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LETTER TO THE EDITOR

A simple method to extract resonance information from the Harris energy eigenvalues and eigenvectors

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Abstract. Within the framework of the J-matrix method of scattering, a given multichannel potential is modelled by its restriction on a subspace spanned by a certain set of L^2 functions. The scattering S-matrix is found exactly for this model potential at the Harris eigenvalues which result from the diagonalization of the scattering Hamiltonian in the same subspace. These values are then analytically continued in the complex energy plane. The poles of the S-matrix are then identified with the complex resonance energies. The associated widths for each resonance are then extracted from the residues of the S-matrix elements at the designated energy.

Several methods to find the complex resonance energies of a given scattering Hamiltonian are available. One that is well investigated is the complex rotation method [1] in which the Hamiltonian is diagonalized in a finite rotated square-integrable basis. When the rotation is large enough, the resonance energies are exposed as the stable eigenvalues against variation in the size of the basis set and other free scale parameters. Other methods are based on fitting the calculated cross section or related quantities to a Breit–Wigner form near the resonance to extract the position and width of the resonance [2, 3]. The direct method, however, is the one based on the definition of the resonances as the poles of the scattering S-matrix in the complex energy plane. In fact, a knowledge of the S-matrix in a certain region of its domain of analyticity allows the analytic continuation to other regions of the complex energy plane. A search of the poles of the analytically continued S-matrix leads to the location of the complex resonance energy whose real and imaginary parts are related to the position and total width of the resonance. Furthermore, it is a fact [4] that the S-matrix element $S_{\alpha\beta}$, has near the resonance energy, ε_r, the separable form

$$S_{\alpha\beta}=S_{\alpha\beta}^{bg}-i\frac{\gamma_\alpha\bar{\gamma}_\beta^*}{E-\varepsilon_r} \tag{1}$$

where $S_{\alpha\beta}^{bg}$ is the background part of the S-matrix and γ_α is related to the partial width Γ_α via the relation $\Gamma_\alpha=|\gamma_\alpha\bar{\gamma}_\alpha^*|$. Thus, it is easy to compute the partial width from the residues of the S-matrix elements at the designated resonance energy.

The purpose of this letter is to show that the J-matrix method of scattering is well suited to utilize the last scheme described above. Given a multichannel scattering potential, the J-matrix solves the scattering problem exactly for a model potential

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obtained from the restriction of the matrix representation of the given potential in a certain L^2-space. The diagonalization of the full scattering Hamiltonian in the subspace where the model potential is non-zero yields what we refer to as the Harris eigenvalues and eigenvectors [5]. The S-matrix elements at the Harris energy eigenvalues, as will be shown, involve only the associated eigenvectors and some basic J-matrix functions [6]. These elements are then analytically continued in the complex energy plane to extract resonance information as outlined above. The method proposed here completely avoids any integration over complex wavefunctions as required by the methods that use the definition of the resonance width as the modulus squared of a golden rule matrix element of the scattering potential involving the resonance wavefunction at the complex resonance energy [7]. Hence, it also avoids any discussion of the difficulty with the problem of normalization of such complex wavefunctions [7, 8].

Consider the scattering of a structureless particle by a target that has M internal states labelled by the threshold energies $E_1, E_2, \ldots, E_M$. The multichannel Schrödinger equation can now be written as

$$\sum_{\beta=1}^{N_c} [\{H_0-(E-E_\beta)\}\delta_{\alpha\beta}+V^{\alpha\beta}]|\psi_{\beta\alpha}\rangle=0 \tag{2}$$

where H_0 is the projectile reference Hamiltonian that may include, in addition to the lth partial wave kinetic energy, the Coulomb term (z/r). The indices α and β designate the target entrance channel and the exit channel, respectively.

The feature that characterizes the J-matrix method of scattering is its use of the complete set of L^2 basis vectors $\{|\varphi_n^{(\alpha)}\rangle\}_{n=0}^{\infty}$, which render the matrix representation of the operator

$$J^{(\alpha)}(E)=H_0-(E-E_\alpha) \tag{3}$$

tridiagonal. When the scattering potential, $V^{\alpha\beta}$, is identically zero, the channels are decoupled, and the J-matrix method solves the channel Schrödinger equation exactly by giving an explicit representation of the sine-like solution $|\mathscr{S}^{(\alpha)}(E)\rangle$, and the cosine-like solution $|\mathscr{C}^{(\alpha)}(E)\rangle$ as

$$\begin{aligned}|\mathscr{S}^{(\alpha)}(E)\rangle&=\sum_{n=0}^{\infty} s_n^{(\alpha)}(E)|\varphi^{(\alpha)}\rangle\\ |\mathscr{C}^{(\alpha)}(E)\rangle&=\sum_{n=0}^{\infty} c_n^{(\alpha)}(E)|\varphi^{(\alpha)}\rangle.\end{aligned} \tag{4}$$

The Fourier-like coefficients $\{s_n^{(\alpha)}(E), c_n^{(\alpha)}(E)\}_{n=0}^{\infty}$ have been found explicitly [6, 9] in the case of the Laguerre and oscillator bases

$$\varphi_n^{(\alpha)}(r)=(\lambda_\alpha r)^{l+1}\,\mathrm{e}^{-\lambda_\alpha r/2}L_n^{2l+1}(\lambda_\alpha r)$$

or (5)

$$\varphi_n^{(\alpha)}(r)=(\lambda_\alpha r)^{l+1}\,\mathrm{e}_n^{-\lambda_\alpha^2 r^2/2}L^{l+1/2}(\lambda_\alpha^2 r^2)$$

$n=0,1,2,\ldots$, respectively. Here λ_α is a free scale parameter for channel α, and $L_n^{\nu}(x)$ is the Laguerre polynomial.

If, on the other hand, $V^{\alpha\beta}$ does not vanish identically, then the J-matrix method solves the scattering problem exactly for the model potential, $W^{\alpha\beta}$, which is an approximate version of $V^{\alpha\beta}$ in the following sense:

$$W^{\alpha\beta}=P_\alpha^{+}V^{\alpha\beta}P_\beta \tag{6}$$

where P_α is the projection operator defined as

$$P_\alpha = \sum_{n=0}^{N_\alpha - 1} |\varphi_n^{(\alpha)}\rangle\langle\bar{\varphi}_n^{(\alpha)}| \tag{7}$$

and P_α^+ is its adjoint [10]. Also, the set $\{|\bar{\varphi}_n^{(\alpha)}\rangle\}_{n=0}^{\infty}$ is the orthogonal complement to the basis given in (5); i.e.

$$\langle\varphi_n^{(\alpha)}|\bar{\varphi}_m^{(\alpha)}\rangle = \langle\bar{\varphi}_n^{(\alpha)}|\varphi_m^{(\alpha)}\rangle = \delta_{nm}. \tag{8}$$

Effectively, the matrix representation of $W^{\alpha\beta}$ is a truncated version of the matrix representation of $V^{\alpha\beta}$ in function space analogous to truncating the potential to an inner configuration space in the R-matrix method of scattering.

With the proposed solution to the Schrödinger equation (2) written as

$$|\psi_{\beta\alpha}(E)\rangle = \sum_{n=0}^{N_\beta - 1} |\varphi_n^{(\beta)}\rangle b_n^{\beta\alpha} + \sum_{n=N_\beta}^{\infty} |\varphi_n^{(\beta)}\rangle \left\{ \frac{s_n^{(\beta)}(E)}{\sqrt{k_\beta}}\,\delta_{\beta\alpha} + \frac{c_n^{(\beta)}(E)}{\sqrt{k_\beta}}\,R_{\beta\alpha} \right\} \tag{9}$$

the function, $R_{\beta\alpha}$, is just the reactance matrix from which the scattering S-matrix can be constructed as

$$S = (1 - \mathrm{i}R)^{-1}(1 + \mathrm{i}R). \tag{10}$$

It turns out [11, 12] that R itself is a solution of the equation

$$\mathscr{A}R = -\mathscr{B} \tag{11}$$

where matrices $\mathscr{A}$ and $\mathscr{B}$ have the explicit forms

$$\begin{aligned} \mathscr{A}_{\beta\alpha}(E) &= \frac{c_{N_\alpha - 1}^{(\alpha)}}{\sqrt{c_\alpha}}\,\delta_{\alpha\beta} + g_{N_\beta - 1, N_\alpha - 1}^{(\beta,\alpha)}(E) J_{N_\alpha - 1, N_\alpha}^{(\alpha)}(E)\,\frac{c_{N_\alpha}^{(\alpha)}}{\sqrt{k_\alpha}} \\ \mathscr{B}_{\beta\alpha}(E) &= \frac{s_{N_\alpha - 1}^{(\alpha)}}{\sqrt{k_\alpha}}\,\delta_{\alpha\beta} + g_{N_\beta - 1, N_\alpha - 1}^{(\beta,\alpha)}(E) J_{N_\alpha - 1, N_\alpha}^{(\alpha)}(E)\,\frac{s_{N_\alpha}^{(\alpha)}}{\sqrt{k_\alpha}}. \end{aligned} \tag{12}$$

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

$$g_{N_\beta - 1, N_\alpha - 1}^{(\beta,\alpha)}(E) = \sum_{\mu=1}^{N_c} \frac{\Lambda_{N_\beta - 1,\mu}^{(\beta)} \Lambda_{N_\alpha - 1,\mu}^{(\alpha)}}{E_\mu - E} \tag{13}$$

where E_μ is a Harris energy eigenvalues and

$$(\Lambda_{0,\mu}^{(1)}, \Lambda_{1,\mu}^{(1)}, \ldots, \Lambda_{N_1 - 1,\mu}^{(1)}, \Lambda_{0,\mu}^{(2)}, \ldots, \Lambda_{N_2 - 1,\mu}^{(2)}, \ldots, \Lambda_{0,\mu}^{(N_M)}, \ldots, \Lambda_{N_M - 1,\mu}^{(N_M)}) \tag{14}$$

is the associated Harris energy eigenvector, while

$$N_c = \sum_{\alpha=1}^{M} N_\alpha$$

is the dimension of the Hamiltonian matrix that 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, $\mathscr{A}$ and $\mathscr{B}$, as

$$S = (\mathscr{B} + \mathrm{i}\mathscr{A})^{-1}(\mathscr{B} - \mathrm{i}\mathscr{A}). \tag{15}$$

Table 1. The resonance energy E_r and its total width Γ for the potential $V=-0.8\,e^{-0.16r^2}+4.0\,e^{-0.04r^2}$ studied by Csoto *et al* [15] with $\lambda=3.0$ and different basis size, compared with the results reported in [15].

N	E_r	Γ
20	1.6440	0.3744
25	1.6276	0.2590
30	1.6321	0.2462
35	1.6322	0.2458
[15]	1.6323	0.2458

The proposed method is based on the fact that this expression for the S-matrix has a well-defined limit at the real Harris energy eigenvalues $\{E_\mu\}_{\mu=1}^{N_c}$ which involves only the Harris eigenvalues, the associated eigenvectors, and the basic J-matrix functions, $s_n^{(\alpha)}(E)$ and $c_n^{(\alpha)}(E)$. For example, in the single-channel case, the S-matrix has the simple form

$$S(E_\mu)=\frac{c_N(E_\mu)-is_N(E_\mu)}{c_N(E_\mu)+is_N(E_\mu)}. \tag{16}$$

On the other hand, the expression for the S-matrix elements at the Harris energy eigenvalues in the multi-channel case can be readily derived [13]. These values are continued in the complex energy plane using the point-wise rational fraction technique of Schlessinger [14]. A numerical search for the poles of any of the elements of the S-matrix yields the complex resonance energies. At a designated resonance energy, ε_r, the partial width, Γ_α associated with channel α is then found from the residue of the element, $S_{\alpha\alpha}(E)$, at the location of the resonance, namely

$$\Gamma_\alpha=\left|\lim_{E\to\varepsilon_r}(E-\varepsilon_r)S_{\alpha\alpha}(E)\right|. \tag{17}$$

The proposed scheme has been applied to the scattering of an s-wave by the potential

$$V=-0.8\,e^{-0.16r^2}+4.0\,e^{-0.04r^2} \tag{18}$$

which is known [15] to possess a resonance at the energy $\varepsilon_r=1.632-i\,0.1229$. It is usual to parameterize the complex resonance energy ε_r by E_r, the (real) resonance energy, and Γ, its total width, as

$$\varepsilon_r=E_r-i\Gamma/2. \tag{19}$$

Table 1 gives the calculated values for E_r and Γ, when the Laguerra basis with different sizes $N=20$, 25, 30 and 35 are used with scale parameter $\lambda=3.0$. The results compare well with the reported value [15].

The utility of the scheme to extract resonance information in the multi-channel case is exhibited by its application to the scattering of a structureless particle with charge z off a two-state target having a unit positive charge and threshold energies $E_1=0.0$ and $E_2=0.1$ au. The matrix elements of the interaction potential are taken to be the one-term separable Yukawas

$$V^{\alpha\beta}=|\zeta_\alpha\rangle V_0^{\alpha\beta}\langle\zeta_\beta| \tag{19}$$

Table 2. The resonance energy E_r its total width Γ and the partial widths for model two-channel of separable Yukawa potentials using the Laguerre basis with $\lambda=0.9$ for charge $z=0$ and $\lambda=1.4$ for $z=-1$, and different basis size $N_1=N_2=N$, compared with the exact results.

z	N	E_r	Γ	Γ_1	Γ_2
0	10	3.5040	0.7486	0.0288	0.7098
	15	3.4891	0.7844	0.0310	0.7426
	20	3.4857	0.7681	0.0308	0.7277
	Exact	3.4859	0.7672	0.0307	0.7292
−1	15	2.9478	0.2036	0.0096	0.2000
	20	2.9483	0.2109	0.0086	0.2080
	25	2.9463	0.2162	0.0087	0.2147
	Exact	2.9484	0.2174	0.0085	0.2176

where

$$\langle r|\zeta_\alpha\rangle=\frac{e^{-\zeta_\alpha r}}{r}. \tag{20}$$

The potential strengths are chosen to be

$$V=\begin{pmatrix}-0.01 & 0.02\\ 0.02 & 0.075\end{pmatrix} \tag{21}$$

with $\zeta_1=0.10$ and $\zeta_2=0.15$. The case of charge $z=0$ and $z=-1$ has been investigated using the Laguerre basis with several values of N_1 (taken to be equal to N_2) and $\lambda_1=\lambda_2=0.9$. As this model is soluble exactly, table 2 compares the results obtained for the location of the resonance and the partial widths for the two channels with the exact values. It is worth noting that it is a virtue of the J-matrix method of scattering to be able to account for the Coulomb term exactly while approximating only the short-range potential V.

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