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Eigenvalues of the time-delay matrix in overlapping resonances

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Abstract

We discuss the properties of the lifetime or the time-delay matrix $Q(E)$ for multichannel scattering, which is related to the scattering matrix $S(E)$ by $Q = i\hbar S(\mathrm{d}S^{\dagger}/\mathrm{d}E)$. For two overlapping resonances occurring at energies E_ν with widths $\Gamma_\nu (\nu = 1, 2)$, with an energy-independent background, only two eigenvalues of $Q(E)$ are proved to be different from zero and to show typical avoided-crossing behaviour. These eigenvalues are expressible in terms of the four resonance parameters (E_ν, Γ_ν) and a parameter representing the strength of the interaction of the resonances. An example of the strong and weak interaction in an overlapping double resonance is presented for the positronium negative ion. When more than two resonances overlap $(\nu = 1, \ldots, N)$, no simple representation of each eigenvalue has been found. However, the formula for the trace of the Q-matrix leads to the expression $\delta(E) = -\sum \arctan[(\Gamma_\nu/2)/(E - E_\nu)] + \delta_\mathrm{b}(E)$ for the eigenphase sum $\delta(E)$ and the background eigenphase sum $\delta_\mathrm{b}(E)$, in agreement with the known form of the state density. The formulae presented in this paper are useful in a parameter fitting of overlapping resonances.

1. Introduction

The presence of a resonance is associated with a rapid increase in the scattering phase shift $\delta(E)$ with respect to small increase in the collision energy E. Recall that, for narrow isolated resonance with a single open channel, $\delta(E)$ may be parametrized in terms of the resonance position E_ν and width Γ_ν by the Breit–Wigner one-level formula

$$\tan[\delta(E) - \delta_\mathrm{b}(E)] = -(\Gamma_\nu/2)/(E - E_\nu), \tag{1}$$

where the background phase shift $\delta_b(E)$ has a slow variation in energy close to the resonance. The subscript ν will take many integer values in the later discussion, but here we may assume $\nu = 1$. The phase shift may be calculated and fitted to (1) to obtain the parameters E_ν and Γ_ν as well as the function $\delta_b(E)$. The equivalent form for the S-matrix is given by the relation $S(E) \equiv \exp(2i\delta) = S_b^{1/2}[1 - i f_\nu]S_b^{1/2}$, where $S_b(E) = \exp(2i\delta_b)$ denotes the background contribution, and where the function

$$f_\nu(E) = \Gamma_\nu/(E - \mathcal{E}_\nu) = \Gamma_\nu/(E - E_\nu + i\Gamma_\nu/2) \tag{2}$$

represents a simple pole at $E = \mathcal{E}_\nu \equiv E_\nu - i\Gamma_\nu/2$.

When two or more open channels are coupled to an isolated resonance, a matrix

$$S_\nu(E) = I - i f_\nu(E) P_\nu \tag{3}$$

may be introduced, and the S-matrix may be partitioned in the manner [1–4]

$$S(E) = V S_\nu V^T = S_b - i f_\nu(E) V P_\nu V^T \tag{4}$$

with a slowly-varying background scattering matrix $S_b(E) = V V^T$, and a rapidly-varying resonance term. The matrix I in (3) is the unit matrix and the superscript T indicates the transpose. The symmetric matrix P_ν in the symmetric unitary matrix S_ν has the meaning of a projection matrix, and can be written as $P_\nu = \mathbf{c}_\nu \mathbf{c}_\nu^\dagger$ with the real, normalized vector $\mathbf{c}_\nu$ having elements $c_{\nu,i} = (\Gamma_{\nu,i}/\Gamma_\nu)^{1/2}$. Here, $\Gamma_{\nu,i}$ is the partial width, which is proportional to the rate of decay into the channel i. The total width is their sum: $\Gamma_\nu \equiv \sum_i \Gamma_{\nu,i}$. In the usual Breit–Wigner form of $S(E)$ [5], the background S_b-matrix is often assumed to be energy-independent and diagonal, which means that no inelastic scattering occurs in the background. Then, the matrix V is diagonal with elements $V_{ii} = \exp(i\phi_i)$, where the background phase shifts ϕ_i are constants. Although this assumption simplifies the theoretical formalism to a great extent, it is often unrealistic.

A simple parametrization of the S-matrix in the form (4) might appear impractical when many channels, and hence many fitting parameters $\{\Gamma_{\nu,i}\}$ and E_ν, are involved. However, Hazi [6] showed that equation (1) still applies to a multichannel problem if Γ_ν is understood as the total width and if $\delta(E)$ and $\delta_b(E)$ are taken to be the eigenphase sum and the background eigenphase sum, respectively. Thus, by diagonalizing the S-matrix, we define eigenphases $(\delta)_j$ by writing the diagonal elements as $\exp[2i(\delta)_j]$, and similarly the background eigenphases $(\delta_b)_j$ by diagonalizing the background S-matrix, S_b. The (background) eigenphase sum is defined as their sum: $\delta(E) \equiv \sum_j (\delta)_j$, $\delta_b(E) \equiv \sum_j (\delta_b)_j$.

Another important perspective of resonance scattering may be gained from the lifetime matrix or the time-delay matrix $Q(E)$, defined by Smith [7] as a generalization of the time delay in single-channel scattering [8, 9]. Smith showed that, for multichannel scattering, one can prove that

$$Q(E) = i\hbar S \frac{dS^\dagger}{dE} = -i\hbar \frac{dS}{dE} S^\dagger = Q^\dagger(E), \tag{5}$$

where the dagger indicates the Hermitian conjugate. For single-channel scattering, the substitution of the expression $S = \exp(2i\delta)$ in terms of the phase shift δ into (5) leads immediately to the formula $Q = 2\hbar(d\delta/dE)$, which is the additional time spent by the projectile in the collision compared with a passage in the absence of any interaction with the target [8, 9]. For multichannel scattering, the diagonal elements Q_{ii} are real and have the physical meaning of the average time delay, over all possible exit channels, starting from the initial channel i. A matrix analysis proves that the trace of the time-delay matrix Q is related to the eigenphase sum $\delta(E)$ by

$$2\hbar \frac{d\delta}{dE} = \mathrm{Tr}\, Q(E), \tag{6}$$

for the $S(E)$-matrix or the eigenphase sum $\delta(E)$ of *any* functional form, either in the presence or in the absence of resonances [10][5].

The main purpose of the present work is to discuss the eigenvalues of the time-delay matrix for overlapping resonances. These resonances are difficult to treat theoretically in a practically useful manner. Even the representation of the S-matrix is very complex for overlapping resonances as compared with the Breit–Wigner one-level formula, and various alternative proposals are found in the literature, as was reviewed recently [11]. Other aspects of overlapping resonances are found in the review articles [12, 13]. In the present paper, we pay attention to the time-delay matrix and develop, in the following section, a theory of overlapping resonances in multichannel scattering; a special case of two overlapping resonances is treated in detail in section 2.3, which leads to an instructive result. Numerical examples of resonances in positronium negative ions are analysed in terms of this theory in section 2.4. Section 3 summarizes this work.

2. Multichannel overlapping resonances

The construction of an explicitly unitary and symmetric S-matrix having a number of closely lying poles, $\nu = 1, \ldots, N$, is a difficult problem and there is a long history of approaching this from various avenues [11]. Simonius [14] proposed an explicitly unitary representation of the S-matrix in the product form

$$S(E) = V \left(\prod_{\nu=1}^{N} S_\nu \right) V^{\mathrm{T}} \tag{7}$$

in terms of the unitary and symmetric matrices S_ν, defined in (3) and now generalized for $\nu = 1, \ldots, N$. Each S_ν has a simple pole at $E = \mathcal{E}_\nu = E_\nu - \mathrm{i}\Gamma_\nu/2$.

Note that the unit vector $\mathbf{c}_\nu$ in the definition of S_ν is now a complex vector and is no longer expressible in terms of the partial widths $\Gamma_{\nu,i}$ as was the case for isolated resonances. Instead, $\mathbf{c}_\nu$ should be interpreted as a vector characterizing the mixing of the channels. The projection matrix $P_\nu = \mathbf{c}_\nu \mathbf{c}_\nu^\dagger$ satisfies the relations

$$P_\nu^2 = P_\nu = P_\nu^\dagger, \qquad \mathrm{Tr}\left(P_\nu^2\right) = \mathrm{Tr}\, P_\nu = 1. \tag{8}$$

In general, there is no commutation of P_ν nor of the S_ν matrices:

$$[P_\nu, P_{\nu'}] \neq 0, \qquad [S_\nu, S_{\nu'}] \neq 0 \qquad \text{for} \quad \nu \neq \nu'. \tag{9}$$

Therefore, equation (7) is in general asymmetric and fails to satisfy time-reversal invariance. The symmetry of S may be enforced by an appropriate choice of vectors $\{\mathbf{c}_\nu\}$, although this is difficult in practice. Nonetheless, the matrix (7) is quite a general unitary representation having poles at the right places, and is often useful when $\mathbf{c}_\nu$ need not be determined, as will be seen below.

2.1. Preliminary

For later use, we now introduce a Lorentzian function $G_\nu(E)$

$$G_\nu(E) \equiv \tau_\nu |f_\nu(E)|^2 = \frac{\hbar\Gamma_\nu}{(E - E_\nu)^2 + (\Gamma_\nu/2)^2}. \tag{10}$$

[5] Equation (6) might appear trivial at the first sight if S and $S^\dagger$ in (5) are diagonalized by a unitary matrix U. However, one should note that $\mathrm{d}U/\mathrm{d}E$ is not zero in general and that its contribution to Tr Q must be examined.

While $f_\nu(E)$ of (2) is dimensionless, the function $G_\nu(E)$ has the dimension of time and takes a maximum value of four times the lifetime $\tau_\nu = \hbar/\Gamma_\nu$ at $E = E_\nu$. The functions $f_\nu(E)$ and $G_\nu(E)$ satisfy the relations

$$1 - \mathrm{i} f_\nu(E) = (E - \mathcal{E}_\nu^*)/(E - \mathcal{E}_\nu) \equiv \exp[2\mathrm{i}\delta_\nu(E)], \tag{11}$$

$$G_\nu(E) = -\hbar f_\nu'(E)[1 + \mathrm{i} f_\nu^*(E)]. \tag{12}$$

The phase $\delta_\nu(E)$ defined by (11) is easily seen to satisfy a Breit–Wigner-type formula

$$\tan\delta_\nu(E) = -\frac{\Gamma_\nu/2}{E - E_\nu}, \qquad 2\hbar\frac{\mathrm{d}\delta_\nu}{\mathrm{d}E} = G_\nu(E). \tag{13}$$

The time-delay matrix Q_ν corresponding to an S-matrix of the form $V S_\nu V^T$ may be expressed as

$$\begin{aligned} Q_\nu &= -\mathrm{i}\hbar(V S_\nu V^T)'(V S_\nu V^T)^\dagger \\ &= -\mathrm{i}\hbar\big[V S_\nu' S_\nu^\dagger V^\dagger + V' V^\dagger + V S_\nu (V^T)'(V^T)^\dagger S_\nu^\dagger V^\dagger\big] \\ &= G_\nu V P_\nu V^\dagger - \mathrm{i}\hbar\big[V' V^\dagger + V S_\nu (V^\dagger V')^T S_\nu^\dagger V^\dagger\big], \end{aligned} \tag{14}$$

where use has been made of the relation

$$-\mathrm{i}\hbar S_\nu' S_\nu^\dagger = G_\nu P_\nu, \tag{15}$$

which follows from equations (3) and (12). Then clearly,

$$\begin{aligned} \mathrm{Tr}\, Q_\nu &= G_\nu(E) - \mathrm{i}\hbar\,\mathrm{Tr}[V' V^\dagger + (V^\dagger V')^T] \\ &= G_\nu(E) - 2\mathrm{i}\hbar\,\mathrm{Tr}(V' V^\dagger) \\ &= G_\nu(E) + 2\hbar(\mathrm{d}\delta_\mathrm{b}/\mathrm{d}E). \end{aligned} \tag{16}$$

Here, the second term in the last expression has been derived by noting that the unitary matrix V is expressible as $V = U_\mathrm{b}^\mathrm{T} O^{1/2}$ in terms of the orthogonal matrix U_b that diagonalizes S_b as $O = U_\mathrm{b} S_\mathrm{b} U_\mathrm{b}^\mathrm{T}$.

2.2. The time-delay matrix

The Q-matrix for the S-matrix of (7) can be written as

$$\begin{aligned} Q &= -\mathrm{i}\hbar\sum_{\nu=1}^{N} V\Pi_{\nu-1} S_\nu' S_{\nu+1}\cdots S_N V^T (V^T)^\dagger S_N^\dagger \cdots S_1^\dagger V^\dagger - \mathrm{i}\hbar[V' V^\dagger S + S(V^T)^\dagger (V^T)'] S^\dagger \\ &= \sum_{\nu=1}^{N}[G_\nu V\Pi_{\nu-1} P_\nu (\Pi_{\nu-1})^\dagger V^\dagger] - \mathrm{i}\hbar[V' V^\dagger + S(V' V^\dagger)^T S^\dagger] \end{aligned} \tag{17}$$

with

$$\Pi_{\nu-1} \equiv S_1 \cdots S_{\nu-1} \quad \text{for} \quad \nu \geqslant 2, \qquad \Pi_{\nu-1} \equiv I \quad \text{for} \quad \nu = 1, \tag{18}$$

where equation (15) has been used. This leads to a simple expression for its trace

$$\begin{aligned} \mathrm{Tr}\, Q &= \mathrm{Tr}\sum_{\nu=1}^{N} G_\nu P_\nu - \mathrm{i}\hbar\,\mathrm{Tr}[V' V^\dagger + (V' V^\dagger)^T] \\ &= \sum_{\nu=1}^{N} G_\nu(E) - 2\mathrm{i}\hbar\,\mathrm{Tr}(V' V^\dagger) \\ &= \sum_{\nu=1}^{N} G_\nu(E) + 2\hbar\frac{\mathrm{d}\delta_\mathrm{b}}{\mathrm{d}E} \end{aligned} \tag{19}$$

due to (8) and (16). This is a slight generalization of the result derived by Lyuboshitz [15], and also agrees with the result for the state density [12].

Since Tr Q is proportional to the derivative $\mathrm{d}\delta/\mathrm{d}E$ of the eigenphase sum δ according to the general theorem (6), the integration of (19) with respect to the energy E (with the proper consideration of the constant of integration) leads to the formula

$$\delta(E) = \sum_{\nu=1}^{N} \delta_\nu(E) + \delta_{\mathrm{b}}(E) = -\sum_{\nu=1}^{N} \arctan \frac{\Gamma_\nu/2}{E - E_\nu} + \delta_{\mathrm{b}}(E), \tag{20}$$

which is a generalization of the Hazi formula (1) [6] for overlapping resonances. Equation (20) and its derivative (19) involve much less parameters and are much more useful in parameter fitting, than that for the S-matrix elements.

2.3. Overlapping double resonance

The case of two overlapping resonances is tractable in an explicit way. In particular, if the background scattering matrix S_{b} is independent of energy, then the Q-matrix of (17) reduces to

$$Q = G_1 V P_1 V^\dagger + G_2 V S_1 P_2 S_1^\dagger V^\dagger. \tag{21}$$

Then consider the unitary transform

$$\overline{Q} \equiv S_1^\dagger V^\dagger Q V S_1 = G_1 P_1 + G_2 P_2, \tag{22}$$

where the commutativity of P_ν and S_ν has been used. Clearly this has the same eigenvalues and trace as Q, that is Tr Q = Tr $\overline{Q} = G_1 + G_2$ in agreement with (19).

Now consider the eigenvectors of $\overline{Q}$ in the form of a linear combination of the vectors $\mathbf{c}_1$ and $\mathbf{c}_2$. This approach is a generalization of that of [16] for isolated resonances. The eigenvalue equation for $\overline{Q}$ can be written as

$$0 = [\overline{Q} - q]\mathbf{x} = \left[G_1 \mathbf{c}_1 \mathbf{c}_1^\dagger + G_2 \mathbf{c}_2 \mathbf{c}_2^\dagger - q\right](a_1 \mathbf{c}_1 + a_2 \mathbf{c}_2). \tag{23}$$

Multiplication of (23) by $\mathbf{c}_1^\dagger$ and by $\mathbf{c}_2^\dagger$ from the left results in the coupled equations

$$\begin{pmatrix} G_1 - q & \alpha G_2 \\ \alpha^* G_1 & G_2 - q \end{pmatrix} \begin{pmatrix} a_1 + \alpha a_2 \\ \alpha^* a_1 + a_2 \end{pmatrix} = 0 \tag{24}$$

for the coefficients a_1 and a_2. Here we have defined the inner product $\alpha \equiv \mathbf{c}_1^\dagger \mathbf{c}_2$. The non-trivial solutions require that

$$(G_1 - q)(G_2 - q) - \beta G_1 G_2 = 0 \tag{25}$$

with $\beta \equiv |\alpha|^2$ and $0 \leqslant \beta \leqslant 1$. Thus, we have Q eigenvalues given by

$$q = q_\pm \equiv \frac{G_1 + G_2}{2} \pm \frac{[(G_1 - G_2)^2 + 4\beta G_1 G_2]^{1/2}}{2}. \tag{26}$$

The corresponding mixing ratios $r_\pm \equiv a_2/a_1$ are given by

$$q_\pm = (1 + \alpha r_\pm)\, G_1 = \left(1 + \alpha^* r_\pm^{-1}\right) G_2. \tag{27}$$

The sum of the two eigenvalues in (26) reduces to $q_+ + q_- = G_1 + G_2$, which is equal to the trace. On the other hand, the matrix $\overline{Q}(E)$ is positive definite since

$$\mathbf{u}^\dagger \overline{Q} \mathbf{u} = G_1 |\mathbf{u}^\dagger \mathbf{c}_1|^2 + G_2 |\mathbf{u}^\dagger \mathbf{c}_2|^2 \geqslant 0 \tag{28}$$

for any vector $\mathbf{u}$ with the appropriate number of elements. Therefore, the eigenvalues of Q other than $q_\pm$ are all zero. The eigenvectors corresponding to these zero eigenvalues are orthogonal to both $V S_1 \mathbf{c}_1$ and $V S_1 \mathbf{c}_2$.

Each eigenvector defines a linear combination of the original physical channels, a new channel that may be called an eigenchannel associated with the Q-matrix, rather than the S-matrix, or simply a Q-matrix eigenchannel. If the scattering process starts from the Q-matrix eigenchannel associated with the eigenvalue q_+ (or q_-), the average time delay is q_+ (or q_-) and shows a resonance behaviour to be elaborated on in the following. No average time delay occurs for scattering starting from any other Q-matrix eigenchannel.

The pair $q_\pm$ of (26) shows typical avoided-crossing behaviour. The strength of the resonance interaction (avoidance) is determined by two kinds of overlap: (i) that between the two Lorentzian profiles $G_1(E)$ and $G_2(E)$ and (ii) the parameter $\beta = \left|\mathbf{c}_1^\dagger \mathbf{c}_2\right|^2$. The product $G_1(E)G_2(E)$ is almost zero for any E if the two resonances are well separated. Then one of the two eigenvalues $q_\pm$ will be nearly equal to $G_1(E)$ and the other to $G_2(E)$. When $G_1(E)$ and $G_2(E)$ overlap each other significantly, the two limiting cases of (26) are

$$\begin{aligned} &\beta \to 0: \quad q_\pm \to G_i(E), && i = 1, 2 \\ &\beta \to 1: \quad q_+ \to G_1(E) + G_2(E), && q_- \to 0. \end{aligned} \tag{29}$$

In the limit of weak overlap β, the two eigenvalues cross each other. For strong interaction of the resonances, i.e. for $\beta = 1$ (or $\mathbf{c}_1 = \mathbf{c}_2$), q_+ will be the only nonzero eigenvalue of the time-delay matrix. In this limit, the two projection matrices are the same ($P_1 = P_2$), and it follows that $\overline{Q}(E) = [G_1(E) + G_2(E)]P_1$. Thus the rank of $\overline{Q}$ is 1. This leads to the case of single-channel resonance with a double-Lorentzian profile. Both of the two resonances are associated with the same Q-matrix eigenchannel defined by the eigenvector $V S_1 \mathbf{c}_1$. Scattering starting from any other Q-matrix eigenchannel has no average time delay.

Note that equation (26) contains only five parameters, namely, the resonance parameters E_1, Γ_1, E_2 and Γ_2 and the overlap parameter β. Details of the vectors $\mathbf{c}_i$ are irrelevant to the Q-matrix eigenvalues for the case of two overlapping resonances with a constant background scattering matrix. Thus, equation (26) affords a convenient and physically transparent parametrization procedure, as will be illustrated in the following subsection.

2.4. Numerical examples of strongly and weakly avoided crossing

Overlapping quantum resonances are common not only in nuclear physics, but also in atomic and molecular systems; see [17–19] for some recent examples. Here we take up the positronium negative ion Ps^- consisting of an electron and a positronium Ps, the latter being a bound state between an electron e^- and a positron e^+. The system Ps^- is equivalent to its charge conjugate system, positronium positive ion $Ps^+ = e^+e^-e^+$. Multichannel continuum states have been calculated by solving close-coupling equations in terms of the hyperspherical coordinates; see [18, 19] for computational details and results. In this example, the two extremes of overlapping resonances are apparent: (a) resonances for the symmetry $^1P^o$ in the energy region just below the threshold $E = -0.027\,78$ au for the break-up into $e^- + Ps(n = 3)$, where n is the principal quantum number, and (b) resonances of symmetry $^1D^e$ just above this threshold. All channels breaking up asymptotically into $e^- + Ps(n \leqslant 4)$ have been included in the close-coupling calculations.

The solid curves in figures 1(a) and (b) represent the two largest calculated eigenvalues of the Q-matrix. Those in figure 1(a) for $Ps^-(^1P^o)$ illustrate the case typical of strong interaction, $\beta \simeq 1$. The upper eigenvalue q_1 looks like a mere superposition of two Lorentzian profiles, one quite narrow and strong and the other much broader and weak. The lower eigenvalue q_2 is much smaller than q_1. Indeed, a choice of $\beta = 0.95$, $(E_1, \Gamma_1) = (-2.8125\times10^{-2}\,\text{au}, 6.24\times10^{-7}\,\text{au})$ and $(E_2, \Gamma_2) = (-2.8097 \times 10^{-2}\,\text{au}, 3.33 \times 10^{-5}\,\text{au})$ in equation (26) results in the broken curves, which show a very good fit to the solid curves. The upper broken curve is hardly

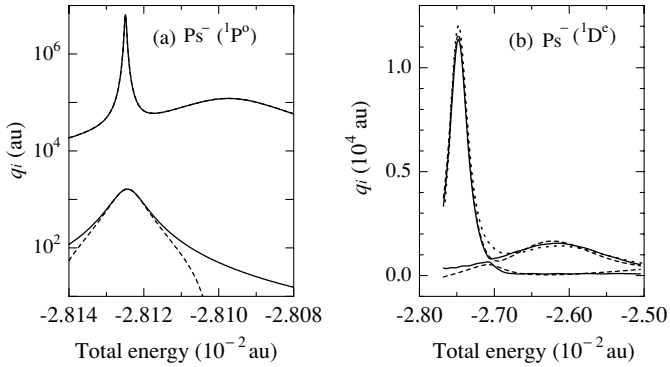

Figure 1. Examples of the eigenvalues q_i of the time-delay matrix $Q(E)$ in the region of an overlapping double resonance in the positronium negative ion $Ps^- = e^+e^-e^-$. The small eigenvalues irrelevant to the avoided crossing are excluded. (a) The strong avoidance case with $\beta = 0.95$ in the symmetry $^1P^o$. Solid curves: hyperspherical close-coupling calculations. Broken curves: fitting of equation (26). The upper broken curve is indistinguishable from the solid curve. (b) The weak avoidance case with $\beta = 0.10$ in the symmetry $^1D^e$. Solid curves: hyperspherical close-coupling calculations. Broken curves: fitting of equation (26) with a weak background augmented; see the text.

distinguishable from the solid curve and from the calculated values of Tr Q. The difference between the solid and broken curves for the lower eigenvalue looks appreciable because of the logarithmic scale, but the absolute difference is quite small. These results also confirm that the background variation is almost negligible in this case.

The solid curves in figure 1(b) for $Ps^-(^1D^e)$ exhibit a typical avoided crossing between narrow and broad resonances, illustrating $\beta \ll 1$. However, a trial fit of (26) immediately suggests the presence of an appreciable background. Thus we add a correction term linear in E to (26). The first step is to fit $f_+(E) \equiv q_+ + q_- + C_0 + C_1E$ to the calculated values of $q_1 + q_2$ to determine the parameters $E_1, \Gamma_1, E_2, \Gamma_2, C_0$ and C_1 since f_+ is independent of β. The second step is to fit $f_-(E) \equiv q_+ - q_- + C_1' + C_2'E$ to $q_1 - q_2$ keeping the already determined values of $(E_i, \Gamma_i, i = 1, 2)$ as they are, to determine the three parameters β, C_1' and C_2'. The values $\beta = 0.10, (E_1, \Gamma_1) = (-2.7480 \times 10^{-2}\text{au}, 3.15 \times 10^{-4}\text{au})$ and $(E_2, \Gamma_2) = (-2.627 \times 10^{-2}\text{au}, 1.7 \times 10^{-3}\text{au})$ yield the broken curves in fairly good agreement with the solid curves. In fact, Tr Q for this case (which is close to $q_+ + q_-$ in the resonance region) was analysed in [19] in terms of the Gaussian-sum formula with a significant background taken into account. The background in this case shows a typical divergence behaviour towards the threshold of $Ps(n = 3)$ due to the dipole field, which was included explicitly in the fitting formula [19]. The resonance parameters obtained were $(E_1, \Gamma_1) = (-2.7480 \times 10^{-2}$ au, 3.1×10^{-4} au) and $(E_2, \Gamma_2) = (-2.617 \times 10^{-2}$ au, 2.1×10^{-3} au), which are quite close to the values extracted from q_+ and q_-.

3. Conclusion

No convenient representation of the multichannel S-matrix for overlapping resonances that is explicitly unitary and symmetric appears to be known in the literature [11]. The explicitly unitary form proposed by Simonius [14] is often useful in the formal theory of overlapping resonances, although the many parameters involved in it make parameter fitting for S-matrix elements almost impossible in practice. However, considerable simplification is attained by

dealing with the lifetime or time-delay matrix $Q(E)$ derived by Smith [7]. Its trace Tr $Q(E)$, which is proportional to the energy derivative of the eigenphase sum $\delta(E)$ (see (6)), is expressible as the sum of the Lorentzian resonance profiles with different heights and widths, plus a term proportional to the energy derivative of the background eigenphase sum $\delta_b(E)$; see (19). This result reduces to $\delta(E)$ expressed as the sum of the Breit–Wigner one-level formulae and $\delta_b(E)$; see (20).

The parametrization of each eigenvalue of the Q-matrix for overlapping resonances is difficult and impractical in general. However, the case of a double resonance with a constant background scattering matrix is easily tractable. We find that only two eigenvalues $q_1(E)$ and $q_2(E)$ are different from zero. They take a form (26) of avoided crossing of two Lorentzian profiles, the strength of the avoidance being represented by a mixing parameter β in this expression, which ranges from 0 to 1. The limit as $\beta \to 0$ is the case of no avoidance, and two Lorentzian profiles cross each other. For $\beta \to 1$, the maximum avoidance occurs with a result that the smaller of the two eigenvalues $q_1(E)$ and $q_2(E)$ tends to zero and the larger becomes the sum of two Lorentzian profiles. Examples close to these two extreme cases, found in the positronium negative ion, have been presented. In conclusion, both the eigenphase sum formulae for the general overlapping resonances and the Q-matrix eigenvalue formula for a double resonance are quite useful in parametrization of overlapping resonances.

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