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# Extrapolation and emulation techniques for few-body resonances

S König

Department of Physics, North Carolina State University, Raleigh, NC 27695, USA

**Abstract.** Quantum resonances, i.e., metastable states that decay over time, are a fascinating phenomenon relevant in different areas of physics. In nuclear physics, they not only appear as excited states of various atomic nuclei, but they can also constitute the ground state of exotic nuclei near the edges of nuclear stability. Characterized by being strongly coupled to the continuum, resonances are notoriously challenging to describe theoretically and to compute numerically, especially when they appear as genuine few-body states. This article summarizes how the complex-augmented eigenvector continuation (CA-EC) method can be used to track resonance states as the underlying interaction governing them is varied. In particular, CA-EC is able to robustly extrapolate states all the way from being bound to becoming resonances. Such extrapolations were originally demonstrated to work well for two-body states, and recent work established that this remains true for few-body systems. In particular, CA-EC can be combined with different techniques used to construct non-Hermitian Hamiltonians, and it therefore provides a path towards scalable resonance calculations for nuclear many-body systems.

## 1 Introduction

Resonances, i.e., metastable quantum states that behave similarly to bound states but decay after a finite lifetime, play an important role not only in nuclear physics—and there in particular for understanding exotic nuclei near the boundary of stability [1, 2]—but also in other areas of physics such as hadron physics or cold atomic systems. Making reliable theoretical predictions for broad many-body resonances continues to be a major challenge in quantum physics, and the exact nature of states, such as for example that of experimentally observed neutron-rich helium isotopes [3, 4], can consequentially remain controversial among theorists [5, 6].

Many theoretical approaches employ a quasi-stationary formalism in which resonances become manifest as complex energy eigenvalues of a non-Hermitian time-independent Hamiltonian. While elegant, such calculations for many-body systems suffer not only from a steep scaling of the numerical cost as the number of particles increases (which is generally true already for pure bound-state calculations), they also require the reliable identification of resonance energies within the complex spectrum of the Hamiltonian—a complicated task since most established eigenvalue algorithms for large matrices are designed or optimized to find extremal real eigenvalues.

The introduction of the eigenvector continuation (EC) technique [7], a form of a reduced-basis method (see Ref. [8] for a recent review), has opened interesting new avenues to address

this difficulty. Eigenvector continuation works by taking a Hamiltonian that is controlled by a set of parameters and represented in a given (typically very high-dimensional) Hilbert space to construct a low-dimensional subspace out of "training vectors" that are eigenstates of the original Hamiltonian at certain values of the parameters. It has been shown that diagonalizing the Hamiltonian projected into this small Hilbert space can provide highly accurate eigenstates at parameter values outside of the training set, and that it is even possible to extrapolate to regions in parameter space where direct "high-resolution" calculations in the original large Hilbert space would be difficult or impossible [7]. This property of EC is what enables the construction of highly accurate "emulators," i.e., small programs that can approximate otherwise expensive calculations at a small fraction of what the numerical cost would be otherwise [9]. This capability enables robust uncertainty quantification for theory predictions and detailed sensitivity studies; see for example Ref. [10] for an early demonstration. There are by now many other applications of EC emulators, with the status as of 2023 reviewed in Ref. [8].

The original EC method was introduced in Ref. [7] to efficiently approximate the eigenvalues $E(c)$ and eigenvectors $|\psi(c)\rangle$ of a Hermitian Hamiltonian $H(c)$, depending smoothly on the parameter $c$ (which can collectively represent multiple parameters). This is achieved by projecting the Hamiltonian $H(c_*)$ for the target parameter(s) $c_*$ of interest onto the reduced space spanned by a set of training states $\{|\psi_i\rangle : i = 1, \cdots, n_{\rm EC}\}$ and by then solving the generalized eigenvalue problem

$$H_{\rm EC}\,|\psi(c_*)\rangle_{\rm EC} = E(c_*)_{\rm EC}\,N_{\rm EC}\,|\psi(c_*)\rangle_{\rm EC} \tag{1}$$

with

$$(H_{\rm EC})_{ij} = \langle\psi(c_i)|H(c_*)|\psi(c_j)\rangle\ , \tag{2a}$$

$$(N_{\rm EC})_{ij} = \langle\psi(c_i)|\psi(c_j)\rangle\ . \tag{2b}$$

The first extension of EC to non-Hermitian Hamiltonians was presented in Ref. [11], which showed that not only can EC be applied to construct emulators for resonance states, but also that it is possible to use an extension of EC to extrapolate a state from the parameter regime where it is bound all the way to where it becomes a resonance. Further applications of EC, with a different focus, were later studied in Refs. [12–14]. This article will proceed to summarize the main findings of Ref. [11], and in particular the recent follow-up work that establishes a path towards bound-to-resonance extrapolations for few- and many-body systems [15].

## 2 Complex-Augmented Eigenvector Continuation

The first step towards developing EC for resonances is to construct a non-Hermitian extension of the Hamiltonian $H(c)$. Among the various ways to achieve this, the so-called "uniform complex scaling method" (see Ref. [16] for a review of complex scaling in general) stands out for its simplicity. For a two-body system with relative coordinate $\mathbf{r}$ and conjugate momentum $\mathbf{p}$, it amounts to the transformation

$$\mathbf{r} \to \mathbf{r}e^{i\phi}\,, \tag{3a}$$

$$\mathbf{p} \to \mathbf{p}e^{-i\phi}\,, \tag{3b}$$

where $\phi > 0$ is a real phase parameter. Therefore, under complex scaling, the Hamiltonian $H(c)$ transforms into

$$H(c) \to H_\phi(c) = \frac{\mathrm{e}^{-2\mathrm{i}\phi}\mathbf{p}^2}{2\mu} + V(c; \mathbf{r}\mathrm{e}^{\mathrm{i}\phi}) \,. \tag{4}$$

For few- and many-body applications, one can start by applying the complex scaling to the underlying single-particle coordinates and, possibly (depending on the particular method), propagating the scaling to the appropriate set of relative coordinates. As noted in Ref. [15], the free Hamiltonian $H_0$ will always pick up a scalar factor $\mathrm{e}^{-2\mathrm{i}\phi}$, while the potential energy operator needs to be evaluated with complex scaled arguments. For example, if $V$ is a local central two-body potential and $\mathbf{r}_{ij}$ is the relative distance between particles $i$ and $j$, then complex scaling is implemented as

$$V(\mathbf{r}_{ij}) \to V(\mathbf{r}_{ij}\mathrm{e}^{\mathrm{i}\phi}) \equiv V(|\mathbf{r}_{ij}|\mathrm{e}^{\mathrm{i}\phi}) \,. \tag{5}$$

Notably, the complex phase enters *after* calculating relative separations between particles.

Complex scaling turns an originally Hermitian Hamiltonian into a complex-symmetric one (in an assumed finite Hilbert space used to represent all operators as matrices, e.g., by discretization of continuous coordinates or by picking a discrete basis). As such, it can have complex eigenvalues, and resonance states appear as normalizable states in the spectrum. Specifically, one gains access to energy eigenstates with $\arg E < \phi$ in this manner, i.e., $\phi$ needs to be chosen large enough to "reveal" the states of interest (but small enough to prevent the complex-scaled potential to become pathological). The complex energies $E = E_R - \mathrm{i}\Gamma/2$ encode both the resonance position $E_R$ and the decay width $\Gamma$.

A two-body state with energy $E$ (for a system with reduced mass $\mu$) is characterized by an asymptotic momentum scale (or wave number) $k$ that is related to the energy as $E = k^2/(2\mu)$. Outside the range of the interaction (assuming a spherically symmetric pure short range potential), the reduced radial wave function in coordinate representation becomes

$$u_{l,k}(r) \sim \hat{h}_l^+(kr) \tag{6}$$

for a state with angular momentum $l$, where $\hat{h}_l^+(kr)$ is a Riccati-Hankel function that, in turn, behaves like an exponential $\mathrm{e}^{\mathrm{i}kr}$ for large $r$. If $E$ is complex, so is $k$, and a decaying resonance—located in the fourth quadrant of both the complex $E$ and $k$ planes—leads to an exponentially growing amplitude of the asymptotic wave function.[1] Complex scaling works because the rotation of $r$ with an angle $\phi > \arg E$ counteracts this exponential growth and renders the wave function normalizable when expressed along the rotated axis; this is illustrated in Fig. 1.

One peculiarity of complex scaling is that working with eigenstates of the complex-symmetric Hamiltonian requires that one replaces the standard inner product on the Hilbert space with the so-called "c-product" [17], which can be defined as

$$(\psi|\phi) = \langle\psi^*|\phi\rangle \,, \tag{7}$$

i.e., the c-product effectively *omits* the complex conjugation otherwise included for bra-side arguments. Although it is strictly not a proper inner product (it does not satisfy the positive-definiteness requirement and it is even possible to have self-orthogonal states), it has been shown that the eigenstates of the complex-scaled Hamiltonian are orthogonal and complete with respect to the c-product; see Refs. [18, 19] for a detailed discussion of the c-product.

[1] In the scattering ($S$) matrix for the system, taken as a function of complex momentum $k$, the resonance is associated with a pair of poles located at $k$ and $-k^*$, both appearing on the second Riemann sheet.

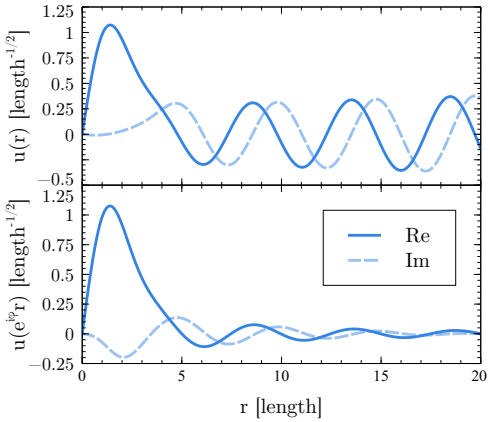


**Figure 1.** Radial resonance wave function calculated without (top panel) and with (bottom panel) complex scaling. Calculated wave function courtesy of N. Yapa.

As long as one stays entirely within the resonance regime (a range of values of $c$ for which a given state of interest remains a resonance throughout, only with varying position and width), Ref. [11] showed that EC can be trivially generalized to complex states by merely replacing the normal inner products in Eqs. (2) with the c-product. This enables the construction of emulators for resonance states, and in particular it is possible to extrapolate reliably from narrow (small $\Gamma \ll E_R$) to broad resonances ($\Gamma \sim E_R$) in this way.

Bound-state eigenvalues remain real under complex scaling [18, 19], but their wave functions become genuinely complex (i.e., they acquire a non-uniform complex phase). It was furthermore shown in Ref. [11] that a naive attempt to use EC with the c-product to extrapolate from bound states to resonances necessarily fails because $H_{\rm EC}$ will be real symmetric despite the underlying Hamiltonian being complex symmetric due to complex scaling. However, Ref. [11] furthermore introduced a strikingly simple way to circumvent this problem: by augmenting the EC subspace with the complex conjugates of all bound training states, reliable extrapolations from bound states to resonances become possible. For two-body states, Ref. [11] explained why this "complex-augmented eigenvector continuation (CA-EC)" works by analyzing the effective asymptotic wave numbers of the bound-state wave functions and their complex conjugates. It is not difficult to see that the complex conjugate states equip the EC subspace with the basis states necessary to represent the (complex-scaled) resonance wave function at the target point in the asymptotic region, while the interior part of the target resonance wave function can be represented equally well with either the original bound states or their complex conjugates (although the description of the interior part in general also benefits from having a larger EC subspace).

In Ref. [15] this argument was refined and extended to general few-body states: a bound eigenstate $|\psi\rangle$ that in coordinate space is described by a wave function $\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots)$ (with a suitable set of coordinates $\mathbf{r}_i$ with corresponding mass factors $\mu_i$) satisfies

$$H\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots) = -\sum_{i=1}^{n-1} \frac{\nabla_i^2}{2\mu_i} \psi(\mathbf{r}_1, \mathbf{r}_2, \cdots) = E\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots) \quad \text{as} \quad |\mathbf{r}_i| \to \infty \tag{8}$$

in the asymptotic regime, where all interactions can be neglected. For simplicity, the parametric dependence on $c$ is not written explicitly here. Under complex scaling, indicated with

a subscript $\phi$ on $H$ and $\psi$, this becomes

$$H_\phi \psi_\phi(\mathbf{r}_1, \mathbf{r}_2, \cdots) = -\mathrm{e}^{-2\mathrm{i}\phi} \sum_{i=1}^{n-1} \frac{\nabla_i^2}{2\mu_i} \psi_\phi(\mathbf{r}_1, \mathbf{r}_2, \cdots) = E\psi_\phi(\mathbf{r}_1, \mathbf{r}_2, \cdots) \quad \text{as} \quad |\mathbf{r}_i| \to \infty \,. \tag{9}$$

Taking the complex conjugate of this equation (noting the $E$ is real for a bound state even with complex scaling), and multiplying both sides by $\mathrm{e}^{-4\mathrm{i}\phi}$ gives

$$H_\phi \psi_\phi^*(\mathbf{r}_1, \mathbf{r}_2, \cdots) = \mathrm{e}^{-4\mathrm{i}\phi} E\, \psi_\phi^*(\mathbf{r}_1, \mathbf{r}_2, \cdots) \quad \text{as} \quad |\mathbf{r}_i| \to \infty \,. \tag{10}$$

This equation shows that in the asymptotic regime, the complex scaled bound-state wave function behave just like decaying resonance, and therefore including these complex scales bound states in the EC subspace basis enables extrapolations to such states.

## 3 Numerical Implementations

In Ref. [11], complex scaling and EC for resonances was implemented using a momentum-space formulation of the two-body Schrödinger equation. One obtains wave functions the rotated line of complex momentum modes (up to some maximum momentum $p_{\max}$ the choice appropriate choice of which depends on the properties of the potential), by solving the Schrödinger equation in integral form, turned into a linear matrix equation upon discretization.

This initial proof of concept was extended in Ref. [15] to the few-body sector using several different numerical techniques. This work shows that resonance EC and, in particular, CA-EC for extrapolating from bound states to resonances perform well independent of the particular method used to construct the non-Hermitian Hamiltonian. Specifically, Ref. [15] used a discrete variable representation (DVR) in finite volume (for which complex scaling has been developed in Ref. [20]) as well as a configuration interaction (CI) method based on harmonic oscillator (HO) states. In addition, a Berggren basis [21, 22] was used in both a direct construction for a three-body model system, as well as in a Gamow Shell Model (GSM) [23] calculation.

## 4 Examples

As mentioned above, if one stays entirely within the resonance regime for both training and target points, EC works for resonances with no modifications other than using the c-product for computing the matrix elements of $H_{\mathrm{EC}}$ and $N_{\mathrm{EC}}$. In Ref. [11], this was demonstrated for resonances generated by a potential of the form

$$V(c; r) = c\left[-5\mathrm{e}^{-r^2/3} + 2\mathrm{e}^{-r^2/10}\right], \tag{11}$$

where $c$ is the tunable parameter used for EC. The ranges and widths of the two Gaussians in Eq. (11) have been chosen arbitrarily, and their precise values do not matter much for the demonstration: one only needs to find a suitable combination of attractive and repulsive terms to generate an S-wave ($l = 0$) resonance, and in higher partial waves ($l > 0$) one can also use a purely attractive potential, with repulsion provided by the centrifugal barrier. In Ref. [11], the momentum-space version of Eq. (11) was used for the numerical calculations, one example of which is reproduced here in Fig. 2. For these calculations, five training points were randomly drawn from the region $c \in (0.45, 0.78)$, and for each target point this extrapolation was repeated multiple times in order to obtain the results with estimated uncertainties. It is evident from the figure, that this procedure works very well.

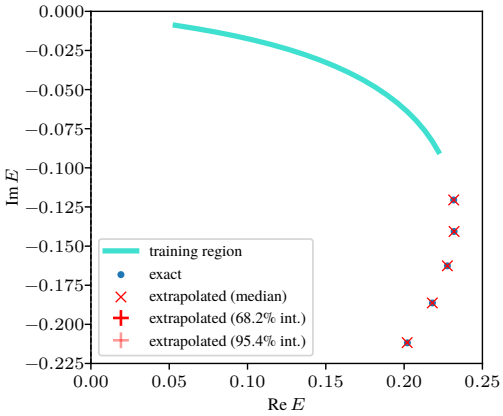


**Figure 2.** Application of EC for resonance-to-resonance extrapolation; see text for details.

For the same potential as given in Eq. (11), one can choose values for $c$ that generate a bound state and train the EC emulator in that regime only. Ref. [11] found that with a naive approach this procedure will only give extrapolated energies that are also real, but CA-EC can be used to obtain accurate results at target values of $c$ where the exact calculation yields a complex-energy resonance state. This is demonstrated in Fig. 3, which shows the case where training points were randomly drawn from the region $c \in (0.9, 1.3)$, using five training points for each extrapolation, and producing an uncertainty estimate by averaging over multiple such evaluations.

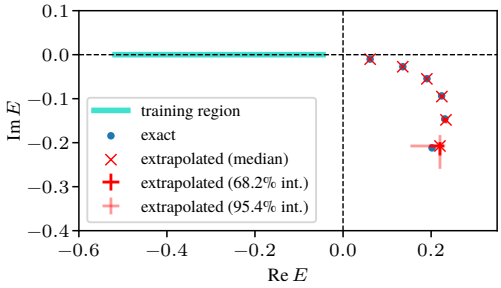


**Figure 3.** Bound-state-to-resonance extrapolation performed with CA-EC; see text for details.

As mentioned previously, Ref. [15] generalized CA-EC to the few- and many-body sector, based on arguing that complex-conjugated bound-state wave functions behave similar to decaying resonances in the domain of coordinate space where all interactions between particles can be neglected, as summarized above in Eqs. (8) to (10). This is relevant because for a state comprised out of more than two particles, its energy can no longer be associated with a single momentum scale that alone determines the asymptotic behavior of the wave function. Instead, there are in general multiple scales corresponding to the various different ways in which the constituents can be separated. In this sense, extending CA-EC from two- to three-body systems presents the most important step, with not much further difficulty to

be expected beyond that (other than, of course, the fact that numerical calculations with fully dynamical degrees of freedom become increasingly challenging as the number of particles grows).

Ref. [15] studied the performance of CA-EC for three-body systems based on assuming that the interaction between any pair of particles is given by

$$V(r) = 2\,\mathrm{e}^{-\left(\frac{r-3}{1.5}\right)^2}. \tag{12}$$

This form was chosen because Refs. [20, 24] showed that with this interaction the system supports a bosonic three-body resonance near $\mathrm{Re}\,E \approx 4.1$. Moreover, this is a genuine three-body resonance because the potential does not support any bound two-body subsystems. To provide bound training states for CA-EC, one can add an attractive term so that the total interaction becomes

$$V(r) = 2\,\mathrm{e}^{-\left(\frac{r-3}{1.5}\right)^2} - c\,\mathrm{e}^{-\left(\frac{r}{3}\right)^2}, \tag{13}$$

with $c$ controlling the degree of the added attraction. Results for CA-EC extrapolations performed for this system are shown in Fig. 4, comparing numerical implementations with three different methods: (a) complex-scaled CI using a HO basis, (b) finite-volume DVR, and (c) a Berggren basis. All these approaches, along with original references, are discussed in more detail in Ref. [15]. Repeating the calculation for the same system with these different methods is useful to demonstrate that indeed CA-EC works well and reliably independent of the concrete details of how it is implemented: as can be seen in Fig. 4, the performance is similar for all three different approaches. These calculations were performed using five bound-state training points, corresponding to $c = -2.6, -2.4, -2.2, -2.0, -1.8$, and the extrapolated results shown are, from left to right in the plots, for $c = -1.2, -0.8, -0.4, -0.2, 0.0$.

In addition to performing this important benchmark, Ref. [15] furthermore demonstrated that CA-EC continues to work well also for a three-body resonance that decays into a two-body bound state plus a third particle, and, to highlight the path towards scalable many-body calculations of resonances, that the method also works with the GSM. That last point is demonstrated by tuning the $^6$He system in such a way that its ground state becomes a resonance.

## 5 Conclusion and Outlook

References [11] and [15] have established CA-EC—and more generally EC for resonances using a non-Hermitian formulation—as a powerful method for few- and many-body calculations. Not only has it been shown that emulators for resonances can be constructed within the non-Hermitian realm, CA-EC in particular makes it possible to reliably extrapolate a state all the way from being bound to becoming a resonance. This is not only fascinating in itself, it is also relevant for practical calculations: in a non-Hermitian large-scale calculation, it can be very difficult to identify resonance states of interest within the overall complex spectrum. Bound states, on the other hand, can easily be identified as extremal (and real) eigenvalues with established numerical methods such as Arnoldi iteration. Eigenvector continuation can then be used to track states that were made bound by some artificially added attraction back to the physical point of interest, in a rigorous manner. Therefore, CA-EC opens the door to scalable calculations of nuclear many-body resonances.

Performing such calculations, in particular for potential exotic nuclear states identified in systems such as $^9$N [25], will be a very interesting application of the technique. To that end, a further extension to systems with multiple charged particles (where consequently the

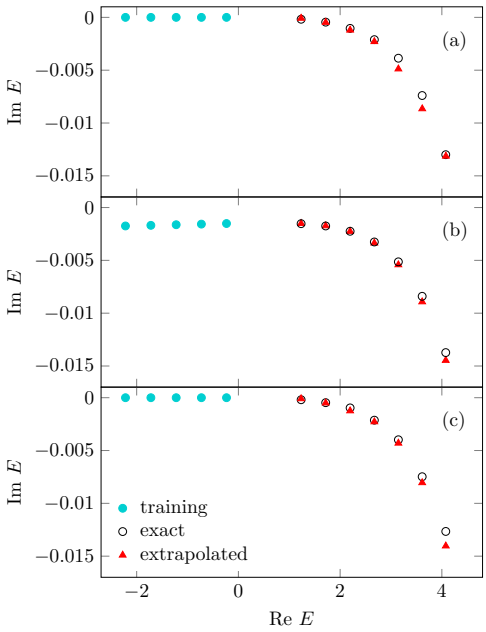


**Figure 4.** Bound-to-resonance extrapolation for the three-boson system carried out under (a) complex-scaled CI in HO basis, (b) complex-scaled finite-volume basis and (c) Berggren basis; see text for details.

Coulomb interaction plays a role for describing their A asymptotic wave functions) is required, and currently work in progress. It also remains to be investigated whether EC can be useful for studying anti-bound (virtual) states.

Beyond these aspects, it is also relevant to explore how CA-EC (and EC in general) can be useful in connection with effective field theories (EFTs). In particular, it has been observed that in some scenarios (see, for example, Refs. [26–28]), a state that is bound for relatively low values of the EFT regulator scale (e.g., a momentum cutoff) may disappear into a threshold as the regulator scale is increased, presumably to become a resonance at that point. Eigenvector Continuation, applied to the regulator scale as relevant parameter—along with the low-energy constants of the theory that "run" with the regulator scale according to the renormalization group (RG)—could provide an elegant way to explicitly track such states from the bound-state to the resonance regime. Of course, the feasibility of such an investigation remains predicated on the availability of a suitable non-Hermitian extension for the relevant computational method. In addition, it will be very interesting to study how EC can be applied in an EFT context beyond leading order, where maintaining RG invariance generally requires that higher-order interactions be treated in perturbation theory [29].

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