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Fano resonances in scattering: an alternative perspective

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Abstract. In a previous paper it has been shown that the interference of the first and second order pole of the Green's function at an exceptional point, as well as the interference of the first order poles in the vicinity of the exceptional point, gives rise to asymmetric scattering cross section profiles. In the present paper we demonstrate that these line profiles are indeed well described by the Beutler-Fano formula, and thus are genuine Fano resonances. Also further away from the exceptional points excellent agreement can be found by introducing energy dependent Fano parameters.

1 Introduction

Fano resonances were first discovered in atomic physics [1,2]. In cross sections in nuclear physics they also appear and are called Feshbach resonances [3,4]. The characteristic features of these resonances are asymmetric line shapes, caused by the interaction between a discrete state and a continuum of states, as described by the formula derived by Fano in his landmark work in 1961 [5]. Later Fano himself developed the subject further in numerous papers, review articles [6], and a book [7].

To date Fano resonances have been observed in a wide array of different subfields of physics. They have been found, to give just a few examples, in mesoscopic condensed matter systems [8], in light scattering by finite obstacles [9], in nanoscale structures [10], in wave transmission through resonant scattering structures[11], in broadband atto-second-pulsed XUV light experiments [12, 13], and in coupled plasmonic systems [14–17].

In this paper we take a different theoretical perspective on Fano resonances. Similar to the well-established description of an isolated resonance by a pole in the complex plane of the scattering function, we here propose an understanding of Fano resonances by specific singularities denoted as exceptional points (EPs) [18].

There is a host of literature about exceptional points [19–21] and references quoted therein (see also, e.g., [22–24]). In our context the important point is the occurrence of an additional pole of second order in the scattering function at the EP. As a consequence, the cross section (the modulus squared of the scattering function) is then characterised by the all important interference of the poles of first and second order. This has been hinted at in a previous paper [21]. The present paper implements this claim with substantial numerical evidence.

We demonstrate that both at and in the vicinity of the exceptional point the cross sections indeed give rise to Fano profiles locally, and therefore can be interpreted as *genuine* Fano resonances. Moreover, the cross sections can globally be described by the Beutler-Fano formula, if energy-dependent Fano parameters are introduced. As an aside we demonstrate that specific parametrisations traditionally used [25] are bound to fail at the EP, since the two peaks of the cross section cannot be associated with individual resonances.

2 The model

For the reader's convenience we briefly review the model introduced in [21]. The model is inspired by work of Joe et al. [26], who had pointed out an analogy between quantum interference in Fano resonances and classical resonances in coupled oscillators (see also [27,28]). The system consists of two one-dimensional harmonic oscillators with unperturbed eigenfrequencies ω_1, ω_2 and damping constants k_1, k_2, coupled by a spring with spring constant f and damping constant g, and periodically driven by an external force with frequency ω. We note that in the literature the model is used to describe the plasmonic response of coupled plasmonic structures (cf. [16,17]).

After setting up the equations of motion in phase space, $(\dot{\boldsymbol{p}}, \dot{\boldsymbol{q}})^{\mathrm{T}} = \mathcal{M}(\boldsymbol{p}, \boldsymbol{q})^{\mathrm{T}} + \boldsymbol{c}\exp(\mathrm{i}\omega t)$, resonant solutions with real frequency ω are found by the roots of the characteristic polynomial of the matrix $\mathcal{M}$. Additional singularites, called exceptional points, occur for complex values of ω where in addition the first derivative of the characteristic polynomial vanishes. This leads

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to 4 real-valued equations for the 8 real parameters $\omega_1, \omega_2, k_1, k_2, g, f, \Re(\omega), \Im(\omega)$. If we provide specific values for the eigenfrequencies and damping constants, we are left with 4 equations for the 4 unknowns $g, f, \Re(\omega), \Im(\omega)$, which in general have to be solved numerically. However, in the special case that the individual oscillators are undamped, $k_1 = k_2 = 0$, as used in the following, the exceptional points can be given in analytical form:

$$\Re[\omega_{\rm EP}] = \frac{1}{2\sqrt{2}}\sqrt{\frac{(3\omega_1^2+\omega_2^2)(\omega_1^2+3\omega_2^2)}{\omega_1^2+\omega_2^2}},$$
$$\Im[\omega_{\rm EP}] = \frac{-1}{2\sqrt{2}}\frac{|\omega_1^2-\omega_2^2|}{\sqrt{\omega_1^2+\omega_2^2}},$$
$$g_{\rm EP} = -\Im[\omega_{\rm EP}] = \frac{1}{2\sqrt{2}}\frac{|\omega_1^2-\omega_2^2|}{\sqrt{\omega_1^2+\omega_2^2}},$$
$$f_{\rm EP} = \frac{(\omega_1^2-\omega_2^2)^2}{4(\omega_1^2+\omega_2^2)}.$$

In close vicinity of an exceptional point the higher dimensional eigenvalue problem can be reduced to an effective two-channel scattering problem. The advantage of the reduction is the analytic availability of the Green's function and thus the scattering amplitudes both near and at the exceptional point. From the Green's function the T matrix can be calculated, and from it the cross sections $|T_{11}|^2$, $|T_{22}|^2$. For details we refer the reader to [21].

3 Fano profiles

3.1 Fits with one Fano profile

To prove that the asymmetric line profiles found in [21] around exceptional points are actual Fano resonances, we first recall the Beutler-Fano formula (see e.g. [7])

$$\sigma(\epsilon) = \frac{(\epsilon+q)^2}{\epsilon^2+1}. \tag{1}$$

It quite generally describes line profiles for a physical process where a continuum state interacts with a bound state embedded in the continuum. In (1)

$$\epsilon = \frac{E-E_{\rm R}}{\Gamma/2} \tag{2}$$

is the reduced energy which measures the energy relative to the position of the resonance $E_{\rm R}$ in units of the half-width $\Gamma/2$ being the width of the quasi-bound state in the continuum (note that the interaction endows the quasi-bound state with a width). The parameter q determines the shape of the resonance and depends on the ratio of the transition matrix elements linking the initial state to the discrete and continuum parts of the final state.

In the following we assume no damping of the individual oscillators and choose $\omega_1 = 2.00$ and $\omega_2 = 2.10$. The exceptional point then appears at $f_{\rm EP} = 0.005$, $g_{\rm EP} = 0.0499$, and $\omega_{\rm EP} = 2.0500-0.04999i$. In Figure 1 we illustrate Fano fits of the cross sections at and near the exceptional point. The fitting parameters are $E_{\rm R}$, Γ, and q, in addition we have a scaling factor in front of equation (1) to scale the height of the resonance and a global shift of the cross section to account for a background. Numerical values of the fitting parameters are given in Table 1.

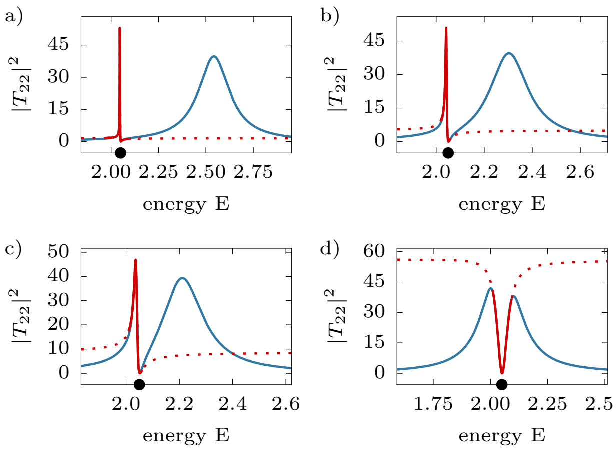

Fig. 1. Fano fits (red) of the cross sections at and near the exceptional point. The parameters are $\omega_1 = 2.00$ and $\omega_2 = 2.10$, $k_1 = k_2 = 0$, the exceptional point appears at $f_{\rm EP} = 0.005$, $g_{\rm EP} = 0.0499$, and $\omega_{\rm EP} = 2.0500 - 0.04999i$. (a) $f = f_{\rm EP} + 1.0$, (b) $f = f_{\rm EP} + 0.5$, (c) $f = f_{\rm EP} + 0.3$, (d) $f = f_{\rm EP}$.

Table 1. Resonance energies $E_{\rm R}$, widths Γ, and asymmetry parameter q of the Fano profiles around the exceptional point shown in Figure 2.

	$E_{\rm R}$	Γ	q
(a)	2.04628	0.00078	−6.43165
(b)	2.04242	0.00289	−3.03946
(c)	2.03899	0.00623	−2.09385
(d)	2.04917	0.02755	−0.06180

It is evident from Figure 1 that both at and further away from the exceptional point the Beutler-Fano formula locally describe the asymmetric line profiles perfectly. It thus confirms that they are Fano resonances.

3.2 Fits with two Fano parameters

If one allows for *two* sets of energy dependent Fano parameters the two peaks in the cross sections and the asymmetric line profile can indeed be modelled over a far wider range of the energy. Examples are shown in Figure 2, the fitting parameters are listed in Table 2. It can be seen that further away from the exceptional point the profiles are locally well described by two Fano forms. This, however, is not surprising since by their very nature each of the separate resonances, one with a larger and one with a smaller width, should be describable by Fano profiles, with different parameters. It is remarkable to see that the

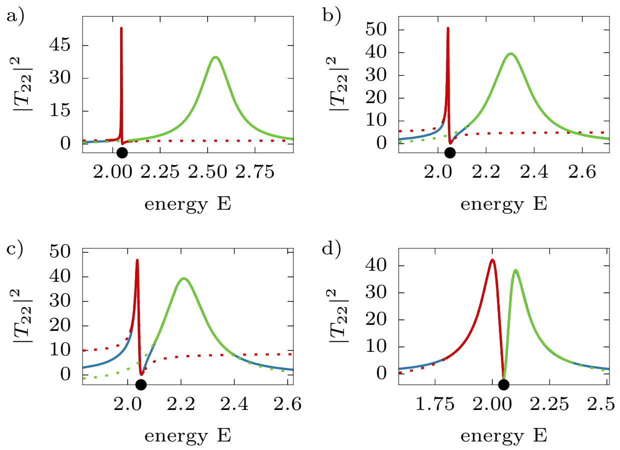

Fig. 2. Fano fits of the cross sections shown in Figure 1 with two sets of Fano parameters.

Table 2. Resonance energies, widths, and asymmetry parameters of the two Fano profiles shown in Figure 2.

	E_1	Γ_1	q_1	E_2	Γ_2	q_2
(a)	2.0463	0.0008	−6.4770	2.5416	0.0995	299.0411
(b)	2.0424	0.0029	−3.1026	2.2997	0.0969	36.6894
(c)	2.0390	0.0062	−2.1014	2.2028	0.0934	12.1206
(d)	2.0244	0.0438	−1.8446	2.0785	0.0440	1.8728

peaks retain Fano profiles even closer to and in particular at the exceptional point, where the interference terms become increasingly important.

3.3 Fit with energy dependent Fano parameters

The idea of energy dependent Fano parameters has been discussed also in the context of q reversals in Rydberg series and multiphotoionisation [29,30]. Here we follow the formulation put forward by Magunov et al. [25] in their study of overlapping resonances. Starting from the S matrix with two isolated resonances $\tilde{E}_k = E_k - \mathrm{i}\Gamma_k/2$ $(k = 1, 2)$, and a smooth reaction background described by a phase shift 2δ, they show that the cross section can be brought into the Beutler-Fano form

$$\sigma(E) = 4\sin^2\eta(E)\frac{(\varepsilon_1 + q(E))^2}{\varepsilon_1^2 + 1}, \tag{3}$$

with

$$\eta(E) = \delta - \operatorname{arccot}(\varepsilon_2), \quad \varepsilon_k = 2(E - E_k)/\Gamma_k,$$

and the *energy dependent* Fano parameter

$$q(E) = -\cot\eta(E).$$

Apart from the scale factor for the height of the cross section, in the extended ansatz (3) the fitting parameters are E_1, Γ_1, E_2, Γ_2 and the phase δ.

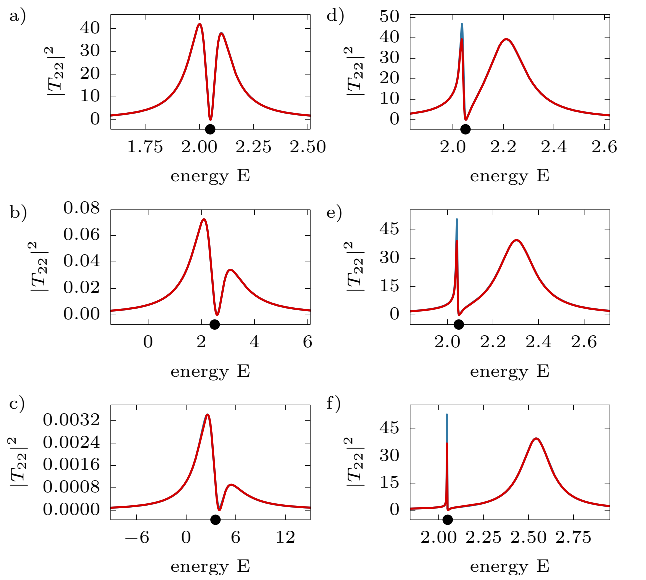

Fig. 3. Fano fits of cross sections at and in the vicinity of exceptional points using equation (4). The blue curves are the calculated cross sections, the red curves denote the fits. The left-hand column shows the results for $\omega_1 = 2.00$ and $\omega_2 = 2.10, 3.00, 5.00$ (from top to bottom) at the respective exceptional point (black dots), while in the right-hand column $\omega_1 = 2.00$, $\omega_2 = 2.10$, and the distance from the exceptional point is successively increased, $\Delta f = 0.3, 0.5, 1$ (from top to bottom).

In all our fits the numerical value of δ turned out to be close to π up to the first five digits. Since δ enters into the S matrix by the factor $\exp(i2\delta)$, this implies that in our model there is no background phase, and we could have chosen $\delta = 0$ from the outset. In this case (3) simplifies to

$$\sigma(E) = \frac{1}{(\epsilon_2^2 + 1)}\frac{(\epsilon_1 + \epsilon_2)^2}{(\epsilon_1^2 + 1)}. \tag{4}$$

The comparison with (1) then shows that ϵ_2 formally assumes the role of an energy dependent asymmetry parameter $q(E)$ for resonance 1, and vice versa.

Examples for fits of the cross sections with energy dependent asymmetry parameters at and in the vicinity of exceptional points are shown in Figure 3. The agreement between the calculated cross section and the energy dependent Fano fit is found to be perfect over the complete energy range.

The fitting parameters required for this excellent agreement are listed in Table 3. For sufficient distance from the EP (rows (d)–(f)), where the interference term plays a minor role, this is to be expected as we encounter essentially two independent and well separated resonances associated with poles the positions of which are given in the table. In contrast, at the EP (rows (a)–(c)) the two peaks cannot be identified as two separated resonances; in fact, here the interference term is crucial to produce the two peaks (see [21]). It therefore comes as no surprise that the best fits produce results – negative widths – that can no longer be interpreted as physical resonances.

Table 3. Fitting parameters for the cross sections shown in Figure 3 calculated using equation (4).

	E_1	Γ_1	E_2	Γ_2
(a)	2.04970	0.10792	2.04990	−0.09239
(b)	2.49559	1.04493	2.50780	−0.91573
(c)	3.47188	3.20257	3.62857	−2.28382
(d)	2.03912	0.01471	2.20748	0.18673
(e)	2.04252	0.00680	2.30187	0.19218
(f)	2.04626	0.00196	2.54172	0.19923

This clearly indicates that the treatment [25] by energy dependent Fano parameters fails at an EP. In fact, the double pole invoked by the EP is different in character from the double pole as considered in [25]: the two-dimensional coefficient matrix of the double pole at the EP does not have full rank but rank unity (see [20]) meaning that the entries are correlated in a particular way. In this context, we also note that our scattering matrices are not unitary as the underlying Hamiltonian is not hermitian.

4 Summary

Starting from the fact that in scattering systems exceptional points give rise to a second order pole in the Green's function, we have investigated the effect on the shape of the scattering cross section as one approaches the exceptional point. In this paper we have demonstrated that the asymmetric line profiles in the neighbourhood of the exceptional point are to be interpreted as Fano resonances. Moreover, by allowing for energy dependent Fano parameters the cross sections can also globally be described as actual Fano profiles.

In our analysis we have adopted an alternative perspective on Fano resonances. On the one side there is the mathematical mechanism of two coalescing eigenvalues – an EP – on the other the physical origin of two interacting near resonances where the one can be a single particle resonance and the other a bound state in the continuum that, owing to the interaction, has acquired itself a width. This is the typical Fano-Feshbach scenario. Whether or not all resonances that can be fitted by the traditional Fano-Feshbach procedure have their origin in an EP cannot be shown. In fact, the particular type and relative strength of the interaction must be taken into account. Yet we believe that the mechanism proposed here should be representative quite generally.

It should be stressed that, in spite of the simplicity of the underlying classical problem, the generic behaviour of line profiles studied in this paper near exceptional points applies to any physical two-channel scattering or transmission problem. Therefore we did establish the direct link between the appearance of asymmetric Fano profiles and the occurrence of exceptional points in parameter space.

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