State Flip at Exceptional Points in Spectra of the Hydrogen Atom in External Fields

Bachelor Thesis

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INTRODUCTION

The concept of *exceptional points* was first defined by Kato (1995) in 1966 in a mathematical context as part of the perturbation theory of a non-Hermitian operator with complex eigenvalues (The physically more relevant definition of exceptional point is made by Heiss, for a reference see Heiss (2012)). An exceptional point can appear in parameter-dependent systems. They describe points in an at least two-dimensional parameter space at which two (or more) eigenvalues and their corresponding eigenstates become identical. In physics operators appear in quantum theory in the form of a Hamiltonian. Usually this Hamiltonian is Hermitian and has purely real eigenvalues, which are associated with a measurable energy. This is a sufficient description of a closed quantum system. A very effective description of open quantum systems interacting with an environment is often possible in terms of non-Hermitian Hamiltonians. These non-Hermitian operators possess in general complex eigenvalues. Due to their non-Hermiticity they may exhibit exceptional points. The imaginary part of an eigenvalue is interpreted as a decay rate of the corresponding state. An example is the hydrogen atom in crossed external electric and magnetic fields. Various exceptional points were identified in that system by Cartarius (2008) which were also published by Cartarius et al. (2007; 2009). This thesis deals with the temporal evolution of states at an exceptional point in the hydrogen atom as an extension to the works mentioned before. Uzdin et al. (2011) and Berry and Uzdin (2011) found that the temporal evolution of resonances, when transported around an exceptional point, has to be considered very carefully. For a closed loop around an exceptional point it is known that the two resonances connected with the exceptional point interchange. However, if a resonance is populated and then transported around the exceptional point, this exchange is not always visible. In particular, it could be shown that for sufficiently slow traversals of the parameter space loop the final population always ends up in the same state. There are suggestions to exploit this fact for technical applications, e.g. purification schemes, cf. Gilary, Mailybaev, et al. (2013), Atabek et al. (2011), and Gilary and Moiseyev (2012). However, Leclerc et al. (2013) showed that also the non-adiabatic exchange is only visible for isolated resonances. In real physical systems transitions to other resonances not connected to the exceptional point are always possible and can influence the dynamics. It is the purpose of this thesis to study this influence. Furthermore we investigate for the first time the transport of a populated resonance around a third-order exceptional point.

Before the hydrogen atom is studied a matrix model proposed by Uzdin et al. (2011) is investigated. An eigenstate is transported along a closed loop in parameter space in its instantaneous basis. It turns out that the initial population does not need to end up in the same state. This phenomenon is called *adiabatic flip*. The time evolution is solved numerically exact. The result is compared to the adiabatic approximation.

The main topic of this thesis is the application of the insights gained from Uzdin et al. (2011) on a physical system, viz. the hydrogen atom in crossed external electric and magnetic fields. A numerical method for calculating the eigensystem of the Hamiltonian was implemented by Cartarius (2008) and is extended in this thesis by means of the

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transport of populations along a parameter space trajectory. For reference a second-order exceptional point is encircled and the transport of resonances around it is discussed. The main focus is set on a third-order exceptional point. The transport around this point is observed in dependence of various parameters. The loop around the exceptional point is traversed in both directions and a phase offset is introduced. The initial population is set in all three resonances involved. Resonances in the vicinity of the exceptional point are taken into respect in the temporal evolution. Based on the results by Uzdin et al. (2011) it is discussed whether or not an adiabatic flip occurs.

EXCEPTIONAL POINTS

2.1. ANALYTICAL FUNCTIONS

A function $f(z) : \mathbb{C} \to \mathbb{C}$ is called analytic in z_0 if the power series of f converges in a vicinity of z_0 . An analytic function is called *single valued* if the value $f(z_0)$ at every point z_0 is independent of the path of the analytic continuation to reach it. In contrast, a *multiple valued* (or multivalued) function can map two or more points in its range to a single value in its domain. A simple example for the difference between those two kinds of functions is $f : z \to z^n$ with $n \in \mathbb{Z}$ for single valued and $f : z \to \sqrt[n]{z}$ for multiple valued functions. To account for the ambiguity of solutions it is best to introduce the *Riemann* surface. For illustration purposes we show a little example.

EXAMPLE 2.1:

Let $f : \mathbb{C} \to \mathbb{C}$ with the specification $f(z) = z^2$. We choose a value $f(z) = e^{i\phi}$. Thus two possible values for z can be obtained.

$$z_1 = e^{i\phi/2}$$

 $z_2 = e^{i(\phi/2 + \pi)}$
(2.1)

Branch point singularities are points at which several branches merge together. Hence the branches have to share a common function value (the function becomes single valued).

2.2. OCCURRENCE AND PROPERTIES

An exceptional point (abbr.: EP) is defined as a branch point singularity of a parameterdependent function. Let T be a matrix of arbitrary dimension of which the entries depend on a complex parameter γ . Hence the eigenvalues of $T(\gamma)$ also depend on this parameter. Suppose that two eigenvalues which belong to two branches of the some analytic function are degenerate for a given value of γ . Then this point is called an exceptional point.

If an exceptional point is encircled in the parameter space of γ , the eigenvalues permute in a cyclic manner, e.g. in a two level system the two eigenvalues interchange. The corresponding eigenvectors also permute but they pick up a geometric phase. To get back to the two level example, the phase is expressed in terms of the sign of the eigenvectors χ_i as in

$$[\boldsymbol{\chi}_1, \boldsymbol{\chi}_2] \stackrel{\text{circle}}{\to} [\boldsymbol{\chi}_2, -\boldsymbol{\chi}_1].$$
(2.2)

In the previous text we have always referred to examples consisting of two levels or similar. This can of course be expanded to n levels and an m dimensional parameter space.



Figure 2.1. (a): Circle in the complex parameter space given by (2.6) with $r = 5 \cdot 10^{-5}$. The start/end point is marked with a filled bullet, the exceptional point is marked with a small triangle. (b): Behaviour of the eigenvalues when encircling the exceptional point in the parameter space. The eigenvalues interchange their positions. The analytical expressions for all quantities are plotted using dashed lines.

► EXAMPLE 2.2: [From Kato (1995, p. 64).]

Here we show an analytic example of how these exceptional points are found and how encircling them operates on the eigenvalues. Please note that this Hamiltonian is *non-Hermitian*! This is a necessary condition for the existence of exceptional points. Let $\kappa \in \mathbb{C}$ and

$$\mathcal{H}(\kappa) = \begin{pmatrix} 1 & \kappa \\ \kappa & -1 \end{pmatrix} \tag{2.3}$$

with the eigenvalues

$$E_{\pm}(\kappa) = \pm \sqrt{1 + \kappa^2}.$$
(2.4)

The right hand side eigenvectors read

$$|\psi_{\pm}(\kappa)\rangle = \begin{pmatrix} -\kappa \\ 1 \pm \sqrt{1 + \kappa^2} \end{pmatrix}.$$
 (2.5)

From $E_{\pm}(\kappa)$ one can easily see that two exceptional points exist for $\kappa_{\pm} = \pm i$, respectively. In this case the eigenvectors read $|\psi(\pm i)\rangle = (\mp i, 1)^{\top}$. If the parameter κ is circled around one of these exceptional points, e.g. by

$$\kappa = \mathbf{i} + r \, \mathrm{e}^{\mathbf{i}\phi},\tag{2.6}$$

where $\phi \in [0, 2\pi)$, the eigenvalues interchange their position. This is best viewed in figure 2.1.

Because the path of a single eigenvalue matches a semicircle it is not closed. If the cycle in parameter space is traversed twice the eigenvalues interchange again and the loop

is closed. For this two-level system an analytical approximation can be found. Inserting (2.6) into (2.4) and assuming $r\ll 2$ yields

$$\tilde{E}_{1,2} = \pm \sqrt{1 + (\mathbf{i} + r \,\mathrm{e}^{\mathbf{i}\phi})^2}$$

$$= \pm \sqrt{r} \,\mathrm{e}^{\mathbf{i}\phi/2} \sqrt{2\mathbf{i} + r \,\mathrm{e}^{\mathbf{i}\phi}}$$

$$\approx \pm \sqrt{2r} \,\mathrm{e}^{\mathbf{i}(\pi/4 + \phi/2)}.$$
(2.7)

These analytical solutions have been plotted in figure 2.1 using dashed lines.

2.2.1. Geometric Phases

In the previous text we have seen that the eigenvalues and eigenvectors permute if an exceptional point is encircled. Another important consequence is the appearance of a *geometric phase*. In the case of a complex symmetric matrix the geometric phase is expressed in terms of a sign change of the eigenvectors as in

$$[\boldsymbol{\chi}_1, \boldsymbol{\chi}_2] \stackrel{\text{circle}}{\to} [\boldsymbol{\chi}_2, -\boldsymbol{\chi}_1].$$
(2.2)

Important is the behaviour for multiple circles. Repeated circles lead consequently to

$$\begin{aligned} & [\boldsymbol{\chi}_1, \boldsymbol{\chi}_2] \stackrel{2 \text{ circles}}{\to} [-\boldsymbol{\chi}_1, -\boldsymbol{\chi}_2], \\ & [\boldsymbol{\chi}_1, \boldsymbol{\chi}_2] \stackrel{4 \text{ circles}}{\to} [\boldsymbol{\chi}_1, \boldsymbol{\chi}_2]. \end{aligned}$$
 (2.8)

Hence it only takes two loops to bring the eigenvalues to their original state, but due to the geometric phase that accumulates while circling, the eigenvectors need four loops to be restored.

ADIABATIC STATE FLIPS GENERATED BY EXCEPTIONAL POINTS

In this chapter the reproduction of the results presented in Uzdin et al. (2011) is shown and discussed. First of all, the model used in this publication will be introduced. Next, the algorithms and methods needed for the reproduction are devised. The following sections are named and structured very similar to those in the paper to maintain comparability.

3.1. FORMALISM

The model used in the following is a two-level non-Hermitian symmetric Hamiltonian \mathcal{H} depending on a parameter $\lambda(t) = (\lambda_1, \lambda_2)$ where $\lambda_i \in \mathbb{R}$. The spectrum has an exceptional point at $\lambda = 0$.

3.1.1. Instantaneous Basis

We define the *instantaneous* basis $|\Phi_{a,b}(\boldsymbol{\lambda})\rangle$ where

$$\mathcal{H}(\boldsymbol{\lambda}) |\Phi_{a,b}(\boldsymbol{\lambda})\rangle = E_{a,b}(\boldsymbol{\lambda}) |\Phi_{a,b}(\boldsymbol{\lambda})\rangle$$
(3.1)

with the instantaneous energies $E_{a,b}(\lambda)$. This representation is also called *adiabatic* basis because it is, as will become clear later, the solution of the Schrödinger equation with the non-adiabatic couplings neglected.

The spectral decomposition of a quantum mechanical state allows us to expand it into a set of basis vectors and corresponding expansion coefficients. The ultimate goal is to obtain a time evolution of these expansion coefficients. The time is introduced in the parameter λ thus every quantity depending on λ also depends on time. The parameter traverses a closed loop in parameter space. This is explained later in detail.

Because we choose the instantaneous basis, the basis vectors are time dependent, hence the coefficients also have to depend on time. Thus we can express any state in the form

$$|\psi(\boldsymbol{\lambda}(t))\rangle = a(t) |\Phi_a(\boldsymbol{\lambda}(t))\rangle + b(t) |\Phi_b(\boldsymbol{\lambda}(t))\rangle.$$
(3.2)

To eliminate the decay of both states due to the non-Hermeticity of \mathcal{H} , we choose \mathcal{H} to have trace 0. Therefore only the relative loss and gain remain. Because we have only two states, gain/loss of one state are proportional to loss/gain of the other state.

3.1.2. Adiabatic Approximation

The adiabatic approximation of the expansion coefficients of the solution of the Schrödinger equation is given by

$$a_{\rm ad}(t) = a(0) \exp\left(-\frac{i}{\hbar} \int_0^t E_a(t') dt'\right),$$

$$b_{\rm ad}(t) = b(0) \exp\left(+\frac{i}{\hbar} \int_0^t E_a(t') dt'\right),$$
(3.3)

because $E_b = -E_a$. See appendix A.2 for a derivation. From here on, a will always refer to the state with adiabatic gain, while b refers to the state with adiabatic loss.

If $a(t) \gg b(t)$ for $0 \le t \le T$ the system has performed an *adiabatic flip*. In accordance with the original paper we will use the same notation for initial conditions where the index denotes the initial set of parameters:

$$\{a_1(t), b_1(t)\} \quad \leftrightarrow \quad \{a_1(0) = 1, b_1(0) = 0\}, \{a_2(t), b_2(t)\} \quad \leftrightarrow \quad \{a_2(0) = 0, b_2(0) = 1\}.$$

$$(3.4)$$

If the time evolution was adiabatic a(t) and b(t) would remain in their initial state for all times and the populations would be transported around the exceptional point with no loss. Nevertheless, non-adiabatic couplings are present and result in an exchange of the populations.

3.1.3. Flip Error

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The *flip errors* are defined as follows:

gain state flip error:
$$R_1 = \left| \frac{a_1(T)}{b_1(T)} \right|,$$
 (3.5)

loss state flip error:
$$R_2 = \left| \frac{b_2(T)}{a_2(T)} \right|.$$
 (3.6)

With these quantities at hand one can also define the *flip error product* $R_1 \cdot R_2$.

Looking at the definitions of the flip errors one immediately sees that they are given in terms of the "population of the initially occupied state divided by that of the initially unoccupied". Please note that the representation (3.2) is used and that the states $|\Phi_a\rangle$ and $|\Phi_b\rangle$ interchange during the circle. Hence, in the adiabatic approximation we expect the errors to diverge since, e.g. $b_1(T) = 0$ and $a_1(T) \neq 0$ for a temporal evolution according to (3.3), i.e. no flip occurred.

3.1.4. Hamiltonian

To simulate an explicit system we will need a Hamiltonian which satisfies all required properties. Hence

$$\mathcal{H} = \mathcal{H}_0 + \sum_{j=1}^2 \lambda_j(t) \mathcal{H}_j = \begin{bmatrix} 1 & i \\ i & -1 \end{bmatrix} + \sum_{j=1}^2 \lambda_j(t) \mathcal{H}_j$$
(3.7)

is chosen, where \mathcal{H}_{i} are symmetric coupling matrices that do not commute with \mathcal{H}_{0} .

To perform a loop in the parameter space we need to choose appropriate parameters. A good choice is

$$\boldsymbol{\lambda}(t) = \begin{bmatrix} \lambda_1(t) \\ \lambda_2(t) \end{bmatrix} = \begin{bmatrix} \alpha_1 + \beta_1 \cos\left(\frac{2\pi}{T}t + \phi\right) \\ \alpha_2 + \beta_2 \sin\left(\frac{2\pi}{T}t + \phi\right) \end{bmatrix},\tag{3.8}$$

because we move and deform the loop by changing the parameters. To move the centre $\alpha_{1,2}$ are used and $\beta_{1,2}$ adjust the semiaxes of the ellipse. The angle ϕ defines the starting point in terms of an offset angle. For the coupling matrices the Pauli matrices are chosen, namely $\mathcal{H}_1 = \sigma_x$ and $\mathcal{H}_2 = \sigma_z$. Then (3.7) is

$$\mathcal{H} = \begin{bmatrix} 1 + \alpha_2 + \beta_2 \sin\left(\frac{2\pi}{T}t + \phi\right) & i + \alpha_1 + \beta_1 \cos\left(\frac{2\pi}{T}t + \phi\right) \\ i + \alpha_1 + \beta_1 \cos\left(\frac{2\pi}{T}t + \phi\right) & -1 - \alpha_2 - \beta_2 \sin\left(\frac{2\pi}{T}t + \phi\right) \end{bmatrix}.$$
(3.9)

3.2. NUMERICAL CALCULATIONS

There are several methods to compute the desired quantities. To calculate the flip errors we need to obtain the time evolution of the expansion coefficients a and b. From above we know that an arbitrary state reads

$$|\psi(\boldsymbol{\lambda}(t))\rangle = a(t) |\Phi_a(\boldsymbol{\lambda}(t))\rangle + b(t) |\Phi_b(\boldsymbol{\lambda}(t))\rangle.$$
(3.2)

There are several different ways of getting the time evolution of the coefficients.

3.2.1. Instantaneous Basis

The time-dependent Schrödinger equation reads

$$i\hbar\partial_t |\psi\rangle = \mathcal{H} |\psi\rangle.$$
 (3.10)

Inserting the state $|\psi\rangle$ from above yields

$$i\hbar\partial_t \big[a(t) |\Phi_a(\boldsymbol{\lambda}(t))\rangle + b(t) |\Phi_b(\boldsymbol{\lambda}(t))\rangle \big] = \mathcal{H} \big[a(t) |\Phi_a(\boldsymbol{\lambda}(t))\rangle + b(t) |\Phi_b(\boldsymbol{\lambda}(t))\rangle \big].$$
(3.11)

Now we use (3.1) to obtain

$$\dot{a}(t) |\Phi_a\rangle + a(t)\partial_t |\Phi_a\rangle + \dot{b}(t) |\Phi_b\rangle + b(t)\partial_t |\Phi_b\rangle = -\frac{\mathrm{i}}{\hbar} \left[a(t)E_a |\Phi_a\rangle + b(t)E_b |\Phi_b\rangle \right].$$
(3.12)

This can be seen as a set of two equations because multiplying with either $\langle \Phi_a | \text{ or } \langle \Phi_b |$ and using $\langle \Phi_a | \Phi_a \rangle = 1$ and $\langle \Phi_a | \Phi_b \rangle = 0$, results in

$$\dot{a}(t) = -\frac{i}{\hbar}a(t)E_a - a(t)\langle\Phi_a|\partial_t\Phi_a\rangle - b(t)\langle\Phi_a|\partial_t\Phi_b\rangle,$$

$$\dot{b}(t) = -\frac{i}{\hbar}b(t)E_b - a(t)\langle\Phi_b|\partial_t\Phi_a\rangle - b(t)\langle\Phi_b|\partial_t\Phi_b\rangle.$$
(3.13)

Calculation of $\partial_t |\Phi_{a,b}\rangle$ There are two methods to calculate $\partial_t |\Phi_{a,b}\rangle$, an analytical one and a numerical one. The numerical method is rather easy, as we just use the differential quotient to get an approximation for the derivative. We could have used a higher order approximation with smaller truncation error, but the results of the first order method were already quite similar to those produced by the analytical solution.

$$\partial_t |\Phi_{a,b}(\boldsymbol{\lambda}(t))\rangle \approx \frac{|\Phi_{a,b}(\boldsymbol{\lambda}(t+h))\rangle - |\Phi_{a,b}(\boldsymbol{\lambda}(t))\rangle}{h} + \mathcal{O}(h).$$
(3.14)

An analytical solution can be obtained by differentiating both sides of the Schrödinger equation with respect to t and applying the product rule.

$$\frac{\partial}{\partial t} \left(\mathcal{H}(\boldsymbol{\lambda}(t)) \left| \Phi_{a,b}(\boldsymbol{\lambda}(t)) \right\rangle \right) = \frac{\partial}{\partial t} \left(E_{a,b}(\boldsymbol{\lambda}(t)) \left| \Phi_{a,b}(\boldsymbol{\lambda}(t)) \right\rangle \right) \\ \left(\partial_t \mathcal{H} \right) \left| \Phi_{a,b} \right\rangle + \mathcal{H} \partial_t \left| \Phi_{a,b} \right\rangle = \left(\partial_t E_{a,b} \right) \left| \Phi_{a,b} \right\rangle + E_{a,b} \partial_t \left| \Phi_{a,b} \right\rangle$$

This set of equation can be written in a matrix form, which reads

$$\begin{bmatrix} \mathcal{H} - \begin{bmatrix} E_{a,b} & 0\\ 0 & E_{a,b} \end{bmatrix} & |\Phi_{a,b}\rangle \\ \hline \langle \Phi_{a,b}| & 0 \end{bmatrix} \begin{bmatrix} \partial_t |\Phi_{a,b}\rangle \\ \partial_t E_{a,b} \end{bmatrix} = \begin{bmatrix} -(\partial_t \mathcal{H}) |\Phi_{a,b}\rangle \\ 0 \end{bmatrix}.$$
(3.15)

Solving this set of equation yields the vector $(\partial_t | \Phi_{a,b} \rangle, \partial_t E_{a,b})^{\top}$, where we dismiss $\partial_t E_{a,b}$.

3.2.2. Natural Basis

To avoid the calculation of derivatives for the eigenvectors we do a basis transform. We choose $|\psi\rangle$ to be

$$|\psi(\boldsymbol{\lambda}(t))\rangle = a(t) |\Phi_a(\boldsymbol{\lambda}(t))\rangle + b(t) |\Phi_b(\boldsymbol{\lambda}(t))\rangle = c_1(t) |\uparrow\rangle + c_2(t) |\downarrow\rangle \equiv \begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix}, \quad (3.16)$$

where the whole time dependency is contained in c_i and constant basis vectors are used. These basis vectors, $|\uparrow\rangle$ and $|\downarrow\rangle$, are the eigenvectors of σ_z . The states $|\Phi_i\rangle$ can also be represented by means of this basis with

$$|\Phi_i(\boldsymbol{\lambda}(t))\rangle = \Phi_{i,1}(\boldsymbol{\lambda}(t)) |\uparrow\rangle + \Phi_{i,2}(\boldsymbol{\lambda}(t)) |\downarrow\rangle.$$
(3.17)

Now the differential equations for the time evolution are fairly easy and read

$$\dot{c}_{1}(t) = -\frac{1}{\hbar} \Big[\mathcal{H}_{11}c_{1}(t) + \mathcal{H}_{12}c_{2}(t) \Big],
\dot{c}_{2}(t) = -\frac{i}{\hbar} \Big[\mathcal{H}_{21}c_{1}(t) + \mathcal{H}_{22}c_{2}(t) \Big],$$
(3.18)

where \mathcal{H}_{ij} are the matrix elements of \mathcal{H} in σ_z -representation as given in (3.9).

The tricky thing remaining is that we want to get the time evolution of a and b, but got the time evolution of c_1 and c_2 . Thus we will need to map these back. This is done by multiplying $|\psi\rangle$ with either $\langle \Phi_a(\boldsymbol{\lambda}(t))|$ to obtain a(t) or $\langle \Phi_b(\boldsymbol{\lambda}(t))|$ to obtain b(t):

$$a(t) = \left\langle \Phi_a(\boldsymbol{\lambda}(t)) \middle| \begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} \right\rangle, \quad b(t) = \left\langle \Phi_b(\boldsymbol{\lambda}(t)) \middle| \begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} \right\rangle.$$
(3.19)

3.2.3. Interaction picture

The interaction picture helps us to solve problems of the form

$$i\hbar\partial_t |\psi\rangle = \left[\mathcal{H}_0 + V(t)\right] |\psi\rangle \tag{3.20}$$

by simplifying this to

$$i\hbar\partial_t \left|\psi\right\rangle_I = V_I(t) \left|\psi\right\rangle_I \tag{3.21}$$

with

$$\begin{aligned} |\psi\rangle_I &= e^{\frac{i}{\hbar}\mathcal{H}_0 t} |\psi\rangle \,,\\ V_I(t) &= e^{\frac{i}{\hbar}\mathcal{H}_0 t} V(t) e^{-\frac{i}{\hbar}\mathcal{H}_0 t}. \end{aligned} (3.22)$$

We insert $V_I(t)$ and substitute $V(t) = \mathcal{H} - \mathcal{H}_0$ where we chose, in contrast to (3.7), $\mathcal{H}_0 = \sigma_z$. Also we set $|\psi(t)\rangle_I = (d_1(t), d_2(t))^\top$ and obtain

$$\partial_t \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = -\frac{\mathbf{i}}{\hbar} \mathbf{e}^{\frac{\mathbf{i}}{\hbar}\sigma_z t} (\mathcal{H} - \sigma_z) \mathbf{e}^{-\frac{\mathbf{i}}{\hbar}\sigma_z t} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}.$$
(3.23)

One can show that this is equivalent to

$$\partial_t \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = -\frac{i}{\hbar} \begin{bmatrix} (\mathcal{H}_{11} - 1)d_1 + \mathcal{H}_{12}e^{\frac{i}{\hbar}2t}d_2 \\ \mathcal{H}_{21}e^{-\frac{i}{\hbar}2t}d_1 + (\mathcal{H}_{11} + 1)d_2 \end{bmatrix}.$$
 (3.24)

For a more extensive calculation see appendix A.3.

As before for the natural basis we will need to map these coefficients back to a(t) and b(t). The first step is to obtain $c_1(t)$ and $c_2(t)$ by inverting $|\psi\rangle_I$:

$$\begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} = e^{-\frac{i}{\hbar}\mathcal{H}_0 t} \begin{bmatrix} d_1(t) \\ d_2(t) \end{bmatrix} = \begin{bmatrix} e^{-\frac{i}{\hbar}t} d_1(t) \\ e^{\frac{i}{\hbar}t} d_2(t) \end{bmatrix}$$
(3.25)

This result can then be used in (3.19).

3.2.4. Initial Conditions

In the previous section we transformed to other bases. This introduces the need to calculate the initial conditions for the new coefficients as these do not represent a(0) and b(0). We will now take a look at the initial conditions for $c_1(t)$ and $c_2(t)$. We know from (3.19) that

$$a(0) = \left\langle \Phi_a(0) \left| \begin{bmatrix} c_1(0) \\ c_2(0) \end{bmatrix} \right\rangle, \quad b(0) = \left\langle \Phi_b(0) \left| \begin{bmatrix} c_1(0) \\ c_2(0) \end{bmatrix} \right\rangle. \tag{3.26}$$

We need to solve this system of equations for $c_1(0)$ and $c_2(0)$. The solution reads

$$c_1(0) = \left. \frac{b\Phi_{a,2} - a\Phi_{b,2}}{\Phi_{a,2}\Phi_{b,1} - \Phi_{a,1}\Phi_{b,2}} \right|_{t=0}, \quad c_2(0) = \left. \frac{a\Phi_{b,1} - b\Phi_{a,1}}{\Phi_{a,2}\Phi_{b,1} - \Phi_{a,1}\Phi_{b,2}} \right|_{t=0}, \quad (3.27)$$

where $\Phi_{i,j}$ denotes the *j*-th component of Φ_i in the σ_z -basis.

The initial conditions $d_1(0)$ and $d_2(0)$ are the same as $c_1(0)$ and $c_2(0)$ because $e^{\alpha \cdot 0} = 1$ for all $\alpha \in \mathbb{C}$.

3.2.5. The Process

The eigenvalues and eigenvectors were calculated using the LAPACK library for FORTRAN by Anderson et al. (1999), and a classical 4-th order Runge-Kutta integrator was used to solve the differential equations for the expansion coefficients.

To complete one circle of cycle time T_i 1000 steps were performed. For the flip error 100 calculations were run between T = 0 and the maximum cycle time of $T_{\text{max}} = 20$.

3.3. RESULTS

3.3.1. Parameter Sets

Calculations were run for two different sets of parameters describing two different trajectories in parameter space. The first is a circular loop with the coefficients

$$S_{\text{circle}} = \{ \alpha_1 = 0, \alpha_2 = 0, \beta_1 = 0.8, \beta_2 = 0.8, \phi = \pi \}$$
(3.28)

used in the circle defined by (3.8). The resulting interchange of the eigenvalues is plotted in figure 3.1 alongside with the trajectories in parameter space.

With the second set an elliptic parameters space loop is done:

$$S_{\text{ellipse}} = \{ \alpha_1 = 0, \alpha_2 = 0.3, \beta_1 = 0.45, \beta_2 = 0.9, \phi = \pi \}$$
(3.29)

The same quantities as for the circle are plotted in figure 3.2.

3.2.4



Figure 3.1. In (a) the behaviour of the eigenvalues when encircling the exceptional point with the trajectory in parameter space as plotted in (b) is shown. The starting points have been marked with a filled square. The trajectory of $\lambda(t)$ has the form of a circle as described in (3.28) — not plotted proportionally to maintain comparability to the elliptic trajectory.



Figure 3.2. In (a) the behaviour of the eigenvalues when encircling the exceptional point with the trajectory in parameter space as plotted in (b) is shown. The starting points have been marked with a filled square. The trajectory of $\lambda(t)$ has the form of an ellipse as described in (3.29).

3.3.2. Time Evolution for One Cycle

Now, for both sets of parameters we do a cycle of time T = 10 in parameter space and evaluate the expansion coefficients. The expansion coefficients are calculated using all of the methods described above. Except for the adiabatic approximation all of them are equivalent and should produce the same results. The results are displayed in figure 3.3 (circle) and 3.4 (ellipse). The two expansion coefficients a(t) and b(t) are distinguished by different colours. The various methods used are marked with different symbols. The coefficients computed by means of the *instantaneous basis* are marked with solid lines,



Figure 3.3. Time evolution of the expansion coefficients for a whole cycle of time T = 10 for the circular trajectory (3.28) in parameter space. The two plots represent two different initial conditions: (a) is the plot for the system initially in the gain state, hence a(0) = 1, b(0) = 0; (b) is for an initial population in the loss state, meaning a(0) = 0, b(0) = 1. The coefficient a(t) is plotted in red, b(t) in blue. The various symbols distinguish between the methods used. Solid lines were calculated in the instantaneous basis, filled squares in the natural basis, filled dots by means of the interaction picture and the empty squares are the adiabatic approximation which is only shown in (a) since only this initial condition behaves approximately adiabatic.

those of the *natural basis* with filled squares, those calculated in the *interaction picture* with filled dots and those of the *adiabatic approximation* with empty squares. The first three methods perfectly match and all solutions reside on top of each other. For the initial condition $\{a(0) = 1, b(0) = 0\}$ the adiabatic approximation was also evaluated which matched the curves as well.

The adiabatic approximation suggests that the initially unpopulated state remains at zero population, but due to non-adiabatic transitions which are possible in the full temporal evolution of the Schrödinger equation (c.f. matrix elements $\langle \Phi_a | \partial_t | \Phi_b \rangle$ and $\langle \Phi_b | \partial_t | \Phi_a \rangle$ in (3.13)) it is excited as well and gains in amplitude. The evolution shown in figures 3.3 (a) and 3.4 (a) can still be considered to be adiabatic because the amplitude of a(t) is about one to two orders of magnitude larger than that of b(t).

This only holds for the initial condition $\{a(0) = 1, b(0) = 0\}$. For the other condition the result differs heavily. In this case a(t) shows the same growth behaviour as b(t) in the first case and b(t) decays, cf. figure 3.3 (b). After some time $(t \approx 3) \ b(t)$ starts to grow. However, it never reaches an amplitude larger than that of a(t). Still at the end of the circle the distance between the two curves is about one order of magnitude, so in the end we obtained a majority population of the same state as for the other initial condition.

This is an important result of the simple example. The adiabatic state flip expected at an exceptional point is not found in the full time evolution. Instead we found that at the end of a closed loop around an exceptional point the system ends up in the same eigenstate!



Figure 3.4. Time evolution of the expansion coefficients for a whole cycle of time T = 10 for the elliptic trajectory (3.29) in parameter space. The two plots represent two different initial conditions: (a) is the plot for the system initially in the gain state, hence a(0) = 1, b(0) = 0; (b) is for an initial population in the loss state, meaning a(0) = 0, b(0) = 1. The coefficient a(t) is plotted in red, b(t) in blue. The various symbols distinguish between the methods used. Solid lines were calculated in the instantaneous basis, filled squares in the natural basis, filled dots by means of the interaction picture and the empty squares are the adiabatic approximation.

3.3.3. Flip Error and Flip Error Product

The cycles were also done for varying cycle time $T_i \in [0, 20]$ and the flip error was computed. The flip errors for the different paths and different initial conditions can be viewed in figures 3.5 (circle) and 3.6 (ellipse). As expected for $T_i \to 0$ the flip error diverges because the exceptional point is encircled so fast that only a non-adiabatic behaviour is possible.

Since the state at the end of a circle is always the same (up to a multiplicative prefactor independent of the initial condition) for sufficiently large cycle times the flip error product converges to one for $T \to \infty$.



Figure 3.5. Flip errors and flip error product for the circular trajectory. In (a) the flip errors are shown; we recall that R_1 is the flip error for the initial condition a(0) = 1, b(0) = 0 and R_2 corresponds to a(0) = 0, b(0) = 1. In (b) the flip error product $R_1 \cdot R_2$ is plotted.



Figure 3.6. Flip errors and flip error product for the elliptical trajectory. In (a) the flip errors are shown. In (b) the flip error product $R_1 \cdot R_2$ is plotted.

EXCEPTIONAL POINTS IN THE SPECTRA OF THE HYDROGEN ATOM

The present chapter will deal with the basic behaviour of the hydrogen atom in crossed external electric and magentic fields. We will discuss the structure of the Hamiltonian and show the transition to a matrix representation given by the well known creation and annihilation operators of the two-dimensional harmonic oscillator. This chapter follows the discussion in Cartarius (2008, Chapter 5).

4.1. HAMILTONIAN

In static external electric and magnetic fields additional terms to the unperturbed hydrogen atom's Hamiltonian need to be considered. In the following text we will assume a static and homogeneous electric field to point in x direction while a static and homogeneous magnetic field is directed along the z direction. Therefore the expressions for those read

$$\boldsymbol{E} = E\boldsymbol{e}_x , \quad \boldsymbol{B} = B\boldsymbol{e}_z, \tag{4.1}$$

where e_i denotes the cartesian unity vector in direction *i*.

The Hamiltonian without relativistic corrections and finite nuclear mass effects can be written as

$$\mathcal{H} = \frac{1}{2m_e} p^2 - \underbrace{\frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}}_{(C)} + \underbrace{\frac{1}{2} \frac{e}{m_e} BL_z}_{(P)} + \underbrace{\frac{1}{8} \frac{e^2}{m_e} B^2(x^2 + y^2)}_{(D)} + \underbrace{eEx}_{(E)}, \tag{4.2}$$

with p denoting the kinetic momentum of the electron, r the distance vector from the origin (here nucleus) and L_z the component of the angular momentum parallel to the external magnetic field. The Hamiltonian contains, besides the kinetic energy, the Coulomb potential (C), a paramagnetic term (P), a diamagnetic term (D) and a potential raised by the electric field (E).

To simplify the representation of the Hamiltonian we introduce atomic Hartree units (cf. appendix B) such that the Hamiltonian reads

$$\mathcal{H} = \frac{1}{2}\boldsymbol{p}^2 - \frac{1}{r} + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2 (x^2 + y^2) + fx \tag{4.3}$$

with the scaled field strengths $f = E/E_0^h$ and $\gamma = B/B_0^h$ (cf. table B.1).

For the numerical calculations to be carried out more easily, the Hamiltonian is transformed to dilated semiparabolic coordinates, see Cartarius (2008, Appendix B) for a more extensive calculation. The main transformation rules are summarised here:

$$\mu = \frac{1}{b}\sqrt{r+z} , \quad \nu = \frac{1}{b}\sqrt{r-z} , \quad \varphi = \arctan\frac{y}{x}.$$
(4.4)

For the sake of brevity only the transformed equation will be presented here:

$$\left\{ \nabla^2_{\mu} + \nabla^2_{\nu} - \left(\mu^2 + \nu^2\right) + b^4 \gamma \left(\mu^2 + \nu^2\right) i \frac{\partial}{\partial \varphi} - \frac{1}{4} b^8 \gamma^2 \mu^2 \nu^2 \left(\mu^2 + \nu^2\right) - 2b^6 f \mu \nu \left(\mu^2 + \nu^2\right) \cos \varphi + 4b^2 \right\} \left|\psi\right\rangle = \lambda \left(\mu^2 + \nu^2\right) \left|\psi\right\rangle \quad (4.5)$$

with the dilated semiparabolic coordinates μ , ν , φ , and the free dilation parameter *b*. In a matrix form this equation corresponds to a generalised eigenvalue problem with the eigenvalue

$$\lambda = -(1 + 2b^4 E). \tag{4.6}$$

To abbreviate the regularised Hamiltonian further we introduce several terms which will help finding a matrix form. First of all the two harmonic oscillators are contracted,

$$\nabla_{\mu}^{2} + \nabla_{\nu}^{2} - \left(\mu^{2} + \nu^{2}\right) = \frac{1}{\mu} \frac{\partial}{\partial \mu} \mu \frac{\partial}{\partial \mu} + \frac{1}{\mu^{2}} \frac{\partial^{2}}{\partial \varphi^{2}} + \frac{1}{\nu} \frac{\partial}{\partial \nu} \nu \frac{\partial}{\partial \nu} + \frac{1}{\nu^{2}} \frac{\partial^{2}}{\partial \varphi^{2}} - \left(\mu^{2} + \nu^{2}\right)$$
$$= -2\mathcal{H}_{0}.$$
(4.7)

The analogy to the two-dimensional harmonic oscillator is obvious, hence a good choice for the basis set is a basis of two two-dimensional harmonic oscillators with a common angular momentum due to the appearance of the same φ in both oscillator terms,

$$|n_{\mu}, n_{\nu}, m\rangle = |n_{\mu}, m\rangle \otimes |n_{\nu}, m\rangle, \qquad (4.8)$$

where $|n_{\mu}, m\rangle$ and $|n_{\nu}, m\rangle$ are eigenstates of the commuting operators

$$N = a_1^{\dagger} a_1 + a_2^{\dagger} a_2,$$

$$L = i(a_1 a_2^{\dagger} - a_1^{\dagger} a_2) = (q_1 p_2 - q_2 p_1)$$
(4.9)

of the two-dimensional harmonic oscillator. The operators are a_i and a_i^{\dagger} the well known ladder operators of the one-dimensional harmonic oscillator, see Messiah (1991).

To calculate the resonances of the system a complex rotation is applied. Complex rotation permits to calculate resonances. These appear as additional discrete eigenvalues. They possess an imaginary part, which takes the role of a decay rate. The complete calculation is done in Cartarius (2008, Section 3.4) and will not be presented here. In summary the complex scaling parameter as introduced in (4.4)

$$b^2 = |b^2| \mathrm{e}^{\mathrm{i}\vartheta} \tag{4.10}$$

performs the complex rotation

$$r \to r \,\mathrm{e}^{\mathrm{i}\vartheta}.$$
 (4.11)

The complex scaled Schrödinger equation reads

$$\begin{cases} -2\mathcal{H}_{0}+|b|^{4}\mathrm{e}^{\mathrm{i}2\vartheta}\gamma\left(\mu^{2}+\nu^{2}\right)\mathrm{i}\frac{\partial}{\partial\varphi}-\frac{1}{4}|b|^{8}\mathrm{e}^{\mathrm{i}4\vartheta}\gamma^{2}\mu^{2}\nu^{2}\left(\mu^{2}+\nu^{2}\right)\\ -2|b|^{6}\mathrm{e}^{\mathrm{i}3\vartheta}f\mu\nu\left(\mu^{2}+\nu^{2}\right)\cos\varphi+4|b|^{2}\mathrm{e}^{\mathrm{i}\vartheta}+\left(\mu^{2}+\nu^{2}\right)\\ \end{cases} e^{-\mathrm{i}2\vartheta}\left|\psi\right\rangle=2|b|^{4}E\left(\mu^{2}+\nu^{2}\right)\left|\psi\right\rangle. \tag{4.12}$$

1

A non-Hermitian matrix representation is obtained by evaluating the matrix elements of the Schrödinger equation with the basis (4.8) and reads

$$\mathcal{A}(\gamma, f) |\psi\rangle = 2|b|^4 E \mathcal{B} |\psi\rangle, \qquad (4.13)$$

where $\mathcal{A}(\gamma, f)$ is the time-dependent complex-symmetric Hamiltonian and \mathcal{B} is a real symmetric positive-definite metric.

The operators mentioned above have a banded structure if written in matrix form. Thus, both $\mathcal{A}(\gamma, f)$ and \mathcal{B} will have a banded structure as well. The matrices were built using up to 17 300 states resulting in a band width of approximately 1200 elements. Resonances were then computed using the ARPACK library, cf. Lehoucq et al. (1998).

4.2. EXCEPTIONAL POINTS

The procedure of searching for exceptional points is described in detail in Cartarius (2008, Section 5.2). The Hamiltonian derived previously depends on two parameters, viz. γ and f. To encircle an exceptional point in the parameter space these parameters need to be adjusted to create a looping trajectory. A good choice is a simple "circle" given by the set

$$\gamma(\varphi) = \gamma_0 (1 + \delta \cos \varphi),$$

$$f(\varphi) = f_0 (1 + \delta \sin \varphi)$$
(4.14)

with the centre (γ_0, f_0) of the circle and a "relative" radius δ . The time is represented by the angle φ .

Because in this work time-dependent transport of encircling exceptional points is investigated and a large number of them is already known we use those listed in table 4.1, which were taken from Cartarius (2008, p. 69), but were published in Cartarius et al. (2009) as well.

4.3. EXPANSION COEFFICIENTS

As already discussed in chapter 3 we are interested in the expansion coefficients of an initial state with respect to a given basis during a parameter space circle. First of all we will derive the differential equation for the coefficients in extension of the procedure introduced in section 3.2.2. We start from the matrix respresentation of the Schrödinger equation,

$$\mathcal{A}(\gamma, f) |\psi\rangle = 2|b|^4 E \mathcal{B} |\psi\rangle \tag{4.15}$$

and insert

$$|\psi(t)\rangle = \sum_{i} \xi_{i}(t) |\phi_{i}\rangle$$
(4.16)

with the eigenvectors $|\phi_i\rangle$ of the Hamiltonian at the starting point on the circle. We will keep these basis states fixed for the whole temporal evolution. Please note that they are

#	γ	f	$\operatorname{Re}(E)$	$\operatorname{Im}(E)$
01	0.002335	0.0001177	-0.01767	-0.000103
02	0.002575	0.000117114	-0.015067	-0.0000823
03	0.002752	0.0001298	-0.015714	-0.00022637
04	0.0030152	0.0001231	-0.01209	-0.000099
05	0.003045	0.0001332	-0.015812	-0.0001896
06	0.0030460	0.000127302	-0.017624	-0.000087
07	0.0037915	0.0001535	-0.01240	-0.000164
08	0.004604	0.0002177	-0.022135	-0.00006878
09	0.004714	0.00021529	-0.01394	-0.00010
10	0.00483	0.000213	-0.01255	-0.00030
11	0.00529	0.0002011	-0.0150	-0.000136
12	0.00537	0.000214	-0.01884	-0.0000679
13	0.005388	0.0002619	-0.02360	-0.00015
14	0.00572	0.000256	-0.01984	-0.000258
15	0.00611	0.000256	-0.01593	-0.00024
16	0.00615	0.000265	-0.0158	-0.000374
17	0.00776	0.000301	-0.0179	-0.000756

Table 4.1. List of exceptional points in the spectrum of the hydrogen atom in crossed external electric and magentic field. The values are given in atomic units, numbers are used to reference the exceptional points in the text.

not eigenstates of the Hamiltonian for other points (γ, f) on the circle. We obtain

$$\begin{split} E\mathcal{B} \left| \psi \right\rangle &= \frac{1}{2|b|^4} \mathcal{A}(\gamma, f) \left| \psi \right\rangle, \\ \mathrm{i}\hbar \partial_t \mathcal{B} \left| \psi \right\rangle &= \frac{1}{2|b|^4} \mathcal{A}(\gamma, f) \left| \psi \right\rangle, \\ \partial_t \mathcal{B} \left| \psi \right\rangle &= -\frac{\mathrm{i}}{\hbar} \frac{1}{2|b|^4} \mathcal{A}(\gamma, f) \left| \psi \right\rangle, \\ \partial_t \mathcal{B} \sum_i \xi_i(t) \left| \phi_i \right\rangle &= -\frac{\mathrm{i}}{\hbar} \frac{1}{2|b|^4} \mathcal{A}(\gamma, f) \sum_i \xi_i(t) \left| \phi_i \right\rangle \end{split}$$

Now we choose ξ_j by multiplying with $\langle \phi_j |$,

$$\partial_t \xi_j(t) = -\frac{\mathrm{i}}{\hbar} \frac{1}{2|b|^4} \sum_i \langle \phi_j | \mathcal{A}(\gamma, f) | \phi_i \rangle \ \xi_i(t) \ .$$
(4.17)

To obtain this formula the orthogonality of the eigenstates with regard to the matrix ${\cal B}$ was used, i.e.

$$\langle \phi_i | \mathcal{B} | \phi_i \rangle = 1 , \quad \langle \phi_i | \mathcal{B} | \phi_j \rangle = \delta_{ij} .$$
 (4.18)

STATE FLIP FOR RESONANCES OF THE HYDROGEN ATOM

5.1. PRELIMINARIES

Before we begin to evaluate the simulations we need to make clear some facts. First of all we investigate the decay of states. Consider the time evolution of a pure state's density matrix,

$$\partial_t \varrho(t) = \partial_t (|\psi(t)\rangle \langle \psi(t)|), = |\partial_t \psi(t)\rangle \langle \psi(t)| + |\psi(t)\rangle \langle \partial_t \psi(t)|$$

where we use the time-dependent Schrödinger equation $i\hbar \partial_t |\psi\rangle = H |\psi\rangle$,

$$= -\frac{\mathrm{i}}{\hbar}H |\psi(t)\rangle \langle \psi(t)| + \frac{\mathrm{i}}{\hbar} |\psi(t)\rangle \langle \psi(t)| H^{\dagger}.$$

In case that $|\psi\rangle$ also fulfils the stationary Schördinger equation $H|\psi\rangle = E|\psi\rangle$ we obtain

$$\partial_{t} \varrho(t) = -\frac{i}{\hbar} E |\psi(t)\rangle \langle \psi(t)| + \frac{i}{\hbar} |\psi(t)\rangle \langle \psi(t)| E^{*}$$

$$= -\frac{i}{\hbar} (E - E^{*}) |\psi(t)\rangle \langle \psi(t)|$$

$$= -\frac{i}{\hbar} 2i \operatorname{Im} E |\psi(t)\rangle \langle \psi(t)|$$

$$\partial_{t} \varrho(t) = \frac{2}{\hbar} \operatorname{Im} E \varrho(t) . \qquad (5.1)$$

This is a first-order ordinary differential equation with the somewhat trivial solution

$$\varrho(t) = \varrho(t_0) \,\mathrm{e}^{2\,\mathrm{Im}\,E\,t/\hbar}.\tag{5.2}$$

Because resonances have a negative imaginary part this corresponds to a decay. Obviously one has that resonances with smaller absolute imaginary part decay slower. Because we defined

$$|\psi(t)\rangle = \sum_{i} \xi_{i}(t) |\phi_{i}\rangle$$
(5.3)

the density matrix is proportional to products of the expansion coefficients of a state $|\psi\rangle$. Therefore also the expansion coefficients will incorporate a decay term

$$\xi_i(t) \sim \mathrm{e}^{\mathrm{Im}\,E_i\,t}.\tag{5.4}$$

We will keep that result in mind for a moment and carry on to the weighted coefficients.

To illustrate the relative gain and loss we define the weighted coefficients $\bar{\xi}$

$$\bar{\xi}_i = |\xi_i|^2 \left(\sum_{j=1}^N |\xi_j|^2\right)^{-1} = \left(\sum_{j=1}^N \frac{|\xi_j|^2}{|\xi_i|^2}\right)^{-1},\tag{5.5}$$

where N is the total number of states taken into account. In this representation there is a term $|\xi_i|^2/|\xi_i|^2$. Hence the decay of ξ_i cancels out.

We already saw the representation of a state $|\psi\rangle$ by its spectral decomposition (5.3) but have so far not chosen a basis. The basis vectors are chosen to be the eigenvectors of the resonances at the beginning of a parameter space circle, i.e.

$$\mathcal{H}(0) \left| \phi_i(0) \right\rangle = E_i(0) \left| \phi_i(0) \right\rangle.$$
(5.6)

In accordance with Klett (2014) we will call this basis set "zero"-basis.

5.2. STATE FLIP AT AN EXCEPTIONAL POINT

In this section the behaviours of the expansion coefficients at an exceptional point are discussed. In figure 5.1 a map of resonances at exceptional points is shown. In total three resonances and their paths in the complex energy plane for a closed loop in the parameter space (γ, f) are depicted. In the inset of subfigure (a) three different paths traversed are shown. The symbols placed on the parameter space path denote the starting point and can also be used to identify the corresponding energy map, e.g. the loop marked with a triangle in the inset corresponds to subfigure (c) because there the starting points are also marked with triangles. Note that all energy maps plotted in figure 5.1 apply for a parameter set where the parameter loop is traversed in mathematically positive direction.

The exceptional points were encircled with different parameter sets. Therefore the field strengths were modified a little and read

$$\gamma(\varphi) = \gamma_0 \{ 1 + \delta \cos[\chi(\varphi + \varphi_0)] \},$$

$$f(\varphi) = f_0 \{ 1 + \delta \sin[\chi(\varphi + \varphi_0)] \},$$
(5.7)

with γ_0 and f_0 being the field strengths at the centre of the circle, the relative radius δ , the chirality χ and the offset φ_0 . In this section a superposition of the following parameters will be

$$\delta = 10^{-2} , \quad \chi = \begin{cases} 1 \\ -1 \end{cases} , \quad \varphi_0 = \begin{cases} 0 \\ \pi/4 \end{cases} .$$
 (5.8)

The parameters set in use is denoted in the form $S = \{\chi, \varphi_0\}$. The eigenvalues E_i , eigenvectors $|\phi_i\rangle$ and expansion coefficients ξ_i are numbered. If any numerical values are given for the coefficients the mantissa is always rounded to four decimal digits.

5.2.1. Second-order Exceptional Point

Exceptional point #15 from table 4.1 was chosen for the procedure. In figure 5.1 (b) a map is displayed showing the two resonances interchanging their position while encircling the exceptional point. A third resonance in the vicinity does not take part in the exchange process. The parameter set chosen is $S = \{\chi = 1, \varphi_0 = 0\}$.

The temporal evolution of the corresponding expansion coefficients is visible in figure 5.2 on page 24. No matter what the initial state is, the evolution always ends with the weighted population in $\xi_1(t)$ (red). In some stages also ξ_2 (green line) gains in



Figure 5.1. Map of a structure with two exceptional points with which in total three resonances are connected and the trajectories traversed. In the three figures the exceptional points are encircled in different manners, in (a) both #15 and #16, in (b) #15, and in (c) #16. The inset displays the path in parameter space. The symbols for the starting points are the same as in corresponding energy diagram, e.g. the path with the square on it corresponds to (a) because there also squares are used. This case is very similar to a third-order exceptional point.

amplitude while ξ_3 does not really play a role. Even when the initial population is set up in ξ_3 it all passes over to the other two resonances. The fact that the same end state for initial states is encountered may seem familiar with respect to chapter 3, where this behaviour was already observed. We need to exercise caution here, because in chapter 3 all calculations were done in the instantaneous basis or when done in another basis at least projected back on it. In this case the results are still in the "zero"-basis hence we cannot associate the time evolution of the expansion coefficients with the path traversed in the energy plane. For a more detailed discussion see Klett (2014).

5.2.2. Third-order Exceptional Point

As previously published by Cartarius et al. (2009) the exceptional points #15 and #16 form a third-order exceptional point if encircled at once. We will investigate the behaviour of the transport of populations along a closed parameter space loop.

In figure 5.1 (a) a map of the resonances with a third-order exceptional point exchange behaviour is shown together with the paths traversed in parameter space. The symbols placed on the parameter paths denote the starting points. The same symbols are also used in the energy maps to highlight the starting point. For the different parameter sets the loop in parameter space changes slightly and so does the energy diagram. The altered 24



Figure 5.2. Time evolution of the expansion coefficients for encircling a second-order exceptional point with the centre $(\gamma, f) = (6.11 \cdot 10^{-3}, 2.57 \cdot 10^{-4})$, the relative radius $\delta = 10^{-2}$, a chirality of $\chi = 1$, and a phase offset of $\varphi_0 = 0$. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .



Figure 5.3. Energy space trajectories for the different sets of parameters. In the first row one can see that if the chirality is inverted the only effect is that the path is being traversed in reverse. In the lower row a phase offset is introduced. This phase offset is always in the direction of movement, i.e. the phase offset $\varphi_0 = \pi/4$ in case of $\chi = 1$ corresponds to a phase of $-\pi/4$ in the mathematical positive direction, cf. inset of figure 5.1 (a). The meaning of the circles is explained later in the text.

diagram with the corresponding parameter set can be viewed in figure 5.3.

A. Chirality $\chi = 1$, Phase $\varphi_0 = 0$. The first parameter set to be discussed is $S_1 = \{\chi = 1, \varphi_0 = 0\}$, cf. figure 5.3 (a). The temporal evolution of the expansion coefficients is plotted in figure 5.4 on page 27. The three different initial conditions are displayed. First of all it is noted that no matter which state was prepared initially the major part of the population left after the circle always ends up in ξ_1 (red line). For the parameter set in use the eigenvalues move according to figure 5.3 (a), i.e. the major part of the population is in the state marked with a circle at the end of a loop. For picture (b-1) the distribution of the relative final populations is

$$\bar{\xi}_1(T) = 0.9935, \quad \bar{\xi}_2(T) = 0.5175 \cdot 10^{-2}, \quad \bar{\xi}_3(T) = 0.1288 \cdot 10^{-2}.$$
 (5.9)

The difference between the three initial populations is that the time evolution shows a different behaviour during propagation but always ends up in the same final population distribution. In left column—(a-1), (a-2), and (a-3)—the actual populations are plotted. After the cycle time of 100 000 all populations are decayed below 10^{-18} . In principle, it would be better to use shorter times but then the effect in the relative populations would not be visible that clearly, i.e. the final population would be in a superposition instead of in a unique state. The temporal evolution of the population seems counterintuitive at first, because in the energy map in figure 5.1 it seems as if E_3 (blue line) is decaying slower than the others integrated over the whole time. Obviously this statement is not

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that trivial and it is necessary to perform the explicitly time-dependent calculation. Still, in simple cases, where the trajectory of the eigenvalues in energy space are trivial like a semi-circle and without any crossings, then an intuitive connection can be derived from the populations. The correspondence is discussed thoroughly for various cases by Klett (2014).

For the case discussed above a calculation with a shorter total evolution time of 25 000 instead of 100 000 was carried out. The result is displayed in figure 5.5 on page 28. In contrast to the evolution with cycle time 100 000 one can observe in the left column that the decay has not progressed that far and the actual population is still conserved up to the order of 10^{-6} . In the right column the relative populations are plotted. We see that the transition to a single state has not yet fully completed and at the end of the cycle the system remains in a superposition state. Even though it looks like this superposition state is equal for all initial conditions it is not exactly the same. The difference is little and included in the following numerical values as a standard deviation

$$\bar{\xi}_1(T) = 0.8101(160), \quad \bar{\xi}_2(T) = 0.0815(64), \quad \bar{\xi}_3(T) = 0.1083(96).$$
 (5.10)

B. Chirality $\chi = -1$, Phase $\varphi_0 = 0$. Next in line is a slightly altered parameter set $S_2 = \{\chi = -1, \varphi_0 = 0\}$ in that sense that the parameter space path is traversed in the opposite direction, cf. figure 5.3 (b). The temporal evolution is plotted in figure 5.6 on page 29. Again it can be observed that the final state is independent of the initial population with the difference that with this parameter set the population of ξ_3 (blue line) outruns the others instead of ξ_1 (red line), cf. figure 5.4 on page 27. Another aspect is that this altered final state emerges from a different exchange behaviour along the path. But as well as for the first parameter set the major part of the population ended up in ξ_1 (red line) and for $\chi = -1$ it ended up in ξ_3 (blue line) but never in ξ_2 (green line). This is due to the fact that the end point for $\xi_1|_{\chi=1}$ and $\xi_3|_{\chi=-1}$ are the starting point of ξ_2 in any case and the resonances never end up in their starting point after one circle. For reference the relative populations at the end of the cycle are given here

$$\bar{\xi}_1(T) = 0.1553 \cdot 10^{-2}, \quad \bar{\xi}_2(T) = 0.5727 \cdot 10^{-2}, \quad \bar{\xi}_3(T) = 0.9927.$$
 (5.11)

C. Chirality $\chi = 1$, Phase $\varphi_0 = \pi/4$. Another possible parameter set is $S_3 = \{\chi = 1, \varphi_0 = \pi/4\}$ where a phase is introduced. This phase is an offset on the circle in the direction of movement on the circular trajectory in parameter space. An offset in mathematical positive direction does not have that much of an impact on the positions of the start and end points of the paths in energy space, cf. figure 5.3 (c). Hence the distance between the point marked with a circle in figure 5.3 (a) and (b) and the new starting point of ξ_2 or the end point of ξ_1 is small. Based on the previous observations we expect the major part of the final population to remain in ξ_1 (red line) which is eminently satisfied, cf. figure 5.7 on page 30. All in all the exchange behaviour is pretty similar to that of the previous parameter sets.

D. Chirality $\chi = -1$, Phase $\varphi_0 = \pi/4$. The last parameter set to be discussed is $S_4 = \{\chi = -1, \varphi_0 = \pi/4\}$. Now the phase rotates the start point in the other direction and the loop is passed through in reverse. Even though the absolute value of the phase is the same as before the results differ seriously. All end points of the paths of the eigenvalues in figure 5.3 (d) are not even close to the points marked with a circle in figure 5.3 (a) and



Figure 5.4. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = 1$, and a phase offset of $\varphi_0 = 0$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .

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Figure 5.5. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = 1$, and a phase offset of $\varphi_0 = 0$. The total time of the evolution is 25 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .



Figure 5.6. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = -1$, and a phase offset of $\varphi_0 = 0$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .

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Figure 5.7. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = 1$, and a phase offset of $\varphi_0 = \pi/4$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .



Figure 5.8. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = -1$, and a phase offset of $\varphi_0 = \pi/4$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .

(b). As plotted in figure 5.8 on page 31 the population now ends up in a superposition state. The explicit population distribution for all initial populations is given by

$$\bar{\xi}_1(T) = 0.2042 \cdot 10^{-2}, \quad \bar{\xi}_2(T) = 0.7502, \quad \bar{\xi}_3(T) = 0.2477.$$
 (5.12)

This is a good example for the serious dependence on the parameter set used. The result can not be trivially estimated from the path traversed in energy space. It was already mentioned that in such a nontrivial case a complete temporal evolution is necessary to relate the energy diagram to the temporal evolution of the populations. For this state additional calculations with shorter total evolution times of 10 000 and 25 000 instead of 100 000 were carried out. The result is displayed in figure 5.9 on page 33. As before, for $S_1 = \{\chi = 1, \varphi_0 = 0\}$, in the case of a total time of 25 000 the final states' occupation does not differ visually (although they do but only by probabilities of ≈ 0.02), cf. right column in the figure. This behaviour changes for even shorter cycle times, in this case 10 000. Now the exceptional point is encircled so fast that the transition cannot even get close to complete during one cycle. This can be seen best in subfigures (a-2) and (a-3) where the red state dominates at the end while for longer cycle times like in subfigures (b-2) and (b-3) clearly the green state dominates. Also the final states tremendously differ visually.

5.3. IMPACT OF NEARBY RESONANCES

Not only these three resonances were taken into account but in further calculations also three others in the vicinity in energy space. This was done to study the influence of the resonances, with which those of the exceptional points will always couple in a realistic physical system. An expanded energy map can be viewed in figure 5.10 again with the loops in parameter space as an inset. One of the additional resonances is a (nearly) bound state with an imaginary part of approximately $5 \cdot 10^{-5}$, i.e. at the end of a cycle all the population will most likely end up in that state and its weighted expansion coefficient should converge towards 1.

5.3.1. Second-order Exceptional Point

We now evaluate the statement made before that all population should switch to the bound state for #15. To do so, the exceptional point is encircled using the parameter set $S_1 = \{\chi = 1, \varphi_0 = 0\}$. In figure 5.11 on page 35 the resonances involved in the exchange process of the exceptional point are drawn using solid, those not involved with dashed lines. We find that the statement is met perfectly because $\xi_4(T) = 0.9999$ (purple line) even though the initial population was never placed in ξ_4 and it does not take part in any exchange process.

5.3.2. Third-order Exceptional Point

The statement is also evaluated for the third-order exceptional point formed when #15 and #16 are encircled together. The parameter set in use is $S_2 = \{\chi = -1, \varphi_0 = 0\}$. Again the resonances involved in the exchange process of the exceptional point are drawn using solid, those not involved with dashed lines, cf. figure 5.12 on page 36. The conjecture that the final population will be completely in this state still holds. We find that this matched perfectly for a third-order exceptional point with $\xi_4(T) = 0.9999$ (purple line).

Another interesting result is that the speed of the dissipation to ξ_5 depends on the distance of the initially populated resonance to the bound state. The closer the initially populated state is to the bound state in energy space the fast the dissipation, i.e. E_3



Figure 5.9. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = -1$, and a phase offset of $\varphi_0 = \pi/4$. In the left column the weighted coefficients for a total evolution time of 10 000 are displayed, in the right column for a total evolution time of 25 000. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 .

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Figure 5.10. Map of a structure with two exceptional points with which in total three resonances are connected and the trajectories traversed. In the three figures the exceptional points are encircled in different manners, in (a) both #15 and #16, in (b) #15, and in (c) #16. The inset displays the path in parameter space. The symbols for the starting points are the same as in corresponding energy diagram, e.g. the path with the square on it corresponds to (a) because there also squares are used. In addition to the resonances already shown in figure 5.3, three further resonances, depicted here, were taken into account.

(blue square) is closest to E_4 (purple square) in figure 5.10 (a), and hence the transition from ξ_3 to ξ_4 is rapid in figure 5.12 (b-3) while the transition from E_1 (red square) which is farther away is much slower, cf. figure 5.12 (b-1). The observed behaviour is a clear proof for the existence of non-adiabatic transitions.

This result is important because in a in realistic system always many other resonances are in the vicinity of an exceptional point. If the adiabatic/non-adiabatic behaviour of resonances at an exceptional point is to be studied or exploited this will not be possible if other "disturbing" resonances are in the vicinity.

5.4. ACCURACY OF THE RESULTS

In this section we will discuss the behaviour of the scalar product when encircling an exceptional point. This is important since it directly quantifies the expected accuracy of the calculations done in the "zero"-basis.

For the system presented chapter 3 we used *all* eigenvectors of the system to calculate the expansion coefficients. For the hydrogen atom there are unfortunately infinitely many, hence we cannot calculate them all and take them into account when computing



Figure 5.11. Time evolution of the expansion coefficients for encircling a second-order exceptional point with the centre $(\gamma, f) = (6.11 \cdot 10^{-3}, 2.57 \cdot 10^{-4})$, the relative radius $\delta = 10^{-2}$, a chirality of $\chi = 1$, and a phase offset of $\varphi_0 = 0$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 . Dashed lines indicate resonances not belonging to the exceptional point.



Figure 5.12. Time evolution of the expansion coefficients for encircling a third-order exceptional point with the centre $(\gamma, f) = (6.09 \cdot 10^{-3}, 2.61 \cdot 10^{-4})$, the relative radius $\delta = 3.0 \cdot 10^{-2}$, a chirality of $\chi = -1$, and a phase offset of $\varphi_0 = 0$. The total time of the evolution is 100 000. In the left column the unweighted coefficients are displayed, in the right column the weighted ones. The various initial conditions are stacked up in rows, i.e. row one is equivalent to an initial population in ξ_1 . Dashed lines indicate resonances not belonging to the exceptional point.



Figure 5.13. Conservation of the scalar product in the three-dimensional and six-dimensional subspace dependent on the radius of the parameter cycle. The solid lines are calculated in the three-dimensional basis, the dashed lines in the six-dimensional basis.

the expansion coefficients. Therefore it was proposed to fall back to an n-dimensional subspace, where n is the number of resonances accounted for in the coefficients.

To be correctly described the resonances must not move out of the plane which they initially, i.e. at the starting point of the parameter space loop, created. Since the vectors $|v_i(0)\rangle$ are used as basis states in the "zero"-basis. That is, we have to check that

$$\sum_{j} \langle v_i(t) | v_j(0) \rangle^2 \stackrel{!}{=} 1.$$
 (5.13)

is fulfilled for all times t. During a cycle the basis vectors may change but only if their projection on the initial basis is preserved, otherwise our description is not correct. Please note that we only use the square instead of the square modulus in the calculation of the projection because we are dealing with a complex symmetric matrix, and this is the correct inner product of the non-Hermitian system (cf. the C-product introduced in Moiseyev (2011)).

Now we are examining this condition for the hydrogen atom. The completeness condition (5.13) was checked for different radii and the projection of $v_1(t)$ on the initial basis. The numerical evaluation, illustrated in figure 5.13, revealed that this condition is met for small radii or a large basis. In case of the second-order exceptional point the maximum deviations from 1 were $3.1085 \cdot 10^{-3}$ for a basis of three resonances and $1.3653 \cdot 10^{-3}$ for a basis of six resonances. This corresponds to a maximum deviation of approximately 0.3%. For the third-order exceptional point the result is not that unique. For a basis set of three resonances, viz. those involved in the exchange process the maximum deviation is about $9.2295 \cdot 10^{-2}$, i.e. approximately 9%. This is definitely not acceptable. However, the calculation has only been done to investigate how a third-order exceptional point behaves *in principle* for a solution of the time-dependent Schrödinger equation. The quantitative results in section 5.2.2 are not out main interest. If precise quantitative values are required, a numerically more expensive calculation

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in an instantaneous basis as explained in section 3.1.1 can be done. For a basis of six resonances the deviation is much smaller with only $1.7897 \cdot 10^{-2}$, which corresponds to 1.7%.

The quite huge error for the set of three resonances at the third-order exceptional point is due to the large relative radius of $\delta = 3 \cdot 10^{-2}$. In contrast this does not have a crucial impact on the results obtained as we already discussed that it is necessary to take nearby resonances into account because of non-adiabatic transitions to (nearly) bound states.

SUMMARY

The main topic of this work was to analyse the transport of populations of resonances along a closed cycle in the parameter space of the hydrogen atom in crossed external electric and magnetic fields. Therefore the spectral decomposition of an arbitrary state in the "zero"-basis was inserted in the Schrödinger equation and a differential equation for the expansion coefficients was derived, cf. (4.17). The differential equation was solved for one cycle around an exceptional point in a finite basis approximation, viz. a three-dimensional and a six-dimensional subspace. To illustrate the exchange behaviour at a second-order exceptional point the point #15 from table 4.1 was encircled. The main result was that the final state does not depend on the initial state of the system. This demonstrates the finding of Uzdin et al. (2011) that an adiabatic state exchange at exceptional points is not observable. Due to non-adiabatic couplings always a population of both states at the exceptional point will be present. For a sufficiently slow traversal of the parameter space loop the slowest decaying state will have a predominant occupation at the end of the circle.

As previously published by Cartarius (2008) and Cartarius et al. (2009) the points #15 and #16 form a third-order exceptional point when encircled at once. This was exploited to study the exchange behaviour of populations for different parameter sets. For an isolated exceptional point, i.e. in the three-dimensional basis approximation, the same result as for the second-order exceptional point could be detected. The final state does not depend on the initial state for sufficiently long cycle times. Still the final state depends on the direction in which the parameter loop is traversed as well as on a phase offset which moves the starting point. From the energy diagram and the fact that resonances with greater modulus of the imaginary part decay faster one could get the impression that the final population will never end up in a state with a large imaginary part is of a non-trivial nature. It is important to study the whole cycle and to add up the decay for all times.

Another question to be answered was if this exchange behaviour could be observed in a real system. First of all it is to say that if we look at the absolute populations after a cycle time of 100 000 we see that most of the populations have vanished and only a fraction of the order of 10^{-20} is left. On the other hand if we reduce the total cycle time under a small threshold the effect reduces or, e.g. for a cycle time of 10 000, completely disappears. In a real system the exceptional point is not isolated but surrounded by a vast number of other resonances and even almost bound states. To include this effect three other resonances in the vicinity of the exceptional point were taken into account in a six-dimensional basis approximation. One of these resonances was a (nearly) bound state with a very low imaginary part of the order of $5 \cdot 10^{-5}$. The result was that nearly all of the other populations had dissipated to this bound state at the end of a cycle.

In total we found that the non-adiabatic exchange phenomenon as discussed by Uzdin et al. (2011) and Berry and Uzdin (2011) needs some care. It will only be observable if the two or three resonances forming an exceptional point will be sufficiently isolated. In all

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simulations discussed in this thesis at the end of a parameter space loop only the slowest decaying resonance was populated. This effect dominates the exchange of resonances for circles around exceptional points completely.

Future works in this direction could carry out the time-dependent calculation of the expansion coefficients in an instantaneous basis instead of the "zero"-basis approximation. Also it would be advantageous to study systems with better controllable time scale than the hydrogen atom where we are dealing with times of the order of picoseconds.

AUXILLIARY MATERIAL

In this chapter you will find all calculations, which have been postponed in the previous text.

A.1. LEFT AND RIGHT EIGENVECTORS

►LEMMA A.1:

In case of a complex symmetric matrix $\mathcal{H} = \mathcal{H}^{\top}$ the left eigenvectors $\langle \tilde{\psi}_n |$ are the right eigenvectors transposed, mathematically speaking

$$\mathcal{H} = \mathcal{H}^{\top} \implies |\tilde{\psi}_n^*\rangle = |\psi_n\rangle.$$
(A.1)

Proof: The left eigenvectors $\langle \tilde{\psi}_n |$ and right eigenvectors $|\psi_n \rangle$ satisfy the relations

Transposing the first line and using $(\langle \tilde{\psi}_n |)^\top = | \tilde{\psi}_n^* \rangle$ yields

$$\mathcal{H}^{\top} \left| \tilde{\psi}_{n}^{*} \right\rangle = \lambda \left| \tilde{\psi}_{n}^{*} \right\rangle. \tag{A.3}$$

With the assumption $\mathcal{H}=\mathcal{H}^\top$ we obtain

$$\mathcal{H} \left| \psi_n^* \right\rangle = \lambda \left| \psi_n^* \right\rangle, \tag{A.4}$$

i.e.

$$|\tilde{\psi}_n^*\rangle = |\psi_n\rangle \iff (\langle \tilde{\psi}_n |)^\top = |\psi_n\rangle.$$
 (A.5)

A.2. ADIABATIC THEOREM

► LEMMA A.2:

The adiabatic approximation of an expansion coefficient of the solution of the timedependent Schrödinger equation was given earlier by

$$a_{\rm ad}(t) = a(0) \exp\left(-\frac{\mathrm{i}}{\hbar} \int_0^t E_a(t') \,\mathrm{d}t'\right). \tag{A.6}$$

Derivation: Consider the time-dependent Schrödinger equation

$$i\hbar\partial_t |\psi(t)\rangle = \mathcal{H}(t) |\psi(t)\rangle.$$
 (A.7)

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The spectral decomposition of any state $|\psi(t)\rangle$ reads

$$|\psi(t)\rangle = \sum_{i} a_{i}(t) |i(t)\rangle$$
, where $\mathcal{H}(t) |i(t)\rangle = E_{i}(t) |i(t)\rangle$. (A.8)

Inserting the spectral decomposition into (A.7) and applying the product rule yields

$$\sum_{i} \dot{a}_{i}(t) \left| i(t) \right\rangle + a_{i}(t) \partial_{t} \left| i(t) \right\rangle = -\frac{i}{\hbar} \sum_{i} E_{i}(t) a_{i}(t) \left| i(t) \right\rangle.$$
(A.9)

Now we choose the state j by multiplying (A.9) with $\langle j(t) |$:

$$\dot{a}_j(t) + \sum_i a_i(t) \langle j(t) | \partial_t | i(t) \rangle = -\frac{\mathrm{i}}{\hbar} E_j(t) a_j(t).$$
(A.10)

The *adiabatic approximation* now is to neglect all terms $\langle j(t) | \partial_t | i(t) \rangle$ because for a slowly traversed path in parameter space the basis changes only a little or not at all,

$$\dot{a}_j(t) = -\frac{\mathrm{i}}{\hbar} E_j(t) a_j(t). \tag{A.11}$$

This ordinary differential equation can be solved by separation of variables,

$$a_j(t) = a_j(t_0) \exp\left(-\frac{\mathrm{i}}{\hbar} \int_{t_0}^t E_j(t') \,\mathrm{d}t'\right). \tag{A.12}$$

A.3. TRANSFORMATION OF THE HAMILTONIAN IN THE INTERACTION PICTURE

►LEMMA A.3:

For arbitrary $\alpha \neq \beta$ and $\tau \in \mathbb{R}$ one has

$$e^{-i\tau\sigma_{\alpha}}\sigma_{\beta}e^{i\tau\sigma_{\alpha}} = \sigma_{\beta}\cos(2\tau) + \varepsilon_{\alpha\beta\gamma}\sigma_{\gamma}\sin(2\tau), \qquad (A.13)$$

where we do not use Einstein's summation convention on the left-hand side. The symbols σ_{α} denote the Pauli matrices.

Sketch of a proof: For the proof we use the commutator relation for the Pauli matrices

$$[\sigma_{\alpha}, \sigma_{\beta}] = 2i\varepsilon_{\alpha\beta\gamma}\sigma_{\gamma}, \tag{A.14}$$

as well as Hadamard's lemma

$$e^{A}Be^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_{n}$$
 (A.15)

with the n-commutator

$$[A, B]_n = [A, [A, B]_{n-1}].$$
(A.16)

Let $A = -i\tau\sigma_{\alpha}$ and $B = \sigma_{\beta}$, such that with (A.15) one has

$$e^{A}Be^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_{n}$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} [-i\tau\sigma_{\alpha}, \sigma_{\beta}]_{n}$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-i\tau)^{n} [\sigma_{\alpha}, \sigma_{\beta}]_{n} .$$
(A.17)

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Calculating the first few terms of the n-commutator yields

$$\sum_{n} [\sigma_{\alpha}, \sigma_{\beta}]_{n} = \sigma_{\beta} + \underbrace{[\sigma_{\alpha}, \sigma_{\beta}]}_{=(A.14)} + \underbrace{[\sigma_{\alpha}, i\varepsilon_{\alpha\beta\gamma}\sigma_{\gamma}]}_{=i\varepsilon_{\alpha\beta\gamma}} + \underbrace{[\sigma_{\alpha}, -\sigma_{\beta}]}_{=-2i\varepsilon_{\alpha\beta\gamma}\sigma_{\gamma}} + \ldots$$

Thus, (A.17) can be split up into even and odd terms

$$e^{A}Be^{-A} = \sum_{n=0}^{\infty} \frac{1}{(2n)!} (-2i\tau)^{2n} \sigma_{\beta} + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} (-2i\tau)^{2n+1} i\varepsilon_{\alpha\beta\gamma} \sigma_{\gamma}$$
$$= \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2n)!} (2\tau)^{2n} \sigma_{\beta} + \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2n+1)!} (2\tau)^{2n+1} \varepsilon_{\alpha\beta\gamma} \sigma_{\gamma}$$
$$= \sigma_{\beta} \cos(2\tau) + \varepsilon_{\alpha\beta\gamma} \sigma_{\gamma} \sin(2\tau) . \quad \blacksquare$$

Now we will use this lemma to transform equation (3.23). The time-dependent part of the Hamiltonian can be expressed using Pauli matrices:

$$V(t) = \mathcal{H} - \sigma_z = (\mathbf{i} + \lambda_1)\sigma_x + \lambda_2\sigma_z.$$
(A.18)

Equation (3.23) reads

$$\partial_t \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = -\frac{\mathbf{i}}{\hbar} \mathbf{e}^{\frac{\mathbf{i}}{\hbar} \mathcal{H}_0 t} (\mathcal{H} - \sigma_z) \mathbf{e}^{-\frac{\mathbf{i}}{\hbar} \mathcal{H}_0 t} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix},$$
$$= -\frac{\mathbf{i}}{\hbar} \mathbf{e}^{\frac{\mathbf{i}}{\hbar} \mathcal{H}_0 t} ((\mathbf{i} + \lambda_1) \sigma_x + \lambda_2 \sigma_z) \mathbf{e}^{-\frac{\mathbf{i}}{\hbar} \mathcal{H}_0 t} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}.$$

With (A.13) and $\alpha = z, \ \beta = x$ and $\tau = -t/\hbar$ one has

$$= -\frac{\mathrm{i}}{\hbar} \left[(\mathrm{i} + \lambda_1) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \mathcal{H}_0 t} \sigma_x \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \mathcal{H}_0 t} + \lambda_2 \sigma_z \right] \begin{bmatrix} d_1 \\ d_2 \end{bmatrix},$$

$$= -\frac{\mathrm{i}}{\hbar} \left\{ (\mathrm{i} + \lambda_1) \left[\sigma_x \cos\left(-\frac{\mathrm{i}}{\hbar} 2t\right) + \sigma_y \sin\left(-\frac{\mathrm{i}}{\hbar} 2t\right) \right] + \lambda_2 \sigma_z \right\} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}.$$

Knowing σ_x and σ_y and the relation $e^{ix} = \cos x + i \sin x$ we get

$$= -\frac{\mathrm{i}}{\hbar} \left\{ (\mathrm{i} + \lambda_1) \begin{bmatrix} 0 & \mathrm{e}^{\frac{\mathrm{i}}{\hbar}2t} \\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}2t} & 0 \end{bmatrix} + \lambda_2 \sigma_z \right\} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}.$$

We can identify (A.18) and rewrite this to

$$= -\frac{\mathrm{i}}{\hbar} \begin{bmatrix} (\mathcal{H}_{11} - 1) & \mathcal{H}_{12} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} 2t} \\ \mathcal{H}_{21} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} 2t} & (\mathcal{H}_{11} + 1) \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix},$$
$$= -\frac{\mathrm{i}}{\hbar} \begin{bmatrix} (\mathcal{H}_{11} - 1)d_1 + \mathcal{H}_{12} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} 2t} d_2 \\ \mathcal{H}_{21} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} 2t} d_1 + (\mathcal{H}_{11} + 1) d_2 \end{bmatrix}.$$

APPENDIX B

ATOMIC UNITS

Throughout this work most of the calculations are carried out in atomic Hartree units. Atomic Hartree units are defined in terms of four arbitrary constants. As base units we choose:

- 1. The electron mass m_e is used as mass base unit.
- 2. Charges are measured in units of the elementary charge e.
- 3. The unit of angular momentum is Planck's constant $\hbar = h/(2\pi)$.
- 4. Lengths are measured in units of the Bohr radius $a_0 = 4\pi\varepsilon_0 \hbar^2/(m_e e^2)$.

Always listing the set of definitions is tedious, therefore it is common practice to abbreviate this by just writing

$$\hbar = a_0 = m_e = e = 1, \tag{B.1}$$

which is perfectly equivalent to the assignment

$$\hbar = 4\pi\varepsilon_0 = m_e = e = 1. \tag{B.2}$$

Table B.1 contains an extensive list of atomic Hartree units with their corresponding value in SI units.

Quantity	Atomic Hartree unit	Value in SI units [*]
angular momentum	$\hbar = h/(2\pi)$	$1.054571726(47)\cdot 10^{-34}\mathrm{Js}$
charge	e	$1.602176565(35)\cdot10^{-19}\mathrm{C}$
electric field	$E_0^h = E_h / (e a_0)$	$5.14220652(11)\cdot10^{11}\mathrm{Vm^{-1}}$
energy	$E_h = \alpha^2 m_e c^2$	$4.35974434(19)\cdot10^{-18}{\rm J}$
length	$a_0 = 4\pi\varepsilon_0\hbar^2/(m_e e^2)$	$0.52917721092(17)\cdot10^{-10}\mathrm{m}$
magnetic flux density	$B_0^h = \hbar/(ea_0^2)$	$2.350517464(52)\cdot10^5\mathrm{T}$
mass	m_e	$9.10938291(40)\cdot 10^{-31}\mathrm{kg}$
momentum	\hbar/a_0	$1.992851740(88)\cdot10^{-24}\rm kgms^{-1}$
time	\hbar/E_h	$2.418884326502(12)\cdot 10^{-17}\mathrm{s}$

 Table B.1. Atomic Hartree units

*Mohr et al. (2012)

RUNGE-KUTTA METHODS

The coefficients are defined by means of ordinary differential equations

1

$$\dot{y} = f(t, y). \tag{C.1}$$

After discretising these equations a numerical solver can be used to integrate the trajectory.

To propagate the coefficients in time a 4-th order Runge-Kutta-Method was used, as devised by Press et al. (2007, pp. 907 sqq.).

$$y_{n+1} = y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4) + \mathcal{O}(h^5)$$

$$t_{n+1} = t_n + h$$
 (C.2)

where

$$k_1 = f\left(t_n, y_n\right),\tag{C.3a}$$

$$k_{2} = f\left(t_{n} + \frac{1}{2}h, y_{n} + \frac{h}{2}k_{1}\right),$$
(C.3b)

$$k_3 = f\left(t_n + \frac{1}{2}h, y_n + \frac{h}{2}k_2\right),$$
 (C.3c)

$$k_4 = f(t_n + h, y_n + hk_3).$$
 (C.3d)

This set of equations is also called *classical Runge-Kutta*. For application in the present case there is still a downside. The step size h needs to be chosen wisely to ensure short runtime by making as few steps as possible as well as good convergence at any point of the trajectory to maintain accuracy over long integration times.

ZUSAMMENFASSUNG

Das Hauptthema dieser Arbeit war die Analyse des Populationstransports von Resonanzen entlang einer geschlossenen Bahn im Parameterraum für das Wasserstoffatom in gekreuzten externen elektrischen und magnetischen Feldern. Dafür wurde die Spektralzerlegung für einen festen Parametersatz ("zero"-Basis) eines allgemeinen Zustandes in die Schrödingergleichung eingesetzt und eine Differentialgleichung für die Entwicklungskoeffizienten abgeleitet, vgl. (4.17). Diese Differentialgleichung wurde für eine Umrundung des exzeptionellen Punktes in der Näherung einer endlichen Basis gelöst, hier ein dreidimensionaler und ein sechs-dimensionaler Unterraum. Um das Vertauschungsverhalten an einem exzeptionellen Punkt zweiter Ordnung darzustellen, wurde der Punkt #15 aus Tabelle 4.1 umrundet. Das wesentliche Ergebnis war, dass der Endzustand nicht vom Anfangszustand des Systems abhängt. Dies demonstriert die Erkenntnisse von Uzdin et al. (2011), dass eine adiabatische Zustandsvertauschung an einem exzeptionellen Punkt nicht beobachtbar ist. Auf Grund nichtadiabatischer Kopplungen bleibt die Population stets in beiden Zuständen des exzeptionellen Punktes. Für ausreichend langsame Durchläufe der Parameterbahn wird am Ende des Kreises immer der am langsamsten zerfallende Zustand die größte Besetzung haben.

Wie bereits von Cartarius (2008) und Cartarius et al. (2009) publiziert, bilden die Punkte #15 und #16 einen exzeptionellen Punkt dritter Ordnung, wenn sie gemeinsam umrundet werden. Dies wurde ausgenutzt, um das Vertauschungsverhalten von Populationen mit verschiedenen Parametersätzen zu untersuchen. Für einen isolierten exzeptionellen Punkt, d.h. in der drei-dimensionalen Näherung, konnte das gleiche Ergebnis wie für den exzeptionellen Punkt zweiter Ordnung gefunden werden. Der Endzustand hängt für ausreichend lange Umrundungszeiten nicht vom Anfangszustand ab. Dennoch hängt der Endzustand sowohl von der Richtung, in die der Parameterkreis durchlaufen wird, als auch von einer Phasenverschiebung, die den Startpunkt ändert, ab. Aus dem Energiediagramm und aus der Tatsache, dass Resonanzen mit größerem Betrag des Imaginärteils schneller zerfallen, könnte man den Eindruck gewinnen, dass sich die Endpopulation nie in einem Zustand mit größerem Imaginärteil befinden wird. Unglücklicherweise ist diese Aussage falsch und die Abhängigkeit vom Imaginärteil nicht trivial. Es ist wichtig, den gesamten Durchlauf zu betrachten und den Zerfalle aufzusummieren.

Eine andere Frage, die es zu beantworten galt, war, ob dieses Vertauschungsverhalten in einem realen System beobachtet werden kann. Zunächst ist zu bemerken, dass wenn wir die absolute Populationen nach einem Durchlauf der Zeit 100 000 betrachten, wir sehen, dass der Großteil der Populationen zerfallen ist und nur ein Bruchteil der Größenordnung 10^{-20} verblieben ist. Wenn wir jedoch die gesamte Umrundungszeit unter eine gewisse Grenze senken, wird der Effekt reduziert oder verschwindet, z.B. für eine Umrundungszeit von 10 000, komplett. In einem realen System ist der exzeptionelle Punkt nicht isoliert, sondern von einer großen Anzahl an anderen Resonanzen und sogar fast gebundenen Zuständen umgeben. Um diesen Effekt miteinzubeziehen, wurden drei weitere Resonanzen in der Nähe des exzeptionellen Punktes in einer sechs-dimensionalen Näherung berücksichtigt. Eine dieser Resonanzen war ein (nahezu) gebundener Zustand mit einem verschwindend geringen Imaginärteil der Größenordnung $5 \cdot 10^{-5}$. Das Ergebnis war, dass zum Ende des Kreises nahezu alle anderen Populationen in diesen gebundenen Zustand übergangen waren.

50 ZUSAMMENFASSUNG

Zusammenfassend wurde herausgefunden, dass die nichtadiabatischer Zustandsvertauschung wie bei Uzdin et al. (2011) und Berry und Uzdin (2011) mit Vorsicht zu betrachten ist. Sie wird nur beobachtbar sein, wenn die zwei oder drei Resonanzen, die einen exzeptionellen Punkt bilden, ausreichend isoliert sind. In allen Simulationen, die in dieser Arbeit diskutiert wurden, war am Ende der Parameterbahn nur die am langsamsten zerfallende Resonanz besetzt. Die Effekt überwiegt den Austausch von Resonanzen für Kreise um einen exzeptionellen Punkt bei weitem.

Zukünftige Arbeiten auf diesem Gebiet könnten die zeitabhängige Rechnung der Entwicklungskoeffizienten in einer instantanen Basis statt der "zero"-Basis-Näherung durchführen. Außerdem wäre es von Vorteil, ein System zu untersuchen, dessen Zeitskala besser kontrollierbar ist als die des Wasserstoffatoms, bei der wir uns auf einer Zeitskala von Picosekunden bewegen.

Ehrenwörtliche Erklärung

Ich erkläre,

- dass ich diese Bachelorarbeit selbständig verfasst habe,
- dass ich keine anderen als die angegebenen Quellen benutzt und alle wörtlich oder sinngemäß aus anderen Werken übernommenen Aussagen als solche gekennzeichnet habe,
- dass die eingereichte Arbeit weder vollständig noch in wesentlichen Teilen Gegenstand eines anderen Prüfungsverfahrens gewesen ist,
- dass ich die Arbeit weder vollständig noch in Teilen bereits veröffentlicht habe, es sei denn, der Pr
 üfungsausschuss hat die Veröffentlichung vorher genehmigt
- und dass der Inhalt des elektronischen Exemplars mit dem des Druckexemplars übereinstimmt.

Stuttgart, 18. August 2014

Henri Menke

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