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# Resonance information from the analytically continued $S$-matrix

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**Abstract.** The $J$-matrix method of scattering is used to calculate the scattering $S$-matrix at the set of energy eigenvalues of the full Hamiltonian matrix constructed from a finite set of square-integrable basis functions. The $S$-matrix is then analytically continued in the complex energy plane via a point-wise rational fraction scheme of Schlessinger. Numerical search techniques are then used to locate the poles of the $S$-matrix, which are identified with the resonance energies. Partial widths are easily calculated from the residues of the $S$-matrix at the designated complex resonance energies.

## 1. Introduction

Recently, the authors introduced a simple method [1] for extracting resonance information from the Harris energy eigenvalues and eigenvectors [2] resulting from the diagonalization of the scattering Hamiltonian in a finite set of $L^2$ bases. The method is based on the formalism of the $J$-matrix method of scattering [3–5] which finds the exact solutions to a model multichannel scattering potential, $\tilde{V}$. The model potential is obtained from the given potential, $V$, by restricting its infinite matrix representation in a complete $L^2$ basis to a finite representation. The basis chosen in each channel $\alpha$ is either the Laguerre basis

$$\phi_n^{(\alpha)}(r) = (\lambda_\alpha r)^{(\nu+1)/2} e^{-\lambda_\alpha r/2} L_n^\nu(\lambda_\alpha r) \tag{1}$$

or the oscillator basis

$$\phi_n^{(\alpha)}(r) = (\lambda_\alpha r)^{\nu+1/2} e^{-\lambda_\alpha^2 r^2/2} L_n^\nu(\lambda_\alpha^2 r^2). \tag{2}$$

In both cases, $\lambda_\alpha$ is a free-scale parameter, and $L_n^\nu(x)$ are the generalized Laguerre polynomials of order $n$. In terms of this basis and the given potential $V$, the model potential $\tilde{V}$ is defined as

$$\tilde{V}^{\alpha\beta} = \sum_{n=0}^{N_\alpha - 1} \sum_{m=0}^{N_\beta - 1} |\bar{\phi}_n^{(\alpha)}\rangle \langle \phi_n^{(\alpha)} | V^{\alpha\beta} | \phi_m^{(\beta)} \rangle \langle \bar{\phi}_m^{(\beta)}| \tag{3}$$

where $\{|\bar{\phi}_n^{(\alpha)}\rangle\}_{n=0}^\infty$ is the orthogonal complement to the basis $\{|\phi_n^{(\alpha)}\rangle\}_{n=0}^\infty$ in the $\alpha$th channel in the sense that $\langle \bar{\phi}_n^\alpha | \phi_m^\alpha \rangle = \langle \phi_n^\alpha | \bar{\phi}_m^\alpha \rangle = \delta_{nm}$. This modelling procedure is analogous to the approach of the $R$-matrix method of scattering which models the given scattering potential

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by a cut-off potential restricted to an inner configuration space [3]. Heller [6] has shown that this approximation scheme, which is ever improvable by enlarging the representation, does not lead to spurious resonances. Thus, the resonances that the $J$-matrix method yields approximate, in a well defined fashion, real resonances.

The scheme for calculating resonance energies is based on the definition of resonances as the poles of the $S$-matrix in the second sheet of the complex energy plane. The $J$-matrix method allows the exact evaluation of the $S$-matrix at the Harris energy eigenvalues which result from the diagonalization of the full Hamiltonian in the subspace where the model potential $\tilde{V}$ is non-zero. Since the real energy axis is in the domain of analyticity of the $S$-matrix, these values can be analytically continued in the complex energy plane. Standard numerical search routines can then be used to locate the poles of the $S$-matrix, which are identified as the complex resonance energies, $\epsilon_r, r = 1, 2, \ldots$. Usually, each resonance is parametrized by $E_r$, the real resonance position, and $\Gamma$, the resonance total width, in the following way:

$$\epsilon_r = E_r - \mathrm{i}\frac{\Gamma}{2}. \tag{4}$$

For each resonance, the partial width $\Gamma_\alpha$, associated with each channel $\alpha$, can be extracted from the residues of the $S$-matrix at the energy $\epsilon_r$. This is possible because the $S$-matrix has the form

$$S_{\alpha\alpha} = S_{\alpha\alpha}^{\mathrm{bg}} - \mathrm{i}\frac{\Gamma_\alpha \mathrm{e}^{\mathrm{i}\theta_\alpha}}{E - \epsilon_r} \tag{5}$$

In the neighbourhood of the $\epsilon_r$ [7]. Here $S_{\alpha\alpha}^{\mathrm{bg}}$ is the background part of the $S$-matrix which behaves regularly at $E = \epsilon_r$, and $\theta_\alpha$ is a real phase.

The purpose of this paper is to show how to calculate the $S$-matrix at the Harris energy eigenvalues and, subsequently, how to analytically continue it in the complex energy plane. This turns out to be a non-trivial problem since the $S$-matrix is a product of two operators, one having a zero and the other having a pole at the Harris energy eigenvalues. In section 2 we use the $J$-matrix method of scattering to derive the general expression for the $S$-matrix. In section 3 we state a sufficient condition for the energy to be a resonance energy. This turns out to be the vanishing of a function, $G(E)$, derivable from the determinant of the $S$-matrix. We find the values of $G(E)$ at the Harris energy eigenvalues. In section 4 we show how to calculate the diagonal elements of the multichannel $S$-matrix at the Harris eigenvalues and how to derive from these elements the partial widths for each resonance. In section 5 we explain how to apply the rational fraction scheme of Schlessinger [8] to analytically continue $G(E)$ and the diagonal elements of the $S$-matrix in the complex plane. We also explain how to use some numerical search techniques to locate resonances in the complex energy plane. In the last section we give results of the application of the proposed method to finding the resonance energy and partial widths for model one- and three-channel scattering problems.

## 2. The $S$-matrix in the scattering region

We consider the scattering of a structureless spinless particle by a target with $M$ internal states labelled by the threshold energies $E_1, E_2, \ldots, E_M$. We assume that the given scattering potential, $V^{\alpha\beta}$, is short range. We also assume that the reference Hamiltonian of

the projectile, $H_0$, may include, in addition to the $l$th partial wave kinetic energy operator, the Coulomb term $(z/r)$, that is,

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{z}{r}. \tag{6}$$

Thus, the multichannel Schrödinger equation for the given scattering problem is

$$\sum_{\beta=1}^{M}\{[H_0 - (E - E_\beta)]\delta_{\alpha\beta} + V^{\alpha\beta}\}|\psi_{\beta\alpha}) = 0. \tag{7}$$

The matrix representation of the operator

$$J^{(\alpha)} = H_0 - (E - E_\alpha) \tag{8}$$

is tridiagonal in the Laguerre basis if we choose $\nu = 2l + 1$, and in the oscillator basis if we choose $z = 0$ and $\nu = l + \frac{1}{2}$. Therefore, the Fourier-like coefficients $\{s_n^{(\alpha)}\}_{n=0}^{\infty}$ of the expansion of the sine-like eigenvector of $H_0$ satisfy the three-term recursion relation

$$J_{n,n-1}^{(\alpha)}s_{n-1}^{(\alpha)} + J_{n,n}^{(\alpha)}s_n^{(\alpha)} + J_{n,n+1}^{(\alpha)}s_{n+1}^{(\alpha)} = 0 \tag{9}$$

for $n \geqslant 1$ and the initial two-term recursion relation

$$J_{0,1}^{(\alpha)}s_1^{(\alpha)} + J_{0,0}^{(\alpha)}s_0^{(\alpha)} = 0. \tag{10}$$

Here

$$J_{nm}^{(\alpha)}(E) = \langle\phi_n^{(\alpha)}|J^{(\alpha)}(E)|\phi_m^{(\alpha)}\rangle. \tag{11}$$

The explicit solutions for the above recursion relations are already known [3, 5]. Similarly, it has been shown [5] that a second solution $\{c_n^{(\alpha)}\}_{n=0}^{\infty}$ of equation (8) with the initial condition

$$J_{0,1}^{(\alpha)}c_1^{(\alpha)} + J_{0,0}^{(\alpha)}c_0^{(\alpha)} = \frac{W}{2s_0^{(\alpha)}} \tag{12}$$

are the coefficients of a vector that behaves asymptotically cosine-like. Here $W$ is the Wronskian of the regular and irregular solution of the $\alpha$th channel potential-free Schrödinger equation. The coefficients $\{c_n^{(\alpha)}, s_n^{(\alpha)}\}_{n=0}^{\infty}$ have already been found explicitly and have been tabulated [5, 9].

Equipped with these coefficients, we may find the exact solution to the Schrödinger equation (7) but with $\tilde{V}^{\alpha\beta}$, as given by equation (3), replacing $V^{\alpha\beta}$. The vector $|\psi_{\beta\alpha}(E))$, which describes the projectile entering the scattering region in channel $\alpha$ with momentum $k_\alpha$ and exiting the region in channel $\beta$ with momentum $k_\beta$, can be expanded in the $\beta$-channel basis $\{|\phi_n^{(\beta)})\}_{n=0}^{\infty}$ as

$$|\psi_{\beta\alpha}(E)) = \sum_{n=0}^{N_\beta-1}|\phi_n^{(\beta)})b_n^{\beta\alpha} + \sum_{n=N_\beta}^{\infty}|\phi_n^{(\beta)})\left\{\frac{s_n^{(\beta)}(E)}{\sqrt{k_\beta}}\delta_{\beta\alpha} + \frac{c_n^{(\beta)}(E)}{\sqrt{k_\beta}}R_{\beta\alpha}\right\}. \tag{13}$$

This suggested solution resembles that of the $R$-matrix method in that outside the range of the cut-off potential the wavefunction is a linear combination of the sine-like and cosine-like

solutions. Therefore, the $R_{\beta\alpha}$ is just the reactance matrix from which the $S$-matrix can be constructed using the relation

$$S(E) = (1 - \mathrm{i}\hat{R})^{-1}(1 + \mathrm{i}\hat{R}) \tag{14}$$

where $\hat{R}$ is the open-channel part of the reactance matrix $R$. Broad and Reinhardt [10, 11] have shown that $\hat{R}$ is a solution of the equation

$$\hat{\mathcal{A}}\hat{R} = -\hat{\mathcal{B}} \tag{15}$$

where $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ are the open part of the matrices $\mathcal{A}$ and $\mathcal{B}$ which have the explicit forms

$$\begin{aligned}
\mathcal{A}_{\beta\alpha}(E) &= \frac{c^{(\alpha)}_{N_\alpha - 1}}{\sqrt{k_\alpha}}\delta_{\alpha\beta} + g^{(\beta,\alpha)}_{N_\beta - 1, N_\alpha - 1}(E) J^{(\alpha)}_{N_\alpha - 1, N_\alpha}(E)\frac{c^{(\alpha)}_{N_\alpha}}{\sqrt{k_\alpha}} \\
\mathcal{B}_{\beta\alpha}(E) &= \frac{s^{(\alpha)}_{N_\alpha - 1}}{\sqrt{k_\alpha}}\delta_{\alpha\beta} + g^{(\beta,\alpha)}_{N_\beta - 1, N_\alpha - 1}(E) J^{(\alpha)}_{N_\alpha - 1, N_\alpha}(E)\frac{s^{(\alpha)}_{N_\alpha}}{\sqrt{k_\alpha}}.
\end{aligned} \tag{16}$$

The quantity $g$ is the inverse of the total Hamiltonian matrix, and $g^{(\beta,\alpha)}_{N_\beta - 1, N_\alpha - 1}(E)$ is the $(N_\beta - 1, N_\alpha - 1)$ element of the $(\beta, \alpha)$ submatrix of $g$. More explicitly, this element can be written as

$$g^{(\beta,\alpha)}_{N_\beta - 1, N_\alpha - 1}(E) = \sum_{\mu=1}^{N_c} \frac{\Lambda^{(\beta)}_{N_\beta - 1, \mu}\Lambda^{(\alpha)}_{N_\alpha - 1, \mu}}{E_\mu - E} \tag{17}$$

where $E_\mu$ is a Harris energy eigenvalue and

$$(\Lambda^{(1)}_{0,\mu}, \Lambda^{(1)}_{1,\mu}, \ldots, \Lambda^{(1)}_{N_1 - 1, \mu}, \Lambda^{(2)}_{0,\mu}, \ldots, \Lambda^{(2)}_{N_2 - 1, \mu}, \ldots, \Lambda^{(M)}_{0,\mu}, \ldots, \Lambda^{(M)}_{N_M - 1, \mu}) \tag{18}$$

is the associated Harris energy eigenvector. Here, $N_c = \sum_{\alpha=1}^{M} N_\alpha$ is the dimension of the Hamiltonian matrix. This is the same as the total number of $L^2$ functions used to diagonalize the scattering Hamiltonian [9]. It is now straightforward to write the scattering $S$-matrix in terms of the two matrices $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ as

$$S = (\hat{\mathcal{B}} + \mathrm{i}\hat{\mathcal{A}})^{-1}(\hat{\mathcal{B}} - \mathrm{i}\hat{\mathcal{A}}). \tag{19}$$

This equation is valid for real energies above the lowest channel threshold. In particular, $S$ has a well defined value even at the Harris energy eigenvalue despite the fact that $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ are both singular at the Harris energy eigenvalue. This problem is solved in the following sections.

## 3. The condition for resonance

Each element of the $S$-matrix is singular at the complex resonance energy $\epsilon_r$. From equation (19) it is clear that a necessary condition for resonance is that

$$\det(\hat{\mathcal{B}} + \mathrm{i}\hat{\mathcal{A}}) = 0. \tag{20}$$

Since the two operators $(\hat{B} \pm i\hat{A})$ cannot both vanish at a point in the complex energy space, a sufficient condition for resonance is

$$G(E) = \frac{\det(\hat{B} + i\hat{A})}{\det(\hat{B} - i\hat{A})} = 0 \qquad \text{at } E = \epsilon_r. \tag{21}$$

This form for the condition for resonance has two favourable properties. First, $G(E)$ has a well defined value at the Harris energy eigenvalue. Second, $G(E)$ has similar analytic properties as the $S$-matrix itself. Hence the values of $G(E)$ at the Harris eigenvalue can be analytically continued in the complex energy plane.

By writing $g^{(\alpha\beta)}$ for $g^{(\alpha\beta)}_{N_\alpha-1,N_\beta-1}$, $J^{(\beta)}$ for $J^{(\beta)}_{N_\beta-1,N_\beta}$, and $R^{(\beta)}_{\pm}$ for $(c^{(\beta)}_{N_\beta} \pm is^{(\beta)}_{N_\beta})/(c^{(\beta)}_{N_\beta-1} \pm is^{(\beta)}_{N_\beta-1})$, we find it more convenient in subsequent analysis to cast the matrices $(\hat{B} \pm i\hat{A})$ in the form

$$(\hat{B} \pm i\hat{A}) = (1 + F_\pm)D_\pm \tag{22}$$

where

$$(F_\pm)_{\alpha\beta} = g^{(\alpha\beta)} J^{(\beta)} R^{(\beta)}_{\pm} \tag{23}$$

and

$$(D_\pm)_{\alpha\beta} = \frac{1}{\sqrt{k_\beta}} (c^{(\beta)}_{N_\beta-1} \pm is^{(\beta)}_{N_\beta-1})\delta_{\alpha\beta}. \tag{24}$$

Thus, we can write the resonance condition of equation (21) equivalently as

$$G(E) = \frac{\det(D_+)}{\det(D_-)} \frac{\det(1 + F_+)}{\det(1 + F_-)} = 0 \qquad \text{at } E = \epsilon_r. \tag{25}$$

More explicitly, we note that

$$\det(1 + F_\pm) = \begin{vmatrix} 1 + g^{(11)}J^{(1)}R^{(1)}_{\pm} & g^{(12)}J^{(2)}R^{(2)}_{\pm} & \dots & g^{(1M_0)}J^{(M_0)}R^{(M_0)}_{\pm} \\ g^{(21)}J^{(1)}R^{(1)}_{\pm} & 1 + g^{(22)}J^{(2)}R^{(2)}_{\pm} & \dots & g^{(2M_0)}J^{(M_0)}R^{(M_0)}_{\pm} \\ \dots & \dots & \dots & \dots \\ g^{(M_01)}J^{(1)}R^{(1)}_{\pm} & g^{(M_02)}J^{(2)}R^{(2)}_{\pm} & \dots & 1 + g^{(M_0M_0)}J^{(M_0)}R^{(M_0)}_{\pm} \end{vmatrix}. \tag{26}$$

Here, $M_0$ denotes the number of open channels at the energy $E$ of interest. The above determinant is a function of various products of the elements of the matrix $g^{(\alpha\beta)}$, each of which has a first-order pole at the energy $E = E_\mu$. However, because of the form of the residue of $g^{(\alpha\beta)}(E)$ at $E = E_\mu$, we find that all higher-order poles except first order vanish identically. It is not hard to show that, typically, near the energy $E_\mu$, we have

$$\begin{vmatrix} g^{(\alpha_1\beta_1)} & g^{(\alpha_1\beta_2)} & \dots & g^{(\alpha_1\beta_m)} \\ g^{(\alpha_2\beta_1)} & g^{(\alpha_2\beta_2)} & \dots & g^{(\alpha_2\beta_m)} \\ \dots & \dots & \dots & \dots \\ g^{(\alpha_m\beta_1)} & g^{(\alpha_m\beta_2)} & \dots & g^{(\alpha_m\beta_m)} \end{vmatrix} = \frac{Q^{(\alpha_1\dots\alpha_m,\beta_1\dots\beta_m)}(E_\mu)}{(E_\mu - E)} + U^{(\alpha_1\dots\alpha_m,\beta_1\dots\beta_m)}_\mu(E) \tag{27}$$

where $U^{(\alpha_1\dots\alpha_m,\beta_1\dots\beta_m)}_\mu(E)$ is a function that behaves regularly at $E = E_\mu$, and the residue $Q$ has the explicit value

$$Q^{(\alpha_1\dots\alpha_m,\beta_1\dots\beta_m)}(E_\mu) = \sum_{(\nu_1>\nu_2>\dots>\nu_{m-1})} \frac{T^{\alpha_1,\alpha_2,\dots,\alpha_m}_\mu T^{\beta_1,\beta_2,\dots,\beta_m}_\mu}{(E_{\nu_1} - E_\mu)(E_{\nu_2} - E_\mu)\dots(E_{\nu_{m-1}} - E_\mu)} \tag{28a}$$

where

$$T_{\mu}^{\alpha_1,\alpha_2,\ldots,\alpha_m} = \begin{vmatrix} \Lambda^{(\alpha_1)}_{N_{\alpha_1}-1,\mu} & \Lambda^{(\alpha_2)}_{N_{\alpha_2}-1,\mu} & \cdots & \Lambda^{(\alpha_m)}_{N_{\alpha_m}-1,\mu} \\ \Lambda^{(\alpha_1)}_{N_{\alpha_1}-1,\nu_1} & \Lambda^{(\alpha_2)}_{N_{\alpha_2}-1,\nu_1} & \cdots & \Lambda^{(\alpha_m)}_{N_{\alpha_m}-1,\nu_1} \\ \cdots & \cdots & \cdots & \cdots \\ \Lambda^{(\alpha_1)}_{N_{\alpha_1}-1,\nu_{m-1}} & \Lambda^{(\alpha_2)}_{N_{\alpha_2}-1,\nu_{m-1}} & \cdots & \Lambda^{(\alpha_m)}_{N_{\alpha_m}-1,\nu_{m-1}} \end{vmatrix}. \tag{28b}$$

The sum in equation (28*a*) is over the indices $\nu_1, \nu_2, \ldots, \nu_{m-1}$, each ranging from 1 to $N_c$ provided that each is different from the index $\mu$. To take advantage of the properties of the various determinants of the matrix $\{g^{(\alpha\beta)}\}$, we recast equation (25) in the form

$$G(E) = \frac{\det(D_+F_+)}{\det(D_-F_-)} \frac{\det(1+F_+^{-1})}{\det(1+F_-^{-1})}. \tag{29}$$

Now the elements of $F_{\pm}^{-1}$ are just the ratio of such determinants. In fact,

$$\lim_{E\to E_\mu}[1+F_{\pm}^{-1}(E)] = \begin{pmatrix} 1+\frac{1}{J^{(1)}R_{\pm}^{(1)}}\frac{Q_\mu^{(11)}}{Q_\mu^{(M_0)}} & \frac{-1}{J^{(1)}R_{\pm}^{(1)}}\frac{Q_\mu^{(12)}}{Q_\mu^{(M_0)}} & \cdots & \frac{(-1)^{M_0-1}}{J^{(1)}R_{\pm}^{(1)}}\frac{Q_\mu^{(1M_0)}}{Q_\mu^{(M_0)}} \\ \frac{-1}{J^{(2)}R_{\pm}^{(2)}}\frac{Q_\mu^{(21)}}{Q_\mu^{(M_0)}} & 1+\frac{1}{J^{(2)}R_{\pm}^{(2)}}\frac{Q_\mu^{(22)}}{Q_\mu^{(M_0)}} & \cdots & \frac{(-1)^{M_0}}{J^{(2)}R_{\pm}^{(2)}}\frac{Q_\mu^{(2M_0)}}{Q_\mu^{(M_0)}} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{(-1)^{M_0-1}}{J^{(M_0)}R_{\pm}^{(M_0)}}\frac{Q_\mu^{(M_01)}}{Q_\mu^{(M_0)}} & \frac{(-1)^{M_0}}{J^{(M_0)}R_{\pm}^{(M_0)}}\frac{Q_\mu^{(M_02)}}{Q_\mu^{(M_0)}} & \cdots & 1+\frac{1}{J^{(M_0)}R_{\pm}^{(M_0)}}\frac{Q_\mu^{(M_0M_0)}}{Q_\mu^{(M_0)}} \end{pmatrix} \tag{30a}$$

where $M_0$ is now the number of open channels at energy $E_\mu$ and

$$Q_\mu^{(\alpha_i\beta_j)} = Q_\mu^{(12\ldots\alpha_{i-1}\alpha_{i+1}\ldots M_0,12\ldots\beta_{j-1}\beta_{j+1}\ldots M_0)}(E_\mu) = Q_\mu^{(\beta_j\alpha_i)} \tag{30b}$$

while

$$Q_\mu^{(M_0)} = Q_\mu^{(12\ldots M_0,12\ldots M_0)}(E_\mu). \tag{30c}$$

On the other hand, the ratio of the determinants of $D_\pm F_\pm$ in equation (29) reduces to the simple products

$$\frac{\det(D_+F_+)}{\det(D_-F_-)} = \prod_{\alpha=1}^{M_0} \frac{(c_{N_\alpha}^{(\alpha)} + \mathrm{i}s_{N_\alpha}^{(\alpha)})}{(c_{N_\alpha}^{(\alpha)} - \mathrm{i}s_{N_\alpha}^{(\alpha)})}. \tag{31}$$

The above two equations give us the set $\{G(E_\mu)\}_{\mu=1}^{N_c}$ exclusively in terms of the Harris energy eigenvalues and eigenvectors and the $J$-matrix basic functions $\{c_{N_\alpha-1}^{(\alpha)}, c_{N_\alpha}^{(\alpha)}, s_{N_\alpha-1}^{(\alpha)}, s_{N_\alpha}^{(\alpha)}\}_{\alpha=1}^{M_0}$, which are involved in the formation of $\{R_\pm^{(\alpha)}\}_{\alpha=1}^{M_0}$. The set can then be analytically continued in the complex energy plane. A resonance is a zero of the analytically continued $G(E)$. In the next section we show how a similar analysis yields the values of the $S$-matrix elements at the Harris energy eigenvalues and how the partial widths can be extracted from the analytically continued $S$-matrix elements.

## 4. The partial widths

Once a resonance is identified by its complex energy $\epsilon_r$, the partial widths, $\Gamma_\alpha$, associated with channel $\alpha$ is obtained from equation (5) as

$$\Gamma_\alpha = |\lim_{E\to\epsilon_r}(E-\epsilon_r)S_{\alpha\alpha}(E)|. \tag{32}$$

In terms of previously defined functions, the $S$-matrix can be written as

$$S(E) = D_+^{-1}(E)\tilde{S}(E)D_-(E) \tag{33}$$

where

$$\tilde{S}(E) = (1+F_+)^{-1}(1+F_-). \tag{34}$$

Careful analysis of the form of the matrix resulting from the operations on the right-hand side of equation (34) shows that the diagonal elements of the $\tilde{S}$-matrix can be written as

$$\tilde{S}_{\alpha\alpha}(E) = \frac{\det(1+K_\alpha)}{\det(1+F_+)} \tag{35}$$

where $K_\alpha$ is identical to $F_+$ except that $R_+^{(\alpha)}$ is replaced by $R_-^{(\alpha)}$. Also, for the same reasons given before, we cast the above equation in the more convenient form

$$\tilde{S}_{\alpha\alpha}(E) = \frac{\det(K_\alpha)}{\det(F_+)}\frac{\det(1+K_\alpha^{-1})}{\det(1+F_+^{-1})}. \tag{36}$$

The first factor is simply

$$\frac{\det(K_\alpha)}{\det(F_+)} = \frac{R_-^{(\alpha)}}{R_+^{(\alpha)}}. \tag{37}$$

The limit value of $\det(1+K_\alpha^{-1})$ at the Harris energy eigenvalues can be obtained by an identical procedure as in equation (30) for $\det(1+F_+^{-1})$ except that in the $\alpha$th row the factor $R_+^{(\alpha)}$ is replaced by $R_-^{(\alpha)}$. Combining the above relations and using the fact that the matrices $D_\pm$ are diagonal, we finally obtain

$$S_{\alpha\alpha}(E) = \frac{(c_{N_\alpha}^{(\alpha)} - is_{N_\alpha}^{(\alpha)})}{(c_{N_\alpha}^{(\alpha)} + is_{N_\alpha}^{(\alpha)})}\frac{\det(1+K_\alpha^{-1})}{\det(1+F_+^{-1})}. \tag{38}$$

Now the set $\{S_{\alpha\alpha}(E_\mu)\}_{\mu=1}^{N_c}$ can be used to analytically continue the diagonal elements of the $S$-matrix in the complex plane in preparation for taking the limit shown in equation (32) at the resonance energy and the subsequent extraction of the partial widths.

## 5. Analytic continuation and search procedure

The set $\{G(E_\mu)\}_{\mu=1}^{N_c}$, as found using the procedure outlined above, is interpolated in energy using the point-wise rational fraction scheme of Schlessinger [8]. A function $G^{ac}(E)$, which has the continued fraction form

$$G^{ac}(E) = \frac{G(E_1)}{1+}\frac{(E-E_1)a_1}{1+}\cdots\frac{(E-E_{N_c})a_{N_c}}{1} \tag{39}$$

is required to coincide with $G(E_\mu)$ at the Harris eigenvalue $E_\mu$. This fixes the coefficients $\{a_n\}_{n=1}^{N_c}$ in the continued fraction as

$$a_\nu = \frac{1}{(E_\nu - E_{\nu+1})}\left\{1 + \frac{(E_{\nu+1}-E_{\nu-1})a_{\nu-1}}{1+}\frac{(E_{\nu+1}-E_{\nu-2})a_{\nu-2}}{1+} \cdots \frac{(E_{\nu+1}-E_1)a_1}{1-[G(E_1)/G(E_{\nu+1})]}\right\} \tag{40a}$$

and

$$a_1 = \{G(E_1)/G(E_2) - 1\}/(E_2 - E_1). \tag{40b}$$

The function $G^{ac}(E)$ is now used as the analytic continuation of $G(E)$ in the complex energy plane.

Resonances are sought as the zeros of $G^{ac}(E)$ in the second sheet of the complex energy plane. Standard numerical techniques may be employed in the search effort. A preliminary step is to evaluate the absolute value, $|G^{ac}|$, of $G^{ac}(E)$ along lines of constant $\mathrm{Im}(E)$. At some value of $\mathrm{Im}(E)$, the plot of $|G^{ac}|$ versus $\mathrm{Re}(E)$ will show a minimum structure at some value of $\mathrm{Re}(E)$. This is shown in figure 1(*a*). The process may be repeated, but this time for $|G^{ac}|$ versus $\mathrm{Im}(E)$, for the above chosen $\mathrm{Re}(E)$. More pronounced minimum structure is likely to appear in the plot at a new $\mathrm{Im}(E)$, as shown in figure 1(*b*). At any stage the point $E = (\mathrm{Re}(E), \mathrm{Im}(E))$ may be used as a starting point for the application of the Newton–Raphson method [12]. When the starting point is close enough to a zero of $|G^{ac}|$, this method converges very quickly, as shown in table 1. A resonance energy, $\epsilon_r$, is recognized as being the energy at which $|G^{ac}|$ is several orders of magnitude smaller than $|G^{ac}|$ values in its immediate neighbourhood, as shown in figures 1(*c*) and 1(*d*). In rare occasions when the starting energy is still far away from the resonance energy as evidenced by the non-convergence of the Newton–Raphson method, the situation may greatly be improved by the utilization of the Ward method [13]. This method iteratively compares the value of $|G^{ac}|$ at the corners of a square of a chosen side length. As the scheme converges, the side length may be reduced so that the energy where a minimum of $|G^{ac}|$ occurs is approached with higher and higher accuracy. Some experience with the use of the Ward method helps in identifying the stage at which the energy may be successfully used as a starting point in the application of the Newton–Raphson method. The search scheme outlined above has been used successfully to locate the resonance energies discussed in the next section.

In a similar fashion, the set $\{S_{\alpha\alpha}(E_\mu)\}_{\mu=1}^{N_c}$ can be analytically continued in the complex energy plane by a function $S_{\alpha\alpha}^{ac}(E)$ which coincides with $S_{\alpha\alpha}(E)$ at the Harris energy eigenvalues. The limiting process required to find the partial widths is essentially equivalent to finding the derivative of $S_{\alpha\alpha}^{ac}(E)$ at the chosen resonance energy $\epsilon_r$. In practice the derivative is evaluated numerically. Alternatively, one may analytically continue the set $\{(E_\mu - \epsilon_r)S_{\alpha\alpha}(E_\mu)\}_{\mu=1}^{N_c}$ and then evaluate the result at $E = \epsilon_r$. Both methods have been used and were found to yield comparable results.

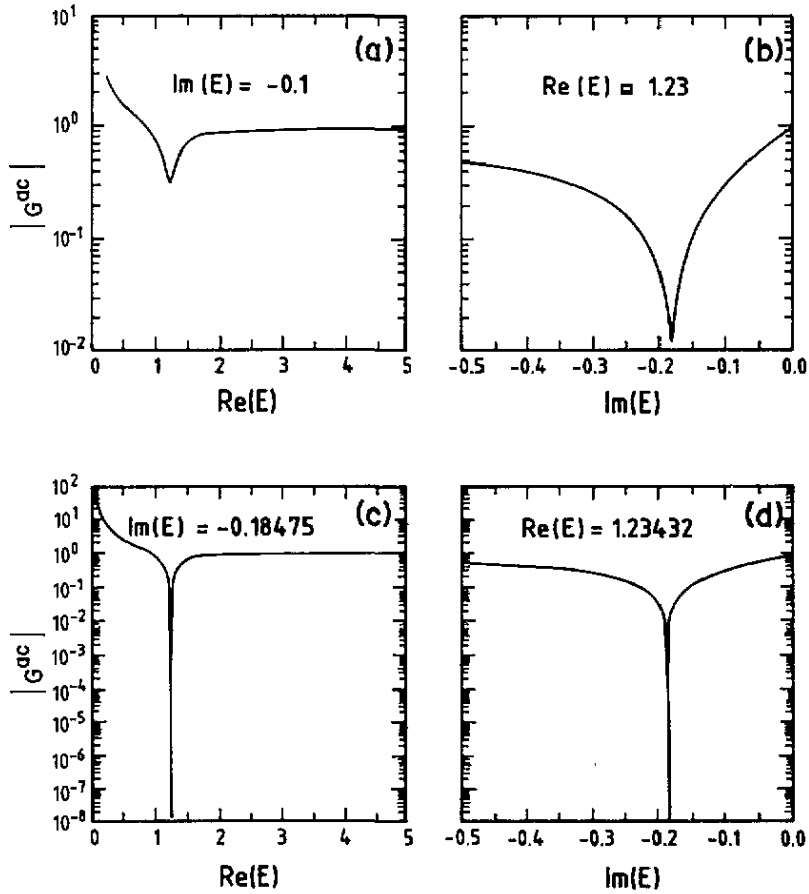


**Figure 1.** Implementation of the search strategy of the zeros of $|G^{ac}(E)|$ in the complex energy plane.

**Table 1.** Resonance search for the potential $V(r) = 2r^2e^{-r}$ (the $z = 0$ case) using the Newton–Raphson method starting with the initial complex energy $E = (1.23, -0.1845)$. The basis size $N$ is 20 and the scale parameter $\lambda$ is 2.0.

| Re($E$) | Im($E$) | $\lvert G^{ac}\rvert$ |
|---|---|---|
| 1.230 000 000 | −1.845 000 000 | 1.21E − 02 |
| 1.234 302 733 | −1.847 964 099 | 1.35E − 04 |
| 1.234 316 686 | −1.847 499 617 | 1.72E − 08 |
| 1.234 316 682 | −1.847 499 661 | 9.90E − 16 |

## 6. Examples

We have applied the method to the $s$-wave scattering by the potential

$$V(r) = 2r^2e^{-r} \tag{41}$$

for the three cases where the charge $z$ may have any of the values 0, −1 or +1. The $z = 0$ case is known [14] to have a resonance at the energy $\epsilon_r = 1.2342 - i0.1872$. We have used

Table 2. The resonance energy, $E_r$, and total width, $\Gamma$, for the potential $V(r) = 2r^2e^{-r}$ for $z = 0, -1$ and $+1$, scale parameter $\lambda = 2.0$ and as a function of basis size $N$, compared to the results of [14] in the $z = 0$ case, and to complex rotation calculation in the $z = -1$ and $+1$ cases.

| $z$ | $N$ | $E_r$ | $\Gamma$ |
|---|---|---|---|
| 0 | 20 | 1.2343 | 0.3695 |
| | 25 | 1.2341 | 0.3745 |
| | 30 | 1.2343 | 0.3744 |
| | 35 | 1.2342 | 0.3745 |
| | From [14] | 1.2342 | 0.3745 |
| −1 | 20 | 0.2361 | 0.0062 |
| | 25 | 0.2380 | 0.0056 |
| | 30 | 0.2359 | 0.0057 |
| | 35 | 0.2359 | 0.0057 |
| | Complex rotation | 0.2359 | 0.0057 |
| +1 | 20 | 1.9106 | 1.1062 |
| | 25 | 1.9038 | 1.1282 |
| | 30 | 1.9036 | 1.1258 |
| | 35 | 1.9038 | 1.1244 |
| | Complex rotation | 1.9040 | 1.1246 |

this model to illustrate the search strategy outlined in the previous section and illustrated in figure 1.

It is a strength of the $J$-matrix method of scattering that the situation when the reference Hamiltonian $H_0$ includes the Coulomb term $(z/r)$ can be handled just as easily as the $z = 0$ case. We give in table 2 the resonance parameters for the cases where $z = 0, -1$ and $+1$ as a function of basis size used. Since these models with $z = -1$ and $+1$ have not been considered by other workers, we compare our results, using the Laguerre basis and different $N$, with the complex rotation method [15].

We also apply the method to a model three-channel problem with $z = 0$ having an interaction potential of the separate form

$$V^{\alpha\beta} = |\zeta_\alpha\rangle V_0^{\alpha\beta}\langle\zeta_\beta| \tag{42}$$

where

$$\langle r|\zeta_\alpha\rangle = e^{-\zeta_{\alpha^2}r^2}. \tag{43}$$

The model has the potential parameters

$$V_0^{\alpha\beta} = \begin{pmatrix} 0.1 & 0.2 & 0.1 \\ 0.2 & -0.3 & 0.1 \\ 0.1 & 0.1 & -1.0 \end{pmatrix} \tag{44}$$

with $\zeta_1 = \zeta_2 = \zeta_3 = 0.5$. The threshold energies are $E_1 = 0$, $E_2 = 2.0$ and $E_3 = 3.0$.

This model may be solved exactly. It possesses a resonance of total width $\Gamma = 0.2245\text{E} - 01$ occurring at $E_r = 3.9404$. The exact associated partial widths are found to be $\Gamma_1 = 0.1493\text{E} - 03$, $\Gamma_2 = 0.1611\text{E} - 01$ and $\Gamma_3 = 0.6050\text{E} - 02$. This model has been solved by the proposed method using the oscillator basis with the same size and scale parameter for all the three channels. Table 3 compares the results of the method with the exact result. It is clear that the method reproduced the resonance parameters very accurately.

**Table 3.** The resonance energy, $E_r$, total width, $\Gamma$, and partial width for a model three-channel problem described in the text as a function of basis size $N$ which has been taken as the same for all three channels. The oscillator basis is used with $\lambda = 1.0$ for all channels. The results of the method are compared with the exact results.

| $N$ | $E_r$ | $\Gamma$ | $\Gamma_1$ | $\Gamma_2$ | $\Gamma_3$ |
|---|---|---|---|---|---|
| 10 | 3.9404 | 0.2228E − 01 | 0.1496E − 03 | 0.1614E − 01 | 0.6004E − 02 |
| 15 | 3.9494 | 0.2245E − 01 | 0.1492E − 03 | 0.1611E − 01 | 0.6050E − 02 |
| 20 | 3.9404 | 0.2245E − 01 | 0.1492E − 03 | 0.1611E − 01 | 0.6050E − 02 |
| Exact | 3.9404 | 0.2245E − 01 | 0.1493E − 03 | 0.1611E − 01 | 0.6050E − 02 |

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