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The complex-scaling method using a complete L^2 -basis

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Abstract. A complete set of square-integrable basis functions is used to find the matrix elements of the rotated model Hamiltonian in which the reference Hamiltonian is fully taken into account while the interchannel potential is approximated by its representation in the finite subset of the complete basis. Since the spectrum of the model Hamiltonian satisfies the Aguilar–Balslev–Combes theorem, the only discrete eigenvalues of the complex-scaled Hamiltonian are the system's bound states and complex resonance energies. We propose an efficient method to locate these resonance energies and show that they converge faster than the eigenvalues of the complex-scaled Hamiltonian using a finite basis, while being less sensitive to the variation of the rotation angle.

The complex-scaling method has been one of the most successful methods for studying resonances. Its basis is rigorously supported by the Aguilar–Balslev–Combes (ABC) theorem [1, 2]. Given a dilation analytic potential, one transforms the Hamiltonian $H = H_0 + V$ into what is termed a complex-scaled Hamiltonian $H_\theta = U(\theta)HU^{-1}(\theta)$, where $U(\theta)$ acts on any function $f(r)$ as

$$U(\theta)f(r) = e^{i\theta/2}f(re^{i\theta}). \quad (1)$$

The ABC theorem in essence states that the bound states of H remain unchanged even after transformation while the continuous spectrum is rotated by an angle of 2θ . The significant implication of the ABC theorem is that the complex resonance energy $\varepsilon_r = E_r - i\Gamma/2$ ($\Gamma > 0$) will be an isolated eigenvalue of the Hamiltonian, H_θ , provided it is exposed by rotation; i.e. $\theta > \theta_c$ where the critical angle $\theta_c = |\arg \varepsilon_r|/2$.

The most practical implementation of the complex-scaling method is by utilizing a finite set of square-integrable basis $\{|\phi_n\rangle\}_{n=0}^{N-1}$ to construct an $N \times N$ matrix representation of H_θ . This construction is accomplished either by calculating the quantities $\{\langle\phi_n|H_\theta|\phi_m\rangle\}_{n,m=0}^{N-1}$ or alternatively the matrix elements $\{\langle\phi_n^\theta|H|\phi_m^\theta\rangle\}_{n,m=0}^{N-1}$, where the complex basis is given by $|\phi_n^\theta\rangle = U^{-1}(\theta)|\phi_n\rangle$. This last alternative method has the advantage of dealing easily with non-analytic potentials such as the square well [3]. The question of convergence of the computed resonance energy as θ and N vary is not as straightforward for the complex-scaled Hamiltonian as it is for the non-rotated self-adjoint Hamiltonian due to the lack of a bounding principle, similar to the Hylleraas–Undheim theorem, to impose on the computed

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eigenvalues [4]. Nonetheless, several empirical techniques have been used to suggest when the choices of parameters are optimum [5–7]. An important point to note in the use of the complex-scaling method is that the ABC theorem is a statement about the Hamiltonian operator, H_θ , while actual implementation of the method deals with \tilde{H}_θ , the finite matrix representation of H_θ . The only discrete energy eigenvalues of the operator, H_θ , are the system bound states and the exposed complex resonance energies, while the spectrum of \tilde{H}_θ is totally discrete. The set of discrete complex energies of \tilde{H}_θ mimicking the rotated continuum of H_θ does not exactly lie on the line of the rotated continuum except in the limit of high matrix size, N [6]. While this causes little confusion in identifying the resonance energy, the use of a complete set of basis functions that fully accounts for the reference Hamiltonian, H_0 , leads to a truly rotated continuous spectrum while the discrete spectrum is then limited to the system bound states and resonance energies.

In this paper, we show that the J -matrix method [8,9] of scattering provides a setting for the rigorous application of the ABC theorem. The method utilizes a complete square-integrable basis which renders the representation of the reference Hamiltonian,

$$H_0 = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2r^2} \quad (2)$$

tridiagonal. The given short-range potential, V , is replaced by a model \tilde{V} whose matrix elements are defined as

$$\langle \phi_n | \tilde{V} | \phi_m \rangle = \begin{cases} \langle \phi_n | V | \phi_m \rangle & 0 \leq n, m \leq N-1 \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

In fact, \tilde{V} is the approximate potential considered in the usual complex-scaling method, which also subjects the reference Hamiltonian, H_0 , to the same approximation. Additionally, the use of the complete basis simply means that the part of the reference Hamiltonian that is left out in the usual finite basis calculation is now accounted for. Thus, the location of the resonance will be more accurate although not substantially modified. This means that we may use the approximate location of the resonance, as given by the finite basis calculation, as a seed to an appropriate search scheme for the resonance associated with the complete basis calculation.

It is convenient to define such a search scheme by using the J -matrix method set up in the orthonormal oscillator basis $\{|\phi_n\rangle\}_{n=0}^\infty$ where

$$\langle r | \phi_n \rangle = \phi_n(r) = a_n (\lambda r)^{\ell+1} e^{-\lambda^2 r^2/2} L_n^{\ell+1/2}(\lambda^2 r^2). \quad (4)$$

Here, λ is a free scale parameter, $L_n^v(x)$ are the generalized Laguerre polynomials of order n , and $a_n = \sqrt{2\lambda n! / \Gamma(n + \ell + 3/2)}$ to ensure orthonormality; i.e.

$$\langle \phi_n | \phi_m \rangle = \delta_{nm}. \quad (5)$$

The model potential, \tilde{V} , may now be written in the form

$$\tilde{V} = P V P \quad (6)$$

where the projection operator, P , is given by

$$P = \sum_{n=0}^{N-1} |\phi_n\rangle \langle \phi_n|. \quad (7)$$

Unlike the usual complex-scaling method which also models the reference Hamiltonian, H_0 , as \tilde{H}_0 , we now consider it in its entirety.

In fact, we are able [9, 10] to find a sine-like eigenvector for H_0

$$|S(\varepsilon)\rangle = \sum_{n=0}^{\infty} s_n(\varepsilon)|\phi_n\rangle \tag{8}$$

and also an asymptotically cosine-like eigenvector

$$|C(\varepsilon)\rangle = \sum_{n=0}^{\infty} c_n(\varepsilon)|\phi_n\rangle \tag{9}$$

with known coefficients $\{s_n, c_n\}_{n=0}^{\infty}$. Details have already been given elsewhere [11, 12].

We now proceed by considering the poles of the S -matrix in the second sheet of the complex energy plane as the definition of resonances. Equivalently, the complex resonance energy is the zero of the Fredholm determinant $\tilde{D}^{(+)}(\varepsilon)$, where

$$\tilde{D}^{(+)}(\varepsilon) = \det(1 + G_0^{(+)}(\varepsilon)\tilde{V}) \tag{10}$$

and $G_0(\varepsilon) = (H_0 - \varepsilon)^{-1}$. By utilizing the form of the potential V given by equation (6), we find that the determinant has the simpler form

$$\tilde{D}^{(+)}(\varepsilon) = \det(1_{PP} + (G_0^{(+)})_{PP}(\varepsilon)\tilde{V}_{PP}) \tag{11}$$

where $A_{PP} = PAP$ for an operator A . This form can be evaluated *exactly*. In fact with $J(\varepsilon) = (H_0 - \varepsilon)$, we may write

$$\begin{aligned} J_{PP}(G_0)_{PP} + J_{PQ}(G_0)_{QP} &= 1_{PP} \\ J_{QP}(G_0)_{PP} + J_{QQ}(G_0)_{QP} &= 0 \end{aligned} \tag{12}$$

where $Q = 1 - P$. Since J has a tridiagonal matrix representation in the basis $\{|\phi_n\rangle\}_{n=0}^{\infty}$, it is not hard to show that

$$(G_0^{(+)})_{PP} = [J_{PP} - |\phi_{N-1}\rangle J_{N-1,N} Z_{NN}^{(+)} J_{N,N-1} \langle\phi_{N-1}|]^{-1} \tag{13}$$

where $Z = (J_{QQ})^{-1}$ and $J_{N-1,N} = \langle\phi_{N-1}|J|\phi_N\rangle$. Thus, we may write

$$\tilde{D}^{(+)}(\varepsilon) = \frac{\det(J + V)_{PP}}{\det(J)_{PP}} \frac{\det(1_{PP} - Y_{PP}^{(+)})}{\det(1_{PP} - (Y_0^{(+)})_{PP})} \tag{14}$$

where $Y_{PP}^{(+)} = g_{PP}|\phi_{N-1}\rangle J_{N-1,N} Z_{NN}^{(+)} J_{N,N-1} \langle\phi_{N-1}|$ with $g_{PP} = [J_{PP} + V_{PP}]^{-1}$. Also $(Y_0^{(+)})_{PP}$ is the potential-free version of $Y_{PP}^{(+)}$ with the correspondence $(g_0)_{PP} = (J_{PP})^{-1}$.

Several points can be made regarding the above expression for $\tilde{D}^{(+)}(\varepsilon)$.

(1) Because it is a determinant, it can be evaluated in any basis including the complex rotated basis. Of course, we have to be careful to identify the domain of validity of the resulting determinant in the complex energy plane.

(2) The quantity $\det(J_{PP} + V_{PP})$ and $\det(J_{PP})$ are the finite products $\prod_{i=0}^{N-1} (\varepsilon_i - \varepsilon)$ and $\prod_{i=0}^{N-1} ((\varepsilon_0)_i - \varepsilon)$, respectively, where $\{\varepsilon_i\}_{i=0}^{N-1}$ is the set of the eigenvalues of the finite Hamiltonian matrix, \tilde{H} , and $\{(\varepsilon_0)_i\}_{i=0}^{N-1}$ is the set of eigenvalues of \tilde{H}_0 in the chosen basis.

(3) The finite matrices, g and g_0 , are the inverse of $(\tilde{H} - \varepsilon)$ and $(\tilde{H}_0 - \varepsilon)$ in the same basis, respectively. Thus they have poles at corresponding eigenvalues of \tilde{H} and \tilde{H}_0 .

(4) The denominator of the above expression for the Fredholm determinant $\tilde{D}^{(+)}(\varepsilon)$ is a product of two quantities, one having zeros at $\{(\varepsilon_0)_i\}_{i=0}^{N-1}$ and the other having poles at the same points coming from g_0 . The overall result is that the denominator does not vanish at $\{(\varepsilon_0)_i\}_{i=0}^{N-1}$. Furthermore, it is a smooth function of energy except for the branch cut associated with Z . This is the same branch cut associated with G_0 and becomes rotated when a complex-scaled basis is used.

(5) The numerator of the above expression does not have zeros at the set of energy points $\{\varepsilon_i\}_{i=0}^{N-1}$, for an analogous reason as in the previous point.

However, it has a zero at the complex energies where

$$\det(1_{PP} - Y_{PP}^{(+)}) = 0. \tag{15}$$

These energies are the system's bound states and resonance energies. Equation (15) also provides a computational tool to define our search scheme for the complex resonance energies. In fact, the operator, $(1_{PP} - Y_{PP})$, has a simple $N \times N$ matrix representation in the finite basis $\{|\phi_n\rangle\}_{n=0}^{N-1}$: it has a non-trivial last column but otherwise has unity along the diagonal. Thus

$$\det(1_{PP} - Y_{PP}) = \{1 - g_{N-1,N-1} J_{N-1,N} Z_{NN}^{(+)} J_{N,N-1}\}. \tag{16}$$

Furthermore, we have shown previously [13] that $J_{N-1,N} Z_{NN}^{(+)} = -R_N^{(+)}$ where

$$R_N^{(+)} = \begin{pmatrix} c_N + is_N \\ c_{N-1} + is_{N-1} \end{pmatrix}. \tag{17}$$

Thus the resonances are the complex energies satisfying

$$[1 + g_{N-1,N-1} J_{N-1,N} R_N^{(+)}] = 0 \tag{18}$$

in the second sheet of the complex energy plane. This equation can be solved using the very fast Newton–Raphson search technique starting with the approximate resonance given by the finite basis calculation as a seed.

The generalization to multi-channel scattering is straightforward. We consider the scattering of structureless spinless particles from a target with M internal states labelled by the channel threshold energies $\tilde{E}_1, \tilde{E}_2, \dots, \tilde{E}_M$. We associate with each channel a complete set of basis $\{|\phi_n^{(\alpha)}\rangle\}_{n=0}^{\infty}$ with an associated scale parameter, λ_α , which may be different for each channel. The projection operator, P_α , is defined as in equation (7) for each channel in terms of the channel basis. We model the given physical potential, $V^{\alpha\beta}$, by the potential, $\tilde{V}^{\alpha\beta}$, as

$$\tilde{V}^{\alpha\beta} = P_\alpha V^{\alpha\beta} P_\beta. \tag{19}$$

The multi-channel Fredholm determinant can be defined in an analogous manner to the one-channel potential case. The condition for the resonance equation (15) is the same, while its explicit form is a generalization of equation (18), namely,

$$\det \begin{pmatrix} 1 + g_{N_1-1,N_1-1}^{(1,1)} J_{N_1-1,N_1}^{(1)} R_{N_1}^{(+)} & g_{N_1-1,N_2-1}^{(1,2)} J_{N_2-1,N_2}^{(2)} R_{N_2}^{(+)} & \dots \\ g_{N_2-1,N_1-1}^{(2,1)} J_{N_1-1,N_1}^{(1)} R_{N_1}^{(+)} & 1 + g_{N_2-1,N_2-1}^{(2,2)} J_{N_2-1,N_2}^{(2)} R_{N_2}^{(+)} & \dots \\ \dots & \dots & \dots \\ g_{N_M-1,N_1-1}^{(M,1)} J_{N_1-1,N_1}^{(1)} R_{N_1}^{(+)} & g_{N_M-1,N_2-1}^{(M,2)} J_{N_2-1,N_2}^{(2)} R_{N_2}^{(+)} & \dots \\ \dots & g_{N_1-1,N_M-1}^{(1,M)} J_{N_M-1,N_M}^{(M)} R_{N_M}^{(+)} & \dots \\ \dots & g_{N_2-1,N_M-1}^{(2,M)} J_{N_M-1,N_M}^{(M)} R_{N_M}^{(+)} & \dots \\ \dots & \dots & \dots \\ \dots & 1 + g_{N_M-1,N_M-1}^{(M,M)} J_{N_M-1,N_M}^{(M)} R_{N_M}^{(+)} & \dots \end{pmatrix} = 0. \tag{20}$$

Here, $J^{(\alpha)} = H_0 - (E - \tilde{E}_\alpha)$ and $R_{N_\alpha}^{(+)} = ((c_{N_\alpha}^{(\alpha)} + is_{N_\alpha}^{(\alpha)}) / (c_{N_\alpha-1}^{(\alpha)} + is_{N_\alpha-1}^{(\alpha)}))$ and $g^{(\alpha,\beta)}$ is the (α, β) submatrix of the finite matrix, $(\tilde{H} - \varepsilon)^{-1}$. The Newton–Raphson search technique can also be used to find the resonance energy as the solution of equation (20).

We have applied the method to the two-channel potential problem

$$V^{\alpha\beta} = V_0^{\alpha\beta} r^2 e^{-r}$$

where

$$V_0^{\alpha\beta} = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix} \quad (21)$$

which has recently been used in the literature [14]. This potential possesses many resonances. We choose to focus our attention on the one located at $\varepsilon_r = 7.2412 - i0.7559$, where the critical angle $\theta_c = 0.052$ rad. In tables 1–3 we compare the behaviour of the position of the resonance, as given by complex scaling with finite and complete oscillator bases, in terms of the relevant parameters, namely the rotation angle, θ , the scale parameter, λ , and the size of the potential matrix size, N . In table 1 we see that complex scaling with a complete basis gives an accurate value of the resonance energy as soon as θ exceeds the critical value, θ_c , while complex scaling with a finite basis requires θ to be distinctively larger than θ_c before yielding comparably accurate results. Even when θ is far away from θ_c , table 2 shows complex scaling with a complete basis is less sensitive to the choice of scale parameter, λ , while the range of λ giving accurate values is narrower for the finite basis. In table 3, we find that complex scaling with a complete basis converges faster than complex scaling with a finite basis as a function of the potential matrix size, N . The difference is more pronounced when $\theta = 0.1$ rad, which is closer to θ_c than the choice $\theta = 0.2$ rad.

Table 1. The resonance energy $\varepsilon = E_r - i\Gamma/2$ for the potential (21) using a complex-scaled oscillator basis with free scale parameter $\lambda = 1.0$ and $N = 30$, and different rotation angles obtained by using both finite and complete bases.

θ (rad)	Finite basis		Complete basis	
	E_r	$\Gamma/2$	E_r	$\Gamma/2$
0.055	6.9652	0.5028	7.2794	0.7975
0.06	6.9742	0.5462	7.2619	0.7846
0.07	6.9984	0.6312	7.2487	0.7687
0.08	7.0345	0.7123	7.2443	0.7617
0.09	7.0922	0.7853	7.2426	0.7586
0.10	7.1870	0.8129	7.2419	0.7572
0.12	7.2352	0.7658	7.2414	0.7562
0.14	7.2399	0.7578	7.2413	0.7560
0.16	7.2409	0.7563	7.2413	0.7560
0.18	7.2412	0.7560	7.2412	0.7560
0.20	7.2412	0.7560	7.2412	0.7560
0.25	7.2412	0.7560	7.2412	0.7560
0.30	7.2412	0.7559	7.2412	0.7559

To understand the above behaviour, we note that using a complex-scaled basis as given by equation (4) is equivalent to using the basis with complex scale parameter, λ ; i.e. $\lambda \rightarrow |\lambda|e^{i\theta}$. This means that the basis diffuseness is controlled by the parameter, $|\lambda|\sqrt{\cos 2\theta}$, rather than $|\lambda|$ alone. Thus, for a given λ , θ and N the finite basis has to represent well the short-range potential, especially within its range, and also the reference Hamiltonian, H_0 , whose influence extends far beyond the limit range of the potential. For the complete basis, the parameters λ , θ and N have to permit the first N members of the basis to represent well the potential. The rest of the complete basis is able to represent H_0 fully, regardless

Table 2. The resonance energy $\varepsilon = E_r - i\Gamma/2$ for the potential (21) using a complex-scaled oscillator basis with $N = 30$, rotation angle $\theta = 0.2$ rad, and different free scale parameters obtained by using both finite and complete bases.

λ	Finite basis		Complete basis	
	E_r	$\Gamma/2$	E_r	$\Gamma/2$
0.6	7.2429	0.7546	7.2414	0.7559
0.7	7.2416	0.7557	7.2414	0.7559
0.8	7.2414	0.7559	7.2414	0.7559
1.0	7.2412	0.7560	7.2412	0.7560
1.2	7.2411	0.7559	7.2412	0.7560
1.4	7.2417	0.7561	7.2412	0.7560
1.6	7.2420	0.7574	7.2412	0.7560
1.8	7.2458	0.7567	7.2413	0.7560
2.0	7.2376	0.7458	7.2414	0.7554
2.2	7.2482	0.7809	7.2403	0.7576
2.4	7.2149	0.7242	7.2407	0.7510
2.6	7.3024	0.7232	7.2523	0.7595

Table 3. The resonance energy $\varepsilon = E_r - i\Gamma/2$ for the potential (21) using a complex-scaled oscillator basis with free scale parameter $\lambda = 1.0$ and rotation angles $\theta = 0.1$ and 0.2 rad, and different basis size obtained by using both finite and complete bases.

θ (rad)	N	Finite basis		Complete basis	
		E_r	$(\Gamma/2)$	E_r	$(\Gamma/2)$
0.1	10	7.3065	0.5635	7.2819	0.6991
	20	7.2445	0.6783	7.2385	0.7528
	30	7.1870	0.8129	7.2419	0.7572
	40	7.2388	0.7914	7.2416	0.7562
	50	7.2254	0.7588	7.2411	0.7562
	60	7.2445	0.7480	7.2411	0.7559
	70	7.2387	0.7617	7.2412	0.7560
	80	7.2444	0.7540	7.2412	0.7560
0.2	5	7.1720	0.6827	7.2459	0.7906
	10	7.2520	0.7467	7.2454	0.7495
	15	7.2409	0.7568	7.2409	0.7560
	20	7.2413	0.7558	7.2412	0.7560
	25	7.2412	0.7559	7.2412	0.7560
	30	7.2412	0.7560	7.2412	0.7559

of the parameters λ and θ . Thus complex scaling with a complete basis is less sensitive to the parameters λ and θ , and converges faster in the parameter N .

The method outlined above may also be set up in terms of the non-orthogonal Laguerre basis

$$\phi_n(r) = b_n(\lambda r)^{\ell+1} e^{-\lambda r/2} L_n^{2\ell+2}(\lambda r) \quad (22)$$

with $b_n = \sqrt{\lambda n! / \Gamma(n + 2\ell + 2)}$.

The matrix representation of the kinetic operator of equation (2) is tridiagonal in this basis [9, 10]. Furthermore, the overlap matrix $\langle \phi_n | \phi_m \rangle$ is itself tridiagonal. What is also of interest, is the fact that the matrix element of the Coulomb term (z/r) is actually diagonal

in this basis [9, 10]. The above facts give the non-orthogonal Laguerre basis the advantage over the orthogonal oscillator basis of equation (4) of being able to account fully for the kinetic energy operator plus the Coulomb term, (z/r) . In the case of scattering of a charged projectile off a charged target, the Hamiltonian contains a Coulomb term and an additional short-range potential. In this case, the reference Hamiltonian, H_0 , contains, in addition to the kinetic energy term of equation (2), the Coulomb term, (z/r) . This reference Hamiltonian can be solved *exactly* in the non-orthogonal Laguerre basis. The additional short-range potential is approximated as in the scheme described in equation (6). Of course $J_{N_\alpha-1, N_\alpha}$ and $R_{N_\alpha}^{(+)}$ for each channel are to be calculated in the above Laguerre basis.

As an example, we again consider the potential (21) with $z = -1.0$ and $+1.0$. Here we focus our attention on the resonances located at $\varepsilon_r = 6.3861 - i0.3517$ and $6.2780 - i1.843E-2$ for $z = -1.0$ and $+1.0$, respectively. Table 4 shows that the conclusion reached in the oscillator case regarding convergence is also valid in the Laguerre case.

Table 4. The resonance energy $\varepsilon = E_r - i\Gamma/2$ for the potential (21) for the cases $z = \pm 1.0$, using a complex-scaled Laguerre basis with free scale parameter $\lambda = 3.0$ and rotation angle $\theta = 0.1$ rad, and different basis size obtained by using finite and complete bases.

z	N	Finite basis		Complete basis	
		E_r	$(\Gamma/2)$	E_r	$(\Gamma/2)$
-1.0	10	6.6126	0.3134	6.3484	0.4163
	20	6.2961	0.4906	6.3766	0.3511
	30	6.4188	0.3513	6.3867	0.3539
	40	6.3788	0.3429	6.3862	0.3511
	50	6.3886	0.3553	6.3861	0.3517
	60	6.3855	0.3502	6.3861	0.3516
+1.0	10	6.2749	2.279×10^{-2}	6.2750	1.814×10^{-2}
	20	6.2767	1.806×10^{-2}	6.2780	1.830×10^{-2}
	30	6.2778	1.872×10^{-2}	6.2780	1.843×10^{-2}
	40	6.2781	1.844×10^{-2}	6.2780	1.844×10^{-2}
	50	6.2780	1.842×10^{-2}	6.2780	1.843×10^{-2}
	60	6.2780	1.842×10^{-2}	6.2780	1.843×10^{-2}

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