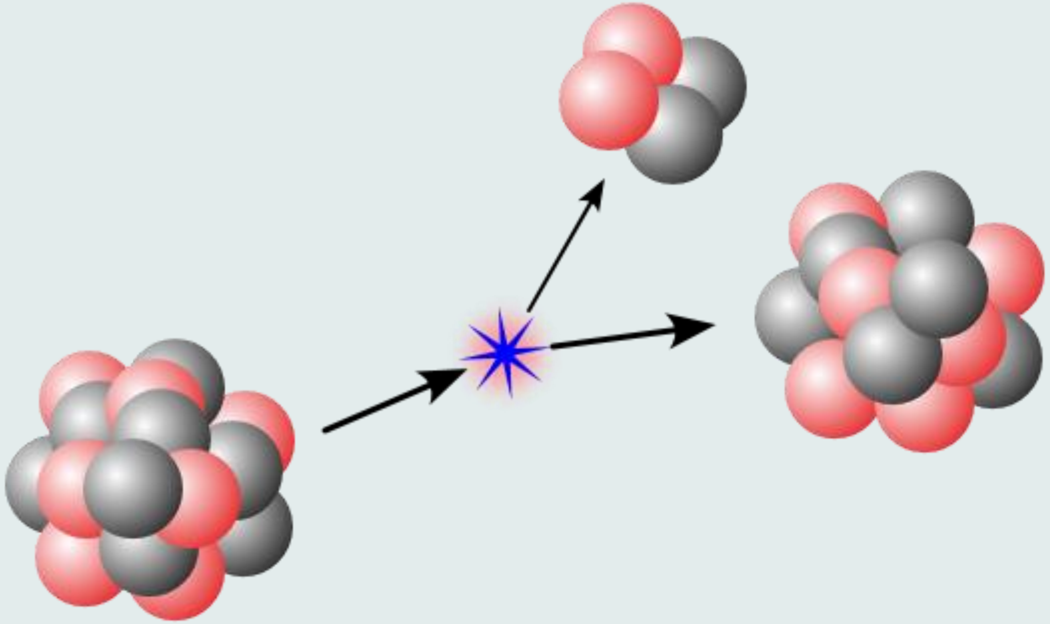
Reduced basis methods (RBMs) for few-body resonances in nuclei



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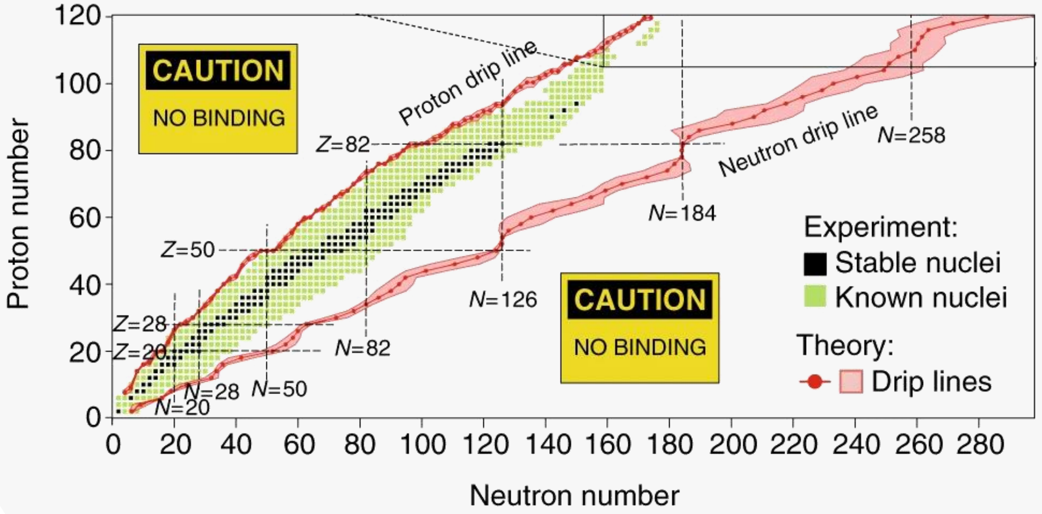
Overview

- Introduction to nuclear resonances / Gamow states
- Non-Hermitian methods
  - Complex scaling
  - Berggren basis
- Eigenvector continuation (EC) as a reduced basis method
  - Resonance EC (narrow–to–broad)
  - Extrapolating across threshold (bound–to–resonance)
- Results for ^{6}He and ^{6}Be

Motivation



Nazarewicz, W. The limits of nuclear mass and charge. *Nature Phys* **14**, 537–541 (2018).

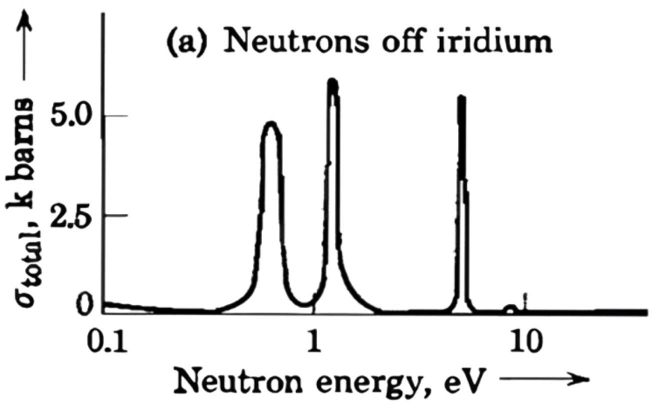
- Studying drip lines (edges of stability)
- Exotic decay modes / cluster radioactivity

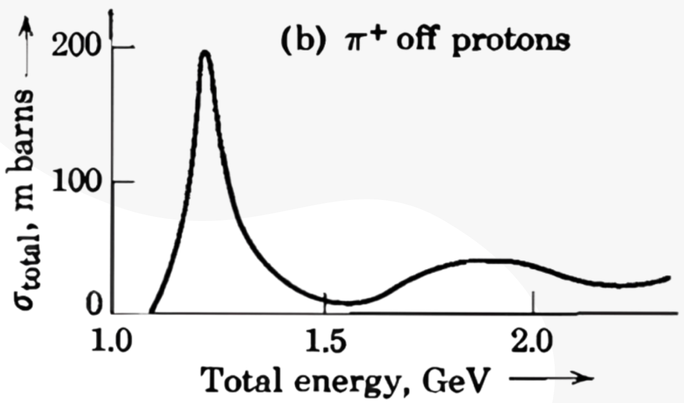
  e.g.: $^{223}\mathrm{Ra} \rightarrow {}^{14}\mathrm{C} + {}^{209}\mathrm{Pb}$
- Broad resonances

  e.g.: $^{7}\mathrm{B}$, $^{8}\mathrm{C}$, $^{9}\mathrm{N}$ or $4\mathrm{n}$

What are resonances?

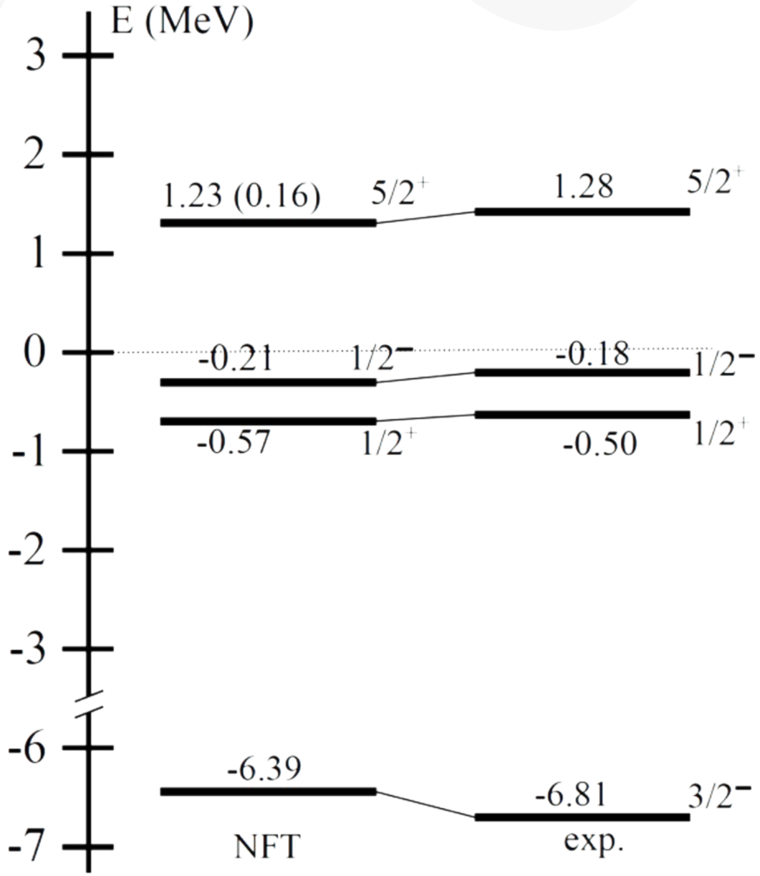
Resonances are peaks of the scattering cross section observed in experiments:

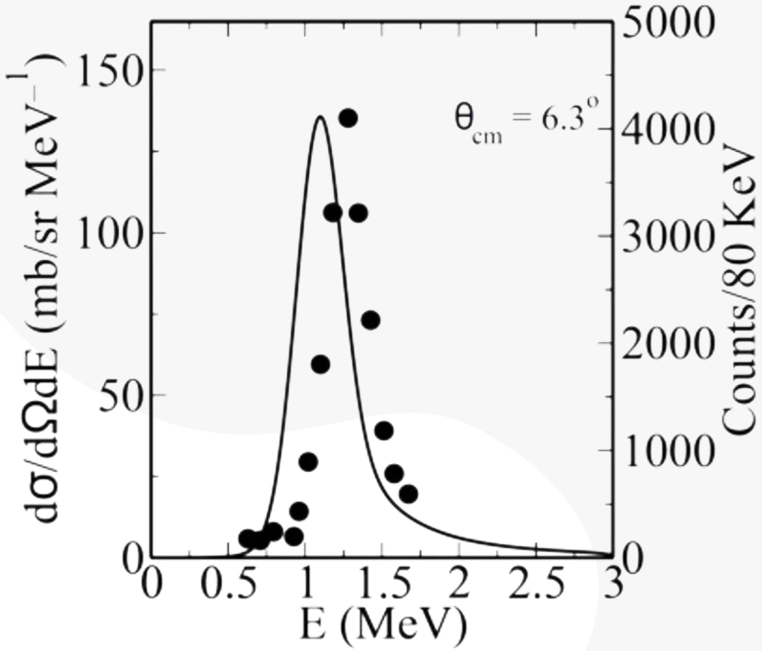




J. R. Taylor, *Scattering Theory: The Quantum Theory of Nonrelativistic Collisions* (Dover Publications, Newburyport, 2012).

What are resonances?





F. Barranco, G. Potel, R. A. Broglia, and E. Vigezzi, *Structure and Reactions of ^{11}Be: Many-Body Basis for Single-Neutron Halo*, Phys. Rev. Lett. **119**, 082501 (2017).

Gamow states

Solutions of the time-independent Schrödinger equation

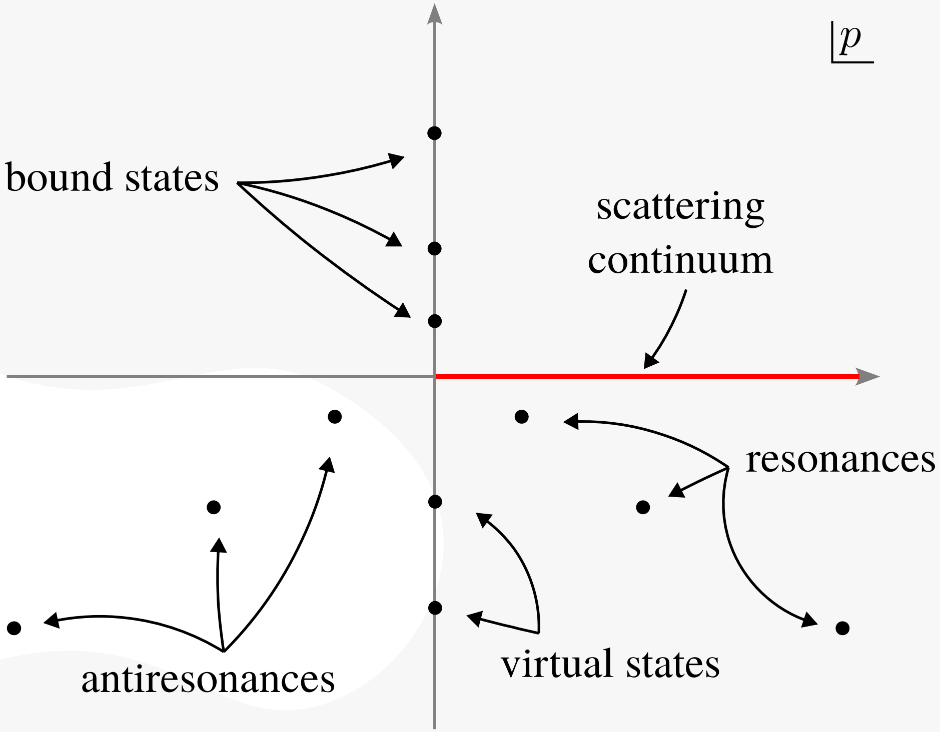
$$\left[\frac{1}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{2\mu r^2} - V(r) + E\right] u_{l,p}(r) = 0$$

with complex eigenvalues

$$E = E_R - \frac{\mathrm{i}\Gamma}{2}$$

$\mathrm{Im}(E) < 0 \Rightarrow$ state decays with time evolution $e^{-iHt/\hbar}$ while the width Γ determines the half-life via $T_{1/2} = \frac{\ln 2}{\Gamma}$.

$$p = \sqrt{2\mu E}$$

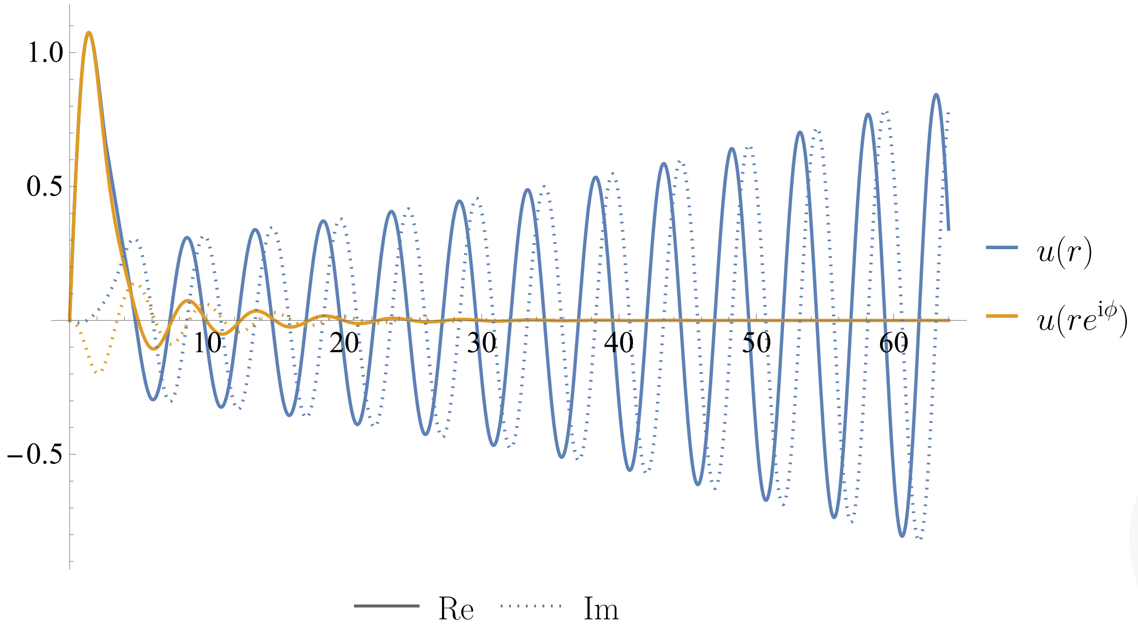


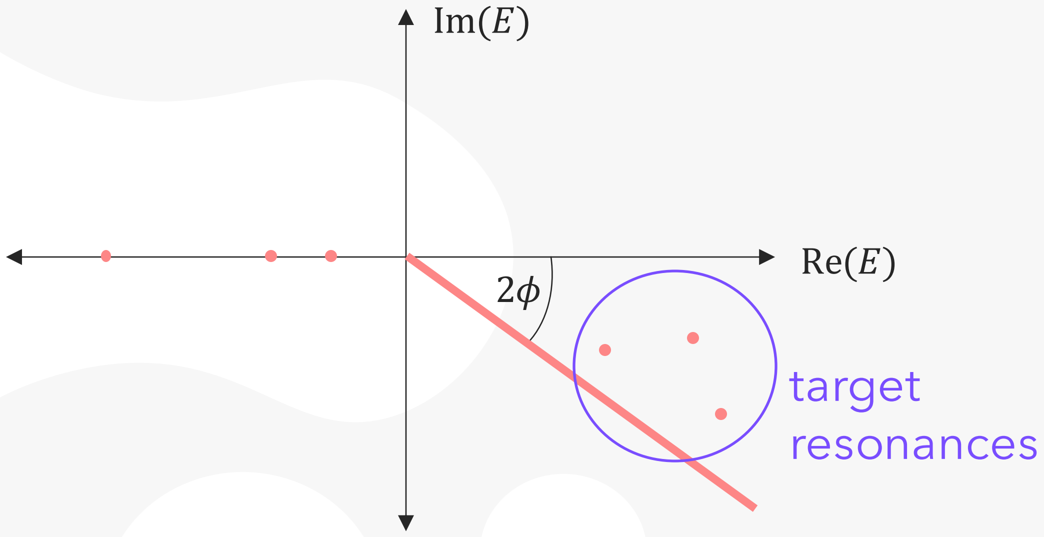
Complex-scaling method (CSM)

Aguilar, Balslev and Combes (1971): transform $r \to re^{i\phi}$ for some $\phi > \arg p$

Or equivalently $k \to ke^{-i\phi}$ (since $[r, k] = \left[r\, e^{i\phi}, k\, e^{-i\phi}\right] = i$)

Need to be careful as ϕ too large might cause $V(r)$ to diverge

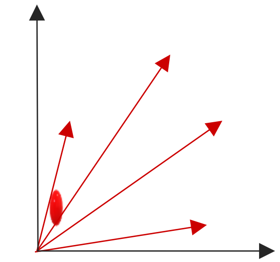




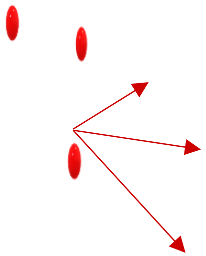
Extension to few-body systems

Choice of coordinate system:

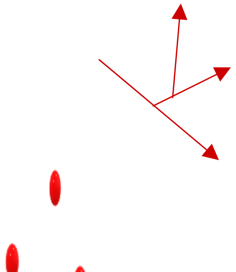
1. Single-particle coordinates



2. Simple relative coordinates

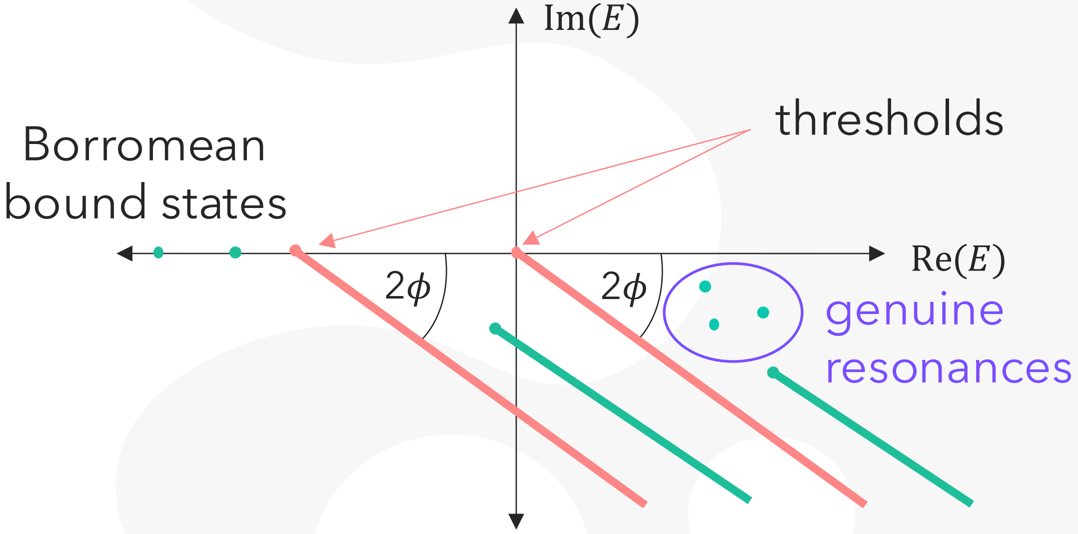


3. Jacobi coordinates



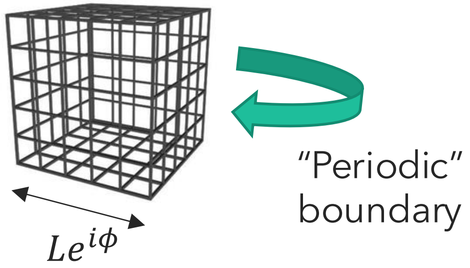
All of them can be expressed as linear transformations ⇒ CSM is implemented via

$$\vec{r}_j \to \vec{r}_j \, e^{i\phi} \text{ for j} = 1, \dots, n-1$$



Complex-scaling in various bases

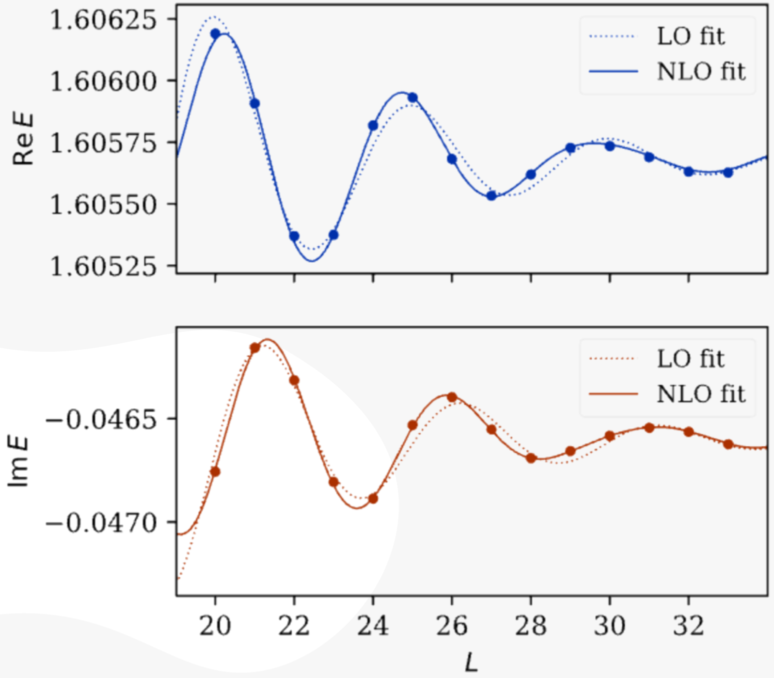
Finite-volume (FV) basis with a simple lattice discretization can be complex-scaled trivially.



E has dependence on box size L but converges at $L \to \infty$.

Lüscher-type formalism can be employed to derive a correction term

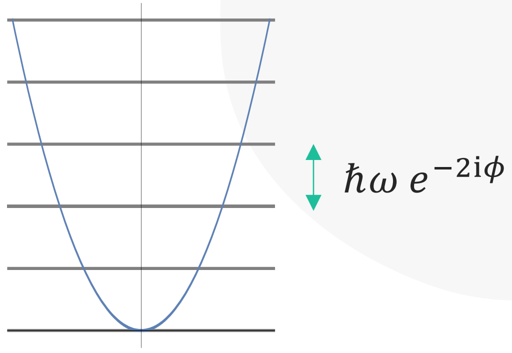
$$\Delta E(L,\phi) \approx \frac{3\gamma^2}{\mu e^{i\phi} L} \exp(i p_\infty e^{i\phi} L) \qquad \text{up to LO}$$



H. Yu, N. Yapa, and S. König, Phys. Rev. C **109**, 014316 (2024).

Complex-scaling in various bases

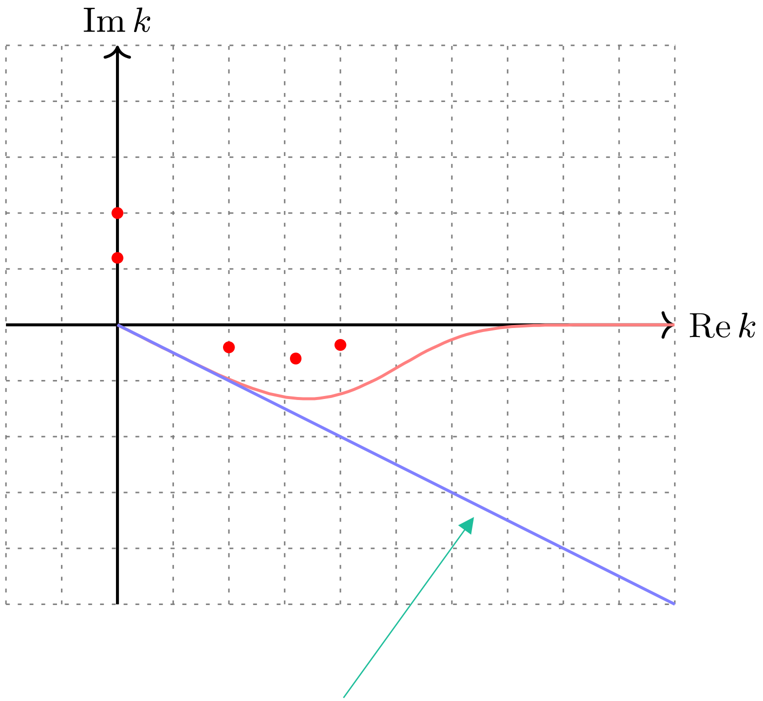
In harmonic oscillator (HO) basis, $r \rightarrow re^{i\phi}$ is equivalent to $\omega \rightarrow \omega e^{-2i\phi}$



This can be seen from the eigenfunctions

$$\langle\vec{r}|n,l,m\rangle = \sqrt{\frac{\omega^{l+3/2}}{\sqrt{\pi}}\frac{2^{n+l+2}\,n!}{(2n+2l+1)!!}}\,r^{l+1}\exp\left(-\frac{\omega r^2}{2}\right)L_n^{\left(l+\frac{1}{2}\right)}(\omega r^2)\,Y_l^m(\hat{r})$$

Berggren basis



Complex-scaled contour for comparison

Straight line contour → Curved contour

Generator potential gives basis poles

$$\mathbb{1} = \sum_B |B\rangle\langle B| + \sum_R |R\rangle\langle R| + \int_c dk\ |k_+\rangle\langle k_+|$$

The poles offload some weight off the continuum ⟹ can use a coarser discretization for the contour

Berggren basis + shell model = Gamow shell model (GSM)

Non-Hermitian QM

Either method breaks the $\mathcal{PT}$-symmetry $\Rightarrow H \neq H^\dagger$ (non-Hermitian)

Transpose symmetry is still preserved $\Rightarrow H = H^T$ (complex & symmetric)

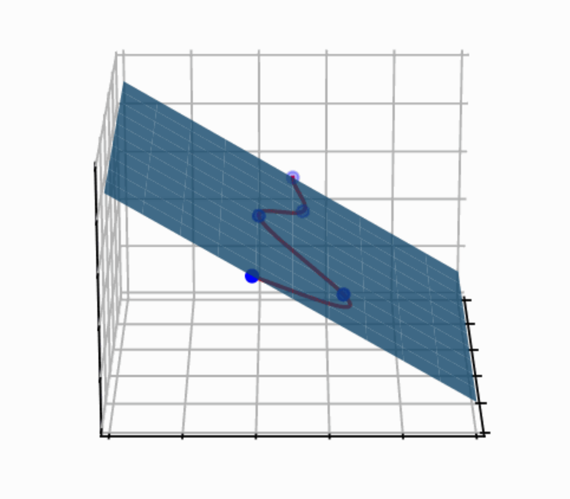
∴ use "c-product" in place of the inner product

$$\langle \psi_1 | \psi_2 \rangle \to (\psi_1 | \psi_2) = \int dx\ \psi_1(x)\, \psi_2(x)$$

no-complex conjugation

Beware of self-orthogonal states: $(\psi|\psi) = 0$

Eigenvector continuation (EC) as a reduced basis method (RBM)



Motivation: Extremal eigenvectors only explore a small subspace of the large Hilbert space, to a good approximation.

"Learn" the subspace explored by eigenvectors

Exactly calculate few eigenvectors $|\psi(c_i)\rangle$ (training points)

↓

Build a reduced basis $\{|\varphi_i\rangle\}$

Orthonormalize $\{|\psi(c_i)\rangle\}$ via Gram-Schmidt or SVD

↓

Construct $H(c_{new})$ and project onto subspace

$$H_{EC}(c_{new})_{ij} = \langle\varphi_i|H(c_{new})|\varphi_j\rangle$$

↓

Diagonalize $H_{EC}(c_{new})$ instead of $H(c_{new})$

$$H_{EC}(c_{new})|\psi(c_{new})\rangle_{EC} = E_{EC}(c_{new})|\psi(c_{new})\rangle_{EC}$$

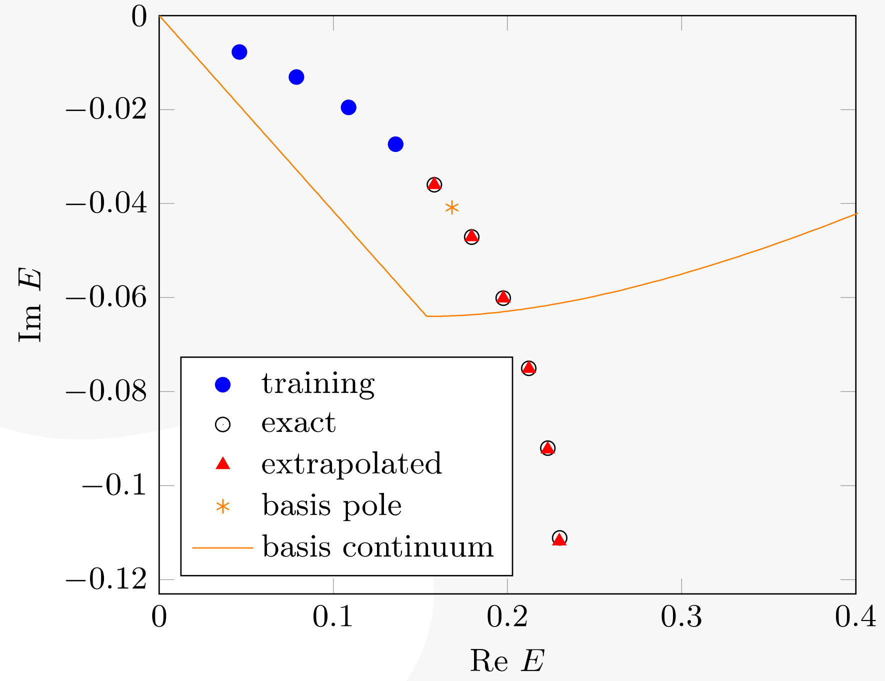
Resonance EC

Narrow-to-broad extrapolation for a 2-body toy model

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

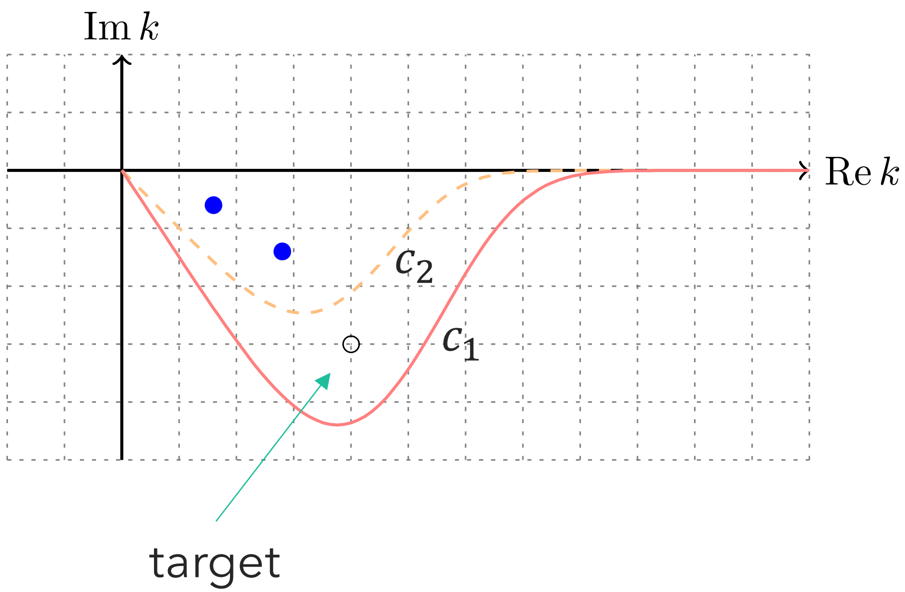
Beyond the contour, reduced basis outperforms the original basis!

Reason: Any information about the original basis (contour + poles) is lost after the projection.



N. Yapa, S. König, and K. Fossez, arXiv:2409.03116 (2024).

Resonance EC



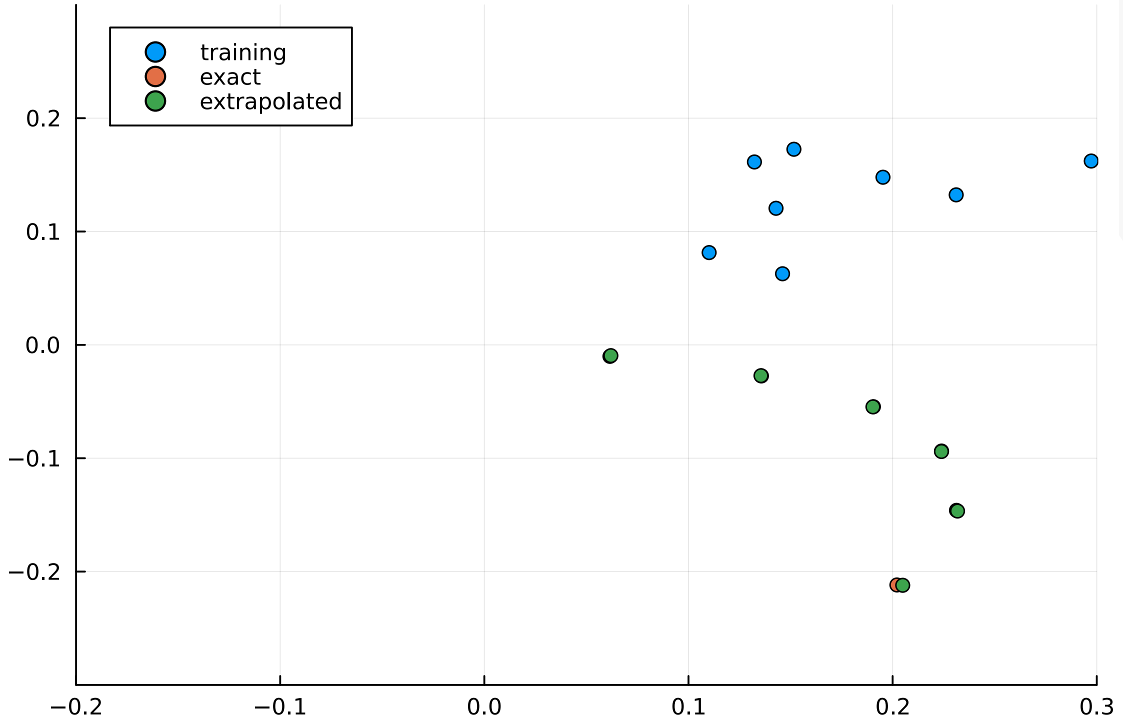
The projected matrix elements

$$\langle\psi_i|H|\psi_j\rangle = \sum_B \dots + \sum_R \dots + \int_c dE \ \dots$$

do not depend on the contour $c = c_1, c_2$ due to the Cauchy integral theorem.

Extrapolation with c_1 should work ⇒ so should c_2.

Training in 1st quadrant



$$H = H_0 + c\,V$$

Complexify c to move the pole into the 1st quadrant

$$c \to c - i\epsilon$$

and pick a random sample in the neighborhood.

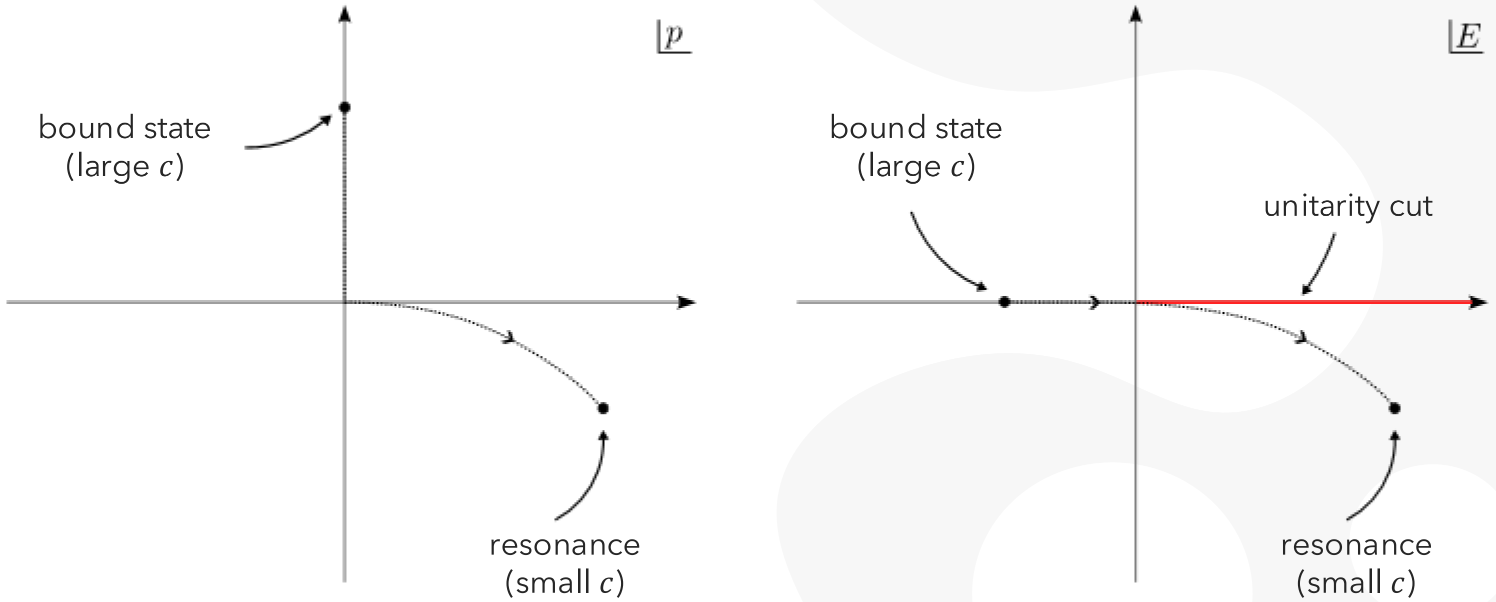
Somewhat similar to recent work by X. Zhang (2024)

Bound states and resonances across the threshold

A bound state can become a resonance (and vice versa) across the threshold when a parameter is tuned (eg: a coupling constant c in $H = H_0 + c\,V$).

Exceptional point at $p = 0$ (threshold)

"Universal" behavior near threshold: $p \approx \pm i\alpha\sqrt{c - c_0}$

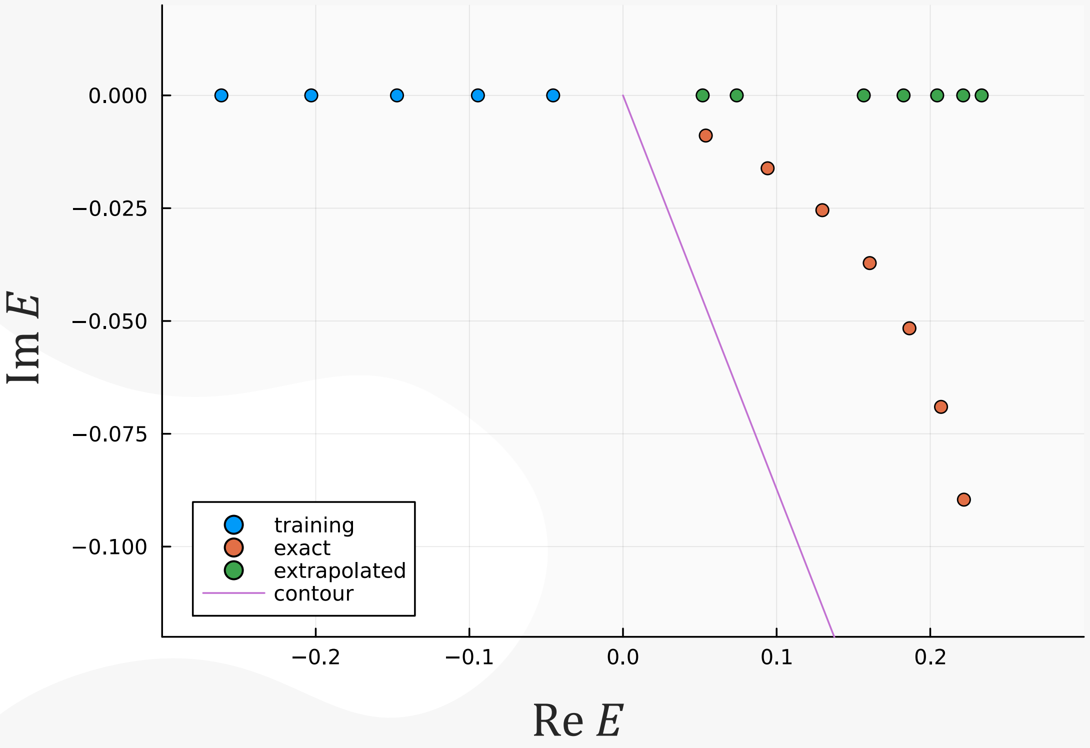


Naïve bound–to–resonance EC

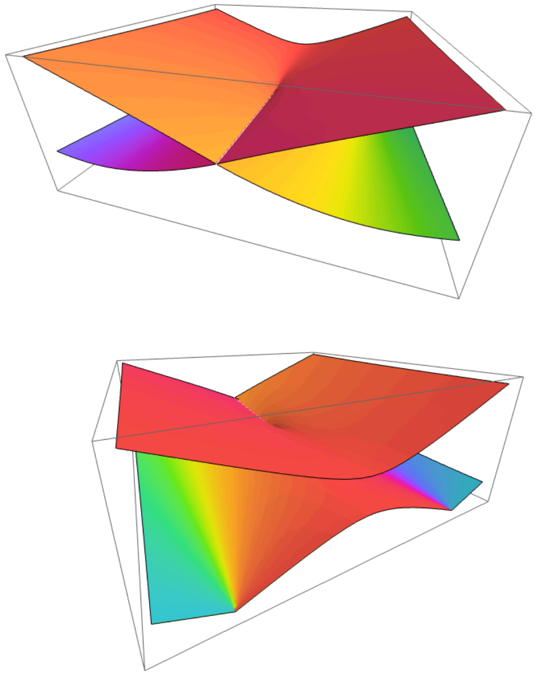
$$
\begin{aligned}
(H_{\text{EC}})_{ij} &= \langle \psi_i | H(c_{new}) | \psi_j \rangle \\
&= \oint dr \oint dr' \, \psi_i(r) \, \langle r | H(c_{new}) | r' \rangle \, \psi_i(r') \\
&= \int_0^\infty dr \int_0^\infty dr' \, \psi_i(r) \, \underbrace{\langle r | H(c_{new}) | r' \rangle}_{\text{real}} \, \psi_i(r') \in \mathbb{R}
\end{aligned}
$$

∴ Extrapolated eigenvalues will be real

The orthonormalization transformation $\{|\psi_i\rangle\} \to \{|\varphi_i\rangle\}$ does not affect this.



More on exceptional points



Square-root-like Reimann surface with a branch point singularity at $p = 0$

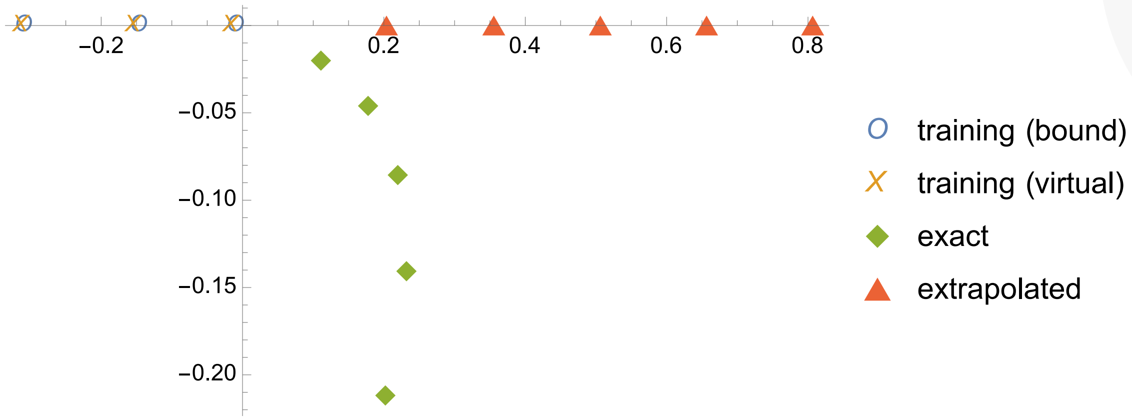
$$p \approx \pm i\alpha\sqrt{c - c_0}$$

Both eigenvectors and eigenvalues coincide at $p = 0$

(in contrast to degeneracy)

EC is known to breakdown across singularities

Bound/virtual–to–resonance EC



$(H_{\mathrm{EC}})_{ij} = \langle \psi_i | H(c_{new}) | \psi_j \rangle \in \mathbb{R}$ still holds.

Cannot use CSM for virtual states. Calculation done in in real r-space using Zeldovich regularization:

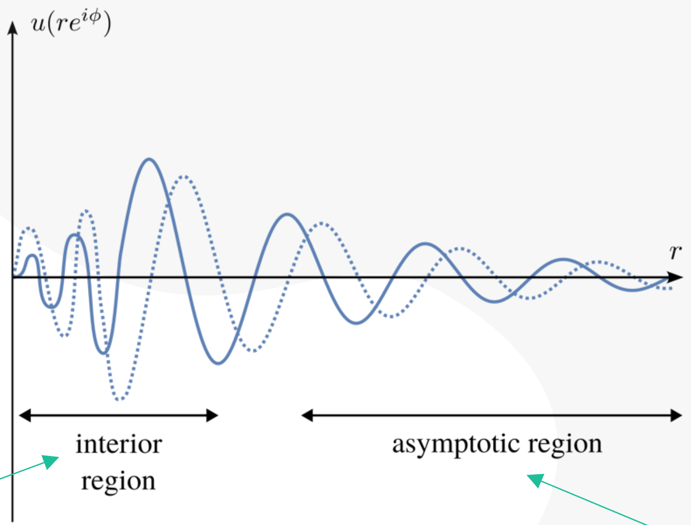
$$\langle \psi_1 | \psi_2 \rangle = \lim_{\mu \to 0} \int_0^\infty e^{-\mu r^2} u_1(r) u_2(r) \, \mathrm{d}r$$

regulator

Complex–augmented EC (CA–EC)

Problem: Interior region can be emulated by training vectors, but asymptotic region cannot.

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - 2\mu V(r) - \frac{l(l+1)}{r^2} + p^2\right] u_{l,p}(r) = 0$$



dominated by $2\mu V(r) + \frac{l(l+1)}{r^2}$

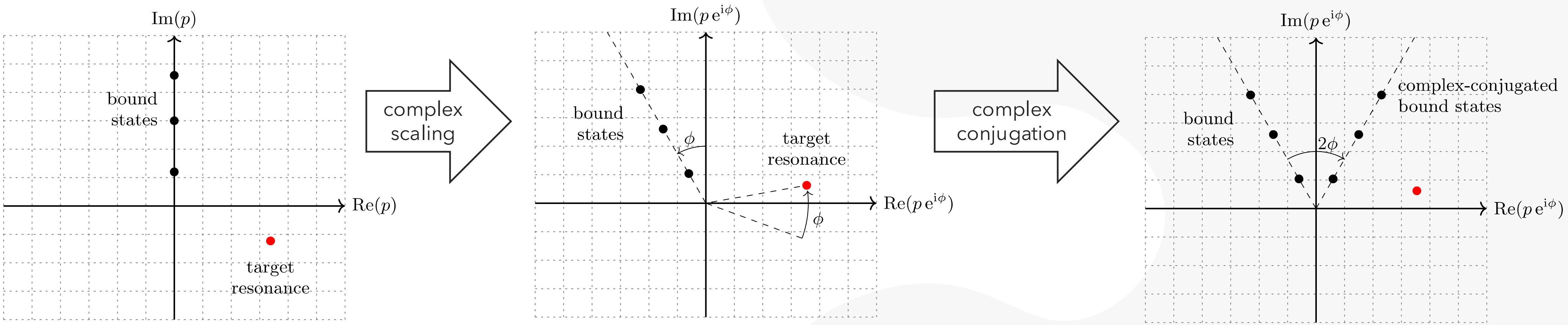
dominated by p^2

Fix: Augment the EC basis by taking the complex conjugate of the training vectors.

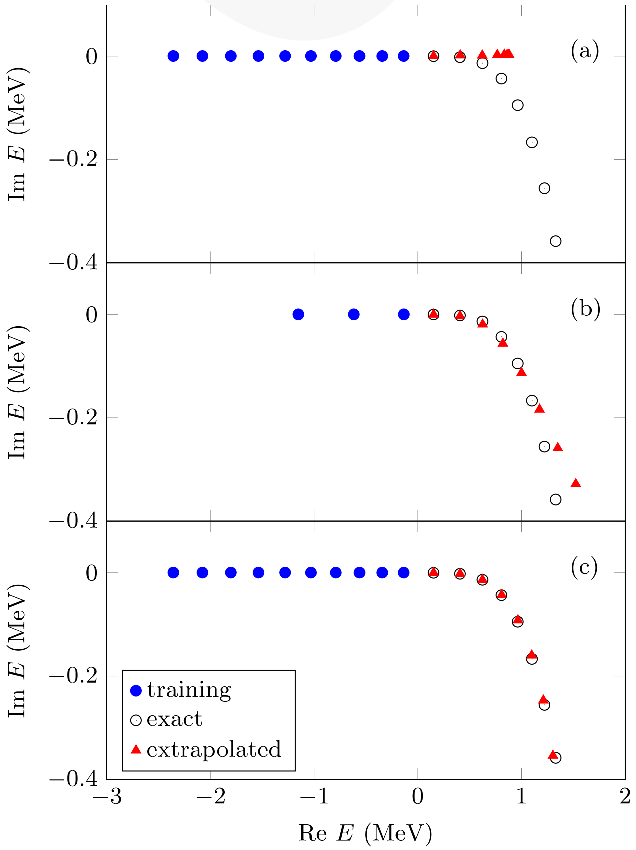
Complex–augmented EC (CA–EC)

Complex conjugation of training states results in $p \to pe^{-2i\phi}$ or $E \to Ee^{-4i\phi}$.

They are now much closer to the target resonance.



Bound–to–resonance extrapolation results: ^{6}He



$^4\text{He} + n + n$ system

Core-nucleon interaction = Woods-Saxon fitted to ^4He–n phase shifts

n–n interaction = regularized contact interaction in $(S, T) = (0,1)$ channel

$$\langle S = 0, T = 1, r | V | S = 0, T = 1, r \rangle = c\, f(r)$$

parameter to be varied

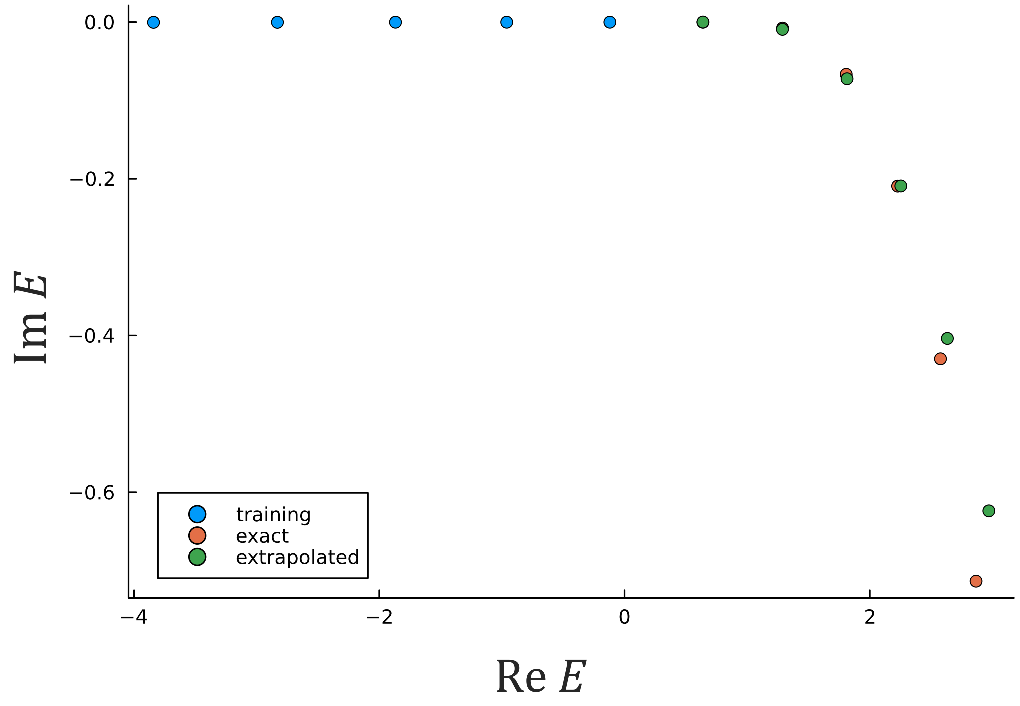
Top: Naïve EC with 10 training states

Middle: CA-EC with 3 training states

Bottom: CA-EC with 10 training states

N. Yapa, S. König, and K. Fossez, arXiv:2409.03116 (2024).

Bound–to–resonance extrapolation results: ^{6}Be



Preliminary

Similar interaction as before, but for a $^4\mathrm{He} + p + p$ system

⇒ works well enough for Coulomb interaction (not short-ranged)

Next goal: Attempt $^7\mathrm{N}$ (5 proton emitter)

Thank you!

My collaborators:

Kévin Fossez

Sebastian König

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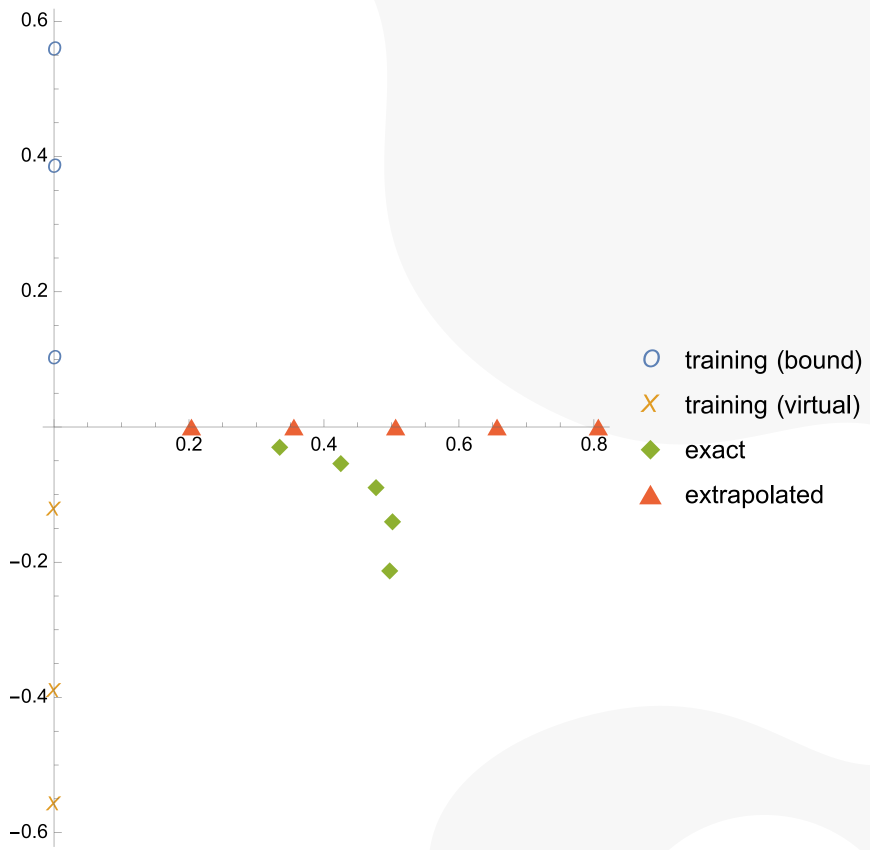
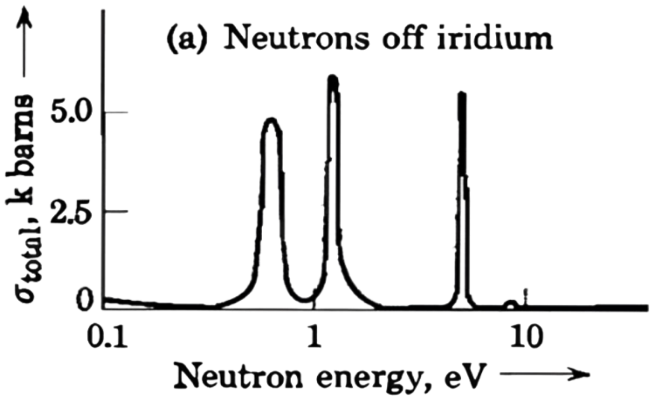
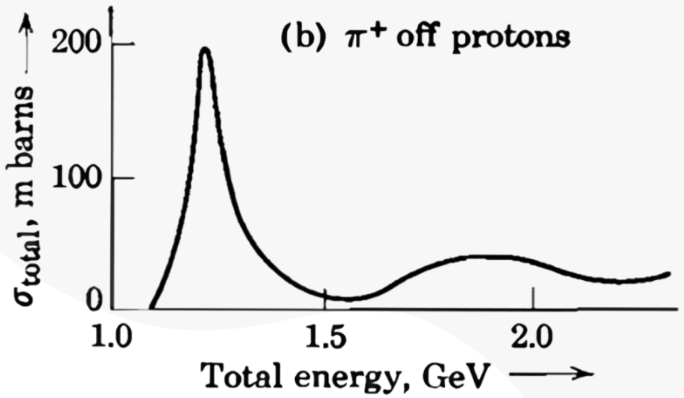
Backup: BV2R in p-space



Backup: What are resonances?

Resonances are peaks of the scattering cross section observed in experiments:





J. R. Taylor, *Scattering Theory: The Quantum Theory of Nonrelativistic Collisions* (Dover Publications, Newburyport, 2012).

Some nuclei created in the lab are observed to be unbound resonances (e.g. $^{27}\mathrm{O}$, $^{28}\mathrm{O}$).

Also occur as metastable states of many nuclei (e.g. $^{11}\mathrm{Be}$) encountered in decay chains.