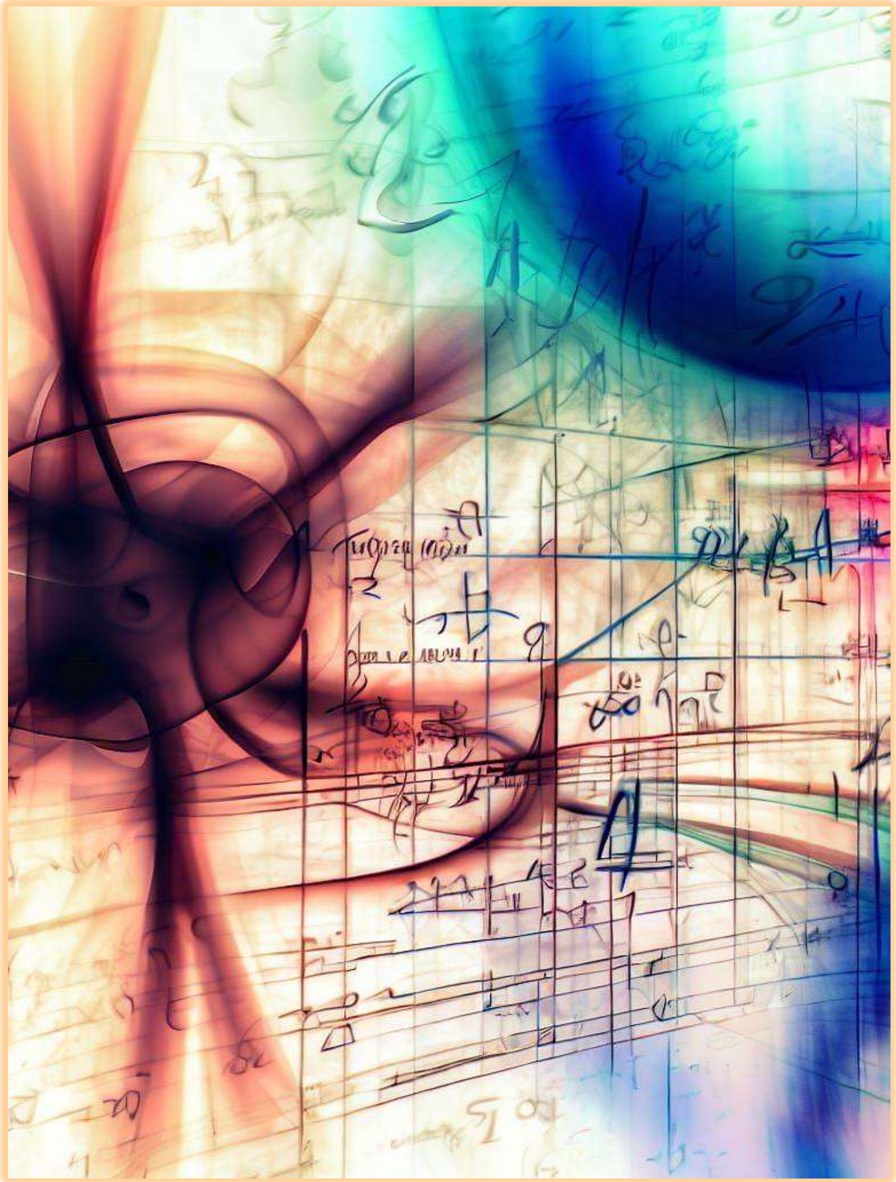

Eigenvector Continuation for Few-Body Resonances

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Outline

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Part I

Finite Volume Eigenvector Continuation (FVEC)

Part II

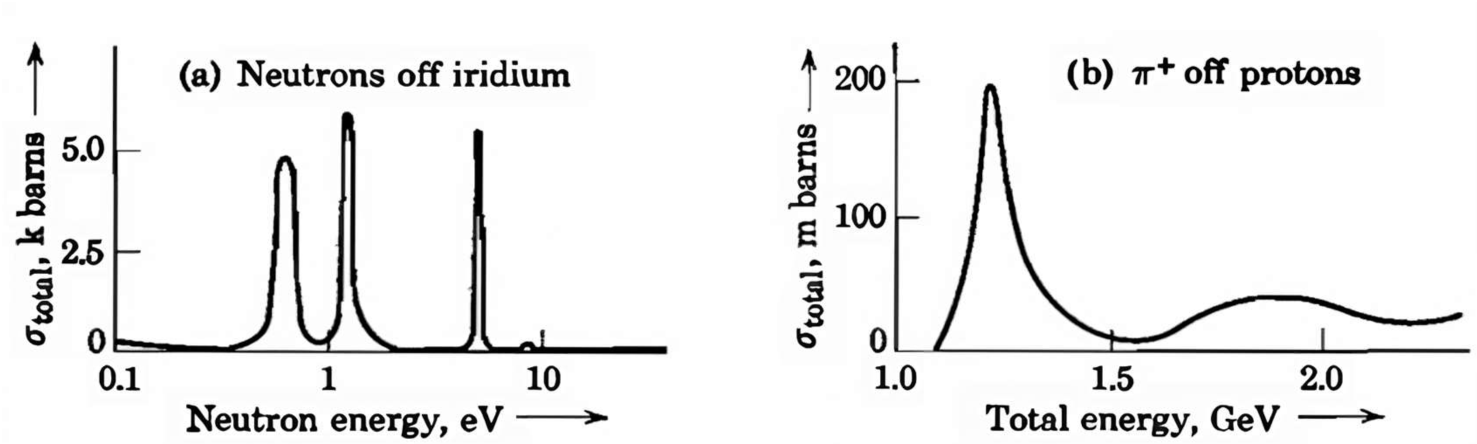
Bound-state-to-resonance EC via complex-scaling

Prelude

Introduction to resonances

Resonances

Resonances appear as large peaks in the scattering cross-section.



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

Furthermore, the scattering phase shift $\delta(k)$ jumps rapidly by π across a resonance.

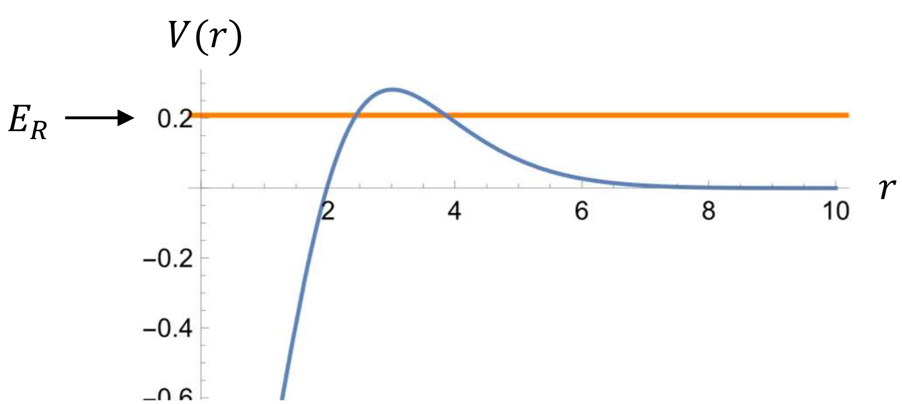
Resonances

Potentials with a repulsive barrier may support resonances.

E.g.: For S-wave ($l = 0$), the potential

$$V(r) = -\frac{5}{2}\exp\left(-\frac{r^2}{3}\right) + \exp\left(-\frac{r^2}{10}\right)$$

supports a resonance at $E_R = 0.209$.

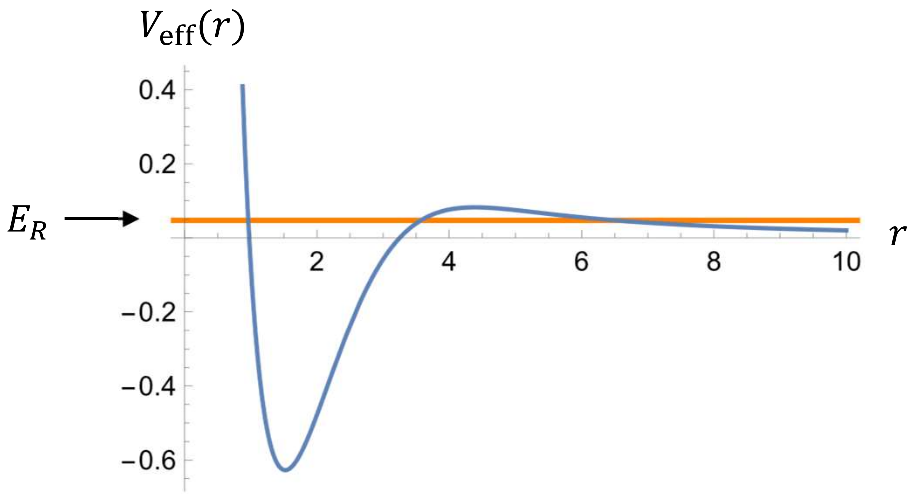


States with $l > 0$ could be trapped by the centrifugal barrier $\frac{l(l+1)}{r^2}$.

E.g.: For P-wave ($l = 1$), the potential

$$V(r) = -\frac{8}{2}\exp\left(-\frac{r^2}{4}\right)$$

supports a resonance at $E_R = 0.0471$.



Gamow states

George Gamow (1904 – 1968) explained alpha decayed as quantum tunneling through the nuclear potential.

The metastable state formed by the alpha-daughter system corresponds to a complex-E solution of the time independent Schrödinger equation – a Gamow state.

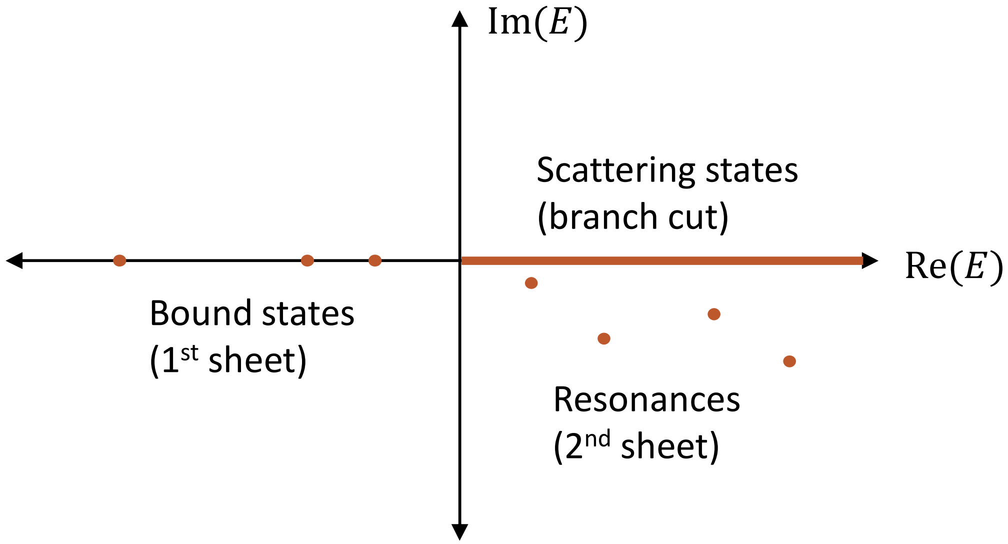
Time delay

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

$\mathrm{Im}(E) < 0 \Rightarrow$ state decays with time evolution $e^{-iHt/\hbar}$.

Gamow states

Gamow states correspond to poles in the second Reimann sheet of the S-matrix, They deform their vicinities in the complex S-matrix-plane and if close enough, can give rise to the peaks on the physical scattering line (positive real line).



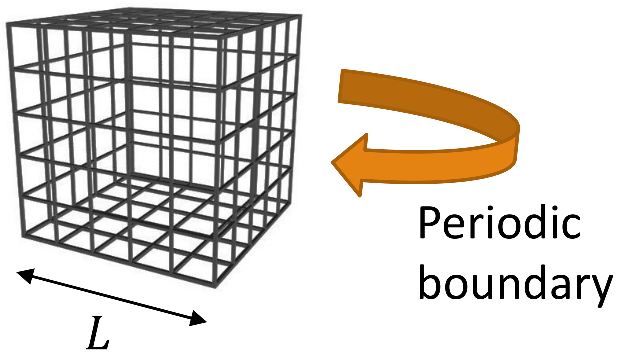
Pole in the S-matrix $\Leftrightarrow$ Jost function $= 0$ $\Leftrightarrow$ Purely outgoing boundary condition

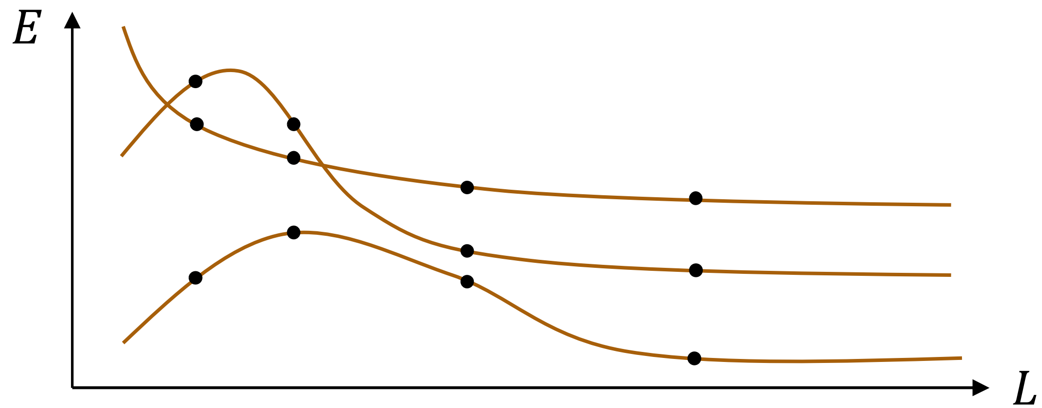
Part I

Finite Volume Eigenvector Continuation (FVEC)

Why finite volume EC?

Sometimes, we have to calculate E vs. L (energy spectrum for varying box size)





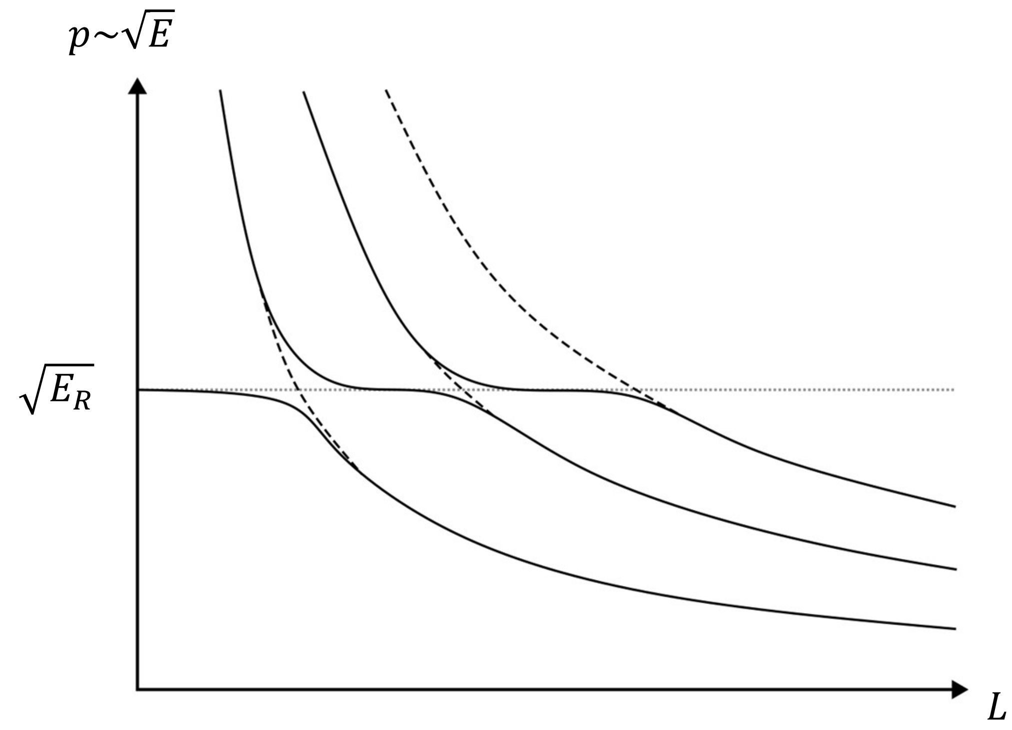
Useful for

1. Infinite volume properties via Lüscher formalism
2. Identifying resonances via avoided crossings ← In this talk

Identifying resonances (avoided crossings)

How do we get avoided crossings?

- $pL = 2\pi n$ for periodic boundary
- $pL + 2\delta(p) = 2\pi n$ when a scattering potential is present
- When $\delta(p)$ goes from 0 to π, the boundary condition changes
  from $\quad pL = 2\pi n$
  to $\quad pL = 2\pi(n-1)$
- We see energy levels "crossing" a step



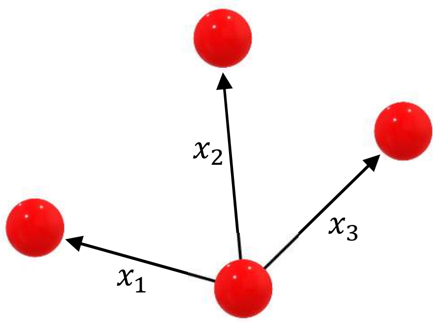
U.J. Wiese, Identification of resonance parameters from the finite volume energy spectrum (1989)

Finite volume construction

Few-body Hamiltonian without the center-of-mass energy:

$$H = \sum_i \frac{p_i^2}{2m} + V(r_i) - \frac{1}{2nm}\left(\sum_i p_i\right)^2$$

We use simple relative coordinates: $x_i = \begin{cases} r_i - r_n & ; i < n \\ \frac{1}{n}\sum r_i & ; i = n \end{cases}$



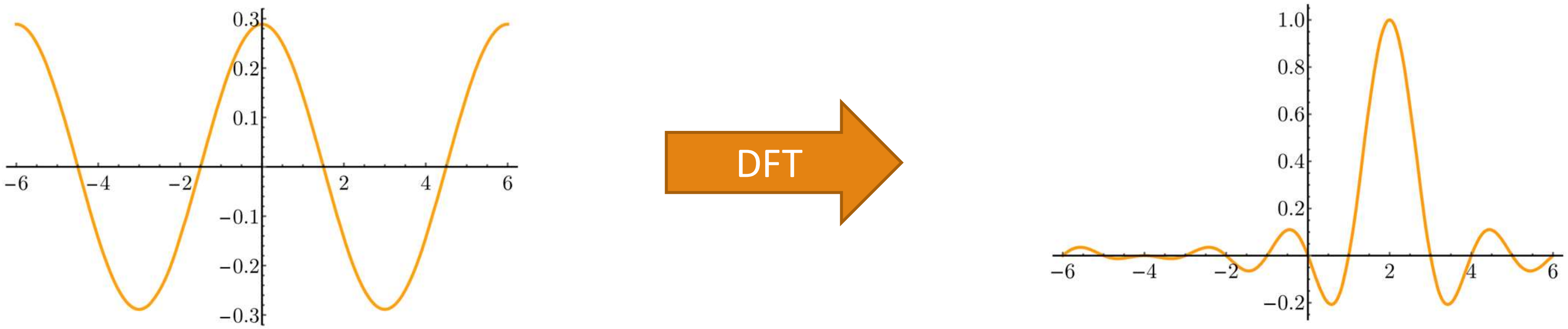
After this canonical transformation, the Hamiltonian becomes

$$H = \sum_i \sum_{j \le i} \frac{q_i \, q_j}{2\mu} + V(r_i)$$

where q_i are the conjugate momenta to x_i and $\mu = \frac{m}{2}$ is the reduced mass.

Finite volume construction

Discrete Variable Representation (DVR): Discrete Fourier Transform of a discrete momentum basis.



n plane waves
(discrete momenta)

n Kronecker-δ functions
("almost" discrete positions)

Periodic by construction.

Finite volume construction

Kinetic energy matrix elements $\langle k|K|l\rangle$ can be calculated exactly because the derivative ∂ is exact.

$$\langle l|\partial|k\rangle = \frac{\pi}{L}\begin{cases} -i & ; k = l \\ (-1)^{k-l}\dfrac{\exp\left(-i\,\dfrac{\pi(k-l)}{n}\right)}{\sin\left(\dfrac{\pi(k-l)}{n}\right)} & ; k \neq l \end{cases}$$

Potential energy matrix elements $\langle k|V|l\rangle$ are diagonal, but an approximation.

$$|k\rangle \approx \left|x = \frac{kL}{n}\right\rangle$$

$$\langle k|V|l\rangle \approx V\left(x = \frac{kL}{n}\right)\delta_{kl}$$

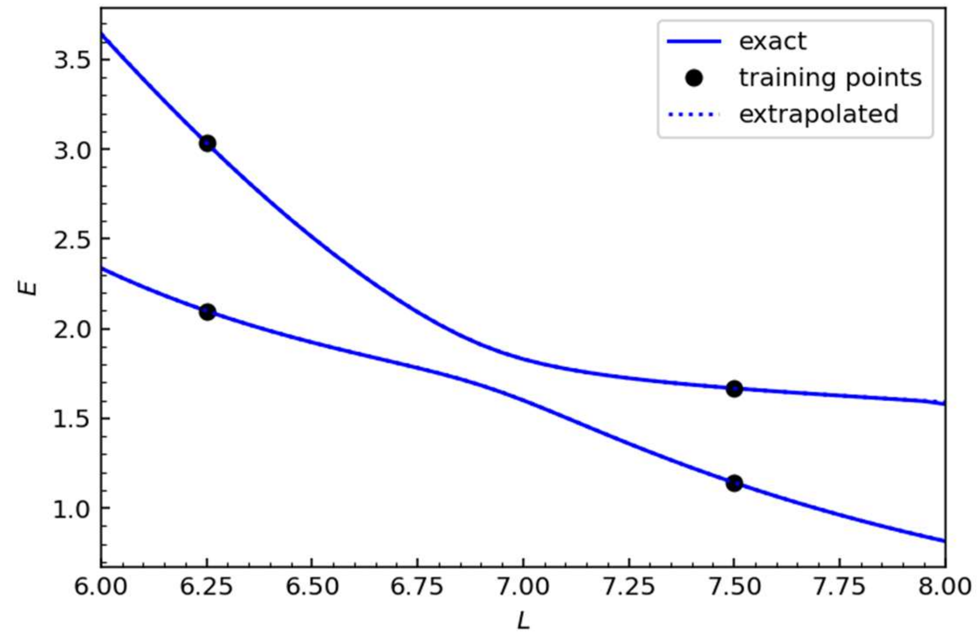
Finite Volume Eigenvector Continuation (FVEC): 2-body example

Two identical particles with $m = 1$ interacting via the potential

$$V(r) = V_0 \exp\left(-\left(\frac{r-a}{R_0}\right)^2\right)$$

where $V_0 = 2.0$, $R_0 = 1.5$, $a = 3$.

Has a known resonance with energy $E_R = 1.606$ and half-width $\Gamma = 0.097$.

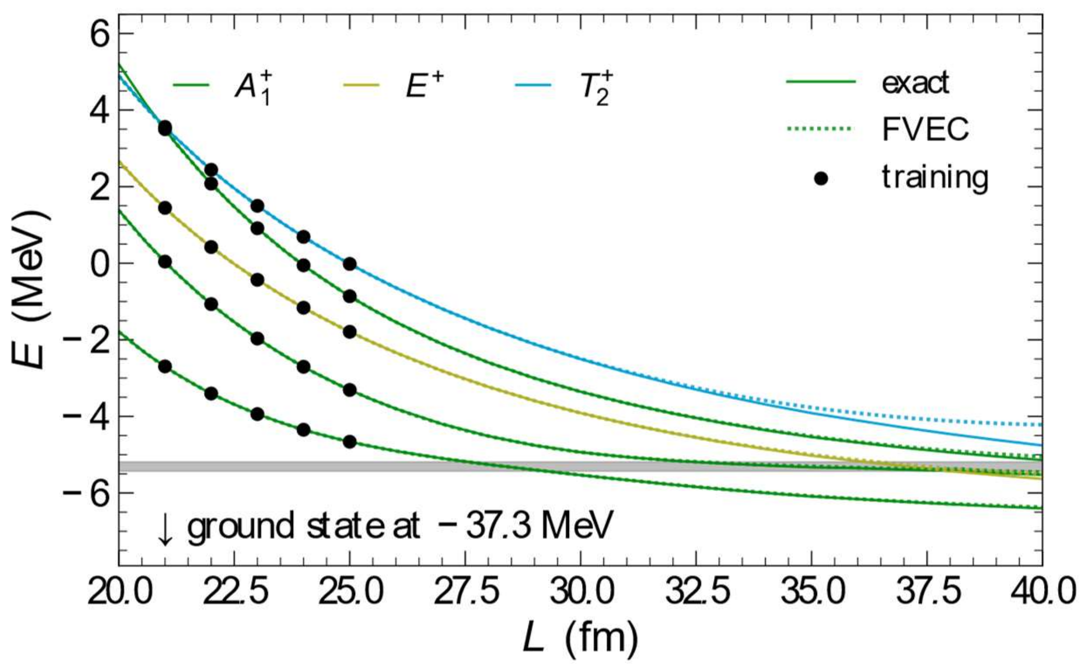


Finite Volume Eigenvector Continuation (FVEC): 3-body example

Three identical spin-0 bosons
with $m = 939.0$ MeV
interacting via the two-body potential

$$V(r) = V_0 \exp\left(-\left(\frac{r}{R_0}\right)^2\right) + V_1 \exp\left(-\left(\frac{r-a}{R_1}\right)^2\right)$$

where $V_0 = -55$ MeV, $V_1 = 1.5$ MeV, $R_0 = \sqrt{5}$ fm, $R_1 = 10$ fm, $a = 5$ fm.



Has a known resonance with energy $E_R = -5.31$ MeV and half-width $\Gamma = 0.12$ MeV.

Does FVEC make sense?

$$H_{ij} = \left\langle \psi_{L_i} \middle| H_{L_*} \middle| \psi_{L_j} \right\rangle$$

$$N_{ij} = \left\langle \psi_{L_i} \middle| \psi_{L_j} \right\rangle$$

Inner products and matrix elements between different Hilbert spaces!

Solution: Periodic Matching

Define the **dilatation operator** $D_{L,L'}$ by $\left(D_{L,L'} f\right)(x) = \sqrt{\frac{L}{L'}} f\left(\frac{L}{L'} x\right)$

Now, the inner product can be redefined as $\left\langle \psi_{L_i} \middle| \psi_{L_j} \right\rangle = \int_{-L_j/2}^{L_j/2} \left(D_{L_j,L_i} \psi_{L_i}\right)(x)^* \, \psi_{L_j}(x) dx$

The matrix element can be defined in a similar manner.

Part II

Bound-state-to-resonance EC via complex-scaling

Partial wave projection

We work with spherically symmetric potentials in the partial wave basis where the radial Schrodinger equation becomes

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

$$[q^2 + k^2]\psi_{l,k}(q) - 2\mu \int \mathrm{d}q'\, V_l(q, q')\psi_{l,k}(q') = 0$$

where $k = \sqrt{2\mu E}$,
$\psi_{l,k}$ is the reduced radial wavefunction, and
l is the angular-momentum quantum number.

Reduces the 3D problem into a 1D problem.

Complex-scaling method (CSM)

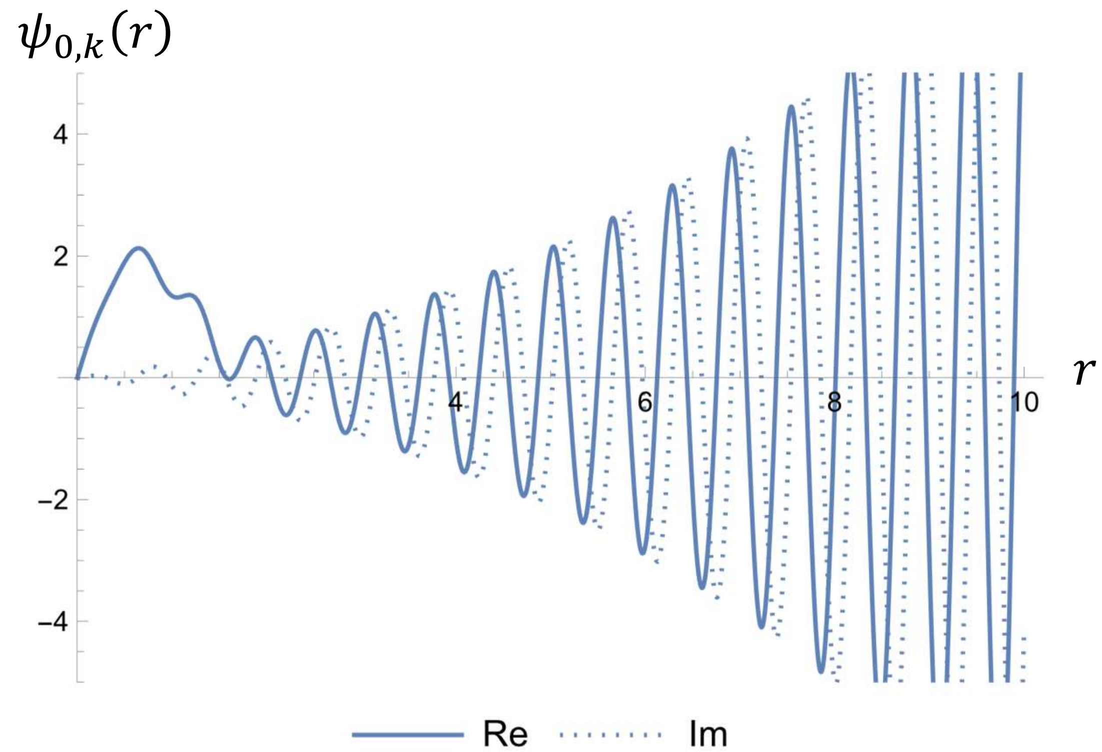
For bound states and resonances,
$\psi_{l,k}(r) \sim \hat{h}_l^+(kr) = ikr\, h_l^{(1)}(kr)$ at $r \to \infty$

$\hat{h}_l^+(z)$ are the Riccati-Hankel functions of the first kind.

$h_l^{(1)}(z)$ are the spherical Hankel functions of the first kind.

For bound states $k = i\kappa$ with $\kappa > 0$
For resonances $\mathrm{Re}(k) > 0$ and $\mathrm{Im}(k) < 0$

For example, $l = 0$ gives $\psi_{l,k}(r) \sim \exp(ikr)$ asymptotically.



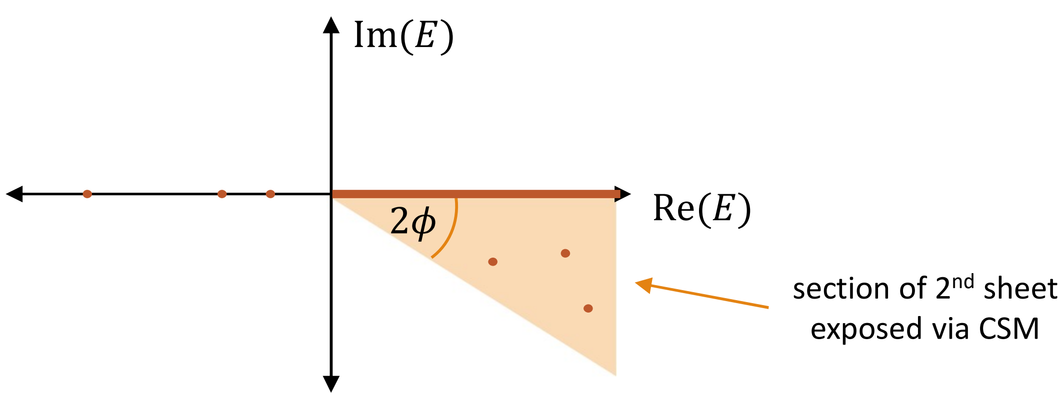
Complex-scaling method (CSM)

CSM involves the transformation

$$r \to re^{i\phi}$$

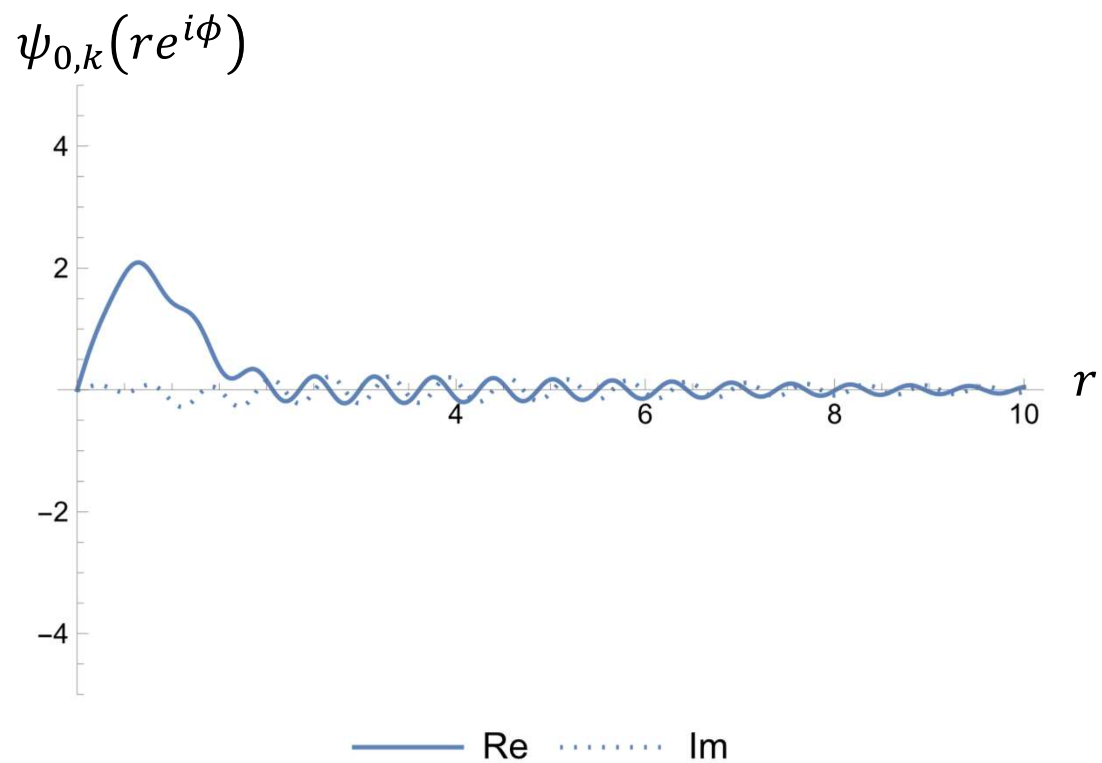
where ϕ is some angle such that $\phi > \frac{\arg}{2}$

This is equivalent to $q \to qe^{-i\phi}$ in momentum space, which exposes a section of the 2nd sheet.



Then $\exp(ikr) \to \exp(ikr\, e^{i\phi})$.

The growing tail turns into a decaying one.



Non-hermiticity and c-product

In traditional QM, non-degenerate eigenvectors of a Hamiltonian are orthogonal under the inner product (scalar product).

$$\langle \psi_1 | \psi_2 \rangle = \int dx \;\; \psi_1^*(x)\, \psi_2(x)$$

However, with CSM, the Hamiltonian is no longer Hermitian, and the eigenvectors are only orthogonal under the "c-product".

$$(\psi_1 | \psi_2) = \int dx \;\; \psi_1(x)\, \psi_2(x)$$

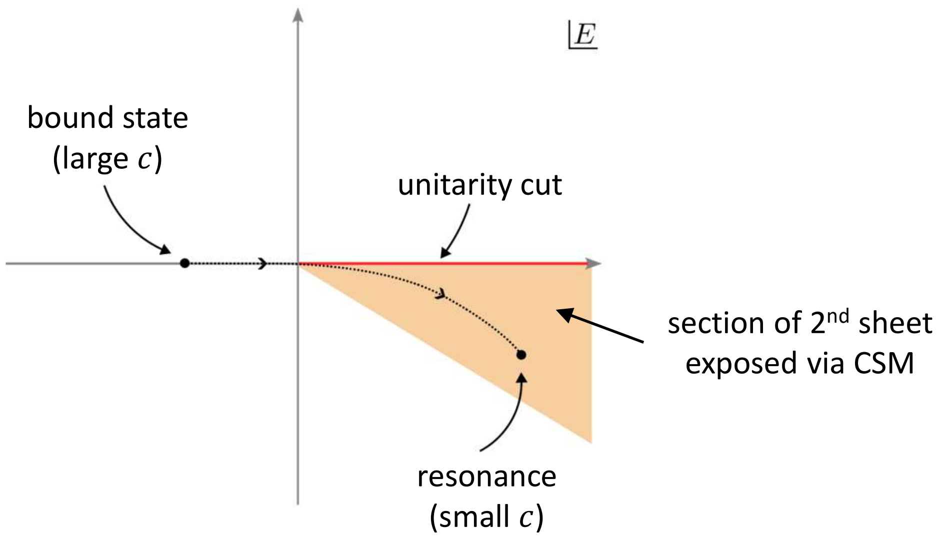
Traditional QM	Non-Hermitian QM
$H = H^\dagger$	$H = H^T$
Inner product	c-product
Real eigenvalues	Complex eigenvalues
Unitary time evolution	States can decay/grow

S-matrix pole trajectory

A bound state may become a resonance when the interaction is made weaker.

$$\hat{H} = \hat{H}_0 + c\,\hat{V}$$

this coupling parameter is gradually decreased



Note: This may or may not happen depending on the details of the potential. Purely attractive potential cannot support S-wave resonances. They will instead become virtual (anti-bound) states.

Resonance-to-resonance extrapolation

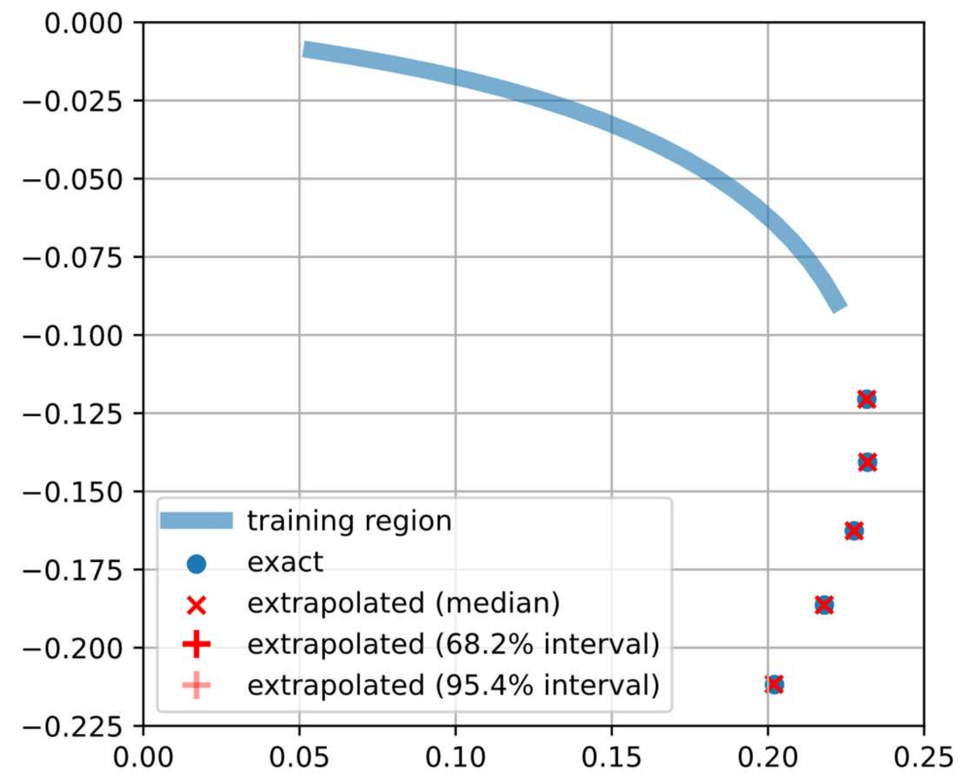
Consider a 2-body system with $m = 1$:

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

in the S-wave ($l = 0$) partial wave.

Uncertainties are estimated by repeating the calculation 128 times while randomizing the location of 5 training points.

EC for resonance-to-resonance extrapolation works out of the box with the only caveat being the c-product.



Bound-state-to-resonance extrapolation

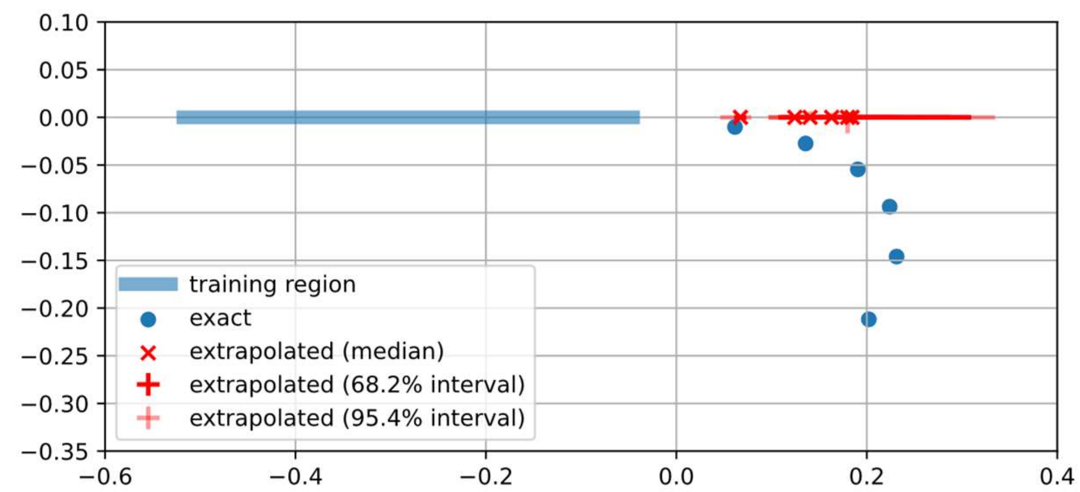
However, naively using EC to extrapolate from bound states to resonances fails.

In fact, it can be easily shown that

$$(N_{EC})_{ij} = (\psi_i|\psi_j) \in \mathbb{R}$$

$$(H_{EC})_{ij} = (\psi_i|H|\psi_j) \in \mathbb{R}$$

and that N_{EC} and H_{EC} are symmetric under c-product.



Conjugate-Augmented Eigenvector Continuation (CA-EC)

Bound-state-to-resonance extrapolation can be accomplished with one simple extra step:

Double the EC basis by including the complex-conjugates of the original training vectors

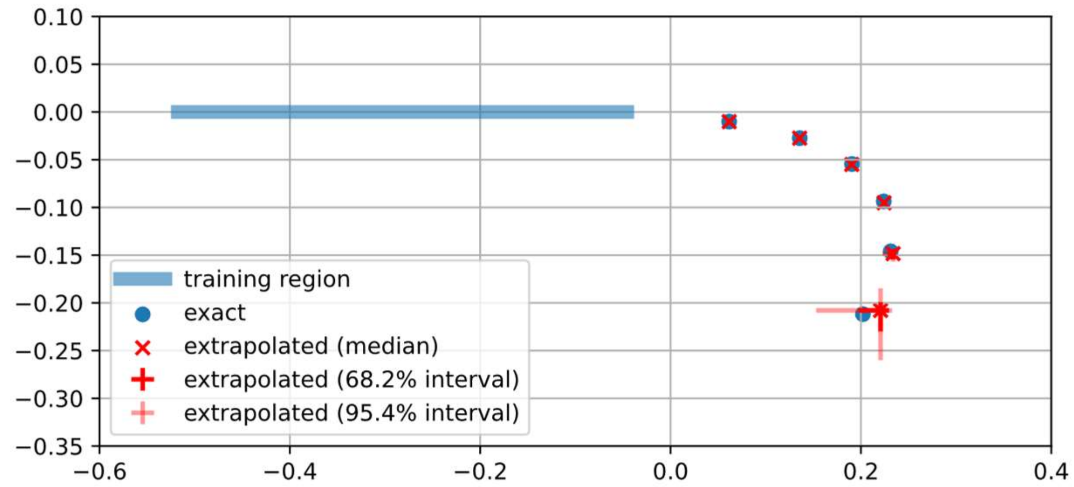
That is, include ψ_i^* for each $\psi_i \quad (i = 1, \ldots, N_{EC})$

Or, alternatively, separate the real and imaginary parts of the EC vectors, with no additional memory usage,

$$\psi_i \rightarrow \{\mathrm{Re}(\psi_i), \mathrm{Im}(\psi_i)\}$$

because,

$$\mathrm{span}\{\mathrm{Re}(\psi_i), \mathrm{Im}(\psi_i)\} = \mathrm{span}\{\psi_i, \psi_i^*\}$$

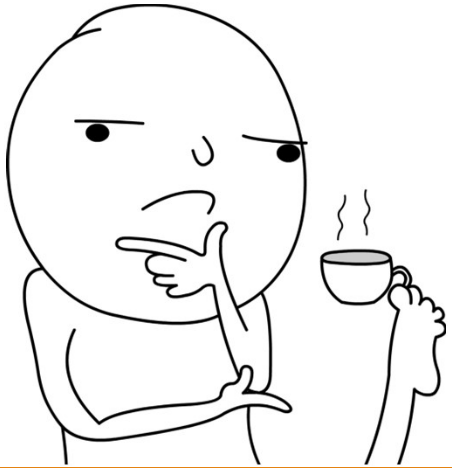


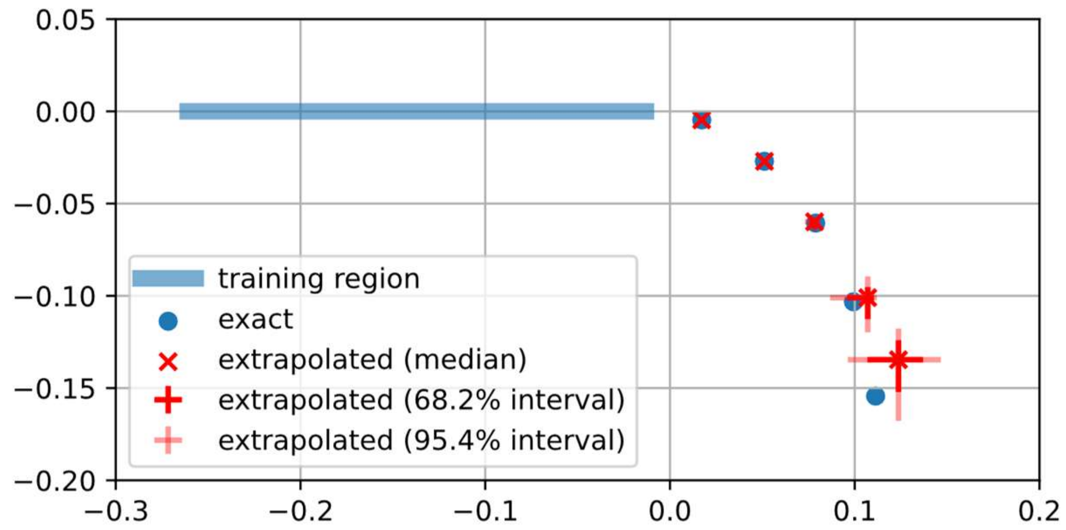
Conjugate-Augmented Eigenvector Continuation (CA-EC)

P-wave ($l = 1$) example:

$$V(r) = -c \exp\left(-\frac{r^2}{4}\right)$$

So, why does CA-EC work so well?





Why does CA-EC work?

Short answer:

Complex-conjugated vectors have better asymptotics for emulating resonances.

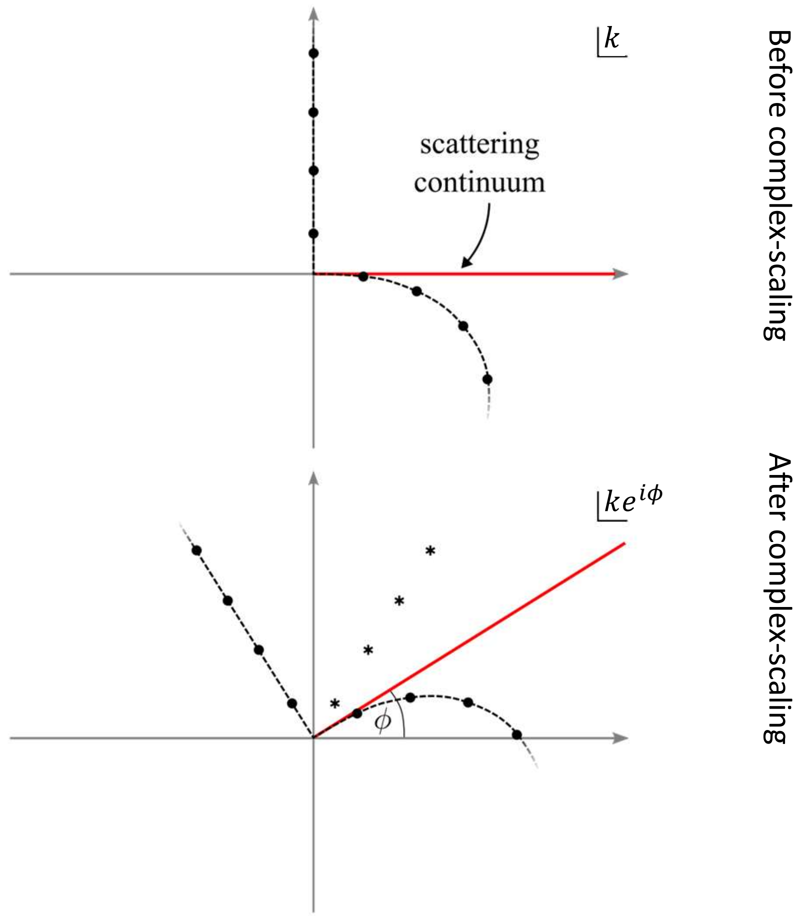
Long answer:

Consider the asymptotic tail of the complex-scaled wavefunction under complex conjugation:

$$e^{ikr\, e^{i\phi}} \to e^{-i\,(-k)\, r\, e^{-i\phi}}$$

which is equivalent to $k \to k\, e^{-2i\phi}$.

These values (indicated by $*$ in the figure) have a positive real part and are closer to the resonant region in the complex-k plane.



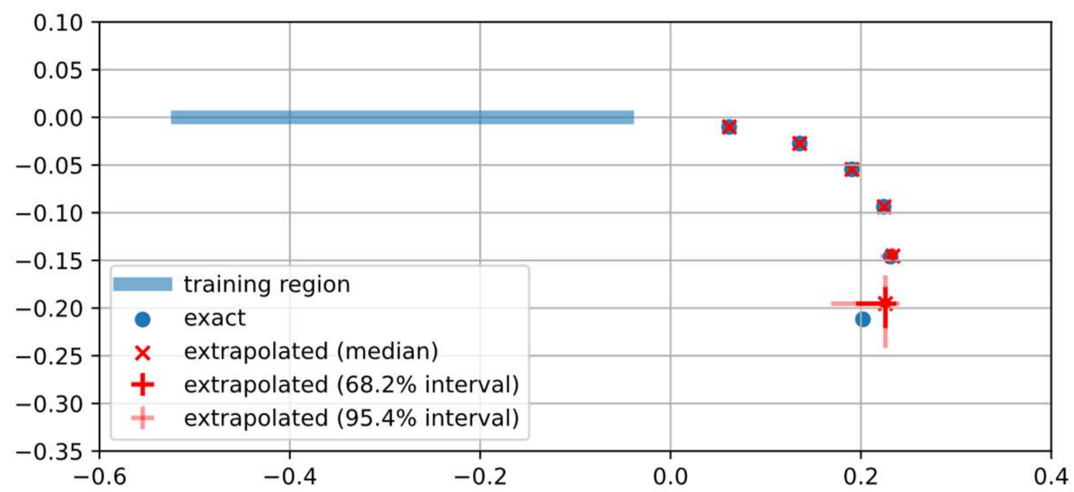
Why does CA-EC work?

Proof:

Instead of adding complex-conjugated vectors, let’s try augmenting the basis with Riccati-Hankel functions

$$\hat{h}_l^+(kr) = ikr\, h_l^{(1)}(kr)$$

with the same k values corresponding to the complex-conjugated vectors.



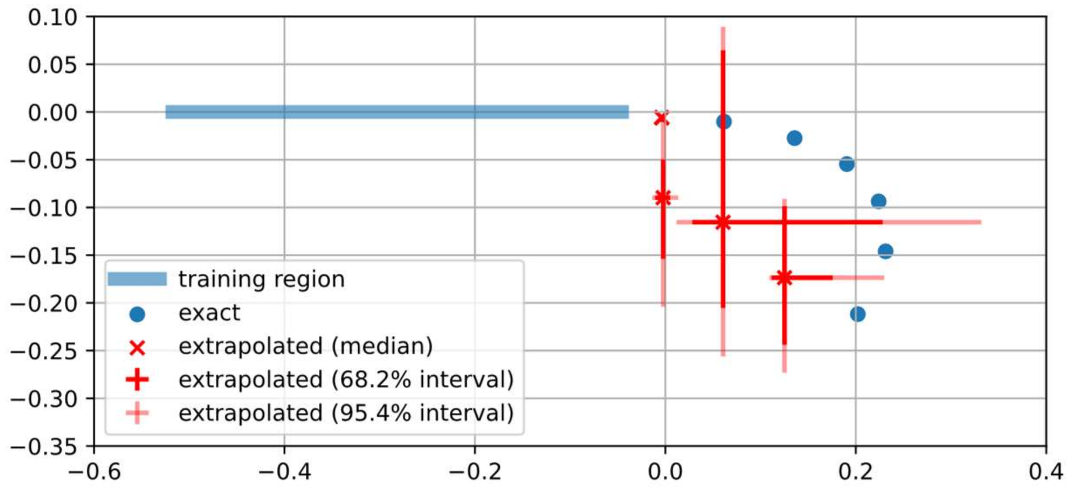
Why does CA-EC work?

Proof:

To verify that original training vectors are also contributing, we can repeat the previous extrapolation after removing them.

In summary, we can conclude that,

1. Original training vectors are contributing to the internal part of the wavefunction.
2. Complex-conjugated vectors are contributing to the asymptotic part of the wavefunction.



Analytic continuation of the wavefunction

In the case when $\psi(r)$ or $\psi(q)$ is only known along the real line, for CA-EC to applicable, we need to continue it on to a complex-scaled contour. This can be done with the integral Schrodinger equation (homogenous) equation.

$$\psi(qe^{-i\phi}) = \int_0^\infty q'^2 \, dq' \, \frac{1}{E - \frac{q'^2}{2\mu}} V(qe^{-i\phi}, q')\psi(q')$$

Therefore, we can lay out a plan for implementing CA-EC:

1. Using exact methods, calculate bound wavefunctions $\psi_i(q)$ of $H(c_i)$ for a set of $c_i > c_{\text{th}}$.
2. Analytically continue $\psi_i(q) \to \psi_i(qe^{-i\phi})$ via the above method.
3. Construct the EC basis with CA-EC. That is, include $\psi_i^*(qe^{-i\phi})$ for each $\psi_i(qe^{-i\phi})$.
4. Extrapolate resonances of $H(c_i)$ for $c_i < c_{\text{th}}$.

Futures goals

1. Extend for few-body systems.
2. Implement offline/online decomposition because $H(c)$ has affine dependence on c.
3. A better uncertainty estimation scheme.

   Note: $\sqrt{\frac{\langle\psi_{EC}|[H - E_{EC}]^2|\psi_{EC}\rangle}{\langle\psi_{EC}|H^2|\psi_{EC}\rangle}}$ doesn't work because of the non-hermiticity!

Thank you for listening!

References and further reading:

1. P. Klos, S. König, H.-W. Hammer, J. E. Lynn, and A. Schwenk. “Signatures of Few-Body Resonances in Finite Volume.” *Physical Review C* 98, no. 3 (September 24, 2018): 034004. https://doi.org/10.1103/PhysRevC.98.034004.

2. Nuwan Yapa, and Sebastian König. “Volume Extrapolation via Eigenvector Continuation.” *Physical Review C* 106, no. 1 (July 18, 2022): 014309. https://doi.org/10.1103/PhysRevC.106.014309.

3. Nuwan Yapa, Kévin Fossez, and Sebastian König. “Eigenvector Continuation for Emulating and Extrapolating Two-Body Resonances.” arXiv, March 10, 2023. https://doi.org/10.48550/arXiv.2303.06139.