Double poles of the $S$-matrix in a two-channel model

W Vanroose†, P Van Leuven‡, F Arickx† and J Broeckhove†
† Departement Wiskunde-Informatica, Universiteit Antwerpen, B-2020 Antwerpen, Belgium
‡ Departement Natuurkunde, Vrije Universiteit Brussel, B-1050 Brussel, Belgium

Received 3 April 1997

Abstract. The poles of the $S$-matrix for a two-channel model with square well potentials are calculated. It is found that the trajectories of these poles in the complex $k$-plane for varying coupling strength show avoided crossings. At the critical parameters the poles coincide to form a double pole. Its presence is revealed by a symmetry property of the cross section.

1. Introduction

In this paper we address the problem of degeneracy of two resonant states or, more generally, to the occurrence of double complex poles of the $S$-matrix.

In recent literature a number of cases of interfering resonances leading to degeneracy have been described. Hernandez and Mondragon [1] considered a doublet of unbound states in $^8$Be as an example of accidental degeneracy of resonances. Kylstra and Joachain [2] discussed double poles in the case of laser-assisted electron–atom scattering. Latinne et al [3] studied degeneracies involving autoionizing states in complex atoms. Double poles have been investigated as examples of non-exponential decay laws. Lassila and Ruuskanen [4] examined atomic resonance fluorescence using a parametrized form of the $T$-matrix. Bell and Goebels [5] proposed a one-channel double well potential model and a Lee-type model of unstable particles as cases with double poles.

Here we describe another scenario for the origin of double poles using a simple two-channel model with square well potentials. Although, in the past, such a model has been used [6] in the context of resonance scattering theory, it has, to our knowledge, not been reported in connection with double poles. We focus our investigation on the role of the coupling strength in the generation of double poles. We present a study of the trajectories of the poles of the $S$-matrix and show that critical values exist of the model parameters which give rise to a double pole.

The situation of coupled channels, one of which is closed, is encountered a.o. in the study of continuum effects of monopole and quadrupole degrees of freedom in $^4$He [7]. It reveals the appearance of Feshbach resonances above the monopole but below the quadrupole threshold. However, the relation with the quadrupole eigenstates (in the uncoupled problem) is not clear: some give rise to a resonance, some do not. In order to gain insight into this situation we turn to an exactly soluble model, in particular one that allows us to vary the coupling strength between the channels because we feel this strength will be a determining factor. Indeed, the trajectory as a function of the coupling strength of a pole of the $S$-matrix reveals the relation of resonances in the coupled problem to states (bound or continuum) in the uncoupled problem. Changing the potential parameters (other than the coupling
strength) modifies the aforementioned trajectories, but we do observe regimes for which the trajectories exhibit a similar topological structure. The occurrence of a double pole at a critical potential parameter value signals the transition from one such regime to another.

2. Model

We consider a two-channel square well model with a single coordinate $x$ and mass $m$. We denote the channel potentials by $U_i$ ($i = 1, 2$) and the coupling matrix element by $U_{12} = U_{21}$. Taking a two component vector $\Psi_i$ for the wavefunction, the Schrödinger equation has the following matrix representation (using units such that $\hbar = 1$ and $m = 1$):

$$\begin{pmatrix}
\frac{-\frac{1}{2} \frac{d^2}{dx^2} + U_1}{U_{21}} & U_{12} \\
U_{12} & \frac{-\frac{1}{2} \frac{d^2}{dx^2} + U_2}
\end{pmatrix}
\begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix} = E
\begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix}.
$$

We recall that the coordinate $x$ can be interpreted either as a one-dimensional Cartesian coordinate (in which case the potentials have an infinite wall at $x = 0$) or, equivalently, as a three-dimensional radial coordinate (in which case the potentials are spherically symmetric and we consider s-waves only). For the potentials $U_i$ we choose square wells with depth $V_i$ and equal range $a$ and we suppose the coupling $U_{12}$ to be square also with height $C$ and the same range $a$. We assume further that the bottom of $U_2$ is shifted by $D$ against $U_1$.

We are interested in elastic scattering resonances and assume channel 1 to be open and channel 2 to be closed. The origin of the energy scale is chosen at the threshold of channel 1 and we denote $E = \frac{1}{2} k^2$, where $k$ is the momentum of the incoming wave.

Resonances are related to the poles of the analytically continued $S$-matrix in the complex plane. The $S$-matrix for momentum $k$ is introduced as usual by writing the asymptotic form of the wavefunction as

$$\Psi_1(x \to \infty) \sim e^{-ikx} - S(k)e^{ikx}.$$  

For the square well model under consideration the $S$-matrix can be calculated exactly with the help of the logarithmic derivative in the inner region. The solution of (1) in the inner region ($0 < x < 1$) can be found by explicit calculation and has the form (using a unit of length such that $a = 1$)

$$\Psi_i = A_i \sin(Kx) + B_i \sin(Lx)$$

with

$$K^2 = k^2 + 2V_1 - D + \sqrt{D^2 + 4C^2}$$

$$L^2 = k^2 + 2V_1 - D - \sqrt{D^2 + 4C^2}.$$  

In this section we restrict ourselves to a simple two-parameter version of the model by assuming that both square wells have the same bottom energy ($D = 0$) and the well in the closed channel to have infinite depth ($V_2 = \infty$). With this simplification, the condition for $k$ to be a pole of the $S$-matrix in the complex $k$-plane is found to be:

$$K \cot K + L \cot L - 2ik = 0.$$  

We shall see later that the parameters $D$ and $V_2$ do not essentially alter the qualitative features of the scenario of double pole generation that are presented here.
3. Results

The main purpose of this paper is to study the position of the poles in the complex plane and to search for double poles by variation of the model parameters. As solutions of (6) the poles constitute a two-parameter family of points in the $k$-plane. In the discussion of scattering phenomena it is sufficient to consider only the fourth quadrant where $\text{Re}(k) \geq 0$ and $\text{Im}(k) \leq 0$.

For $C = 0$, the channels are uncoupled and the problem is that of scattering by the square well in the first channel. This case is well known and has been studied in detail by Nussenzveig [8]. The $S$-matrix poles in the complex plane describe trajectories as the potential strength $V_1$ is increased from 0 to $\infty$. The poles in the lower half of the $k$-plane form symmetric pairs (mirror images with respect to the imaginary axis) which will move towards each other and, for a specific potential depth, coalesce into a double pole (virtual state) on the imaginary axis. Apart from these exceptional situations all poles of the $S$-matrix for the square well potential are single poles.

In the coupled case two types of poles occur. The first type (hereafter referred to as type 1) corresponds to the poles of the uncoupled square well and can be classified by the integer $n$ according to their limiting position for $C \to 0$ and $V_1 \to 0$

$$\lim_{V_1 \to 0, C \to 0} k_n^{(1)} = n\pi - i\infty. \quad (7)$$

The second type of poles (referred to as type 2) are associated with the bound states in the closed channel. For weak coupling they appear as sharp resonances at a position determined by the energy of the bound states of $U_2$. These resonances can be labelled with an integer $m$ according to their limiting position for $C \to 0$ (in our case the bound states of an infinite square well)

$$\lim_{C \to 0} k_m^{(2)} = \sqrt{(m\pi)^2 - 2V_1} - i0. \quad (8)$$

Equation (6) is solved by a numerical procedure. The method of steepest descent is used to locate the zero minima of the modulus of the left-hand side of (6) for a specific parameter set. For small $V_1$ the two types of poles for the same integer label lie in the same region of the complex plane. This permits a local study of the behaviour of $k_n^{(1)}(V, C)$ and $k_n^{(2)}(V, C)$ in this particular region of the $k$-plane.

We consider the trajectories for constant potential depth and increasing coupling. The type 1 pole starts, for $C = 0$, at a position determined by Nussenzveig’s solution of the uncoupled system. The type 2 pole starts, for weak coupling, near the real axis at a position (see (8)) determined by a bound state of the closed channel. For increasing coupling both trajectories first approach each other and then, for larger $C$, they show an ‘avoided crossing’. What happens next depends on the value of $V_1$. Figure 1(a) shows the trajectories for $V_1 = 2$. The type 1 pole moves towards the imaginary axis where it coincides with its image of the third quadrant. This is an analogous behaviour to Nussenzveig’s uncoupled case. The type 2 trajectory bends back towards the real axis and it reaches, for a large $C$, a bound state in the continuum, i.e. where $\text{Im}(k) \to 0$. In figure 1(c), the trajectories for potential strength $V_1 = 3$ are plotted. We note that poles interchange their identity at the avoided crossing. Now the type 1 trajectory deviates towards the positive real axis and the pole leads to a bound state in the continuum, whereas the type 2 trajectory approaches the negative imaginary axis and produces a virtual state. For a critical value of $V_1$ both trajectories collide into a double, fully degenerate, pole at a critical value of $C$. This is shown in figure 1(b). We note that for a range of non-critical values of $V_1$ we obtain ‘half’ degeneracies, i.e. poles with equal $\text{Re}(k)$ or $\text{Im}(k)$. These occur at the same $C$-value as the
Figure 1. Trajectories of $S$-matrix poles for the coupled channel model with fixed potential strength $V_1$ and variable coupling strength $C$ (indicated by dots). (a) $V_1 = 2$, type 1 and type 2 trajectories have an avoided crossing; (b) $V_1 = 2.1$, both types of poles coincide; (c) $V_1 = 3$, type 1 and type 2 trajectories interchange identity at the avoided crossing. The open circles indicate the degenerate poles.

double poles and correspond to the point of closest approach of the trajectories as seen in figure 1.

4. Discussion

A characteristic feature of the degeneracy of both type of poles is apparent in the cross section. At the critical parameters the cross section $\sigma$ (divided by the unitarity limit $4\pi/k^2$) is a symmetric function of $k$ about a momentum window close to the real part of the double pole. To illustrate this symmetry we plot $\sigma(k)k^2/4\pi$ in figure 2 at the critical potential. This result is similar to the cross section in laser-assisted electron–atom scattering obtained by Kylstra and Joachian and is also reported in connection with non-exponential decay by Lassila and Ruuskanen. In contrast to the assertion in [2], the symmetry of the cross section is not in general a unique signature of the double poles. Indeed, in the case of so-called ‘half degeneracies’, where only the real part or imaginary part of both poles are equal, the
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Figure 2. The cross section $\sigma(k)k^2/4\pi$ for critical potential depth $V_1 = 2.1$ and different couplings. (a) $C = 2.1$, (b) $C = 3.1$, (c) $C = 4.1$. For the critical coupling (case b), the two peaks are symmetric in an interval around the window momentum.

Table 1. Critical parameters for different branches and the position of the double pole at Re($k$) and Im($k$).

<table>
<thead>
<tr>
<th></th>
<th>$n = 1$</th>
<th>$n = 2$</th>
<th>$n = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V^{cr}$</td>
<td>2.1</td>
<td>2.9</td>
<td>3.4</td>
</tr>
<tr>
<td>$C^{cr}$</td>
<td>3.1</td>
<td>5.7</td>
<td>8.5</td>
</tr>
<tr>
<td>Re($k$)</td>
<td>3.3</td>
<td>5.8</td>
<td>9.3</td>
</tr>
<tr>
<td>Im($k$)</td>
<td>−0.9</td>
<td>−1.1</td>
<td>−1.2</td>
</tr>
</tbody>
</table>

cross section is also symmetric (see figure 3).

In section 3 we presented the mechanism of formation of double poles using the first branch ($n = 1$) of the solutions of equation (6). The same scenario also applies to the other branches in other regions of the complex $k$-plane. This happens at other (higher) critical values of the parameters $V$ and $C$. In table 1 we list the values of the critical parameters for different $n$.

So far we have used the simplified model with $D = 0$ and $V_2 = \infty$. We have tested the results given above and found them to be robust against the variation of these parameters. If the bottom of $U_2$ is displaced relative to $U_1$ the only effect is to shift the position of
5. Conclusion

We have calculated the poles of the $S$-matrix in a two-channel model where the channel potentials and the coupling are chosen as square wells with the same range. We looked at the elastic scattering region where one channel is open and the other is closed. We have two types of poles: one is associated with the resonances of the uncoupled problem, the other with the bound states of the closed channel. The trajectories of the poles in the complex $k$-plane show avoided crossings as the coupling strength is changed. At critical values of the model parameters the two types of poles are fully degenerate and form a double pole. The cross section corresponding to the critical case has two peaks symmetric with respect to a window momentum. The cross section corresponding to the case of half degeneracy also shows symmetric behaviour.

In the particular model used here the double poles lie far from the real axis and can therefore not readily be associated with well pronounced resonances. Also, the double pole occurs at a large value of the coupling strength. This calculation is a presentation of a...
simple mechanism that provides insight into the generation and behaviour of double poles. We cannot conclude as yet that the scenario presented here is a generic one. However, the results suggest a more detailed study of a two-channel model with more realistic potentials.

Acknowledgments

The authors are indebted to J Joachain and N Kylstra for interesting discussions. This work was supported by the ‘Fonds voor Wetenschappelijk Onderzoek Vlaanderen’.

References