Fano-Feshbach resonances in two-channel scattering around exceptional points

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Abstract. It is well known that in open quantum systems resonances can coalesce at an exceptional point, where both the energies and the wave functions coincide. In contrast to the usual behaviour of the scattering amplitude at one resonance, the coalescence of two resonances invokes a pole of second order in the Green’s function, in addition to the usual first order pole. We show that the interference due to the two pole terms of different order gives rise to patterns in the scattering cross section which closely resemble Fano-Feshbach resonances. We demonstrate this by extending previous work on the analogy of Fano-Feshbach resonances to classical resonances in a system of two driven coupled damped harmonic oscillators.

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1. Introduction

When a quantum state in the continuum interacts with another discrete state, the two states give rise to a resonance in the continuum channel showing an asymmetric line profile in the cross section. The theoretical description of these resonances was developed independently by Feshbach [1] in nuclear physics using projection operator techniques, and by Fano [2] in atomic physics using the language of superposition of wave functions. These Fano-Feshbach resonances are ubiquitous in physics, and have more recently also been found in mesoscopic condensed matter systems [3] and nanoscale structures [4]). They have also been used in Bose-Einstein condensates to tune the scattering interaction [5]. Joe et al. [6] have pointed out that one can even draw an analogy between quantum interference of Fano-Feshbach resonances and classical resonances in a system of two driven coupled damped oscillators; one of the oscillators exhibits the standard enhancement of the amplitude near its eigenfrequency, while near the eigenfrequency of the second oscillator the amplitude acquires an asymmetric profile, and at a certain frequency of the driving force it can even become zero. Effectively there are two driving forces acting on the first oscillator which are out of phase and may cancel each other. This example demonstrates one of the basic features of the Feshbach-Fano resonance, namely resonant destructive interference.

The same classical system has also been analyzed [7] to exemplify typical behaviour of quantum systems with non-Hermitian operators. These operators occur for example in open quantum systems, which are in contact with an environment, and where resonances with complex energies appear. Other examples of systems which can be described by non-Hermitian operators can be found, e. g., in Ref. [8]. It is well known that resonances show characteristic effects not observable in Hermitian quantum systems. Among these effects are exceptional points (EPs) [9] being isolated points in an (at least) two-dimensional parameter space at which two or even more eigenstates coalesce. EPs exhibit distinct features and usually influence in their vicinity the behaviour in parameter space in a specific way [10]. They show particular properties such as the permutation of eigenstates for a closed adiabatic loop in parameter space [11], a special geometric phase for the one only eigenstate at the EP [12], or a linear term in the time evolution of the wave function besides the usual exponential behaviour [13]. EPs feature in quantum mechanical as well as in classical systems, examples can be found in Ref. [14].

A further important property of EPs is the appearance of a pole of second order in the Green’s function [15,16] when an EP is approached in parameter space; this second order pole occurs in addition to the pole of first order usually associated with resonances. It is the purpose of this paper to demonstrate how the approach of these poles of first order and their merger with an additional pole of second order impacts on the scattering cross section. We demonstrate that it is even already in the vicinity of the merging of the two poles where the specific Fano-Feshbach-like features in the cross section occur. As shown in Refs. [17] the generic behaviour of systems in the vicinity of an EP can be stripped down to a two-dimensional matrix eigenvalue problem, irrespective of the concrete classical or quantum system under consideration. In the present paper we use the above mentioned driven classical system of two coupled oscillators with damping to mimic the general behaviour of a two-channel $T$ matrix in open quantum systems when an EP is approached; note that the open system implies non-unitarity of $T$. In Sect. 2 we briefly review the classical problem. In Sect. 3 we present the results and relate them to the ongoing literature. In Sect. 4 we draw
conclusions and give an outlook.

2. The model

In line with the previous discussion, and for the reader’s convenience, we briefly review the model of two coupled classical oscillators. Denoting by \( p_1, p_2, q_1, q_2 \) the momenta and spatial coordinates of two point particles of equal mass the equations of motion read for the driven system

\[
\frac{d}{dt} \begin{pmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix} = \mathcal{M} \begin{pmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ 0 \\ 0 \end{pmatrix} \exp(i\omega t) \tag{1}
\]

with

\[
\mathcal{M} = \begin{pmatrix} -2g - 2k_1 & 2g & -f - \omega_1^2 & f \\ 2g & -2g - 2k_2 & f & -f - \omega_2^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{2}
\]

where \( \tilde{\omega}_j - ik_j, \ j = 1, 2, \) with \( \tilde{\omega}_j = \sqrt{\omega_j^2 - k_j^2} \), are the unperturbed damped frequencies while \( f \) and \( g \) are the coupling spring constant and damping of the coupling, respectively. The driving force is assumed to be oscillatory with one single frequency and acting on each particle with amplitude \( c_j \). Here we are interested only in the stationary solution being the solution of the inhomogeneous equation which reads

\[
\begin{pmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix} = (i\omega - \mathcal{M})^{-1} \begin{pmatrix} c_1 \\ c_2 \\ 0 \\ 0 \end{pmatrix} \exp(i\omega t). \tag{3}
\]

Resonances occur for the real values \( \omega \) of the complex solutions of the secular equation

\[
\text{det} |i\omega - \mathcal{M}| = 0 \tag{4}
\]

and EPs occur for the complex values \( \omega \) where

\[
\frac{d}{d\omega} \text{det} |i\omega - \mathcal{M}| = 0 \tag{5}
\]

is fulfilled simultaneously together with Eq. (4). We choose the parameter \( f \) as the second variable needed to enforce the simultaneous solution of Eqs. (4) and (5) and keep the other parameters of \( \mathcal{M} \) fixed. Thus we encounter the problem of finding the EPs of the matrix problem

\[
\mathcal{M}_0 + f \mathcal{M}_1 \tag{6}
\]

with

\[
\mathcal{M}_0 = \begin{pmatrix} -2g - 2k_1 & 2g & -\omega_1^2 & 0 \\ 2g & -2g - 2k_2 & 0 & -\omega_2^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{7}
\]

and

\[
\mathcal{M}_1 = \begin{pmatrix} 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{8}
\]
Note that $M_0$ and $M_1$ are not symmetric. In the numerical search for the EP we enforce $f$ to be real. This is achieved by adjusting accordingly the value of the real parameter $g$. In other words, instead of the two parameters of a complex $f$ we choose the two real values for $f$ and $g$. This choice is of course motivated on physical grounds.

In the neighbourhood of the EP we reduce the actual problem to an effective two-channel scattering problem. It is well known that a higher dimensional eigenvalue problem can be reduced to a two-dimensional matrix problem in close vicinity of an EP [17]. The advantage lies in the analytic availability of the Green’s function and thus of the scattering amplitudes. It enables the understanding of the effects of the EP upon the pattern of the scattering at and in close vicinity of an EP. In fact, as mentioned above the coalescence of two resonance poles – i.e. at the EP – leads to a pole of second order [10,15,16] besides the usual first order pole. This is made explicit in the reduced matrix which can be written in the form

$$H(f) = H_0 + fV = \begin{pmatrix} \Omega_1 & 0 \\ 0 & \Omega_2 \end{pmatrix} + f \begin{pmatrix} \epsilon_1 & \delta_1 \\ \delta_2 & \epsilon_2 \end{pmatrix}$$

(9)

where all entries are obtained numerically from the original physical parameters in Eq.(2). One finds the EPs at

$$f_{\text{EP}} = \frac{-i(\Omega_1 - \Omega_2)}{i(\epsilon_1 - \epsilon_2) \pm 2\sqrt{\delta_1 \delta_2}}$$

(10)

with the Green’s function

$$G(E) = (E - H(f_{\text{EP}}))^{-1} = \frac{1}{E - \omega(f_{\text{EP}})} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{i\sqrt{\delta_1 \delta_2}f_{\text{EP}}}{(E - \omega(f_{\text{EP}}))^2} \begin{pmatrix} 1 & i\sqrt{\frac{\delta_1}{\delta_2}} \\ i\sqrt{\frac{\delta_2}{\delta_1}} & -1 \end{pmatrix}.$$  

(11)

The explicit form for $\omega(f_{\text{EP}})$ can be found in [14]. We emphasise that the values of the EPs of the matrices in Eq.(9) and Eq.(6) coincide and so do the energy trajectories in the vicinity of the EPs.

When calculating the scattering amplitudes $T(E) = V + VG(E)V$ and a cross section from $|T_{1,1}|^2$ or $|T_{2,2}|^2$ the interference term between the second and first order pole terms turns out to be of crucial importance. Moreover, even when moving slightly away from the EP by choosing $f$ somewhat different from $f_{\text{EP}}$ the interference of the two resonance poles appearing now yields two peaks in $|T_{1,1}|^2$ or $|T_{2,2}|^2$ that cannot be identified with either individual pole term. Quantitative results of this striking phenomenon will be discussed in the following section.

3. Results and discussion

For a first discussion we use the parameter set $\omega_1 = 2.8$, $\omega_2 = 3$, $k_1 = k_2 = 0$. A physically acceptable EP is found at $\omega_{\text{EP}} = 2.9 - 10.1$ for $f_{\text{EP}} = 0.02$ and $g_{\text{EP}} = 0.1$ (the actual numerical values are obtained at much higher precision). Using these values the plot of $|T_{2,2}|^2$ versus the energy is shown on top of Fig.1 (the corresponding plot for $T_{1,1}$ looks similar). The distinct two peaks are not related to an individual pole of first
or second order, the whole pattern is rather brought about by the sum of the moduli squared of the two pole terms plus the interference term; in particular, the zero of the scattering function between the two peaks is invoked by the interference term. To illustrate the dramatic effect we display on the bottom of Fig.1 the interference term; note the difference in scale by an order of magnitude. Of course the contributions from the individual pole terms – at the same position – are of similar order of magnitude.

The obvious follow-up question is: how does the pattern change under a small variation of, say, $f$? When $f$ is moved away from $f_{\text{EP}}$, two individual resonance pole terms emerge from the EP, one with a larger width (imaginary part) and the other with a smaller width. In fact, for $f = f_{\text{EP}} + 0.2$, the pole moving to the left has diminished its width while the width of the pole moving to the right has grown larger. For $f = f_{\text{EP}} - 0.2$ it is just the other way around. The illustration in Fig.2 where the two cases are displayed seems to confirm this by comparing the widths of the peaks of the left and the right figure. However, it would be fallacious to associate either of the two peaks with one of the two resonance poles as the interference term still has its notable effect. The two poles without interference could not even be resolved as they would be two overlapping resonances. Rather, not only the zero between the peaks but also their width and position is effected by the interference term. This is illustrated in Fig.3 where all terms are illustrated for the two cases.

Moving even further away with $f$ from $f_{\text{EP}}$, the scattering gradually assumes a form where each peak can be associated with one resonance pole as the interference term has become small in comparison with the pole terms. And yet, for our parameters the interference term still forces the vanishing of scattering between the two peaks. The illustrations in Fig.4 for $f = f_{\text{EP}} \pm 1$ are to clarify this point. We mention that the zero, meaning no scattering at this energy point, has also been observed in a similar setting for complex scattering potentials modelling wave guides with $\mathcal{PT}$-symmetric gain and loss [18,19].
When instead of changing \( f \) other parameters are changed, the pattern is qualitatively similar. One notable difference is caused by giving the unperturbed frequencies a finite width denoted above by \( k_1 \) and \( k_2 \). If either one or both are different from zero the zero between the peaks of the scattering function disappears, there remains a dip without touching the zero line. A similar behaviour has been observed by Joe et al. [6] for the amplitudes of their oscillator system. In actual experiments showing Fano-Feshbach resonances this is the rule. There are in fact experiments where the asymmetry and the depth of the dip can be tuned by varying an experimental parameter, for example the magnetic field in an Aharanov-Bohm interferometer with a quantum dot [20].

Common to all illustrations is the ubiquitous asymmetry inherent in Fano-Feshbach resonances. It is caused by the different widths of the pole terms and by the interference term, most pronounced in Fig.4 even though there the interference term is small in comparison with the contributions of the two pole terms.

The energy trajectories illustrated in Fig.5 for \(-1 < f < +1\) clearly indicate the changing of the widths when \( f \) is varied over the specified range (we recall that the trajectories are in perfect agreement over the range considered irrespective of the full (6) or the reduced problem (9)). When the interference becomes larger while approaching the EP (Fig.2 and Fig.3), the asymmetry is always discernible and caused to an increasing extent by the interference term while the pole terms become more and more equal until they coalesce at the EP (Fig.1). There the most remarkable feature are the two (unequal) peaks, where neither of them can be associated with a single resonance pole. In all cases considered the interference term produces the zero scattering at an energy between the two peaks or – for different parameters – a minimum.
Figure 4. Interference term (blue), moduli squared of the two pole terms (green and pink) and $|T_{22}|^2$ (thick line) vs. energy for $f = f_{EP} + 1$ (left) and $f = f_{EP} - 1$ (right). For clarity the contributions of the individual pole terms are displayed in the bottom row.

Figure 5. Trajectories in the complex energy plane when $f$ is varied in the interval [-1,1]. The EP occurs at $E = 2.9 - 0.099$ where the trajectories bounce off each other. The red and green dots indicate the starting points for $f = -1$.

4. Summary and Conclusions

Starting from the fact that in scattering systems EPs give rise to a second order pole in the Green's function, in addition to the usual first order pole, we have investigated the impact on the shape of the scattering cross section as one approaches the EP. We have demonstrated that the merging of the two poles results in manifestly asymmetric line profiles closely resembling Fano-Feshbach resonances. We have demonstrated that it is the interference term of the poles which generates the asymmetric line profiles. In particular, at a certain energy it can produce a zero in the cross section, i.e. with no scattering at all, or just a minimum. We have used a simple classical system of two coupled oscillators with damping driven by an external force to highlight the effect of the interference term, but our findings apply quite generally to scattering cross sections close to an EP in open quantum systems.

The present paper has established a close link between the appearance of Fano-Feshbach-like line profiles and the occurrence of EPs in parameter space. The review article [4] describes numerous experiments where in recent years asymmetric Fano-
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Feshbach-like line profiles have been observed, among them experiments with the interaction of light with structured matter, matter-wave scattering in Bose-Einstein condensates, light scattering by nanoparticles, and plasmonic micro cavities, to name just a few. From our findings it can be conjectured that all these asymmetric line profiles may be related to the occurrence of EPs in the parameter spaces of the corresponding experiments. To verify this conjecture in actual experiments remains a challenge for the analysis of such experiments.

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