Variational search for control pulses suppressing decoherence

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> vorgelegt von Daniel Spannenkrebs geboren in Witten

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- 1. Gutachter: Prof. Dr. Götz S. Uhrig
- 2. Gutachter: Prof. Dr. Joachim Stolze

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C Simulation Fits

Abstract

Suppression of decoherence is a necessary prerequisite for quantum computation and NMR spectroscopy. In these areas of research control pulses play an important role because they are used to perform necessary operations. The influence of a pulse on decoherence can be investigated via the central spin model. An important task is the search for pulse shapes which suppress the decoherence effectively.

This work addresses the search for decoherence suppressing pulses. To describe the physical situation a semiclassical form of the central spin model with a cusp-like autocorrelation is used. We introduce a variational search method which leads after analytical calculations to an Euler-Lagrange equation. For amplitude-modulated pulses analytical and numerical methods to find solutions of the Euler-Lagrange equation are presented. The pulse which we assume to be the most important outcome of these methods in terms of decoherence suppression is tested via a simulation program written by Stanek. In addition the variational method is applied to frequency-modulated pulses but the Euler-Lagrange equation is not solved within this work.

Zusammenfassung

Dekohärenzunterdrückung ist eine notwendige Voraussetzung für Quanteninformationsverarbeitung und NMR-Spektroskopie. In diesen Forschungsbereichen spielen Kontrollpulse eine wichtige Rolle weil sie für notwendige Operationen verwendet werden. Der Einfluss eines Pulses auf die Dekohärenz kann im Zentralspinmodell untersucht werden.

Diese Arbeit beschäftigt sich mit der Suche nach dekohärenzunterdrückenden Pulsen. Um die physikalische Situation zu beschreiben, wird eine semiklassische Form des Zentralspinmodelles mit einer spitzen Autokorrelation verwendet. Wir stellen eine Variationsrechnung als Suchmethode vor, die nach analytischen Rechnungen zu einer Euler-Lagrange Gleichung führt. Für amplitudenmodulierte Pulse werden analytische und numerische Methoden vorgestellt, um die Lösungen zu finden. Der Puls, den wir für das wichtigste Ergebnis dieser Methoden bezüglich der Dekohärenzunterdrückung halten, wird mit einem von Stanek geschriebenen Simulationsprogramm getestet. Als Ergänzung wird die Variationsmethode auch auf frequenzmodulierte Pulse angewendet, aber die Euler-Lagrange Gleichung wird in dieser Arbeit nicht gelöst.

1 Introduction and Motivation

Control pulses are a fundamental part of quantum computation and NMR spectroscopy. An important tool to of the theoretical description of these topics is the central spin model in all of its different versions. Typical examples of these versions are the quantum mechanical central spin model and the semiclassical central spin model.

Since the realization of devices using quantum information processing seems to be a possible task in the foreseeable future, the central spin model has undergone an intensive development. The idea of storing information in quantum systems exists principally almost since the beginning of quantum mechanics [1] but significant investigations aiming into the direction of devices based on quantum information processing started mainly in 1982. In that year Benioff did some considerations about the simulation of a classical system by a quantum system [2] and Feynman did some considerations on the opposite case, namely the simulation of a quantum system by a classical system [3]. The application of pulses in NMR spectroscopy is used since 1949, three years after the development of NMR spectroscopy [4].

Quantum information processing in comparison with classical information processing has besides other advantages the main advantage of the so called quantum parallelism [1]. It is the potential of a quantum computer to perform multiple operations at the same time whereas a classical computer has to perform the same operations one after another. This is not an advantage from which a quantum computer benefits in every case. This advantage can be used just for suitable problems and the algorithms have to be written in such a way that they make use of this advantage. But if these conditions are fulfilled, the advantage can be huge in comparison with a classical computer. There are several examples for algorithms written for quantum computers.

A famous example for a quantum algorithm is the Shor algorithm [5] which factorizes a number in polynomial time, that means, the run time depends polynomial on the bit length log(N) of the input number N. The Shor algorithm is not just a test algorithm for quantum computers but rather a good example for an algorithm which could be really used for practical purposes. Data cryptography is based on factorization [1] and hence the Shor algorithm or similar quantum algorithms could become very useful in the field of cryptography, if an efficient quantum computer will be build.

In general every quantum system with two different energy values can be used as a quantum bit [1]. Possible realizations are electrons in a magnetic field captured in electron traps or quantum dots. The requirements that a physical system as a candidate for a quantum computer has to fulfill are summarized under the five DiVincenzo criteria [6].

One of these criteria is the necessity of low decoherence times of the quantum bits. The ground steps of a quantum algorithms are operations depending on the states of one or two quantum bits, so called quantum gates. Decoherence causes errors, that means, deviation in the ground steps from the predicted operations. For a working quantum computer a total avoidance of errors is not necessary. Instead it is enough to hold the errors per

quantum gate under a certain threshold according to the quantum threshold theorem [7]. The relevance of the central spin model for the field of quantum information processing lies in the understanding of the decoherence of a quantum bit. Decoherence is caused by different interactions of the central spin with its environment especially by the hyperfine interaction of the central spin with the nuclei in its surrounding material [8]. The relation of the central spin model to the decoherence lies in the fact that you can understand the central spin as a quantum bit and the bath spins as the disturbing environment, i.e. the nuclei in the surrounding material.

In this work we use the semiclassical form of the central spin model. This means we treat just the central spin quantum mechanically and we use an averaged classical fluctuating field for the bath. This does not consider the quantum mechanical effects in the bath and is hence further afar from the reality than a quantum mechanical central spin model, but the advantage is, that the semiclassical central spin model has a much easier mathematical representation and makes computational approaches much faster, because it reduces the states of a big number of bath spins to a single variable. The averaged field is known under the title Overhauser field and it is already attested that it is a justified simplification of the bath [9, 10].

The situation which we want to investigate in this work is the decoherence under extern pulses with the aim to find pulse shapes which suppress the decoherence. This is interesting because in a quantum computer you have to perform operations on the qubits. These operations have to turn the direction of the spin in the Bloch sphere by an angular of π , $\frac{\pi}{2}$ and $\frac{\pi}{4}$ for the Hadamard gate. These operations are a necessity because they represent the ground steps of every quantum algorithm [1, 21]. Hence control pulses are a fundamental part of quantum computation and it is vital to suppress decoherence during the application of a pulse as effectively as possible. A typical idea for quantum computers is to implement these operations via magnetic pulses.

Further relevance of control pulses lies in the fact that pulses are used in sequences for the suppression of decoherence. This is known under the title dynamical decoupling and was initiated by the discovery of the Hahn Echo, which was demonstrated in 1950 [12]. Dynamical decoupling is investigated for sequences of equidistant and non-equidistant pulses [13]. Examples are the Carr-Purcell-Meiboom-Gill sequence [14] with preparatory work from [15] and the Uhrig-dynamical-decoupling sequence [16, 17, 18, 19].

The investigations in this work which are new within the research field of the semiclassical central spin model are mainly two points. The first one is that we use a variational approach for the pulse search. To our knowledge the method which we use is new in this research area. A variational approach to the topic of decoherence was already done by Gordon and Kurizki in 2008 [20] but they addressed a sequence of pulses while we vary the shape of a single pulse. Variational approaches are for example common in analytical mechanics or path integral methods to minimize functionals. We investigate just π -pulses. For our method we define a reasonable functional which we want to minimize and auxiliary conditions which we want to fulfill. Hence we treat a typical optimization problem.

The second investigation in this work lies in the noise model which we use. Previous works mainly used a Gauß distribution for the autocorrelation of the noise while we use a cusp. This is not the first work that investigates a cusp as the autocorrelation, see for example [21] which is the most important forerunner of this work. But this noise model is much less investigated than a Gauß distribution and further research is necessary. A special feature of the cusp-like autocorrelation is a term in the expansion of the Frobenius norm that does not exist under a Gauß distribution as autocorrelation. This term was just in [21] discovered and this work continues the investigation.

A further noteworthy aspect of this work is that we search for pulses which minimize the docoherence under an assumed energy limitation which can be caused for example by device-limits or a certain energy value that you do not want to exceed because of a limited energy supply. The forerunner of this work [21] presents the pulses under two aspects, namely an upper limit of the amplitude and a lower limit of the pulse duration. Such a limitation is a typical aspect of the search for new pulses because without any limitation it would be no problem to create a perfectly decoherence suppressing pulse and in practice you have limitations in every case. The reasons for our choice of a limited energy are rather conceptional reasons concerning the practicability of the variational approach than reasons concerning physical questions. To show the quality of the pulses that we find within this work we show all the features of the new pulses in comparison with the already known pulses CORPSE and SCORPSE [22, 23] while SCORPSE is also called UPi in [24].

This work is structured as follows. In this chapter we give at first in chapter 1.1 an overview of the model including the semiclassical central spin model and the cusp-like noise model. Then in chapter 1.2 we present all the mathematics that we need for the pulse search.

Chapter 2 is the main part of this work where the variational calculation for amplitudemodulated pulses is presented. In chapter 2.1 we apply the ansatz to the problem and we do the first calculations which lead to an Euler-Lagrange equation. The next two chapters 2.2 and 2.3 contain the solutions of the Euler-Lagrange equation. In chapter 2.2 we present analytical solutions of a simplified form of the Euler-Lagrange equation and in chapter 2.3 we present numerical solutions of the general form of the Euler-Lagrange equation.

Chapter 3 contains a test of the best solution to verify it. The test is done by simulating the time evolution of a spin under the new discovered pulse with a program written in the forerunner work [21] which is described in chapter 3.1. In chapter 3.2 we present the results of the test and in chapter 3.3 we discuss these results.

Chapter 4 is an additional part where we apply an analogue variational approach to frequency modulated pulses but we follow this approach just until we get a raw form of an Euler-Lagrange equation because as you can see in chapter 4 problems arise which make the calculations much more difficult than for amplitude-modulated pulses. In chapter 4.1 we explain the aims of the approach. Further we present the Lagrangian in chapter 4.2 and the Euler-Lagrange equation in chapter 4.3 and in chapter 4.4 we discuss the situation. Chapter 5 is the conclusion and the outlook of this work where we discuss the results within the research field of the central spin model.

1.1 Model

The model that is used in this work is the semiclassical form of the central spin model, which is presented in chapter 1.1.1. Because the semiclassical model contains a field which fluctuates statistically obeying an specific autocorrelation it is necessary to make a choise for the autocorrelation which is done in chapter 1.1.2. The formulas are from [25, 21].

1.1.1 Semiclassical central spin model

According to [25, 21] the central spin model consists of a central spin and a bath of spins arranged around the central spin. The central spin can be created by applying a static magnetic field to a spin- $\frac{1}{2}$ particle, for example an electron, so that the particle has two different energy eigenvalues in the magnetic field due to the Zeeman interaction. Without loss of generality the magnetic field and hence the axis of precession is arranged along the z-direction of the coordinate system. The contributing interactions are the interaction between the central spin and the bath spins and the interactions between the bath spins among each other.

In addition in order to do operations on the central spin an applied high-frequency pulse is included into the system and causes an interaction with the central spin. The pulse turns the direction of the spin by a predefined angular where we treat just π -pulses. The interaction between the bath spins and the pulse is neglected in this work.

In general there is also a contribution to the Hamiltonian of the static magnetic field, but to simplify the Hamiltonian the rotating wave approximation is used [25] so that this contribution is not noticeable in the coordinate system which we use. The pulse has the same frequency as the spin-precession around the static magnetic field. Then you can divide the pulse into two fields, which rotate into opposite directions with the frequency of the precession. One of these parts $V_{res}(t)$ rotates into the same direction as the precession and the other part $V_{non-res}(t)$ rotates into the opposite direction. Rotating wave approximation means that $V_{non-res}(t)$ is neglected because it rotates with a very high frequency in the rotating coordinate system. The legitimization of this approximation and a further description can be seen in [26].

At first we write down the pulse shape within the non-rotating coordinate system. The pulse is applied within the time interval $0 \le t \le \tau_p$ where t is the actual time and τ_p is the pulse duration. The resulting time-dependent pulse amplitude in the static coordinate

system is calculated in (1) according to [25]:

$$V(t) = 4V_0(t)\cos(\omega_{ref} \cdot t + \Omega(t) + \Phi_p)\vec{e}_x$$

$$= V_{res}(t) + V_{non-res}(t)$$

$$= 2V_0(t)[\cos(\omega_{ref} \cdot t + \Omega(t) + \Phi_p)\vec{e}_x + \sin(\omega_{ref} \cdot t + \Omega(t) + \Phi_p)\vec{e}_y]$$

$$+ 2V_0(t)[\cos(\omega_{ref} \cdot t + \Omega(t) + \Phi_p)\vec{e}_x - \sin(\omega_{ref} \cdot t + \Omega(t) + \Phi_p)\vec{e}_y].$$
(1)

 $V_0(t)$ is the maximum amplitude of the field, ω_{ref} is the angular velocity of the precession and hence of $V_{res}(t)$, $\Omega(t)$ is a time-dependent phase and Φ_p is a time-independent phase. For amplitude-modulated pulses a modulation of $V_0(t)$ is used and for frequency-modulated pulses a modulation of $\Omega(t)$ is used.

Now we apply the rotating wave approximation. We ignore the second line in the result of (1) and transfer the first line, which represents the remaining rotation direction, into the rotating coordinate system. The remaining field of an amplitude-modulated pulse after the rotating wave approximation seems to be static in the rotating coordinate system and can be written in the rotating coordinate system according to (2) without loss of generality because of the freedom of choice of the phase of the rotating coordinate system.

$$V_{rot}^a(t) = 2V_0(t)\vec{e}_y \tag{2}$$

For frequency-modulated pulses the field is

$$V_{rot}^f(t) = 2V_0 \left[\cos\left(\Omega(t)\right) \vec{e}_x + \sin\left(\Omega(t)\right) \vec{e}_y \right].$$
(3)

The semiclassical form of the central spin model uses a simplification for the interaction between the central spin and the bath spins. In the Gaudin-model [27, 28] without the simplification the interaction has the Hamiltonian (4) according to [9] in which the bath is represented as a sum over the bath spins.

$$H_{I}^{q} = \vec{S_{0}} \sum_{i=1}^{N} J_{i} \vec{S_{i}}$$
(4)

 S_0 is the central spin, S_i are the bath spins, J_i is a coupling constant and N is the number of bath spins in the model. In the semiclassical model [8, 29] the sum over the bath spins, which is a quantum mechanical object, is replaced by a fluctuating scalar-field $\vec{\eta}(t)$, which is a classical object. This neglects indeed all the quantum mechanical effects within the bath but it is a justified model for a bath which is large enough on short time scales where the bath can be assumed as frozen. The computational effort is reduced enormously because the semiclassical model replaces the 2^N bath-dimensions for N bath spins by just one classical variable.

The interaction between the central spin and the bath is included in the model just as an interaction with the z-direction of the central spin because a rotation symmetrical noise model around the z-axis is used. This is explained in detail in chapter 1.1.2. The complete

Hamiltonian is written as

$$H = H_B + H_I(t) + H_P(t)$$

$$= H_B + \vec{\sigma} \cdot \vec{\eta}(t) + \vec{\sigma} \cdot \vec{v}(t).$$
(5)

If we stick to amplitude-modulated pulses, which are treated mainly in this work, we can simplify (5) to

$$H = H_B + \sigma_z \cdot \eta_z(t) + \sigma_y \cdot v_y(t).$$
(6)

As described above the static magnetic field does not appear in (6). The term H_B is a formal term which is written just for now in the more general Hamiltonian. In chapter 1.2.1 we show that this term leads to the time evolution of the bath field $\vec{\eta}(t) = e^{iH_B t} \vec{\eta} e^{-iH_B t}$ (we set $\hbar = 1$). In chapter 1.1.2 we introduce a noise model which captures the time evolution of the bath field in a statistical way. The more general time evolution with H_B will be replaced by this statistical model and henceforth H_B will not appear anymore in the equations.

1.1.2 Noise model

The semiclassical model contains a field which fluctuates according to an autocorrelation. Hence a choice for a specific function describing the autocorrelation is necessary. The accordance between the real world and the semiclassical model depends on this choice. The easier task is to chose an expectation value of the field. Due to its statistical character generated by a big number of fluctuations the probability for different values of the field is usually a Gaussian distribution around an expectation value, such as it it used in [21]. Because of the static magnetic field the z-direction is the only direction with a special feature and for the rest the model is rotational symmetric around the z-direction. Hence (7) is a reasonable choice according to [25].

The effect of this rotation symmetry is that we reduce the decoherence to effects due to pure dephasing and we ignore any effects due to longitudinal relaxation. Pure dephasing alone does not bring a quantum bit closer to the state $|0\rangle$ or $|1\rangle$ but that happens in the combination of pure dephasing and the applied pulse. When the phase of the two states is changed the pulse causes another effect on the spin than it was initially planned and this effect can change the direction of the spin in every possible way and hence it can change the probability to measure the state $|0\rangle$ or $|1\rangle$. Now an autocorrelation describing the correlation of the field with itself between two times t_1 and t_2 has to be chosen. Because of the symmetry concerning time shifts the noise and its autocorrelation should be only dependent of the difference $\Delta t = t_2 - t_1$. According to [25] a formal description of the autocorrelation $g(t_1, t_2)$ is written in (8) where $W_1(\eta_1, t_1)$ is a Gaussian distribution with the variance σ^2 .

$$g(t_1, t_2) = g(\Delta t) = \langle \eta(t_1) \cdot \eta(t_2) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \eta_1 \eta_2 W_2(\eta_2, t_2, \eta_1, t_1) d\eta_1 d\eta_2 \qquad (8)$$
$$\int_{-\infty}^{\infty} W_2(\eta_2, t_2, \eta_1, t_1) d\eta_2 = W_1(\eta_1, t_1)$$
$$W_1(\eta_1, t_1) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2} \left(\frac{\eta_1 - \bar{\eta}}{\sigma}\right)^2}$$

In many preceding works the autocorrelation is considered as a Gaussian distribution. A quite new approach [21] which is followed also in this work considers the autocorrelation as a cusp. This cusp typically arises due to an Ornstein-Uhlenbeck process [21, 30]. This process is a result of highly energetic fluctuations in the bath and is dominant on short time scales. Hence it is a model which captures the physics especially at high temperatures. Such fluctuations can be for example spin-orbit couplings. An example is [21] where both, a Gaussian distribution and a Cusp are considered in a simulation. The autocorrelation assumed here is given as

$$g(\Delta t) = \bar{\eta}^2 + g_0 e^{-\nu \Delta t} = \bar{\eta}^2 + g_0 - g_0 \nu |\Delta t| + \frac{g_0}{2} \nu^2 |\Delta t|^2 + O\left(|\Delta t|^3\right).$$
(9)

The Taylor series expresses the autocorrelation in powers of $|\Delta t|$. This will play a role in the chapters 1.2.3 and 1.2.4 because the conditions for pulses of the first two orders are a consequence of the orders zero and one of this Taylor series. A special term in (9) that we want to pay attention to is the term linear in $|\Delta t|$ because this term concerns the new investigations to which this work belongs to. This term is a special feature of a cusp-like autocorrelation in comparison with a Gauß distribution. In many previous works a Gauß distribution was used as the autocorrelation where the term does not exist due to the vanishing derivation of a Gauß distribution in its maximum. The importance of this term lies in the fact that it leads to an order in the Frobenius norm that was just in [21] discovered. You can see the derivation of this order in chapter 1.2.3. A plot of the autocorrelation can be seen in figure 1.



Figure 1: Cusp-like autocorellation in dependence of the time distance

1.2 Supression of decoherence

The aim of this chapter is to set up a quantitative definition of the pulse quality in terms of decoherence suppression. At first we set up the time evolution operator for the interaction between the central spin and the bath following the way of the calculations in [31]. This is needed in order to set up the so called Frobenius norm of a pulse. The Frobenius norm describes the difference between the actual pulse and the theoretically ideal pulse. The ideal pulse would be a delta peak [31] but it is not realizable in experiments because of its infinite big amplitude and its infinite short pulse duration. Hence the Frobenius norm is a quantification for the quality of a pulse and we get mathematical expressions which we need for the pulse search. The Frobenius norm will be expressed in orders of the pulse duration. The idea to let these orders vanish in ascending order leads to conditions that the pulses shall fulfill.

The shapes of the pulses, the conditions and the Frobenius norm will be expressed at first in dependence of the pulse duration. This is shiftable into expressions in dependence of the maximum amplitude or the energy of a pulse, so that the pulses are in every case expressed in dependence of one variable. The expressions in different variables are just different sights on the same pulse and do not mean a change of the physics. But an aspect which is physically important is the choice of the variable which we try to minimize. That means we search for a pulse which is good under the definition of quality that we set up in chapters 1.2.3 and 1.2.4 and in addition minimizes the value of one of the three variables. The effect which we want to reach is that the pulse is optimized under a certain value of one of these variables which can be for example a limit due to the devices which create the pulse. An example is the limitation of the amplitude. It is clear that an infinitely big amplitude is not implementable. We are interested in finding the best pulse under a restriction which we choose.

1.2.1 Time evolution operator

To set up the time evolution operator we follow the calculations of [31]. The most general formulation of the time evolution operator over the whole pulse duration $U_p(\tau_p, 0)$ is given by

$$U_p(\tau_p, 0) = e^{-i\tau_p H_B} T\{e^{-i\vec{\sigma} \cdot \int_0^{\tau_p} \vec{v}(t)dt}\} U_I(\tau_p, 0).$$
(10)

The first exponential function is the time evolution of the bath, the second exponential function is the time evolution induced by the pulse and $U_I(\tau_p, 0)$ is the time evolution induced by the interaction between the central spin and the bath which is the disturbing part in the system that we want to have as close to the identity operator as possible. The time evolution for the applied pulse \hat{P}_t can be rearranged as

$$\hat{P}_{t} := T\{e^{-i\vec{\sigma}\cdot\int_{0}^{t}\vec{v}(t')dt'}\}$$

$$= e^{-i\vec{\sigma}\cdot\hat{a}(t)\frac{\psi(t)}{2}}.$$
(11)

This formulation represents a rotation around the pulse field in the rotating wave approximation [32]. $\hat{a}(t)$ is the axis of rotation and $\psi(t)$ is the angle of rotation. The Schrödinger equation for the pulse is

$$i\partial_t \hat{P}_t = H_P(t)\hat{P}_t.$$
(12)

 $\vec{v}(t)$ written in dependence of $\vec{a}(t)$ and $\psi(t)$ is

$$2\vec{v}(t) = \dot{\psi}(t)\vec{a}(t) + \dot{\vec{a}}(t)\sin\psi(t) - [1 - \cos\psi(t)]\left[\dot{\vec{a}}(t) \times \vec{a}(t)\right]$$

$$\Leftrightarrow \vec{v}(t) \cdot \vec{a}(t) = \frac{\dot{\psi}(t)}{2}.$$
(13)

The calculations of (13) can be seen in detail in [25]. The total time evolution obeys the Schrödinger equation

$$i\partial_t U_p(t,0) = [H_B + H_I + H_P] U_p(t,0)$$
(14)

From a combination of (12) and (14) we get

$$i\partial_t U_I(t,0) = G(t)U_I(t,0) \tag{15}$$

$$G(t) = e^{iH_B t} \hat{P}_t^{-1} \left(\vec{\sigma} \cdot \vec{\eta}\right) \hat{P}_t e^{-iH_B t}$$

$$\tag{16}$$

The Schrödinger equation (15) leads to the interaction part of the time evolution operator over the whole pulse duration

$$U_I(\tau_p, 0) = T\{e^{-i\int_0^{\tau_p} G(t)dt}\}.$$
(17)

Now we calculate the time evolution of the bath and the pulse separately. We define according to [31] H_{qb}

$$G(t) = e^{iH_B t} H_{qb} e^{-iH_B t} \tag{18}$$

$$H_{qb} = \hat{P}_t^{-1} \left(\vec{\sigma} \cdot \vec{\eta} \right) \hat{P}_t$$
(19)
= $\vec{\sigma} \cdot \vec{\eta} \cos \psi(t) - \vec{\sigma} \cdot [\vec{a}(t) \times \vec{\eta}] \sin \psi(t) + 2 [\vec{a}(t) \cdot \vec{\eta}] [\vec{\sigma} \cdot \vec{a}(t)] \frac{\sin^2 (\psi(t))}{2}.$

The calculations in (18) can be seen in detail in [31]. Further we define according to [31]

$$\vec{S}(t) := \hat{P}_t^{-1} \vec{\sigma} \hat{P}_t = D_{\hat{a}}(\psi) \vec{\sigma}.$$
(20)

The meaning of (20) is that the influence of the pulse is captured in a rotation of the Pauli matrices vector $\vec{\sigma}$ where $D_{\hat{a}}(\psi)$ is the corresponding 3×3 rotation matrix. Now we shift the expression of the rotation from the pauli matrices vector $\vec{\sigma}$ to the field $\vec{\eta}$ so that $\vec{\sigma}$ will be static in our picture.

$$H_{qb} = \hat{P}_t^{-1} \left(\vec{\sigma} \cdot \vec{\eta} \right) \hat{P}_t = \vec{S}(t) \vec{\eta} = \left[D_{\hat{a}}(\psi) \vec{\sigma} \right] \cdot \vec{\eta} = \left[D_{\hat{a}}(-\psi) \vec{\eta} \right] \vec{\sigma} := \vec{n}_{\eta}(t) \cdot \vec{\sigma}$$
(21)

(18) and (21) lead to

$$\vec{n}_{\eta}(t) = \vec{\eta}\cos\psi(t) - [\vec{a}(t)\times\vec{\eta}]\sin\psi(t) + \vec{a}(t)\left[\vec{a}(t)\cdot\vec{\eta}\right]\left[1 - \cos\psi(t)\right].$$
(22)

Now we include the time evolution of the bath into our calculations, e.g. we calculate G(t). This has an effect only on η :

$$\vec{\eta}(t) = \vec{\eta}_t = e^{iH_B t} \vec{\eta} e^{-iH_B t} \tag{23}$$

As described in chapter 1.1.1 H_B is captured in the time evolution of $\vec{\eta}$ and hence H_B is henceforth no longer in our equations because this time evolution is replaced by the statistical noise model presented in chapter 1.1.2.

Now we want to transform (17) into a mathematical expression that we can work with in the pulse search. In order to do this we expand the exponent with a Magnus expansion. The Magnus expansion builds up a power series expression of an exponent, in this case a series of powers of the pulse duration τ_p . This is a description which is needed for the variational pulse search technique because we must be able to see the effect of a small variation on the pulse quality in a quantitative way. A detailed description such as a proof of the Magnus expansion can be seen in [33]. The Magnus expansion of (17) is given by

$$U(\tau_p, 0) = e^{-i\left(\int_0^{\tau_p} G(t)dt - \frac{i}{2}\int_0^{\tau_p} dt_1 \int_0^{t_1} dt_2[G(t_1), G(t_2)] + O(\tau_p^{3})\right)}.$$
(24)

If we insert $G(t) = \vec{n}_{\eta_t}(t) \cdot \vec{\sigma}$ where η_t is the statistical fluctuating field, we get

$$U(\tau_p, 0) = e^{-i\left(\int_0^{\tau_p} \vec{n}_{\eta_t}(t) \cdot \vec{\sigma} dt - \frac{i}{2} \int_0^{\tau_p} dt_1 \int_0^{t_1} dt_2 \left[\vec{n}_{\eta_t}(t_1) \cdot \vec{\sigma}, \vec{n}_{\eta_t}(t_2) \cdot \vec{\sigma}\right] + O(\tau_p^3)\right)}$$
(25)
= $e^{-i\left(\vec{\mu}^{(1)} \cdot \vec{\sigma} + \vec{\mu}^{(2)} \cdot \vec{\sigma} + O(\tau_p^3)\right)}.$

We are interested in the first order of the Magnus expansion. The following calculations can be seen in detail in [25].

Now we calculate the first order of the Magnus expansion for amplitude-modulated pulses. The axis of rotation is

$$\vec{a}(t) = \begin{pmatrix} 0\\1\\0 \end{pmatrix} \tag{26}$$

and (13) leads to the differential equation

$$v(t) = \frac{\dot{\psi}(t)}{2} \tag{27}$$

which is analytically solvable. The first order for amplitude-modulated pulses is

$$\vec{\mu}^{(1)} \cdot \vec{\sigma} = \int_{0}^{\tau_p} \vec{n}_{\eta}(t_1) \cdot \vec{\sigma} dt \qquad (28)$$
$$= \sigma_z \int_{0}^{\tau_p} \eta(t) \cos \psi(t) dt - \sigma_x \int_{0}^{\tau_p} \eta(t) \sin \psi(t) dt.$$

For frequency-modulated pulses the situation is more difficult. The axis of rotation is

$$\vec{a}(t) = \begin{pmatrix} \sin\left(\theta(t)\right)\cos\left(\phi(t)\right) \\ \sin\left(\theta(t)\right)\sin\left(\phi(t)\right) \\ \cos\left(\theta(t)\right) \end{pmatrix}.$$
(29)

and (13) leads to the system of equations

$$\frac{\partial \psi(t)}{\partial t} = 2V_0 \sin\left(\theta(t)\right) \left[\sin\left(\Omega(t)\right) \sin\left(\phi(t)\right) + \cos\left(\Omega(t)\right) \cos\left(\phi(t)\right)\right] \tag{30}$$

$$\frac{\partial \phi(t)}{\partial t} = V_0 \frac{\cos\left(\frac{\psi(t)}{2}\right) \sin\left(\Omega(t) - \psi(t)\right) - \sin\left(\frac{\psi(t)}{2}\right) \cos\left(\theta(t)\right) \cos\left(\Omega(t) - \phi(t)\right)}{\sin\left(\frac{\psi(t)}{2}\right) \sin\left(\theta(t)\right)}$$
(31)

$$\frac{\partial \theta(t)}{\partial t} = V_0 \frac{\cos\left(\frac{\psi(t)}{2}\right)\cos\left(\theta(t)\right)\cos\left(\Omega(t) - \phi(t)\right) + \sin\left(\frac{\psi(t)}{2}\right)\sin\left(\Omega(t) - \psi(t)\right)}{\sin\left(\frac{\psi(t)}{2}\right)}.$$
 (32)

The system of equations is not analytically solvable. This is a problem that makes the variational calculation for frequency-modulated pulses more complicated than the variational calculation for amplitude-modulated pulses as you can see in chapter 4. $\theta(t)$ and $\phi(t)$ are functions, which appear because of the non-static rotation axis. These functions and $\psi(t)$ are auxiliary functions which are not part of the underlying mathematical problem. In theory the problem could be described completely without these functions, but these functions still stand as placeholders in the equations because there is no analytical solution of the system of the equations (30), (31) and (32). The first order for frequency-modulated pulses is according to [25]

$$\vec{\mu}^{(1)} \cdot \vec{\sigma} = \int_{0}^{\tau_{p}} \vec{n}_{\eta}(t_{1}) \cdot \vec{\sigma} dt$$

$$= \bar{\eta} \sigma_{x} \int_{0}^{\tau_{p}} (-a_{y}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{x}(t)a_{z}(t)) dt$$

$$+ \bar{\eta} \sigma_{y} \int_{0}^{\tau_{p}} (a_{x}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{y}(t)a_{z}(t)) dt$$

$$+ \bar{\eta} \sigma_{y} \int_{0}^{\tau_{p}} (\cos(\psi(t)) + (1 - \cos(\psi(t)))a_{x}^{2}(t)) dt.$$
(33)

Because it is important in chapter 4, we write down the second order, too. It is

$$\mu^{(2)} = 2i\vec{\sigma} \int_{0}^{\tau_{p}} \int_{0}^{t_{1}} (\vec{n}_{\eta}(t_{1}) \times \vec{n}_{\eta}(t_{2})) dt_{2} dt_{1}$$

$$= 2i\sigma_{x} \left(\bar{\eta}^{2} + g_{0}\right) \int_{0}^{\tau_{p}} \int_{0}^{t_{1}} (n_{yz}(t_{1})n_{zz}(t_{2}) - n_{zz}(t_{1})n_{yz}(t_{2})) dt_{2} dt_{1}$$

$$= 2i\sigma_{y} \left(\bar{\eta}^{2} + g_{0}\right) \int_{0}^{\tau_{p}} \int_{0}^{t_{1}} (n_{zz}(t_{1})n_{xz}(t_{2}) - n_{xz}(t_{1})n_{zz}(t_{2})) dt_{2} dt_{1}$$

$$= 2i\sigma_{z} \left(\bar{\eta}^{2} + g_{0}\right) \int_{0}^{\tau_{p}} \int_{0}^{t_{1}} (n_{xz}(t_{1})n_{yz}(t_{2}) - n_{yz}(t_{1})n_{xz}(t_{2})) dt_{2} dt_{1}$$

$$= 2i\sigma_{z} \left(\bar{\eta}^{2} + g_{0}\right) \int_{0}^{\tau_{p}} \int_{0}^{t_{1}} (n_{xz}(t_{1})n_{yz}(t_{2}) - n_{yz}(t_{1})n_{xz}(t_{2})) dt_{2} dt_{1}$$

with the abbreviation

$$\vec{n}_{\vec{\eta}}(t) = \eta(t) \begin{pmatrix} -a_y(t)\sin(\psi(t)) + (1 - \cos(\psi(t)))a_x(t)a_z(t) \\ -a_x(t)\sin(\psi(t)) + (1 - \cos(\psi(t)))a_y(t)a_z(t) \\ \cos(\psi(t)) + (1 - \cos(\psi(t)))a_x^2(t) \end{pmatrix}.$$
(35)

1.2.2 Frobenius norm

After the calculation of the time evolution operator of the disturbance we follow a calculation of Stanek of which a short version can be found in [21] in order to get a quantified expression for the pulse quality. The deviation between the ideal pulse with the density matrix ρ_{id}^{γ} and the real pulse with the density matrix ρ_{re}^{γ} is expressed in the density matrix

$$\rho^{\gamma} := \rho_{id}^{\gamma} - \rho_{re}^{\gamma} \tag{36}$$

(37)

with

$$\rho_{id}^{\gamma} = \hat{P}_{\tau_p} \rho_0^{\gamma} \hat{P}_{\tau_p}^{\dagger}$$

$$\rho_{re}^{\gamma} = \hat{P}_{\tau_p} U_I(\tau_p) \rho_0^{\gamma} U_I^{\dagger}(\tau_p) \hat{P}_{\tau_p}^{\dagger}$$
(38)

The density matrices ρ_0^{γ} represent totally polarized states of the central spin in the direction of the axis γ . They are given by

$$\rho_0^{\gamma} = \frac{1}{2} \left[\mathbb{1} + \sigma^{\gamma} \right] \tag{39}$$

The square of the Frobenius norm Δ_F is defined as

$$\Delta_F^2 := \frac{1}{3} \sum_{\gamma=x,y,z} Tr\left(\rho^\gamma\right)^2.$$
(40)

After carrying out the square and exploiting the properties of the time evolution and the rotation operator according to [21] (40) leads to

$$\Delta_F^2 := 2 \left[1 - \frac{1}{3} \sum_{\gamma=x,y,z} Tr\left(\rho_{id}^{\gamma} \rho_{re}^{\gamma}\right) \right].$$
(41)

It is helpful to write the time evolution operators of the interaction as

$$U_I(\tau_p) = \mathbb{1} \cdot \cos|\vec{\mu}| - i \frac{\vec{\mu} \cdot \vec{\sigma}}{|\vec{\mu}|} \sin|\vec{\mu}|.$$
(42)

We will use

$$\left(\sigma_{\gamma}(\vec{\mu}\cdot\vec{\sigma})\right)^{2} = \mu_{\gamma}^{2} - \sum_{\alpha=x,y,z}^{\alpha\neq\gamma} \mu_{\alpha}^{2}$$

$$\tag{43}$$

$$\left(\vec{\mu}\cdot\vec{\sigma}\right)^2 = |\vec{\mu}|^2 \tag{44}$$

$$Tr\left(2\sigma_{\gamma}\left(\vec{\mu}\cdot\vec{\sigma}\right)^{2}\right)=0.$$
(45)

With these equations we calculate the trace in (41) using $\hat{P}_{\tau_p}^{\dagger}\hat{P}_{\tau_p} = \mathbb{1}$ and cyclical permutation under the trace:

$$Tr\left(\rho_{id}^{\gamma}\rho_{re}^{\gamma}\right) = Tr\left(\hat{P}_{\tau_{p}}\rho_{0}^{\gamma}\hat{P}_{\tau_{p}}^{\dagger}\hat{P}_{\tau_{p}}U_{I}(\tau_{p})\rho_{0}^{\gamma}U_{I}^{\dagger}(\tau_{p})\hat{P}_{\tau_{p}}^{\dagger}\right)$$
(46)
$$= \cos|\vec{\mu}|^{2} + \frac{\sin^{2}|\vec{\mu}|}{4|\vec{\mu}|^{2}} \cdot Tr\left((\vec{\mu}\cdot\vec{\sigma})^{2} + 2\sigma_{\gamma}(\vec{\mu}\cdot\vec{\sigma})^{2} + (\sigma_{\gamma}(\vec{\mu}\cdot\vec{\sigma}))^{2}\right)$$
$$= \cos|\vec{\mu}|^{2} + \frac{\sin^{2}|\vec{\mu}|}{|\vec{\mu}|^{2}}\mu_{\gamma}^{2}$$

We insert this trace into the Frobenius norm:

$$\begin{split} \Delta_F^2 &= 2 \left[1 - \frac{1}{3} \sum_{\gamma = x, y, z} Tr\left(\rho_{id}^{\gamma} \rho_{re}^{\gamma}\right) \right] \\ &= 2 \left[1 - \cos |\vec{\mu}|^2 - \frac{1}{3} \frac{\sin |\vec{\mu}|^2}{|\vec{\mu}|^2} \left(\mu_x^2 + \mu_y^2 + \mu_z^2\right) \right] \\ &= \frac{4}{3} \left[1 - \cos^2 |\vec{\mu}| \right]. \end{split}$$
(47)

Until this point we have calculated the Frobenius norm exactly. Now we are going to make an approximation. We insert the Taylor series of the cosine into (47) and thus we get according to the calculations of Stanek

$$\Delta_F^2 \approx \frac{4}{3} \left[1 - (1 - \frac{1}{2} |\vec{\mu}|^2)^2 \right] = \frac{4}{3} |\vec{\mu}|^2 + O\left(|\vec{\mu}|^4 \right).$$
(48)

In the next two sections we are going to deduce conditions for amplitude-modulated and frequency-modulated pulses from (48) and from the boundary conditions.

1.2.3 Conditions for amplitude-modulated pulses

For the conditions we use just the first order of the Magnus expansion. We calculate the contribution of this order to Δ_F by inserting it into (48) according to [25].

$$\overline{\mu_x^{(1)^2}} + \overline{\mu_z^{(1)^2}} \tag{49}$$

$$= \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \sin(\psi(t_1)) \sin(\psi(t_2)) dt_1 dt_2$$

$$+ \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \cos(\psi(t_1)) \cos(\psi(t_2)) dt_1 dt_2$$

$$= \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \cos(\psi(t_1) - \psi(t_2)) dt_1 dt_2$$

We insert the Taylor series (9) of the autocorrelation.

$$\overline{\mu_x^{(1)^2}} + \overline{\mu_z^{(1)^2}}$$

$$= \int_0^{\tau_p} \int_0^{\tau_p} \left(\bar{\eta}^2 + g_0 - g_0 \nu |\Delta t| + \frac{g_0}{2} \nu^2 |\Delta t|^2 + O\left(|\Delta t|^3\right) \right) \cos\left(\psi(t_1) - \psi(t_2)\right) dt_1 dt_2$$
(50)

Now there are different orders of $|\Delta t|$. Note that there are two reasons for different orders in Δ_F and their combination leads to the actual orders. One reason is the Magnus expansion of the time evolution operator and the other one is the Taylor series of the autocorrelation. At first we look at the first order of the Taylor series. We set up the demand on the pulses that the order from the first order of the Magnus expansion and the first order of the Taylor series vanishes completely:

$$\int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \bar{\eta}^{2} \cos\left(\psi(t_{1}) - \psi(t_{2})\right) dt_{1} dt_{2} = 0 \qquad (51)$$
$$\bar{\eta}^{2} \left[\int_{0}^{\tau_{p}} \sin(\psi(t_{1})) dt_{1} \int_{0}^{\tau_{p}} \sin(\psi(t_{2})) dt_{2} + \int_{0}^{\tau_{p}} \cos(\psi(t_{1})) dt_{1} \int_{0}^{\tau_{p}} \cos(\psi(t_{2})) dt_{2} \right] = 0$$

According to [25] we get the two conditions (52) and (53). Further we deduce a boundary condition from the usage of π -pulses [25]. We know that the difference between the initial angular $\psi(0)$ and the final angular $\psi(\tau_p)$ has to be π and hence we can write down the condition (54).

$$\int_{0}^{\tau_p} \sin\left(\psi(t)\right) dt = 0 \tag{52}$$

$$\int_{0}^{\tau_p} \cos\left(\psi(t)\right) dt = 0 \tag{53}$$

$$\psi(\tau_p) - \psi(0) = \pi \tag{54}$$

The biggest contribution to the decoherence on the central spin is due to the first order of the Frobenius norm. Thus the fulfillment of the conditions (52) and (53) is a reasonable first step in order to suppress decoherence. Further we look at the second order of the Taylor series in (50) and define

$$X = -\int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} |t_{1} - t_{2}| \cos\left(\psi(t_{1}) - \psi(t_{2})\right) dt_{1} dt_{2}.$$
(55)

As explained in chapter 1.2.2 this term is a recently discovered [21] special feature of the cusp-like autocorrelation in comparison with a Gauß distribution where this order does not exist. The meaning of this term is that it is the order τ_p^3 with its prefactor in Δ_F^2 . After we let the first order vanish via the conditions (52) and (53) it would be nice to let the second order vanish, too. But this is not possible because of the No-Go theorem. It is shown in [15] that it is impossible to let (55) vanish at the same time when the conditions (52), (53) and (54) are fulfilled. Thus the best what we can try to reach is to create a pulse, which makes (55) as small as possible while (52), (53) and (54) are fulfilled.

1.2.4 Conditions for frequency-modulated pulses

For frequency-modulated pulses we set up conditions in analogy to the condition for amplitude-modulated pulses such as in [25]. We use (33) to calculate

$$\begin{aligned} \overline{\mu_x^{(1)^2}} + \overline{\mu_y^{(1)^2}} + \overline{\mu_z^{(1)^2}} \end{aligned} \tag{56} \\ = \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \left(-a_y(t_1) \sin\left(\psi(t_1)\right) + \left(1 - \cos\left(\psi(t_1)\right)\right) a_x(t_1) a_z(t_1) \right) \\ \left(-a_y(t_2) \sin\left(\psi(t_2)\right) + \left(1 - \cos\left(\psi(t_2)\right)\right) a_x(t_2) a_z(t_2) \right) dt_1 dt_2 \\ + \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \left(a_x(t_1) \sin\left(\psi(t_1)\right) + \left(1 - \cos\left(\psi(t_1)\right)\right) a_y(t_1) a_z(t_1) \right) \\ \left(a_x(t_2) \sin\left(\psi(t_2)\right) + \left(1 - \cos\left(\psi(t_2)\right)\right) a_y(t_2) a_z(t_2) \right) dt_1 dt_2 \\ + \int_0^{\tau_p} \int_0^{\tau_p} g(t_1 - t_2) \left(\cos\left(\psi(t_1)\right) + \left(1 - \cos\left(\psi(t_1)\right)\right) a_x^2(t_1) \right) \\ \left(\cos\left(\psi(t_2)\right) + \left(1 - \cos\left(\psi(t_2)\right)\right) a_x^2(t_2) \right) dt_1 dt_2. \end{aligned}$$

We insert the Taylor series (9):

$$\begin{aligned} \overline{\mu_x^{(1)^2}} + \overline{\mu_y^{(1)^2}} + \overline{\mu_z^{(1)^2}} \end{aligned} \tag{57} \\ = \int_0^{\tau_p} \int_0^{\tau_p} \left(\bar{\eta}^2 + g_0 - g_0 \nu |\Delta t| + \frac{g_0}{2} \nu^2 |\Delta t|^2 + O\left(|\Delta t|^3\right) \right) \\ \left(-a_y(t_1) \sin\left(\psi(t_1)\right) + (1 - \cos\left(\psi(t_1)\right)) a_x(t_1) a_z(t_1)\right) \\ \left(-a_y(t_2) \sin\left(\psi(t_2)\right) + (1 - \cos\left(\psi(t_2)\right)) a_x(t_2) a_z(t_2)\right) dt_1 dt_2 \\ + \int_0^{\tau_p} \int_0^{\tau_p} \left(\bar{\eta}^2 + g_0 - g_0 \nu |\Delta t| + \frac{g_0}{2} \nu^2 |\Delta t|^2 + O\left(|\Delta t|^3\right) \right) \\ \left(a_x(t_1) \sin\left(\psi(t_1)\right) + (1 - \cos\left(\psi(t_1)\right)) a_y(t_1) a_z(t_1)\right) \\ \left(a_x(t_2) \sin\left(\psi(t_2)\right) + (1 - \cos\left(\psi(t_2)\right)) a_y(t_2) a_z(t_2)\right) dt_1 dt_2 \\ + \int_0^{\tau_p} \int_0^{\tau_p} \left(\bar{\eta}^2 + g_0 - g_0 \nu |\Delta t| + \frac{g_0}{2} \nu^2 |\Delta t|^2 + O\left(|\Delta t|^3\right) \right) \\ \left(\cos\left(\psi(t_1)\right) + (1 - \cos\left(\psi(t_1)\right)) a_x^2(t_1) \right) \\ \left(\cos\left(\psi(t_1)\right) + (1 - \cos\left(\psi(t_1)\right)) a_x^2(t_1) \right) \\ \left(\cos\left(\psi(t_2)\right) + (1 - \cos\left(\psi(t_2)\right)) a_x^2(t_2) \right) dt_1 dt_2 \end{aligned}$$

In analogy to the amplitude-modulated pulses we want to let the order from the first order of the Magnus expansion and the first order of the Taylor series vanish. We derive the first order conditions from (57). Further there are boundary conditions for the frequencymodulated pulses which you can see in [25]. Altogether we get the following conditions:

$$\int_{0}^{\tau_{p}} (-a_{y}(t)\sin\left(\psi(t)\right) + (1 - \cos\left(\psi(t)\right))a_{x}(t)a_{z}(t)) dt = 0$$
(58)

$$\int_{0}^{\tau_{p}} (a_{x}(t)\sin(\psi(t)) + (1 - \cos(\psi(t)))a_{y}(t)a_{z}(t)) dt = 0$$
(59)

$$\int_{0}^{\tau_{p}} \left(\cos\left(\psi(t)\right) + (1 - \cos\left(\psi(t)\right))a_{x}^{2}(t) \right) dt = 0$$
(60)

$$\psi(\tau_p) - \psi(0) = \pi \tag{61}$$

$$\theta(\tau_p) = \frac{\pi}{2} \tag{62}$$

 Δ_F in the second order of the Taylor series is derived in chapter 4 because it is a newly derived formula in this work.

2 Variational Calculation for Amplitude-Modulated Pulses

This chapter contains the central investigations of this work for amplitude modulatedpulses. At first we give an overview of the ansatz and start with the essential calculations of the variation in chapter 2.1 where we finally come to the central differential equation which we want to solve. This differential equation will be solved in two main steps. The first step is to set one Lagrange multiplier to zero and solve the remaining equation analytically in chapter 2.2. The second step is the extension of the solution to a solution of the general equation with a numerical method in chapter 2.3.

2.1 Variational ansatz

We start with an explanation of the variational ansatz. Our initial situation consists of conditions which we want to fulfill. One of them is (54) which is the boundary condition of a π -pulse and the others are (52) and (53) which we want to fulfill because of the reasonable idea to make the orders of the Frobenius norm vanish in ascending order. As described above the next order is X in (55) which we cannot make vanish at the same time with the fulfillment of the conditions because of the No-Go Theorem [34]. Thus the best we can try to reach is to make X as small as possible while we fulfill the three conditions.

In addition to these aims stemming from the wanted pulse quality we want to set up a further aim which leads to a good realizability of the pulse in an experiment or further a device such as a quantum computer. Previous works such as [21] aim at a big pulse duration or a small amplitude. Both of these ideas are hardly integrable into our variational calculus due to the fact that it is difficult to include a discrete limitation of such values and thus we have to think about something different. The idea is to minimize the energy of a pulse given by

$$E = \frac{1}{2} \int_0^{\tau_p} v^2(t).$$
 (63)

E and X can be minimized with different weightings to each other via a Lagrange multiplier that you will see in the formulas. The minimization of the energy is reasonable because of two aspects. The first one is that it can be beneficial to use pulses with a low energy due to a limited energy supply and heating. The second one is that the deviation of the actual spin angle $\dot{\psi}(t)$ which is contained in the energy corresponds to the amplitude of a pulse and thus we get a special form of an amplitude minimization in our method, too. The energy is suitable to our variational calculation because we can insert it easily into the functional I. In total we have two terms X and E that we want to minimize while we want to fulfill the three conditions (52), (53) and (54). This is a typical optimization problem and a variational calculation is a good suggestion for the solution of such a problem.

A variational calculation is generally used to find the static points and thus the maxima, minima or saddle points of a functional $I(\vec{q}(t), \dot{\vec{q}}, t)$. In the argument of the functional stand the functions $\vec{q}(t)$, their first deviations $\dot{\vec{q}}(t)$ and the variable t. Hence the initial equation of a variational calculation is

$$\delta I(\vec{q}(t), \dot{\vec{q}}(t), t) = 0. \tag{64}$$

The functional is written as an integral over a Lagrange function \mathcal{L} :

$$I = \int \mathcal{L}\left(\vec{q}(t), \dot{\vec{q}}(t), t\right) dt.$$
(65)

Finally the solutions are reached over the Euler-Lagrange equations for every single function $q_i(t)$:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i(t)} - \frac{\partial \mathcal{L}}{\partial q_i(t)} = 0.$$
(66)

2.1.1 Functional

Now we want to adjust our problem to a variational calculation as described above. With (52), (53), (55) and (63) we define the functional

$$I = \frac{1}{8} \int_{0}^{\tau_{p}} \dot{\psi}^{2}(t) dt + \lambda_{1} \int_{0}^{\tau_{p}} \sin(\psi(t)) dt + \lambda_{2} \int_{0}^{\tau_{p}} \cos(\psi(t)) dt$$

$$+ \lambda_{3} \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} |t_{1} - t_{2}| \cos(\psi(t_{1}) - \psi(t_{2})) dt_{1} dt_{2}.$$
(67)

 λ_1 , λ_2 and λ_3 are Lagrange multipliers.

2.1.2 Lagrangian

To set up a Lagrangian at first we have to identify the coordinates and the variable in (65) for our problem. Our problem is one dimensional and thus there is just one Euler-Lagrange equation. The coordinate that we use is the angle $\psi(t)$ depending on the variable t. Note that we are finally searching for a pulse shape defined by (27) which depends on $\dot{\psi}(t)$. This will play an important role later in this work because when we know any general solutions for $\psi(t)$ depending on a number of variables the solutions for v(t) depend on one variable less because one variable gets lost by the derivation.

We set up the Lagrangian for our problem by identifying \mathcal{L} in (65). This is easy for the three terms in (67) which consist of one integral where the terms contributing to the Lagrangian are just the integrands. For the term consisting of two integrals it is not that easy. It is easily comprehensible that one integral must stay in \mathcal{L} after removing the integral which you see in (65) but we cannot just remove one of the two integrals to get the contribution to \mathcal{L} . In fact both integrals are equal before a formulation such as \mathcal{L} . This leads to a prefactor. To get this prefactor we trace the mathematical derivation of the general Euler-Lagrange equations. We call the integrand of X

$$f(\psi(t_1), \dot{\psi}(t_1), \psi(t_2), \dot{\psi}(t_2)) = |t_1 - t_2| \cos\left(\psi(t_1) - \psi(t_2)\right).$$
(68)

Then we derive the Euler-Lagrange equation and we can identify the contribution to \mathcal{L} .

$$\delta \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} f(\psi(t_{1}), \dot{\psi}(t_{1}), \psi(t_{2}), \dot{\psi}(t_{2})) dt_{1} dt_{2} = 0$$

$$\Leftrightarrow \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(f(\psi(t_{1}) + \delta\psi(t_{1}), \dot{\psi}(t_{1}) + \delta\dot{\psi}(t_{1}), \psi(t_{2}) + \delta\psi(t_{2}), \dot{\psi}(t_{2}) + \delta\dot{\psi}(t_{2})) \right) \\ - f(\psi(t_{1}), \dot{\psi}(t_{1}), \psi(t_{2}), \dot{\psi}(t_{2})) \right) dt_{1} dt_{2} = 0$$

$$\Leftrightarrow \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{1})} \delta\psi(t_{1}) + \frac{\partial f}{\partial \dot{\psi}(t_{1})} \delta\dot{\psi}(t_{1}) + \frac{\partial f}{\partial \dot{\psi}(t_{2})} \delta\psi(t_{2}) + \frac{\partial f}{\partial \dot{\psi}(t_{2})} \delta\dot{\psi}(t_{2}) \right) dt_{1} dt_{2} = 0$$

$$\Leftrightarrow \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \frac{\partial f}{\partial \psi(t_{1})} \delta\psi(t_{1}) dt_{1} dt_{2} + \int_{0}^{\tau_{p}} \left[\delta\psi(t_{1}) \frac{\partial f}{\partial \dot{\psi}(t_{2})} \right]_{0}^{\tau_{p}} dt_{2} - \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \delta\psi(t_{1}) \frac{d}{dt_{1}} \frac{\partial f}{\partial \dot{\psi}(t_{2})} dt_{1} dt_{2}$$

$$\int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \frac{\partial f}{\partial \psi(t_{2})} \delta\psi(t_{2}) dt_{1} dt_{2} + \int_{0}^{\tau_{p}} \left[\delta\psi(t_{2}) \frac{\partial f}{\partial \dot{\psi}(t_{2})} \right]_{0}^{\tau_{p}} dt_{1} - \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \delta\psi(t_{2}) \frac{d}{dt_{2}} \frac{\partial f}{\partial \dot{\psi}(t_{2})} dt_{1} dt_{2} = 0$$

$$\Leftrightarrow \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{1})} \delta\psi(t_{1}) + \delta\psi(t_{1}) \frac{d}{dt_{1}} \frac{\partial f}{\partial \dot{\psi}(t_{1})} \right) dt_{1} dt_{2}$$

$$+ \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{2})} \delta\psi(t_{2}) + \delta\psi(t_{2}) \frac{d}{dt_{2}} \frac{\partial f}{\partial \dot{\psi}(t_{2})} \right) dt_{1} dt_{2} = 0$$

The single integrals in the last step vanish due to the fact that $\delta \psi(t)$ is zero in the starting and the ending point t = 0 and $t = \tau_p$. The integrands are completely symmetrical in t_1 and t_2 because X is symmetrical in t_1 and t_2 as you can see in (55). Further the range of integration is equal for t_1 and t_2 and hence we get:

$$\int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{1})} \delta \psi(t_{1}) + \delta \psi(t_{1}) \frac{d}{dt_{1}} \frac{\partial f}{\partial \dot{\psi}(t_{1})} \right) dt_{1} dt_{2}$$

$$= \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{2})} \delta \psi(t_{2}) + \delta \psi(t_{2}) \frac{d}{dt_{2}} \frac{\partial f}{\partial \dot{\psi}(t_{2})} \right) dt_{1} dt_{2}.$$
(70)

Thus we can write:

$$\delta \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} f(\psi(t_{1}), \dot{\psi}(t_{1}), \psi(t_{2}), \dot{\psi}(t_{2})) dt_{1} dt_{2}$$

$$= 2 \int_{0}^{\tau_{p}} \int_{0}^{\tau_{p}} \left(\frac{\partial f}{\partial \psi(t_{1})} \delta \psi(t_{1}) + \delta \psi(t_{1}) \frac{d}{dt_{1}} \frac{\partial f}{\partial \dot{\psi}(t_{1})} \right) dt_{1} dt_{2}$$

$$= \int_{0}^{\tau_{p}} \left(\frac{\partial \left(2 \int_{0}^{\tau_{p}} f dt_{2} \right)}{\partial \psi(t_{1})} \delta \psi(t_{1}) + \delta \psi(t_{1}) \frac{d}{dt} \frac{\partial \left(2 \int_{0}^{\tau_{p}} f dt_{2} \right)}{\partial \dot{\psi}(t_{1})} \right) dt_{1}.$$

$$(71)$$

Now we can identify the contribution to \mathcal{L} in comparison with (65) as

$$\mathcal{L}_X(\psi(t), \dot{\psi}(t), t) = 2 \int_0^{\tau_p} f dt_2 = 2 \int_0^{\tau_p} |t - t_2| \cos\left(\psi(t) - \psi(t_2)\right) dt_2.$$
(72)

Then we have all the terms that we need to write down the Lagrangian as

$$\mathcal{L}(\psi(t), \dot{\psi}(t), t)$$

$$= \frac{1}{8} \dot{\psi}(t)^{2} + \lambda_{1} \sin(\psi(t)) + \lambda_{2} \cos(\psi(t)) + 2\lambda_{3} \int_{0}^{\tau_{p}} |t - t_{2}| \cos(\psi(t) - \psi(t_{2})) dt_{2}.$$
(73)

2.1.3 Euler-Lagrange equation

The next step is to derive the Euler-Lagrange equation from the Lagrangian. We insert (73) into (66):

$$\frac{d}{dt}\frac{\partial\mathcal{L}(\psi(t),\dot{\psi}(t),t)}{\partial\dot{\psi}(t)} - \frac{\partial\mathcal{L}(\psi(t),\dot{\psi}(t),t)}{\partial\psi(t)} = 0$$

$$\frac{d}{dt}\frac{\partial\frac{1}{8}\dot{\psi}^{2}(t)}{\partial\dot{\psi}(t)} - \frac{\partial\left(\lambda_{3}2\int_{0}^{\tau_{p}}|t-t_{2}|\cos\left(\psi(t)-\psi(t_{2})\right)dt_{2}+\lambda_{1}\sin\left(\psi(t)\right)+\lambda_{2}\cos\left(\psi(t)\right)\right)}{\partial\psi(t)} = 0$$

$$\psi''(t) + 8\lambda_{3}\int_{0}^{\tau_{p}}|t-t_{1}|\sin\left(\psi(t)-\psi(t_{2})\right)dt_{2}+4\lambda_{2}\sin\left(\psi(t)\right)-4\lambda_{1}\cos\left(\psi(t)\right) = 0.$$
(74)

Now we want to capture the last two terms within one term. We calculate:

$$\begin{aligned} \lambda_{2}\sin(\psi(t)) - \lambda_{1}\cos(\psi(t)) & (75) \\ &= -\lambda_{2}\frac{i}{2}\left(e^{i\psi(t)} - e^{-i\psi(t)}\right) + \lambda_{2}\frac{1}{2}\left(e^{i\psi(t)} - e^{-i\psi(t)}\right) \\ &= -\frac{1}{2}\left(\lambda_{2} + i\lambda_{1}\right)e^{i\psi(t)} - \frac{1}{2}\left(\lambda_{2} - i\lambda_{1}\right)e^{-i\psi(t)} \\ &= \frac{\lambda_{2}}{2}\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}\frac{1 + i\frac{\lambda_{1}}{\lambda_{2}}}{\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}}e^{i\psi(t)} + \frac{\lambda_{2}}{2}\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}\frac{1 - i\frac{\lambda_{1}}{\lambda_{2}}}{\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}}e^{-i\psi(t)} \\ &= \frac{\lambda_{1}}{2}\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}e^{i\left(\psi(t) + \arctan\frac{\lambda_{1}}{\lambda_{2}}\right)} + \frac{\lambda_{2}}{2}\sqrt{1 + \frac{\lambda_{1}^{2}}{\lambda_{2}^{2}}}e^{-i\left(\psi(t) + \arctan\frac{\lambda_{1}}{\lambda_{2}}\right)} \\ &= \sqrt{\lambda_{2}^{2} + \lambda_{1}^{2}}\cos\left(\psi(t) + \arctan\frac{\lambda_{1}}{\lambda_{2}}\right) \\ &= \sqrt{\lambda_{2}^{2} + \lambda_{1}^{2}}\sin\left(\psi(t) + \arctan\frac{\lambda_{1}}{\lambda_{2}} + \frac{\pi}{2}\right) \end{aligned}$$

Thus we can rewrite (74) as:

$$\ddot{\psi}(t) + 4\sqrt{\lambda_2^2 + \lambda_1^2} \sin\left(\psi(t) + \arctan\frac{\lambda_1}{\lambda_2} + \frac{\pi}{2}\right)$$

$$+ 8\lambda_3 \int_0^{\tau_p} |t - t_2| \sin\left(\psi(t) - \psi(t_2)\right) dt_2 = 0$$

$$(76)$$

Before we start to solve the Euler-Lagrange equation (76) we want to think about a few general aspects of the solutions and the physical meaning of these aspects.

(76) is a differential equation of the second order. This means that the solution for $\psi(t)$ contains two integration constants which will be variables in the solution. Further there are three Lagrange multipliers in (76) and thus these three Lagrange multipliers are variables in the solution, too. Hence altogether there are five variables in the general solution for $\psi(t)$.

But an important point is that in the end we are not searching for a solution of $\psi(t)$. We are searching for a solution of the pulse shape v(t) which is defined by (27) in dependence of the derivation $\dot{\psi}(t)$. This is important because one of the variables in the solution gets lost due to the derivation and thus the solution of v(t) contains just four variables.

Then an adjustment of the solution to the auxiliary conditions is necessary. Every auxiliary condition determines one of the variables. Hence after adjusting the solution to the auxiliary conditions three variables are determined and just one free variable is left in the solution.

But because of the way in which we express the solution this variable will not appear in our equation. We will choose specific values for λ_3 and we will plot the functions that we want to investigate against λ_3 . This means we just look at solutions for fix values of λ_3 . For a fix value of λ_3 the solutions depend on no further variables. But this does not mean that there is just one solution for a fix value of λ_3 because different solutions in discrete steps are possible. This stems from the discrete different possibilities to adjust the general solution to the auxiliary conditions. The different discrete solutions will play an important role in this work because we will look at first at the symmetric solution which is one of these discrete solutions but rather we look at asymmetric solutions which are further solutions of these discrete steps.

Another important aspect is the meaning of λ_3 . This Lagrange multiplier is the weighting of X against the energy E in the minimization. This means if we choose λ_3 to be zero and we solve (76), we get the pulses with a minimized energy but there is absolutely no minimization of the term X. If we make λ_3 bigger we get pulses with a mix of a minimized energy E and the minimized term X. The bigger λ_3 is the stronger is the minimization of X in comparison with the minimization of E. If we let λ_3 grow to infinity we reach the opposite case of $\lambda_3 = 0$ asymptotically. In this case we get a pulse with the minimized function X but almost no minimization of the energy E is included in our calculation.

In the differential equation (76) you can see a periodicity in $\psi(t)$ with the period 2π . This means the differential equation stays exactly the same if we add a phase of 2π to the function $\psi(t)$.

Now we want to solve the Euler-Lagrange equation while we fulfill the conditions (52), (53) and (54). This is a typical optimization problem known from mathematics.

The best what we can try to reach is to get an analytical solution because in comparison to a numerical solution it delivers a formula as the solution which gives us more general information.

The problem is that (76) is to our knowledge not analytically solvable. The main problem which prevents us from finding an analytical solution is the term with the integral. Without this term (76) would be analytically solvable. Because we prefer an analytical solution to a numerical one it seems to be a good idea to solve as much of (76) as we can analytically and include the rest numerically into the solution. That means concretely that we want to solve the equation in the following two steps. In the first step we ignore the difficult term with the integral by setting $\lambda_3 = 0$ and thus we get the differential equation:

$$\ddot{\psi}(t) + 4\sqrt{\lambda_3^2 + \lambda_2^2} \sin\left(\psi(t) + \arctan\frac{\lambda_2}{\lambda_3} + \frac{\pi}{2}\right) = 0$$
(77)

or with other constants λ and Φ corresponding to the amplitude and the angular in polar coordinates:

$$\ddot{\psi}(t) + 4\lambda \sin\left(\psi(t) + \Phi + \frac{\pi}{2}\right) = 0.$$
(78)

This term is a form of the Sine-Gordon equation. We solve this equation analytically. Further we have to adjust the solution to the auxiliary conditions (52), (53) and (54). This is done in chapter 2.2.2. The analytical solution is not just a preparation step in order to solve the general Euler-Lagrange equation (76), but rather it has an own physical meaning which is worth to have a look at. Neglecting the term with the integral is equal to setting λ_3 to zero and as explained above the solution of (77) hence corresponds to a pulse with minimized energy. In the second step we include the term with the integral numerically so that we get solutions for (76). To do this we let λ_3 raise in small steps within an algorithm which is described in detail in chapter 2.3. This means that we shift the weighting in the minimization starting from a pure energy minimization in small steps to a growing focus on the minimization of the term X in comparison to the minimization of the energy E.

The analytical part is nice to have on its own but an additional advantage is that the numerical treatment in the second step is at an advantage in comparison with a pure numerical treatment of the whole problem because with the analytical solution of the first step we have an exact starting point for the numerical calculation and because the part of the whole problem which we capture numerically is smaller than in a pure numerical treatment.

As a preparation for the analytical solution we write down three qualitative features which a solution of the differential equation fulfilling the auxiliary conditions must have under the restriction $\lambda_3 = 0$ under which we set up analytical solutions. This restriction does not concern statement 2, which is generally valid.

Statement 1

A solution $\psi(t)$ must be antisymmetrical around the points $\psi(t) = -\Phi - \frac{\pi}{2} + n \cdot 2\pi$ with $n \in \mathbb{Z}$.

Due to the periodicity we look at n = 0 without loss of generality. Now we think about the areas to the left and to the right of the point where we have $\psi(t) = -\Phi - \frac{\pi}{2}$. We see in the differential equation (78) that the second derivation $\ddot{\psi}(t)$ depends just on a sine which is negative in the interval $-\Phi - 3\frac{\pi}{2} < \psi(t) < -\Phi - \frac{\pi}{2}$ and positive in the interval $-\Phi - \frac{\pi}{2} < \psi(t) < \Phi + \frac{\pi}{2}$. Further it is obvious that for two points t_1 and t_2 we have $\ddot{\psi}(t_1) = -\ddot{\psi}(t_2)$ if the corresponding functions $\psi(t_1)$ and $\psi(t_2)$ have equal distances to the value $\psi(t) = -\phi - \frac{\pi}{2}$ on different sides of this value, that means $\psi(t_1) = -\Phi - \frac{\pi}{2} - (\psi(t_2) - (-\Phi - \frac{\pi}{2})) = -2\Phi - \pi - \psi(t_2)$. When we now imagine that we move from a point with $\psi(t) = -\Phi - \frac{\pi}{2}$ to the left side and to the right side in equally infinitesimal small steps then it is obvious that $\psi(t)$ must be antisymmetrical around this point because we start with the same derivation $\dot{\psi}(t)$ and the second derivation $\ddot{\psi}(t)$ is all the time the negative of each other when we compare the left side with the right side.

Statement 2

A solution which fulfills the auxiliary conditions cannot be an injective function.

That means there must be points with $\dot{\psi}(t) < 0$. This can be explained with the fact that a function still fulfills the auxiliary conditions (52) and (53), if you add any constant to the function. This can be shown as follows. At first we write down the conditions with a constant phase ϕ .

$$\int_{0}^{\tau_{p}} \sin \left(\psi(t) + \phi\right) dt = 0 \tag{79}$$

$$\int_{0}^{\tau_{p}} \cos \left(\psi(t) + \phi\right) dt = 0$$

Now we apply a trigonometric formula which leads to

$$\cos(\phi) \int_{0}^{\tau_{p}} \sin(\psi(t))dt + \sin(\phi) \int_{0}^{\tau_{p}} \cos(\psi(t))dt = 0$$
(80)
$$\cos(\phi) \int_{0}^{\tau_{p}} \cos(\psi(t))dt - \sin(\phi) \int_{0}^{\tau_{p}} \sin(\psi(t))dt = 0$$

Here we can read that the conditions with any constant are fulfilled at the same time when the conditions without a constant are fulfilled and hence we can use any shifted function $\psi(t)$ with the same justification. If we assume an injective function, the function values must be in an interval of the range π because this is the range which is given by the boundary conditions and if a function exceeds this range it has just a chance to fulfill the boundary condition if it is not injective. Now we shift the interval of the function by a vertical translation in the graph to the interval $-\frac{\pi}{2} < \psi(t) < \frac{\pi}{2}$. We see easily that a function within the interval $-\frac{\pi}{2} < \psi(t) < \frac{\pi}{2}$ cannot fulfill the condition (53) because the cosine is positive within the interval and hence $\int_{0}^{\tau_{p}} \cos(\psi(t))$ must be positive.

Statement 3

A solution function must stay within one of the intervals $-\Phi - \frac{\pi}{2} + n \cdot 2\pi < \psi(t) < -\Phi + \frac{\pi}{2} + n \cdot 2\pi$ with $n \in \mathbb{Z}$.

The different intervals stem from the periodicity of the differential equation described above and for simplicity we chose n = 0. The restriction to the interval is due to the boundary conditions that we have to fulfill. To show this we think about what happened, if the solution would start within the interval and then leaves the interval. At the first look it is conceivable that the solution leaves the interval and later comes back so that it is possible that it fulfills the boundary condition. But this is a misconception. The following consideration about the differential equation reveals that a solution which leaves the interval over the upper or lower border must be an injective raising or sinking function, which cannot fulfill the auxiliary conditions as explained above. In the upper half of the interval the sine in the differential equation (78) is positive and in the lower half the sine is negative. This is a necessity for a non-injective function because a function that crosses the middle of the interval has behind this crossing point a derivation leading away from the middle and thus it needs a negative second derivation $\ddot{\psi}(t) < 0$ in the upper half or a positive second derivation $\ddot{\psi}(t) > 0$ in the lower half to turn its direction. This turn must happen before it reaches the borders of the interval. We explain the reason for the upper border because the explanation for the lower border is exactly analogue. If we assume that the function reaches the upper border with a positive first derivation $\dot{\psi}(t) > 0$ then it gets into the lower half of the next interval where the second derivation is positive $\ddot{\psi}(t) > 0$. This means that the function will necessarily rise with a growing derivation and hence reach the middle of this interval. Then the function raises on with a decreasing derivation but because the symmetry argument explained above, which is valid in every interval, the function will reach the upper border of this interval with the same derivation as it had on the lower border and the same shape of the function is repeated in the next interval and so on.

Our aim as explained above is to reach a mix of a minimization of the Energy E and of the term X, but that is just a qualitative formulation. Before we start to search for solutions we have to write down a quantitative formulation of our aim.

We express the shape of pulses over the pulse duration τ_p . We know that a pulse gets better if the pulse duration decreases. It would be nice to minimize a function which does not depend on the pulse duration so that we can say something about the pulse quality in general without referring to specific values of the pulse duration. To find such a function we look at the dependence of E and X of the pulse duration τ_p :

$$E = \frac{1}{2} \int_{0}^{\tau_p} v^2(t) dt \sim \frac{1}{\tau_p}$$
(81)

$$X = \int_{0}^{1} \int_{0}^{p} |t_1 - t_2| \cos\left(\psi(t_1) - \psi(t_2)\right) dt_1 dt_2 \sim \tau_p^3$$
(82)

$$A = v_{max} \sim \frac{1}{\tau_p} \tag{83}$$

This is due to the fact that $\psi(t)$ has no physical magnitude and hence its derivation is proportional to $\frac{1}{\tau_p}$ which leads to the proportionality of the energy while it is quite obvious that t and dt are proportional to τ_p . A is the amplitude of a pulse corresponding to the highest value of v(t) within the pulse shape. To construct a function without a physical magnitude we define:

$$Z = XE^3. ag{84}$$

In addition we have a look at the function

 τ_n τ_r

$$Z_A = XA^3. ag{85}$$

This function is interesting for us because it is independent of the pulse duration τ_p , too, due to the proportionality $X \sim \tau_p^3$ and $A \sim \frac{1}{\tau_p}$. We do not minimize the maximum amplitude A of a pulse in a direct way and so we do not expect that XA^3 is minimized in the same effective way as XE^3 , but the minimization of the energy can be interpreted as a minimization of the amplitude in some averaging way over the whole pulse. Hence it is worth to have a look at the minimization of XA^3 .

2.2 Analytical solutions

In this chapter we write down the different analytical solutions of the simplified Euler-Lagrange equation (77). In chapter 2.2.1 we show the general analytical solution of the differential equation and in chapter 2.2.2 we show the analytical solutions under the auxiliary conditions.

2.2.1 General solution function

(77) represents a reduced form with just one parameter, namely the time t, of the Sine-Gordon equation. The general Sine-Gordon equation with two parameters has different solutions, which are called solitons and can be seen for example in [35]. For our needs we are interested in a general form of the solution of the reduced Sine-Gordon equation.

A useful form of the solution which we want to use for our work is given in [36]. The problem discussed in [36] is the mathematical pendulum, which has physically nothing to do with our problem, but the mathematical equations are the have the same form as in our case. In [36] there are no phase factors in the sine as we have in the equations (77) and (78). This is not a problem because it is obvious how these phase factors can be included into the solution. In the equations (77) and (78) you can see that the phase factors are just added on $\psi(t)$ within the sine and thus when we set up our formulation of the solution we just have to subtract these phase factors from the solution given in [36]. According to [36] regarding the explained aspect the general form of the solution is given by:

$$\psi(t) = 2 \arcsin\left(k \cdot \sin\left(\sqrt{4\sqrt{\lambda_2^2 + \lambda_1^2}}(t - t_0)|k\right)\right) - \arctan\frac{\lambda_1}{\lambda_2} + \frac{\pi}{2}$$
(86)

$$\psi(t) = 2 \arcsin\left(k \cdot \sin\left(\sqrt{4\lambda}(t-t_0)|k\right)\right) - \Phi + \frac{\pi}{2}.$$
 (87)

We define $m = \sqrt{4\lambda}$. The two emerging integration constants are k and t_0 . t_0 has obviously the meaning of a shift in the t-direction. Note that the solution (86) contains four constants, not five, because we have chosen $\lambda_3 = 0$. The emerging function sn is one of the elliptic Jacobi functions.

2.2.2 Solutions under the auxiliary conditions

At first we want to find symmetrical solutions. Symmetrical means that the solution v(t) is symmetrical around the point $t_{\frac{1}{2}} = \frac{\tau_p}{2}$ and hence that the solution for $\psi(t)$ is point symmetrical or antisymmetrical around the point $t_{\frac{1}{2}}$. We reach this by determining one constant in the solution in such a way that the solution must be symmetrical. This seems at the first look as a reduction of the generality of the solution not just in the different discrete functions that fulfill the auxiliary conditions but rather in a reduction of the free eligible variables. This is not the case as we can see when we include the auxiliary conditions into our considerations. A symmetrical around the point $\frac{\pi}{2}$. That means we determine one constant but we fulfill one condition in the same step, too. That is what we initially planned to do to fulfill the conditions so in the end determining one variable to make the solution symmetrical does not lead to a reduction of the free constants in the solution under the auxiliary conditions.

The solution is periodical with a period that consists of two halves in every period which are antisymmetrical to each other. If we look into the general solution, we see that the solution is antisymmetrical around the point t_0 . This means we can create a solution which is antisymmetrical in $\psi(t)$ and thus symmetrical in v(t) by choosing t_0 in the middle between our boundary points $t_0 = \frac{1}{2}\tau_p$. Now we do not have to care about the condition (53), which is automatically fulfilled, and we just have to adjust the solution to the conditions (52) and (54).

At first we adjust the solution to the boundary condition. Due to the periodicity of the solutions we can fulfill the boundary condition with different numbers of periods between the boundary points where we can start with a positive or negative derivation $\dot{\psi}(t)$. We will look at different solutions starting with a solution that has less than one oscillation period between the boundary points. At first we want to write down a general equation which describes the solution under the boundary conditions. Later we look at specific numbers of periods within the boundary points. We get

$$\psi(\tau_p) = \pi$$

$$\Leftrightarrow 2 \arcsin\left(k \operatorname{Sn}(m(\tau_p - \frac{1}{2}\tau_p))\right) = \frac{\pi}{2}$$

$$\Leftrightarrow \operatorname{Sn}(m\frac{1}{2}\tau_p|k) = \frac{1}{\sqrt{2}k}$$

$$\Leftrightarrow \frac{1}{2}m\tau_p = \operatorname{arcSn}\left(\frac{1}{\sqrt{2}k}|k\right)$$

$$\Leftrightarrow m_1 = 2\operatorname{arcSn}\left(\frac{1}{\sqrt{2}k}|k\right) + 4\operatorname{K}(k) \cdot j$$

$$m_2 = 4\operatorname{K}(k) - 2\operatorname{arcSn}\left(\frac{1}{\sqrt{2}k}|k\right) + 4\operatorname{K}(k) \cdot j.$$
(88)

K(k) is an elliptic Integral and $j \in \mathbb{N}$ including j = 0. j describes the numbers of

whole periods within the solution between the boundary points. Note that this does not mean that there is an integer number of periods between the boundary points because in every solution there is a non-completed period in addition to the number of whole periods described by j. m_1 describes the solutions starting with a positive derivation $\dot{\psi}(t) > 0$ and m_2 describes the solutions starting with a negative derivation $\dot{\psi}(t) < 0$. Note that there is no solution for m_1 with j = 0 which fulfills the auxiliary conditions. The reason lies in statement 2. The solution of the differential equation for m_1 with j = 0 is injective with a positive derivation and thus according to statement 2 it can not fulfill the auxiliary conditions.

Further we adjust the solution to the remaining condition (52). This means we determine the remaining constant k. This is analytically difficult. We do it numerically by treading equation (52) as a root finding task, which we can solve easily with an interval method similar to the methods described in [37]. The tables 1 and 2 show the calculated values of the solutions. Appendix A explains the graphical meaning of these solutions. The figures 2 and 4 show the solutions for the angular and 3 and 5 show the solutions for the pulse shape.

Pulse	m	k
1	$4\mathbf{K}(k) - 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2k}} k\right)$	0.85509241
2	$4\mathbf{K}(k) + 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2}k} k\right)$	0.94140311
3	$-8\mathrm{K}(k) + 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2k}} k\right)$	0.88579264
4	$-8\mathrm{K}(k) - 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2}k} k\right)$	0.92698697
5	$12\mathrm{K}(k) - 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2k}} k\right)$	0.89417815
6	$12\mathrm{K}(k) + 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2}k} k\right)$	0.92142142
7	$-16\mathrm{K}(k) + 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2}k} k\right)$	0.89809898
8	$-16\mathrm{K}(k) - 2\mathrm{arcSn}\left(\frac{1}{\sqrt{2}k} k\right)$	0.91847486

Table 1: The first eight analytical solutions

Pulse	$E\left[\frac{1}{\tau_p}\right]$	$X\left[\tau_p^3\right]$	XE^3	$A\left[\frac{1}{\tau_p}\right]$	XA^3
1	4.583	0.150535	14.493	5.384410	23.499
2	27.723	0.039648	844.762	11.279234	56.893
3	35.100	0.023843	1031.065	13.911100	64.187
4	81.517	0.012659	6857.364	19.746023	97.464
5	93.751	0.009353	7707.136	22.370874	104.715
6	163.413	0.006155	26859.794	28.195976	137.976
7	180.517	0.004961	29182.336	30.818857	145.216
8	273.415	0.003628	74156.607	36.639920	178.456

Table 2: Function values of the first eight analytical solutions


Figure 2: Angular of analytical solutions in dependence of the time



Figure 3: Pulse shape of analytical solutions in dependence of the time



Figure 4: Angular of further analytical solutions in dependence of the time



Figure 5: Pulse shape of further analytical solutions in dependence of the time

Further we want to think about asymmetrical solutions. As explained above the symmetrical solution is one of the discrete possibilities to adjust the general solution to the auxiliary conditions. We assume that there are asymmetrical solutions for the general differential equation. The question is if there are asymmetrical solutions for the simplified differential equation, too. This is not the case. In the following we proof that no asymmetric solution for the reduced differential equation exists.

To set up the proof at fist we use the fact that we can add any phase to the function $\psi(t)$ in the equations (52) and (53) as it is shown in statement 2. We add $\Phi + \frac{\pi}{2}$ so that the sine in condition (52) has the same argument as the sine in the differential equation. Then we use statement 1 which tells us that a solution of the differential equation must be antisymmetrical around the points where we have $\psi(t) = -\Phi - \frac{\pi}{2} + n \cdot 2\pi$. Due to the antisymmetry the only possibility to get an asymmetrical solution is to place the boundary points asymmetrically around such a symmetry point. But this is not possible because of the conditions (52) and (53). Due to the shift the sine in equation (52) is antisymmetrical around the solution, too. Further it can shange its sign only in symmetry points. To fulfill condition (52) the positive and the negative part in the integrand must have the same volume. Due to the symmetry of the sine in condition (52) this is just possible if the boundary points are symmetrically arranged around a symmetry point and hence it follows that every solution which fulfills the auxiliary conditions is forced to be symmetrical.

Note that this proof is just valid for the reduced Euler-Lagrange equation (77). The whole Euler-Lagrange equation (76) is another differential equation and thus we can say at this point nothing about the existence of asymmetrical pulses as solutions of the whole Euler-Lagrange equation. As you will see in chapter 2.3.3 there are indeed asymmetrical solutions of the whole Euler-Lagrange equation which we find in that chapter with a numerical approach.

2.3 Numerical solutions

In this chapter we want to solve the whole differential equation (76). That means we use the analytic solution of the preceding chapter for the simplified Euler-Lagrange equation and we extend the solution to different values of λ_3 numerically. The integral in (76) is not analytically solvable and thus we can not change the differential equation to a form without an integral. There are many different methods to solve differential equations numerically but a typical feature of the most methods is that they are based on a stepwise walk along the values of the variable in the differential equation, in our case the time from 0 to τ_p . The integral term prevents us from applying such a method directly because in the integral we need information about the whole function $\psi(t)$ while a stepwise method has in every step just the information about the preceding steps but not about the following steps. In order to solve the differential equation we use a method that is generally based on a standard method for which we chose the Runge-Kutta algorithm of fourth order but the method uses several runs over the whole Runge-Kutta algorithm.

Further we want to search for asymmetrical pulses. To do this we change the program so that we get a second program which is similar to the first one.

The scheme of the programs is explained in the following chapter. The purpose of this chapter is to find a solution with lower value of XE^3 in comparison with the analytical solution. This is possible because we expect that the energy E has a vanishing derivation in $\lambda_3 = 0$ because the analytical calculus aimed on a pure minimization of the energy. If the term X has a non-vanishing derivation in $\lambda_3 = 0$ its shrinkage will outperform the growths of E at least in a short area around $\lambda_3 = 0$. We expect that X has a non-vanishing derivation in $\lambda_3 = 0$ because the analytical calculus ignores the minimization of X completely.

2.3.1 Scheme of the programs

Here we explain the function scheme of the programs that we use for the search for symmetrical and asymmetrical pulses. At first we look at the program for the search for symmetrical pulses. Due to the fact that the integral term in (76) requires knowledge of the whole solution the following idea seems to be a useful approach.

The first clear point is that we have to discretize the function $\psi(t)$ along the t-axis due to the numerical stepwise moving Runge-Kutta algorithm. We chose 2000 steps. We calculate solutions by rising values of the Lagrange multiplier λ_3 i.e. by concrete weightings of the minimization of the term X to the minimization of the energy E. We start by $\lambda_3 = 0$, which corresponds the analytically solved problem in chapter 2.2. The advantage of this starting point is that in this point we know the solution with high precision. Then we raise λ_3 in small steps. In every single step we use the solution of the preceding step as the function $\psi(t_2)$ in (76) over which we integrate in the differential equation. This solves the problem that a standard method delivers just knowledge of the preceding steps. In every single step in λ_3 we apply a loop which lets the solution converge to the solution by the specific value of λ_3 . The idea of the loop is to apply the Runge-Kutta algorithm to (76) at first with the solution of the preceding step within the integral. To improve the efficiency of the program the Runge-Kutta algorithm runs from the middle by $t_{\frac{1}{2}} = \tau_p$ to the end by τ_p instead of running over the whole pulse shape. The left half is adjusted antisymmetrically to the right half because we restrict this first program to symmetrical pulses. Then we get a new solution $\psi(t)$ from the Runge-Kutta algorithm which we use in a second application of the Runge-Kutta algorithm within the integral. Further in every step of the loop we use the solution of the preceding step as the function within the integral as $\psi(t_2)$.

When we change the differential equation and thus the solution it is expectable that the new solution will not fulfill the auxiliary conditions under the same Lagrange multipliers. We have to adjust the new solution numerically to the auxiliary conditions in every single step of the loop again by determining the Lagrange multipliers. This is a problem which corresponds to a root search. One of the auxiliary conditions (53) is automatically fulfilled due to the fact that we restrict ourselves to symmetrical pulses with $\lambda_3 = 0$. Then we have two remaining conditions (52) and (54) which we want to fulfill by determining two parameters. One of these parameters is λ_2 , But we need a second parameter. We use the starting derivation $\dot{\psi}(t_{\frac{1}{2}})$ which is quite more easy to handle numerically than the variable k from the analytical solution. The method that we use in the root search is the Broyden's algorithm taken from the numerical recipes [38]. The Broyden's algorithm is a quasi-Newton method and it is based on the secant method.

Alltogether in every single step of the loop we do a root search with the solution function $\psi(t)$ from the preceding loop step and we get a new solution in the actual loop step when the auxiliary conditions are fulfilled more exactly than a numerical threshold, which we set for the root search. We need a second threshold for the loop, which repeats the Runge-Kutta algorithm. We expect that the loop converges to the solution under the chosen variables in each step so that the difference between consecutive solutions becomes smaller and smaller. We use the norm $||\vec{\psi}_n(t) - \vec{\psi}_{n+1}(t)||_2$ for the definition of the difference between two consecutive solutions. The indices define the number of the step within the loop and the functions $\psi(t)$ are vectors containing the values of $\psi(t)$ at the discretized points of this function. The loop ends when the difference between two consecutive solutions becomes smaller then a threshold that we set. A pseudocode version of this program can be seen in Appendix B.

In addition we want to search for asymmetrical pulses. To do this we use a program that is quite similar to the program which searches for symmetrical pulses. Due to the fact that we do not know if asymmetrical solutions exist and by which values of λ_3 asymmetrical solutions exist we do not write a program which raises λ_3 in small steps and uses for the initial solution in every step the solution of the previous one. Instead we write a program which searches in bigger steps in λ_3 and uses in every step the same solution as the initial guess for example the asymmetrical CORPSE pulse or the analytical solution from chapter 2.2 which led to the results below. In every step the program does in general the same process as the program which searches for symmetrical solutions with a few differences. The first difference is that the Runge-Kutta algorithm does not run from the middle to $t = \tau_p$. Instead it runs from t = 0to $t = \tau_p$. Another difference is that the Lagrange multiplier λ_2 , which was chosen to be zero in the solution for symmetrical pulses, has not anymore a predefined value. The program does not perform a root search in two but instead in three variables. We use a representation such as (78) of the Euler-Lagrange equation containing the integral term from (76) and we use the amplitude λ and the angular Φ instead of λ_1 and λ_2 . Hence the three variables for the root search are λ , Φ and the initial derivation $\dot{\psi}(0)$.

Here lies a big disadvantage in the program performance in comparison with the first search program. In addition the initial values of the three variables are in general much more far away from the solution because as explained there are no small steps in λ_3 where one step delivers the initial solution for the following one.

2.3.2 Symmetrical solutions

In this chapter we present the symmetrical solutions. The main aim is to find the solution with the minimal value of the function XE^3 and as a secondary aim the solution with the minimal value of the function XA^3 because these functions are independent of the pulse duration τ_p . At first plots of E and X alone are shown. In figure 6 you can see the plot of E against the Lagrange multiplier λ_3 which is raised in steps of $\Delta\lambda_3 = 0.05$.



Figure 6: Energy in dependence of λ_3

For raising values of λ_3 the energy gets worse and worse. This is expectable when you remember that the Lagrange multiplier λ_3 can be interpreted as the weight of the minimization of the term X in comparison with the minimization of the energy E. That means the bigger λ_3 grows the less is E minimized and that is exactly what you can see in figure 6. Further the fact that we see a local minimum of E in figure 6 in the point $\lambda_3 = 0$ due to the vanishing derivation of the energy in this point is what we wanted to reach in chapter 2.2 for the analytical solution. Hence figure 6 can be seen as a verification of the results in chapter 2.2. It shows that the analytical method worked well and led indeed to a local minimum.

In figure 7 you can see a plot of the term X against the Lagrange multiplier λ_3 .



Figure 7: X in dependence of λ_3

As you can see in figure 7 the term X has a non-vanishing derivation in the point $\lambda_3 = 0$. This is what we hoped and thus the function XE^3 has a minimum of XE^3 which we find with the numerical calculation. Another point is that the graph of X looks for big values of λ_3 as if it gets closer to an asymptote. This is according to the No-Go theorem because we know that a pulse which fulfills the auxiliary conditions can not make X to zero at the same time. Hence there must be a minimum point of X which the graph can not cross. Figure 8 shows a plot of the function XE^3 against λ_3 over a big range.



Figure 8: XE^3 in dependence of λ_3

For a better visualization figure 9 shows the same graph as figure 8 but a smaller area around the minimum of XE^3 .



Figure 9: A smaller frame of XE^3 in dependence of λ_3

In figure 9 you can see the position of the minimum of XE^3 in the point $\lambda_3 = 10.25$. The minimum is the smallest value that we reach within this work and thus the pulse at this point is the most important outcome of this work under all the presented pulses.

A disadvantage is that this pulse has a value XE^3 which is very close to the value of the analytical solution. Hence we win not very much shrinkage in XE^3 . Further we look at the pulse which minimizes the function XA^3 . At first we plot the maximum amplitude A in figure 10. A has a non-vanishing derivation in $\lambda_3 = 0$. This is expectable because in the analytical solution we did no direct minimization of A.



Figure 10: Maximum amplitude in dependence of λ_3

In figure 11 the function XA^3 is shown. As expected we see that it has a minimum which is an interesting point to have a look at.



Figure 11: XA^3 in dependence of λ_3

At first we want to have a look at the general development of the pulse shape under a raising λ_3 . In tabular 3 the function values for pulses at some points of λ_3 are shown and in the figures 12 and 13 you can see the angular and the shape of these pulses.

λ_3	$E\left[\frac{1}{\tau_p}\right]$	$X\left[\tau_p^3\right]$	XE^3	$A\left[\tau_p^3\right]$	XA^3
25	4.626	0.147318	14.583	4.874125	17.059
50	4.803	0.142703	15.809	4.283410	11.215
75	5.223	0.136068	19.386	4.179140	9.932
100	6.017	0.127058	27.680	4.639220	12.686

Table 3: Numerical solutions for raising λ_3



Figure 12: Angular in dependence of the time for raising values of λ_3



Figure 13: Pulse shape in dependence of the time for raising values of λ_3

In tabular 4 you can see the values of the relevant functions for our pulses in comparison with CORPSE and SCORPSE.

Pulse	$E\left[\frac{1}{\tau_p}\right]$	$X\left[\tau_p^3\right]$	XE^3	$A\left[\frac{1}{\tau_p}\right]$	XA^3
XE^3 min	4.590	0.149288	14.438	5.184094	20.799
XA^3 min	5.049	0.138516	17.828	4.123058	9.709
SCORPSE	6.717	0.127612	38.671	3.665191	6.283
CORPSE	23.166	0.029884	371.541	6.806784	9.425

Table 4: Numerical solutions of the functions minimizing XE^3 and XA^3 in comparison with CORPSE and SCORPSE

In figure 14 the time-dependent angular $\psi(t)$ of the central spin to its initial position of the pulses in the minima of XE^3 and XA^3 in comparison with the already known CORPSE and SCORPSE [22, 23, 24] is shown and in 15 the pulse shapes are shown.



Figure 14: Angular in dependence of the time of the XE^3 and XA^3 minimizing pulses and for comparison of the already known pulses SCORPSE and CORPSE



Figure 15: Pulse shape in dependence of the time of the XE^3 and XA^3 minimizing pulses and for comparison of the already known pulses SCORPSE and CORPSE

2.3.3 Asymmetrical solutions

Further we evaluate the solutions of the program which searches for asymmetrical solutions. Because we had not initially idea by which values of the parameters asymmetrical solutions could be we have just a few evaluated points due to the big step ranges and we show just a few points in λ_3 . We start the program with the analytical symmetrical solution of chapter 2.2 and move over to asymmetrical solutions by the initial choice of the parameters. We find some asymmetrical solutions for which we show the function values in tabular 5 and plot $\psi(t)$ and v(t) in the figures 16 and 17.

λ_3	$E\left[\frac{1}{\tau_p^3}\right]$	$X\left[\tau_p^3\right]$	XE^3	$A\left[\frac{1}{\tau_p}\right]$	XA^3
0	4.590	0.14929	14.438	5.1740	20.678
7.14285	4.598	0.15003	14.587	5.3179	22.564
14.2857	4.646	0.14927	14.964	5.2564	21.679
21.42855	4.732	0.14819	15.705	5.2042	20.887
28.57145	4.867	0.14672	16.913	5.1677	20.247
35.7143	5.058	0.14478	18.732	5.1561	19.846

Table 5: Asymmetrical numerical solutions



Figure 16: Angular in dependence of the time of a few asymmetric pulses



Figure 17: Pulse shape in dependence of the time of a few asymmetric pulses

As you can see the asymmetrical solutions are for small values of λ_3 very similar to the symmetrical analytical solution and for growing values of λ_3 they get probably continuously away from the analytical solution. The steps of the shapes in the figures 16 and 17 stem from the stepwise choice of λ_3 which is not a parameter of the root search.

2.3.4 Discussion

The variational calculations in chapter 2.1 run quite straightforward and are not a big difficulty for amplitude-modulated pulses.

For the solutions in the chapters 2.2 and 2.3 the comparison with the already known pulses CORPSE and SCORPSE is interesting because it proves the quality of the new pulses. In chapter 2.2 the analytical solution leads to a series of pulses which are divided discretely from each other. We see that the best pulse of this series is the first one which has the lowest number of oscillations between its boundary points.

A few qualitative considerations let us understand this aspect. A pulse which oscillates often between the boundary points has to have a bigger average amplitude than a pulse that oscillates less often. This is due to (27) which implies that the traveled angular into both directions is proportional to the integral over the pulse shape from t = 0 to $t = \tau_p$. This means that a big traveled angular leads to a big average amplitude and thus a big pulse energy. The qualitative statement that we can make is that keeping the traveled angular small is one of the features of a pulse which makes the energy small and leads thus to a small function XE^3 . In the series of the analytical solutions the first one is the pulse which has the smallest travelled angular and hence fulfills this idea best. In comparison with the pulses CORPSE and SCORPSE the best analytical pulse has a lower energy and a lower function XE^3 .

A surprising result that was not clear beforehand is that already the analytical pulse has a lower function XE^3 than CORPSE and SCORPSE because the analytical calculation contains absolutely no minimization of the term X. The energy minimization alone was successful enough to reach this.

The next stage was the numerical calculation in which the minimization of the term X was included to find the minimum of the function XE^3 . The pulse which we found minimizes the function XE^3 a little bit more than the analytical solution. The solution in the minimum of the function XE^3 is the most important new pulse in this work because this minimum of XE^3 is the smallest value that we found and thus the pulse is the best pulse regarding to our definition of decoherence suppression quality. The disadvantage is that the difference to the value of XE^3 of the analytical solution is really small. This means that the numerical method in fact led to an improvement but to an improvement much smaller than we hoped to reach. But in the end it is important that the new pulse performs well in comparison with CORPSE and SCORPSE and the advantage in the minimization of XE^3 is big in comparison.

A remarkably point is the qualitative similarity between the new pulse at the minimum of XE^3 and SCORPSE. The similarities between these two pulses are the three intervals

where the spin moves backwards in the first interval, forward in the second interval and again backwards in the third interval. Further the points where the pulse shape crosses the value zero are close to each other. The differences are in the quantitative pulse shape. For the reason of this outcome we can just set up assumptions but it could have something to do with the fact that the minimization of the energy and the minimization of the maximum amplitude are not completely independent of each other. This is due to the fact that the energy contains an integral over the square of the amplitude and thus depends in some way of the average value of $v^2(t)$. Then the outcome leads to the idea that the qualitative puls shape with these three intervals of the new pulse and SCORPSE could be in some way ideal for such problems because two independent methods led to this qualitative pulse shape. But note that this idea is not more than an assumption for the reason of this outcome.

In addition we looked at the pulse in the minimum of XA^3 . This pulse has a bigger value of XA^3 than the SCORPSE pulse but a smaller value of XE^3 . Hence this pulse is an interesting outcome of this work, too.

In the end we had a look at asymmetrical pulses, not because we really expected better performances than for the symmetrical pulses, but rather for further understanding of possible solutions of the Euler-Lagrange equation. The asymmetrical pulses have a bigger function XE^3 than the symmetrical solution. Thus they are indeed just relevant for considerations concerning understanding of the equations and not for considerations concerning quality for practical purposes.

3 Simulation of the Pulses

The pulse in the minimum of XE^3 is the most important result for practical purposes in this work. Thus we want to do a further verification of its quality. In order to do this we use a program of Stanek [21]. He wrote a program which calculates the Frobenius norm for a default pulse under the cusp-like autocorrelation. In the end the program delivers a plot of the Frobenius-norm against the pulse duration τ_p or the maximum amplitude A. We will present those plots but more interesting for us is a plot of the Frobenius norm against the energy which is easily calculable starting from one of the first two plots.

In chapter 3.1 we present the scheme of the program and explain how it works. In chapter 3.2 the results are presented and in chapter 3.3 we discuss the results. What we hope to see is that the results of the simulation coincide with the results of the values of XE^3 and XA^3 in chapter 2 because this would underline the correctness of the calculations in chapter 2.

3.1 Scheme of the program

The idea of Stanek's [25] program is to calculate an averaged Frobenius norm of a pulse via the calculation of the time evolution under fluctuations created by a random number generator which obeys the Noise model described in chapter 1.1.2. Using more fluctuations within the pulse duration improves the statistical accuracy of the results but it causes a higher computation time. We use 5 runs of 100000 fluctuations for our calculations. The calculation of the time evolution itself is not time intensive because just simple integrals have to be carried out. Stanek [21] reduces the error of the integration for the timedependent Hamiltonian with the method of CFETs (commutator-free exponential time propagators) [39, 40] but this does not increase the run-time significantly. The main difficulty is the sampling of the fluctuations $\eta(t)$ which obey the autocorrelation. To do this Stanek [21] writes down a differential equation for the noise

$$\dot{\eta} = -\nu\eta + h(t). \tag{89}$$

h(t) represents white noise. The solution is given by:

$$\eta(t) = \left[\int_{0}^{t} dt' h(t') e^{\nu t'} + \eta_0\right] e^{-\nu t}.$$
(90)

This is what is the time dependence which is needed for the noise but further the values h_0 and η_0 have to be determined. To do this the autocorrelation is used. Stanek comes to the result:

$$h_0 = 2\nu g_0^2 \tag{91}$$

$$\bar{\eta}_0 = 0 \tag{92}$$

$$\operatorname{Var}(\eta_0) = g_0^2 \tag{93}$$

3.2 Results

Now we present the results of the simulation for the pulse in the minimum of XE^3 in comparison with CORPSE and SCORPSE. At first we have a look at plots of the Frobenius norm plotted against the pulse duration τ_p which we produce directly as an outcome of the program. Then we translate this plot over the relationship between τ_p , A and E to a plot of the Frobenius norm against the inverse amplitude and the inverse energy. A demonstrative understanding of these plots is that for every point on the x-scale which you chose to look at you compare the three pulses with the same pulse duration, amplitude or energy. In figure 18 you can see the plot of the Frobenius norm against the pulse duration, in figure 19 against the inverse amplitude and in figure 20 against the inverse energy.



Figure 18: Frobenius norm of the XE^3 minimizing pulse in comparison with the Frobenius norm of the pulses SCORPSE and CORPSE in dependence of the pulse duration τ_p



Figure 19: Frobenius norm of the XE^3 minimizing pulse in comparison with the Frobenius norm of the pulses SCORPSE and CORPSE in dependence of the maximum amplitude A



Figure 20: Frobenius norm of the XE^3 minimizing pulse in comparison with the Frobenius norm of the pulses SCORPSE and CORPSE in dependence of the energy E

The first important point that should be said to avoid confusion is that the cutoff values of the Frobenius norm for the new pulse, i.e. the value below which the Frobenius norm is not calculable, has nothing to do with physics. It is just a numerical effect and if you are interested in the physics and not numeric, you should focus on the graphs on the right side of the kink where the Frobenius norm is above of this cutoff value. Below at fist we discuss the physics and in the end we do a few considerations on the numerical cutoff.

What you can see in figure 18 is exactly what we expected. The new pulse is worse than CORPSE and SCORPSE plotted against the pulse duration. This is due to the fact that the new pulse is not directly constructed to be good under this definition of quality and this coincides with the results in chapter 2. Plotted against the inverse amplitude in figure 19 the new pulse is worse than CORPSE and SCORPSE and this coincides with our results in chapter 2 again.

The most important plot is figure 20 because this plot shows the quality under our definition of quality. In chapter 2 the results showed that we reached this aim with success because the new pulse had a smaller function XE^3 than CORPSE and SCORPSE. Thankfully picture 20 confirms this result. As you can see the Frobenius norm of the new pulse plotted against the inverse energy stays always below the Frobenius norm of CORPSE and SCORPSE.

Fits through the graphs on the right side of the kink can be seen in Appendix C where fits for the XA^3 minimizing pulse, which we do not plot in the graphs for reasons of clarity, are shown, too.

Now we want to think about the numerical cutoff. The cutoff is due to the fact that the new pulse is divided into a certain number of intervals between t = 0 and $t = \tau_p$. To do investigations concerning this cutoff we tested the program with different numbers of

intervals. Until this point the new pulse was described with 2000 intervals all over this work but now we want to test the simulation with 100 till 2000 intervals ascending in steps of 100 intervals with 1000 fluctuations. The result can be seen in 21 where the cutoff is plotted against the number of intervals.



Figure 21: Limitation value of the numerically calculated Frobenius norm in dependence of the numerical discretization of the pulses

A fit of the function $\Delta_F^{Limit}(N) = \frac{a}{N^b}$ in Figure 21 reveals $a = 3.35104 \pm 0.001167$ and $b = 2.00172 \pm 0.00007483$. Hence we assume that the cutoff value of the Frobenius norm has an inverse quadratic dependence of the number of intervals N:

$$\Delta_F^{Limit} \sim \frac{1}{N^2} \tag{94}$$

The cutoff value has no noticeable dependence of the number of digits at double precision which are used within the values of the intervals. Thus we can say that the variable which determines the cutoff value is the number of intervals N alone in our case. This is not a general statement because if we would raise the number of intervals much higher it is expectable that the number of digits in the interval values will become the variable which determines the cutoff. Making the cutoff value smaller is hence just a question of computation time because more pulse intervals raise the computation time of the numerical program from chapter 2.2 which calculates the pulse and the computation time of the simulation program.

It is unclear if a smaller cutoff value is really necessary. Within this work the areas in the plots above the cutoff value tell us everything what we want to know because the double logarithmical plots show straight lines which allow a clear comparison of the pulse qualities. The reason that there is no cutoff for CORPSE and SCORPSE is that these pulses are known exactly. The amplitude and the switching times are exact values described in units of the known constant π .

3.3 Discussion

The simulation worked well and verified the results of chapter 2. This is an important validation in order to present a pulse as the outcome of this work which could have a theoretical and practical use for decoherence suppression. All the qualitative graphs agree with the calculated values in chapter 2 and thus we have determined the quality of the new pulse in comparison with CORPSE and SCORPSE over two independent ways. In the three graphs we can see clearly the growth of the Frobenius norm with the exponent $\frac{3}{2}$ which is due to the mixed term in the Frobenius norm under the cusp-like autocorrelation. This result under the cusp-like autocorrelation was already plotted in the work of Stanek [21].

4 Variational Ansatz for Frequency-Modulated Pulses

The main part of this work was the application of a variational approach to the search for decoherence suppressing amplitude-modulated pulses. Now we try to apply a similar approach with the difference that we want to search for frequency modulated pulses instead of amplitude modulated pulses.

The most important difference between the two approaches lies in the fact that for frequencymodulated pulses there are four instead of one varied function which are dependent of each other such that they could be described theoretically by one varied function, too. Note that there is one instead of two functions for amplitude-modulated pulses because the dependence between $\psi(t)$ and v(t) is analytically solvable. But we have no analytical solution for the coupling equations (30), (31) and (32). The approach would be absolutely analogue, if we could solve these equations analytically. We know that the functions $\psi(t)$, $\phi(t)$ and $\theta(t)$ are dependent of $\Omega(t)$ and thus if we had a solution for the coupling equations, we could write down all the formulas as functionals in dependence of $\Omega(t)$ just as we can write the equations in dependence of v(t) or alternatively $\psi(t)$ in the search for amplitude-modulated pulses. The fact that we have no analytical solution makes this way impossible. What we can do instead is doing a variational calculation with four functionals instead of one functional and with the coupling equations as three auxiliary conditions which couple the functionals.

This way of the variational calculation is not as easy as the variational calculation for amplitude modulated pulses because it can not be done straightforward following the known standard way of a variational calculation. Instead we have to backtrace the whole derivation of the Euler-Lagrange formalism starting from the postulation of a stationary action. This is done in chapter 4.3 where you can see that the dependence of the four functionals of each other indeed changes the way of the calculations for the derivation of an Euler-Lagrange equation. Due to the arising difficulties we just write down the calculations until we have an Euler-Lagrange equation for the search for frequency modulated pulses. We do not give solutions for these equations because it would be a difficult task to search for solutions and we do not start this within this work.

4.1 Minimized functions

As described in chapter 1 there are four conditions (58), (59), (60) and (61) which stem from the minimization to zero of the first order of the Frobenius norm and the boundary condition. In addition we want to minimize the next order of the Frobenius norm. As for amplitude modulated pulses this order is an order proportional to $\tau_p^{\frac{3}{2}}$ for frequency modulated pulses, too.

The difference is that this order does not stem just from the combination of the linear order of the Magnus expansion with the linear order of the Taylor series of the noise. Instead there is a contribution of the combination of the linear and the quadratic order of the Magnus expansion with the constant order of the Taylor series of the noise, too.

The reason that such a contribution does not exist for amplitude modulated pulses is that there is just one second order term in the Magnus expansion which has another direction than the two first order terms. Just terms in the same direction lead to a contribution to the Frobenius norm. For frequency modulated pulses there are three first order terms in the Magnus expansion, one of them in each direction, and three second order terms, one of them in each direction, too. Thus there are indeed combinations of different orders in the same direction, which contribute to the Frobenius norm.

$$\overline{\mu_x^{(1)^2}} + \overline{\mu_y^{(1)^2}} + \overline{\mu_z^{(1)^2}} + \overline{\mu_x^{(1)}} + \overline{\mu_x^{(1)}} + \overline{\mu_y^{(1)}} + \overline{\mu_y^{(1)}} + \overline{\mu_z^{(1)}} + \overline{\mu_z^{(1)}} + \overline{\mu_z^{(2)}}$$

$$= \text{QuadraticOrder} + g_1 \int_0^{\tau_p} \int_0^{\tau_p} |t_1 - t_2| [n_{xz}(t_1)n_{xz}(t_2) + n_{yz}(t_1)n_{yz}(t_2) + n_{zz}(t_1)n_{zz}(t_2)] dt_1 dt_2$$

$$= \overline{\eta} (\overline{\eta}^2 + g_0) \int_0^{\tau_p} \int_0^{\tau_p} \int_0^{\tau_p} \int_0^{t_2} [n_{xz}(t_1)n_{yz}(t_2)n_{zz}(t_3) - n_{xz}(t_1)n_{zz}(t_2)n_{yz}(t_3) + n_{yz}(t_1)n_{zz}(t_2)n_{xz}(t_3)] dt_1 dt_2$$

$$J_{0} J_{0} J_{0}$$

$$-n_{yz}(t_{1})n_{xz}(t_{2})n_{zz}(t_{3}) + n_{zz}(t_{1})n_{xz}(t_{2})n_{yz}(t_{3}) - n_{zz}(t_{1})n_{yz}(t_{2})n_{xz}(t_{3})] dt_{3}dt_{2}dt_{1} + O(\tau_{p}^{4})$$

=QuadraticOrder + $X_{f} + O(\tau_{p}^{4})$

As you can see in (95) we call the term in the Frobenius norm X_f which is trilinear in τ_p . The situation is now similar to the situation for amplitude modulated pulses. We want to make the orders of the Frobenius norm vanish in ascending order. The three first order terms can vanish completely, described within the auxiliary conditions, and further we want to make the next order (95) as small as possible.

Analogue to the approach for amplitude modulated pulses where we minimized the energy we want to minimize a similar term for frequency modulated pulses, too. This term should describe something what describes a practically limited physical size or a physical size that we want to keep small for any reasons. For amplitude modulated pulses we have chosen the energy which is limited by the amplitude for a certain pulse duration and which is wanted to be small. Here we chose the same term $M = \frac{1}{8} \int_{0}^{\tau_{p}} \dot{\psi}^{2}(t) dt$. The reason for which we chose this function is that a quite smooth movement of the angular $\psi(t)$ should be more easy to be implemented by a device than a movement with sudden changes of the movement or peaks of the speed.

Note that the choice of a minimized function is a conceptual question which depends on the practical purposes within an experiment or a produced device. Other functions could be chosen with good justification, too, depending on the purpose. Such as for amplitude modulated pulses one of the minimized functions has a Lagrange multiplier, we set it in front of X_f . This Lagrange multiplier describes the weight of the minimization of X_f in comparison with M.

4.2 Lagrangian

Now we have to write down a Lagrangian for the situation which contains all the terms that we want to eliminate due to the auxiliary conditions or minimize. For simplification we reduce the problem analogously to the reduced analytical solvable problem for amplitudemodulated pulses. That means we neglect the minimization of the term (95) completely by setting its Lagrange multiplier to zero. What is left is the minimization of M under the auxiliary conditions. To derive the Lagrangian we write down the action functional:

$$I = \frac{1}{8} \int_{0}^{\tau_{p}} \dot{\psi}^{2}(t) dt$$

$$+ \lambda_{1} \int_{0}^{\tau_{p}} (-a_{y}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{x}(t)a_{z}(t)) dt$$

$$+ \lambda_{2} \int_{0}^{\tau_{p}} (a_{x}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{y}(t)a_{z}(t)) dt$$

$$+ \lambda_{3} \int_{0}^{\tau_{p}} (\cos(\psi(t)) + (1 - \cos(\psi(t)))a_{x}^{2}(t)) dt$$
(96)

Now we compare the action functional (96) with the formal definition of an action functional over a Lagrangian (65) and we identify the Lagrangian in . The Lagrangian is

$$L = \frac{1}{8} \dot{\psi}^{2}(t)$$

$$+ \lambda_{1} \left(-a_{y}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{x}(t)a_{z}(t)) \right)$$

$$+ \lambda_{2} \left(a_{x}(t) \sin(\psi(t)) + (1 - \cos(\psi(t)))a_{y}(t)a_{z}(t)) \right)$$

$$+ \lambda_{3} \left(\cos(\psi(t)) + (1 - \cos(\psi(t)))a_{x}^{2}(t) \right) .$$
(97)

4.3 Euler-Lagrange equation

In this chapter we describe the derivation of the Euler-Lagrange equation. This part contains the most important differences in comparison with the standard Euler-Lagrange formalism due to the fact that we have four minimized functions which are dependent of each other. What we do now is to add a small variation to the four functions $\Omega(t)$, $\phi(t)$, $\theta(t)$ and $\psi(t)$:

$$\Omega(t) \qquad \Omega(t) + \delta\Omega(t)
\phi(t) \longrightarrow \qquad \phi(t) + \delta\phi(t)
\theta(t) \longrightarrow \qquad \theta(t) + \delta\theta(t)
\psi(t) \qquad \psi(t) + \delta\psi(t)$$
(98)

Without the coupling equations the calculation could be such as the standard variational calculation of the Lagrange formalism of the second kind in analytical mechanics. Then we could compare the four functions $\Omega(t)$, $\phi(t)$, $\theta(t)$ and $\psi(t)$ with four degrees of freedom in the mechanical case and the mathematics would be the same. But the important difference is that the four functions are dependent of each other due to the coupling equations (58), (59) and (60). This situation is thus similar to coordinates in analytical mechanics which are coupled over constraint equations such as within the Lagrange formalism of the first kind. We can start the derivation of the Euler-Lagrange equation similar to the Euler-Lagrange formalism of the second kind but at the point where the independence of the degrees of freedom of each other is used in the Euler-Lagrange formalism of the second kind, we have to leave this way of calculations and then we have to find another solution for the problem.

Note that we know already before we did any calculations that there can be just one Euler-Lagrange equation for our problem and not a higher number of Euler-Lagrange equations. For example you could guess that there must be four of them, one for each of the functions, but that is wrong. This is due to the fact that we have just one independent varied function and just this function should have an Euler-Lagrange equation because just this function represents a physical degree of freedom. The three other functions which could be theoretically expressed in dependence of this one independent function do not have Euler-Lagrange equations because these functions have nothing in common with physical degrees of freedom. They are just mathematical placeholders due to the missing solution of the coupling equations. In the following calculation we backtrace the derivation of the

Euler Lagrange formalism starting from the postulation of a stationary action functional.

$$\delta \int \mathcal{L} \left(\Omega, \dot{\Omega}, \phi, \dot{\phi}, \theta, \dot{\theta}, \psi, \dot{\psi} \right) dt = 0$$

$$\Leftrightarrow \int \left(\mathcal{L} \left(\Omega + \delta \Omega, \dot{\Omega} + \delta \dot{\Omega}, \phi + \delta \phi, \dot{\phi} + \delta \dot{\phi}, \theta + \delta \theta, \dot{\theta} + \delta \dot{\theta}, \psi + \delta \psi, \dot{\psi} + \delta \dot{\psi} \right) = 0$$

$$\Leftrightarrow -\mathcal{L} \left(\Omega, \dot{\Omega}, \phi, \dot{\phi}, \theta, \dot{\theta}, \psi, \dot{\psi} \right) \right) dt = 0$$

$$\Leftrightarrow \int \left(\frac{\partial \mathcal{L}}{\partial \Omega} \delta \Omega + \frac{\partial \mathcal{L}}{\partial \dot{\Omega}} \delta \dot{\Omega} + \frac{\partial \mathcal{L}}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \delta \dot{\theta} + \frac{\partial \mathcal{L}}{\partial \theta} \delta \theta + \frac{\partial \mathcal{L}}{\partial \dot{\theta}} \delta \dot{\theta} + \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \delta \psi + \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \delta \dot{\psi} \right) dt = 0$$
(99)

$$\Leftrightarrow \int \left(\left(\frac{\partial \mathcal{L}}{\partial \Omega} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\Omega}} \right) \delta\Omega + \left(\frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) \delta\phi \\ + \left(\frac{\partial \mathcal{L}}{\partial \theta} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\theta}} \right) \delta\theta + \left(\frac{\partial \mathcal{L}}{\partial \psi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) \delta\psi \right) dt = 0$$

Until this point the calculations do not differ in any way from the calculations of the Euler-Lagrange formalism of the second kind. In the Euler-Lagrange formalism of the first kind the four functions $\Omega(t)$, $\phi(t)$, $\theta(t)$ and $\psi(t)$ would be degrees of freedom which are independent of each other and at this point you would say that the variations $\delta\Omega(t)$, $\delta\phi(t)$, $\delta\theta(t)$ and $\delta\psi(t)$ can be chosen independently of each other and hence you would claim that each of the four braces in (99) has to be zero to fulfill the postulation of a stationary action functional. Thus you would get four Euler-Lagrange equations there.

But this is not possible in our situation and thus we have to find another way to fulfill the postulation. The four variations are not independent of each other. They are coupled over the coupling equations and thus we can not see the Euler-Lagrange equation as easy as in the Euler-Lagrange formalism of the second kind. Instead we follow another way. At first we write all the terms under the integral linear in the variation of the independent function, we chose $\Omega(t)$ to be this. We calculate further:

$$\int \left(\left(\frac{\partial \mathcal{L}}{\partial \Omega} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\Omega}} \right) \delta\Omega + \left(\frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) \frac{\delta\phi}{\delta\Omega} \delta\Omega + \left(\frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) \frac{\delta\psi}{\delta\Omega} \delta\Omega \right) dt = 0$$

$$(100)$$

In (100) we are able to identify the Euler-Lagrange equation, but at first we want to do something else. Now we are able to see the Euler-Lagrange equation in a formal way, but we are not able to write down an explicit form of the Euler-Lagrange equation. We use the same argument as in the Euler-Lagrange formalism of the second kind about the free eligibility of $\delta\Omega(t)$ and say that the postulation of the stationarity of the action functional is fulfilled if the prefactor of $\delta\Omega(t)$ is zero. The formal form of the Euler-Lagrange equation is:

$$\begin{pmatrix} \frac{\partial \mathcal{L}}{\partial \Omega} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\Omega}} \end{pmatrix} + \left(\frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) \frac{\delta \phi}{\delta \Omega}$$

$$+ \left(\frac{\partial \mathcal{L}}{\partial \theta} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\theta}} \right) \frac{\delta \theta}{\delta \Omega} + \left(\frac{\partial \mathcal{L}}{\partial \psi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) \frac{\delta \psi}{\delta \Omega} = 0.$$

$$(101)$$

The formal form of the Euler-Lagrange equation (101) tells us formally how the equation looks like but this form is not enough for concrete calculations. The problem is quite obvious. The braces are not difficult to calculate because we have got a Lagrangian in chapter 4.2 and the braces contain just derivations of the Lagrangian with respect to the four functions or their time derivations. This can produce longer calculations but there are no conceptual problems expected. The problem lies in the fractions behind the braces because these fractions contain time derivations of the varied functions which are dependent of the degree of freedom $\Omega(t)$.

At this point we have no knowledge of the explicit form of these fractions and we have to think about a method to write something mathematical manageable instead of these fractions. To do this we use the four coupling equations. The idea is to make an expansion of the time derivations of the variations linear in the variations. This means we write the time derivations of the variations as:

$$\begin{split} \delta \dot{\phi} &= f_{11} \delta \Omega + f_{12} \delta \phi + f_{13} \delta \theta + f_{14} \delta \psi \qquad (102) \\ \delta \dot{\theta} &= f_{21} \delta \Omega + f_{22} \delta \phi + f_{23} \delta \theta + f_{24} \delta \psi \\ \delta \dot{\psi} &= f_{31} \delta \Omega + f_{32} \delta \phi + f_{33} \delta \theta + f_{34} \delta \psi. \end{split}$$

In the end $\delta \psi(t)$, $\delta \theta(t)$ and $\delta \psi(t)$ must be writable in an expansion as functions which are linear in $\delta \Omega(t)$. Due to (102) the shape of $\delta \Omega(t)$ from the start until the present point in time t is relevant for the shape of $\delta \psi(t)$, $\delta \theta$ and $\delta \phi$. Hence it is clear that these three functions must be writable in a linear expansion as a convolution. We define the vector $\vec{v}(t)$ of the three dependent functions:

$$\vec{v}(t) = \begin{pmatrix} \delta\phi\\ \delta\theta\\ \delta\psi \end{pmatrix}.$$
 (103)

We define the convolution with the for now unknown and just formal function $\vec{\chi}(t, t')$:

$$\vec{v}(t) = \int_0^t dt' \vec{\chi}(t,t') \cdot \delta\Omega(t').$$
(104)

This linear expansion in $\delta\Omega$ has an important advantage concerning the calculation of (101). There is a good justification for throwing away all the terms which are more than linear in the variations. The theory of variational calculations contains putting an infinitesimal small variation on a shape of a function to find the solution for which the minimized function is stationary in such an infinitesimal variation. The fact that the variations are infinitesimal small leads to the justification that we need to throw away all the orders which are more than linear. The quadratic order must be infinitesimal small in comparison with the linear order, the trilinear order must be infinitesimal small in comparison with the quadratic order and so on. Hence we can throw away all orders except of the linear order without causing any problems.

The task is now to find an explicit expression of (104). At first we try to find a linear expansion according to (102). To do this we start from the three coupling equations (58), (59) and (60). In these equations we add a small variation to all the four functions according to (98) on the right sides of these equations so that the left sides have the meaning of $\dot{\phi} + \delta \dot{\phi}$, $\dot{\theta} + \delta \dot{\theta}$ and $\dot{\psi} + \delta \dot{\psi}$. On the right sides we expand all the trigonometric functions in Taylor series until the first order. According the multiplications of trigonometric functions mixed orders will arise which are more than linear in the variations. We throw away all the terms which are more than linear in the variations so that we get an expansion until the first order. Then we substract the to each expansion according non-varied time derivations of the functions $\dot{\phi}$, $\dot{\theta}$ and $\dot{\psi}$ from the expansions. The result is that we get expansions of $\delta \dot{\phi}$, $\delta \dot{\theta}$ and $\delta \dot{\psi}$. This corresponds to (102). We start with the calculation for ψ .

$$\begin{split} \delta \dot{\psi} &(105) \\ = \dot{\psi} + \delta \dot{\psi} - \dot{\psi} \\ = 2V \sin \left(\theta + \delta\theta\right) \left[\sin \left(\Omega + \delta\Omega\right) \sin \left(\phi + \delta\phi\right) + \cos \left(\Omega + \delta\Omega\right) \cos \left(\phi + \delta\phi\right)\right] \\ &- 2V \sin \left(\theta\right) \left[\sin \left(\Omega\right) \sin \left(\phi\right) + \cos \left(\Omega\right) \cos \left(\phi\right)\right] \\ = 2V \left(\sin \left(\theta\right) + \cos \left(\theta\right) \delta\theta\right) \left[\left(\sin \left(\Omega\right) + \cos \left(\Omega\right) \delta\Omega\right) \cdot \left(\sin \left(\phi\right) + \cos \left(\phi\right) \delta\phi\right) \\ &+ \left(\cos \left(\Omega\right) - \sin \left(\Omega\right) \delta\Omega\right) \cdot \left(\cos \left(\phi\right) - \sin \left(\phi\right) \delta\phi\right)\right] \\ &- 2V \sin \left(\theta\right) \left[\sin \left(\Omega\right) \sin \left(\phi\right) + \cos \left(\Omega\right) \cos \left(\phi\right)\right] \\ \approx 2V \cos \left(\theta\right) \left(\sin \left(\Omega\right) \sin \left(\phi\right) + \cos \left(\Omega\right) \cos \left(\phi\right)\right) \delta\theta \\ &+ 2V \sin \left(\theta\right) \left(\sin \left(\Omega\right) \cos \left(\phi\right) - \sin \left(\Omega\right) \cos \left(\phi\right)\right) \delta\Omega \end{split}$$

We do the same calculation for $\phi.$

$$\begin{split} \delta\dot{\phi} & (106) \\ =\dot{\phi} + \delta\dot{\phi} - \dot{\phi} \\ = V \frac{\cos\left(\frac{\psi + \delta\psi}{2}\right) \sin\left(1 + \delta\Omega - \psi - \delta\psi\right) - \sin\left(\frac{\psi + \delta\psi}{2}\right) \cos\left(\theta + \delta\theta\right) \cos\left(\Omega + \delta\Omega - \phi - \delta\phi\right)}{\sin\left(\frac{\psi + \delta\psi}{2}\right) \sin\left(\theta + \delta\theta\right)} \\ - V \frac{\cos\left(\frac{\psi}{2}\right) \sin\left(\Omega - \psi\right) - \sin\left(\frac{\psi}{2}\right) \cos\left(\theta\right) \cos\left(\Omega - \phi\right)}{\sin\left(\frac{\psi}{2}\right) \sin\left(\theta\right)} \\ = V \frac{1}{\sin\left(\frac{\psi + \delta\psi}{2}\right) \sin\left(\theta + \delta\theta\right)} \left[\cos\left(\frac{\psi + \delta\psi}{2}\right) \left(\sin\left(\Omega + \delta\Omega\right) \cos\left(\psi + \delta\psi\right) - \cos\left(\Omega + \delta\Omega\right) \sin\left(\psi + \delta\psi\right)\right) \right] \\ - \sin\left(\frac{\psi + \delta\psi}{2}\right) \cos\left(\theta + \delta\theta\right) \left(\cos\left(\Omega + \delta\Omega\right) \cos\left(\phi + \delta\phi\right) + \sin\left(\Omega + \delta\Omega\right) \sin\left(\phi + \delta\phi\right)\right)\right] \\ - V \frac{\cos\left(\frac{\psi}{2}\right) \sin\left(\Omega - \psi\right) - \sin\left(\frac{\psi}{2}\right) \cos\left(\theta\right) \cos\left(\Omega - \phi\right)}{\sin\left(\frac{\psi}{2}\right) \sin\left(\theta\right)} \\ = V \left(\cot\left(\frac{\psi}{2}\right) - \frac{1}{2\sin^{2}\left(\frac{\psi}{2}\right)}\delta\psi\right) \left(\frac{1}{\sin\left(\theta\right)} - \frac{\cos\left(\theta\right)}{\sin^{2}\left(\theta\right)}\delta\theta\right) \\ \left[\left(\sin\left(\Omega\right) + \cos\left(\Omega\right)\delta\Omega\right) (\cos\left(\psi\right) - \sin\left(\psi\right)\delta\Omega\right) (\cos\left(\phi\right) - \sin\left(\Omega\right)\delta\Omega) (\sin\left(\psi\right) + \cos\left(\psi\right)\delta\psi)\right] \\ - V \left(\cot\left(\theta\right) - \frac{1}{\sin^{2}\left(\theta\right)}\delta\theta\right) \left[(\cos\left(\Omega\right) - \sin\left(\Omega\right)\delta\Omega) (\cos\left(\phi\right) - \sin\left(\phi\right)\delta\phi\right) \\ + (\sin\left(\Omega\right) + \cos\left(\Omega\right)\Omega\Omega) (\sin\left(\phi\right) + \cos\left(\phi\right)\delta\phi\right)\right] \\ - V \frac{\cos\left(\frac{\psi}{2}\right) \sin\left(\Omega - \psi\right) - \sin\left(\frac{\psi}{2}\right) \cos\left(\theta\right) \cos\left(\Omega - \phi\right)}{\sin\left(\frac{\psi}{2}\right) \sin\left(\theta\right)} \\ \approx V \frac{1}{\sin\left(\theta\right)} \left[\cot\left(\frac{\psi}{2}\right) (-\sin\left(\Omega\right)\sin\left(\psi\right) - \cos\left(\Omega\right)\cos\left(\psi\right)) \\ - \frac{1}{2\sin\left(\frac{\psi}{2}\right)} \cos\left(\theta\right) \cos\left(\psi\right) - \cos\left(\Omega\right)\sin\left(\psi\right)\right)}{\delta\psi} \\ \frac{V}{\sin\left(\theta^{2}\right)} \left[\cos\left(\Omega\right)\cos\left(\phi\right) + \sin\left(\Omega\right)\sin\left(\phi\right) - \\ \cot\left(\frac{\psi}{2}\right)\cos\left(\theta\right)\cos\left(\phi\right) - \cos\left(\Omega\right)\sin\left(\psi\right)\right)}{\delta\phi} \\ + V \left[\cot\left(\frac{\psi}{2}\right) \frac{1}{\sin\left(\theta\right)} (\cos\left(\psi\right)\cos\left(\psi\right) + \sin\left(\Omega\right)\sin\left(\psi\right)) \\ - \cot\left(\theta\right) (\sin\left(\Omega\right)\cos\left(\phi\right) + \cos\left(\Omega\right)\sin\left(\phi\right)\right)} \right] \delta\Omega \end{split}$$

And now we do the same calculation for $\theta.$

$$\begin{split} \delta\dot{\theta} & (107) \\ =\dot{\theta} + \delta\dot{\theta} - \dot{\theta} \\ = V \frac{\cos\left(\frac{\psi + \delta\psi}{2}\right)\cos\left(\theta + \delta\theta\right)\cos\left(\Omega + \delta\Omega - \phi - \delta\phi\right) + \sin\left(\frac{\psi + \delta\psi}{2}\right)\sin\left(\Omega + \delta\Omega - \psi - \delta\psi\right)}{\sin\left(\frac{\psi + \delta\psi}{2}\right)} \\ - V \frac{\cos\left(\frac{\psi}{2}\right)\cos\left(\theta\right)\cos\left(\Omega - \phi\right) + \sin\left(\frac{\psi}{2}\right)\sin\left(\Omega - \psi\right)}{\sin\left(\frac{\psi}{2}\right)} \\ = V \cot\left(\frac{\psi + \delta\psi}{2}\right)\cos\left(\theta + \delta\theta\right)\cos\left(\Omega + \delta\Omega\right)\cos\left(\phi + \delta\phi\right) + \sin\left(\Omega + \delta\Omega\right)\sin\left(\phi + \delta\phi\right)\right) \\ + V \left(\sin\left(\Omega + \delta\Omega\right)\cos\left(\psi + \delta\psi\right) - \cos\left(\Omega + \delta\Omega\right)\sin\left(\psi + \delta\psi\right)\right) \\ - V \frac{\cos\left(\frac{\psi}{2}\right)\cos\left(\theta\right)\cos\left(\Omega - \phi\right) + \sin\left(\frac{\psi}{2}\right)\sin\left(\Omega - \psi\right)}{\sin\left(\frac{\psi}{2}\right)} \\ = V \left(\cot\left(\frac{\psi}{2}\right) - \frac{1}{2\sin^{2}\left(\frac{\psi}{2}\right)}\delta\psi\right)\left(\cos\left(\theta\right) - \sin\left(\theta\right)\delta\theta\right) \\ \left(\cos\left(\Omega\right) - \sin\left(\Omega\right)\delta\Omega\right)\left(\cos\left(\phi\right) - \sin\left(\phi\right)\delta\phi\right) \\ + V \left(\cot\left(\frac{\psi}{2}\right) - \frac{1}{2\sin\left(\frac{\psi}{2}\right)}\delta\psi\right)\left(\cos\left(\theta\right) - \sin\left(\theta\right)\delta\theta\right) \\ \left(\sin\left(\Omega\right) + \cos\left(\Omega\right)\delta\Omega\right)\sin\left(\phi\right) + \cos\left(\phi\right)\delta\phi\right) \\ + V \left(\sin\left(\Omega\right) + \cos\left(\Omega\right)\delta\Omega\right)\sin\left(\phi\right) + \cos\left(\psi\right)\delta\psi\right) \\ - V \frac{\cos\left(\frac{\psi}{2}\right)\cos\left(\theta\right)\cos\left(\Omega - \phi\right) + \sin\left(\frac{\psi}{2}\right)\sin\left(\Omega - \psi\right)}{\sin\left(\frac{\psi}{2}\right)} \\ \approx - V \left[\frac{\cos\left(\theta\right)}{2\sin^{2}\left(\frac{\psi}{2}\right)}\left(\cos\left(\Omega\right)\cos\left(\phi\right) + \sin\left(\Omega\right)\sin\left(\phi\right)\right) \\ - \sin\left(\Omega\right)\sin\left(\psi\right) - \cos\left(\Omega\right)\cos\left(\phi\right)\right) \\ + \cos\left(\Omega\right)\cos\left(\psi\right) + \sin\left(\Omega\right)\sin\left(\phi\right) \\ + V \left[\cot\left(\frac{\psi}{2}\right)\cos\left(\theta\right)\cos\left(\phi\right)\sin\left(\phi\right) - \sin\left(\Omega\right)\cos\left(\phi\right)\right) \\ + \cos\left(\Omega\right)\cos\left(\psi\right) + \sin\left(\Omega\right)\sin\left(\phi\right)\cos\left(\phi\right) \\ + V \cot\left(\frac{\psi}{2}\right)\sin\left(\theta\right)\cos\left(\phi\right)\cos\left(\phi\right) + \sin\left(\Omega\right)\sin\left(\phi\right)\right)\delta\theta \\ - V \cot\left(\frac{\psi}{2}\right)\sin\left(\theta\right)\cos\left(\phi\right)\cos\left(\phi\right) + \sin\left(\Omega\right)\sin\left(\phi\right)\right)\delta\theta \\ - V \cot\left(\frac{\psi}{2}\right)\sin\left(\theta\right)\cos\left(\phi\right) + \cos\left(\theta\right)\cos\left(\theta\right)\cos\left(\phi\right)\cos\left(\phi\right)\right)$$

Now we have expansions of the time derivations of the variations linear in the variations. This does not already give us an expression of the variations linear in the independent variation $\delta\Omega$. It is analytically difficult to find such an expression and the idea is to do an analytical approach, which is not a part of this work. The next step that we can do easily is to write down an expression of the Euler-Lagrange equation which still contains the variations. This is simply done by inserting the Lagrangian (97) into the formal Euler-Lagrange equation (101) and we get the equation:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \Omega} &+ \frac{\partial \mathcal{L}}{\partial \phi} \frac{\delta \phi}{\delta \Omega} + \frac{\partial \mathcal{L}}{\partial \theta} \frac{\delta \theta}{\delta \Omega} + \left(\frac{\partial \mathcal{L}}{\partial \psi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \psi} \right) \frac{\delta \psi}{\delta \Omega} = 0 \end{aligned} \tag{108} \\ \Leftrightarrow \left(-\lambda_1 \sin\left(\theta\right) \cos\left(\phi\right) \sin\left(\psi\right) + \lambda_1 \left(\cos\left(\psi\right) - 1\right) \sin\left(\theta\right) \cos\left(\theta\right) \sin\left(\phi\right) \\ \lambda_2 \sin\left(\psi\right) \sin\left(\theta\right) \sin\left(\phi\right) + \lambda_2 \left(1 - \cos\left(\psi\right)\right) \sin\left(\theta\right) \cos\left(\phi\right) \cos\left(\theta\right) \\ &+ 2\lambda_3 \left(\cos\left(\psi\right) - 1\right) \sin\left(\theta\right)^2 \sin\left(\phi\right) \cos\left(\phi\right) \right) \frac{\delta \phi}{\delta \Omega} \\ \left(-\lambda_1 \sin\left(\psi\right) \cos\left(\theta\right) \sin\left(\phi\right) + \lambda_1 \left(1 - \cos\left(\psi\right)\right) \cos\left(\phi\right) \left(\cos\left(\theta\right)^2 - \sin\left(\theta\right)^2\right) \\ &+ \lambda_2 \sin\left(\psi\right) \cos\left(\theta\right) \sin\left(\phi\right) + \lambda_2 \left(1 - \cos\left(\psi\right)\right) \sin\left(\phi\right) \left(\cos\left(\theta\right)^2 - \sin\left(\theta\right)^2\right) \\ &+ 2\lambda_3 \left(1 - \cos\left(\psi\right)\right) \sin\left(\theta\right) \cos\left(\theta\right) \cos\left(\phi\right)^2 \right) \frac{\delta \theta}{\delta \Omega} \\ &+ \left(-\frac{1}{4}\psi'' - \lambda_1 \sin\left(\theta\right) \sin\left(\phi\right) \cos\left(\phi\right) + \lambda_1 \sin\left(\psi\right) \sin\left(\theta\right) \cos\left(\phi\right) \cos\left(\phi\right) \\ &+ \lambda_2 \cos\left(\psi\right) \sin\left(\theta\right) \cos\left(\phi\right) + \lambda_2 \sin\left(\phi\right) \sin\left(\theta\right) \cos\left(\phi\right) \sin\left(\phi\right) \\ &- \lambda_3 \sin\left(\psi\right) + \sin\left(\psi\right) \sin\left(\theta\right) \sin\left(\theta\right) \cos\left(\phi\right) \cos\left(\phi\right) \cos\left(\phi\right) \right) \frac{\delta \psi}{\delta \Omega} = 0. \end{aligned}$$

Thus we have an Euler-Lagrange equation which contains the still not calculated variations. It is clear that the linear expansion of the variations in $\delta\Omega$ leads to an Euler-Lagrange equation that does not contain the variations anymore because the fractions behind the braces are then independent of the variations due to the fact that the numerator and the denominator are both linear in $\delta\Omega$. The following task would be now to calculate these braces numerically.

4.4 Discussion

The variational ansatz for the search for frequency-modulated pulses works in theory such as the variational ansatz for the search for amplitude modulated pulses but in practice the not analytically solvable coupling equations lead to difficulties which finally have to be solved numerically. We did not start this numerical treatment but it is expectable that it will not be easy to do. A big disadvantage in comparison with the amplitude modulated pulses is that a partly analytical solution of the resulting Euler-Lagrange equation is probably not possible. The form of the Euler-Lagrange equation is much more complicated than for amplitude modulated pulses which makes an analytical solution not probable. Further a numerical treatment from the start is anyway necessary due to the fractions which contain the variations.

5 Conclusion and outlook

The variational method which we presented worked well according to our expectations for amplitude-modulated pulses.

The first nice aspect is that we have analytical results in chapter 2.1 for the Euler-Lagrange equation with $\lambda_3 = 0$ and without the auxiliary conditions. To include the auxiliary conditions we had to adjust the result to one of these conditions numerically. The numerical error could be made much smaller than in this work due to the fact that the numerical calculation is just a simple interval method and thus the numerical error should not have any effect on practical purposes.

Further the best analytical result, namely the first one in the tables 1 and 2, is according to our aims better than CORPSE and SCORPSE which are presented in table 4. The function XE^3 for the new pulse has a value of 37.477696465 percent of the value for the SCORPSE pulse and 3.900780802 percent of the value for the CORPSE pulse. Note that this good result is reached without any minimization of the term X, we focused just on the minimization of the energy E and we see that this was already enough to reach this result.

The other analytical solutions have very high values of XE^3 . Already the second solution in the tables 1 and 2 has a much higher value of XE^3 than the CORPSE pulse and hence the only interesting pulse according to our aims is the first one. The higher pulses are much worse according to our aims and hence practically not interesting but they are interesting if you want to have a general understanding of the solutions of the Euler-Lagrange equation. In chapter 2.2 symmetrical solutions for eligible values of λ_3 are presented. We searched for a minimum of the function XE^3 and we have found such a minimum in the point $\lambda_3 = 10.25$. The positive aspect is that the numerical method worked in principle as we wanted it to work and that we indeed have found a minimum of XE^3 . The negative aspect is the small improvement through. It has a value of 99.620506451 percent of the value for the best solution from chapter 2.1. For any practical purposes we win very little but the best pulse from chapter 2.2 is still preferable to the best pulse from chapter 2.1. Note that this disadvantage is not a disadvantage concerning the variational method in general. This disadvantage emerged just for our problem and this does not mean that it would occur for a similar variational method with a slightly changed ansatz.

In order to present an overview of further solutions some asymmetrical numerical solutions are presented in chapter 2.3. These solutions are worse than the numerical solutions. We presented a low number of solutions where you can not see clear curves against λ_3 such as in chapter 2.2 due to the fact that we did not know beforehand for which values of λ_3 asymmetrical solutions occur and hence we worked with big steps. If you do such a calculation in smaller steps it is expectable that you can make a plot such as figure 8 where the curve for asymmetrical pulses runs above of the curve for symmetrical pulses. Then it would be advantageous to use the solution of every point as the initial solution for the next point just as in chapter 2.2. We used for every point the first solution from chapter 2.1 within this work. Further it is possible that there is not just one curve of asymmetrical pulses but rather a whole bunch of curves, maybe an infinite number, which we did not find due to our program and the initial values of the parameters, but that is not clear. But note that for any practical purposes the best symmetrical solution is preferable to the asymmetrical solutions due to the quality and hence the asymmetrical solutions are just presented for the completeness' sake.

In chapter 3 a simulation of the best solution from chapter 2.1 is presented and compared with CORPSE and SCORPSE. This simulation worked successful and led to the expected result and thus it validated the result from chapter 2 that the new pulse has a smaller function XE^3 than SCORPSE and CORPSE while these two pulses have smaller functions X and XA^3 .

Further we tried to make an variational ansatz for frequency-modulated pulses in chapter 4. As explained there the problem is principally similar to the problem for amplitudemodulated pulses but due to the missing analytical solution of the equations (30), (31) and (32) the problem is much harder to handle and our result was the Euler-Lagrange equation (108) which we did not solve. We expect that an analytical solution is impossible and that a numerical solution is difficult due to the remaining variations in this equation. Hence the result of this part is that we can just show the principal ansatz but a solution which could be relevant for practical purposes seems to be very difficult to get.

For succeeding research the most relevant part of this work are firstly the shown principles especially concerning the variational ansatz to the problem and secondly for more practical purposes the pulse in chapter 2.2 in the minimum of XE^3 .

The ansatz is interesting because we could show that it works well and changes of such an ansatz for succeeding research are conceivable. For example the minimization of the energy E is something which could be replaced by other minimized functions. The choice of the function which you minimize is a question which has no definite answer because it depends strongly on your aims and the physical situation that you want to address. For example if you have a practical problem such as building a device which works with information stored in quantum bits this question must propably answered with respect to the limitations of the pulses due to the used devices. This is mainly a limitation of the amplitude and a limitation of too fast changes in the pulse shape. This is the reason for which preceding works such as [21] used the amplitude or the inverse pulse duration as the parameter against which they plotted definitions of the pulse quality. If you have more theoretical purposes completely different functions can be conceivable to minimize depending on what you want to show.

The best pulse of this work is a result which could be important for practical purposes if the experimental implementation is well enough possible. The problem could be that the pulse shape changes continuously and it is unclear how well a device can create such a continuous shape. Maybe a device has to divide the pulse into small constant steps such as we did it for the numerical calculations but the steps in this work are probably too small for a device to implement. Bigger steps would have an influence on the pulse quality because all the function values which we calculated within this work would change. The second important question is how important the minimization of the energy is for practical purposes. The most important limitation is probably the limitation of the amplitude and thus the SCORPSE pulse which does this minimization as the best pulse would be the first choice. Maybe a mix of different quality criteria can be interesting, too. Then the pulse which minimizes the function XA^3 could be an interesting candidate because you can see in table 4 that it is worse than the SCORPSE pulse if you look at the function XA^3 but it is much better than the SCORPSE pulse if you look at the function XE^3 . For the pulse which minimizes XA^3 the function XA^3 has a value of 154.528091676 percent of the value of the SCORPSE pulse but the function XE^3 has a value of 0.46101729978 percent of the value of the SCORPSE pulse. Hence in comparison with the SCORPSE pulse the quantitative advantage in the value of XE^3 is much bigger than the disadvantage in the value of XA^3 . The remaining question is how much weight you put on these aspects for practical purposes.

Of course we are not able to suppress decoherence completely and it is probable that this will never be possible, but fortunately this is not necessary. In practice decoherence suppression such as we investigated it within this work is usually used in combination with error correction schemes. Decoherence suppression prohibits errors before they happen and error correction schemes fix errors after they happened. Hence a complete suppression of decoherence is not necessary due to the threshold theorem [7]. Decoherence suppression which is better than a certain threshold is needed and then the correction schemes are able to eliminate the remaining errors. Examples for error correction schemes can be seen in [41, 42, 43, 44].

Appendix

A Analytical solutions

The general solution (86) has a periodical shape independent of the chosed values for the variables. An example is for the solution is shown in figure 22 where the aspect that we want to point out is not the quantitative shape for specific variables but rather the qualitative periodical shape that the solution have for any values. Now we want to show graphically what we calculate in (88) in order to give a deeper understanding of the last step in (88) where the values of m_1 and m_2 are calculated. To adjust the solution to the boundary condition we see quite easily in figure 22 what we have to do. We can stretch and clinch the solution along the t-axis by varying the parameter m and thus we just have to chose those parameters of m for which the solution ends at the points t = 0 and $t = \tau_p$ with a distance of π . Due to the symmetry of the solutions it is enough to move the intercection points with the line at π in figure 22 into the boundary point at $t = \tau_p$. The values of m which you get by doing this are the solutions which we calculate in (86). If a point where the graph has a negative derivation in figure 22 is at the boundary point, the solution corresponds to m_1 , and if a point where the graph has a positive derivation in figure 22 is at the boundary point, the solution corresponds to m_2 .



Figure 22: Frobenius norm of the XE^3 minimizing pulse in comparison with the Frobenius norm of the pulses SCORPSE and CORPSE in dependence of the pulse duration τ_p

B Pseudocode

for (int i=0;i<=Lambda3steps;i++) {

lambda3=0.1*(double)i;

while (!Convergence)(This Loop iterates the Euler-Lagrange equation){

broydn(This function searches for the the parameter-values which fulfill the auxiliary conditions);

}

}

C Simulation Fits

We fit the three functions in the figures 18, 19 and 20 at the right side of the kink. Further we fit the same plot for the pulse minimizing XA^3 , which is not included in the three figures because the figures would become not clear. The fits are done with the function $f(x) = ax^b$ where we expect $b = \frac{3}{2}$. Note that the fit-values should not be taken too seriously because they vary strongly depending on the number of points which we include into the fit. Table 5 shows the fit-values for the figure 18, table 6 shows the fit-values for figure 19 and table 7 shows the fit-values for figure 20.

Pulse	a	b
XEEE	4.03505 ± 0.01612	1.47941 ± 0.001406
XAAA	4.68691 ± 0.00951	1.49088 ± 0.000604
SCORPSE	7.17434 ± 0.00545	1.49948 ± 0.0002105
CORPSE	20.5495 ± 0.04318	1.48623 ± 0.0005264

Table 6: Fits of the Frobenius norm against τ_p

Pulse	a	b
XEEE	4.97087 ± 0.01043	1.48738 ± 0.0006248
XAAA	3.46506 ± 0.006611	1.49088 ± 0.0006038
SCORPSE	2.89281 ± 0.001832	1.49948 ± 0.0002103
CORPSE	3.33553 ± 0.003864	1.48701 ± 0.0004105

Table 7: Fits of the Frobenius norm against 1/A

Pulse	a	b
XEEE	0.429972 ± 0.0004675	1.48738 ± 0.0006233
XAAA	0.419268 ± 0.0004474	1.49088 ± 0.0006026
SCORPSE	0.412543 ± 0.0001506	1.49948 ± 0.0002099
CORPSE	0.192561 ± 0.00007395	1.48701 ± 0.0004094

Table 8: Fits of the Frobenius norm against 1/E

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Eidesstattliche Versicherung

Ich versichere hiermit an Eides statt, dass ich die vorliegende Bachelorarbeit mit dem Titel "Variational search for control pulses suppressing decoherence" selbstständig und ohne unzulässige fremde Hilfe erbracht habe. Ich habe keine anderen als die angegebenen Quellen und Hilfsmittel benutzt, sowie wörtliche und sinngemäße Zitate kenntlich gemacht. Die Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

Ort, Datum

Unterschrift

Belehrung

Wer vorsätzlich gegen eine die Täuschung über Prüfungsleistungen betreffende Regelung einer Hochschulprüfungsordnung verstößt, handelt ordnungswidrig. Die Ordnungswidrigkeit kann mit einer Geldbuße von bis zu 50 000 € geahndet werden. Zuständige Verwaltungsbehörde für die Verfolgung und Ahndung von Ordnungswidrigkeiten ist der Kanzler/die Kanzlerin der Technischen Universität Dortmund. Im Falle eines mehrfachen oder sonstigen schwerwiegenden Täuschungsversuches kann der Prüfling zudem exmatrikuliert werden (§63 Abs. 5 Hochschulgesetz -HG-).

Die Abgabe einer falschen Versicherung an Eides statt wird mit Freiheitsstrafe bis zu 3 Jahren oder mit Geldstrafe bestraft.

Die Technische Universität Dortmund wird ggf. elektronische Vergleichswerkzeuge (wie z.B. die Software "turnitin") zur Überprüfung von Ordnungswidrigkeiten in Prüfungsverfahren nutzen.

Die oben stehende Belehrung habe ich zur Kenntnis genommen.

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