Global and Local Aspects of Exceptional Points

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Exceptional points are singularities of eigenvalues and eigenvectors for complex values of, say, an interaction parameter. They occur universally and are square root branch point singularities of the eigenvalues in the vicinity of level repulsions. The intricate connection between the distribution of exceptional points and particular fluctuation properties of level spacing is discussed. The distribution of the exceptional points of the problem $H_0 + \lambda H_1$ is given for the situation of hard chaos. Theoretical predictions of local properties of exceptional points have recently been confirmed experimentally. This relates to the specific topological structure of an exceptional point as well as to the chiral properties of the wave functions associated with exceptional points.

I. INTRODUCTION

We address the questions: which are the common properties of the *quantum mechanical Hamilton operators* that give rise to spectral properties that are ascribed to quantum chaos. If a matrix representation of a Hamiltonian originating from a classically chaotic analogous case is given, we explore the mathematical mechanism that produces the special statistical features of the spectrum for the particular parameter range where classical chaos is discerned. While classical chaos has no intrinsic statistical property, a further puzzling question is: why can a plain statistical approach, with no physical input (such as GOE or GUE) [1], reproduce the statistical properties of the spectrum so successfully?

We believe that the common root to the answer of these questions lies in what is called the exceptional points [2] (EP) of an operator. Most physical problems in quantum mechanics can be formulated by the Hamiltonian $H_0 + \lambda H_1$ where the parameter λ can play the role of a perturbation parameter, or it may serve to effect a phase transition, or it may under variation steer the system from an ordered into a chaotic regime. The EPs of the full operator are the points λ for which two eigenvalues coalesce. Here we exclude genuine degeneracies of the self-adjoint problem, in other words, the eigenvalues coincide for no real λ. For a hermitian H_0 and H_1 the EPs occur only in the complex λ-plane. Note that the operator $H_0 + \lambda H_1$ is not self-adjoint for complex λ-values.

The definition of EPs is general and applies also to operators in an infinite dimensional space, also when the spectrum of the operator has a continuum part [3]. In the present work we restrict ourselves to finite N-dimensional matrices H_0 and H_1 as in this case the role of the EPs and the associated Riemann sheet structure is thoroughly

understood [4,5]. We do not believe that restriction to matrices has a major impact on our conclusions since virtually all the practical work even in connection with quantum chaos is done in a finite dimensional matrix space.

The physical significance of the EPs is due to their relation with avoided level crossing for real λ-values. The spectrum $E_k(\lambda)$, $k = 1, \ldots, N$ has branch point singularities at the EPs, in fact, any pair of the N levels are generically connected by a square root branch point in the complex λ-plane. If this happens near to the real λ-axis, a level repulsion will occur for the two levels for real λ-values. Globally, all the EPs determine the shape of the whole spectrum. There is a nice analogy to the more widely known connection between the singularities being poles of the scattering function and the shape of the cross section: in a similar way as the positions of the poles including their statistical properties determine the measurable cross section, the EPs determine the shape of the spectrum and in particular the occurrences of avoided level crossings. The distribution of the EPs will therefore determine the fluctuation properties of level spacing.

The positions of the EPs are fixed in the complex λ-plane and are determined solely by H_0 and H_1. For large matrices it is prohibitive to determine the positions of the EPs. However, it is possible to determine the distribution reasonably well from the knowledge of the two operators. Generically, a high density of EPs is a sufficient prerequisite for the occurrence of quantum chaos if they are randomly distributed according to a specific distribution function.

In the following section we recapitulate the basics about EPs. Section three presents matrix models to exemplify the distribution of EPs and level spacing fluctuations. Section four presents two recent experiments where (i) the local topological structure of an EP has been shown to be a physical reality and (ii) where the chiral property of the wave functions at the EP has been demonstrated. Section five presents a summary and outlook.

II. EXCEPTIONAL POINTS AND UNPERTURBED LINES

Avoided level crossings are always associated with EPs [4–7] wherever they occur for the levels $E_k(\lambda)$ of the Hamiltonian $H_0 + \lambda H_1$. We give an elementary example for illustration and briefly list the essential aspects with regard to EPs.

Consider a two dimensional real matrix problem where H_0 is diagonal with eigenvalues ϵ_1 and ϵ_2, while H_1 is represented in the form

$$H_1 = U \cdot D \cdot U^{-1}. \tag{1}$$

Here, the diagonal matrix D contains the eigenvalues ω_1 and ω_2 of the matrix H_1 and U is the rotation

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

The eigenvalues of the problem $H_0 + \lambda H_1$ are

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

where

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

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

$$E_k^0(\lambda) = \epsilon_k + \lambda\omega_k \qquad k = 1,2 \tag{5}$$

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 avoided level crossing occurs. Now the two levels coalesce in the complex λ-plane where R vanishes which happens at the complex conjugate points

$$\lambda_c = -\frac{\epsilon_1 - \epsilon_2}{\omega_1 - \omega_2} \exp(\pm 2i\phi). \tag{6}$$

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.

These considerations carry over to an N-dimensional problem [4]. The diagonal matrix H_0 contains the elements ϵ_k and D the elements ω_k, $k = 1,\ldots,N$; the matrix U is now an N-dimensional rotation which can be parametrized by $N(N-1)/2$ angles ϕ_k. (In the quoted paper a parametrization was chosen so that U is unity when all angles are zero.) The EPs are determined by the simultaneous solution of the equations

$$\det(E - H_0 - \lambda H_1) = 0$$
$$\frac{d}{dE}\det(E - H_0 - \lambda H_1) = 0. \tag{7}$$

There are generically $N(N-1)$ solutions which occur in complex conjugate pairs in the λ-plane. At those points the N levels $E_k(\lambda)$ are connected in pairs by square root branch points when they are analytically continued into

the complex λ-plane. Note that, for the matrix problem, the square root branch points are the only singularities of the spectrum. Since the positions of the singularities determine the shape of the spectrum, and in particular the fluctuation properties, a closer analysis is indicated. As is exemplified in the next section, the essential condition for the occurrence of level statistics ascribed to quantum chaos is a high density of EPs in the complex plane within a small window of real λ-values.

To get an idea about the density of EPs we introduce the concept of *unperturbed lines*. Clearly, when U is the unit matrix (all angles are zero), the spectrum of $H_0 + \lambda H_1 = H_0 + \lambda D$ is given by the lines $\epsilon_k + \lambda\omega_k$ with $k = 1,\ldots,N$. The $N(N-1)/2$ intersection points of the N lines depend on the relative order of the numbers ϵ_k and ω_k. If both sequences are in ascending order, all intersections occur at negative λ-values; conversely, if one sequence is ascending and the other descending all intersections occur at positive λ-values. In general, the order which is appropriate for the actual problem, is expected to lie between the two extremes. To find out the appropriate order we are guided by the asymptotic behavior of the levels $E_k(\lambda)$ of the full problem. For large values of λ the leading terms are given by

$$E_k(\lambda) = \lambda\omega_k + \alpha_k + \ldots \tag{8}$$

where the dots stand for first and higher order terms in $1/\lambda$. Neglecting these terms, Eq.8 yields just the unperturbed lines with the appropriate association of slopes ω_k and intercepts α_k. From perturbation theory we find the latter to be the diagonal elements of the rotated H_0, *viz.*

$$\alpha_k = (U^{-1} \cdot H_0 \cdot U)_{k,k}. \tag{9}$$

III. DISTRIBUTION FUNCTION

We begin with the distribution function of the intersection points of the unperturbed lines as this can be derived rigorously. Assuming a uniform random distribution for the ω_k and the ϵ_k (the eigenvalues of H_1 and H_0, respectively), the intersection points $\lambda_{i,k} = -(\epsilon_i - \epsilon_k)/(\omega_i - \omega_k)$ are distributed according to [8]

$$P(x) = \frac{\text{const}}{x^2}. \tag{10}$$

The fact that $P(x)$ cannot be normalized is due the fact that we assumed a uniform distribution of the ω_k over the whole range of the real numbers; for a finite sample there will therefore be a deviation of $P(x)$ around $x = 0$ from the form given in Eq.(10) as no $|\omega_k|$ is larger than some finite large number and hence an arbitrary small value of $1/\omega$ cannot occur leading to a cut-off of $P(x)$ for $x \in [0, 1/\omega_{\text{max}}]$.

The intersection points are the points of degeneracies of $H_0 + \lambda H_1$ as long as U is equal to the identity matrix. We now gradually switch on the interaction between the levels by switching on the angles ϕ_k randomly of the random orthogonal matrix U [8] but keeping initially the interval from which the angles are chosen very small. In this way the degeneracies become level repulsions as the EPs start moving out into the complex λ-plane, a complex conjugate pair from each degeneracy. We conjecture that their distribution function remains unchanged when they move out into the plane. For small values of the mixing angles in U they will of course be concentrated around the real axis. The distribution function is now a function of two variables, say the real and imaginary part of a complex number. We parametrize this number by $r \exp(i\alpha)$. For a fixed angle α the EPs are distributed according to

$$P(r) = \frac{\text{const}}{r^2}. \tag{11}$$

This has been confirmed numerically in numerous cases and can be shown using a large number of samples of two dimensional matrices. If the mixing angles of U are very small, there is an obvious dependence on α as the EPs cluster around the real axis; yet for fixed α the distribution law is always given by Eq.(11). Moreover, for the nearest neighbor distribution (NND) of the energy levels it turns out that a proper Wigner distribution is obtained only when the EPs have fanned out into the plane in such a way that their distribution becomes independent of the angle α. In Fig.1 it is illustrated how the EPs fan out into the plane when the mixing angles of U are turned on.
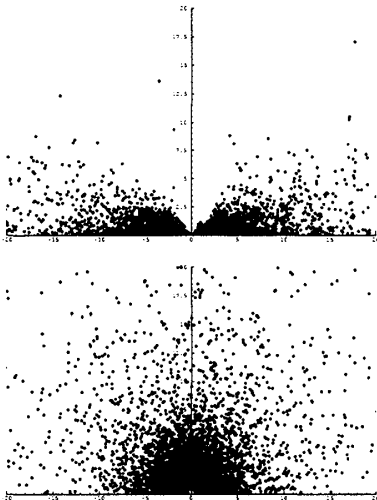

FIG. 1. Exceptional points as they move into the complex λ-plane when the angles in U are switched on. The lower part illustrates hard chaos.

The law of Eq.(11) is verified numerically even if the

EPs originate out of a degeneracy of high multiplicity. In Fig.2 the emergence of EPs out of a point of degeneracy is illustrated. The figure shows the development (top left to bottom right) as a function of the increasing size of the interval from which the angles ϕ_k are randomly chosen. Here, Eq.(11) is obtained once they fill the plane in an isotropic way, that is when the distribution has become independent of α. A further increase of the angles leaves the statistical behaviour unchanged.

To summarize: hard chaos, that is a Wigner distribution for the NND of the energy levels, is associated with a distribution of EPs in the complex plane that is independent of the angle α of the complex number $r \exp(i\alpha)$ and depends only on the distance r according to Eq.(11). If an α-dependence prevails, the NND is not Wigneresque. In the limiting case of no interaction ($U \equiv$ identity) no EP occurs, and the NND of the above example using a random set of ϵ_k and/or ω_k is given by a Poisson distribution.
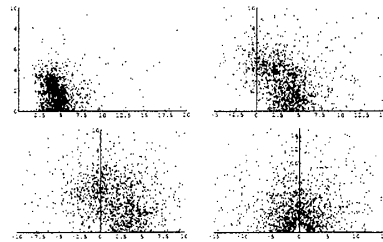

FIG. 2. Exceptional points as they move into the complex λ-plane when the angles in U are switched on. Here a point of degeneracy at $\lambda = 5$ is the starting point. In the figure on the bottom right this information is completely lost and hard chaos prevails.

We only mention that, in special integrable and thus non-generic cases, the EPs are arranged in a geometrically ordered pattern like in the integrable Lipkin model [9]. However, a perturbation no matter how small leads to the generic situation of hard chaos for those values of λ where a high concentration of EPs occurs; for the Lipkin model this is the region around the phase transition [7].

IV. LOCAL PROPERTIES OF EXCEPTIONAL POINTS

The topological structure of the square root branch point associated with an EP has been shown to be a physical reality in a recent experiment [10]. As a particular consequence it has been established experimentally that the phases of the wave functions that take part in the coalescence of the two energy levels show a phase behavior that is *distinctly different* from that of a usual degeneracy, i.e. from that at a diabolic point [11]. We emphasize that one major signature, contrasting an EP from a de-

generacy, is the lack of two independent eigenfunctions; there is in fact only one eigenfunction: the EPs are the points where the Jordan form of the operator does not give a diagonal matrix [2]. This is sometimes overlooked in the literature [12,13]. They can also occur in the continuum as the coalescence of two resonances [14]. In the quoted paper the behaviour of the corresponding scattering matrix has been discussed: an exceptional point occurs as a pole of second order in the S-matrix.

The crucial experiment [10] yielded three major results which have been predicted in [15]:

1. If a loop is performed in the λ-plane around the EP, the eigenenergies E_1 and E_2 are interchanged.

2. The wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ are interchanged by the loop and, in addition, one of them changes sign. In other words, a loop in the λ-plane transforms the pair $\{\psi_1, \psi_2\}$ into $\{-\psi_2, \psi_1\}$. Therefore the two possible directions of looping yield different phase behavior. In fact, encircling the EP a second time in the same direction, we obtain $\{-\psi_1, -\psi_2\}$ while the next loop yields $\{\psi_2, -\psi_1\}$ and only the fourth loop restores the original pair. It follows that by going in the opposite direction, one finds after the first loop what is obtained after three loops in the former direction. This finding confirms the fourth root character of singularity for the wave functions.

3. The eigenvalues E_1, E_2 have been studied as functions of λ for two paths that were not closed. One path was just above, the other one just below λ_c. The results were different. Calling the real part of an eigenvalue the resonance energy and its imaginary part the resonance width. On one of the paths, the widths cross while the resonance energies avoid each other. On the other path, the resonance energies cross while the widths avoid each other.

We conclude the discussion with a further important local property of EPs. The single and unique (up to a global factor) wave function at the EP has always a specific chiral behavior [16]. A recent experiment at the TU-Darmstadt [17] has directly confirmed this feature. In similar context this has been discussed for acoustic waves in a medium [18] and indirectly observed in optics [19]. The latter has been explained in terms of EPs in [20]. The essential finding of [16] is the unique form of the wave function at the EP. For a complex symmetric matrix it is given by the following superposition

$$|\psi_{EP}\rangle = |\psi_1\rangle \pm i|\psi_2\rangle \tag{12}$$

and no other superposition can occur. Here the plus or minus sign refers to a specific EP. The $|\psi_i\rangle$ are the two wave functions that coalesce at the EP. No other superposition is possible, irrespective of a particular physical

situation such as driving the dissipating system. For a time dependent problem this signals chiral behavior. If the two wave functions relate to different parities or to different linear polarizations, the superposition is obviously chiral; in the latter case it is a circularly polarized wave of specific orientation. We recall that here H_0 and H_1 are assumed to be real symmetric. If the two operators are complex but still hermitian [21] or altogether non-hermitian [22] there is still a unique superposition but Eq.(12) has to be modified. If H_0 or H_1 are non-hermitian, the EPs may lie on the real λ-axis [22].

V. SUMMARY AND OUTLOOK

Exceptional points are a fascinating subject of theoretical physics. As they are the only singularities of the spectrum for a matrix problem, they 'make' the spectrum, so to speak. They are directly associated with level repulsion. As a consequence, they govern the time evolution of wave packets [23] and the transition rates of Landau-Zener transition [24]. Their statistical properties relate directly to that of the spectrum itself. Integrable systems give rise to a geometrical ordering while chaotic systems relate to disordered arrangements, yet with a specific distribution function.

The local behavior is fascinating on its own. The topological structure of a square root branch point is a physical reality with all its consequences for the wave functions. In addition, with its intrinsic chiral behavior it may even hold some promise to shed light on the ubiquitous left-right asymmetry of our macroscopic world. In fact, any EP gives an indication about the relation between chirality and dissipation as it is accessible and manifests itself only for dissipative systems. We conclude on a speculative note: the kinematic relation $E = \pm\sqrt{\vec{p}^2 + m^2}$ bears all properties of an EP at $|\vec{p}| = \pm im$. It was this relationship that led Dirac to his famous equation including the properties of chirality of a spin system.

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