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Phases of wave functions and level repulsion

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Abstract. Avoided level crossings are associated with exceptional points which are the singularities of the spectrum and eigenfunctions, when considered as functions of a complex coupling parameter. It is shown that the wave function of *one* state changes sign but not the other, if the exceptional point is encircled in the complex plane. An experimental setup is suggested where this peculiar phase change could be observed.

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The phase of the wave function changes in a characteristic way, if a self-adjoint Hamiltonian has an energy degeneracy at specific values in some parameter space and if a loop around the point of degeneracy is described in parameter space [1]. In the simple case of a real symmetric Hamiltonian two parameters are needed to get a *diabolic point*. In this case Berry's phase is π when looping around the degeneracy in the two-dimensional parameter space.

If a self-adjoint Hamiltonian depends only on one parameter, its variation will in general give rise to level repulsion [2]. Associated with a level repulsion is a pair of exceptional points [3] which are the points where the two levels actually coalesce when continued analytically into the complex plane of the parameter [4]. In the present letter we discuss the behaviour of the wave functions and their phases when an exceptional point is encircled. We suggest an experimental situation where such behaviour could be measured. It is distinctly different from a diabolic point where Berry's phase occurs. In particular, an exceptional point must not be confused with a coincidental degeneracy of resonance states, considered in [5] as a generalization of Berry's phase.

The difference between a diabolic point and an exceptional point is due to the self-adjointness of the Hamiltonian in the former and the lack of it in the latter case. Also, when continuing into the complex parameter plane we are faced with analytic functions of a complex variable implying a more rigid mathematical structure. In the references quoted above a thorough discussion is given of the spectrum and eigenfunctions, when one parameter of the Hamiltonian is continued into the complex plane. The parameter chosen can be an interaction strength, but other choices are possible [6]. In the present paper we consider the problem of the form $H_0 + \lambda H_1$ (with H_0 and H_1 symmetric) and analytically continue the spectrum and the eigenfunctions into the complex λ-plane where the exceptional points occur. Generically, an N-dimensional matrix problem yields $N(N-1)$ exceptional points. For an infinite-dimensional problem, an infinite number usually occurs [7]. Depending on the particular structure of H_1, this infinite number of exceptional points can have an accumulation point in the finite λ-plane which may be associated with a phase transition occurring at $\Re\lambda \approx \lambda_{\text{accum}}$ [8]. In very special cases like the single-particle spectrum of the Hulthen potential [9] the exceptional points may be absent altogether.

All essential aspects of exceptional points can be illustrated on an elementary level with a two-level model. In fact, for finite or infinite-dimensional problems an isolated exceptional point can be described locally by a two-dimensional problem [10]. In other words, even though a high or infinite-dimensional problem is globally more complex than the two-dimensional problem, we do not loose generality for our specific purpose when the restriction to a two-dimensional problem is made. For easy illustration we therefore confine ourselves to the discussion of

$$H = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} + \lambda U \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} U^\dagger \,, \tag{1}$$

with

$$U = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}. \tag{2}$$

This is, up to a similarity transformation, the most general form of a real two-dimensional Hamilton matrix of the type $H_0 + \lambda H_1$. The particular dependence on the parameter λ has been chosen as it is of a nature widely used in physical applications. We emphasize that our aim is not in particular directed at a physical model that is describable by a two-dimensional problem although there may exist

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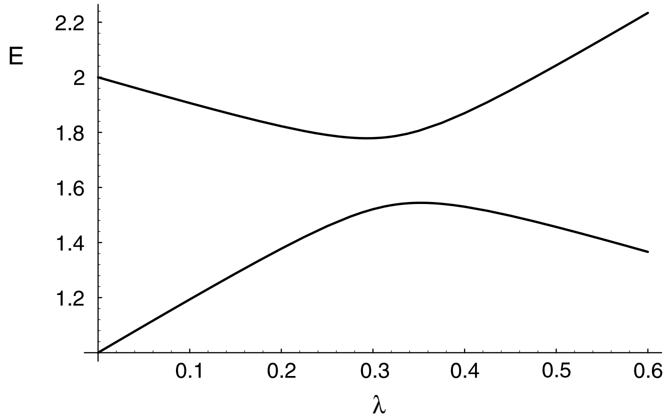

Fig. 1. Level repulsion using in equation (3) $\epsilon_1 = 1$, $\epsilon_2 = 2$, $\omega_1 = 2$, $\omega_2 = -1$ and $\phi = \pi/25$.

interesting problems in our special context. The example has been chosen for illustration, while the physical application that we have in mind is an infinite-dimensional situation.

The eigenvalues of H are given by

$$E_{1,2}(\lambda) = \frac{\epsilon_1 + \epsilon_2 + \lambda(\omega_1 + \omega_2)}{2} \pm R\,, \tag{3}$$

where

$$R = \left\{ \left(\frac{\epsilon_1 - \epsilon_2}{2}\right)^2 + \left(\frac{\lambda(\omega_1 - \omega_2)}{2}\right)^2 + \frac{1}{2}\lambda(\epsilon_1 - \epsilon_2)(\omega_1 - \omega_2)\cos 2\phi \right\}^{1/2}. \tag{4}$$

Clearly, when $\phi = 0$ the spectrum is given by the two lines

$$E_k^0(\lambda) = \epsilon_k + \lambda\omega_k, \quad k = 1, 2$$

which intersect at the point of degeneracy $\lambda = -(\epsilon_1 - \epsilon_2)/(\omega_1 - \omega_2)$. When the coupling between the two levels is turned on by switching on ϕ, the degeneracy is lifted and an avoided level crossing occurs as is illustrated in Figure 1. Now the two levels coalesce in the complex λ-plane where R vanishes. This happens at the complex conjugate points

$$\lambda_c = -\frac{\epsilon_1 - \epsilon_2}{\omega_1 - \omega_2}\exp(\pm 2i\phi). \tag{5}$$

At these points, the two levels $E_k(\lambda)$ are connected by a square root branch point; in fact the two levels are the values of one analytic function on two different Riemann sheets. In Figure 2a we display contours in the complex energy plane for each level, obtained if a loop in the complex λ-plane does not encircle the exceptional point. Accordingly, Figure 2b shows the corresponding contours, if the exceptional point is encircled. In this case only a double loop in the λ-plane yields a closed loop in the energy plane.

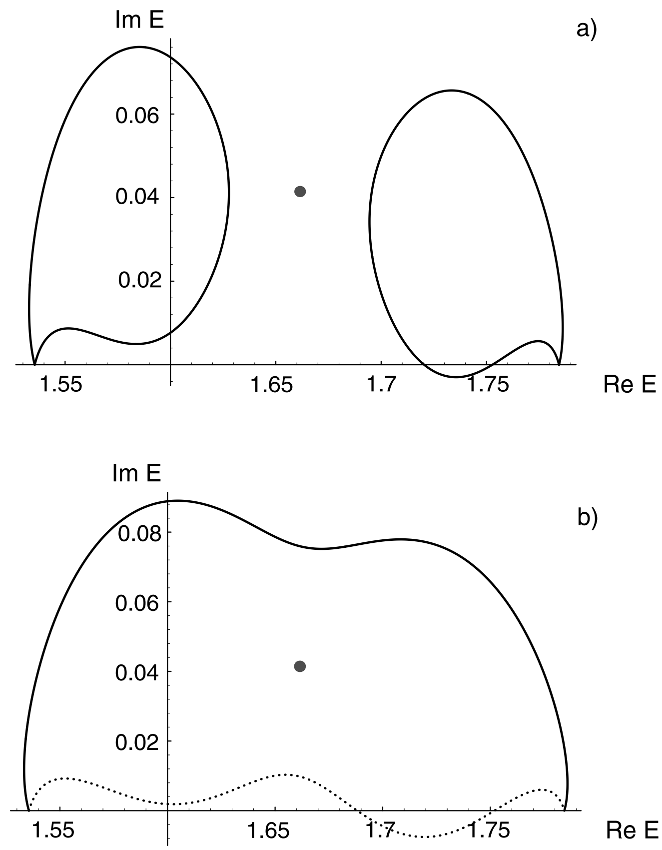

Fig. 2. Contours in the complex energy plane. The top illustrates contours for each level, if a closed loop is described in the λ-plane without encircling the exceptional point. The bottom illustrates the energy contour produced by two (equal) closed loops in the λ-plane, which encircle the exceptional point. The solid line corresponds to the first closed loop in the λ-plane and the dotted line to the subsequent loop. The solid dot is the position where the contours would meet, if the loops crossed the exceptional point in the λ-plane.

Obviously, this connection is not of the type encountered at a genuine diabolic point.

The difference has a bearing also on the scattering matrix [11] and on the wave functions $\psi_1(\lambda)$ and $\psi_2(\lambda)$. In [11], although the notion *exceptional points* is not used, the pertinent distinction between a genuine degeneracy of two resonances and the analytic coalescence (exceptional point) of two (complex) eigenvalues is nicely discussed. A usual degeneracy of two resonances still gives rise to a simple pole in the scattering matrix or Green's function, while an exceptional point produces a double pole. With regard to the eigenfunctions, we recall that for complex λ the Hamiltonian is no longer self-adjoint. This means that the eigenfunctions are no longer orthogonal. We rather have a bi-orthogonal system which can be normalized as

$$\langle\tilde{\psi}_1(\lambda)|\psi_2(\lambda)\rangle = \delta_{1,2}\,, \tag{6}$$

where $|\psi_k\rangle$ and $\langle\tilde{\psi}_k|$ are the right-hand and left-hand eigenvectors of H, respectively. Note that equation (6) causes problems at the exceptional point, since it is exactly at this point where two linearly independent eigenfuctions no longer exist. This is in contrast to a genuine degeneracy of a self-adjoint operator where a k-fold degeneracy always gives rise to a k-dimensional eigenspace. At the exceptional point not only the eigenvalues but also the eigenfunctions coalesce. As a consequence the orthogonality conflicts with the normalization. In other words, if equation (6) is enforced globally (*i.e.* also at $\lambda = \lambda_c$), the components of the wave function have to blow up. This can be made explicit by parametrizing the wave functions by the complex angle θ, *viz.*

$$\psi_1(\lambda) = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \quad \psi_2(\lambda) = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \tag{7}$$

with

$$\tan^2\theta(\lambda) = \frac{E_1(\lambda) - E_2(\lambda) - (\epsilon_1 - \epsilon_2) - \lambda(\omega_1 - \omega_2)\cos 2\phi}{E_1(\lambda) - E_2(\lambda) + (\epsilon_1 - \epsilon_2) + \lambda(\omega_1 - \omega_2)\cos 2\phi}. \tag{8}$$

At $\lambda = \lambda_c$ we have $E_1 = E_2$ and hence $\tan^2\theta = -1$ implying $|\cos\theta| = |\sin\theta| = \infty$, that is the components of the wave functions blow up. (Note that $\tan^2\theta \equiv 0$ in the trivial case $\phi = 0$.) The increase of the components of the wave functions while approaching exceptional points has been used in similar context as a theoretical signature of a phase transition [8], but we do not believe that it has observational consequences.

We now study the behaviour of the wave functions in more detail for two contours in the λ-plane which start, say, at $\lambda = 0$ and end at large real values of λ, but enclose an exceptional point between the two contours. For the complex angle θ we choose an expression which is more convenient for this purpose, *viz.*

$$\tan\theta(\lambda) = \frac{\lambda(\omega_1 - \omega_2)\sin 2\phi}{E_1(\lambda) - E_2(\lambda) + \epsilon_1 - \epsilon_2 + \lambda(\omega_1 - \omega_2)\cos 2\phi}. \tag{9}$$

The first path can be taken along the real λ-axis. From equation (9) we read off the expected result that $\theta(0) = 0$ and $\theta(\lambda) \to \phi$ for $\lambda \gg |(\epsilon_1 - \epsilon_2)/(\omega_1 - \omega_2)|$. In obtaining this result use is made of $E_1 - E_2 = 2R \to \lambda(\omega_1 - \omega_2)$ for $\lambda \gg |(\epsilon_1 - \epsilon_2)/(\omega_1 - \omega_2)|$. For the second path we move into the upper λ-plane in order to pass above the exceptional point before returning down to the real axis again. Using again equation (9) we now have to observe that we crossed into the other sheet which means $E_1 - E_2 = -2R \to -\lambda(\omega_1 - \omega_2)$. As a consequence we find this time $\tan\theta = -\cot\phi = \tan(\phi + \pi/2)$. Surely we would expect the wave functions to interchange just like the energies, if an exceptional point is encircled. But our finding indicates that *one wave function has changed its sign.* In fact, we obtain along the second path

$$\psi_1 \to \psi_2, \quad \psi_2 \to -\psi_1. \tag{10}$$

Note that this result is equally obtained, if a closed contour surrounding the exceptional point is described in the λ-plane. Of interest is the result of a double loop in the λ-plane. This yields

$$\psi_1 \to -\psi_1, \quad \psi_2 \to -\psi_2 \tag{11}$$

which is, in accordance with the corresponding single loop in the energy plane, just Berry's phase retrieved. We mention that this implies that, if the wave functions are parametrized as in equation (7), then they have an algebraic singularity that is determined by a fourth root at the exceptional point; only a four-fold loop in the λ-plane restores completely the original situation as far as the wave functions are concerned.

Next we address the question concerning the physical significance of these findings. It boils down to the problem of varying a *complex* interaction parameter in the laboratory. Problems of a similar nature have been discussed in connection with Berry's phase for dissipative systems [12], but not as yet for exceptional points. We are guided by the phenomenological description of open quantum systems [8] and submit as one suggestion a strongly absorptive system, where the parameter λ in equation (1) is traditionally replaced by $-iG$ with real absorption parameter G. With the replacement the eigenvalues acquire imaginary parts which are related to the inverse life times of the states of the open system. The exceptional points appear now in the complex G-plane at

$$G_c = -\frac{\epsilon_1 - \epsilon_2}{\omega_1 - \omega_2}\exp(\pm 2i\phi + i\pi/2). \tag{12}$$

If the coupling of the two channels is equal, that is if $\phi = \pi/4$, the two exceptional points lie on the real G-axis at

$$G_c = \pm\frac{\epsilon_1 - \epsilon_2}{\omega_1 - \omega_2}.$$

If the coupling is nearly equal, they lie just above or below the real axis depending on the coupling being slightly weaker or stronger ($\phi < \pi/4$ or $\phi > \pi/4$). Controlling the absorption parameter G *and* the relative coupling enables one to pass the exceptional point on a path below and above, which is the situation described above. The wave functions will change according to equation (10).

A setup similar to the one proposed by Berry [1] and implemented in [13] provides a further possibility for experimental verification. In a two-dimensional electromagnetic resonator consider two suitable levels which display level repulsion under variation of a judiciously chosen control parameter, such as a change of the geometry of the resonator [13,14]. The absorption can be controlled by radiation losses, regulated by an absorber used in the resonator or by suitable antennas. For the final analysis it is immaterial whether the description uses a complex parameter λ (as discussed in the previous paragraph) or phenomenological widths for the unperturbed energies ϵ_k. In fact, equation (5) can also be used with the replacement $\epsilon_k \to \epsilon_k - i\Gamma_k$, which results in a shift of one of the exceptional points towards the real axis or beyond (the other exceptional point moves further away into the λ-plane). Variation of the parameter λ, achieved by changing the geometry of the resonator, and the use of different values of the absorption allows the experimenter to pass the exceptional point on its left- or right-hand side. Fortuitously, in the spirit of the experiment performed by [13] the adiabatic change of the parameters is not essential, since it is the movement of the nodes of the wave functions (the electric field in the case considered) that are being observed under parameter variation [14]. Possible jumps of the phases do therefore not affect the result of interest. Again we stress that the exceptional point which is associated with the level repulsion under consideration is not to be confused with a genuine degeneracy of resonances: the latter has no effect upon the wave functions whereas the former is a singular point of the spectrum and can be discerned by equations (10). Note that, for large values of the absorption, one state may be much broader than the other [8].

We emphasize again that the occurrence of exceptional points is a generic mathematical feature associated with any system that has avoided level crossing. While this presentation used a two-dimensional illustration, the results can be immediately generalized. In fact, if more than one exceptional point is encircled, the resulting phase change is simply a combination of several two-dimensional cases. The findings presented in this paper therefore appear to have universal significance.

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