Some Features of Exceptional Points

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Abstract A short resumé of the essentials of exceptional points of second order is given. We then concentrate on a discussion of specific features of exceptional points of third order. While general properties of these singularities have been expounded extensively in the literature, we here concentrate on some specific aspects, that is the occurrence of 'hidden' or 'concealed' third order exceptional points. They occur under specific circumstances when an apparent second order exceptional point is accompanied by a third eigenvalue being equal to the other two at the singularity.

1 Introduction

When physical phenomena are described in terms of mathematical functions it is usually the singularities of such functions that point to particular physical phenomena. For instance, in scattering theory it is the pole terms in the complex energy plane of the scattering function that describe resonance phenomena observable at real energies. During the past two decades a different type of singularities has given rise to much attention. The Exceptional Points (EPs), so named by Kato [1], are spectral singularities giving rise to a great variety of physical phenomena. They occur generically in eigenvalue problems when eigenvalues and eigenfunctions depend on parameters and are thus potentially encountered in almost any problem of physical interest. As such they occur in classical as well as in quantum mechanical problems. In fact, the classical damped harmonic oscillator provides for a prime example being presented below. While there are numerous classical phenomena, in the literature most applications and effects seem to relate to quantum mechanical problems. Some of the more important ones, in our opinion, are briefly described in the following section.

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In the subsequent section we present a rehash of the basic properties of EPs followed by a short discussion of some major phenomena associated with EPs. This part is aimed at the general reader and not at the experts. In Sect. 3 we present a few special facts and examples in connection with EPs of higher order with an emphasis on 'hidden' third order EPs.

2 Exceptional Points of Second Order

2.1 Formal Properties

Consider one of the simplest problem in classical mechanics: the damped classical oscillator. In suitable units it is described by the differential equation

$$\ddot{x} + 2k\dot{x} + \omega^2 x = 0 \tag{1}$$

with the two linearly independent solutions

$$x_{1,2}(t) = \exp(\mathrm{i}\,\tilde{\omega}_{1,2}t) \quad \text{where} \quad \tilde{\omega}_{1,2} = \mathrm{i}k \pm \sqrt{\omega^2 - k^2}. \tag{2}$$

Obviously, for $k = \omega$ the two solutions coalesce and here we encounter an EP in its simplest form. It is well known that in this case the additional independent solution bears the factor t being multiplied to the exponential function $\exp(-kt)$. In this context see also [2–5].

We next confine our discussion to the eigenvalues of a two-dimensional matrix where the direct connection of an EP and the phenomenon of level repulsion is easily demonstrated. Consider the problem

$$\begin{aligned} H(\lambda) &= H_0 + \lambda V \\ &= \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} + \lambda \begin{pmatrix} \omega_1 & \delta \\ \delta & \omega_2 \end{pmatrix} \end{aligned} \tag{3}$$

where the parameters ϵ_k and ω_k determine the non-interacting resonance energies $E_k = \epsilon_k + \lambda\omega_k,\ k = 1, 2$ being two crossing lines as a function of λ. We may choose all parameters complex and we require $[H_0, V] \neq 0$ to avoid the problem from being trivial. Owing to the interaction invoked by the matrix elements δ the two levels do not cross but repel each other. However, the two levels *coalesce* at specific values of λ in the vicinity of the level repulsion, that is at the two EPs

$$\lambda_{1,2} = \frac{(\epsilon_1 - \epsilon_2)}{(\omega_2 - \omega_1) \pm 2i\delta}. \tag{4}$$

For $\delta \neq 0$ the energy levels have a square root singularity as a function of λ and read

$$E_{1,2}(\lambda) = \frac{1}{2}\left(\epsilon_1 + \epsilon_2 + \lambda(\omega_1 + \omega_2) \pm \sqrt{(\omega_1 - \omega_2)^2 + 4\delta^2}\sqrt{(\lambda - \lambda_1)(\lambda - \lambda_2)}\right). \tag{5}$$

We use the term *coalesce* as the pattern is distinctly different from a degeneracy usually encountered for Hermitian operators. Note that $H(\lambda)$ is Hermitian if all parameters in (3) are real. However, in this case, λ_1 and λ_2 are complex, in other words, at the EP the Hamiltonian is non-Hermitian. In fact, an EP cannot occur for a Hermitian matrix or any Hamiltonian. This becomes obvious when looking at the eigenfunctions. At $\lambda = \lambda_1$ there is only one eigenvector which reads (up to a factor)

$$|\phi_1\rangle = \begin{pmatrix} +i \\ 1 \end{pmatrix} \tag{6}$$

and similar at $\lambda = \lambda_2$

$$|\phi_2\rangle = \begin{pmatrix} -i \\ 1 \end{pmatrix}. \tag{7}$$

Since H is non-Hermitian at the EPs, we have to use the bi-orthogonal basis. The corresponding left hand eigenvector of H are at λ_1 and λ_2

$$\langle\tilde{\phi}_{1,2}| = (\pm i, 1), \tag{8}$$

respectively. Note that the norm—that is the scalar product $\langle\tilde{\phi}_k|\phi_k\rangle,\ k = 1, 2$—vanishes which is often referred to as self-orthogonality [6]. Note that, for a (complex) symmetric Hamiltonian as in (3), the eigenvector at the EP is independent of parameters occurring in (3).

At the EP the difference between a degeneracy and a coalescence is clearly manifested by the occurrence of only *one* eigenvector instead of the familiar two in the case of a genuine twofold degeneracy. Note, however, that a non-Hermitian operator can also have a genuine degeneracy which is, of course, not an EP. The important point is the converse: a Hermitian operator can never have an EP.

The existence of only one eigenvector with vanishing norm is related to the fact that for $\lambda = \lambda_1$ or $\lambda = \lambda_2$ the matrix $H(\lambda)$ cannot be diagonalised [1]. At these points the Jordan decomposition reads

$$H(\lambda_1) = S\begin{pmatrix} E(\lambda_1) & 1 \\ 0 & E(\lambda_1) \end{pmatrix} S^{-1} \tag{9}$$

with

$$S = \begin{pmatrix} i & \frac{2i\delta - \omega_1 + \omega_2}{(\epsilon_1 - \epsilon_2)\delta} \\ 1 & 0 \end{pmatrix} \tag{10}$$

and $E(\lambda_1)$ being the eigenvalue at the EP. Similar expressions hold at $\lambda = \lambda_2$. We mention that the second column of S is often referred to as an associate vector obeying $(H(\lambda_1) - E(\lambda_1))|\psi_{assoc}\rangle = |\phi_1\rangle$.

The consideration of a two dimensional problem covers all aspect of an EP, since the vanishing of the norm of the eigenvectors allows to reduce a high dimensional problem approximately to two dimensions in close vicinity of an EP (see for instance [7]).

2.2 Physical Effects

To the best of our knowledge, the first direct experimental verification of the analytic properties of an EP has been achieved by the Darmstadt group some fifteen years ago. In two papers [8] an encircling of the square root branch point was performed using a microwave cavity. The expected behaviour, i.e. the interchange of the energies as well as the interchange of the corresponding eigenfunctions including their global phase change has been verified experimentally. Moreover, the phase difference $\pi/2$ between the two components of the eigenstate at the EP (see (6)) has been established experimentally. There are many more physical effects related to EPs as discussed in the literature (see a survey e.g. in [9]), the list is still continuously expanding. They cover classical as well as quantum mechanical problems.

Three more general aspects deserve to be mentioned. The idea of $\mathcal{PT}$-symmetric Hamiltonians suggested in [10] has given rise to a host of literature during the past few years. The point of $\mathcal{PT}$-symmetry breaking under parameter variation is an EP. In other words, the specific non-Hermitian Hamiltonians being symmetric under the combined action of parity and time reversal can have a real spectrum. In this case the eigenfunctions are also symmetric under $\mathcal{PT}$. At a particular point of some suitable parameter the symmetry gets broken, the eigenvalue becomes complex and the eigenfunction ceases to be $\mathcal{PT}$-symmetric. Usually two real eigenvalues coalesce and move into the complex plane when such parameter sweeps over the symmetry breaking point. This point has all characteristics of an EP. Note that owing to the non-hermiticity from the outset of the Hamiltonian such parameters and in particular the energy is real at the EP being impossible, as we recall, for a Hermitian Hamiltonian.

The second aspect refers to the combined effect of many EPs in many body problems. As has been points out many years ago [11] quantum phase transitions are related to singularities of the partition function. This has been elaborated in detail using the Lipkin model [12] where the role of EPs and their accumulation in the thermodynamic limit is demonstrated. Moreover, when such models are perturbed the onset of chaos, especially in the transitional region, can be understood by the irregular trajectories of the EPs under a perturbation. The connection between chaos and EPs in many body problems has been pointed out earlier in [13].

The third aspect, being more of theoretical interest, is the role of EPs in approximation schemes. The Random Phase Approximation, often used in the past to calculate excited states in a mean field approach [14], yields an approximate Hamiltonian that is non-Hermitian. The instability point which occurs when the particle-hole interaction is increased is in fact an EP, where two energies coalesce and then move into the complex plane. Yet, in some cases, this point can be interpreted as the onset of a phase transition of the many body system. Being singularities the EPs also affect the convergence radius of power expansions in, say, a strength parameter. A typical case in point are the "intruder" states introduced in [15] in a shell model approach of an effective interaction.

3 Exceptional Points of Third Order

Exceptional points of higher order are possible if sufficient parameters are at one's disposal. For the special case of (complex) symmetric matrices the occurrence of an EPN (Nth order EP) requires $(N^2 + N - 2)/2$ parameters for the N-dimensional matrix, and even more parameters for a more general N-dimensional matrix. As an implementation in the laboratory would require a very special experimental effort for $N > 3$ we restrict ourselves to EP3s. Some general properties have been discussed in [16, 17] where the latter paper also gives special examples of particular simple matrices giving rise to an EP3. Here we focus upon the study of some special cases which we like to denote as *concealed* EP3: the spectrum has three *equal* eigenvalues at some parameter value that seem to appear as an EP2 in addition to an incidentally coinciding third eigenvalue, whereas for some specific perturbation the three eigenvalues turn out to be an EP3. A situation of this nature occurred in the study of a Bose system by the Pitaevski equation being a non-linear problem [18].

It is obvious that the spectrum alone of three equal eigenvalues cannot give any indication as to whether we encounter a degeneracy or an EP of second or third order. Recall that it is the eigenfunctions that distinguish between a coalescence and a degeneracy. Related to this is the Jordan form J of the full original matrix problem involving the interaction between the levels: if J is diagonal the three equal eigenvalues constitute a true degeneracy, if one element of the (upper) side diagonal is unity we expect an EP2 and an EP3 if both elements of the side diagonal are unity.

As an example consider the y-dependent eigenvalue problem of the matrix

$$H = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ y & -2-y & 3 \end{pmatrix}. \tag{11}$$

Its Jordan-decomposition $H = SJS^{-1}$ yields

$$J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\sqrt{1-y} & 0 \\ 0 & 0 & 1+\sqrt{1-y} \end{pmatrix} \tag{12}$$

with

$$S = \begin{pmatrix} 1 & 1-\sqrt{1-y} & 1+\sqrt{1-y} \\ 1 & (1-\sqrt{1-y})^2 & (1+\sqrt{1-y})^2 \\ 1 & (1-\sqrt{1-y})^3 & (1+\sqrt{1-y})^3 \end{pmatrix}. \tag{13}$$

At first superficial glance this might appear to be an EP2 as by going around the branch point at $y = 1$ the eigenvalues and eigenfunctions simply interchange. An indication for the richer structure is the rank drop of S at $y = 1$: the rank drop is 2 while for a genuine EP2 it should be only 1. In fact, when y is put equal to unity from the outset in H, the Jordan form turns out to be

$$J_{H(y=1)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$

clearly suggesting an EP3. The actual patterns become clear when we perturb H and consider instead

$$H_\epsilon = \begin{pmatrix} \epsilon & 1 & 0 \\ 0 & 0 & 1 \\ y & -2-y & 3 \end{pmatrix}. \tag{15}$$

We expand the eigenvalues of H_ϵ in powers of ϵ and obtain

$$E_1 = 1 + \frac{y}{1-y}\,\epsilon + O(\epsilon^2) \tag{16}$$

$$E_2 = 1 - \sqrt{1-y} + \frac{1-y-\sqrt{(1-y)^3}}{2(1-y)^2}\,\epsilon + O(\epsilon^2) \tag{17}$$

$$E_3 = 1 + \sqrt{1-y} + \frac{1-y+\sqrt{(1-y)^3}}{2(1-y)^2}\,\epsilon + O(\epsilon^2) \tag{18}$$

again confirming our finding from above as long as $y \neq 1$; for $y = 1$ the expansion fails. If, however, y is set equal to unity from the outset in H_ϵ we this time obtain the expansions

$$E_1 = 1 + \epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{19}$$

$$E_2 = 1 + \exp\left(\frac{2\pi i}{3}\right)\epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{20}$$

$$E_3 = 1 + \exp\left(\frac{4\pi i}{3}\right)\epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{21}$$

clearly indicating the sprouting out of the three solutions from the EP3 at $y = 1$. Any perturbation of a similar kind yields the same qualitative result, while the coefficients of the powers of ϵ may be different.

There are, however, specific non-generic perturbations of H that do not give rise to an EP3. If we replace H by $H + \epsilon Ptb$ where each row of the perturbing matrix Ptb contains the same number of the same element (say unity) irrespective of their position while the other elements are zero, then the perturbed matrix $H + \epsilon Ptb$ cannot have an EP3. To show this analytically consider the transformed matrix

$$S^{-1}(H + \epsilon Ptb)S = D + \epsilon\, S^{-1} Ptb\, S$$

with D the diagonal form of H and keeping in mind that $\det[H + \epsilon Ptb] = \det[S^{-1}(H + \epsilon Ptb)S]$. The first column of S can always be arranged to contain only unities, hence the first column of the product $Ptb\, S$ contains likewise the same element under the condition made for Ptb. As a consequence, the first column of $S^{-1} Ptb\, S$ has the form $\{c, 0, 0\}^T$ with c a non-zero number. Thus, also $D + \epsilon\, S^{-1} Ptb\, S$ has this form of the first column (with different first element $\tilde{c} = 1 + \epsilon c$). The eigenvalues are obtained from the characteristic polynomial in E, i.e. from $\det(D + \epsilon\, S^{-1} Ptb\, S - E\, I) = 0$ which factors into $(\tilde{c} - E) \times Q_2(E)$, with $Q_2(E)$ being a second order polynomial yielding an EP2 and making an EP3 impossible.

It may be of interest to contrast the matrix in (11) with the slightly modified form

$$h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ -1 + y & -y & 2 \end{pmatrix} \tag{22}$$

which has the same spectrum (diagonal form) as H but the corresponding similarity transformation is now

$$s = \begin{pmatrix} 1 & 0 & 0 \\ 1 & (1 - \sqrt{1 - y}) & (1 + \sqrt{1 - y}) \\ 1 & (1 - \sqrt{1 - y})^2 & (1 + \sqrt{1 - y})^2 \end{pmatrix}. \tag{23}$$

The rank drop of s at $y = 1$ is now 1, it implies that h has no ‘hidden’ EP3 at the singularity which is just an EP2. In fact, the Jordan form of h at $y = 1$ is

$$J_{h(y=1)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{24}$$

Of course, the similarity transformation to obtain this form cannot be identified with s in (23) by setting $y = 1$ as s^{-1} does not exist; as usually in such case s contains an associate vector.

To summarise: whether or not three equal eigenvalues correspond to a threefold degeneracy or to a coalescence of two or even three eigenvalues can only been decided by looking at the full problem, that is the type of interaction between the three states. A singularity like the square root behaviour of levels as a function of an external parameters must also occur in the eigenfunctions to ensure the characteristics of an EP. An important criterion is the rank of the matrix listing the three eigenvectors. If it keeps its full rank when approaching the apparent singularity there is no EP but a genuine degeneracy, if the rank drop is 1 or 2 there is an EP2 or an EP3, respectively. This principle can be spun further to higher dimensions implying of course a rapidly increasing number of different possibilities. While the Jordan decomposition at the singularity yields all information at the singularity, the physically interesting aspect is the analytic behaviour when by variation of an external parameter the particular singularity is approached. Note that such limit is not uniform for the eigenvectors. In fact, owing to the rank drop of the matrix listing the eigenvectors at the singularity, its inverse does not exist. It is here where the associate vectors come into play for the Jordan decomposition.

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