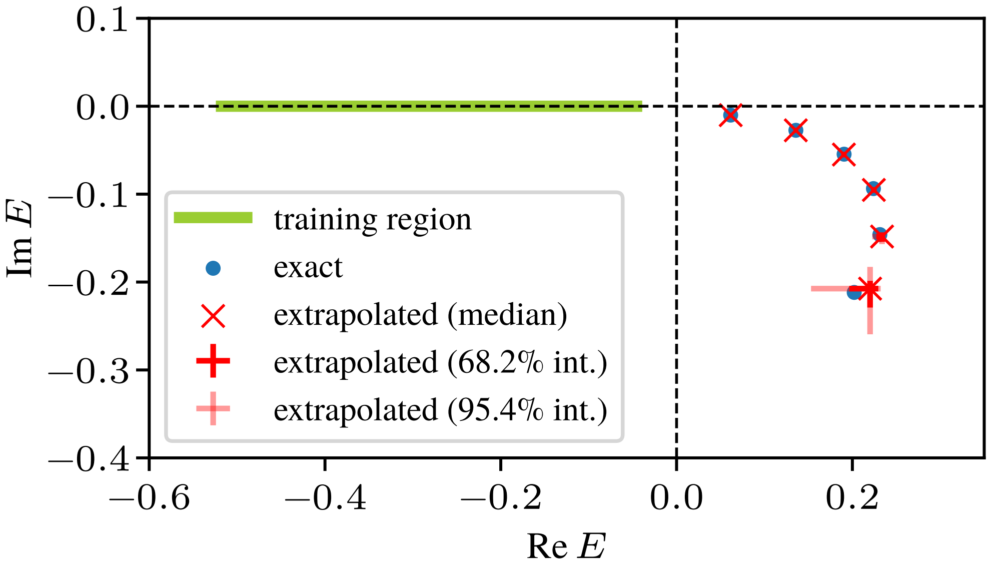
- **bound-state-to-resonance extrapolation fails with naive approach...**




- it can be shown that for bound states, the EC Hamiltonian is real symmetric
  - this is a consequence of using the c-product for complex-scaled bound states
  - as such, it can have only real eigenvalues

# Bound-state-to-resonance continuation

- **however, there is a way to make this work!**




- we introduced **complex-augmented eigenvector continuation (CA-EC)**
  - in addition to the training wave functions, include also their complex conjugates
  - this provides the key information to describe the long-distance asymptotics
  - doubles EC basis size at (almost) zero cost

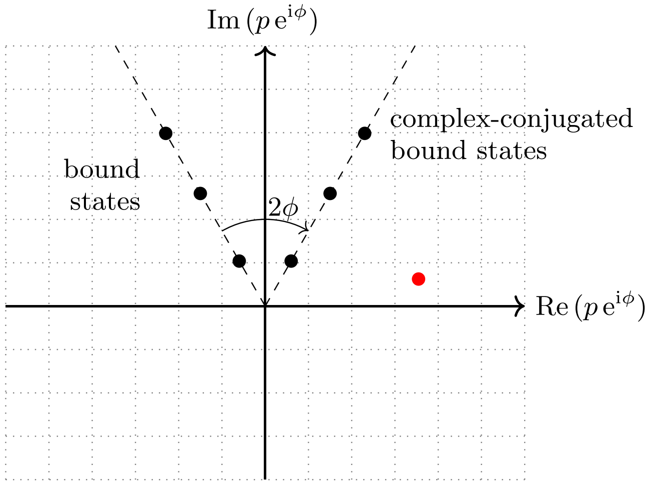
Yapa, Fossez, SK, PRC **107** 064316 (2023)

# Why does this work?

# Complex-augmented EC

## Intuitive explanation

- bound-state energies CS-invariant
- but asymptotic wave numbers change
- complex conjugation moves them into the right quadrant for describing resonances




## Formal explanation

- consider the Schrödinger equation for the complex-conjugated bound state
- evalulate it at large distances, where the potential becomes negligible:

$$-\mathrm{e}^{2\mathrm{i}\phi}\,\frac{\nabla^2}{2\mu}\psi(\mathbf{r}) = E\,\psi(\mathbf{r}) \quad \text{for} \quad |\mathbf{r}| \to \infty$$

- multiplication with $\mathrm{e}^{-4\mathrm{i}\phi}$ yields $H_\phi\psi^*(\mathbf{r}) = \mathrm{e}^{-4\mathrm{i}\phi}E\,\psi^*(\mathbf{r})$

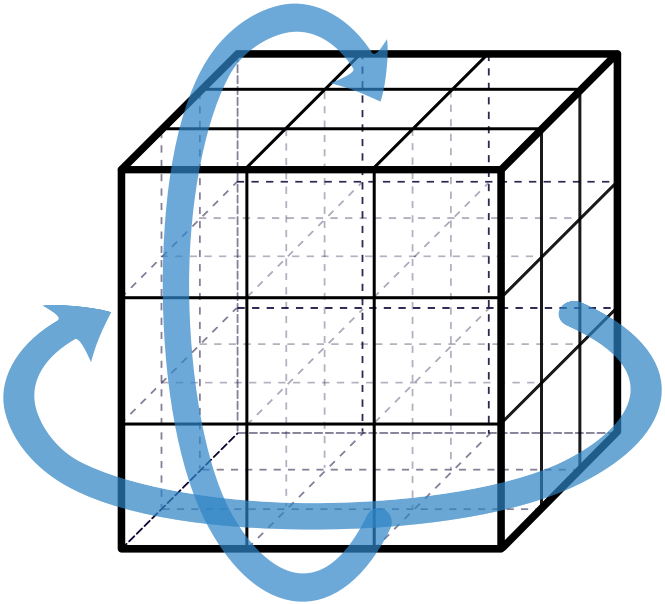
Yapa, SK, Fossez, PRC **111** 064318 (2025)

# What about more than two particles?

**Benchmark different few-/many-body methods**

# Complex scaling in finite volume

**Consider a cubic peridioc boundary condition:**



- useful to directly extract observables from volume dependence of energy levels
  - asymptotic normalization coefficients, resonance positions, radii
    ..., Yu, SK, Lee, PRL **131** 212502 (2023); Klos, SK el al., PRC **98** 034004 (2018); Taurence + SK, PRC **109** 054315 (2024)
- **but also as a generic and powerful few-body technique**

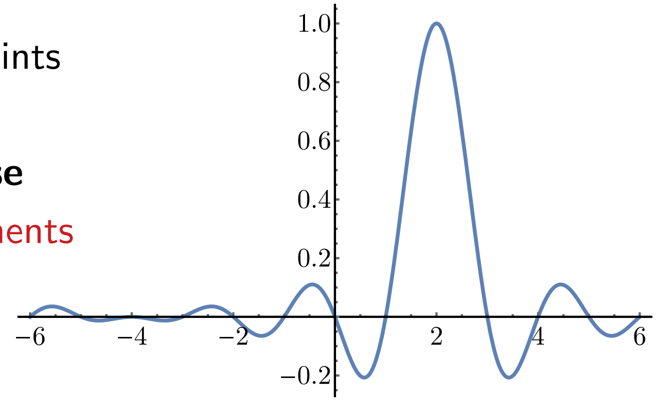
# Discrete variable representation

## Efficient calculation of 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

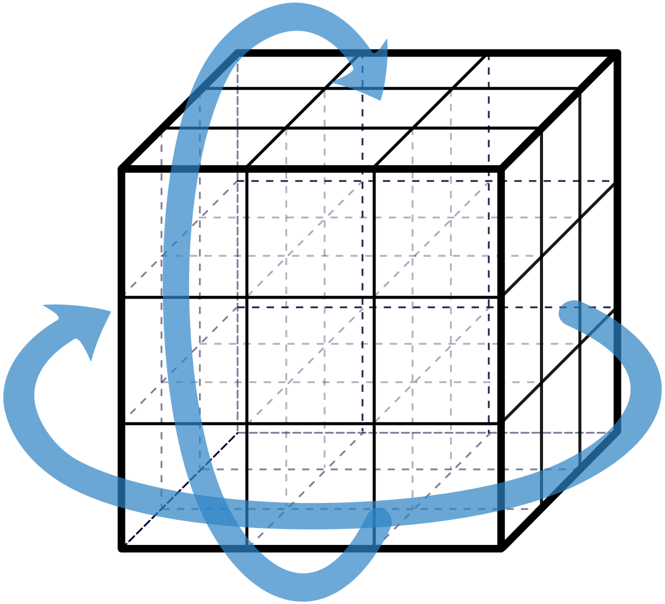



- periodic boundary condistions ↔ plane waves as starting point
- **efficient implementation for large-scale calculations**
  - handle arbitrary number of particles (and spatial dimensions)
  - numerical framework scales from laptop to HPC clusters Klos, SK et al., PRC **98** 034004 (2018)
  - recent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

Dietz, SK et al., PRC **105** 064002 (2022); SK, JP Conf. Ser. **2453** 012025 (2023)

# Complex scaling in finite volume

**Consider a cubic peridioc boundary condition:**



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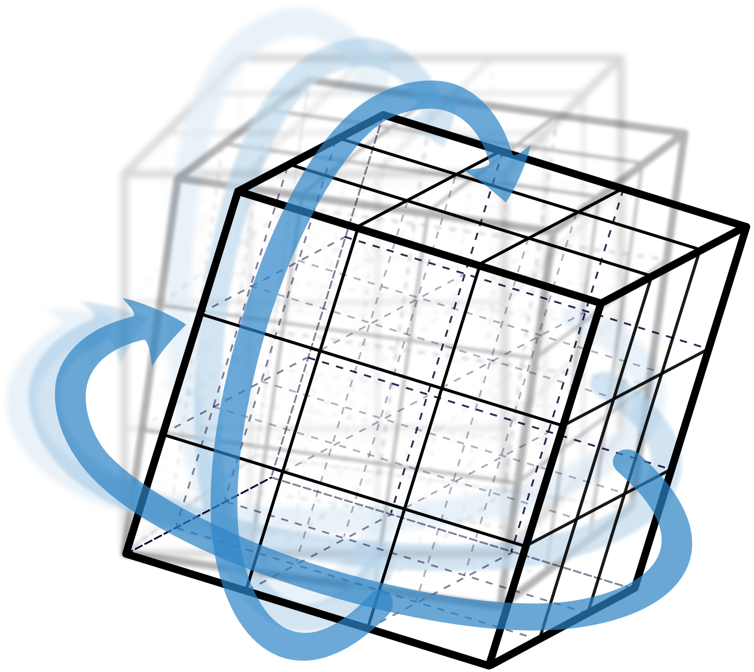


**Now imagine it in terms of complex-scaled coordinates!**

# Complex scaling in finite volume

## Key idea

Yu, Yapa, SK, PRC **109** 014316 (2023)

- **put system into a box, apply peridioc boundary condition along rotated axes**

## Volume dependence

- resonances, like bound states, correspond to isolated S-matrix poles
- complex scaling renders their wave functions normalizable
- we can adapt bound-state techniques to derive their volume dependence

$$\Delta E(L) = \frac{3\gamma_\infty^2}{\mu\zeta L}\left[\exp(\mathrm{i}\zeta p_\infty L) + \sqrt{2}\exp(\mathrm{i}\sqrt{2}\zeta p_\infty L) + \frac{4\exp(\mathrm{i}\zeta\sqrt{3}p_\infty L)}{3\sqrt{3}L}\right] + \mathcal{O}\left(\mathrm{e}^{\mathrm{i}2\zeta p_\infty L}\right)$$

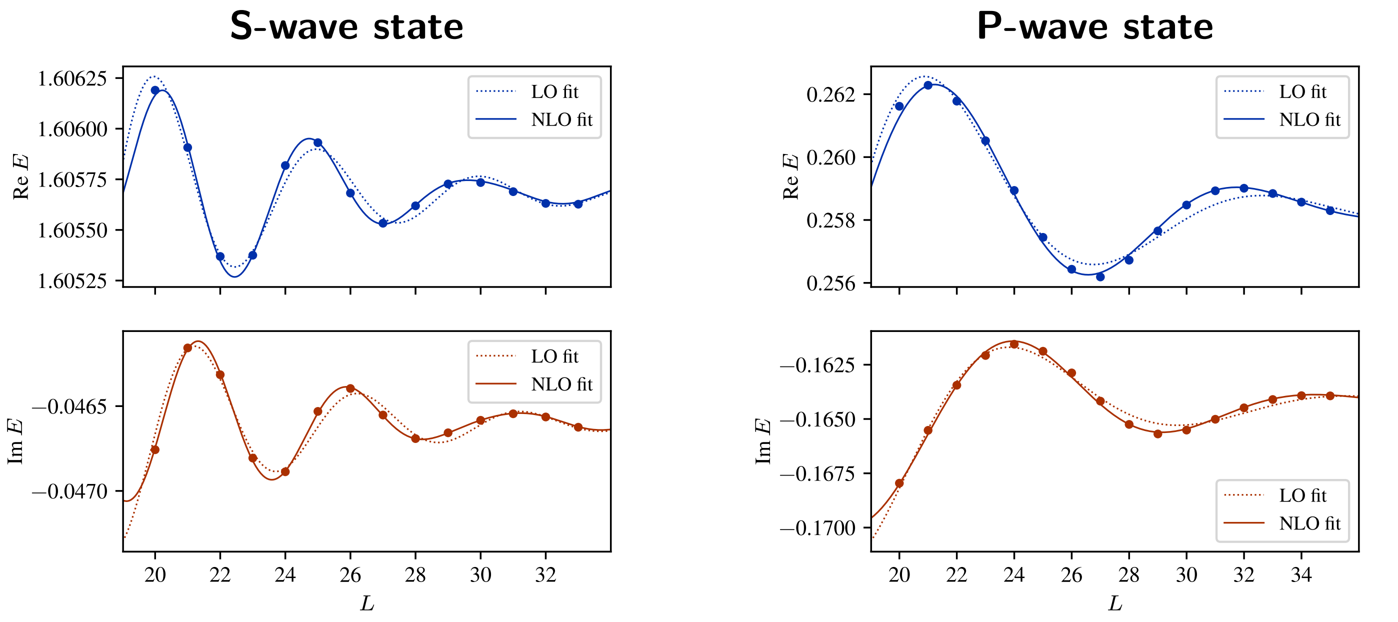
- in this equation $\zeta = \mathrm{e}^{\mathrm{i}\phi}$, $p_\infty = \sqrt{2\mu E(\infty)}$
- explicit form for leading term (LO) and subleading corrections (NLO)
- **note:** dependence on volume $L$ and complex-scaling angle $\phi$

## Numerical implementation

- DVR method can be adapted to this scenario (scaling of $x, y, z \rightsquigarrow$ scaling of $r$)

# Resonance examples

- two-body calculations are in excellent agreement with derived volume dependence
  - S-wave resonance generated via explicit barrier
  - P-wave resonance from purely attractive potential

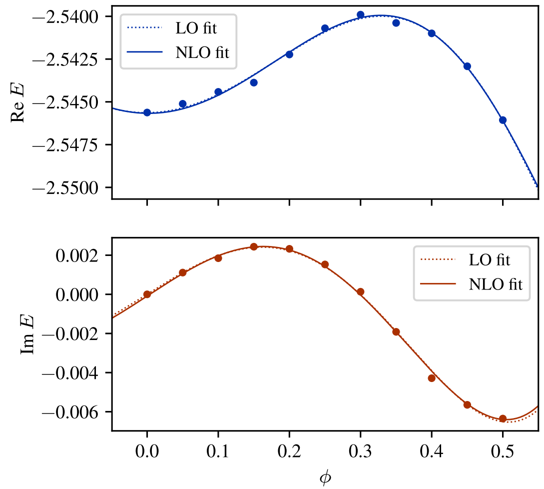



- **fitting the $L$ dependence yields physical resonance position and lifetime!**

# More applications

## Single-volume bound-state fitting

- bound-state energies normally remain real under complex scaling (strictly true in infinite volume)
- the finite-volume, however, induces a non-zero imaginary part
- $\mathrm{Re}\, E$ and $\mathrm{Im}\, E$ oscillate as a function of $L$
  - **and also as a function of $\phi$**
- possible to fit $\phi$ dependence at fixed volume!



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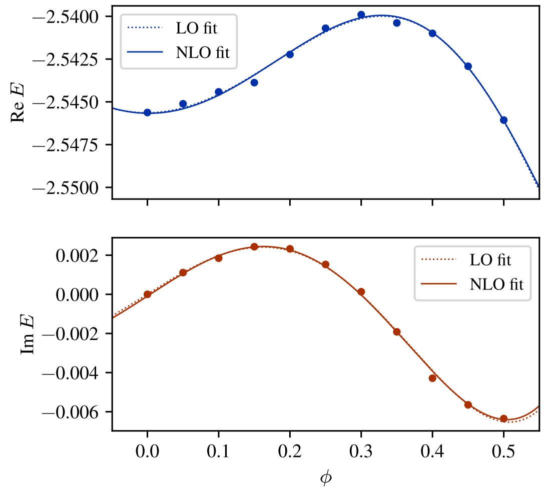
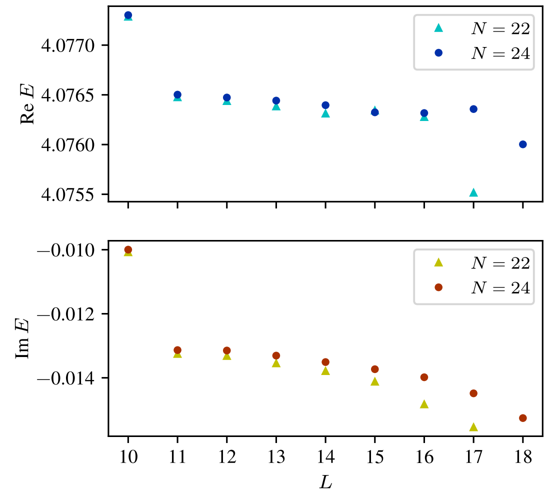
  - **and also as a function of $\phi$**
- possible to fit $\phi$ dependence at fixed volume!




## Three-body resonance

- the exact volume dependence is only known for two-body system
- the complex scaled FV-DVR can however be used to study more particles
- three-boson example in good agreement with previous avoided-crossings analysis

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

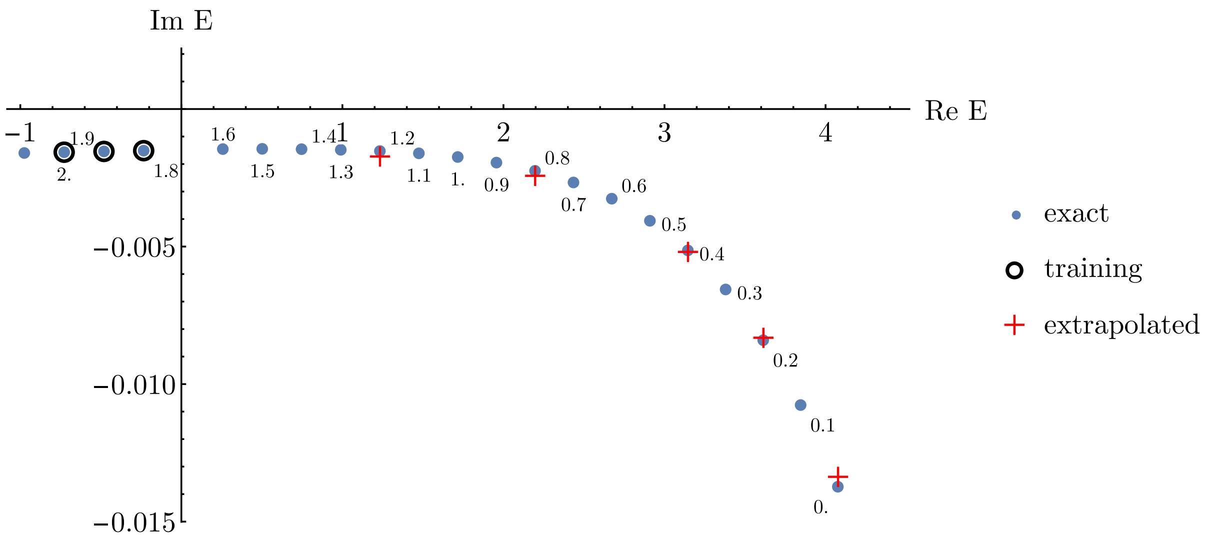


# Three-boson resonance trajectory

- take potential from before that generates a (genuine) three-body resonance
  - established via avoided level crossings (purely real spectrum)
- add attractive two-body potential to bind system
- **use eigenvector continuation (via complex scaling in FV) to extrapolate**

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

$$V(r) = 2\exp\left[-\left(\frac{r-3}{1.5}\right)\right] + V_0 \exp\left(-(r/3)^2\right)$$

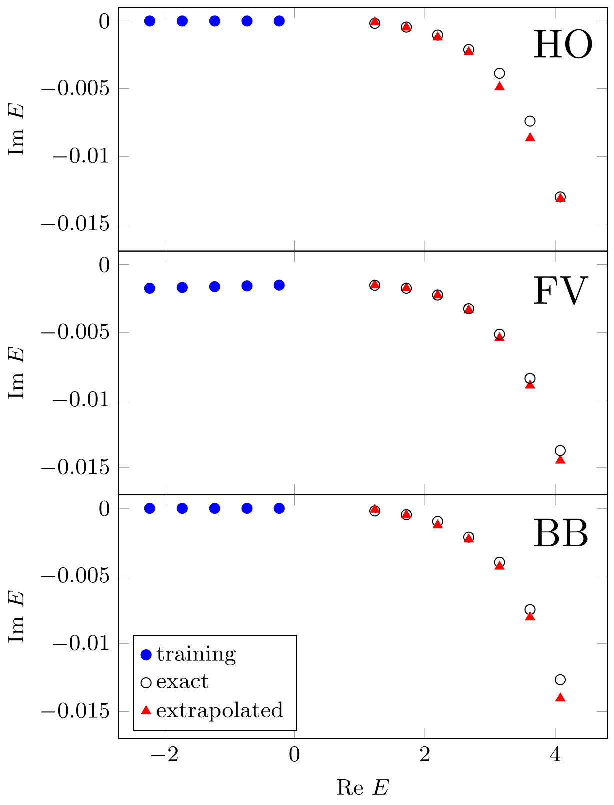


# Resonance EC for few/many-body systems

**CA-EC can be implemented with different numerical methods:**

Yapa, SK, Fossez, PRC **111** 064318 (2025)

- Finite-Volume (FV) DVR
  - just discussed
- Harmonic Oscillator (HO) basis (complex freq.)
  - equivalent to complex scaling
- Berggren Basis (BB)
  - deformed contour plus selection of poles
- Gamow Shell Model
  - path towards many-body applications




## Comparison / Benchmark

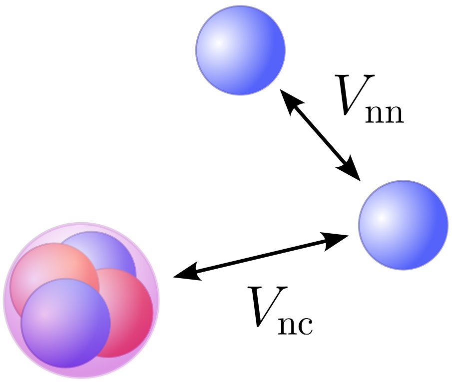
- three-boson system with...
  - HO basis
  - FV-DVR calculation
  - Berggren Basis

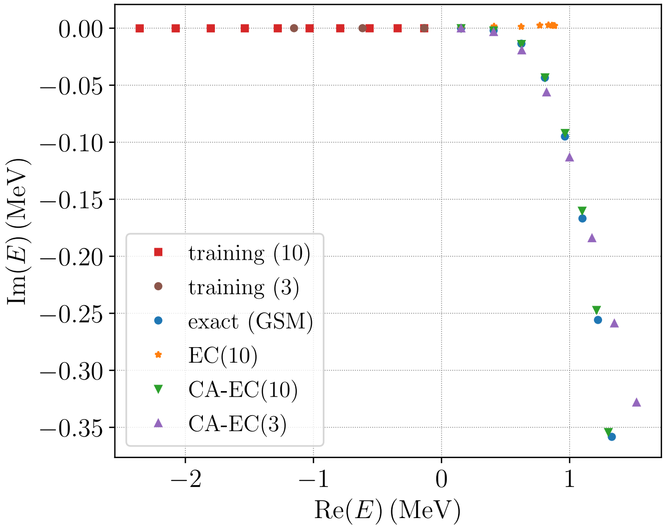
⇝ **excellent agreement overall!**

# Realistic physics application

- consider Gamow Shell Model (GSM) for $^6$He system
  - $^4$He core plus two neutrons
  - Woods-Saxon potential for core-neutron interaction, fit to $^4$He-$n$ phase shifts
  - contact interaction between neutrons
- **reduce strength of $nn$ interaction to make system unbound**

Fossez et al., PRC **98** 061302 (2018)




**CA-EC works nicely also for this system!**

Yapa, SK, Fossez, PRC **111** 064318 (2025)

# Conclusion

## Summary

- complex scaling method can be combined with eigenvector continuation
- possible to construct emulators for resonance states
- resonance-to-resonance extrapolation is straightforward
- conjugate-augmented EC enables bound-state-to-resonance extrapolation
- method initially developed for two-body resonances
- extension to three-body resonances recently established
- method works independent of particular numerical framework
- GSM application paves way towards extrapolating many-body resonances

## Outlook

- inclusion of Coulomb force important to treat charged-particles resonances
- application to recently discoverd exotic resonances, such as $^{9}$N
- consider possible extensions to handle virtual ("anti-bound") states

# Thanks...

## ...to my students and collaborators...

- N. Yapa (NCSU → FSU); K. Fossez (FSU); H. Yu (NCSU → Tsukuba)
- A. Schwenk, H.-W. Hammer, K. Hebeler (TU Darmstadt); P. Klos, J. Lynn
- D. Lee (FRIB/MSU), R. Furnstahl (OSU)
- A. Ekström (Chalmers U.), T. Duguet (CEA Saclay)

## ...for support, funding, and computing time...

FRIB Theory Alliance U.S. DEPARTMENT OF ENERGY Office of Science NSF

- Jülich Supercomputing Center
- NCSU High-Performance Computing Services

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## ...and to you, for your attention!