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Characterization of resonances using an exact model S-matrix

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Abstract. The S-matrix, which is exact for a model potential that can be made to closely approximate a given physical potential, is found in closed form as a function of complex system energy. This allows a calculation of the density of resonance states for real scattering energies, from which real resonance position, total widths, and partial widths can easily be extracted. Alternatively, a direct search of the poles of the S-matrix in the complex energy plane locates the complex resonance energies while the residues of the S-matrix elements at each pole yield the resonance partial widths.

The work reported here is in continuation of the authors' effort [1, 2] to utilize the advantages of the J-matrix method of scattering [3–7] in the calculation of resonance parameters, a subject of growing recent interest [8–11]. This method, which uses only square-integrable basis functions, has two desirable properties. First, it finds the exact S-matrix for a model problem that closely approximates the given physical problem. The second is that this S-matrix is given in closed form in terms of an arbitrary value of the scattering energy E. By considering the energy parameter E to be complex, one has a natural closed form analytic continuation of the S-matrix in the complex energy plane valid in the vicinity of the real energy axis. This allows us to use the J-matrix method of scattering to calculate the resonance parameters of narrow resonances using either the indirect or the direct approaches with equal ease. In the first approach one carries out a complete real energy calculation of a relevant physical quantity such as the cross sections or the eigenphase shifts near a resonance. One then extracts information on the real resonance position E_r and total width Γ by fitting the result to a Breit–Wigner form plus background [11–13]. Here we propose to use the S-matrix to calculate directly the density of resonance states $\rho(E)$ using the collision life-time matrix Q [8, 14, 15]:

$$\rho(E) = \frac{1}{2\pi}\,\mathrm{Tr}[Q] \qquad Q = \mathrm{i}S\frac{\mathrm{d}S^{\dagger}}{\mathrm{d}E}. \tag{1}$$

Near the real resonance energy E_r, the density $\rho(E)$ has the form

$$\rho(E) = \frac{1}{\pi}\frac{\Gamma/2}{(E-E_r)^2+\Gamma^2/4}. \tag{2}$$

In the multi-channel case, we can extract the partial widths from the open-channel contribution to the trace, namely

$$\frac{1}{2\pi}Q_{\alpha\alpha} = \frac{1}{\pi}\frac{\Gamma_\alpha/2}{(E-E_r)^2+\Gamma^2/4} \tag{3}$$

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where Γ_α is the partial width associated with channel α.

In the direct approach, the complex resonance energy $\epsilon_r = E_r - i\Gamma/2$ is an isolated point in the complex energy plane with special properties. It is either the eigenvalue of a complex dilated Hamiltonian [10, 16] or equivalently the pole of the Green's function, T-matrix, or the S-matrix. Here we search for ϵ_r as the poles of the exact model S-matrix in the second sheet of the complex energy plane. In a multi-channel case the S-matrix has, near the complex resonance pole, the form [17]:

$$S_{\alpha\beta}(E) = S^{bg}_{\alpha\beta}(E) - i\frac{\gamma_\alpha \overline{\gamma}^*_\beta}{E - \epsilon_r} \tag{4}$$

where $S^{bg}_{\alpha\beta}(E)$ is the background part of the S-matrix that behaves regularly at the pole and γ_α is related to the partial width via the relation $\Gamma_\alpha = |\gamma_\alpha \overline{\gamma}^*_\alpha|$. Thus once we find ϵ_r we can obtain the partial widths as

$$\Gamma_\alpha = \lim_{E \to \epsilon_r} |(E - \epsilon_r) S_{\alpha\alpha}(E)|. \tag{5}$$

In the single-channel case, the J-matrix method of scattering uses a complete set of square-integrable basis functions to solve *exactly* the zero-order Schrödinger equation

$$H_0 \Psi^0(E, r) = E \Psi^0(E, r) \tag{6}$$

where

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{z}{r}. \tag{7}$$

The basis may be either the Slater basis

$$\phi_n(r) = (\lambda r)^{l+1} e^{-\lambda r/2} L_n^{2l+1}(\lambda r) \qquad n = 0, 1, \ldots \tag{8}$$

or the oscillator basis (the case $z = 0$ only)

$$\phi_n(r) = (\lambda r)^{l+1} e^{-\lambda^2 r^2/2} L_n^{l+1/2}(\lambda^2 r^2) \qquad n = 0, 1, \ldots \tag{9}$$

where λ is a free scale parameter and $L_n^\nu(x)$ is the generalized Laguerre polynomial [18]. The coefficients that make the wavefunction

$$\Psi^0_s(E, r) = \sum_{n=0}^{\infty} s_n(E) \phi_n(r) \tag{10}$$

solve the Schrödinger equation (6) and behave asymptotically sine-like are already known [4, 7]. Similarly the coefficients that make the function

$$\Psi^0_c(E, r) = \sum_{n=0}^{\infty} c_n(E) \phi_n(r) \tag{11}$$

behave asymptotically cosine-like and are already known.

Now, given a short-range potential V, the method finds the exact solution to the model potential W derivable from V by restricting the matrix representation of the latter to the first N members of the complete basis; i.e.

$$W_{n,m} = \langle \phi_n | W | \phi_m \rangle = \begin{cases} \langle \phi_n | V | \phi_m \rangle & \text{for } 0 \leqslant n, m \leqslant N-1 \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

This is similar to the modelling scheme followed in the R-matrix method of scattering [19] which replaces the short-range potential by a cut-off potential restricted to an inner configuration space. Heller has shown [20] that this modelling procedure does not lead to spurious resonances that plagued variational calculations. Furthermore, the resonances associated with the model potential approximate in a well defined and improvable fashion the resonances of the real problem.

Now, the J-matrix method solves the Schrödinger equation

$$(H_0 + W)\Psi(E, r) = E\Psi(E, r) \tag{13}$$

exactly. The solution satisfying an outgoing boundary condition is

$$\Psi(E, r) = \sum_{n=0}^{N-1} d_n(E)\phi_n(r) + \sum_{n=N}^{\infty} [(c_n(E) - \mathrm{i}s_n(E)) - S(E)(c_n(E) + \mathrm{i}s_n(E))]\phi_n(r) \tag{14}$$

in complete analogy to the form of the R-matrix wavefunction where the solution in the outer region of configuration space is a combination of an incoming wave and an outgoing wave modified by the S-matrix. The set $\{d_n\}_{n=0}^{N-1}$ contains the coefficients of wavefunction in the inner space to which the potential is restricted. These coefficients as well as the S-matrix can be solved exactly by equating the projection on both sides of the Schrödinger equation (13) on each member of the complete basis. The S-matrix, which is the quantity of interest to us, has the *exact* solution

$$S(E) = \frac{(c_{N-1}(E) - \mathrm{i}s_{N-1}(E)) + g_{N-1,N-1}(E)J_{N-1,N}(E)(c_N(E) - \mathrm{i}s_N(E))}{(c_{N-1}(E) + \mathrm{i}s_{N-1}(E)) + g_{N-1,N-1}(E)J_{N-1,N}(E)(c_N(E) + \mathrm{i}s_N(E))}. \tag{15}$$

Here the matrix $\{g_{n,m}\}_{n,m=0}^{N-1}$ is the inverse of the matrix $\{(H_0 + V - E)_{n,m}\}_{n,m=0}^{N-1}$. Also the matrix $J_{n,m} = \langle \phi_n | (H_0 - E) | \phi_m \rangle$ happens to be tridiagonal. The previous effort [1, 2] made use of the fact that the above expression for $S(E)$ has a simple form at the N Harris energy eigenvalues which are the poles of $g_{N-1,N-1}(E)$. The set of N values of $S(E)$ is then analytically continued in the complex energy plane using the point-wise rational fraction technique of Haymaker and Schlessinger [21]. In this effort we use the analytic expression as given directly by equation (15) to provide a natural analytic continuation of $S(E)$ valid in the vicinity of the real energy axis. In addition, we note the following interesting points about the above expression for $S(E)$:

(i) It is *exact* for the N-term separable potential W which closely approximates the physical potential,

(ii) it is a closed-form solution in terms of the scattering energy parameter E,

(iii) it is *unitary* for real positive energies E,

(iv) The inversion of the $N \times N$ matrix $\{(H_0 + V - E)_{n,m}\}_{n,m=0}^{N-1}$ to obtain the $N \times N$ matrix $\{g_{n,m}\}_{n,m=0}^{N-1}$ is carried out only once in the calculation, independent of the energy parameter E, and finally

(v) the Coulomb term (z/r) is fully taken into account in the Slater basis, a distinction for the J-matrix method.

We have used this S-matrix to calculate the density of resonance states for the potential $V(r) = 7.5r^2e^{-r}$ which is already known [8,22] to support an s-wave resonance at $E_r = 3.426$ having total width $\Gamma = 2.56 \times 10^{-2}$ for the case where $z = 0$. The result of fitting $\rho(E)$ to a Breit–Wigner form is shown in figure 1. We have also repeated the same calculation for the case where the zero-order Hamiltonian contains the attractive Coulomb term $(-1/r)$. We compare our results with that obtained using the complex rotation method [16, 17].

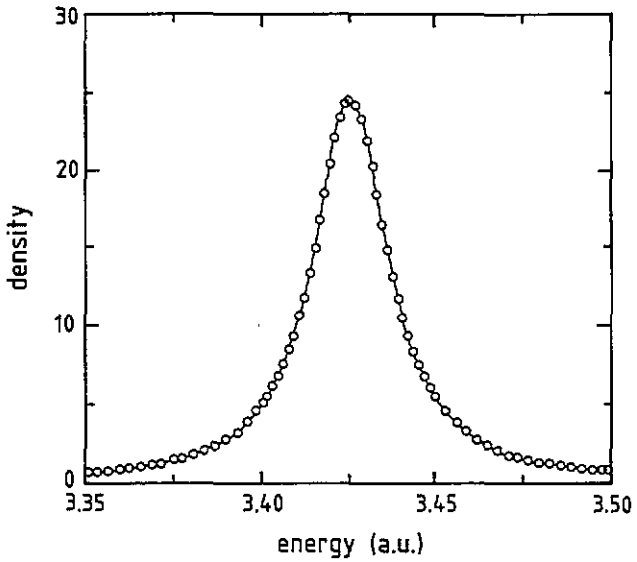

Figure 1. The density of resonance states $\rho(E)$ for the s-wave scattering from the potential $V(r) = 7.5r^2e^{-r}$ ($z = 0$ case), calculated using equation (1) (open circles), with $N = 30$ Slater basis and $\lambda = 5.5$. The Lorentzian (continuous curve) has $E_r = 3.426$ and $\Gamma = 2.58 \times 10^{-2}$ a.u.

On the other hand, by considering E in $S(E)$ to be complex we may search for the poles ϵ_r of $S(E)$ in the complex energy plane. The search strategy has previously been described in detail [2]. Table 1 gives the results of such a search for the cases mentioned above as a function of the model size N.

The generalization to multi-channel scattering is straightforward. We assume a target of discrete internal states having energies $E_1, E_2, \ldots, E_M$. The projectile is structureless and spinless. The channel potentials $V^{\alpha\beta}$ are short range with any possible Coulomb terms included in the zero-order Hamiltonian in each channel. The basis $\{\phi_n^{(\alpha)}(r)\}_{n=0}^{N_\alpha-1}$ in each channel α may either be of the Slater or the oscillator type, where λ_α may be different for each channel. The model potential $W^{\alpha\beta}$ is obtained from $V^{\alpha\beta}$ in an analogous fashion to the single-channel case, namely

$$W_{n,m}^{\alpha\beta} = \langle\phi_n^{(\alpha)}|W|\phi_m^{(\beta)}\rangle = \begin{cases} \langle\phi_n^{(\alpha)}|V|\phi_m^{(\beta)}\rangle & 0 \leqslant n \leqslant N_\alpha - 1,\ 0 \leqslant m \leqslant N_\beta - 1 \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

The multi-channel generalization of the single-channel S-matrix has been given in detail elsewhere [2]. It satisfies similar properties to those given by (i) to (v) above. What is

Table 1. Resonance parameters resulting from the complex energy search for the poles of the S-matrix of equation (15) for the potential $V(r) = 7.5r^2 e^{-r}$, for the cases $z = 0$ and $z = -1$ as a function of model size N for Slater basis and $\lambda = 5.5$. The results of Mandelshtam *et al* [8] (for the $z = 0$ case) are included. For the case $z = -1$, the complex rotation method has been used with a 30 Slater basis having $\lambda = 5.5$ and $\theta = 0.2$ rad.

z	N	E_r	Γ
0	15	3.426	2.17×10^{-2}
	20	3.426	2.79×10^{-2}
	25	3.427	2.45×10^{-2}
	30	3.426	2.58×10^{-2}
	Mandelshtam *et al*	3.426	2.56×10^{-2}
−1	15	1.7805	8.62×10^{-5}
	20	1.7805	9.19×10^{-5}
	25	1.7805	9.44×10^{-5}
	30	1.7805	9.58×10^{-5}
	Complex rotation	1.7805	9.57×10^{-5}

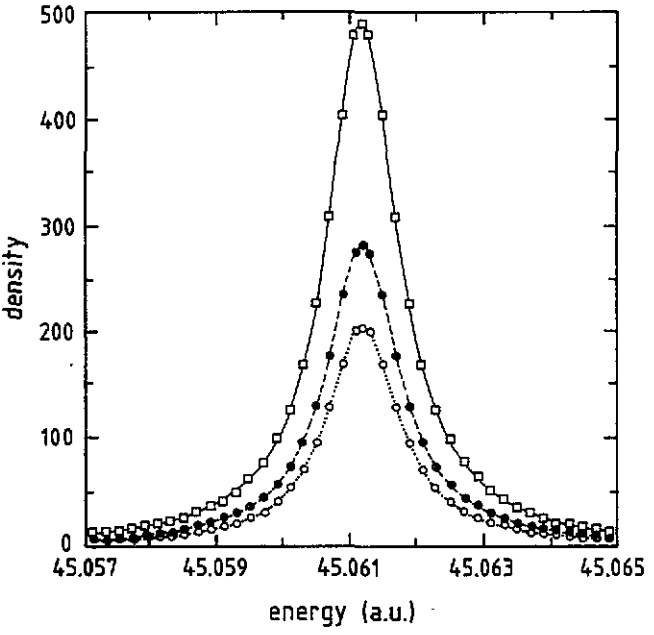

Figure 2. The density of resonance states $\rho(E)$ for the three-channel problem defined in equation (17) in the text, calculated using equation (1) (squares), with $N = 30$ oscillator basis in each channel having the same $\lambda = 3.97$. The Lorentzian (continuous curve) has $E_r = 45.061$ and $\Gamma = 1.30 \times 10^{-3}$. The contributions of channel 1 (open circles) and channel 2 (solid circles) are fitted to Lorentzians with the same E_r and with $\Gamma_1 = 5.40 \times 10^{-5}$ and $\Gamma_2 = 7.47 \times 10^{-5}$, respectively.

important is that the exact multi-channel J-matrix expression for the S-matrix can be used as its own analytic continuation in the complex energy plane valid in the vicinity of the real energy axis.

We have used the oscillator basis to calculate the exact model S-matrix for the three-

Table 2. Resonance parameters resulting from the complex energy search for the poles of the S-matrix of equation (15) for the three-channel problem defined in equation (17) in the text, as a function of model size N, taken to be the same for all channels with the same $\lambda = 3.97$. The results of Fels and Hazi [23] are included.

N	E_r	Γ	Γ_1	Γ_2
20	45.076	1.24×10^{-3}	4.80×10^{-4}	7.58×10^{-4}
25	45.066	1.36×10^{-3}	5.94×10^{-4}	7.66×10^{-4}
30	45.068	1.30×10^{-3}	5.37×10^{-4}	7.65×10^{-4}
Fels and Hazi	45.068	1.29×10^{-3}	5.29×10^{-4}	7.60×10^{-4}

channel problem coupled by square-well potentials, an example often used as a testing ground for new schemes [11, 13, 17, 23]. The target threshold energies are $E_1 = 0.0$, $E_2 = 37.5$, and $E_3 = 50.0$ a.u., while the potential parameters are

$$V^{\alpha\beta}(r) = \begin{cases} \left[\dfrac{U^{\alpha\beta}}{2}\right] & \text{for } 0 \leqslant r \leqslant 1 \\ 0 & \text{otherwise} \end{cases} \qquad U = \begin{pmatrix} 10.0 & 0.1 & 1.0 \\ 0.1 & 2.0 & 0.1 \\ 1.0 & 0.1 & -16.0 \end{pmatrix}. \tag{17}$$

This problem is known to support an s-wave resonance at $E_r = 45.086$ having total width $\Gamma = 1.29 \times 10^{-3}$. We calculated the density of resonance states $\rho(E)$ and the contribution of the two open channels to them from the calculated S-matrix in equations (2) and (3). In figure 2 we fitted the results to Breit–Wigner forms with the same position and width. The extracted information on the resonance position, total width, and partial widths compares well with that of Fels and Hazi [23].

Alternatively, we have used the same model S-matrix $S(E)$ but now with E considered to be complex to search for its poles in the complex energy plane. Table 2 shows the computed values of the resonance parameters as a function of model size.

It is clear that the reason the J-matrix method of scattering is able to characterize resonances directly or indirectly is the availability of an exact model S-matrix in closed form as a function of the complex energy parameter E.

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