Rydberg systems in parallel electric and magnetic fields: an improved method for finding exceptional points

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Abstract

Exceptional points are special parameter points in spectra of open quantum systems, at which resonance energies become degenerate and the associated eigenvectors coalesce. Typical examples are Rydberg systems in parallel electric and magnetic fields, for which we solve the Schrödinger equation in a complete basis to calculate the resonances and eigenvectors. Starting from an avoided crossing within the parameter-dependent spectra and using a two-dimensional matrix model, we develop an iterative algorithm to calculate the field strengths and resonance energies of exceptional points and to verify their basic properties. Additionally, we are able to visualise the wave functions of the degenerate states. We report the existence of various exceptional points. For the hydrogen atom these points are in an experimentally inaccessible regime of field strengths. However, excitons in cuprous oxide in parallel electric and magnetic fields, i.e., the corresponding hydrogen analogue in a solid state body, provide a suitable system, where the high-field regime can be reached at much smaller external fields and for which we propose an experiment to detect exceptional points.

Keywords: exceptional points, hydrogen, exciton, parallel fields

(Some figures may appear in colour only in the online journal)

1. Introduction

Rydberg systems in external fields are important examples of quantum systems which can be accessed theoretically via numerical calculations as well as experimentally in various cases (see [1] and references therein). A feature, found numerically, of the open quantum system of a hydrogen atom in crossed electric and magnetic fields is the occurrence of exceptional points (EPs) within the high-field regime [2]. At these special points in the two-dimensional parameter space, spanned by the strengths of the external magnetic and electric field, not only two resonances become degenerate, but also the two corresponding eigenvectors coalesce [3]. Encircling an EP in parameter space leads to a typical exchange behaviour of the corresponding resonances within the complex energy plane [4]. Here, isolated parameter values on a closed loop with small distances in-between are sufficient to observe the exchange behaviour of the eigenvalues (see, e.g., [5]). As shown in [2] the complex eigenvalues can be extracted from the resonance spectra via the harmonic inversion method. Thus an adiabatic propagation of a wave packet (as, e.g., in [6]) is not required. The continuous connection of the eigenvalues in the complex energy plane leads to a clear and unambiguous proof of an EP. Theoretically, the occurrence of EPs has been shown for, e.g., atomic spectra [2, 7–9] and molecular spectra [10], optical waveguides [11] or resonators [12, 13], and they have been found experimentally, e.g., in microwave cavities [5, 14, 15], electronic circuits [16], metamaterials [17], and exciton-polariton resonances [18]. Exceptional points in open quantum systems can be used to transfer population between the related resonances as has been done, e.g., for vibrational modes of the H$_2^+$ ion and the Na$_2$ molecule [19, 20]. In addition, a laser-controlled rotational cooling of Na$_2$ could be realised based on exceptional
points [21]. In a completely different application, EPs have shown to be extremely important for the enhancement of the sensitivity of optical detectors [13, 22]. EPs may also be used to generate Majorana bound states in superconductors [23].

An experimental validation of the predicted EPs for the hydrogen atom seems currently out of reach because the strength of the external magnetic field needed to access the high-field regime is in the order of several ten to hundreds of Tesla [2], which yet cannot be realised experimentally. On the other hand, due to computational limits, precise numerical calculations for the hydrogen atom are only possible at high fields, which are strong enough to lead to the coalescence of levels at low energies. The ability to search for EPs numerically at higher levels and therefore at lower fields within the spectrum of the hydrogen atom is limited by the increasing number of states to be taken into account. This short-coming may be overcome with the help of recent high resolution absorption experiments with Rydberg excitons in cuprous oxide (Cu$_2$O), which exhibit a hydrogen-like spectrum up to a principal quantum number of $n = 25$ [24, 26]. Here, the common description of excitons similar to a hydrogen atom with a Coulomb interaction between a negatively charged electron and a positively charged hole (see, e.g., [27]) seems to be appropriate. In Cu$_2$O the strengths of the external fields to enter the high-field regime are much smaller compared to the hydrogen atom [28]. Hence, it provides a system that is appropriate to check theoretical predictions experimentally.

In this paper we will demonstrate the occurrence of EPs for Rydberg systems in parallel electric and magnetic fields. We verify several EPs by the typical exchange behaviour of the associated eigenvectors [4], and then try to locate the precise position of these EPs within the parameter space spanned by the strengths of the external magnetic and electric field. Using the recently proposed three-point method of Uzdin and Lefebvre [29] we are in principle able to locate these positions, however, with a huge amount of computational effort. Therefore, we develop a new and much less expensive method, the octagon method (OM), which is based on a two-dimensional matrix model to describe the vicinity of the two states forming an EP. Using the OM, we are able to calculate the precise position of a variety of EPs within the cylindrically symmetric system of a Rydberg atom in parallel electric and magnetic fields. Additionally, the OM allows us to simulate the exchange behaviour of the two associated resonances and their paths in the complex energy plane while encircling an EP in parameter space without further time-consuming quantum-mechanical calculations. For Rydberg excitons in Cu$_2$O these EPs are located in an experimentally accessible regime of the external field strengths. Therefore we propose an experiment to verify our theoretical predictions by measurements of photoabsorption spectra in cuprous oxide.

A second purpose of this paper is to visualise the two states associated with an EP. At an EP the two probability distributions of the (numerically) degenerate states do not coincide exactly as a result of limited computational accuracy. They differ by various sets of structured lines. These lines show the same exchange behaviour when encircling the EP in parameter space as has already been demonstrated experimentally, e.g., for microwave cavities in [5]. By averaging the eigenvectors of the associated states we compute the probability distribution of the degenerate states directly at the EP.

The paper is organised as follows: in section 2 we present the modelling of Rydberg systems in parallel electric and magnetic fields and discuss the similarities and differences between hydrogen and cuprous oxide. In subsection 2.1 follows the theory for the computation of eigenstates. In subsection 2.2 we use a two-dimensional matrix model to develop the OM as an iterative algorithm to find the exact position of an EP in the parameter space as well as its precise complex resonance energy. Section 2.3 deals with the question how the points of convergence of this new method can be verified as EPs without unnecessary time-consuming calculations. In section 3 all results are presented. The EPs found are listed and discussed, and we also visualise the associated states directly at the EP.

2. Methods and theoretical background

The Hamiltonian of the hydrogen atom in parallel electric ($F$) and magnetic ($B$) fields, which are both orientated along the $z$-axis, reads

$$H_{\text{hyd}} = \frac{\mathbf{p}^2}{2m_0} - e^2 - \frac{1}{4\pi\varepsilon_0} \frac{1}{r} + \frac{eB}{2m_0} L_z + \frac{e^2 B^2}{8\mu_0} (x^2 + y^2) + e F z,$$

(1)

where $e$ denotes the elementary charge, $\mathbf{p}$ the relative momentum, and $r = \sqrt{x^2 + y^2 + z^2}$ is the distance between the electron with mass $m_0$ in free space and the proton with approximately infinite mass. The vacuum permittivity is denoted by $\varepsilon_0$, and $L_z$ is the $z$-component of the angular momentum operator.

To set up a Hamiltonian similar to equation (1) for a Rydberg exciton in Cu$_2$O we use the simple band model [27]. The external fields are included via minimal substitution. We introduce relative and centre-of-mass coordinates and set the pseudomomentum of the centre of mass to zero. The resulting Hamiltonian for a Rydberg exciton in Cu$_2$O reads [30]

$$H_{\text{ex}} = \frac{\mathbf{p}^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 \varepsilon} \frac{1}{r} + \frac{eB}{2\mu} \frac{m_h - m_e}{m_h + m_e} L_z + \frac{e^2 B^2}{8\mu} (x^2 + y^2) + e F z,$$

(2)

with the effective masses $m_e = 0.99 m_0$ for the electron, $m_h = 0.62 m_0$ for the hole, and $\mu = 0.38 m_0$ being the reduced mass [31]. Note that in equation (2) we have not included a band gap energy. Therefore, the energies need to be corrected by an offset of $E_{\text{gap}} = 2.17208 \text{ eV}$ [24].

For reasons of symmetry due to the parallel fields, the angular momentum is a good quantum number\(^1\); so the angular momentum operator $L_z$ can be replaced by its quantum number $m$. Hence, the corresponding paramagnetic

\(^1\) For Cu$_2$O this is also true in the simple band model, since the cubic group is a group of very high symmetry [27, 22].
term \( H_0 \) (the third term in equation (2)) describes a \( B \)-dependent shift of the zero point energy. For this reason we can neglect this term in the following and treat only the Hamiltonian \( H' = H - H_0 \). To reduce the two equations (1) and (2) to the same form we introduce appropriate units with material dependent constants \( B_0 \) and \( F_0 \), where \( \gamma = B/B_0 \) is the reduced magnetic flux density and \( f = F/F_0 \) the reduced strength of the electric field (see appendix A). Consequently, the Hamiltonian of relative motion for a hydrogen-like system in parallel electric and magnetic fields reads

\[
H' = \frac{1}{2} p^2 - \frac{1}{r} + \frac{1}{8} \gamma^2 (x^2 + y^2) + f z, \tag{3}
\]

Hence, equation (3) becomes independent of the material parameters of the system (atomic or solid state). The respective properties are absorbed in the constants \( B_0 \) and \( F_0 \). For the hydrogen atom holds \( B_0 = 2.350 \times 10^3 \) and \( F_0 = 5.142 \times 10^3 \) for \( \text{Cu}_2\text{O} \) we obtain \( B_0 = 603.4 \) and \( F_0 = 1.760 \times 10^8 \) (see appendix A).

### 2.1. Computation of eigenstates

Due to the electric fields and the complex scaling we obtain resonances as eigenstates of the non-Hermitian Hamiltonian (3). In contrast to bound states, which have a real energy and infinite lifetime, the energies of the decaying resonance states become complex, whereupon the imaginary part describes the width of the resonance or its inverse lifetime [33]. Resonances can be introduced by non-Hermitian operators using the complex rotation of the real semiparabolic Hamiltonian of relative motion for a hydrogen-like system [34, 33]. The Hamiltonian for parallel electric and magnetic fields we make use of the fact that level repulsion is induced a complex rotation of the real semiparabolic coordinates \( \mu, \nu \). The purpose of this article is to verify the existence of EPs for Rydberg systems in parallel external fields and to locate their precise position in the parameter space spanned by the electric field strength \( f \) and the magnetic field \( \gamma \). Here \( E' \) is the energy of the respective quantum state and corresponds to the Hamiltonian \( H' \) in equation (3). The Hamiltonian \( H_0 = H' + H_r \) in equation (5) is the sum of two two-dimensional harmonic oscillators \( H_r \) with \( \rho \in \{ \mu, \nu \} \) to be taken as radial coordinate,

\[
H_\rho = \left( -\frac{1}{2} \Delta_\rho + \frac{1}{2} \rho^2 \right), \quad \Delta_\rho = \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{m^2}{\rho^2}, \tag{6}
\]

with \( m \) being the magnetic quantum number. Hence, for the matrix representation of equation (5) the eigenstates \( |n_\rho, m\rangle \) of the two-dimensional harmonic oscillator represent an appropriate basis [37]. Since the angle \( \varphi \) in \( H_r \) and \( H_x \) is the same, just one fixed angular quantum number \( m \) is needed to construct the basis

\[
|n_{\mu}, n_{\nu}, m\rangle = |n_{\mu}, m\rangle \otimes |n_{\nu}, m\rangle \tag{7}
\]

of the total system (we use \( m = 0 \) in the following calculations, which yields \( H = H' \) and \( E = E' \)). The relations needed to calculate the matrix representation of equation (5) within the basis (7) can be found in [38, 39]. Its diagonalization is done using the ARPACK package [40], where we consider only states up to a maximum quantum number of \( n_{\text{max}} = n_\mu + n_\nu \). The value \( n_{\text{max}} = 90 \) has turned out to be sufficient in the following calculations. Convergence is assured by choosing a proper value for the parameter \( b \) of the dilated semiparabolic coordinates [41]. The position space representation of the basis (7) is given by (see, e.g., [39] for a derivation)

\[
\Psi_{n_{\mu}, n_{\nu}, m}(\mu, \nu, \varphi) = \sum_{n_{\mu}, n_{\nu}} \frac{n_{\mu}! n_{\nu}!}{(n_{\mu} + |m|)! (n_{\nu} + |m|)!} \times \frac{1}{\sqrt{2\pi}} f_{n_{\mu}, m}(\mu) f_{n_{\nu}, m}(\nu) e^{im\varphi},
\]

\[
f_{n_{\rho}, m}(\rho) = e^{\frac{\rho^2}{2}} \rho^{|m|} L^{|m|}_{\rho}(\rho^2) \quad \text{for} \quad \rho \in \{ \mu, \nu \}, \tag{8}
\]

with the generalised Laguerre polynomials \( L^{|m|}_{\rho}(\rho) \). Note that the correct inner product for the wave functions of the non-Hermitian Hamiltonian (5) obtained with the complex scaling approach is achieved by complex conjugating only the intrinsically complex parts \( \exp(i \varphi) \rightarrow \exp(-i \varphi) \) and not that originating from the complex parameter \( b \) [33].

We use this complex conjugation throughout this article.

In dilated semiparabolic coordinates the spatial wave functions of a state with energy \( E_i \) read

\[
\Psi_i(\mu, \nu, \varphi) = \sum_{\mu, \nu} c_{i, n_{\mu}, n_{\nu}} \Psi_{n_{\mu}, n_{\nu}, m}(\mu, \nu, \varphi), \tag{9a}
\]

\[
\Psi^*_i(\mu, \nu, \varphi) = \sum_{\mu, \nu} c_{i, n_{\mu}, n_{\nu}}^* \Psi_{n_{\mu}, n_{\nu}, m}(\mu, \nu, \varphi), \tag{9b}
\]

with the expansion coefficients \( c_{i, n_{\mu}, n_{\nu}} \) of the associated eigenvector obtained by the matrix diagonalization of equation (5).

### 2.2. Octagon method for the exact localisation of EPs

The purpose of this article is to verify the existence of EPs for Rydberg systems in parallel external fields and to locate their precise position in the parameter space spanned by the strength \( f \) of the electric field and \( \gamma \) of the magnetic field. A recently proposed iterative algorithm to calculate the exact position of an EP in parallel space is the three-point method of Uzün and Lefebvre [29]. It converges if the initial parameters are chosen close enough to the actual position of the EP. To find initial parameters for an EP in parallel electric and magnetic fields we make use of the fact that level repulsion is associated with the occurrence of EPs [4]. Therefore, the
parameters of an avoided crossing within the energy spectrum provide a good starting point to find an EP. 

By applying the three-point method to the system of an exciton in parallel electric and magnetic fields it turns out that the initial parameters of an avoided crossing are generally not close enough to the actual position of an EP to achieve a convergent behaviour; so further highly expensive numerical calculations are needed [39]. In this regard, we develop an improved method, which is able to converge from the initial parameters of an avoided crossing to the precise position of an EP. To this aim, the basic properties of an EP have to be taken into account.

At an EP not only the two resonances become degenerate, but also the two corresponding eigenvectors coalesce [3]. If an EP is fully encircled in parameter space, its two related resonances exchange their position in the complex energy plane [4]. In the local vicinity around the EP the two related states can be described using a two-dimensional matrix $M$ (see, e.g., [4]). Any coupling to other states is not taken into account here. We assume the elements $M_{ij}$ of $M$ with $k, l \in \{1, 2\}$ to be linear expansions in the strengths $\gamma$ and $f$ of the external fields to describe their influence on the states in the vicinity of a centre-point $(\gamma_0, f_0)$ [42]

$$M_{ij} = a_{ij}^{(0)} + a_{ij}^{(1)} (\gamma - \gamma_0) + a_{ij}^{(2)} (f - f_0).$$

The eigenvalues $E_i$ with $i \in \{1, 2\}$ of $M$ then fulfil

$$\kappa \equiv E_1 + E_2 = \text{tr}(M) = A + B (\gamma - \gamma_0) + C (f - f_0),$$

$$\eta \equiv (E_1 - E_2)^2 = \text{tr}^2(M) - 4 \det(M) = D + E (\gamma - \gamma_0) + F (f - f_0) + G (\gamma - \gamma_0)^2 + H (f - f_0),$$

with complex coefficients $A$ to $I$. In contrast to the three-point method of Uzdin and Lefebvre [29] our approach includes additional quadratic terms in equation (11b). For the Rydberg system in parallel electric and magnetic fields the three-point method turned out to be very sensitive to the initial conditions. To obtain convergence, one has to start very close to $(\gamma_{EP}, f_{EP})$ and huge numerical effort is necessary to get that close [39]. According to [29], EPs appear in the vicinity of an avoided crossing of two states; so it would be useful to have a method that converges when using the rough initial parameters of such an avoided crossing. The inclusion of the quadratic terms in equation (11b) leads to the OM, which can be visualised by means of figure 1. To get simple relations for the coefficients the OM uses nine points in the $(\gamma, f)$ parameter space; eight at the corners of an octagon and one at the centre to compute the coefficients $A$ to $I$ in equations (11). Solving equation (5) at every point $i$ in figure 1 the two eigenvalues $E_{1,i}$ and $E_{2,i}$ associated with the EP need to be calculated. The sum $\kappa_i = E_{1,i} + E_{2,i}$ and the squared difference $\eta_i = (E_{1,i} - E_{2,i})^2$ can be used to determine all coefficients of equation (11), i.e.,

$$A = \kappa_0, \quad B = \frac{\kappa_1 - \kappa_5}{2h_\gamma},$$

$$C = \frac{\kappa_3 - \kappa_7}{2h_f}, \quad D = \eta_0,$$

$$E = \eta_1 - \eta_5, \quad F = \frac{\eta_3 - \eta_7}{2h_f},$$

$$G = \frac{\eta_1 + \eta_5 - 2\eta_0}{2h\gamma}, \quad I = \frac{\eta_3 + \eta_7 - 2\eta_0}{2h_f}.$$  

Having calculated the coefficients (12) we can make an estimation for the position $(\gamma_{EP}, f_{EP})$ of the EP by setting the left-hand side of equation (11b) to zero, which is the condition for the degeneracy of the two eigenvalues. With the abbreviations $x \equiv (\gamma_{EP} - \gamma_0)$ and $y \equiv (f_{EP} - f_0)$ we obtain

$$0 = D + E x + F y + G x^2 + H x y + I y^2.$$  

To find the EP, both the real and the imaginary part of the polynomial in equation (13) must vanish. The resulting system of equations has in general four complex roots $(x, y)$. Only one of these four roots is indeed an estimation for $(\gamma_{EP}, f_{EP})$. The other three (possibly complex) roots arise due to the mathematical structure of approximating the squared energy difference in equation (11b) up to the second order in $\gamma$ and $f$, and therefore have no physical relevance. The formulas needed to calculate the four roots of equation (13) as well as a method to choose the physically correct one are presented in appendix B.

The position estimate $(\gamma_{EP}, f_{EP})$ can be taken as centre-point $(\gamma_0, f_0)$ of a new octagon in parameter space to calculate the eigenvalues of equation (5). Afterwards, a new set of
coefficients (12) can be determined and a new estimation for \((\gamma_{\text{EP}}, f_{\text{EP}})\) can be made. Continuing this procedure step-by-step allows us to develop an iterative algorithm, which converges to the true position of the EP,

\[
\begin{align*}
\gamma_{0}^{(n+1)} &= \gamma_{\text{EP}}^{(n)}, \\
\gamma_{\text{EP}} &= \lim_{n \to \infty} \gamma_{0}^{(n)}, \\
f_{0}^{(n+1)} &= f_{\text{EP}}^{(n)}, \\
f_{\text{EP}} &= \lim_{n \to \infty} f_{0}^{(n)}. \\
\end{align*}
\]

(14)

Here, \((\gamma_{0}^{(n)}, f_{0}^{(n)})\) denotes the centre of the octagon during the \(n\)th iteration step and \(\gamma_{\text{EP}}^{(n)} = \gamma_{0}^{(n)} + x\) and \(f_{\text{EP}}^{(n)} = f_{0}^{(n)} + y\) are the corresponding estimates for the position of the EP obtained by solving for \(x\) and \(y\) in equation (13).

2.3. Verification of found EPs

Once the OM has converged to a specific point in the \((\gamma, f)\)-parameter space, one has to prove that this point actually is an EP. There are two possibilities for this verification. For the first one an EP is fully encircled in parameter space, so the corresponding resonances will undergo an exchange of their position in the complex energy plane [3]. To be able to sort the calculated resonances properly, equation (5) has to be solved successively in small steps on the circle around the EP. Hence, the computational effort is very high. By using the OM this effort can be reduced considerably. Having obtained the coefficients \(A\) to \(I\) by solving equation (5) numerically only at the nine points of the octagon in figure 1 the values of \(\kappa\) and \(\eta\) of equation (11) are well known for all sets of parameters \((\gamma, f)\), which lie in the vicinity of \((\gamma_{0}, f_{0})\) where the approximations (11) hold. Thus, for any point \((\gamma, f)\) on the circle circumscribing the octagon (provided that the radius is small enough), the two resonances \(E_{1}\) and \(E_{2}\) can be calculated using equation (11) without further time-consuming diagonalization of equation (5),

\[
E_{1,2} = \kappa(\gamma, f) \pm \sqrt{\eta(\gamma, f)^{2} - \eta(\gamma, f)}. 
\]

(15)

The arising paths in the complex energy plane can now be visually checked for the exchange behaviour of the corresponding resonances.

Another possibility is the calculation of a winding number that allows for a clear statement about the existence of an EP without the need to visually check the paths of exchanging resonances in the complex energy plane. Here again, the circle around the octagon, \(\gamma(\varphi) = \gamma_{0} + h_{\varphi} \cos(\varphi), f(\varphi) = f_{0} + h_{\varphi} \sin(\varphi),\) is discretized in \(n\) steps, which are denoted by respective angles \(\varphi_{i}\) with \(i \in \{0, \ldots, n\}\) as in the previous method. At each point \((\gamma(\varphi_{i}), f(\varphi_{i}))\) of the discretized circle the squared energy difference \(\eta(\varphi_{i})\) can be calculated easily using equation (11b) with the known coefficients \(D\) to \(I\). The result is a closed curve for \(\eta\) within the complex \(\eta\)-plane. If this \(\eta\)-curve encircles the origin of coordinates, an EP is located within the circle in the \((\gamma, f)\)-space [39]. This can be tested numerically using the residue theorem by which we calculate the winding number of the \(\eta\)-curve for a function with a pole at the origin of coordinates with a discretized formula

\[
W_{\eta=0} = \frac{1}{2\pi i} \sum_{i=1}^{n} \eta(\varphi_{i+1}) - \eta(\varphi_{i}) \frac{\eta(\varphi_{i})}{2\eta(\varphi_{i})}. 
\]

(16)

In case of \(W_{\eta=0} = 1\) at a sufficiently high \(n\) the resonances (15) show the typical exchange behaviour of an EP, which is located within the octagon-circle in the \((\gamma, f)\)-space.

3. Results and discussion

To find initial parameters for the OM, we look at first for avoided crossings between two levels in the term-scheme of the Rydberg system in parallel fields, as level repulsion is associated with the occurrence of EPs [4]. For this purpose, the real part of the resonances’ energy, which is obtained by solving equation (5), can be plotted as a function of the field strength \(\gamma\) keeping the ratio \(\gamma/f\) constant. Figure 2(a) shows an excerpt of such spectra for the ratio \(\gamma/f = 80\), where a maximum quantum number of \(n_{\text{max}} = 90\) has been used. An avoided crossing is marked by a red arrow (we could as well choose the other avoided crossing visible in figure 2(a) as long as the correct eigenvalues related to the avoiding states are used to set up the two-dimensional matrix model). Here we extract the initial parameters \(\gamma_{0} = 1.481 \times 10^{-3}, f = 1.851 \times 10^{-5}\) and \(\text{Re}(E) = -6.90 \times 10^{-3}\) to start our iterative algorithm.

Starting from these initial parameters, the OM converges within 14 iteration steps towards the precise position of an EP in parameter space

\[
\begin{align*}
\gamma_{\text{EP}} &= 8.598 633 574 \times 10^{-4}, \\
f_{\text{EP}} &= 2.005 076 385 \times 10^{-5}, \\
\end{align*}
\]

(17)

at which the two corresponding resonances become degenerate. The closer the centre-point of the octagon gets to the true position of the EP, the smaller becomes the value \(|E_{1,i} - E_{2,i}|\) in each iteration step \(i\), as is displayed in figure 2(b) (red crosses). For a given matrix representation the degeneracy of the two resonances can only be reached down to an energy difference of \(\Delta E = 10^{-10}\). This can be explained by the limited numerical precision when solving equation (5) with the IRAM method of the ARPACK package [40]. To estimate the precise complex energy \(E_{\text{EP}}\) of an EP, the energy of the two corresponding resonances \(E_{1}\) and \(E_{2}\) can be averaged (by calculating \(\gamma_{\text{EP}}\) and \(f_{\text{EP}}\) for \(\eta = 0\) in equation (11b) and applying the results to equation (11a))

\[
E_{\text{EP}} = \frac{E_{1} + E_{2}}{2} + \mathcal{O}(\gamma_{0} - \gamma_{\text{EP}}), (f_{0} - f_{\text{EP}}). 
\]

(18)

Being close to \(\gamma_{\text{EP}}\) and \(f_{\text{EP}}\) within the system, higher-order terms can be neglected. While the degeneracy of the corresponding resonances only goes down to an energy difference of \(\Delta E = 10^{-10}\) (see figure 2(b)), estimation (18) for the complex energy of the EP converges with a considerably higher precision to

\[
E_{\text{EP}} = -7.647 637 585 \times 10^{-3} - 8.461 814 32 \times 10^{-7}i, 
\]

(19)
Figure 2. (a) Real part of the energy of the resonances obtained by solving equation (5) with $\gamma/f = 80$, $m = 0$ and $n_{\text{max}} = 90$. The levels are labelled by their principal quantum numbers $n$ in the limit $\gamma, f \to 0$. Two avoided crossings are visible. The right one (marked as a.c. with a red arrow) between the levels with $n = 10$ and $n = 8$ is taken to obtain a set of initial parameters for the OM to search for an EP in its vicinity (see text). (b) Typical convergence behaviour to an EP with the octagon method. Red crosses: modulus of the energy difference $\Delta E$ of the two resonances $E_{i,\alpha}$ and $E_{i,\beta}$, coalescing to an EP, at iteration step $i$. Blue dots: modulus of the difference $\Delta E$ between the estimation $E_{\text{EP},i} = (E_{i,\alpha} + E_{i,\beta})/2$ for the complex energy of an EP and the estimation $E_{\text{EP},i-1}$ of the precedent iteration step.

Figure 3. Exemplary paths of the resonances in the complex energy plane for the iteration steps $i = 7$ and $i = 9$ of figure 2(b). The crosses mark the resonances calculated by solving equation (5) at the nine points of the octagon (see figure 1). Also shown are the resonance energies at the centre-point of the octagons. While for $i = 7$ these resonances are still clearly separated, for $i = 9$ they coincide within the drawing accuracy. They match the paths that are calculated via equation (15) using the respective coefficients $A$ to $I$ of each iteration step. The path of each resonance is plotted in a different colour. In iteration step seven, each resonance returns to its starting point after a full circle around the octagon. Thus, no EP is located within the respective $(\gamma, f)$ region and the winding number according to equation (16) is $W^{(7)}_{\eta=0} = 0$. In step nine the resonances show the clear exchange behaviour of an EP, which is located close to the centre point of the octagon. The winding number is $W^{(9)}_{\eta=0} = 1$. In contrast to step seven, the two resonances are almost degenerate at the centre point indicating convergence of the algorithm.

during the iteration process (see blue dots in figure 2(b)).

To verify that the point of convergence really is an EP, we calculate for each iteration step in figure 2(b) the resonances $E_1$ and $E_2$ according to equation (15) using the respective coefficients $A$ to $I$ of the OM. As an example we show for an elliptical path circumscribing the octagon in the $(\gamma, f)$-space the resulting paths of the resonances in the complex energy plane (for the two iteration steps $i = 7$ and $i = 9$) in figure 3. While no EP-typical exchange behaviour can be seen in iteration step seven, in step nine the two resonances exchange their position after a full circle of the octagon. This indicates an EP located near the centre-point of the octagon, where the two resonances almost become degenerate. To avoid checking the resulting paths for exchange behaviour visually, the winding number can be calculated using equation (16). While it is still zero in iteration step seven the winding number becomes one in step nine, and thus the occurrence of an EP is verified numerically.

To find more EPs for a Rydberg system in parallel fields we generate spectra as in figure 2(a) for a wider range of parameters, see, e.g., figure 4, in which the spectra are calculated with a ratio $\gamma/f = 120$ and a maximum quantum number of $n_{\text{max}} = 90$. The modulus of the complex dilation parameter $b = |b| \exp(\text{i}\alpha)$ has been chosen to be $|b| = \sqrt{32/35} \gamma^{-1/6}$ (see [41]), whereas $\alpha$ has been varied to ensure convergence of the resonances (converged resonances are independent of the rotation angle $\alpha$). The resulting spectra cover a range of $\gamma$ up to $\gamma = 3 \times 10^{-3}$, which corresponds to $B = 705 \text{T}$ for the hydrogen atom (still far away from being realised experimentally yet) or to $B = 1.8 \text{T}$ for Cu$_2$O, which is fully accessible in a possible experimental realisation (see, e.g., [25]). Figure 4 shows a high number of avoided crossings (most of them are marked by red circles). From each of them an initial set of parameters for the OM can be extracted to start the iterative search for an EP.

With the OM several EPs could be found (see figure 5) in the system described by equation (3). Using the proper constants $F_0$ and $B_0$ as well as the correct energy scaling (see appendix A), the results can be converted to SI-units either for the hydrogen atom or for excitons in Cu$_2$O. A large portion of the EPs shown in figure 5 could be found in a region with $\text{Re}(E) < 0$ (the zero-point of the $\text{Re}(E)$-axis is defined by the threshold between bound states and continuum states in the absence of external fields) and relatively small external fields
The strengths \( g \) and \( f \) are increased simultaneously, keeping the ratio \( \gamma/f = 120 \) constant. A value of \( \gamma = 3 \times 10^{-3} \) either corresponds to \( B = 705 \) T for the hydrogen atom or to \( B = 1.8 \) T for Cu\(_2\)O (see appendix A). Avoided crossings are marked by red circles.

Figure 4. Real part of the energy of the resonances obtained by solving equation (5) with maximum quantum number \( n_{\text{max}} = 90 \). The strengths \( \gamma \) and \( f \) are increased simultaneously, keeping the ratio \( \gamma/f = 120 \) constant. A value of \( \gamma = 3 \times 10^{-3} \) either corresponds to \( B = 705 \) T for the hydrogen atom or to \( B = 1.8 \) T for Cu\(_2\)O (see appendix A). Avoided crossings are marked by red circles.

up to \( \gamma_{\text{EP}} \approx 10^{-2} \), \( f_{\text{EP}} \approx 10^{-4} \). This corresponds to \( \gamma_{\text{EP}} \approx 2.35 \times 10^3 \) T, \( f_{\text{EP}} \approx 5.14 \times 10^5 \) V cm\(^{-1} \) for the hydrogen atom or to \( \gamma_{\text{EP}} \approx 6.03 \) T, \( f_{\text{EP}} \approx 1.76 \times 10^3 \) V cm\(^{-1} \) for Cu\(_2\)O. In figure 5(d) one can see that the EPs found are approximately located along a straight line with \( \gamma_{\text{EP}}/f_{\text{EP}} = 50 \) in this low-field regime (the precise values for \( \gamma_{\text{EP}}/f_{\text{EP}} \) are displayed in figure 5(a), where the accumulation near 50 is less obvious). At higher fields a significant deviation from this behaviour is found. Even though the EPs seem to form two branches if only the magnetic field is considered, see figure 5(b), in this high-field regime such a behaviour cannot be observed for the electric field in figure 5(c). However, both figures show the same behaviour for small fields: the higher the strength of the external fields, the lower are the energies of the resonances of the Rydberg system which interact to form an EP. When reaching the high-field regime, this behaviour changes and EPs with \( \text{Re}(E) > 0 \) can be found, too. It is important to note that figure 5 does not show all existing EPs of a Rydberg system in parallel electric and magnetic fields but just those found within the scope of our work. Therefore, more EPs could be found, which possibly would change the appearance of figure 5 especially in the high-field regime.

In table 1 we present the parameters of selected EPs to compare the significantly differing physical values for the hydrogen atom and Cu\(_2\)O. With regard to the external field strengths of the EPs, the fields for Cu\(_2\)O are about two orders of magnitude smaller than those for the hydrogen atom due to effective masses and the relative dielectric constant of the solid (see appendix A). In contrast to the hydrogen atom, the external fields to detect EPs in Cu\(_2\)O can be realised in an experiment (see, e.g., [26] with \( B \) up to 7 T). Hence, we propose the measurement of photoabsorption spectra of the states associated with an EP in Cu\(_2\)O. Close to the EP these spectra can be analyzed by means of harmonic inversion [2] to detect the exchange behaviour of resonances and to use the OM to locate the precise position of an EP in the real system of Cu\(_2\)O. Extending this method according to [43], even an investigation directly at the EP would be possible.

To find the precise position of an EP in parameter space as well as its exact energy only the eigenvalues of equation (5) are needed. Additionally, using the eigenvectors according to equation (9), the associated states can be calculated. A visualisation of the probability density \( |\Psi|^2 \) for the two states belonging to the EP at \( \gamma = 2.387 \times 10^3 \), \( f = 2.739 \times 10^5 \) with the energy \( E = -6.85886 \times 10^{-3} \) is presented in figure 6(a), which is calculated with \( n_{\text{max}} = 90 \) and \( |h| = 2.6 \) in semiparabolic coordinates. Due to the cylindrical symmetry of a state with \( m = 0 \) in parallel electric and magnetic fields, only the first quadrant of the \((\mu_1, \mu_2)\)-plane is needed to cover the full position space. The angle \( \varphi \) of equation (4) can be chosen arbitrarily and we use \( \varphi = 0 \). To obtain a real-valued probability density, the absolute value of \( \Psi \) has to be taken [44]. The reason for this is the complex rotation, where only the intrinsic complex parts of \( \Psi \) are conjugated in \( \Psi^* \) (see equation (9)) and thus \( \Psi^* \Psi \) stays a complex quantity. According to [3] not only the eigenvalues, but also the eigenvectors coalesce at an EP. The visualisation of the two associated states should therefore look the same, which cannot be verified in figure 6(a). Although the two probability densities have the same extension in the space of semiparabolic coordinates they differ by their nodal line patterns.

If the nodal patterns of the wave functions of the two states are studied for a circle around the EP they show the same exchange behaviour as the eigenvalues. Following a full circle in parameter space around the EP in small steps and calculating and sorting the plots of the probability densities have the same extension in the space of semiparabolic coordinates they differ by their nodal line patterns.

The reason for the difference in the nodal patterns of the two states in figure 6(a), which have been calculated directly at the precise position of the EP can be found by looking at figure 2(b), where the degeneracy of the eigenvalues (red \( \times \)) can only be reached down to an energy difference of \( \Delta E = 10^{-10} \) due to numerical limitations. The same limitations prevent the eigenvectors from degenerating at the EP.

2 The use of the term nodal lines must be considered with caution here because at these lines the probability density is just significantly smaller compared to the surrounding area—it does not go to zero, which would be the common definition for a nodal line.
The accuracy of calculating the exact energy at an EP could be raised by taking the mean value of the two related resonances (see equation (18) and blue dots in figure 2(b)). Extending this approach to the eigenvectors, the guessed (degenerate) eigenvector $|\psi_{EP,\text{guess}}\rangle$ for the two resonances at the EP can be found by

$$|\psi_{EP,\text{guess}}\rangle = |\psi_1\rangle + |\psi_2\rangle,$$

where $|\psi_1\rangle$ and $|\psi_2\rangle$ are the (numerically) not completely degenerate eigenvectors that were used to obtain figure 6(a). The naive expectation is that it should be possible to calculate the wave function at an EP by normalising $|\psi_{EP,\text{guess}}\rangle$. However, this is in principle impossible since the physically correct inner product $\int |\psi|^2 \psi^* d^3r$ of a wave function at the EP vanishes [44]. That is, close to the EP the normalised wave function diverges. This can be observed in figure 6(b). Note that the scale for the modulus of the wave function is two orders of magnitude higher compared to figure 6(a). Consequently, the level of divergence—or in other words the smallness of $\int |\psi|^2 \psi^* d^3r$—is a further indicator of how close $|\psi_{EP,\text{guess}}\rangle$ is to the exact position of the EP.

### 4. Conclusion and outlook

Based on a work on EPs in the hydrogen atom in crossed electric and magnetic fields [2], we started to investigate the appearance of EPs in a generalised and more symmetric model: the hydrogen-like system in parallel electric and magnetic fields. Using appropriate units (see appendix A), our results hold either for the hydrogen atom or for CuO$_2$ (for which a hydrogen-like spectrum of excitons up to a principal quantum number of $n = 25$ has been found recently [24]). The initial points to start an iterative search for the precise position of an EP in parameter space are given by the parameters of an avoided crossing within the spectra because level repulsion is associated with the occurrence of EPs [4]. Since the common three-point method [29] of finding EPs in open quantum systems has to start its iterative search close to an EP’s actual position, it does in general not show convergence with the initial parameters of an avoided crossing. Using a two-dimensional matrix model to describe the two states forming an EP in its local vicinity, we have developed the OM, an iterative method that converges to the precise position of an EP in parameter space. Performing the time-consuming calculation of the resonances at just nine points in parameter space (eight at the corners of an octagon and one at its centre-point), the OM provides a very fast and stable method which only needs the initial parameters of an avoided crossing to converge to the precise position of the related EP in parameter space, and which yields its precise complex energy by taking the mean energy of the two associated resonances. Using the OM, the paths of the associated resonances in the complex energy plane during a circle around the EP in small steps in parameter space can be revealed without further quantum-mechanical (and time-consuming) calculations. The exchange behaviour of these paths can be tested numerically by

Figure 5. EPs found in the system described by equation (3) using the OM. The EPs are presented in the material-independent description of appropriate units. These results can be converted either to values for the hydrogen atom or to values for CuO$_2$ using the relations in appendix A.
calculating a winding number which verifies the existence of an EP. Using the OM, we were able to find a variety of EPs within the open quantum system of an exciton in parallel electric and magnetic fields. In contrast to the hydrogen atom, a variety of the EPs that we predict for Cu$_2$O are in a regime below $B = 10$ T, which is experimentally accessible. Hence, Cu$_2$O provides an appropriate system to verify our theoretical predictions experimentally. A possible experimental realisation would be the measurement of photoabsorption spectra of the states associated with an EP in Cu$_2$O and analyzing them by means of harmonic inversion [2]. Even an extension according to [43] to investigate spectra directly at the EP would be possible.

In the second part of our work we visualised the coalescence of the two wave functions belonging to the resonances which become degenerate at the EP. Calculating the probability densities in semiparabolic coordinates at the precise position of the EP, the exact coalescence could not be confirmed for numerical reasons as the two states differ by their nodal line patterns (these patterns show the exchange behaviour expected for the two resonances since they transform into each other while completely encircling the EP in small steps [39]). Motivated by a mean-value-calculation for the associated complex resonances to determine the precise energy of an EP, we averaged the numerically different eigenvectors of the two resonances directly at the EP and obtained one degenerate eigenvector, of which we calculated the probability density.

In an experiment the realisation of an EP in hydrogen-like resonance spectra seems to be very promising for excitons in semiconductor devices [26, 32]. In this context our work gives clear evidence for the appearance of EPs. However, extensions to some simplifications should be investigated. From a theoretical point of view some work still remains to be done to extend the hydrogen-like model for excitons in Cu$_2$O to a more realistic model. One should, e.g., include a more complex band structure with more than one valence band [25]. Another possibility would be to consider the exchange and correlation effects according to [27] or to include exciton-phonon interaction [25]. Furthermore, we plan to perform calculations for Cu$_2$O in crossed electric and magnetic fields, as it was done for the hydrogen atom in, e.g., [2, 45–50]. For this case, the Hamiltonian (2) for Cu$_2$O cannot be brought to the same form as the Hamiltonian (1) for the hydrogen atom by using an appropriate scaling. Consequently, the results for the hydrogen atom cannot be converted to the results for Cu$_2$O in a simple way and separate calculations need to be done.

### Appendix A. Choice of appropriate units

The use of appropriate units within the course of the present work has the advantage that calculations can be carried out

| Table 1. Parameters of selected EPs of the system described by equation (3). Note that the energies of Cu$_2$O are given without the offset caused by the band gap energy of $E_{\text{gap}} = 2.17208$ eV [24]. |
|---|---|---|---|---|
| **Hydrogen atom** |  |  | **Cu$_2$O** |
| $B$ [T] | $F$ [meV] | $E_i$ [eV] | $E_i$ [meV] | $E_i$ [μeV] |
| 229.64 | 120250 | −0.1904 | −0.6209 | 0.590 | 41.16 | −1.286 | −0.419 |
| 561.26 | 140870 | −0.1866 | −0.2564 | 1.441 | 48.22 | −1.261 | −1.732 |
| 799.69 | 341940 | −0.3886 | −2.072 | 2.053 | 117.0 | −2.625 | −14.00 |
| 1261.3 | 668930 | −0.3996 | −0.5002 | 3.238 | 229.0 | −2.699 | −3.379 |
| 1506.7 | 686310 | −0.5245 | −4.402 | 3.868 | 234.9 | −3.544 | −29.74 |
| 2316.3 | 1096200 | −0.6733 | −0.5999 | 5.946 | 375.2 | −4.549 | −4.054 |
| 3595.7 | 2430880 | −0.4783 | −12.03 | 9.231 | 832.0 | −3.234 | −81.25 |

Figure 6. (a) Visualisation of the probability density $|\psi^*\psi|$ for the two states belonging to the EP at $(\gamma = 2.387819 \times 10^{-3}, f = 2.739422 \times 10^{-5})$ with the energy $E = −0.685886 \times 10^{-2} − 0.942211 \times 10^{-5}$ in the $(\mu_r, \mu_i)$-plane of semiparabolic coordinates. For further details see text. b) Estimation for the probability density $|\psi^*\psi|$ of the degenerate state at the EP of figure 6(a). The distribution is calculated according to equation (9) based on the estimation $|\psi_{\text{EP}}|_{\text{guess}}$ for the degenerated eigenvector (see equation (20)).
without material-dependent parameters (see equation (3)). These parameters are absorbed in the scaling constants \( F_0 \) of the electric and \( B_0 \) of the magnetic field. The numerical value of these constants depends on the system considered; either a hydrogen atom or a Rydberg exciton in Cu2O (see table A1). The difference in these constants can be explained on one hand by the reduced mass \( \mu \). The mass of the proton in the hydrogen atom can be taken as approximately infinite compared to the mass of the electron. Hence, \( \mu \approx m_0 \) here (with \( m_0 \) being the mass of an electron in free space), whereas for Rydberg excitons in Cu2O the reduced mass amounts to \( \mu = 0.38m_0 \) [31]. On the other hand, the Coulomb interaction in Cu2O is screened by the dielectric constant \( \varepsilon_r = 7.50 \) [27].

In the case of a hydrogen atom there is no such screening, and thus \( \varepsilon_r = 1 \).

Having done a calculation in appropriate units the quantities in table A1 can be used to convert the result to either hold for a hydrogen atom or for Rydberg excitons in Cu2O. As an example: a magnetic flux density of \( \gamma = 1 \) in equation (3) corresponds either to \( B_0 = 2.35 \times 10^5 \) T for the hydrogen atom or to \( B_0 = 603 \) T for Cu2O.

### Appendix B. Estimating the position of an EP

In section 2.2 a solution of equation (13) is needed to estimate the position (\( \gamma_{\text{EP}}, f_{\text{EP}} \)) of an EP. Since the coefficients \( D \) to \( I \) are complex, both the real and the imaginary part of the polynomial in equation (13) must be set to zero

\[
0 = \text{Re}(D) + \text{Re}(E) x + \text{Re}(F) y \\
+ \text{Re}(G) x^2 + \text{Re}(H) x y + \text{Re}(I) y^2, \quad (B.1a)
\]

\[
0 = \text{Im}(D) + \text{Im}(E) x + \text{Im}(F) y \\
+ \text{Im}(G) x^2 + \text{Im}(H) x y + \text{Im}(I) y^2. \quad (B.1b)
\]

Dividing equation (B.1a) by \( \text{Re}(I) \) and equation (B.1b) by \( \text{Im}(I) \) and subtracting the resulting equations cancels the \( y^2 \)-term and yields

\[
y(x) = -\frac{W(D, I) + W(E, I) x + W(G, I) x^2}{W(F, I) + W(H, I) x}, \quad (B.2)
\]

where we introduce the abbreviation

\[
W(U, V) \equiv U_i V_j - U_j V_i \quad (B.3)
\]

with \( U_i \equiv \text{Im}(U), U_j \equiv \text{Re}(U) \) and \( U, V \in \{ D, E, F, G, H, I \} \). Inserting equation (B.2) in equation (B.1a) for \( W(F, I) + W(H, I) x = 0 \) yields a fourth-order polynomial of which the roots need to be found:

\[
0 = f_1 W(F, I) + I, W(D, I)^2 \\
+ \{ f_2 W(H, I) + f_3 W(F, I) \} x \\
+ 2l, W(D, I) W(G, I) + I, W(E, I) x^2 \\
+ \{ f_4 W(H, I) + [2l, W(E, I) \} x^3 \\
+ \{ I, W(H, I) + I, W(G, I) W(G, I) \} x^4.
\]

(B.4)

Here, further abbreviations are used

\[
\begin{align*}
\tilde{f}_1 &= D, - F, W(D, I), \\
\tilde{f}_2 &= E, - F, W(E, I) - H, W(D, I), \\
\tilde{f}_3 &= G, - F, W(G, I) - H, W(E, I).
\end{align*}
\]

(B.5a) \( (B.5b) \) \( (B.5c) \)

Having found a root \( x \) of equation (B.4), the corresponding \( y \) can be calculated using equation (B.2).

In general, equation (B.4) has four complex roots \( x, y \in \{1,...,4\} \), in practice there are cases with two or all four solutions being real. Only one of the four roots is indeed a physical estimation for \( \gamma_{\text{EP}} \) (and \( f_{\text{EP}} \)). The other three (possibly complex) roots arise due to the mathematical structure of approximating the squared energy difference in equation (11b) up to the second order in \( g \) and \( f \) and therefore have no physical relevance. To select the physically correct root out of the four possible ones, it proved to be useful not to set the left hand side of equation (13) immediately to zero, but to \( (1 - \varepsilon) D \) with an initial value of \( \varepsilon = 0 \)

\[
(1 - \varepsilon) D_1 = D_1 + E_1 x + F_1 y \\
+ G_1 x^2 + H_1 x y + I_1 y^2, \quad (B.6a)
\]

\[
(1 - \varepsilon) D_2 = D_1 + E_1 x + F_1 y + G_1 x^2 + H_1 x y + I_1 y^2. \quad (B.6b)
\]

Now the \( D \) on the left-hand side of equation (B.6) cancels out that on the right-hand side. Hence, an obvious solution is \( x = y = 0 \), which corresponds to the centre-point of the octagon. If we assume the coefficients \( D \) to \( I \) to describe the system at this point most accurately (as they are calculated for an octagon with this centre-point), it is reasonable to treat the root with \( x = 0 \) at \( \varepsilon = 0 \) as the distinguished one, which can then be followed by rising \( \varepsilon \) in small steps to \( \varepsilon = 1 \). Now the equation again corresponds to equation (13); however, with the difference that the distinguished root resulting from that with \( x = 0 \) at \( \varepsilon = 0 \) can be taken as the true value of \( \gamma_{\text{EP}} \). The
corresponding value for $f_{EP}$ results again from equation (B.2). The approach of selecting the correct solution out of the four possible $x_j$ is illustrated in figure B1 where the paths of the real values of the solutions $x_j$ are plotted as a function of $\varepsilon$. At $\varepsilon = 1$ the physically correct solution is the one that originates from $\text{Re}(x_j) = 0$ at $\varepsilon = 0$ (marked with red bullets). A plot similar to figure B1 for the imaginary part $\text{Im}(x_j)$ of the four solutions shows qualitatively the same behaviour.

Note that even in the sometimes occurring case of all four solutions of equation (13) being complex at $\varepsilon = 1$, it is still possible to make an estimation for the position of the EP by taking the estimation for $\gamma_{EP}$ and $f_{EP}$ at an $\varepsilon$-value smaller than one, where the distinguished root is still real. Sometimes, after a few iteration steps the distinguished solution at $\varepsilon = 1$ becomes real again and in that case the algorithm can converge to an EP.

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