Time behaviour near to spectral singularities

W. D. Heiss

National Institute for Theoretical Physics, Stellenbosch Institute for Advanced Study,
and Institute of Theoretical Physics, University of Stellenbosch, 7602 Matieland, South Africa

Spectral singularities such as exceptional points invoke specific physical effects. The present paper focuses upon the time dependent solutions of the Schrödinger equation. In a simple model it is demonstrated that - depending on initial conditions - within close proximity of exceptional points the time behaviour of the wave function displays characteristic features such as very fast decay or the opposite, i.e. very long life time. At the exceptional point the wave function typically has a linear term in time besides the usual exponential behaviour.

INTRODUCTION

Recently the effects of spectral singularities upon scattering have been discussed in general terms [1]using a particular model for demonstration. It is the exceptional points (EP) [2] that generically occur in Hamiltonians of open systems for specific (complex) values of some parameters [3, 4]. The EPs are associated with the coalescence of two (or more) eigenvalues under variation of appropriate parameters; in contrast to a degeneracy the corresponding eigenstates also coalesce and have zero norm. For that reason they give rise to a double pole in the scattering function [5] and thus to characteristic physical effects. Here we mention atomic and molecular physics [6–8], optics [9], nuclear physics [10] and in different theoretical context $\mathcal{PT}$-symmetric models [11], to name just a few. Depending on the particular situation EPs can signal a phase transition [12, 13]. The topological structure being a square root branch point in the complex plane has been shown experimentally to be a physical reality [14–16].

The present paper resumes the model dealt with in [1], however, from a very different viewpoint. While the scattering deals with a stationary physical situation, we here investigate the effect of EPs upon the time behaviour of solutions of the time dependent Schrödinger equation. Such effects have been seen recently in [17] with optical micro-spirals, in [18] for Rabi oscillations and earlier in [19] for a singular di-electric tensor. It is expected that the rapidly improving experimental techniques of lasers applied for instance to atomic and molecular physics will focus upon time behaviour to an increasing extent [20].

The following section presents the time evolution with the emphasis at or close to an EP. A generic physical example is given in section 3 showing the characteristic and dramatic changes of the time dependent wave function in the proximity of EPs. A summary concludes the paper.

TIME EVOLUTION

The Model

It is well established that, in the close vicinity of an EP, a two-dimensional matrix model suffices to capture all essential features associated with the singularity. We thus begin with the model Hamiltonian

$$
\begin{aligned}
H(\lambda) &= H_0 + H_1(\lambda) = H_0 + \lambda V \\
&= \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \lambda \begin{pmatrix} \epsilon_1 & \delta \\ \delta & \epsilon_2 \end{pmatrix}
\end{aligned}
\tag{1}
$$

where the parameters ω_k and ϵ_k determine the non-interacting resonance energies $E_k = \omega_k + \lambda \epsilon_k$, $k = 1, 2$. The time evolution of a two dimensional state vector $|\psi(t)\rangle$ with the initial condition $|\psi(0)\rangle = \{C_1, C_2\}^T$ is given by

$$
|\psi(t)\rangle = \sum_{k=1,2} \exp(-iE_k(\lambda)t)\langle\phi_k|\psi(0)\rangle|\phi_k\rangle
\tag{2}
$$

with the eigenvalues

$$
E_{1,2}(\lambda) = \frac{1}{2}(\omega_1 + \omega_2 + \lambda(\epsilon_1 + \epsilon_1) \mp D
\tag{3}
$$

$$
D = \sqrt{CC(\lambda - EP1)(\lambda - EP2))}
\tag{4}
$$

$$
CC = 4\delta^2 + (\epsilon_1 - \epsilon_2)^2
\tag{5}
$$

expressed in terms of the EPs

$$
EP1 = \frac{i(\omega_1 - \omega_2)}{-2\delta - i(\epsilon_1 - \epsilon_2)}
\tag{6}
$$

$$
EP2 = \frac{i(\omega_1 - \omega_2)}{+2\delta - i(\epsilon_1 - \epsilon_2)}
\tag{7}
$$

and the normalised eigenvectors

$$
\begin{aligned}
|\phi_1\rangle &= \begin{pmatrix} D + 2\lambda\delta, \\ \omega_1 - \omega_2 + \lambda(\epsilon_1 - \epsilon_2) \end{pmatrix} \\
&\times \frac{1}{\sqrt{(\omega_1 - \omega_2 + \lambda(\epsilon_1 - \epsilon_2))^2 + (2\lambda\delta + D)^2}}
\end{aligned}
\tag{8}
$$

with $|\phi_2\rangle$ obtained from $|\phi_1\rangle$ by the replacement $\delta \to -\delta$. Note that the denominator of $|\phi_k\rangle$ vanishes when $\lambda \to$

$EP1$ or $\lambda \to EP2$, the leading order being $(\lambda - EP)^{1/4}$ [3].

Actually, as in [1], we have chosen for the eigenvectors a basis rotated by the angle $\pi/4$ rather than the basis given by (1). This specific observational basis is essential to ensure that even for the non-interacting case ($\delta = 0$) the two rotated channels feature equally and are observed simultaneously, while - for $\delta = 0$ - the states in the basis given by (1) live in orthogonal spaces. The difference between the two rotated channels appears when δ is switched on as is discussed in the following sections.

Inserting the explicit expressions into (2) we obtain for the components denoted by $z_{1,2}(t)$ of the two component solution

$$|\psi(t)\rangle = \begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix}$$

the result

$$
\begin{aligned}
z_2(t) = \quad & C_2 \left(\frac{\exp(-iE_1 t) + \exp(-iE_2 t)}{2} \right. \\
& + \left. \delta \frac{\exp(-iE_1 t) - \exp(-iE_2 t)}{D} \right) \\
+ C_1 \quad & \frac{\exp(-iE_1 t) - \exp(-iE_2 t)}{2D} \\
\times \quad & (\omega_1 - \omega_2 + \lambda(\epsilon_1 - \epsilon_2)).
\end{aligned}
\tag{9}
$$

The first component $z_1(t)$ is obtained from $z_2(t)$ by the replacements $C_1 \leftrightarrow C_2$ and $\delta \to -\delta$.

Before discussing the detailed behaviour in an actual physical situation we first turn to the analytic solution at an EP.

Time behaviour at an exceptional point

When λ approaches an EP the denominator D in (9) vanishes. So do the corresponding numerators since $E_1 \to E_2$ when $\lambda \to EP$. A finite limit is obtained and reads

$$
\begin{aligned}
z_2^{EP1}(t) = \\
\frac{(\epsilon_1 - \epsilon_2 - 2i\delta + i\delta(\omega_1 - \omega_2)t)C_2 - \delta(\omega_1 - \omega_2)tC_1}{\epsilon_1 - \epsilon_2 - 2i\delta} \\
\times \exp(-it \frac{i(\epsilon_1\omega_2 - \epsilon_2\omega_1) + \delta(\omega_1 + \omega_2)}{i(\epsilon_1 - \epsilon_2) + 2\delta})
\end{aligned}
\tag{10}
$$

and

$$
\begin{aligned}
z_1^{EP1}(t) = \\
\frac{(\epsilon_1 - \epsilon_2 - 2i\delta - i\delta(\omega_1 - \omega_2)t)C_1 - \delta(\omega_1 - \omega_2)tC_2}{\epsilon_1 - \epsilon_2 - 2i\delta} \\
\times \exp(-it \frac{i(\epsilon_1\omega_2 - \epsilon_2\omega_1) + \delta(\omega_1 + \omega_2)}{i(\epsilon_1 - \epsilon_2) + 2\delta}).
\end{aligned}
\tag{11}
$$

The essential point is the linear time dependence occurring in the coefficient of the exponentials. The 'singularity', usually associated with an EP, invokes in the time frame the additional linear time dependence. This is of course no surprise; it is a well known result from the theory of ordinary differential equations. The evolution equation $i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle$ gives rise to linear terms in time if H cannot be diagonalised but has a non-diagonal Jordan normal form; this is precisely the case at an EP. It is here where the associate vector defined by

$$(H(\lambda = EP) - E_{EP})|\phi_{\text{assoc}}\rangle = |\phi_{EP}\rangle$$

plays its role (see for instance [21]). For more details and generalisations (higher order terms in t) we refer to the Appendix.

We note that the linear time dependence at an EP has been noticed in [19] for a non-diagonalisable di-electric tensor, and recently in [17] for asymmetric scattering in optical micro-spirals, and also indirectly in [18] for Rabi oscillations in a microwave cavity.

We mention that these results cannot be obtained easily from a simple Fourier transform of the corresponding Green's function $G(E) = (E - H)^{-1}$ as given in [1]. The reason is due to the fact that (i) the residues blow up owing to the vanishing norm of the eigenfunctions at the EP (actually $G(E)$ has a pole of second order [5]), and (ii) the associate vector does not naturally occur. Of course, the mathematical connection does exist, yet the results in the time domain are much easier obtained by the approach used in the present paper.

A PARTICULAR PHYSICAL CASE

For illustration we use the same parameters as in [1], that is $\omega_1 = 1.55 - 0.007i$, $\omega_2 = 1.1 - 0.007i$, $\epsilon_1 = -0.4 - 0.0006i$, $\epsilon_2 = 0.4 + 0.0005i$ and $\delta = 0.0115i$. For λ we restrict ourselves to the interval [0.53,0.59]; the critical value is $\lambda_c = 0.563$, it is there where a resonance pole comes closest to the real axis. The close proximity of two exceptional points makes the movement of the resonance pole under variation of λ rather swift and dramatic. This is illustrated in Figure 1 where trajectories are drawn in the complex energy plane.

The specific values chosen have no particular significance, they serve to illustrate the principle, that is the effect of a near EP upon the behaviour of resonance poles and thus the time behaviour of the state vectors; any other set that invokes repulsion and coalescence of resonances would serve the same purpose as long as the imaginary parts of the poles are near to the real axis. While we did not specify units for the present illustration, choosing for instance meV for the energies would imply picoseconds as time units in Figures 2 and 3.

Similar in spirit to the procedure in [17] we choose for the initial condition of $\psi(t)$ a specific polarisation
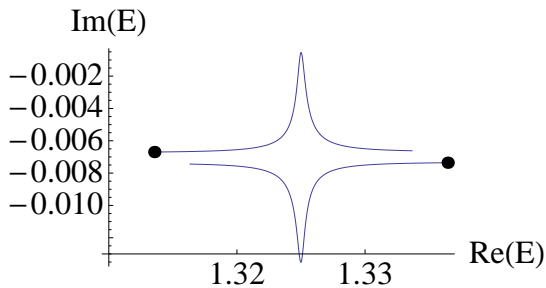
FIG. 1: Energy eigenvalue trajectories when λ sweeps from 0.53 to 0.59. Note that for our choice of parameters the trajectories run in opposite directions, the respective starting points are indicated by a dot.

and consider the two cases $\psi(0) = \{1,0\}^T$ and $\psi(0) = \{0,1\}^T$. In Figure 2 the two components are plotted for the latter case at a value of λ where the two resonances are well separated (the dots in Figure 1). Three main features become obvious: (i) the initial conditions require that the first and second component begin at zero and unity, respectively; (ii) the beat is determined by the frequency difference of the two near resonances while the coupling invokes an amplitude transfer between the two components; (iii) the damping – not to be confused with the beat – is determined by the width (the imaginary part) of the two resonances, $\exp(-t\Gamma)$ gives the envelope of the damped oscillation. Note that for our choice of parameters we find $\Gamma = 0.007$ for the width while the beat frequency $\Delta E = \Re[E_1] - \Re[E_2] = 0.025$ is larger than the width (a few beats can be accommodated under the envelope). Swapping the initial conditions would essentially swap the two components.

A dramatic change occurs when $\psi(t)$ is plotted at the critical point $\lambda_c = 0.563$ being the point where the trajectories peak in Figure 1. Moreover, the change affects the two different initial conditions in a very different and characteristic way. Three important changes are noticed in Figure 3: (i) the beat has disappeared; (ii) for the initial condition $\psi(0) = \{0,1\}^T$ (top row) the leading component is very weakly damped while the other component remains rather small, yet it is also weakly damped; (iii) for the initial condition $\psi(0) = \{1,0\}^T$ (bottom row) the leading component $z_1(t)$ is strongly damped while the
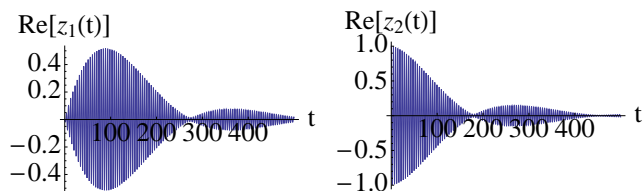

FIG. 2: Time dependence of the two components of the wave function at $\lambda = 0.53$. The corresponding imaginary parts look the same.

other component $z_2(t)$ is essentially like that for the top row (here $z_1(t)$). Again we emphasise that the respective envelopes of $z_2(t)$ (top) and $z_1(t)$ (bottom) are given by the damping related to the widths of the top and bottom peak in Figure 1, the values are $\Gamma_{\text{top}} = 0.0005$ and $\Gamma_{\text{bot}} = 0.013$.

These findings are explained using Figure 1 and (9,10) and (11). At the critical point there is one narrow resonance (top peak in Figure 1) and one broader resonance (bottom peak in Figure 1). As the frequencies (the real parts of the energy) are the same, there is no beat. Now we first turn to $z_2(t)$ of the top row and $z_1(t)$ of the bottom row in Figure 3. As seen from (9) the expression associated with $C_2 = 1$ has two terms: the sum of the exponentials with the two eigenenergies (and the factor $1/2$) and their difference (with the factor δ/D); the two terms are added. Similarly, the corresponding two terms for $z_1(t)$ being associated with $C_1 = 1$, $C_2 = 0$ are subtracted. The conspiring behaviour due to the sum in the one case and the difference in the other becomes evident in (10) (with $C_2 = 1$, $C_1 = 0$) and (11) (with $C_1 = 1$, $C_2 = 0$), respectively. The energies in the exponential are of course different in (9), there is the small and large damping (width). When adding the two terms as for $z_2(t)$, top row of Figure 3, the small damping prevails while subtracting as for $z_1(t)$, bottom row, the large damping is dominant. At the top row $z_1(t)$ is immaterial in comparison with $z_2(t)$, while at the bottom row $z_2(t)$ becomes stronger than $z_1(t)$. We return to this interesting aspect in the last section.

These rather dramatic differences for the time behaviour depending on the initial conditions are expected to be observable as a physical effect; in fact, the polarisation in [17] is just one case in point. The findings discussed in the present paper complement beautifully the results presented in [1]. This is discussed in greater detail in the
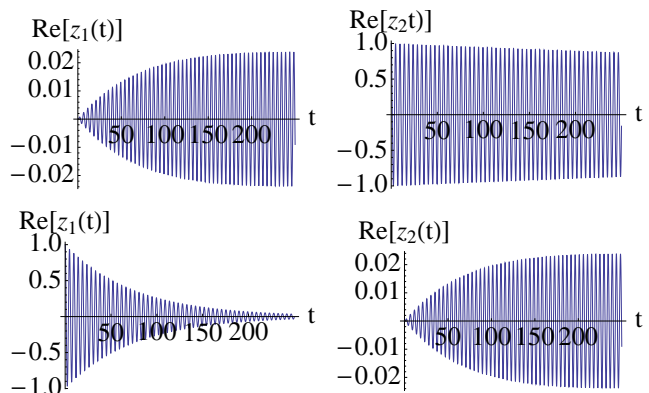

FIG. 3: Time dependence of the two components of the wave function at the critical points $\lambda = 0.563$. The top row is with initial conditions as in Figure 2 while in the second row the initial components are interchanged. Note that the time axis extends only half as far as the one in Figure 2.

following section.

When going beyond the critical point with λ, say at $\lambda = 0.59$, Figure 2 is essentially repeated. The graphs for the imaginary parts of the complex components $z_{1,2}(t)$ look essentially as the ones given.

SUMMARY AND CONCLUSION

In [1] the effect of EPs has been discussed within the same model and parameters as in the present paper, but the emphasis was on resonance scattering, that is a stationary physical situation. Now we focus upon the related time dependent problem, that is the solution of the time dependent Schrödinger equation, which is formally given by

$$|\psi(t)\rangle = \exp(-iHt)|\psi(0)\rangle.$$

For the purpose of the present paper the Hamiltonian is modelled by a 2×2-matrix describing an open system. It depends on a parameter λ and of interest is the behaviour of $|\psi(t)\rangle$ when λ is at an EP or sweeping over a range nearby an EP. Similar to the findings in [1] the variation of λ causes dramatic changes due to the proximity of EPs.

When the resonances are well separated, the time behaviour is damped owing to the widths of the eigenstates, but there is also a beat owing to the difference of the two frequencies. This changes dramatically when a pair of EPs is approached: the beat disappears, and depending on the initial condition the leading component is very weakly or very strongly damped. This is reminiscent of the very sharp resonance peak in the one channel and a broad peak in the other channel in two channel scattering [1]. In addition, while the smaller component remains insignificant for the weakly damped case, it becomes the stronger component for the strongly damped case. In fact, while there the leading component tends quickly to zero due to the larger width, the associated smaller component becomes dominant and is actually weakly damped. This corresponds exactly to the *peak on the broad peak* as detected in [1].

As a general result we noticed that the singular behaviour usually associated with EPs leads to a much milder pattern in the time frame. The 'self-orthogonality' of the eigenstates appears in a less dramatic way: depending on the order of the EP a polynomial in the time variable occurs besides the exponentials; in the simplest case it is just a linear term [17–19].

As an increased activity of experiments using time behaviour in atomic and molecular physics can be expected, the findings of the present paper may be of special relevance.

Appendix

This is a rehash of known facts from linear ordinary differential equations. If the time independent square matrix operator $\mathcal{O}$ is diagonalisable, the evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|\chi(t)\rangle = \mathcal{O}|\chi(t)\rangle$$

with the initial condition $|\chi(0)\rangle$ is solved by

$$|\chi(t)\rangle = \sum_k \exp(E_k t) \frac{\langle \phi_k^l | \chi(0) \rangle | \phi_k^r \rangle}{\langle \phi_k^l | \phi_k^r \rangle}$$

with E_k and $|\phi_k^r\rangle$ and $\langle \phi_k^l|$ forming the right and left hand eigensystem of the operator $\mathcal{O}$. At an EP, when two eigenvalues coalesce, the matrix cannot be diagonalised but has the Jordan decomposition

$$\mathcal{O} = S\,J\,S^{-1}$$

with

$$J = \begin{pmatrix} E_{EP} & 1 & & & \\ 0 & E_{EP} & & 0 & \\ & & E_3 & & \\ & 0 & & \ddots & \\ & & & & E_N \end{pmatrix}$$

where we have listed the two EPs first. Now the solution of

$$\frac{\mathrm{d}}{\mathrm{d}t}|\xi(t)\rangle = J\,|\xi(t)\rangle$$

reads for the initial vector $\{C_1, \ldots, C_N\}^T$

$$|\xi(t)\rangle = \{ \ (C_1 + tC_2)\exp(E_{EP}t), C_2\exp(E_{EP}t), \\ C_3\exp(E_3 t), \ldots, C_N\exp(E_N t)\}^T$$

which can be transformed back into the basis of the original $\mathcal{O}$ using the similarity transformation S. A so-called associate vector related to the eigenvector $|\phi_{EP}\rangle$ by

$$(\mathcal{O} - E_{EP})|\phi_{\text{assoc}}\rangle = |\phi_{EP}\rangle$$

features here in the second column of S. For the special case of Section 2 it can be chosen as in the second column of S which reads

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

This explicit form explains the terms linear in t occurring in (10) and (11).

It is clear how to generalise this when more than two levels coalesce. For k coalescing levels the first component of $|\xi(t)\rangle$ is given by

$$(C_1 + t\,C_2 + t^2/2!\,C_3 + \ldots + t^{k-1}/(k-1)!\,C_k)\exp(E_{EP}t)$$

and accordingly for the following components.

---

[1] W.D. Heiss and R.G. Nazmitdinov Eur.Phys.J. D**58**, 53 (2010).

[2] T. Kato, *Perturbation theory of linear operators* (Springer, Berlin, 1966).

[3] W.D. Heiss, Eur.Phys.J. D**7**, 1 (1999); Phys.Rev. E**61**, 929 (2000); Czech.J.Phys. **54**, 1091 (2004).

[4] U. Günther, I. Rotter, B.F. Samsonov, J.Phys.A: Math.Theor. **40**, 8815 (2007).

[5] E. Hernandez, A. Jaureguit and A. Mondragon, J. Phys. A **33**, 4507 (2000)

[6] E.A. Solov'ev, Sov.Phys.Usp. **32**, 228 (1989).

[7] H. Cartarius, J. Main, G. Wunner, Phys. Rev. A**79**, 053408 (2009).

[8] R. Lefebvre *etal.*, Phys.Rev.Lett. **103**, 123003 (2009).

[9] M.V. Berry, D.H.J. O'Dell, J.Phys.A**31**, 2093 (1998).

[10] J. Okolowicz, M. Ploczajczak, Phys.Rev. C**80**, 034619 (2009).

[11] M. Znojil, Phys.Lett. B**647**, 225 (2007).

[12] W.D. Heiss, F.G. Scholtz, H.B. Geyer, J.Phys.A: Math.Gen. **38**, 1843 (2005).

[13] P. Cejnar, S. Heinze, M. Macek, Phys.Rev.Lett. **99**, 100601 (2007).

[14] C. Dembowski, H.-D. Gräf, H.L. Harney, A. Heine, W.D. Heiss, H. Rehfeld, A. Richter, Phys.Rev.Lett. **86**, 787 (2001).

[15] C. Dembowski, B. Dietz, H.-D. Gräf, H.L. Harney, A. Heine, W.D. Heiss, A. Richter, Phys.Rev. E**69**, 056216 (2004).

[16] S.-B. Lee, J. Yang, S. Moon, S.-Y. Lee, J.-B. Shim, S.W. Kim, J.-H. Lee, K. An, Phys.Rev.Lett. **103**, 134101 (2009).

[17] J. Wiersig, S.W. Kim and M. Hentschel, Phys.Rev. A **78**, 53809 (2008).

[18] B. Dietz *etal.* Phys. Rev. E**75**, 027201 (2007).

[19] M.V. Berry, Current Science **67**, 220 (1994).

[20] Heinrich Schwoerer (Laser Centre, Stellenbosch), private communication

[21] A.A. Mailybaev, O.N. Kirillov, A.P. Seyranian, Phys.Rev. A**72**, 014104 (2005).