

Fingerprints of exceptional points in the survival probability of resonances in atomic spectra

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The unique time signature of the survival probability exactly at the exceptional point parameters is studied here for the hydrogen atom in strong static magnetic and electric fields. We show that indeed the survival probability $S(t) = |\langle \psi(0) | \psi(t) \rangle|^2$ decays exactly as $|1 - at|^2 e^{-\Gamma_{\text{EP}} t / \hbar}$, where Γ_{EP} is associated with the decay rate at the exceptional point and a is a complex constant depending solely on the initial wave packet that populates exclusively the two almost degenerate states of the non-Hermitian Hamiltonian. This may open the possibility for a first experimental detection of exceptional points in a quantum system.

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I. INTRODUCTION

Exceptional points (EPs) [1], i.e., branch point singularities in non-Hermitian physical systems, where two complex eigenvalues degenerate and the corresponding *eigenstates coalesce*, have been shown to exhibit prominent effects not observable in their absence. Most dramatic is the influence of EPs in quantum mechanics, where effects appear which are not possible in the case of Hermitian Hamiltonians with potentials describing bound-state spectra. Although the EPs are single points in an (at least) two-dimensional parameter space, they influence a whole region of parameters and lead to unusual results such as the permutation of eigenstates for a closed adiabatic loop in the parameter space or a special type of geometric phase [2]. Exceptional points have recently been detected in a number of physical applications. Most examples are known for optical systems such as unstable lasers [3], waveguides [4], and optical resonators [5]. In quantum systems the existence of exceptional points has been proven theoretically, e.g., in atomic [6,7] or molecular [8] spectra, in the scattering of particles at potential barriers [9], in atom waves [10,11], and in non-Hermitian Bose-Hubbard models [12,13]. The experimental verification of their physical nature was achieved in microwave cavities [14,15]. Despite this success, an experimental observation in a true quantum system is still lacking. Resonances at an exceptional point exhibit, however, a unique decay behavior [5,13,16–19], and it is the purpose of this paper to demonstrate that this can open the possibility for the first experimental detection of EPs in an atomic quantum system.

The most fundamental quantum objects which contain exceptional points are atoms in static external magnetic and electric fields. As such they are accessible to both experimental and theoretical methods, and thus ideally suited for studying the influence of exceptional points on quantum systems. Indeed, the existence of branch points in the resonance spectra of the hydrogen atom in crossed electric and magnetic fields was found numerically [7,20]. Here the two field strengths

play the role of two controllable parameters necessary to set the system at the exceptional points. In this paper we want to demonstrate that the unique time signature of the survival probability exactly at the exceptional point parameters also appears in a detectable form in spectra of the hydrogen atom.

The paper is organized as follows. In Sec. II we review how in every quantum system exhibiting exceptional points a unique time behavior of the survival probability leads to an unambiguous fingerprint of the branch point singularity. To verify the existence of this signal in a true quantum system we show that it appears for the hydrogen atom in crossed electric and magnetic fields in Sec. III. Conclusions are drawn in Sec. IV.

II. FINGERPRINT OF EXCEPTIONAL POINTS IN THE TIME BEHAVIOR OF THE SURVIVAL PROBABILITY

Let us first explain the motivation of our work. It has been shown theoretically in a two-dimensional model [16], in optical microspirals [5], in a non-Hermitian Bose-Hubbard model [13], and in complex crystals [17,18] as well as experimentally for Rabi oscillations in a microwave cavity [19] that when the spectrum of a non-Hermitian Hamiltonian has an exceptional point then for a broad range of initial conditions the survival probability $S(t) = |\langle \psi(0) | \psi(t) \rangle|^2$ decays exactly as $|1 - at|^2 e^{+2\text{Im}(E_{\text{EP}})t/\hbar}$, where E_{EP} is the complex energy of the resonance state at the EP and a is a complex constant depending solely on the initial wave packet. The resonance decay rate (inverse lifetime) is defined as $\Gamma_{\text{EP}} = -2\text{Im}(E_{\text{EP}}) > 0$. This behavior is in clear contrast to the purely exponential decay far away from an EP, and the special condition is that the initial wave packet should populate *only* the exceptional eigenstate $|\psi_{\text{EP}}\rangle$ and its complementary state $|\chi\rangle$ as obtained from the Jordan chain formalism, such that $|\psi_{\text{EP}}\rangle\langle\chi| + |\chi\rangle\langle\psi_{\text{EP}}| = \hat{1}$ (see a detailed explanation in Sec. 9.2 of Ref. [21], where the closure relations for a non-Hermitian Hamiltonian with an incomplete spectrum are discussed in detail). In this paper we will demonstrate this behavior of the survival probability for a quantum mechanical system.

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Let us give here a simple explanation for this unusual situation. The EP is associated with a situation where $\hat{H}(\lambda)|\psi_j\rangle = E_j|\psi_j\rangle$, such that for $\lambda \rightarrow \lambda_{\text{EP}}$ two eigenvalues are degenerate, $E_j - E_{j'} \rightarrow 0$ (i.e., upon coalescence $E_j = E_{j'} \equiv E_{\text{EP}}$), and also the corresponding eigenstates coalesce $\psi_j \rightarrow \psi_{j'}$ (up to a phase factor i [21], i.e., upon coalescence $\psi_j = i\psi_{j'} \equiv \psi_{\text{EP}}$) such that

$$\hat{M}|\psi_{\text{EP}}\rangle = 0, \quad (1)$$

where

$$\hat{M} = \hat{H} - E_{\text{EP}} \quad (2)$$

and $\Gamma_{\text{EP}} = -2\text{Im}(E_{\text{EP}})$ is the decay rate of the system.

Let us take a basis set consisting of ψ_{EP} and its complementary state χ for the initial wave packet. In this basis the 2×2 matrix representation of \hat{M} is a matrix \mathbf{M} for which $\mathbf{M}^2 = 0$. Therefore

$$\begin{aligned} U(t \leftarrow 0) &= e^{-i\mathbf{H}t/\hbar} = e^{-iE_{\text{EP}}t/\hbar} e^{-i\mathbf{M}t/\hbar} \\ &= e^{-iE_{\text{EP}}t/\hbar} \sum_n \frac{(-i\mathbf{M}t/\hbar)^n}{n!} \\ &= e^{-iE_{\text{EP}}t/\hbar} (\mathbf{I}_{2 \times 2} - i\mathbf{M}t/\hbar). \end{aligned} \quad (3)$$

Consequently, for any initial state $\psi(t=0)$ which is a linear combination of ψ_{EP} and its complementary state χ

$$\begin{aligned} \langle \psi(t=0) | U(t \leftarrow 0) | \psi(t=0) \rangle \\ = e^{-iE_{\text{EP}}t/\hbar} [1 - it \langle \psi(t=0) | \mathbf{M} | \psi(t=0) \rangle / \hbar] \end{aligned} \quad (4)$$

and for real values of $\langle \psi(t=0) | \mathbf{M} | \psi(t=0) \rangle$ the survival probability is given by

$$\begin{aligned} S(t) &= |\langle \psi(t=0) | U(t \leftarrow 0) | \psi(t=0) \rangle|^2 \\ &= \{1 + [\langle \psi(t=0) | \mathbf{M} | \psi(t=0) \rangle / \hbar]^2 t^2\} e^{+2\text{Im}(E_{\text{EP}})t/\hbar}. \end{aligned} \quad (5)$$

For complex values of $\langle \psi(t=0) | \mathbf{M} | \psi(t=0) \rangle$ an additional term linear in t is added. Certainly, the quadratic dependence for short times is not surprising. What is important here is that there are no terms of order higher than t^2 so that the time dependence remains t^2 for all times. This provides a unique fingerprint proving unambiguously the presence of an exceptional point, since the power series expansion of Eq. (3) stopping after the linear term requires the presence of an EP. The effect even remains in a larger vicinity around the branch point singularity. Observations which are similar to exceptional points but not connected to true branch points such as narrow avoided crossings for Wannier-Stark resonances [22] are not sufficient.

III. NONEXPONENTIAL DECAY OF RESONANCES IN SPECTRA OF THE HYDROGEN ATOM

In our study the resonances are calculated numerically exactly by the diagonalization of a matrix representation of the Hamiltonian. Without relativistic corrections and finite nuclear mass effects [23], the Hamiltonian reads in atomic units

$$H = \frac{1}{2} \mathbf{p}^2 - \frac{1}{r} + \frac{1}{2} \gamma L_z + \frac{1}{8} \gamma^2 (x^2 + y^2) + fx, \quad (6)$$

where L_z is the z component of the angular momentum. The strengths of the electric and magnetic fields are labeled f and

γ , respectively. We exploit the fact that the parity with respect to the ($z=0$) plane is a constant of motion and include in all our calculations only resonances with even z parity.

To uncover the decaying unbound resonance states we use the complex rotation method [21,24,25], for which the coordinates of the system \mathbf{r} are replaced with the complex rotated ones $\mathbf{r}e^{i\vartheta}$. For the application of the complex rotation method to hydrogen spectra, see [26]. This procedure renders the resonance wave functions square integrable so that they are automatically included in the spectrum as new discrete eigenstates with complex eigenvalues in the matrix representation. The real parts of the complex energies represent their energies and the imaginary parts their widths (lifetimes). After introduction of complex dilated semiparabolic coordinates [27], the Schrödinger equation of the Hamiltonian (6) assumes in a basis representation the form of a generalized eigenvalue problem,

$$A(\gamma, f)\Psi = 2|b|^4 E \mathbf{B} \Psi, \quad (7)$$

with a complex symmetric matrix $A(\gamma, f)$ and a real symmetric matrix \mathbf{B} . In this equation b is the complex dilation parameter and E the complex resonance energy. The eigenstates can be normalized such that $(\Psi_i | \mathbf{B} | \Psi_j) = \delta_{ij}$, where the parentheses indicate an inner product in which complex parts originating exclusively from the complex dilation parameter b are not conjugated, which is the appropriate inner product for complex scaled wave functions (c-product; cf. Refs. [21,25]). Note that this normalization does not hold at an exceptional point where each of the two states is orthogonal to itself [21].

We first demonstrate that the decay signal of the probability density according to Eq. (4),

$$S_m(t) = \exp[2\text{Im}(E_{\text{EP}})t] |1 - i(\Psi_0 | \mathbf{M} | \Psi_0)t|^2, \quad (8a)$$

can be found in the quantum spectrum of the hydrogen atom in a large region around the exceptional point, where in our case the matrix \mathbf{M} of Eq. (2) is given by

$$\mathbf{M} = A(\gamma, f)/(2|b|^4) - E_{\text{EP}} \mathbf{B}. \quad (8b)$$

The subscript ‘‘m’’ of S_m in Eq. (8a) is given in order to emphasize the fact that the survival probability is calculated here using the matrix representation of the Hamiltonian given by Eq. (8b). This is to distinguish it from the direct evaluation of the survival probability as discussed later [Eq. (13)]. For this purpose we calculate resonance spectra for several small distances δ from the exceptional point at $(f_{\text{EP}}, \gamma_{\text{EP}})$ in the space of the two field strengths, i.e., we use

$$f = f_{\text{EP}}(1 - \delta), \quad \gamma = \gamma_{\text{EP}}(1 - \delta). \quad (9)$$

For small δ the two eigenstates Ψ_1 and Ψ_2 belonging to the branch point singularity can be identified clearly. Note, however, that due to roundoff errors in the numerical calculations δ never strictly attains the value 0 and always $\delta \neq 0$. As we will show in this paper, even when $\delta \neq 0$, i.e., when we have two *almost* degenerate states and the spectrum is *complete*, the fingerprint of the EPs (strictly obtained only exactly at the coalescence of two eigenstates) in the survival probability is still pronounced.

It is well known for exceptional points that Ψ_1 and Ψ_2 converge to the single independent eigenstate with the phase relation

$$\Psi_{\text{EP}} = \Psi_1 = i\Psi_2 \quad (10)$$

for $\delta \rightarrow 0$ [21]. A complete basis in the corresponding two-dimensional subspace is spanned by Ψ_{EP} and the associated vector Ψ_a ,

$$[A(\gamma, f) - 2|b|^4 E_{\text{EP}} \mathbf{B}] \Psi_a = \Psi_{\text{EP}}, \quad (11)$$

where Ψ_a is essential for a decay signal of the form (8a) [16]. Despite the convergence of Ψ_1 and Ψ_2 to the same state it is possible to extract an adequate superposition of Ψ_{EP} and Ψ_a , viz.,

$$\Psi_0 = \sqrt{(1 + 1/\sqrt{\delta})/2} \Psi_1 + \sqrt{(1 - 1/\sqrt{\delta})/2} \Psi_2. \quad (12)$$

As we get closer to the EP when $\delta \rightarrow 0$ the amplitudes of Ψ_1 and Ψ_2 approach infinitely large values. However, the initial wave packet Ψ_0 remains c-normalized. See Ref. [21] for details about use of the complex normalization rather than the conventional scalar product for calculating the norm of a vector state.

We choose the exceptional point labeled 8 in Table I of Ref. [20] at the field strengths $f = 0.0002177$ and $\gamma = 0.004604$, and with the complex energy $E_{\text{EP}} = -0.022135 - 0.00006878i$ (all values in atomic units). The survival probability for the superposition (12) is plotted in Fig. 1 for an offset $\delta = 10^{-5}$. At an exceptional point we expect a decay of the survival probability in the form (8a). The corresponding numerical result is shown with the solid red line in Fig. 1, where we found $(\Psi_0 | M | \Psi_0) = (3.83 - 4.58i) \times 10^{-4}$. Since we use here the c-product [21,25] rather than the regular scalar

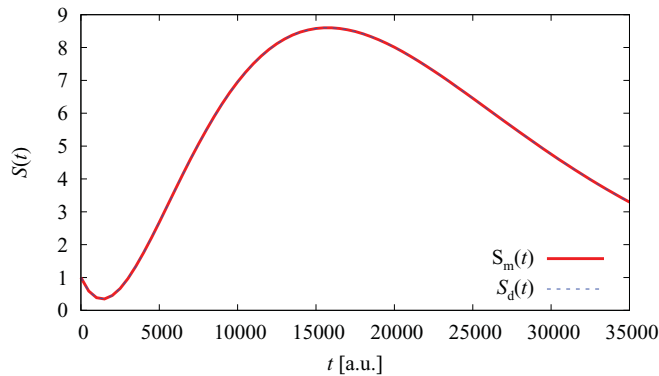


FIG. 1. (Color online) Survival probability for the resonances at the exceptional point labeled 8 in Ref. [20] with an offset of $\delta = 10^{-5}$. Shown are the direct evaluation $S_d(t)$ according to Eq. (13) and the expected form $S_m(t)$ of Eq. (8a) including a linear term in t in addition to the exponential decay. Note that on the scale of the figure the survival probabilities calculated by the two methods are not distinguishable. Since we use here the c-product rather than the regular scalar product, the survival probability can assume values larger than 1. This nonphysical behavior results from the way we normalize Ψ_0 [see Eq. (12)]. As we will show later this problem disappears when the initial wave packet is prepared by using a laser excitation of the field-free ground state. On the c-product, read Refs. [21,25].

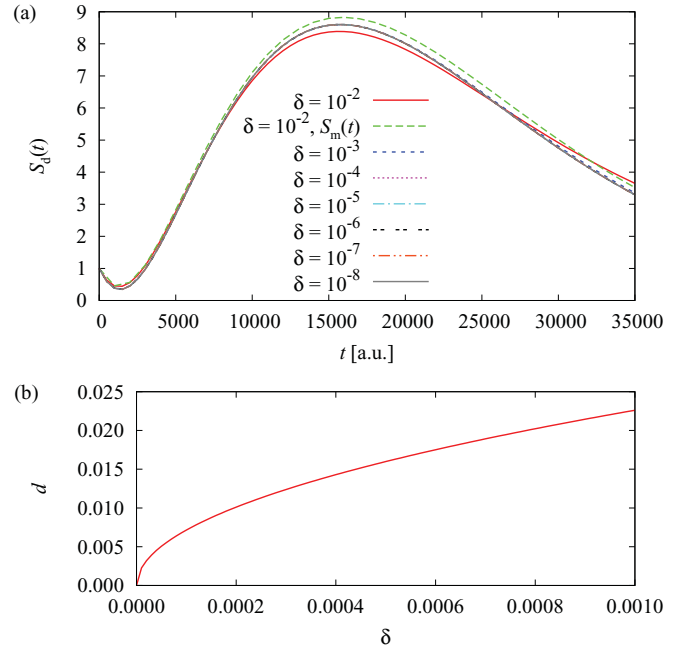


FIG. 2. (Color online) (a) Survival probability $S_d(t)$ for the same exceptional point as in Fig. 1 but for several different offsets $\delta = 10^{-8}, \dots, 10^{-2}$. Small deviations appear only for the largest $\delta = 10^{-2}$. In this case also a small difference from the shape $S_m(t)$ at an exceptional point becomes observable. (b) The modulus $d = \langle \Psi_1 + i\Psi_2 | \Psi_1 + i\Psi_2 \rangle$ vanishes at the exceptional point as is expected due to the phase relation (10).

product, the survival probability can assume values larger than 1 for the mathematical choice given in Eq. (12). Additionally, we calculate the survival probability directly without any assumption about its shape close to an exceptional point, i.e., we evaluate

$$S_d(t) = \left| \sum_i (\Psi_0 | \mathbf{B} | \Psi_i) (\Psi_i | \mathbf{B} | \Psi_0) \exp(-i E_i t) \right|^2, \quad (13)$$

where we use 100 eigenvectors of the matrix diagonalization in the energy vicinity of the EP for the basis states Ψ_i . The blue dashed line in Fig. 1 shows the results of the latter method. As can be seen clearly, the two methods agree very well, which proves that the description of the decay with the linear term in (8a) is correct. Obviously the polynomial contribution influences the decay significantly, i.e., the unique time behavior of the resonances at an exceptional point is a relevant effect in matter waves and can be found unambiguously for atomic resonances.

The typical time signal of an exceptional point is even present at larger distances δ . In Fig. 2(a) we plot the direct evaluation (13) for the same exceptional point as in Fig. 1 but for several different offsets $\delta = 10^{-8}, \dots, 10^{-2}$. For all of these distances the two vectors belonging to the branch point are well defined. Almost all calculations provide exactly the same results. Only for $\delta = 10^{-2}$ do we observe a slight difference from the other calculations. At this distance also the validity of the matrix representation (8a) including only the two components associated with the exceptional point breaks down; however, the differences are still small. The

corresponding line $S_m(t)$ is included in the figure. For all other values of δ shown, we checked that the results of the two methods agree completely, which demonstrates that the structure of Eq. (3), which is only fulfilled in the presence of an exceptional point, survives in a larger vicinity around the branch point. The signal keeps its unique structure. To verify that we obtain the correct vectors Ψ_1 and Ψ_2 in all calculations, we plot the modulus $d = \langle \Psi_1 + i\Psi_2 | \Psi_1 + i\Psi_2 \rangle$ in Fig. 2(b). According to the phase relation (10), d must vanish in the limit $\delta \rightarrow 0$. Exactly this behavior is found.

So far we have demonstrated that it is possible to find an adequate superposition of the two eigenvectors; however, we want to show furthermore that this signal can be excited in a realistic case. Is it possible to occupy such a superposition in an experimental situation? To investigate this question we assume a hydrogen atom in external fields, where the electron is in the orbital $2p$, $m = 0$, for which any perturbation due to the fields we use can be ignored. The eigenstates at the exceptional point are excited with a laser polarized linearly along the direction of the static magnetic field. We use a Gaussian pulse shape of the form

$$E(\omega) \sim \exp[-\sigma(\omega - \omega_0)^2], \quad \omega_0 = \text{Re}(E_{\text{EP}}) - E_I, \quad (14)$$

where E_I is the energy at the initial state Ψ_I ($2p$, $m = 0$). The width was chosen to be $\sigma = 1000/\omega_0$. Then the occupation amplitude for a transition to eigenstate Ψ_i of the Hamiltonian is

$$A_i = \int d\omega E(\omega) \frac{\langle \Psi_I | D | \Psi_i \rangle}{E_I - E_{\text{EP}} + \hbar\omega} \quad (15)$$

with the dipole operator D for the present choice of the light pulse.

Figure 3(a) shows the occupation probability $|A_i|^2$ versus the real part of the energy for the states in the vicinity of the branch point. One can see that the two states connected with the branch point (marked with filled blue circles) have an occupation probability almost three orders of magnitude larger than all other states. This does not tell us, however, whether or not an adequate superposition of the two dominating states similar to the mathematical case in Eq. (12) can be achieved. Thus, we construct the normalized state

$$\Psi_F = \frac{\tilde{\Psi}_F}{\sqrt{\langle \tilde{\Psi}_F | \mathbf{B} | \tilde{\Psi}_F \rangle}}, \quad \tilde{\Psi}_F = \sum_i A_i \Psi_i \quad (16)$$

occupied by the laser with the states shown in Fig. 3(a). The survival probability is calculated according to Eq. (13) with Ψ_F instead of Ψ_0 . Figure 3(b) shows the results. The small oscillations are due to the weaker excitations of the neighboring states. They disappear for a pulse denser in frequency space. The dominating signal is still formed by the two states associated with the exceptional point. The linear part in the time behavior (8a) is weaker than in the mathematical case Ψ_0 of Eq. (12); however, it is present and is expressed in the nonexponential decay. After the division by the exponential part the polynomial contribution of the physical (observable) survival probability calculated for the initial wave packet Ψ_F [see Eq. (16)] is given by

$$S_{\text{d,p}}(t) = S_{\text{d}}(t) / \exp[2\text{Im}(E_{\text{EP}})t]. \quad (17)$$

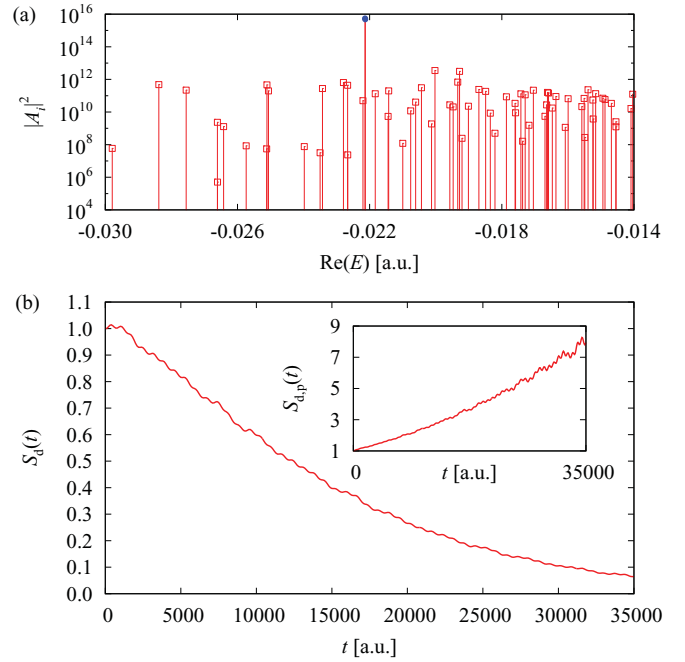


FIG. 3. (Color online) (a) Occupation probabilities $|A_i|^2$ in arbitrary units for resonances in the energy vicinity of the exceptional point. The two resonances connected with the exceptional point are marked with blue (filled) circles. On the scale of our plot the two almost degenerate states are not distinguishable. (b) Survival probability for the excited state Ψ_F , which is prepared by using a laser to excite the field-free ground state [see Eq. (16)]. The division by the exponential part in the inset demonstrates the presence of the polynomial contribution. The behavior of the survival probability as presented here is exactly as in the analytical expression given in Eq. (8a).

To demonstrate that the origin of this signal is in fact the structure (8a) originating from an exceptional point, we calculated the matrix element $\langle \Psi_F | M | \Psi_F \rangle = (0.226 + 5.25i) \times 10^{-5}$. The line $|1 - i\langle \Psi_0 | M | \Psi_0 \rangle t|^2$ is not distinguishable from the full numerical result presented in Fig. 3(b).

IV. CONCLUSION

We proved in this paper that any quantum system exhibiting exceptional points shows a time evolution of the form (3) for two resonances exactly at the EP, i.e., the decay includes a quadratic term as in Eq. (5) which is distinct from the typical exponential decay apart from branch point singularities. Here it is important to note that this effect is not only observable exactly at the parameters of the EP but can rather be seen in a large vicinity. In our study we found it still for a relative offset of the parameters of $\delta = 10^{-2}$.

We were furthermore able to demonstrate that it is possible to excite an adequate superposition of the eigenvector at an exceptional point and its associate counterpart in a realistic physical situation such that the unique time signal becomes observable in atomic spectra. The quadratic term significantly influences the survival probability we found for the hydrogen atom in crossed electric and magnetic fields. It is an effect that leaves clear signatures in the decay of resonances in quantum systems and obviously opens an additional possibility

of detecting an unambiguous fingerprint of an exceptional point accessible with experimental methods. It might thus facilitate the first experimental detection of exceptional points in a true quantum system.

In this paper the time evolution of the resonances excited with the laser pulse (14) is evaluated with the survival probability calculated from the spectrum via the c-product [21,28]. Both its modulus and phase have experimental consequences [29]. In the realistic physical situation shown in Fig. 3 the survival probability describes the decay of a resonance state in time. Thus one has to measure the decaying occupation of such a state. This can presumably be detected with a second laser as already indicated [16]. Furthermore, the extraction of the time signal from the spectrum is possible and has already been used for microwave cavities [19] via a Fourier transform. In this context we should mention that

the ultrastrong magnetic and electric fields we have used in our calculations are due to our computational limitations to exceptional points associated with low-lying resonance positions. However, the phenomenon discussed here appears for highly excited resonances as well. In such cases much weaker and feasible external fields are required to observe the unique survival probability of a wave packet, which initially populates mainly the two almost degenerate states associated with the exceptional point.

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