Resonance scattering at third-order exceptional points

W D Heiss$^{1,2}$, G Wunner$^3$,

$^1$Department of Physics, University of Stellenbosch, 7602 Matieland, South Africa
$^2$National Institute for Theoretical Physics (NITheP), Western Cape, South Africa
$^3$Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

E-mail: dieter@physics.sun.za

Abstract. We analyze scattering cross sections at and near third-order exceptional points (EP3), i.e., points in physical parameter space where three energies and eigenfunctions coincide. At an EP3, the Green’s function contains a pole of third order, in addition to poles of second and first order. We show that the interference of the three pole terms produces a rich variety of line shapes at the exceptional point and in its neighbourhood. This is demonstrated by extending previous work on two harmonic oscillators to a system of three driven coupled damped oscillators. We also discuss the similarities and the differences in the behaviour of the amplitudes in the classical problem and the scattering cross sections in the quantum mechanical problem at the EP3.

PACS numbers: 03.65.Nk, 46.40.Ff, 03.65.Vf, 31.15.-p,

1. Introduction

Specific spectral singularities, that is singularities of eigenvalues of operators, have been dubbed exceptional points (EP) by Kato in his textbook 1966 [1]. In physics we are usually interested in EPs of Hamilton operators. They are isolated points in an (at least) two-dimensional parameter space at which two or even more eigenvalues coalesce. A coalescence is not a degeneracy since the corresponding eigenvectors become aligned meaning that there is no higher dimensional eigenspace. This is of course not possible for hermitian Hamiltonians, but it occurs in open quantum systems, in parity-time symmetric systems [2], systems with loss and gain [3–6] and others. Usual degeneracies may nevertheless also occur in non-hermitian problems. The physical effects of exceptional points of second order (EP2) have been discussed extensively in the literature, we refer the reader to review articles, e. g. [7–9], and references quoted therein.

In recent years, the effects of exceptional points of higher order [10], in particular of third order (EP3s), have received increasing attention. For example, the chirality of EP3s was analyzed bei Heiss [11], the behaviour of eigenfunctions when encircling an EP3 was discussed by Demange and Graefe [12] and Ryu et al. [13], and EP3s were shown to also appear in theoretical studies of Bose-Einstein condensates [14] and the Bloch equations [15].

The present paper studies the effect of poles of higher order in the scattering function at the EP. Our analysis focuses upon scattering cross sections at and near third-order exceptional points (EP3). At an EP3, the Green’s function has a pole of third order, in addition to poles of second and first order. We show that the interference of the three pole terms produces a rich variety of line shapes at the exceptional point and in its neighbourhood. This is demonstrated by extending previous work on two harmonic oscillators [16–19] to a system of three driven coupled damped oscillators. We discuss the similarities and point out at the EP3 the differences between the behaviour of the classical amplitudes and the scattering cross sections of the corresponding quantum mechanical problem.

2. The model

We consider three one-dimensional harmonic oscillators with masses $m_1$, $m_2$, $m_3$, unperturbed eigenfrequencies $\omega_1$, $\omega_2$, $\omega_3$ and damping constants $k_1$, $k_2$, $k_3$ being coupled by springs with spring constants $f_{12}$, $f_{13}$, $f_{23}$ and associated dampings $g_{12}$, $g_{13}$, $g_{23}$. The system is driven by an external force with fixed period $\omega$ at one of the three oscillators. It is an extension of the model discussed in [16, 19, 20]. After setting up the equations of motion in phase space, time-periodic solutions and resonances with real frequency $\omega$ are found by the roots of the characteristic polynomial of the matrix

$$
\mathcal{M} = \begin{pmatrix}
-2g_{12} - 2g_{13} & 2g_{12} & 2g_{13} & -f_{12} - f_{13} & f_{12} & f_{13} \\
2g_{12} & -2g_{12} - 2g_{23} & 2g_{23} & -f_{12} - f_{13} & f_{12} & f_{13} \\
2g_{13} & 2g_{23} & -2g_{13} - 2g_{23} & f_{13} & f_{23} & -f_{13} - f_{23} \\
1/m_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/m_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 1/m_3 & 0 & 0 & 0
\end{pmatrix}.
$$

\begin{document}

\maketitle

Resonance scattering at third-order exceptional points

\section{1. Introduction}

Specific spectral singularities, that is singularities of eigenvalues of operators, have been dubbed exceptional points (EP) by Kato in his textbook 1966 [1]. In physics we are usually interested in EPs of Hamilton operators. They are isolated points in an (at least) two-dimensional parameter space at which two or even more eigenvalues coalesce. A coalescence is not a degeneracy since the corresponding eigenvectors become aligned meaning that there is no higher dimensional eigenspace. This is of course not possible for hermitian Hamiltonians, but it occurs in open quantum systems, in parity-time symmetric systems [2], systems with loss and gain [3–6] and others. Usual degeneracies may nevertheless also occur in non-hermitian problems. The physical effects of exceptional points of second order (EP2) have been discussed extensively in the literature, we refer the reader to review articles, e. g. [7–9], and references quoted therein.

In recent years, the effects of exceptional points of higher order [10], in particular of third order (EP3s), have received increasing attention. For example, the chirality of EP3s was analyzed bei Heiss [11], the behaviour of eigenfunctions when encircling an EP3 was discussed by Demange and Graefe [12] and Ryu et al. [13], and EP3s were shown to also appear in theoretical studies of Bose-Einstein condensates [14] and the Bloch equations [15].

The present paper studies the effect of poles of higher order in the scattering function at the EP. Our analysis focuses upon scattering cross sections at and near third-order exceptional points (EP3). At an EP3, the Green’s function has a pole of third order, in addition to poles of second and first order. We show that the interference of the three pole terms produces a rich variety of line shapes at the exceptional point and in its neighbourhood. This is demonstrated by extending previous work on two harmonic oscillators [16–19] to a system of three driven coupled damped oscillators. We discuss the similarities and point out at the EP3 the differences between the behaviour of the classical amplitudes and the scattering cross sections of the corresponding quantum mechanical problem.

\section{2. The model}

We consider three one-dimensional harmonic oscillators with masses $m_1$, $m_2$, $m_3$, unperturbed eigenfrequencies $\omega_1$, $\omega_2$, $\omega_3$ and damping constants $k_1$, $k_2$, $k_3$ being coupled by springs with spring constants $f_{12}$, $f_{13}$, $f_{23}$ and associated dampings $g_{12}$, $g_{13}$, $g_{23}$. The system is driven by an external force with fixed period $\omega$ at one of the three oscillators. It is an extension of the model discussed in [16, 19, 20]. After setting up the equations of motion in phase space, time-periodic solutions and resonances with real frequency $\omega$ are found by the roots of the characteristic polynomial of the matrix

$\begin{pmatrix}
-2g_{12} - 2g_{13} & 2g_{12} & 2g_{13} & -f_{12} - f_{13} & f_{12} & f_{13} \\
2g_{12} & -2g_{12} - 2g_{23} & 2g_{23} & -f_{12} - f_{13} & f_{12} & f_{13} \\
2g_{13} & 2g_{23} & -2g_{13} - 2g_{23} & f_{13} & f_{23} & -f_{13} - f_{23} \\
1/m_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/m_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 1/m_3 & 0 & 0 & 0
\end{pmatrix}$.
Resonance scattering at third-order exceptional points

Figure 1. Left: Eigenvalue trajectories emerging from the EP3 (red dot) when $f_{12}$ is varied from $f_{EP} = 0.02$ to $f_{12} = 0.92$ (green dots). Right: Trajectories when $g_{12}$ is varied from $g_{EP} = 0.098$ to $g_{12} = 0.25$. Notice the different scales: the red dot has the same coordinates. Choice of parameters see Sec. 3.

EP3s occur for complex values of $\omega$ where the characteristic polynomial of $M$ as well as its first and the second derivatives vanish, i.e.

$$\text{det}(M + i\omega) = 0, \quad \frac{d}{d\omega}\text{det}(M + i\omega) = 0, \quad \frac{d^2}{d^2\omega}\text{det}(M + i\omega) = 0. \quad (1)$$

These equations lead to 6 real-valued equations for the 17 real parameters $\omega_i, k_i, m_i, g_{ij}, f_{ij}, (i, j = 1, 2, 3), \Re(\omega), \Im(\omega)$.

For the special case of undamped oscillators, $k_1 = k_2 = k_3 = 0$, and for vanishing couplings between oscillator 1 and 3, $f_{13} = g_{13} = 0$, we are left with 12 real parameters, and the the above matrix simplifies to

$$M = \begin{pmatrix}
-2g_{12} & 2g_{12} & 0 & -f_{12} - \omega_1^2 & f_{12} & 0 \\
2g_{12} & -2g_{12} - 2g_{23} & 2g_{23} & f_{12} & -f_{12} - f_{23} - \omega_2^2 & f_{23} \\
0 & 2g_{23} & -2g_{23} & 0 & f_{23} & -f_{23} - \omega_3^2 \\
1/m_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/m_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 1/m_3 & 0 & 0 & 0
\end{pmatrix}.$$ 

Equations (1) can be solved only numerically. With further values given for the oscillator frequencies and the masses, complex solutions for the remaining parameters are found in general. It should be noted that complex solutions of (1) always exist. The challenge is to find solutions being physically acceptable, that is the spring and damping constants must be real and positive, i.e. $f_{ij} > 0$, $g_{ij} > 0$, and the width should obey $\Im(\omega) < 0$; we focus on positive frequencies, i.e. $\Re(\omega) > 0$. In addition, solutions should not only be physically acceptable but also of physical interest: for instance, an EP3 lying far away from the real axis cannot yield much structure on the real axis, in other words, a small width is desirable.

Having set the values for $\omega_i$ and $m_i, i = 1, \ldots, 3$ we numerically seek EP3s. Our interest is focused upon the 4-th quadrant in the complex $\omega$-plane where usually a few solutions occur. For given $f_{12} > 0$ and $f_{23} > 0$ we obtain solutions with complex values for $g_{12}, g_{23}$ and $\omega$. Of those we concentrate upon a particular solution that comes closest to the constraints as imposed above. By re-adjusting the values for $f_{12} > 0$ and $f_{23} > 0$ we obtain in certain cases solutions that satisfy the constraints. For the model considered it appears that acceptable solutions (e.g. small width) could not be found for all three masses being equal. In fact, even when two masses are equal,
the width still turned out to be unsuitably large. We cannot claim to have searched
the whole set of parameters. In view of our interest being directed to three-channel
scattering problems a wider search may be sensible and necessary once a specific
experimental setting is realised.

The reduction in the vicinity of the EP3 from the six- to a three-dimensional
problem follows the lines similar to those applied in [19, 20]. In Fig. 1 we display
trajectories of eigenvalues in the $\omega$-plane. For the region considered they coincide
perfectly with those from the original six-dimensional problem. We recall that the
eigenvalues displayed in Fig. 1 give rise to resonances of the classical amplitudes of
the oscillators while they are as well the pole positions, i.e. scattering resonances,
of the Green’s function used for the three-channel scattering problem. Only at the
EP3, where the trajectories coalesce, the scattering problem will be different from the
classical oscillators owing to the all important interference of the third, second and
first order pole terms of the Green’s function at the EP3. These facts will be discussed
in the following Section.

3. Results

Using the parameters $m_1 = 1, m_2 = 3, m_3 = 4$ and $\omega_1 = 1, \omega_2 = 1.4, \omega_3 = 1.7$ we
obtain an acceptable EP3 at $\omega_{EP3} = 0.89 - 10.071$ for the couplings $f_{12} = 0.021, f_{23} =
0.23, g_{12} = 0.098, g_{23} = 0.0095$ (actually the values are obtained at much higher
precision). If one intends to study the vicinity of the EP3, one has to realise an
important characteristic of the EP3: owing to the higher number of parameters there
is a multitude of possibilities to unfold the three eigenvalues when moving away from
the EP3. The trajectories displayed in Fig. 1 using the two different parameters $f_{12}$
and $g_{12}$ are manifestly different. Formally, the decomposition

$$H = M_0 + xM_1,$$

yields different three-dimensional matrices $M_0$ and $M_1$ for different choices of the
parameter $x$ as long as $H$ is taken at an EP3. As a consequence, while the Green’s
function has at the EP3 the form [21]

$$(H - E_{EP3})^{-1} = \frac{I}{\omega - E_{EP3}} + \frac{H - IE_{EP3}}{(\omega - E_{EP3})^2} + \frac{(H - IE_{EP3})^2}{(\omega - E_{EP3})^3}$$

with $I$ being the identity matrix, the scattering matrix element

$$t_{i,k} = (M_1(H - E_{EP3})^{-1}M_1)_{i,k}$$

will also be different for different choices of $x$. Recall that, for the cross section,
$|M_1(H - E_{EP3})^{-1}M_1|^2$ has to be considered giving rise to interference terms from the
poles of different order. In other words the cross section at the EP3 is different
depending on the choice of $x$. Note that this feature renders an experimental
realisation of an EP3 with a rich and challenging structure.

We here present three distinct choices. In Fig. 2 results are illustrated using
$x = f_{12}$.

Similar to the case for an EP2 we recall that the various peaks at the left hand
figure cannot be associated with a particular resonance pole. Also similar to the
case of the EP2 is the zero of the scattering amplitude due to interference; the zero
disappears and becomes a minimum when one or more of the damping constants $k_i$
are switched on. At the EP3, where the scattering amplitude has poles of different
Resonance scattering at third-order exceptional points

Figure 2. Cross section $|t_{11}(\omega)|^2$ for $f_{12} = 0.021$ (the value at the EP3) and for $f_{12} = 0.92$

Figure 3. Individual contributions of the pole and interference terms to the cross sections shown in Fig. (2). Top left: sum only of the pole terms of third, second and first order, all at the same position. Top right: the three individual interference terms. Bottom left: contributions of the individual first order poles; the residue of one of the poles with small width is very small. Bottom right: sum of interference terms.

order at the same position, the pattern is essentially generated by the structure of the various interference terms. The all important role of the interference terms is illustrated in Fig. 3. Only the sum of the interference terms and of the pole terms of different order yields the final pattern as illustrated in Fig. 2. In contrast, moving away from the EP3, the distinct peak at the right hand illustration is clearly caused by a traditional resonance pole term; it is the pole related to the green dot on the right of the left hand panel of Fig. 1. The smaller structure of the right hand panel of Fig. 2 is still due to the combined effect of the interference terms being, however, much smaller and the two poles with smaller width (see left hand panel of Fig. 1). This is illustrated on the bottom row of Fig. 3. The interference shows its effect only at the pole terms with small width.

Let us contrast these results with those obtained by the choice $x = g_{12}$.

It is evident that the displays of Fig. 4 are distinctly different from those in Fig. 2, albeit there is a qualitative similarity, especially on the respective left hand panels (at the EP3). Further away from the EP3 (right hand panel) the gross pattern in Fig. 4 is dominated by the contribution from a distant resonance pole with a large width ($\omega_{\text{res}} = 0.75 - i0.8$, see Fig. 1 right hand panel) while the substructure is caused by the interference terms and the other two poles with small widths.

To underline the variety of possible structures we display in Fig. 5 the result of choosing $x = f_{23}$. The illustration presents a situation where the interference terms are of minor importance. Yet they produce an asymmetry for the sum of the three
pole terms at the EP3. It is obvious that the peak has not the shape of a Lorentzian. We mention that the patterns remain qualitatively unchanged when all the masses are multiplied by the factor 2. Yet, the EP3 then occurs for $\omega_{EP3} = 0.63 - i 0.051$.

The interference terms dominate the whole pattern at the EP3. It is as such a typical quantum mechanical or wave mechanical problem that has no analogy for the three classical oscillators. However, further away from the spectral singularity, where each individual pole of the three poles can produce a resonance, it is of some interest to compare typical classical amplitudes with the corresponding wave scattering phenomena. In Fig. 6 we illustrate the amplitude of the first oscillator (smallest mass) using the initial condition $q_1 = 1$, $q_2 = q_3 = 0$ with all initial momenta equal to zero. The three resonances (green points on left hand panel of Fig. 1) are clearly discernible.

The other oscillators show similar patterns owing to the mutual coupling. However, at the EP3 the classical amplitudes have little or no structure in contrast to the pronounced interference patterns for the scattering amplitudes.

4. Summary

The dominance of interference upon scattering at an EP has been demonstrated for an EP2 in [19, 20]. The present study has clearly shown the by far richer structure of basically the same phenomenon for scattering using parameters giving rise to an
EP3 or its vicinity. In principle, this could be expected as an EP3 can also be seen as the confluence of two EP2s that share a Riemann sheet in the complex energy plane. And it is here where the increased complexity can be visualised. Depending on the choice of the specific parameter that is varied to make the three eigenvalues sprout into three different directions, the respective two EP2s connecting two different pairs of the three levels are themselves arranged and connected differently depending on the parameter choice. Even though the two EP2 are usually not amenable physically - they have non-real coupling constants -, yet it is this mathematical structure that explains the different patterns at the EP3 and its vicinity for variations of different parameters.

To dissolve such rich and delicate structure in the laboratory means of course a considerable challenge for experimentation. As there are a number of cases for the occurrence of an EP3 discussed in the literature (see Introduction), we feel there is a good chance to show that these structures are in fact a physical reality. One realisation could be measuring transmission profiles through three coupled waveguides with gain and loss as suggested in [12]. Another possibility could be an extension of a microwave cavity experiment with three partitions of the cavity instead of the two. After all, it was about 15 years ago when the first encircling of an EP2 was successfully achieved for the two partitions [22].

Acknowledgement

WDH and GW gratefully acknowledge the support from the National Institute for Theoretical Physics (NITheP), Western Cape, South Africa. GW expresses his gratitude to the Department of Physics of the University of Stellenbosch where this work was carried out.

References

Resonance scattering at third-order exceptional points


