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Degeneracy of resonances in a double barrier potential

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Abstract. Degeneracy of resonant states and double poles in the scattering matrix of a double barrier potential are contrived by adjusting the parameters of the system. The cross section, scattering wavefunction and Gamow eigenfunction are computed at degeneracy. Some general properties of the degeneracy of resonances are exhibited and discussed in this simple quantum system.

1. Introduction

In this paper, by means of a simple and elementary example, we will exhibit some characteristic properties of the degeneracy of two resonant states and the concomitant occurrence of a complex double pole in the S-matrix of a quantum system.

The problem of the degeneracy of resonances arises naturally in connection with the Berry phase of resonant states [1–4]. In a previous paper, we have shown that accidental degeneracies of resonant states mixed by a Hermitian interaction give rise to multiple poles in the S-matrix [5]. More recently, a number of cases of interfering resonances leading to degeneracy have been described. We considered a doublet of unbound states in ^{8}Be as an example of accidental degeneracy of resonances [6]. Vanroose *et al* [7] examined the formation of complex double poles of the S-matrix in a two channel model with square well potentials. Kylstra and Joachain [8, 9] discussed double poles of the S-matrix in the case of laser-assisted electron–atom scattering. Latinne *et al* [10, 11] studied degeneracies involving auto-ionizing states in complex atoms. Lassila and Ruuskanen [12] pointed out that Stark mixing in an atom can display double pole decay. Knight [13] examined the decay of Rabi oscillations in a two level system with double poles. Double poles were investigated as examples of non-exponential decay laws by Bell and Goebel [14] who proposed a one channel, double barrier potential model and a Lee-type model of unstable particles as examples showing double poles. The formal theory of multiple pole resonances and resonant states in the rigged Hilbert space formulation of quantum mechanics was developed by Bohm *et al* [15] and Antoniou *et al* [16].

Here, we will discuss the formation of a series of doublets of interfering resonances in the scattering of a beam of particles by a double barrier potential in the model of Bell and Goebel [14]. It will be shown that degeneracies of resonant states and double poles of the S-matrix may be brought about by simply adjusting the parameters of the system, i.e., the strength and position of the two potential barriers. In the particular model discussed here, the double poles lie very close to the real axis and can therefore readily be associated with well pronounced resonances. We solve the degeneracy conditions numerically and compute the phase shift, cross section, scattering wavefunction and the Gamow eigenfunction at degeneracy. We also

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present an approximate analytical solution of the degeneracy conditions which allows us to discuss some properties of the complex energy hypersurfaces at degeneracy in parameter space. Although the discussion is restricted to resonances in this rather schematic model of a potential well with two regions of trapping, we will put emphasis on those characteristic properties of the degeneracy of resonant states of a generic nature which are, in fact, independent of the model.

2. Scattering by a double delta barrier potential

Doublets of resonances and accidental degeneracy of resonant states may occur in the scattering of a beam of particles by a potential well with two regions of trapping. A simple example is provided by two concentric spherical potential barriers which divide space into three regions: an inner spherical cavity inside the first barrier, a second cavity comprised between the two spherical barriers and the outer free space. In what follows, we will consider the conditions for the occurrence of a degeneracy of two resonances in this simple system and some of the properties of the Gamow eigenfunctions near and at a degeneracy of resonances. In order to make the analysis as simple and explicit as possible, we take the potential barriers to be delta functions.

The s-wave radial Schrödinger equation is

$$\frac{\mathrm{d}^2u(k,r)}{\mathrm{d}r^2} + k^2u(k,r) - \left(\frac{\pi}{\alpha}\delta(r-a) + \frac{\pi}{\beta}\delta(r-b)\right)u(k,r) = 0. \tag{1}$$

The external parameters of the system are the strength of the two potential barriers, π/α and π/β, and the ratio b/a of the two barrier positions. The parameters α, β, a and b are real and positive, we will take $b > a$.

The regular solution of (1) normalized to unit slope at the origin, $\phi(k,r)$, is as follows. In the inner region, $0 \leqslant r \leqslant a$,

$$\phi_I(k,r) = \frac{1}{k}\sin kr \tag{2}$$

at $r = a$; $\phi_I(k,r)$ is continuous but its derivative is discontinuous:

$$\phi_I(k,a) = \phi_{II}(k,a) \tag{3}$$

$$\left(\frac{\mathrm{d}\phi_{II}}{\mathrm{d}r}\right)_a = \left(\frac{\mathrm{d}\phi_I}{\mathrm{d}r}\right)_a + \frac{\pi}{\alpha}\phi_I(k,a). \tag{4}$$

Hence, in the middle region, $a \leqslant r \leqslant b$,

$$\phi_{II}(k,r) = \frac{1}{k}\left(\sin kr + \frac{\pi}{(k\alpha)}\sin ka \sin k(r-a)\right). \tag{5}$$

At $r = b$, $\phi(k,r)$ satisfies continuity conditions similar to (4) with β in place of α. Hence, in the outer region, for $r \geqslant b$, we obtain

$$\phi_{III}(k,r) = \frac{1}{k}\left\{\sin kr + \frac{\pi}{k\alpha}\sin ka \sin k(r-a) + \frac{\pi}{k\beta}\left[\sin kb + \frac{\pi}{k\alpha}\sin ka \sin k(b-a)\right]\sin k(r-b)\right\}. \tag{6}$$

The last expression may be written as a combination of an outgoing wave $\exp(\mathrm{i}kr)$ and an incoming wave $\exp(-\mathrm{i}kr)$:

$$\phi_{III}(k,r) = \frac{\mathrm{i}}{2k}[f(-k)\exp(-\mathrm{i}kr) - f^*(-k)\exp(\mathrm{i}kr)] \tag{7}$$

where

$$f(-k) = 1 + \frac{\pi}{k\alpha}\exp(\mathrm{i}ka)\sin ka + \frac{\pi}{k\beta}\exp(\mathrm{i}kb)\sin kb + \frac{\pi^2}{k^2\alpha\beta}\exp(\mathrm{i}kb)\sin ka\sin k(b-a) \tag{8}$$

is the Jost function and $f^*(-k) = f(k)$.

The scattering wavefunction, $\psi(k, r)$, is the solution of (1) which vanishes at the origin and, for values of r larger than the range of the potential, behaves as the sum of a free incoming spherical wave of unit incoming flux plus a free outgoing spherical wave. The coefficient of the outgoing spherical wave is the scattering matrix $S(k)$:

$$\psi(k, 0) = 0 \tag{9}$$

and

$$\lim_{r\to\infty}\{\psi(k, r) - [\exp(-\mathrm{i}kr) - S(k)\exp(\mathrm{i}kr)]\} = 0. \tag{10}$$

Hence, the scattering wavefunction $\psi(k, r)$ and the regular solution $\phi(k, r)$ are related by

$$\psi(k, r) = \frac{-2\mathrm{i}k}{f(-k)}\phi(k, r) \tag{11}$$

and the scattering matrix is given by

$$S(k) = \frac{f^*(-k)}{f(-k)} = \exp(\mathrm{i}2\delta(k)) \tag{12}$$

where the Jost function $f(-k)$ is given by (8). The phase shift $\delta(k)$ may be written as

$$\delta(k) = -\tan^{-1}\left(\frac{\mathcal{N}}{\mathcal{D}}\right) \tag{13}$$

where

$$\mathcal{N} = \frac{\pi}{k\alpha}\sin^2 ka + \frac{\pi}{k\beta}\sin^2 kb + \frac{\pi^2}{k^2\alpha\beta}\sin ka\sin kb\sin k(b-a)$$

and

$$\mathcal{D} = 1 + \frac{\pi}{k\alpha}\sin ka\cos ka + \frac{\pi}{k\beta}\sin kb\cos kb + \frac{\pi^2}{k^2\alpha\beta}\sin ka\cos kb\sin k(b-a).$$

The cross section σ_0

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta(k) \tag{14}$$

is readily computed from (12)–(14); see figure 1.

3. Resonances and resonant states

The zeros of the Jost function

$$f(-k_n) = 1 + \frac{\pi}{k_n\alpha}\sin k_n a\exp(\mathrm{i}k_n a) + \frac{\pi}{k_n\beta}\sin k_n b\exp(\mathrm{i}k_n b) + \frac{\pi^2}{k_n^2\alpha\beta}\sin k_n a\sin k_n(b-a)\exp(\mathrm{i}k_n b) = 0 \tag{15}$$

give poles in the scattering matrix $S(k)$.

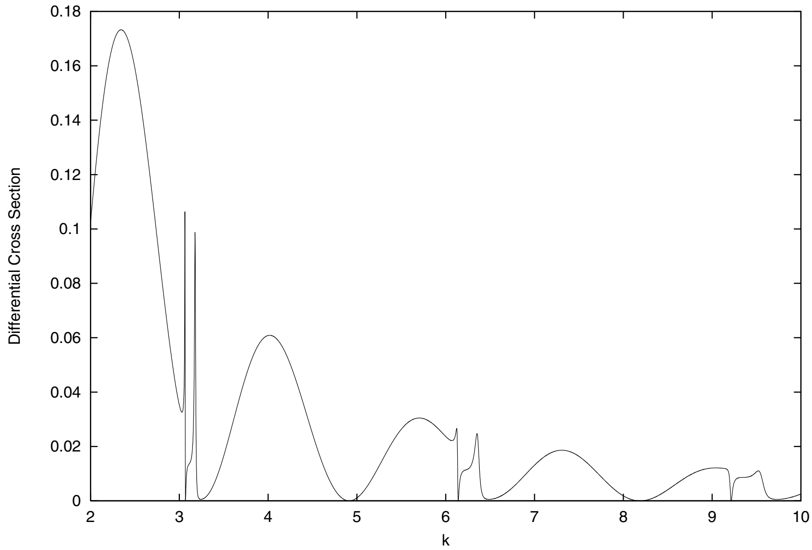

Figure 1. The scattering cross section $\sigma_0(k)$ for $\alpha = 0.05$, $\beta = 0.1$ and $b = 1.95$ (α, β, and b are measured in units of a, k is measured in units of a^{-1}). A series of doublets of narrow resonances, centred at $k \cong n\pi$, $n = 1, 2, 3, \ldots$, is apparent. Off resonance, the wide bumps in the cross section are typical of hard sphere scattering.

Resonant or Gamow eigenfunctions, $u_n(k_n, r)$, are the solutions of (1) which vanish at the origin and behave as purely outgoing spherical waves for values of r larger than the range of the potential:

$$u_n(k_n, 0) = 0 \tag{16}$$

and

$$\lim_{r\to\infty} \left[\frac{\mathrm{d}u_n(k_n, r)}{\mathrm{d}r} - \mathrm{i}k_n u_n(k_n, r) \right] = 0 \tag{17}$$

where k_n is a complex solution of (15) with $\mathrm{Re}\, k_n > 0$ and $\mathrm{Im}\, k_n < 0$.

From (7), (15) and (17), the Gamow eigenfuctions $u_n(k_n, r)$ and the regular solution $\phi(k, r)$ are related by

$$u_n(k_n, r) = \frac{2\mathrm{i}k_n N_n}{f(k_n)} \phi(k_n, r) \tag{18}$$

where N_n is a normalization constant. Then, in the inner region, $0 \leqslant r \leqslant a$, the Gamow eigenfunction is

$$u_n^{(I)}(k_n, r) = N_n \sin k_n r; \tag{19}$$

in the middle region, $a \leqslant r \leqslant b$,

$$u_n^{(II)}(k_n, r) = N_n \left(\sin k_n r + \frac{\pi}{k_n \alpha} \sin k_n a \sin k_n (r - a) \right); \tag{20}$$

and in the outer region, $b \leqslant r < \infty$,

$$u_n^{(III)}(k_n, r) = N_n \left(\sin k_n b + \frac{\pi}{k_n \alpha} \sin k_n a \sin k_n (b - a) \right) \exp(-\mathrm{i}k_n b) \exp(\mathrm{i}k_n r). \tag{21}$$

4. Doublets of resonances

The condition for resonances to occur, equation (15), may be rewritten as

$$\left(k + \frac{\pi}{\alpha}\exp(\mathrm{i}ka)\sin ka\right)\left(k + \frac{\pi}{\beta}\exp(\mathrm{i}k(b-a))\sin k(b-a)\right) \\ -\mathrm{i}k\frac{\pi}{2\beta}\exp(\mathrm{i}2k(b-a))(\exp(\mathrm{i}2ka)-1) = 0. \tag{22}$$

When the second term in the left-hand side of equation (22) is very small,

$$\left|\frac{k\pi}{2\beta}\exp(\mathrm{i}2k(b-a))(\exp(\mathrm{i}2ka)-1)\right| \approx 0 \tag{23}$$

the two trapping regions are weakly coupled. Then, the resonances in the double barrier potential occur as if the two cavities were resonating (almost) independently of each other. The condition (23) is satisfied when

$$ka \approx \pi + u \tag{24}$$

with

$$|u| \ll 1 \tag{25}$$

and

$$\frac{\pi^2 a}{\beta}|u| \ll 1. \tag{26}$$

The two cavities resonate in unison if both factors in the first term in the left-hand side of (22) are also very small for the same values of the parameters.

Computing the first factor in the left-hand side of (22) to leading order in u, gives

$$ka + \frac{\pi a}{\alpha}\exp \mathrm{i}ka \sin ka \approx \pi + \left(1 + \frac{\pi a}{\alpha}\right)u + \mathrm{i}\frac{\pi a}{\alpha}u^2. \tag{27}$$

The resonance condition for the first cavity, i.e. the vanishing of (27), gives u in terms of α:

$$u \approx -\frac{\alpha}{a}\frac{\pi}{\pi + \frac{\alpha}{a}}. \tag{28}$$

Then, the inequalities (25) and (26) become

$$0 < \frac{\alpha}{a} < \frac{\beta}{a\pi^2} \ll 1. \tag{29}$$

Therefore, the condition (23) is satisfied when the inner shell potential at $r = a$ is very strongly repulsive and the outer shell potential at $r = b$ is also strongly repulsive but less so than the inner one. Then, the two cavities resonate almost independently of each other, and the first cavity resonates at

$$ka \approx \pi - \frac{\alpha}{a}\frac{\pi}{\pi + \frac{\alpha}{a}} - \mathrm{i}\frac{\alpha}{a}\frac{\pi^2}{\pi + \frac{\alpha}{a}}. \tag{30}$$

If we want the two cavities to resonate at the same wavenumber, it should be possible to accommodate about the same number of half-wavelengths in each cavity, which may be accomplished if the radial dimensions are similar, that is, if

$$\frac{b}{a} - = 1 - x \tag{31}$$

with

$$|x| \ll 1. \tag{32}$$

The magnitude of x may be estimated from the resonance condition for the second cavity. Computing the second factor in the first term in the left-hand side of (22) to leading order in α/a and x, we obtain:

$$ka + \frac{ka}{\beta} \exp \mathrm{i}ka \left(\frac{b}{a} - 1\right) \sin ka \left(\frac{b}{a} - 1\right) \approx \left(1 - \frac{\alpha}{\beta}\right) \frac{\pi}{\pi + \frac{\alpha}{a}} - \frac{\pi a + \beta}{\beta} x. \tag{33}$$

The resonance condition for the second cavity, i.e. the vanishing of (33), gives

$$x \approx \frac{\beta - \alpha}{a(\pi + \frac{\beta}{a})}. \tag{34}$$

Once we have an order of magnitude estimate for x, we may estimate the resonance wavenumber of the second cavity. From (31),

$$k(b - a) = ka(-x) \tag{35}$$

when the two cavities resonate in unison, ka and x are given by (30) and (34) respectively. Then, the second cavity will resonate at

$$k(b - a) \approx \pi - \frac{\beta}{a} \frac{\pi}{\pi + \frac{\beta}{a}} - \mathrm{i} \frac{\beta}{a} \frac{\pi^2}{\pi + \frac{\beta}{a}}. \tag{36}$$

Therefore, when the inner shell potential is very strongly repulsive, the outer shell potential is also strongly repulsive but less so than the inner one and the radial dimensions of the two cavities are such that they may accommodate about the same number of half-wavelengths; the inner cavity will resonate at

$$k_n a \approx n\pi - n \frac{\alpha}{a} \frac{\pi}{\pi + \frac{\alpha}{a}} - \mathrm{i} n \frac{\alpha}{a} \frac{\pi^2}{\pi + \frac{\alpha}{a}} + \cdots \qquad n = 1, 2, 3, \ldots \tag{37}$$

and the outer cavity will resonate at

$$k_{n'}(b - a) \approx n'\pi - n' \frac{\beta}{a} \frac{\pi}{\pi + \frac{\beta}{a}} - \mathrm{i} n' \frac{\beta}{a} \frac{\pi^2}{\pi + \frac{\beta}{a}} + \cdots \qquad n' = 1, 2, 3, \ldots. \tag{38}$$

Hence, when (23), (29) and (34) are satisfied, we have an infinite series of doublets of resonances.

The most extreme instance of closely spaced resonances is that of an exact coincidence of two resonances, that is, of a double pole in the scattering matrix. Consider, for example, the first doublet of resonances, $n = n' = 1$. If we want the two cavities to resonate exactly at the same wavenumber, one needs to match exactly both the real and imaginary parts of the corresponding resonance wavenumbers. In the following section, it will be shown that small changes in at least two parameters will allow us to tune the two trapping regions so that they will resonate in unison; see figures 2 and 3.

5. Accidental degeneracy of resonances

When the Jost function $f(-k)$ has a double zero at $\tilde{k}$, the scattering matrix $S(k)$ has a double pole at $k = \tilde{k}$. Hence, the condition for the occurrence of a degeneracy of two resonances is that both the Jost function $f(-k)$ and its first derivative $\mathrm{d}f(-k)/\mathrm{d}k$ vanish at $\tilde{k}$. From (8), these conditions become

$$\tilde{k}\left(\tilde{k} + \frac{\pi}{\beta} \exp(\mathrm{i}\tilde{k}b) \sin \tilde{k}b\right) + \frac{\pi}{\alpha} \exp(\mathrm{i}\tilde{k}a) \sin \tilde{k}a \left[\tilde{k} + \frac{\pi}{\beta} \exp(\mathrm{i}\tilde{k}(b - a)) \sin \tilde{k}(b - a)\right] = 0 \tag{39}$$

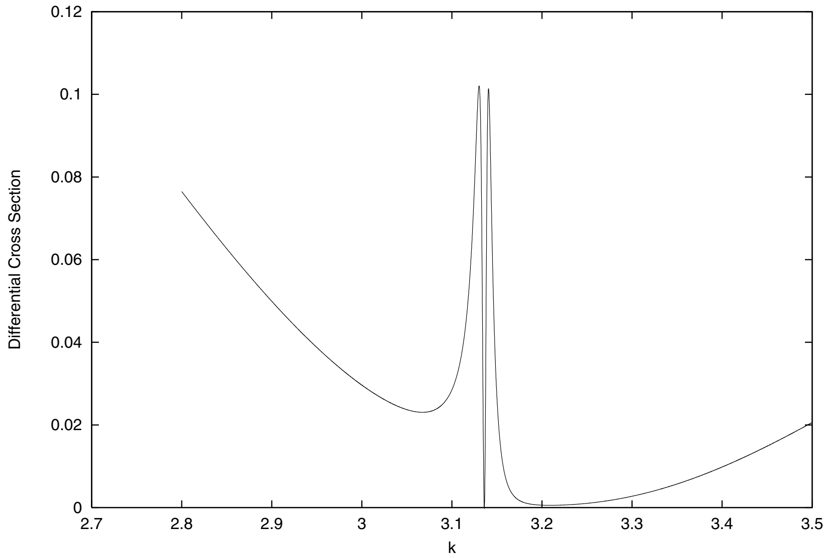

Figure 2. Degeneracy of the first doublet of resonances is brought about at $\tilde{k} = 3.136\,507\,668 - \mathrm{i}0.005\,062\,929$ by fine tuning the parameters of the system to the values $\alpha = 0.005\,077\,3229$, $\beta = 0.101\,86$ and $b = 1.968\,008\,257\,74$. At the double pole degeneracy, the cross section has a narrow split peak.

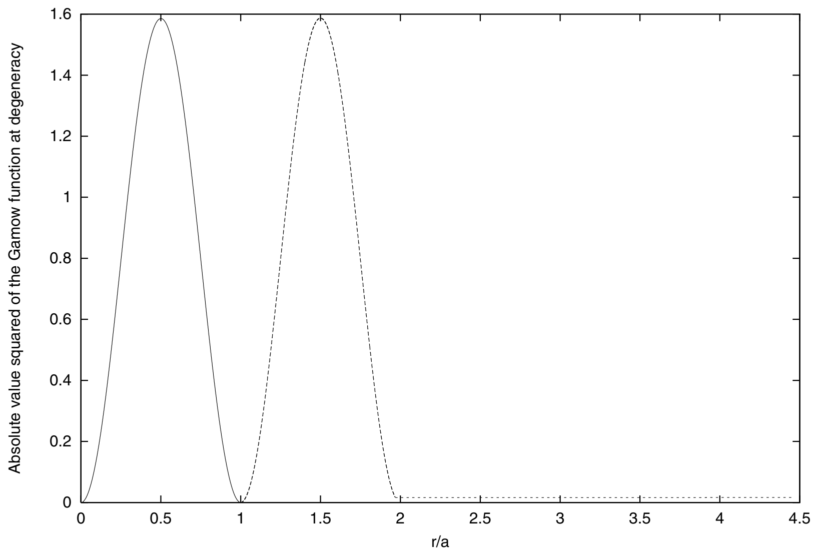

Figure 3. The absolute value squared of the Gamow eigenfunction belonging to the double pole (exact degeneracy) as a function of r. The full curve is the amplitude squared of the wave in the inner region, $0 \leqslant r/a \leqslant 1$. The dashed curve is the amplitude squared of the wave in the middle region, $1 \leqslant r/a \leqslant 1.968\,008\,257\,74$. The short-dashed line is the amplitude squared of the wave in the outer, free space, region; the exponential growth of the amplitude in this region is so slow that it is not apparent in the figure.

and

$$2\tilde{k} + \frac{\pi}{\beta}\exp(\mathrm{i}\tilde{k}b)\sin\tilde{k}b + \tilde{k}\frac{\pi}{\beta}b\exp(\mathrm{i}2\tilde{k}b) + \frac{\pi}{\alpha}\exp(\mathrm{i}\tilde{k}a)\sin\tilde{k}a\left[1 + \frac{\pi}{\beta}(b-a)\exp(\mathrm{i}\tilde{k}2(b-a))\right] + \frac{\pi}{\alpha}a\exp(\mathrm{i}2\tilde{k}a)\left[\frac{\pi}{\beta}\exp(\mathrm{i}\tilde{k}(b-a))\sin\tilde{k}(b-a) + \tilde{k}\right] = 0. \quad (40)$$

We have a system of two coupled independent equations with three real, independent parameters, α/a, β/a and b/a, whose values should be adjusted to satisfy (39) and (40). The coupled equations (39) and (40) were solved numerically. In the numerical computation, length was measured in units of a and the wavenumber k was measured in units of a^{-1}. Accordingly, in the following, we will write α, β, b, k_n and $\tilde{k}$ instead of α/a, β/a, b/a, $k_n a$ and $\tilde{k}a$. Starting from the values $\alpha = 0.005$, $\beta = 0.1$ and $b = 1.968$, we find the first doublet at

$$k_1 = 3.135\,170 - \mathrm{i}0.002\,981$$
$$k_{1'} = 3.139\,813 - \mathrm{i}0.006\,802. \quad (41)$$

By fine tuning the parameters to the values $\alpha = 0.005\,077\,3229$, $\beta = 0.101\,86$ and $b = 1.968\,008\,257\,74$, the first doublet becomes degenerate, with a precision better than one part in 10^8, at

$$\tilde{k} = 3.136\,507\,668 - \mathrm{i}0.005\,062\,929. \quad (42)$$

In the case of a one-channel problem with a short-ranged, local potential and fixed angular momentum, as the example we are considering here, the solution of the radial equation (1), which vanishes at the origin and behaves as a purely outgoing wave at distances larger than the range of the potential, is unique up to a multiplying constant. In other words, for each given set of values of the external parameters $(X_1, X_2, \ldots X_n)$ there is one and only one Gamow eigenfunction $u_n(k_n, r)$ associated to each complex wavenumber eigenvalue k_n. When we move in parameter space from the point $(X_1, X_2, \ldots X_n)$ where all eigenvalues are different to a point $(X_1^*, X_2^*, \ldots X_n^*)$,where two eigenvalues, say k_1 and $k_{1'}$, are equal, the corresponding Gamow eigenfunctions $u_1(k_1, r)$ and $u_{1'}(k_{1'}, r)$ go to a common limit $u_{\tilde{1}}(\tilde{k}, r)$. Hence, at degeneracy, there is only one normal mode, the Gamow eigenfunction $u_{\tilde{1}}(\tilde{k}, r)$, associated to the repeated (degenerate) eigenvalue $\tilde{k}$; see figure 3. However, another, linearly independent, generalized eigenfunction or abnormal mode is provided by the same limiting process that gives rise to the degeneracy. As we move in parameter space from the point $(X_1, X_2, \ldots X_n)$ to the degeneracy point $(X_1^*, X_2^*, \ldots X_n^*)$, the difference of the two eigenvalues that become degenerate vanish, and the difference of the corresponding Gamow eigenfunctions also vanish. Then, by continuity of $k_1(X_1, X_2, \ldots X_n)$ and $k_{1'}(X_1, X_2, \ldots X_n)$ at the common limit $\tilde{k}(X_1^*, X_2^*, \ldots X_n^*)$, the derivative of the Gamow eigenfunction with respect to the wavenumber eigenvalue exists:

$$v_{\tilde{1}}(\tilde{k}, r) = \left(\frac{\mathrm{d}u_1(k_1, r)}{\mathrm{d}k_1}\right)_{\tilde{k}} = \lim_{|k_{1'}-k_1|\to 0} \frac{u_{1'}(k_{1'}, r) - u_1(k_1, r)}{k_{1'} - k_1}. \quad (43)$$

The generalized Gamow eigenfunction, also called Jordan–Gamow eigenfunction, is

$$\hat{u}_{\tilde{1}}(\tilde{k}, r) = \frac{\mathrm{d}u_{\tilde{1}}(\tilde{k}, r)}{\mathrm{d}\tilde{k}} + c(\tilde{k})u_{\tilde{1}}(\tilde{k}, r) \quad (44)$$

where $c(\tilde{k})$ is a function of $\tilde{k}$ but is independent of r. The generalized Gamow eigenfunction $\hat{u}_{\tilde{1}}(\tilde{k}, r)$ is a solution of the inhomogeneous equation

$$\frac{\mathrm{d}^2\hat{u}_{\tilde{1}}(\tilde{k}, r)}{\mathrm{d}r^2} + \tilde{k}^2\hat{u}_{\tilde{1}}(\tilde{k}, r) - \left(\frac{\pi}{\alpha}\delta(r-a) + \frac{\pi}{\beta}\delta(r-b)\right)\hat{u}_{\tilde{1}}(\tilde{k}, r) = -2\tilde{k}u_{\tilde{1}}(\tilde{k}, r) \quad (45)$$

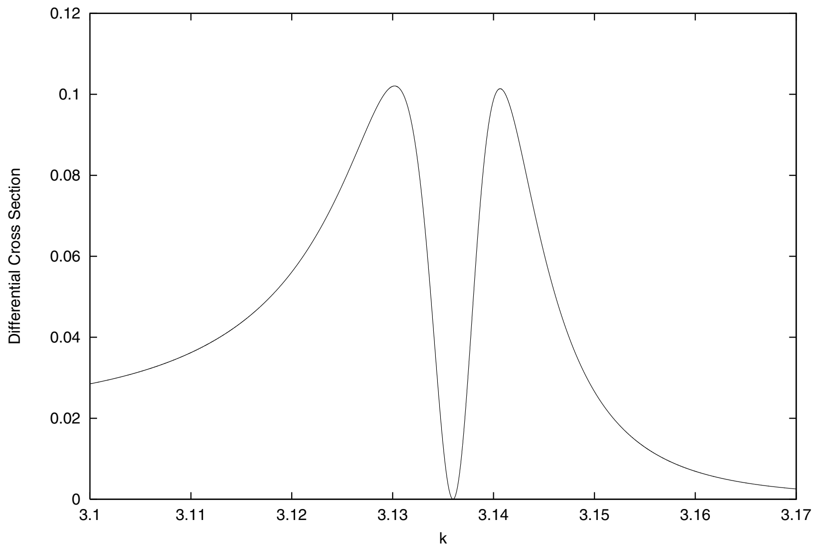

Figure 4. The split peak resonance characteristic of a double pole in the scattering amplitude. At $\tilde{k}_{\mathrm{res}} = 3.135\,98$, the cross section vanishes and the scattering wavefunction, $\psi(k, r)$, in the inner cavity attains its maximum amplitude. Note the enlarged scale in the abscissa.

obtained from (1) taking the derivative with respect to the eigenvalue k. The Jordan–Gamow eigenfunction $\hat{u}_{\tilde{1}}(\tilde{k}, r)$ satisfies the same boundary conditions as the Gamow eigenfunction, that is, it vanishes at the origin and behaves as a purely outgoing wave at distances larger than the range of the potential.

At degeneracy, the number of dimensions of the subspace of eigenfunctions or geometric multiplicity of the degeneracy is smaller than the number of repeated eigenvalues or algebraic multiplicity of the degeneracy. The Gamow eigenfunction and the generalized Gamow eigenfunction form a Jordan cycle of generalized eigenfunctions of length two [17]. These generic properties of a degeneracy of two complex energy eigenvalues and the corresponding Gamow eigenfunctions of the time independent radial Schrödinger operator are also realized at the exceptional points of the spectrum of a self-adjoint Hamiltonian perturbed by a Hermitian interaction with one complex coupling parameter, discussed by Kato [18] and Heiss [19] in connection with the avoided level crossings of bound states.

5.1. Cross section and phase shift at degeneracy

At the resonance degeneracy, the cross section has a characteristic split peak. The splitting occurs because right at the middle of the degenerate resonance, the phase shift goes through π and the cross section vanishes; see figures 4 and 5.

5.2. The scattering wavefunction

When k is far from any resonance value, the scattering wavefunction, $\psi(k, r)$, is a slowly varying function of k. As a function of r, it is very small inside the outer cavity and it is extremely small inside the inner cavity. The scattering is almost pure hard sphere scattering due to the incoming wave bouncing off the outer delta shell potential barrier without being able to penetrate; see figure 6.

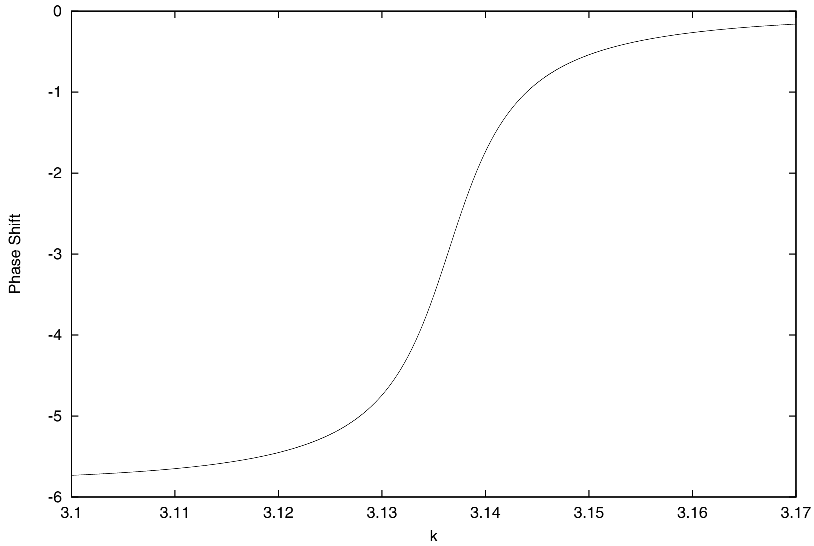

Figure 5. The characteristic sharp increase by 2π of the phase shift $\delta(k)$, as a function of k, produced by a double resonance pole in the scattering amplitude. At the centre of the double pole resonance, $\tilde{k} = 3.135\,98$, the phase shift goes through π.

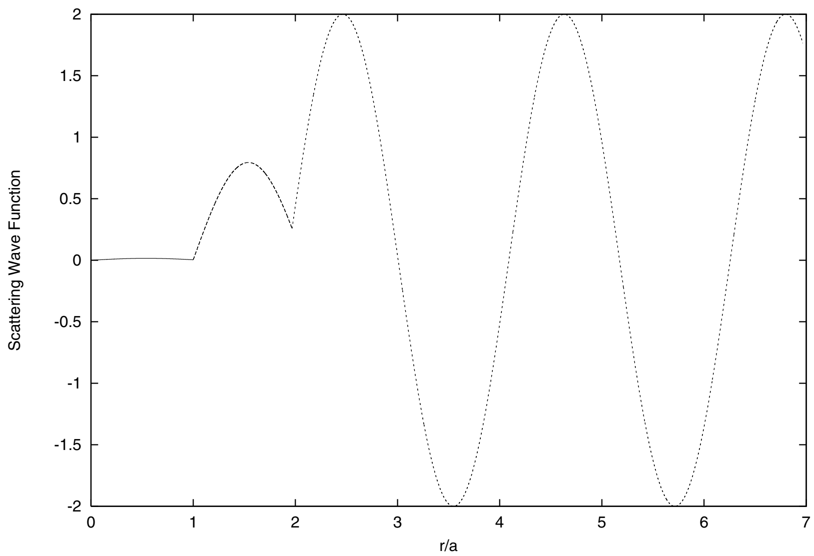

Figure 6. The scattering wavefunction, $\psi(k, r)$, as a function of r, evaluated at $k = 2.9$ on the low energy side of the double pole resonance. In the inner region, the amplitude of the scattering wavefunction is extremely small and is very small in the middle region. Most of the wave bounces off the outer delta shell potential.

Close to a degeneracy of resonances, when k changes from the low energy side to the high energy side of the degenerate resonance value, the scattering wavefunction, $\psi(k, r)$, changes very rapidly with k. At first, as k approaches the resonance value $\tilde{k}_{\text{res}}$ from below, $\psi(k, r)$ grows rapidly in the outer cavity and a small wave begins to be perceptible in the inner cavity;

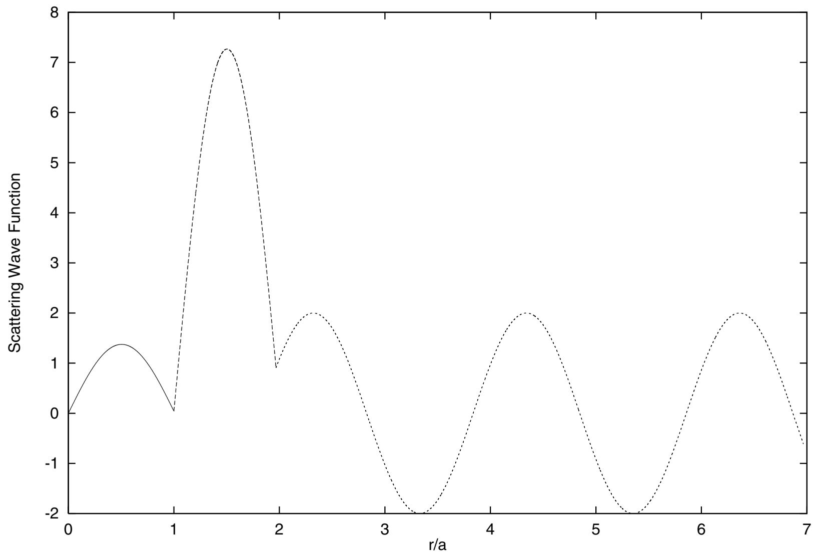

Figure 7. At $k = 3.11$, closer to the double pole resonance, the scattering wavefunction, $\psi(k, r)$, as a function of r, grows in the middle region and a small wave begins to be perceptible in the inner region. Note the change of scale in the ordinate.

see figure 7. As k increases, the amplitude of the wave in the inner cavity increases and the amplitude of the wave in the outer cavity decreases, until the wave in the two cavities resonate with the same amplitude at $k = 3.131\,44$; see figure 8. A further increase in k, at $k = 3.1365$, slightly above the centre of the double resonance, will make the inner cavity resonate at full amplitude while the outer cavity is completely quiet; see figure 9. When k goes to values larger than $\tilde{k}_{\text{res}} = 3.135\,98$, the amplitude of the wave in the inner cavity decreases while the amplitude of the wave in the outer cavity increases again. As k grows even larger the wave in the inner cavity becomes extremely small and the wave in the outer cavity decreases to very small values; see figures 10 and 11.

6. Accidental degeneracy of resonances in parameter space

6.1. The condition for degeneracy

An approximate analytical solution of the condition for degeneracy of two resonances, that is for the occurrence of a double pole in the scattering matrix $S(k)$, equations (39) and (40), may easily be found. When the condition (23) is satisfied, the two resonant poles corresponding to the first doublet of resonances are close to $k_0 a \approx \pi$. Hence, it will be convenient to define new variables δ and ϵ through the equations:

$$ka = \pi + \delta \tag{46}$$

$$k(b - a) = \pi + \delta + \epsilon. \tag{47}$$

As in the previous section, to simplify the notation, length will be measured in units of a and k will be measured in units of a^{-1}, then $a = 1$, $\alpha/a = \alpha$ and $\beta/a = \beta$.

We will make α and ϵ functions of β:

$$\alpha = X(\beta) = X_0\beta^2 + \mathrm{O}(\beta^3) \tag{48}$$

$$\epsilon + \beta = -2Z(\beta) = -2Z_0\beta^2 + \mathrm{O}(\beta^3) \tag{49}$$

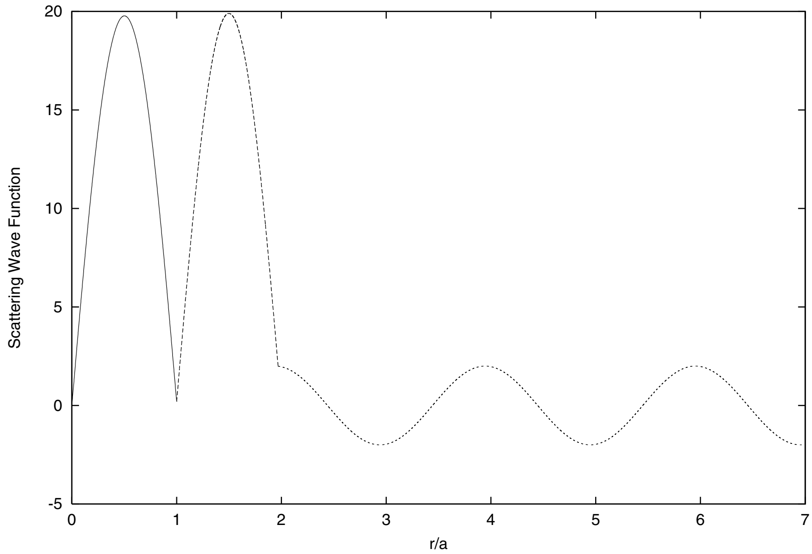

Figure 8. The scattering wavefunction, $\psi(k, r)$, as a function of r at $k = 3.131\,44$, slightly below the centre of the double pole resonance. The two cavities resonate with equal amplitude. Note the change of scale in the ordinate.

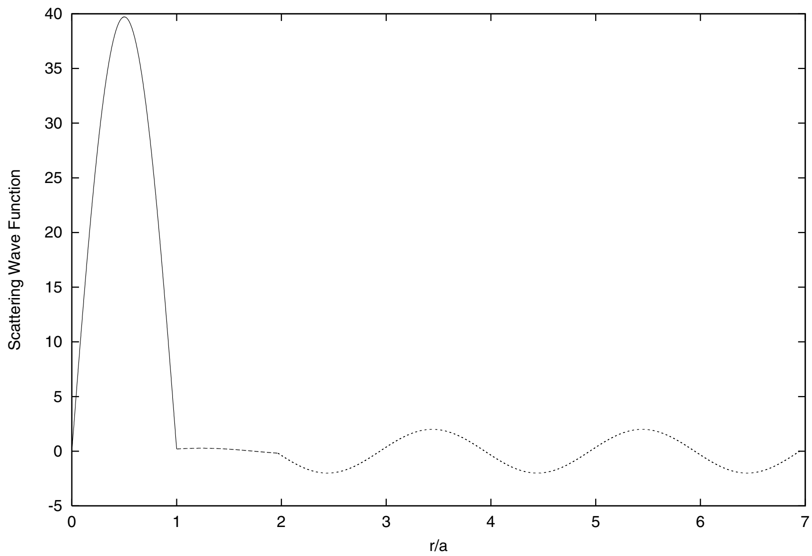

Figure 9. At $k = 3.1365$, slightly above the centre of the double pole resonance, the inner cavity resonates at full amplitude while the outer cavity is completely quiet.

where X_0 and Z_0 are two, free real parameters of order one. Now, we will look for an approximate solution of the conditions of degeneracy, equations (39) and (40), when $\delta = (k - \pi)$ is of order β^2, for small β.

We substitute the expressions (46) and (47) in (39) and (40) and obtain a new set of equations with the arguments of exponential and trigonometric functions written in terms of

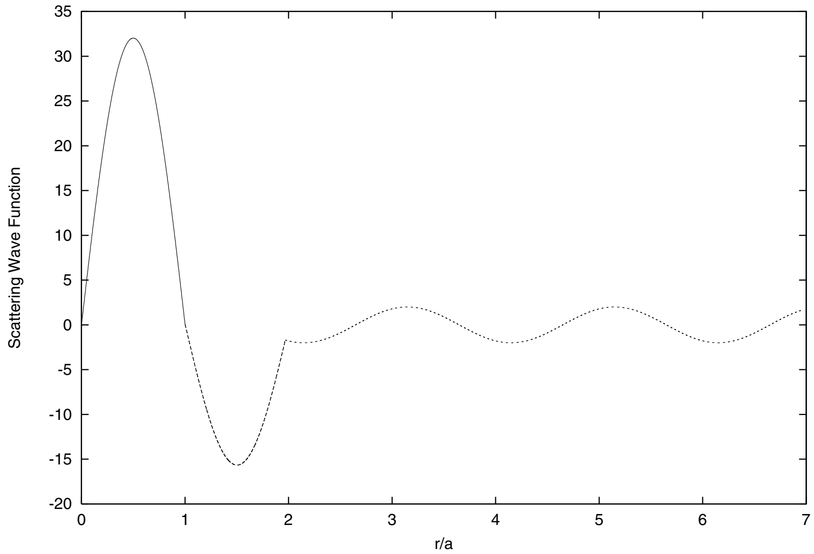

Figure 10. At $k = 3.139$, on the high energy side of the double pole resonance, the amplitude of the scattering wavefunction, $\psi(k, r)$, in the inner cavity decreases, while in the outer cavity it increases again.

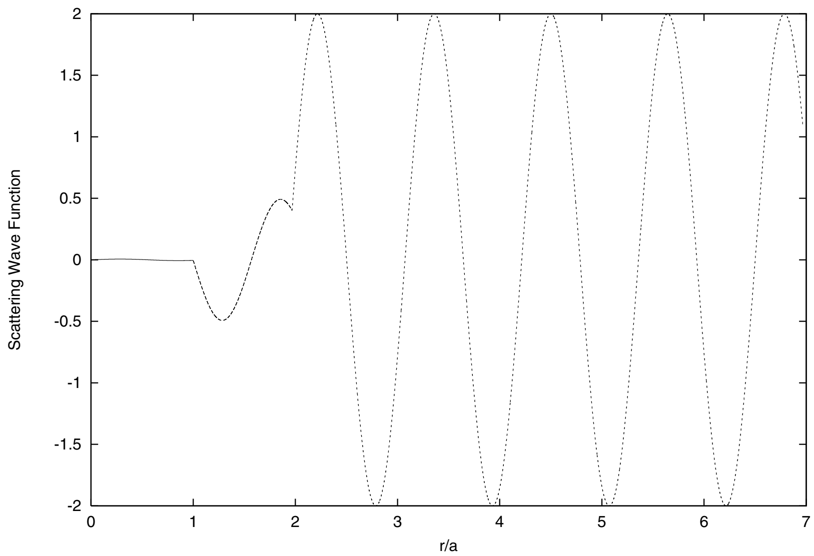

Figure 11. The scattering wavefunction, $\psi(k, r)$, as a function of r, evaluated at $k = 5.5$, on the high energy side of the double pole resonance. In the inner region, the wavefunction is extremely small and, in the middle region, it has a very small amplitude. Most of the wave bounces off the outer shell potential. Note the change of scale in the ordinate.

the small parameters δ and ϵ. According to (48) and (49), for β small, α and ϵ are also small. Linearizing the exponentials and trigonometric functions and neglecting terms of order β^5, the resonance condition, equation (39), becomes:

$$k^2 + 2[-(\pi - \alpha) + \tfrac{1}{2}(\epsilon + \beta) - \mathrm{i}\tfrac{1}{2}\beta\epsilon]k$$
$$+[\pi(\pi - \epsilon) - (2\pi - \epsilon)\alpha - \beta(\pi - \alpha)(1 - \mathrm{i}\epsilon)] = 0. \quad (50)$$

The two roots of this equation give the (approximate) positions of the two resonance poles corresponding to the first doublet of resonances in the fourth quadrant of the complex k-plane:

$$k_{1,2} = \pi - (X(\beta) - Z(\beta)) - \mathrm{i}\Gamma(\beta) + \pm\sqrt{[(X^2(\beta) + Z^2(\beta)) - \tfrac{1}{4}\Gamma^2(\beta)] - \mathrm{i}Z(\beta)\Gamma_z(\beta)} \quad (51)$$

where $\Gamma_z(\beta) = \beta^2$, $\Gamma_x = 0$ and $X(\beta)$ and $Z(\beta)$ were defined in (48) and (49).

Now, we define $R_0^2 = X_0^2 + Z_0^2$ and $\tan\theta = X_0/Z_0$, then setting $R_0 = \frac{1}{2}$ and $\theta = \frac{1}{2}\pi, \frac{3}{2}\pi$, the term under the square root vanishes and the two roots of (40) coincide. Within the approximations stated above, this result clearly indicates that by adjusting the parameters of the system, we can indeed arrange for the two zeros of the Jost function to coincide and produce one double pole of $S(k)$ at $\tilde{k}$:

$$\tilde{k} = \pi - \tfrac{1}{2}\beta^2 - \mathrm{i}\tfrac{1}{2}\beta^2 + \mathrm{O}(\beta^3). \quad (52)$$

This approximate analytical solution and the numerical computation presented in the previous section indicate that the degenerate resonances of the $S(k)$ matrix of the scattering by a double delta barrier potential may be brought about by adjusting the parameters of the system.

Note that:

(1) The positions of the poles in the complex plane are functions of three independent parameters. Therefore, in general, the geometric loci of the poles in the k-plane are not lines (trajectories) but two-dimensional regions.

(2) By making α and b or ϵ functions of β, we force the poles to move in well defined trajectories when β changes. If the functions $\alpha = X(\beta)$ and $-\frac{1}{2}(\epsilon + \beta) = Z(\beta)$ are properly chosen, the two trajectories cross and the two poles coincide at the crossing where a double pole of $S(k)$ is produced.

(3) In general, the position of the double pole in the k-plane is not fixed. In the example just discussed, when β changes the double pole moves on a trajectory which starts at $k_0 = \pi$ as a diagonal line with slope -1 and goes down into the fourth quadrant of the complex k-plane.

7. Resonance degeneracy in parameter space

If the first two zeros of the Jost function are factored out, the scattering matrix takes the form

$$S(k) = S_I^{(\mathrm{res})}(k)\exp(\mathrm{i}2\delta_B(k)) \quad (53)$$

where $\delta_B(k)$ is the background phase shift due to the hard sphere scattering and the contribution of the far away resonances. $S_I^{(\mathrm{res})}(k)$ is the resonating part of $S(k)$ due to the first doublet of resonances

$$S_I^{(\mathrm{res})}(k) = \frac{(k - k_1^*)(k - k_2^*)}{(k - k_1)(k - k_2)} \quad (54)$$

where k_1 and k_2 are the positions of the first two poles corresponding to the first doublet of resonances.

The analytical properties of $S_I^{(\mathrm{res})}(k)$ as a function of the external parameters α, β and b (or X, Z and Γ_z) may be brought out by rewriting $S_I^{(\mathrm{res})}(k)$ as

$$S_I^{(\mathrm{res})}(k) = \mathbf{1} - \mathrm{i}\mathbf{W}\frac{1}{[k\mathbf{1}_{2\times 2} - \mathbf{K}]}\mathbf{W}^\dagger \quad (55)$$

where

$$\mathbf{K} = \mathcal{K} - \mathrm{i}\tfrac{1}{2}\mathbf{W}^{\dagger}\mathbf{W} \tag{56}$$

and

$$\mathcal{K} = \begin{pmatrix} \pi - X + 2Z & X \\ X & \pi - X \end{pmatrix} \tag{57}$$

$$\mathbf{W}^{\dagger}\mathbf{W} = \sqrt{2}\Gamma \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{58}$$

In (55), the matrix $[k\mathbf{1}_{2\times 2} - \mathbf{K}]^{-1}$ plays the role of an effective propagator. The 2×1 row matrix $\mathbf{W}$ is the matrix of the decay amplitudes which couples the elastic channel to the first two resonant states. The form of the anti-Hermitian part of $\mathbf{K}$ ensures the unitarity of $S_I^{(\mathrm{res})}(k)$. The poles of $S_I^{(\mathrm{res})}(k)$ are the eigenvalues of $\mathbf{K}$.

It is convenient to write $\mathbf{K}$ in terms of the Pauli matrix valued vector $(\sigma_x, \sigma_y, \sigma_z)$ as

$$\mathbf{K} = (\tfrac{1}{2}\,\mathrm{tr}\ \mathbf{K})\mathbf{1}_{2\times 2} + (\vec{R} - \mathrm{i}\tfrac{1}{2}\vec{\Gamma}) \cdot \vec{\sigma} \tag{59}$$

where $\vec{R}$ and $\vec{\Gamma}$ are real vectors with Cartesian components $(X, 0, Z)$ and $(0, 0, \Gamma_z)$.

Then, the eigenvalues of $\mathbf{K}$ are given by

$$k_{1,2} = \tfrac{1}{2}\,\mathrm{tr}\,\mathbf{K} \pm \sqrt{(\vec{R} - \mathrm{i}\tfrac{1}{2}\vec{\Gamma})^2}. \tag{60}$$

The eigenvalues k_1 and k_2 coincide when the term under the square root vanishes. Since real and imaginary parts should vanish, we get the pair of equations

$$R_d^2 - \tfrac{1}{4}\Gamma_d^2 = 0 \qquad \vec{R}_d \cdot \vec{\Gamma}_d = 0. \tag{61}$$

To produce a degeneracy of resonant eigenenergies, the two linearly independent conditions, (61), should be satisfied for non-vanishing values of $\vec{R}$ and $\vec{\Gamma}$ (non-vanishing values of X, Z, and Γ_z). Therefore, at least two real independent parameters should be varied.

The degeneracy conditions, equations (61), define a circle of radius $\frac{1}{2}\Gamma_d$ in a plane orthogonal to the vector $\vec{\Gamma}_d$, in parameter space. Since the parameter space of the problem under consideration has only two effective dimensions and the 'circle' is in the one-dimensional subspace OX orthogonal to OZ, *the circle reduces to two points*. In the approximation of equations (48), (49) and (51), the Cartesian coordinates of these two points are $X_{\mathrm{od}} = \pm\frac{1}{2}$, and $Z_{\mathrm{od}} = 0$.

Since the degeneracy conditions, equations (61), are satisfied for non-vanishing values of $\vec{R}_d$ and $\vec{\Gamma}_d$, the matrix $(\vec{R}_d - \mathrm{i}\frac{1}{2}\vec{\Gamma}_d) \cdot \vec{\sigma}$ does not vanish at degeneracy, and the matrix $\mathbf{K}_d$ is not diagonal at degeneracy.

In the approximations of (48), (49) and (51), $\mathbf{K}_d$ becomes

$$\mathbf{K}_d = \tilde{k}\mathbf{1}_{2\times 2} + \tfrac{1}{2}\beta^2 \begin{pmatrix} -\mathrm{i} & 1 \\ 1 & \mathrm{i} \end{pmatrix}. \tag{62}$$

The matrix $\mathbf{K}_d$ may be brought to a Jordan canonical form [17] by means of a similarity transformation

$$\mathbf{M}^{-1}\,\mathbf{K}_d\,\mathbf{M} = \Delta_d = \begin{pmatrix} \tilde{k} & 0 \\ 1 & \tilde{k} \end{pmatrix} \tag{63}$$

with

$$\mathbf{M} = \begin{pmatrix} 1 & -\mathrm{i} \\ 0 & 1 \end{pmatrix}. \tag{64}$$

Off degeneracy, $(k_1 \neq k_2)$, the matrix $\mathbf{K}$ may be brought to diagonal form by means of another similarity transformation

$$\mathbf{N}^{-1}\mathbf{K}\mathbf{N} = \Delta = \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \qquad k_1 \neq k_2. \tag{65}$$

At degeneracy Δ, as a function of the parameters X, Z and Γ_z, is discontinuous, it jumps to the Jordan canonical form (63), and the similarity transformation $\mathbf{N}$ is singular. Hence, the spectral representation $\boldsymbol{\Delta}$ of $\mathbf{K}$ is not appropriate to discuss the geometric properties of the hypersurfaces which represent the complex eigenvalues k_1 and k_2 in parameter space. In contrast, the matrix $\mathbf{K}$ is a continuous function of the parameters X, Z and Γ including those points where $\mathbf{K}$ becomes degenerate (the diabolical circle). This property makes the representation of $S^{(\mathrm{res})}(k)$ defined in equations (55)–(58) adequate to discuss the degeneracy of two resonances in terms of the geometric properties of the hypersurfaces which represent k_1 and k_2 in parameter space [5].

8. Conclusions

In the above sections, we found that double poles can indeed occur in a simple model of the scattering of a beam of particles by a potential well with two regions of trapping. More precisely, we showed that double poles of the scattering matrix of a double barrier potential may be contrived by adjusting the parameters of the system. We solved the degeneracy conditions numerically and computed the phase shift, cross section, scattering wavefunction and the Gamow eigenfunction at degeneracy. We also found an approximate analytical solution of the degeneracy conditions and discussed some properties of the complex energy hypersurfaces at degeneracy in parameter space.

In conclusion, some general properties of a degeneracy of resonances were explicitly exhibited in a simple model of the scattering of a beam of particles by a potential well with two regions of trapping. Among these properties, it is worth mentioning the following:

(i) The minimum number of free, real, independent parameters that should be varied to produce a degeneracy of resonances is two, independent of the time reversal character of the interaction.
(ii) At degeneracy two complex energy eigenvalues are equal and associated with only one Gamow eigenfunction. Completeness of the set of complex energy eigenfunctions requires another independent solution, the generalized energy eigenfunction or Jordan–Gamow eigenfunction. Hence, the double pole of the scattering matrix is associated with two degrees of freedom: the Gamow eigenfunction, or normal mode, and the generalized Jordan–Gamow eigenfunction, or abnormal mode.
(iii) The number of dimensions of the subspace of eigenfunctions associated to the degenerate complex energy eigenvalue or geometric multiplicity of the degeneracy is smaller than the number of repeated eigenvalues or algebraic multiplicity of the degeneracy. The Gamow eigenfunction and the generalized Jordan–Gamow eigenfunction form a cycle of generalized eigenfunctions of length two which is associated to a Jordan canonical form of rank two [17].
(iv) At an accidental degeneracy of resonances, neighbouring complex energy hypersurfaces are connected at two points in parameter space, in contrast with the single conical point typical of a degeneracy of bound states.

We end our paper with a last comment: in the absence of symmetry, degeneracies are called accidental for lack of an obvious reason to explain why two energy eigenvalues, E_1 and

E_2, of a typical Hamiltonian should coincide [20]. In this paper, by means of an elementary example, we have pointed out that, when the Hamiltonian and the Jost function depend on at least two real, independent 'control' parameters, and the conditions for degeneracy are made explicit in terms of these parameters, a degeneracy of resonances may be brought about by simply adjusting the control parameters of the system so as to satisfy the degeneracy conditions. When this situation is realized, degeneracies of resonances are, in fact, not accidental even if at degeneracy no symmetry of the system arises, as is usually the case for bound states.

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