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Computation of Resonances and Bound States Using J-Matrix Approach

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The poles of the S-matrix, which represent both resonances and bound states, are being investigated numerically using the J-matrix approach in an infinite L^2 basis set. These poles are found to be stable against variations in all computational parameters. To test the accuracy and validity of this approach we have implemented our scheme to find the resonance and bound state energies for a well known test potential and compared our results favorably with those obtained previously in the literature.

Keywords: Resonance energies, algebraic scattering, J-matrix, S-matrix.

The study of resonance energies associated with the scattering of a projectile by a target is of fundamental importance for the understanding of both the structure of the target and the nature of the interaction of the projectile-target system [1]. Hence different numerical methods have been devised to compute the resonance energies which are complex in nature. Complex rotation (CR) method has been one of the most successful methods for studying resonances. It is based on the rigorous theoretical work of Aguilar-Balslev-Combes (ABC) theorem [2]. This theorem states in essence that if the original Hamiltonian is transformed under complex rotation $r \rightarrow re^{i\theta}$, where θ is a real angular parameter, then the complex eigenvalues associated with resonances will be isolated and remain unchanged under this transformation while the continuous energy spectrum mimicked by the discrete spectrum will be rotated by - 2θ in the complex energy plane. The key element of the complex rotation method is the extension of the original Hamiltonian into the non-Hermitian domain.

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The associated eigenvalues of the resulting non-Hermitian Hamiltonian are complex in nature, with the real part representing the position of the resonance, and the imaginary part giving the inverse lifetime.

The most direct way to compute the resonances, however, is based on the more accurate definition of the resonances as being the poles of the scattering S-matrix in the complex energy plane.

One can show that each element of the S-matrix is singular at the complex resonance energy E

$$S^{-1}(E) = 0, \qquad E = E_R \pm\ i\ E_I.$$

This condition is sufficient for obtaining the resonance position E_R and width $\Gamma = 2E_I$. Several methods to find the complex resonance energies of a given scattering Hamiltonian are available. There are many techniques that enable us to evaluate the S-matrix, one approach is to use the Jost function and its analytic properties [3-5], in another approach Yamani & Abdelmonem [6] showed how to calculate the S-matrix at the Harris eigenvalues and, subsequently analytically continue it in the complex energy plane and then extract the required resonance information from the analytically continued S-matrix. In our present work we will combine the analytical properties of the S-matrix, the complex rotation and the J-matrix approach [7]. In our previous work [8] we have contented ourselves by using the complex rotation in a finite dimensional space spanned by L^2 basis. Due to the finiteness of the dimensional space the accuracy of our numerical results was limited, any additional improvement request larger spaces and consequently more computational times. Since the objective of all computational schemes is to increase the accuracy and to improve the efficiency in locating the resonance positions and widths without extending the numerical computing resources we have opted in the present work to use the power of the J-matrix approach which enables us to include an infinite tail reflecting the solution of the exactly solvable part of the Hamiltonian, usually referred to as the H_0 problem in the J-matrix literature.

A direct study of resonances is usually done in the complex energy plane. As mentioned above, resonance energies are the subset of the poles of the S-matrix function which are located in the lower half of the complex energy plane. One way to uncover these resonances, which are “hidden” below the real line in the *E*-plane, is to use the complex scaling (complex rotation) method [2]. This method exposes the resonance poles and makes their study easier and manipulation simpler. The subset of eigenvalues that corresponds to resonance spectra remain stable against variations in all computational parameters (including θ, as long as these poles are far enough from the cut “line”).

In the atomic units $\bar{h} = m = e = 1$, the one-particle wave equation for a spherically symmetric potential $V(r)$ in the presence of the Coulomb field reads as follows:

$$(H - E)\,\chi = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2r^2} + \frac{Z}{r} + V(r) - E\right]\chi = 0, \tag{1}$$

where $\chi(r)$ is the wavefunction which is parameterized by the potential parameters, ℓ, Z and *E*. The wavefunction χ will be expanded in an L^2 complete basis set $\{\phi_n\}$ which is chosen to make the matrix representation of the reference Hamiltonian:H_0 ($\equiv H - V$) tridiagonal. We parameterize the basis by a positive length scale parameter λ as $\{\phi_n(\lambda r)\}$to allow for more computational freedom. The following choice of the basis functions [9] is compatible with the domain of the Hamiltonian and satisfies the desired boundary conditions (vanishing of the wavefunction at $r = 0$ and as $r \to \infty$)

$$\phi_n(x) = a_n\, x^\alpha\, e^{-x/2} L_n^\nu(x); n = 0, 1, 2, \ldots \tag{2}$$

where $x = \lambda r$, $\lambda > 0$, $\alpha > 0$, $\nu > -1$, $L_n^\nu(x)$ is the Laguerre polynomial, and a_n is the normalization constant $\sqrt{\lambda\Gamma(n+1)/\Gamma(n+\nu+1)}$. We then require the reference Hamiltonian matrix representation to be tridiagonal in this "Laguerre basis" [10]. This requirement leads to the choice $\alpha = \ell + 1$ and $\nu = 2\ell + 1$ and gives the following tridiagonal matrix representation for H_0 [11]

$$\begin{aligned}(H_0)_{nm} =& \langle\varphi_n(x)| - \frac{\lambda^2}{2}\frac{d^2}{dx^2} + \frac{\lambda^2}{2}\frac{\ell(\ell+1)}{x^2} + \frac{\lambda Z}{x}|\varphi_m(x)\rangle \\ =& \frac{\lambda^2}{8}\left(2n + \nu + 1 + \frac{8Z}{\lambda}\right)\delta_{n,m} + \frac{\lambda^2}{8}\sqrt{n(n+\nu)}\delta_{n,m+1} \\ &+ \frac{\lambda^2}{8}\sqrt{(n+1)(n+\nu+1)}\delta_{n,m-1}.\end{aligned} \tag{3}$$

In the manipulation, we used the differential equation, differential formula, three-term recursion relation, and orthogonality formula of the Laguerre polynomials [10]. Now, the only remaining quantity that is needed to perform the calculation is the matrix elements of the effective potential *V*(*r*). This is obtained by evaluating the integral

$$\begin{aligned}V_{nm} &= \int_0^\infty \phi_n(\lambda r)V(r)\phi_m(\lambda r)dr \\ &= \lambda^{-1}a_n a_m \int_0^\infty x^\nu e^{-x} L_n^\nu(x) L_m^\nu(x)\left[xV(x/\lambda)\right]dx.\end{aligned} \tag{4}$$

The evaluation of such an integral for a general effective potential is almost always done numerically. We use the Gauss quadrature approximation which gives [12]

$$V_{nm} \cong \sum_{k=0}^{N-1} \Lambda_{nk}\Lambda_{mk}\left[\varepsilon_k\, V(\varepsilon_k/\lambda)\right], \tag{5}$$

where ε_k and $\{\Lambda_{nk}\}_{n=0}^{N-1}$ are the respective *N* eigenvalues and normalized eigenvectors of the *N*×*N* tridiagonal overlap symmetric matrix $\langle\phi_n \mid \phi_m\rangle$, whose elements are

$$K_{n,n} = 2n + \nu + 1, \qquad K_{n,n+1} = -\sqrt{(n+1)(n+\nu+1)} \tag{6}$$

The value of N in (5) is chosen in an optimal way to ensure a good sampling of the potential without extending too much the computational time. Therefore, the reference Hamiltonian H_0 in this representation, which is at the heart of the J-matrix approach, is accounted for in full and is handled analytically; not numerically. On the other hand, the effective potential V is approximated by its matrix elements in an adequate subset of the basis.

The potential V is approximated by its representation in a subset of the basis, such that

$$H_{nm} \cong \begin{cases} (H_0)_{nm} + V_{nm}, & n, m \leq N-1; \\ (H_0)_{nm}, & n, m > N-1. \end{cases} \tag{7}$$

Such a representation is the fundamental underlying feature of the J-matrix [7] method. As it is obvious from (7), the reference Hamiltonian is not truncated at all, this full account of the reference Hamiltonian should result in a substantial improvement on the accuracy of the results and this is the real power of the S-matrix approach we are proposing. The direct method, we will be using, to find the resonances is based on the J-matrix. Bound states are associated with negative real eigenvalues while resonances are associated with complex eigenvalues which have positive real parts and negative imaginary parts. The S-matrix in the J-matrix method is defined by [6]

$$\begin{aligned} S(E) &= T_{N-1}(E)\frac{1 + g_{N-1,N-1}(E)J_{N-1,N}(E)R_N^-(E)}{1 + g_{N-1,N-1}(E)J_{N-1,N}(E)R_N^+(E)}, \\ T_n &= \frac{c_n - is_n}{c_n + is_n}, \quad R_n^{\pm} = \frac{c_n \pm is_n}{c_{n-1} \pm is_{n-1}}, \\ g_{N-1,N-1}(z) &= D_\nu^N \sum_{n=0}^{N-1} \frac{\Gamma_{N-1,n}^2}{\varepsilon_n - z} = D_\nu^N \left[\prod_{m=0}^{N-2} (\tilde{\varepsilon}_m - z) \Big/ \prod_{n=0}^{N-1} (\varepsilon_n - z) \right], \\ D_\nu^N &= N + \nu. \end{aligned} \tag{8}$$

Here, $g_{n,m}$ is the inverse of the matrix$(H_0 + V - E)$, εi and ε'_i are the eigenvalues of H and the one truncated by removing the last row and last column, respectively. It should be noted that our definition of $R_N^{\pm}$ is the inverse of the conventional one adapted by the founders of the J-matrix approach [7].

The matrix Λ simultaneously diagonalizes H and the overlap matrix K where $K_{nm} = \langle \psi_n \mid \psi_m \rangle$. $J_{m,n}$ are the J-matrix elements defined by $J_{m,n} = \langle \phi_m | (H_0 - E) | \phi_n \rangle$and are represented by a tridiagonal matrix. The quantities s_n and c_n are just the expansion coefficient of the sine-like and cosine-like functions which constitute the two independent asymptotic solutions of the differential equation $(H_0 - E)\psi = 0$. This terminology is being used in the J-matrix approach where we denote the two independent solutions of the reference Hamiltonian by

$$|S\rangle = \sum_{n=0}^{\infty} s_n |\varphi_n\rangle, \qquad |C\rangle = \sum_{n=0}^{\infty} c_n |\varphi_n\rangle \tag{9}$$

To illustrate this resonance finding approach and demonstrate the ability and accuracy of the proposed J-matrix approach, we use a well known potential which was used heavily in the literature due to its simplicity and the richness of its spectra which includes both shallow and deep resonances. We consider the Hamiltonian with the following potential [3,4,6,13,14]

$$V(r) = 7.5\, r^2 e^{-r}, \tag{10}$$

This potential has already been shown to support s-wave resonances even in the absence of Coulomb potential. Also it can support bound states with negative charge, Z, as it will be shown below. The above approach will be numerically implemented to the study and analysis of resonances for the potential $V(r)$ in the complex E-plane to illustrate the accuracy of this method and determine the advantage of this procedure compared to other numerical approaches.

Before we discuss our numerical results, it is important to mention that the package of MATHEMATICA (Version 5) [15] has been used extensively to perform our calculations. To calculate the roots of S^{-1} matrix, one has to use the built in Newton–Raphson type of iteration procedure. The accuracy of the S-matrix results crucially depends on the accuracy of the seed that we use which originates from the complex rotation approach (CR). So, it is important to use the most accurate seed, having this mind we have decided to use the computational power of MATHEMATICA up to fifty digits while in the final results we showed only the significant ones.

In the following we will give the recipe of our procedure for calculating the bound and resonance energies of our test potential for different values of Z and ℓ. For a given choice of physical parameters, we investigate the stability of the calculated eigenvalues that correspond to bound states and/or resonances as we vary the scaling parameter λ and rotation angle θ until we reach a plateau in λ and θ, independently [8]. Then to improve on the accuracy of the results, we select a values of λ and θ from within their respective plateau and increase the dimension of the space N until the desired accuracy is reached. The digits that are shown italic in the tables correspond to uncertain digits and are kept only for comparison purposes.

Our strategy for calculating the resonances and bound states of the system is based on the following procedure: First we use the CR [8,11] to calculate the bound and resonance states for the given parameters. This step also gives the critical angle or the opening angle for each resonance state, it is usually done using a large value of N, say 100, $\theta \leq \pi/3$, and a suitable value of λ. This step is crucial in our approach since it gives the energies of the bound states, the energies and the widths of the resonance states which constitute our seeds for the S-matrix computations. We start our study by considering the S-wave uncharged system which has been treated in the literature. First we study the range of parameter spaces in λ and θ which ensure the stability of our computations; this phase has been named the

State	**Our work**	**[3]**	**[4]**	**[14]**
R1	3.42639031014825046005 -0.01277448059289562497 i	3.426390331 - 0.012774481 i	3.4263903101 - 0.012774481 i	3.426390310 - 0.012774481 i
R2	4.8348068410964 - 1.117876668867918 i	4.834806841- 1.117876669 i	4.8348068411 - 1.1178766688 i	4.834806841- 1.117876669 i
R3	5.277279863983998- 3.38905329525395 i	5.277279780 - 13.389053178 i	5.2772798640 -3.3890532952 i	5.277279864 - 13.389053295 i
R4	5. 0649296073802 - 5.97603478786563 i		5.064929 6074 - 5.9760347878 i	5.064929 608 - 5.976034788 i
R5	4.268860299262605 - 8.71690843394784491 i		4.2688602993 - 18.7169084339 i	4.268860299 - 8.716908434 i
R6	2.947781600328765 - 11.530514731260112 i		2.9477816003- 11.530514732 i	2.9477816003 - 11.530514731 i
R7	1.1471837382928 - 14.36900713709712 i		1.1471837383 - 14.3690071370 i	1.147183738- 14.369007137 i
R8	-1.096688978956- 17.2010217933 i		-1.0966889789 - 17.2010217933 i	-1.096688979 - 17.201021793 i
R9	-3.7541441226 - 20.0045074966 i		-3.7541441225 - 20.0045074967 i	-3.75414412 - 20.00450749 i
R10	-6.80030388 - 22.76315507 i			-6.800304 - 22.76315 i
R11	-10.2139610 -25.4644312 i			-10.21 - 25.46 i

Table 1: The resonance energies associated with Z = 0 and ℓ =0, while λ *is* ranging from 8-18, θ ranging from 0.5-1.2 and N is ranging from 50 to 70. Comparison with the available literature results is also shown in the last three columns [3, 4, 14].

search for λ-plateau and θ-plateau, respectively, and was treated in details in our previous work [8]. In Table 1 we show only the first eleven resonances associated with this potential. For ease of discussion we refer to the resonances associated with this potential as R1, R2, . . ., R11 starting from the shallow one, R1, to the deepest one, R11, all parameters values were chosen within the corresponding plateau. The dimensional space parameter N was taken to be 70 except for the resonances R1 and R2 for which it was taken to be 50. As usual, to decide about the right number of significant digits we should keep for N =50, say, we perform an additional computation with $N = 51$ (any higher number will do) and keep only the digits that did not change when comparing the results with those with $N = 50$. It is worth mentioning that, in general, the results for the deep resonance are relatively less accurate than those of the shallow one. Comparison with the available literature results is also shown in the last three columns [3, 4, 14] of Table 1. Our results using J-matrix approach are found to be more accurate than those in the literature. We need to mention here that similar calculations can be performed using the oscillator basis [7] for the case of $Z = 0$, however, we noticed that for this particular potential the results obtained using the Laguerre basis are more accurate than those associated with the oscillator basis for the same basis size N. As an example we mention that the resonance R2 in Table 1 is given by R2 = 4.8348068 - 1.11787651 i in the oscillator basis using $\lambda = 2$ and $\theta = 0.5$, hence a reduction from 14 significant figures in the Laguerre basis to 8 significant figures in the oscillator basis for the same value of $N = 50$. It is our conjecture that for potentials which are much shorter in range compared to ours, we expect that the results obtained using the oscillator basis might outperform those using the Laguerre basis.

State (λ, θ)	**Our work**	**[3]**	**[14]**
R1(12,0.5)	1.78052453636230533 - 0.00004785969842869 i	1.780524536 - 0.000047859 i	1.780524536 - 0.0000478597 i
R2(12,0.5)	4.101494946209229 - 0.578627213765913 i	4.101494946 - 0.578627214 i	4.101494946 - 0.578627214 i
R3(12,0.8)	4.663461096660910 - 2.683200770291628 i	4.663461099 - 2.683200769 i	4.663461097 - 2.683200770 i
R4(15,1)	4.561151055148 - 5.206698021694 i		
R5(15,1)	3.849197759911 - 7.908283499740 i		
R6(15,1)	2.5933485088 - 10.6937408173 i		
R7(15,1)	0.84464713 - 13.510954553 i		
R8(15,1)	-1.356846 - 16.3265018 i		
R9(15,1)	-3.978854 - 19.117065 i		
R10(15,1)	-6.9947 - 21.8654 i		

Table 2: Values of the resonances energies obtained using S-matrix for N = 60, $\lambda = 12$, $\ell = 0$, Z = -1, θ = 0.5 (for R1 and R2) and θ = 0.8 (for R3), all other resonances were obtained for θ = 1 and λ = 15. The last two columns show the numerical data available in the literature for comparison [3, 14].

We consider now the effect of the charge through the Coulomb potential Z/r, thus we add to the test potential (10) a Coulomb term Z/r. In this case to obtain bound states we need to have negative *Z,* however large values will generate more bound states and fewer resonances. Here we consider the moderate case with $Z = -1$ and ℓ= 0, which was treated in the literature [3, 14]. Table 2 shows the resonances generated by this potential, we see that our results agree with those in the literature [3,14] and outperform them at high values of N with more significant figures.

a)

N	Ground state energy $\lambda = 5, \theta = 0$
15	-4.47399521(9582)
20	-4.4739952221(02)
25	-4.473995222133
26	-4.473995222133

b)

N	*E* (shallow resonance) $\lambda = 5, \theta = 0.3$	*E* (deep resonance) $\lambda = 14, \theta = 0.8$
30	0.69283206(84321) - 0.0116652519(68029) i	1.842585521(154557) - 1.113181443(3889586) i
40	0.69283206794(35) - 0.01166525198(0639) i	1.84258552122810(2) - 1.1131814432139(644) i
50	0.6928320679440 - 0.011665251982125 i	1.842585521228104 - 1.1131814432139194 i
51	0.6928320679440 - 0.011665251982125 i	1.842585521228104 - 1.1131814432139194 i

Table 3: The energy for the ground state (a) and two of the resonances (b) with $Z = -7$ and $\ell = 1$ for different values of *N*.

Finally, we would like to study the effect of the orbital centrifugal term $\ell(\ell+1)/2r^2$ together with the Coulomb term Z/r, the values ℓ= 1 and $Z = -7$ are being chosen. In this case, 22 bound states and two resonance states have been found. Following the above procedure one can study the variations of the ground state in Table 3a and the two resonance states in Table 3b as a function of the dimensional parameter *N*. The effect of changing ℓ, at fixed Z, could be clearly understood from the comparison of results in Table 4. From this table it can be observed that the ground state energy decreases drastically with increasing ℓ. However, the effect of changing ℓ on the values of the first two resonances state energies is less pronounced.

In summary, we presented the computation of the bound and resonance energy states as being the poles of the S-matrix using the J-matrix technique which includes partial contributions of the Hamiltonian from the infinite dimensional space. To test the validity and accuracy of our approach we have implemented it for a typical short-range scattering potential $V(r) = 7.5\ r^2 e^{-r}$which was widely used in the literature. More accurate results

		ℓ =0 $(\lambda = 12,\ \theta = 0.7)$	ℓ =1 $(\lambda = 5,\ \theta = 0.4)$	ℓ =2 $(\lambda = 3,\ \theta = 0.4)$
Ground state N = 30	B1	- 24.179134460556	- 4.473995222134	- 0.575903594988
Resonances N = 40	R1	0.801994445339-0.036277959631i	0.692832067944-0.011665251982 i	0.405958975050-0.000501309145 i
	R2	1.712768600246-1.341289175693 i	1.842586470829-1.113189558416 i	2.074374194936-0.727438733704 i

Table 4: The energy for the ground state and the first two resonances for $Z = -7$ and different values of l. The values of θ are indicated for the resonances while for bound states it is set to $\theta = 0$.

for the bound and resonant state energies of this test potential were generated and compared favorably with the most recent results in the literature [4,14] for different values for the parameters $Z$and ℓ. Our approach could easily be generalized to handle other short-range potentials such as the Morse potential, the Yukawa potential and the Hulthen potential, to mention only few. The present approach can easily handle non-analytic potentials which, usually, cannot be handled with great accuracy using other numerical approaches.

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