Universiteit Utrecht

Master Thesis Theoretical Physics

Effects of spin inertia on ground-state energies: the spin-instanton

First supervisor:
Prof. dr. R.A. (Rembert) Duine

Second supervisor:
Prof. dr. ir. H.T.C. (Henk) Stoof

Daily supervisor:
Dr. T. (Tim) Ludwig

Author:
Teun Kluck
6152384

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Abstract

Recent experiments have shown that spin dynamics depend on spin inertia [1, 2]. If the spin dynamics are dependent on spin inertia, the energy levels of a single spin could have an inertia-dependence too. In this thesis, we investigate how spin inertia affects the lowest energy levels of a single spin. To find this result, we consider a model of a large spin, with easy-axis anisotropy. Furthermore, the spin is influenced by a magnetic field and we place the spin in a bath of harmonic oscillators, to induce non-zero spin inertia. We consider a spin which can have values in a single direction. We call this model the circular-spin model. To find these lowest energy levels and their eigenenergies, we use instanton calculus. For the circular-spin model, we find the lowest energy levels. This new result tells us how spin inertia affects the lowest energy levels of a spin. We found that these energy levels have a similar dependence on spin inertia as the lowest energy levels of a particle in a double-well potential, depends on the mass of the particle. With this result, we have a better fundamental understanding of the lowest energy levels of spins. Furthermore, this result may provide a new way to experimentally detect spin inertia.

Acknowledgements

I want to thank my supervisors Rembert Duine and Tim Ludwig for guiding me in the right direction. I really appreciate the time Tim saved for me to let me ask all my questions. I want to thank Tim's patience for explaining many physical concepts when I did not understand them fully directly. The work environment I have been working in the last year has been very constructive and motivating. I want to thank my supervisors for making this nice environment. Furthermore, I want to thank my father, Jeroen Kluck, and my supervisors for correcting my drafts and teaching me how to become a better writer. I am very thankful for the understanding of all people around me, the moment that my head was not fully focused on my thesis project when I heard that my mother had cancer. I thank my friends who are working on their theses at the same time as me for making all hours in the Buys-Ballot building fun and motivating me to come to the university every day. Finally, I want to thank my girlfriend, Lucía, for motivating me through the year.

Contents

1 Introduction

Magnetization dynamics play a crucial role in a wide range of applications. For example, electronic data is saved in bits, which are represented by spins pointing either up or down. To control these bits, and to know how to manipulate them, it is important to understand the behaviour of spins. Individual spins aim to align with magnetic fields and are lowest in energy if they are aligned with the effective magnetic field around them. If we include all forces acting on the spin we end up with the dynamics of a spin. The dynamics of a single spin $\mathbf{S}$ are mathematically described by the Landau–Lifshitz–Gilbert (LLG) equation [1],

$$\dot{\mathbf{S}} = \mathbf{S} \times \left(\mathbf{B}_{\text{eff}} - \alpha_0 \dot{\mathbf{S}} \right). \tag{1.1}$$

This equation describes a single macro-spin in an effective magnetic field $\mathbf{B}_{\text{eff}}$. In the effective magnetic field are typically included the external magnetic field and the intrinsic magnetic field, generated by the magnet a spin itself can be part of. If the spin is not isolated, it can dissipate energy into its environment, which leads to the Gilbert damping term with coefficient α_0. The LLG equation describes the dynamics of a spin returning to its equilibrium position after it has been excited. The cross-product between the spin and the effective magnetic field $\mathbf{S} \times \mathbf{B}_{\text{eff}}$, leads to the precession of the spin around the effective magnetic field. The Gilbert damping term, $\mathbf{S} \times \alpha_0 \dot{\mathbf{S}}$, leads to the damping to the equilibrium state (see figure 1a).

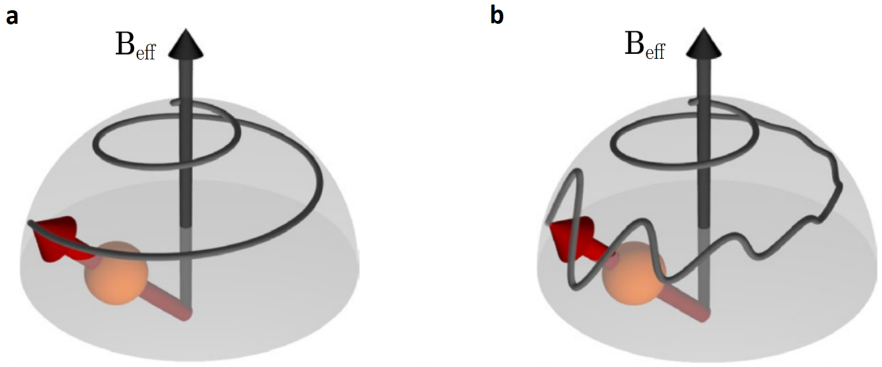

Figure 1: *An illustration of the dynamics of a spin. In (*a*) we see a spin out of its equilibrium position. The equilibrium position is the spin aligned with the effective magnetic field* $\boldsymbol{B}_{\text{eff}}$*. The spin rotates around the equilibrium position, which is called precession. This figure corresponds with the LLG equation (1.1). In (*b*) we see the same plot but now with an extra movement. This is the nutation. This figure corresponds with the ILLG equation (1.2), that includes spin inertia. The frequency of the nutation is usually much larger than the frequency of the precession. The figures are adapted from the paper by K. Neeraj et al. [1].*

Recently, an extra component in the spin dynamic was observed experimentally [1], namely nutation of the spin (see figure 1b). The nutation is described mathematically by

including spin inertia I in the LLG equation [2, 3]

$$\dot{\mathbf{S}} = \mathbf{S} \times \left(\mathbf{B}_{\text{eff}} - \alpha_0 \dot{\mathbf{S}} - I\ddot{\mathbf{S}} \right). \tag{1.2}$$

This equation is also called the Inertial-Landau–Lifshitz–Gilbert (ILLG) equation. The term including spin inertia can arise, for example, from high frequency modes from the environment [4]. In the ILLG equation (1.2) the spin dynamics are dependent on the inertia. To have an intuition of spin inertia, we see the spin inertia as the spin equivalent of mass.

The relation between spin dynamics and spin inertia leads to many new questions. Recently, research has been devoted to a better fundamental understanding of spin inertia, which could result in making use of spin inertia in technology [3, 5, 6]. Some fundamental questions that come to mind have to do with the energy levels of a spin system, which are influenced by spin inertia. We are now interested in the following two questions. Under what circumstances does spin inertia influence the energy levels of a spin? On which variables do the spin energy levels depend? In this thesis, we are going to look specifically at the lowest energy levels: the ground state and the first excited state of a spin.

To answer the questions above, we use a spin model with inertia. This model includes a large spin, which allows us to use semi-classical approximations. This spin is localized and in contact with a bath of harmonic oscillators, as this is a simple model which includes inertia. We use the same bath as in the thesis by M. Gaspar Quarenta [4]. To have a good description of the energy levels of a spin system, we have to take into account quantum effects. This is because we are interested in particles that are so small that quantum effects play a role. However, the ILLG equation does not include any quantum aspects of the spin. To find the quantum mechanical energy levels of a spin, we will use path integrals. With the path integral formulation, we can use the spin-instanton to find the lowest energies of the spin. We find that the lowest energy levels of a spin are dependent on inertia if they are of the following form: the lowest energy levels should be a superposition of multiple potential minima. The reason for this is that only when the lowest energy levels are superpositions, we can describe the ground state by the spin constantly tunneling between the multiple potential minima.

Exactly when the spin tunnels between the potential minima, the spin is influenced by inertia [7]. We can find the tunneling mathematically with the spin-instanton. If the spin would have no inertia dependence, a spin could tunnel infinitely fast through the barrier and that would cost no energy for a spin. In the derivation of the lowest energy levels of a spin we make an assumption, which has the result that we can only use the spin-instantons for a spin with non-zero inertia. A spin-instanton is a quasi-classical trajectory of a spin going from one potential minimum to another. We call any trajectory which includes a spin-instant a spin-instanton trajectory. To prevent confusion, we call a spin-instanton, which trajectory goes once from one potential minimum to another, the single spin-instanton. In this thesis we will therefore introduce the calculation of the ground-state energies of a spin, using instanton calculus.

To have a good understanding of the instanton, we will first look at the ground-state energies of a particle in a double-well potential. These ground-state energies are derived by analyzing the instanton [8] as is reviewed in chapter 2. If readers are familiar with

this derivation, they can skip chapter 2 and start reading chapter 3. In chapter 3 and 4 we study a spin that is macroscopic, localized and in contact with a bath of harmonic oscillators. Also, the spin has easy-axis anisotropy and is influenced by a magnetic field perpendicular to the easy-axis anisotropy. In this model, which we call the spherical-spin model, the ground-state energies of the spin are derived using the spin-instanton.

In a general model, there are many quasi-classical paths to go from one spin-state to another. However, if we look at a spin model with one degree of freedom, we only have to take into account one or two quasi-classical paths between spin states. We will therefore look at the model that we call circular-spin model. This is a model where we fix the y-coordinate of a spin. What we are left with is a model with only one angle dependence and therefore it is called the circular-spin model. The circular-spin model gives us information about the spherical-spin model and we can calculate the ground-state energies of the spin, using the spin-instanton. The derivation is roughly speaking similar to the derivation of the ground-state energies in chapter 2.

2 Ground-state energies of a particle in a double-well potential

In this chapter, we consider a particle in the double-well potential as plotted in figure 2. A remarkable property in quantum mechanics is, that for a particle in the double-well potential, the ground state is a superposition of a particle in the left and right well of the potential. In classical mechanics, a ground state cannot be a superposition. The classical ground states are given by the particle in one of the wells. We can interpret the ground state in quantum mechanics mentioned above as follows: a particle in the double-well potential in the left well is influenced by the right well [9].

Classically, a particle that has not enough energy to cross a potential barrier, cannot travel from one potential minimum to the other. However, in quantum mechanics this is possible because a particle in the double-well potential can tunnel from one well through the potential barrier to the other well. To find the ground-state energy for a particle in the double-well potential, we need to know what the influence of tunneling is on the ground state, as tunneling leads to a non-degenerate ground state. For a particle with a small mass it is relatively easy to tunnel through the potential barrier. Therefore, the ground-state energy of a particle in the double-well potential must have a non-trivial dependence on the mass. The ground state we find with quantum mechanics, has a lower energy than if a particle would be in one potential well only.

The easiest way of finding the lowest energy levels of the double-well potential is with the WKB-method [10]. Another way of finding these states is by using the instanton [11]. In the path-integral description of quantum mechanics, the phenomenon of a particle going from one potential minimum to the other over a high potential barrier is also possible as this event is included as one optional path in the path integral. The path from one potential minimum to the other is called the instanton. A more formal definition of the instanton is: an instanton is a quasi-classical trajectory in Wick-rotated time of a particle going from one potential extremum to the other. We call any trajectory which includes an instanton an instanton trajectory. This gives us the same information as a particle tunneling from one potential minimum to the other [12]. We can therefore find the lowest energy levels of the double-well potential with the instanton.

How we can use exactly the instanton to find the ground-state energy is explained in this chapter. One thing we should note is that the instanton only plays a role in the derivations for an energy level, which is a superposition of two other states, as only then tunneling is relevant.

2.1 The quantum instanton

The double-well potential (see figure 2) is given by the following equation

$$V(q) = \frac{m\omega_0^2}{8a^2}\left(a^2 - q^2\right)^2. \tag{2.1}$$

Here m is the mass of the particle and $\pm a$ are the positions of the minima of the potential. Further, ω_0 is the oscillator frequency, which determines the width of the potential and

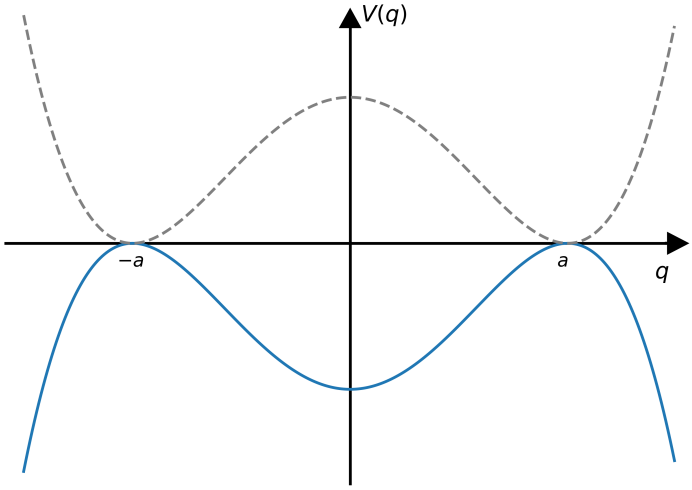

Figure 2: *The double-well potential (in grey), with a Wick rotation of the double-well potential (in blue). The Wick rotation flips the potential around the horizontal axis. This is best to see via the equations of motion, which we get by varying the action in equation (2.2). The equations of motion after the Wick rotation are given by* $-m\ddot{q} + \frac{\partial v(q)}{\partial q} = 0$ *instead of* $m\ddot{q} + \frac{\partial v(q)}{\partial q} = 0$*, which are the equations of motion in real-time. The extra minus sign makes it possible for a particle to have a classical solution for a path from* $q = -a$ *to* $q = a$*. This solution, which is the instanton, can be seen as a particle going from one extremum to the other in imaginary time. In the left well we see the potential of a harmonic oscillator. The harmonic oscillator is a good approximation of the double-well potential in the vicinity of the minima* $q = -a$ *and* $q = a$*.*

corresponds to the energy differences of a particle in a single well with the same curvature as the double-well potential. The oscillation frequency is exactly the frequency of a harmonic oscillator with which we will relate the double-well potential later (see equation (2.14)). We should be aware of the fact that ω_0 and a determine the height of the barrier between the two wells [9].

Once we have the potential, we can write an expression for the action of a particle in the double-well potential after a Wick rotation, $t \to -i\tau$, by

$$\mathcal{S}[q] = \int_0^\tau d\tau' (V(q) - \frac{m}{2}\dot{q}^2). \tag{2.2}$$

The goal of this chapter is to find the ground-state energies of a particle in a double-well potential. To do so we use the following equation, which gives a relation between the eigenenergies of the particle and the action [8]

$$\sum_n \langle q_f|n\rangle\, e^{-E_n\tau}\, \langle n|q_i\rangle = \langle q_f|e^{-\hat{H}\tau}|q_i\rangle = C\int_{q_i}^{q_f} Dq \exp(-\mathcal{S}[q]). \tag{2.3}$$

Here C is a prefactor.[1] A proof of the equation above is in appendix A. Let us explain

[1] We are not interested in the prefactor C. In this thesis the prefactor is not of importance, as only the

this equation in words. The middle term in equation (2.3) is the probability amplitude for a particle that starts at position q_i at imaginary time zero, to be found at position q_f at imaginary time τ later. We work with imaginary time, as this is needed for the instanton.[2] Furthermore, E_n are the eigenenergies of the Hamiltonian $\hat{H}$ with eigenbasis $|n\rangle$. There is no $\hbar$ in this equation as we put in the whole thesis $\hbar = 1$. The right equality in equation (2.3) holds, as this is the path integral between the initial state $|q_i\rangle$ and the final state $|q_f\rangle$. Before we can find an expression for the ground-state energies, we have to find the lowest energy levels for the double-well potential.

2.2 The lowest energy levels

Equation (2.3) is only useful once we take the limit of $\tau \to \infty$. In this case all terms of the form $e^{-E_n\tau}$ go to zero. The terms that go the slowest to zero, are the terms with the lowest energy, E_n. These are the only relevant terms in the equation. We choose to look not only at the ground state but also at the first excited state. We can include these two states if the difference between the eigenenergies of the ground state and the first excited state, $\Delta\epsilon$, is very small compared with the difference between the ground state and second excited state [9]. This requirement holds if $\omega_0 a^2$ is large, as for these values the barrier is large. When the barrier is large, there is relatively little influence from one well to the other and therefore the ground state and the first excited state are nearly the same.

We can find the ground state and first excited state because we know that the double-well potential and the Hamiltonian are symmetric under parity between the right and left well. This means that we can switch all states in one well with all states in the other well in the equations describing the system, and the mathematical results will be the same. If a Hamiltonian is invariant under a certain symmetry, its eigenstates are invariant under the same symmetry. The lowest energy levels which are invariant under parity are the symmetric state $|S\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$ and antisymmetric state $|A\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$ [13]. Calculations show that $|S\rangle$ the ground state and $|A\rangle$ is the first excited state of the Hamiltonian [14]. In this description, $|L\rangle$ and $|R\rangle$ are the local ground states of the left and right well respectively.

The lowest eigenenergies are given by $E_S = \frac{1}{2}(\omega_0 - \Delta\epsilon)$ and $E_A = \frac{1}{2}(\omega_0 + \Delta\epsilon)$. We argue

dependence in the exponential leads to the energy gap between the ground-state energy and first excited state energy. The prefactor leads to the so-called reference energy, $E_{\text{ref}} = \frac{1}{2}(E_0 + E_1)$, however, there is another way to find this prefactor, so for now we ignore it and say only that the probability amplitude is proportional to the path integral.

[2]Let us explain why we have to work with Wick-rotated time when we are looking at instantons. The instanton trajectories, or just instantons, are the quasi-classical trajectories between two potential minima. This means that for an instanton the quantum fluctuations are not included. A particle has to get excited if it goes classically from one well to the other, so if it follows a quasi-classical path between two minima. In the double-well potential we are looking at, this excitation is so high, that we can ignore the contributions from the particle going classically from one well to the other in real-time. However, we can do a Wick rotation. In the Wick-rotated time τ the potential is suddenly flipped over the horizontal axis (See figure 2). This makes it possible to calculate the instanton trajectory in imaginary time, as a particle can now go classically from one extremum to the other. The Wick rotation is a mathematical trick, which makes it possible to calculate the instanton trajectory. We use the same procedure for the Wick rotation as is done in general in physics [8].

why this should be the lowest energies. If the two wells would be infinitely far away from each other and as a result the barrier would be infinitely high, then the two wells would look exactly like a harmonic oscillator with frequency ω_0. In this case $|L\rangle$ and $|R\rangle$ are ground states with eigenenergies $\frac{\omega_0}{2}$. If we are looking at wells closer to each other, so for a finite a, we would look at a finite barrier. Now, a particle in one well is influenced by the other well and can travel passed the barrier and the eigenstates become the symmetric and antisymmetric states. By letting the wells come closer to each other, we do not change the total energy of the system. This means that if the ground-state energy becomes slightly smaller, the first-excited-state energy becomes slightly larger [10]. We find that indeed the lowest eigenenergies are given by $E_S = \frac{1}{2}(\omega_0 - \Delta\epsilon)$ and $E_A = \frac{1}{2}(\omega_0 + \Delta\epsilon)$.

2.3 The path integral

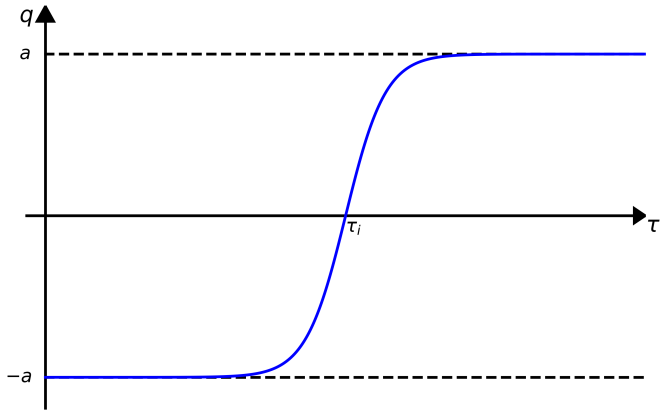

Figure 3: *The trajectory of a particle going from one extremum to the other without quantum fluctuations, also called a single instanton trajectory. The particle starts at $q = -a$ and travels to $q = a$. The path the instanton takes is determined using energy conservation (see appendix B why we can consider energy conservation in Wick-rotated time). The total energy E is given by the sum of kinetic energy $K'(q) = -\frac{m}{2}\dot{q}^2$ and potential energy $V(q)$, $E = K'(q) + V(q)$. The double-well potential in Wick-rotated time is such that $V(\pm a) = 0$. When the particle is on an extremum, it is not moving, so there the kinetic energy in Wick-rotated time is zero, $K'(\pm a) = 0$. This means that the total energy is zero, $E = 0$. On all other positions in the potential, the energy is conserved so $\frac{m}{2}\dot{q}^2 = V(q)$. This is a first-order differential equation, which we can solve. We find that $q(\tau) = a\tanh(\frac{1}{2}(ac_1 + \omega\tau)$. The constant c_1 determines when the particle is moving from one extremum to the other. The single instanton trajectory, which is plotted above, is given by $q(\tau)$.*

We can use the lowest energy levels to write equation (2.3) as follows

$$\lim_{\tau\to\infty} \sum_{n\epsilon\{S,A\}} \langle q_f|n\rangle\, e^{-E_n\tau}\, \langle n|q_i\rangle \propto \lim_{\tau\to\infty} \int_{q_i}^{q_f} Dq \exp(-\mathcal{S}[q]). \tag{2.4}$$

To get a useful result out of this equation, we have approximate the path integral from q_i to q_f. The path integral is calculated by the quasi-classical paths with corrections, as is done

in the saddle-point approximation [8]. These corrections are the quantum fluctuations. This is seemingly a long computation as there are many paths, but we can simplify the problem. First, we say that a particle is nearly all its (Wick-rotated) time τ, fluctuating around the positions $q = \pm a$. Only on rare occasions, a particle is traveling from one extremum to the other (see figure 3).

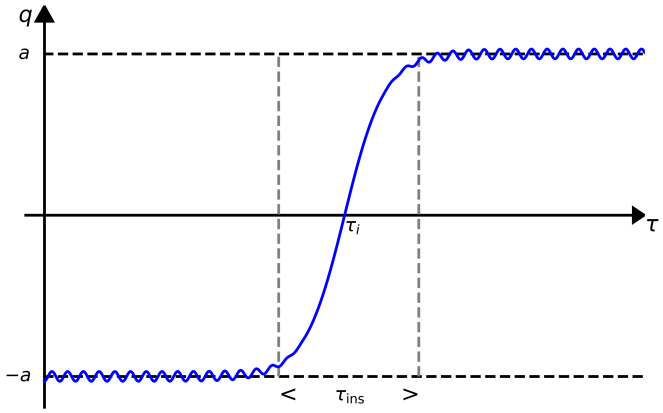

Figure 4: *A single trajectory of a particle going from $q = -a$ to $q = a$ with quantum fluctuations. The position of the particle is plotted against the imaginary time τ. Around the time τ_i the particle moves from position. We make the assumption that the instanton time, τ_{ins}, is very small. The instanton time is the time when the displacement of the particle gives a relevant contribution to the integral in equation (2.8). A particle starts moving from one well to another due to quantum fluctuations. The instanton time is determined by the time between the moment the particle leaves the area dominated by quantum fluctuations and the time it arrives in the area dominated by quantum fluctuations around the other extremum. Further, we see in the plot that the quantum fluctuations are small compared with the displacement from $q = -a$ to $q = a$. We therefore only have to take into account quantum fluctuations when the particle is on an extremum.*

On the parts of the instanton trajectories where the particle flips from potential extremum, the quantum fluctuations are negligible compared with the change in the position of the particle (see figure 4). Because of this reason, with the fact that the particle is mostly on an extremum, we only have to consider quantum fluctuations when a particle is on an extremum.

We make the assumption that the quantum fluctuations are local, which means that they are only changing the path slightly. We can now split the path integral into two parts, the quasi-classical part and the quantum fluctuations. In the quasi-classical part, we only integrate over quasi-classical paths, which are all paths that could happen using only classical principles. For the quantum fluctuations, we consider all the fluctuations around the quasi-classical paths. We call this paths quasi-classical and not classical as we are still considering a quantum system.

We split the path integral in two parts by writing the action as a combination of quasi-

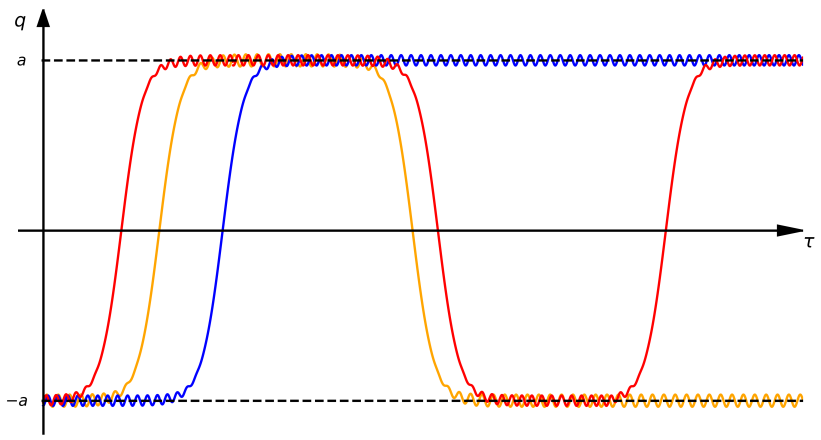

Figure 5: *Three possible paths for a particle starting at $q = -a$. To calculate the eigenenergies of a particle in the double-well potential, we have to integrate over all paths. Luckily there are only some paths relevant as they give a bigger contribution. The particle is highly unlikely to do a random path from $q = -a$ to $q = a$. The only relevant path going from $q = -a$ to $q = a$ once is the single instanton trajectory. As argued in the text, we only have to integrate over all possible quantum fluctuations when a particle is on an extremum and we have to sum over the different moments when a particle can travel from one extremum to the other extremum.*

classical paths with quantum corrections

$$\mathcal{S}[q] = \mathcal{S}[q_{cl} + \delta q]. \tag{2.5}$$

In this equation, we write the position $q = q_{cl} + \delta q$, where q_{cl} is the classical position and δq are fluctuations around q_{cl}. We can therefore write the action in a term with only the quasi-classical paths and separately the corrections which are given by

$$\mathcal{S}_{qu}[\delta q] = \mathcal{S}[q_{cl}] - \mathcal{S}[q_{cl} + \delta q]. \tag{2.6}$$

As we integrate over all paths, we have to integrate over both the quasi-classical paths and the quantum fluctuations (see figure 5). We end up with the following equation

$$\int_{q_i}^{q_f} Dq \exp(-\mathcal{S}[q]) = \sum_{\{q_{cl}\}} C_{cl} e^{-\mathcal{S}[q_{cl}]} \int D\delta q \exp(\mathcal{S}_{qu}[\delta q]). \tag{2.7}$$

Here sum includes all possible quasi-classical paths. In this equation C_{cl} is only a prefactor which we need to add for all different quasi-classical paths. In equation (2.6) we have the instanton trajectories

$$\sum_{\{q_{cl}\}} C_{cl} e^{-\mathcal{S}[q_{cl}]},$$

and the quantum fluctuations

$$\int Dq' \exp(\mathcal{S}_{qu}[q']).$$

We ignore the time that the particle is moving from one extremum to the other for the quantum fluctuations. Ignoring this time only leads to a tiny difference in outcome. Because of this, together with the approximation that we only look at quantum fluctuations when the particle is on an extremum, we can evaluate the quantum fluctuations independently of the quasi-classical paths. Therefore, we can really evaluate the right-hand side of equation (2.7) as two separate integrals.

2.4 The single instanton trajectory

Before we compute the path integral over the classical action, we look at a single instanton trajectory first. A single instanton trajectory is the path of a particle going once from one minimum to the other (see figure 4). Due to symmetry, the single instanton trajectory from $q = -a$ to $q = a$ has the same outcome as from $q = a$ to $q = -a$. We want to calculate the path integral over a single instanton trajectory (I_{inst})

$$I_{\text{inst}} = C_a \exp\left(-\int_0^\infty d\tau' \big(V(q_{cl}) + \frac{m}{2}\dot{q}_{cl}^2\big)\right) = C_a \exp\left(-\mathcal{S}_{\text{inst}}\right), \tag{2.8}$$

where $\dot{q}_{cl} = \frac{\partial q_{cl}}{\partial \tau'}$ and $\mathcal{S}_{\text{inst}}$ is the single instanton action. Further, C_a is a prefactor which results from taking the path integral.

Looking at the single instanton trajectory, the time integral going to infinity seems intimidating. However, it is enough to integrate from zero to a time τ_{ins}, the instanton time. This needs some explanation, as we expect classically that the particle would not even move if it is on an extremum. Due to quantum fluctuations, the particle is often not exactly on an extremum. Secondly, it would take an infinite time to get exactly to the other extremum. However, the particle reaches the area around the extremum, where quantum fluctuations are dominant, after a certain time. This time is called the instanton time τ_{ins} (see figure 4). Once the particle is in the area where the quantum fluctuations dominate, we say that it went from one extremum to the other.

For a particle close to an extremum, its classical contribution to the action is negligible. Indeed for a particle close to an extremum, its velocity is nearly zero and therefore the kinetic term too, $V(q) = 0$ for $q = \pm a$. The contribution from the integral from τ_{ins} to infinity is ignored. We can therefore take the integral from zero to τ_{ins}.

We can find a convenient expression for the single instanton action, by using energy conservation. The total energy is conserved so $\frac{m}{2}\dot{q}^2 = V(q)$. With this we find that

$$\mathcal{S}_{\text{inst}} = \int_0^{\tau_{\text{ins}}} d\tau' \frac{dq_{cl}}{d\tau'}(m\dot{q}_{cl}) = \int_{-a}^{a} dq \big(2mV(q)\big)^{\frac{1}{2}}. \tag{2.9}$$

In the equation above, q is now a dummy variable, so we can integrate over the position. The double-well potential $V(q)$ is given in equation (2.1). We find that

$$\mathcal{S}_{\text{inst}} = \frac{2}{3} m\omega_0 a^2. \tag{2.10}$$

Now the single instanton trajectory can be calculated, as the single instanton action is independent of position. We then find that

$$I_{\text{inst}} \propto \exp\left(-\mathcal{S}_{\text{inst}}\right) = \exp\left(-\frac{2}{3} m\omega_0 a^2\right). \tag{2.11}$$

With this result, we found a convenient expression for the contribution of the mass of a particle and the shape of the well to the single instanton trajectory.

2.5 Classical paths

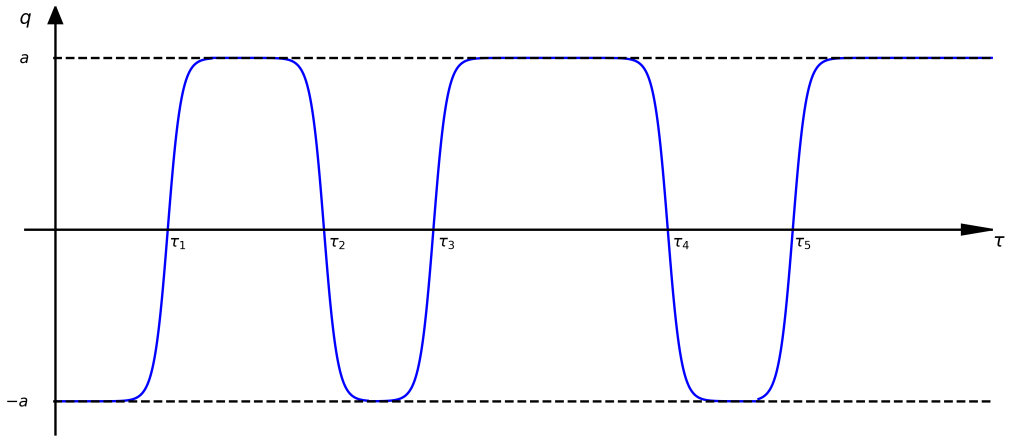

Figure 6: *A possible instanton trajectory without quantum fluctuations. A particle starts at the extremum $q = -a$. Around an imaginary time τ_1 it moves to the other extremum. Then it moves back at τ_2 and so on. We can order the times when the particle moves between extrema. All classically possible paths can be determined in this way.*

In equation (2.7) we integrate over all possible quasi-classical paths from $-a$ to a, including the paths where a particle goes from one extremum to another multiple times (see figure 6). The particle can travel many times from one extremum to another. However, for a particle with mass, a particle is most of the time in one of the extrema. The instanton time multiplied with the number of switches, is small compared with the time a particle is in the extrema. If the particle would be massless, it would have no kinetic energy and it would travel infinitely fast from one extremum to the other, if we ignore relativity. The massless particle could switch infinitely many times from position. In this situation we cannot use the instanton. We need particles to be massive to introduce the instanton.

Now we go back to the classical part of the path integral (2.7). To compute this, we have to look at the main contributions. The classical solutions are always of the following form: A particle starts on a potential extremum $\pm a$, then moves n times from one extremum to the other. The moment it moves is given by τ_i, where the index stands for after how many switches between extrema the particle moves. After a time τ, we stop and see where the particle is. All classically possible paths the particle has taken are the trajectories.

To include all trajectories we have to integrate over all classically relevant paths. We do this by integrating over the times that the particle can go from one extremum to the other τ_i. Now we can calculate all classically relevant paths together. We get that the quasi-classical paths from equation (2.7) are given by the following equation

$$\sum_{\{q_{cl}\}} C_{cl} e^{-\mathcal{S}[q_{cl}]} = \sum_n \int_0^\tau d\tau_1 ... \int_0^{\tau_{n-1}} d\tau_n \left(I_{\text{inst}}\right)^n . \tag{2.12}$$

In this equation, n is the number of single instanton trajectories, as this is the number of switches between extrema the particle has taken. We have used here that all single instanton trajectories give the same contribution. We integrate τ_i from 0 to τ_{i-1} as all instanton trajectories can be ordered in time. Using that $\int_0^\tau d\tau_1 ... \int_0^{\tau_{n-1}} d\tau_n = \frac{\tau^n}{n!}$ gives

$$\sum_{\{q_{cl}\}} C_{cl} e^{-\mathcal{S}[q_{cl}]} = \sum_n \frac{1}{n!} \left(\tau I_{\text{inst}}\right)^n . \tag{2.13}$$

In this expression is convenient, as it only depends on the single instanton trajectory.

2.6 Quantum fluctuations

Now we look at the quantum fluctuations. As said before, we only have to look at the fluctuations when the particle is on an extremum. When we look at the particle in one of the wells we can make the approximation that both wells individually are very similar to a single well. This single well has a potential, which is given by

$$V_{HO}(x) = \frac{m}{2}\omega_0^2 x^2. \tag{2.14}$$

This is the potential for a harmonic oscillator, which is a well-known potential in quantum mechanics. This potential corresponds really well with the double-well potential around the points $q = \pm a$ in the double-well potential. We find the single-well potential after a coordinate shift $q - a = x$ for the left well, and $q + a = x$ for the right well. One can see that the approximation is good by making a Taylor expansion in the double-well potential around $q = \pm a$ and comparing it with the potential for the harmonic oscillator. Up to second order in the Taylor expansion they are identical.

We can now find the quantum fluctuations as we know how to get them for the harmonic oscillator. The quantum fluctuations for a particle being on a potential extremum for a time τ are given by

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = \int_{x_i}^{x_f} Dx \exp\left(-\int_0^\tau d\tau' (V_{HO}(x) + \frac{m}{2}\dot{x}^2)\right). \tag{2.15}$$

We know how to work with the harmonic oscillator in real-time. In appendix C we derive the following result

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C' \sin(-i\omega_0\tau)^{-\frac{1}{2}}, \tag{2.16}$$

where C' is a constant, which is irrelevant for now. To calculate the path integral from equation (2.3), we have to look at all possible paths. We therefore have to look at a particle being in one of the wells for a time $\Delta\tau$, before it travels to the other well. We assume that a particle is much longer on an extremum than the time it takes for a particle to do a single quantum fluctuation. This means mathematically that $\omega_0\Delta\tau >> 1$. With this assumption we can write equation (2.16) as a single exponential

$$\sin(-i\omega_0\Delta\tau) = \frac{1}{2i}(e^{\omega_0\Delta\tau} - e^{-\omega_0\Delta\tau}) \approx \frac{1}{2i}e^{\omega_0\Delta\tau}. \tag{2.17}$$

With this we find that for a particle being on an extremum of the potential for a time $\Delta\tau$, the path integral is given by

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C' e^{-\frac{\omega_0 \Delta\tau}{2}}. \tag{2.18}$$

Notice that this is exactly the same expression as the path integral of a particle being in the ground state of a single-well potential for a time $\Delta\tau$, as the ground-state energy of a particle in a single well potential is given by $E_0 = \frac{\omega_0}{2}$.

Now we want to find the quantum fluctuation for the whole path integral. As the particle is nearly always on the position $q = \pm a$, it is a good assumption to take the quantum fluctuations from the particle on an extremum for the entire time τ. With this assumption, we find that the total contribution from the quantum fluctuations is given by

$$\int D\delta q \exp(-\mathcal{S}_{qu}[\delta q]) = C' e^{-\frac{\omega_0 \tau}{2}}. \tag{2.19}$$

Next, we can use the result of the quantum fluctuations and quasi-classical paths to find a result for the path integral in equation (2.7)

$$\int_{q_i}^{q_f} Dq \exp(-\mathcal{S}[q]) = C' e^{-\frac{\omega_0 \tau}{2}} \sum_n \frac{1}{n!} \tau^n \exp\left(-n\mathcal{S}_{\text{inst}}\right). \tag{2.20}$$

We can combine this with equation (2.4) and we find

$$\lim_{\tau\to\infty} \sum_{n\epsilon\{S,A\}} \langle q_f|n\rangle \, e^{-E_n \tau} \, \langle n|q_i\rangle \propto \lim_{\tau\to\infty} e^{-\frac{\omega_0 \tau}{2}} \sum_n \frac{1}{n!} \tau^n \exp\left(-n\mathcal{S}_{\text{inst}}\right). \tag{2.21}$$

We can use this equation to find the lowest energies of a particle in a double-well potential.

2.7 The energy gap

To see how the lowest energy levels are related to the instanton, we have a look at the left-hand side of equation (2.21). Here the ground state and first excited state are given by the symmetric and antisymmetric eigenstates respectively. These eigenstates have eigenenergies given by $E_S = \frac{1}{2}(\omega_0 - \Delta\epsilon)$ and $E_A = \frac{1}{2}(\omega_0 + \Delta\epsilon)$ [7]. Fortunately, we can relate the energy difference between the ground state and the first excited state $\Delta\epsilon$ with the single instanton (see appendix D). We find that the energy gap between the ground state and the first excited state is given by

$$\Delta\epsilon = I_{\text{inst}}. \tag{2.22}$$

We can combine this with equations (2.10) and (2.11) and we find that

$$\Delta\epsilon \propto \exp\left(-\frac{2}{3} m\omega_0 a^2\right). \tag{2.23}$$

The energy gap is, as expected, dependent on the mass of the particle. The bigger the mass of the particle is, the smaller the energy gap is. This is as expected, because for a particle with a big mass, it is harder to go from one extremum to the other, exactly as it is harder to go from one extremum to the other if the barrier is high. For a high barrier the energy gap is smaller. Similarly, for a higher mass the energy gap is smaller too.

2.8 Conclusion

We found a procedure to get the ground-state energies of a particle in a double-well potential, by using the instanton. This procedure is more complicated than if we would find the ground-state energies via the WKB-method [10]. We found exactly the same result as is found with the WKB-method, namely

$$\Delta\epsilon \propto \exp\left(-\frac{2}{3}m\omega_0 a^2\right). \tag{2.24}$$

This is the same result as in the book by A. Altland *et al.* [8].

We want to note explicitly that the energy gap is proportional to e^{-m}, so the energy gap is getting exponentially smaller for a bigger mass. If the mass would be infinitely large, a particle could not tunnel through the barrier, and therefore the two potentials would be independent of each other. This would lead to two exactly the same single-well potentials and therefore two degenerate ground states.

The reason that we used the instanton in the derivation is that we are now familiar with instanton calculus. We find the ground-state energies for a spin using an instanton in the next chapters. The procedure is the same for the particle in a double-well potential as for a spin, but the spin Hamiltonian has different terms, which makes the derivation more complicated. However, many steps are the same and a good understanding of the instanton for a particle in a double-well potential makes the derivation easier to follow.

After calculating the ground-state energies, we have a better understanding of superpositions, as we know how a particle can move between two wells. We also found the path integral of a particle moving between wells, as this is the single instanton trajectory. In the derivation of the ground-state energies, we assumed that some paths from one well to the other are physically relevant and other paths we neglected. Still, we found the right result for the lowest energy levels of a particle in a double-well potential. This means that our assumption when a path is likely to happen or not, is reasonable. We can conclude that the quasi-classical paths between potential minima are the most relevant paths together with small quantum deviations of these paths.

We found a result which explains the influence of tunneling on ground-state energies. However, tunneling is also interesting for other situations such as potentials where one potential minimum is a lot smaller than another. With tunneling one could find how big the probability is that a particle would go from a higher potential minimum to a lower potential state after crossing a barrier. The instanton could be used for such a problem too.

3 The spherical-spin model

In this chapter we look at spin systems. Where in chapter 2 we reproduced a result which is already known, we now give a new result and we do a derivation which has not been done before. As has been explained in the introduction, we are interested in a spin system with non-zero inertia.

For this system we are looking for the lowest energy levels and the ground-state energies of a spin. We argued in the introduction that the lowest energy levels are dependent on inertia if they are a superposition of multiple potential minima. For such lowest energy levels, tunneling has to be taken into account. We can calculate these lowest energy levels with an instanton, the spin-instanton. For the derivation of the lowest eigenenergies for a spin, we use the same steps as in chapter 2. However, now the derivation is more complicated as even a simple spin system has many variables to take into account. In the following chapters, we consider a large single spin, which is localized.

In this chapter we first create a spin model which has a dependence on inertia. In this model the spin can point in any direction on a sphere. The model is therefore called the spherical-spin model. For this model we use instanton calculus to find the lowest energy levels and the energy gap between the ground state and the first excited state. As it turns out, finding the lowest energies for the spherical-spin model is hard. To make a good derivation of the energy gap between the ground state and the first excited state, we look at a more simple model, namely the circular-spin model. In the circular-spin model the spin can only point in a direction on a circle. This model is explained in chapter 4. In chapter 3, we first explain the spherical-spin model in detail, then we derive the spin action and equations of motion. Finally we discuss what has to be done to find the energy gap between the lowest eigenenergies of the spherical-spin model.

3.1 The spin Hamiltonian

We find an interesting spin model, if we look at a macrospin in a magnet with easy-axis anisotropy. We also add an external magnetic field on the spin. We choose the z-direction such, that it corresponds with the direction of the anisotropy. We choose the external magnetic field to be in the negative x-direction as this is the most convenient choice, so $B_x < 0$. The Hamiltonian which corresponds with this model is given by

$$\hat{H}_{\text{spin}} = -K\hat{S}_z^2 - B_x\hat{S}_x. \tag{3.1}$$

We call this the spin Hamiltonian. In the spin Hamiltonian, K is the anisotropy parameter [15, 16]. The addition of a magnetic field leads to a significant effect if the magnetic field has the same order of magnitude as the anisotropy parameter multiplied with the total spin S, so $-B_x \sim KS$.

The potential corresponding with the spin Hamiltonian, called the spin potential, is given by (see figure 7)

$$V = -KS_z^2 - B_xS_x. \tag{3.2}$$

This potential has two minima. Also, the spin potential and the spin Hamiltonian are invariant under parity in the z-direction S_z. For this model, the lowest energy levels are a

superposition of the spin being both of the potential minima. This means that to find the ground state, we have to take into account the instanton. We now have a model of a spin system which has a relevant spin-instanton dependence.

One might wonder why we have to include a magnetic field in the model. If we look at the same model but with $B_x = 0$, we would be working with the so-called easy-axis Hamiltonian

$$\hat{H}_{\text{ea}} = -K\hat{S}_z^2. \tag{3.3}$$

This Hamiltonian is invariant under parity in the z-direction too. However, after looking at the corresponding potential $V_{\text{ea}} = -KS_z^2$, we see that the potential minima are given by $S_z = S$ and $S_z = -S$. These minima are eigenstates of the easy-axis Hamiltonian. Therefore, the spin does not have to tunnel to the other potential minimum to lower its energy and thus the spin-instanton does not play a role in this system.

By adding the magnetic field in our model, the potential minima are no longer eigenstates of the corresponding Hamiltonian. This has the consequence that the ground state is a superposition of the two potential minima and we need the spin-instanton to find the lowest energy levels.

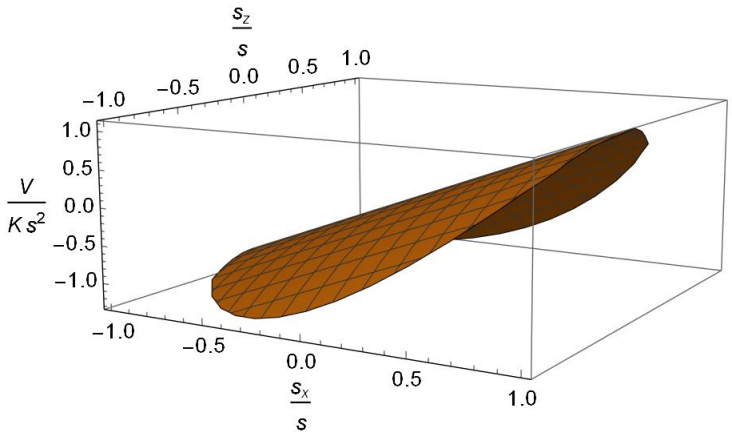

Figure 7: *In this figure the dimensionless spin potential ($\frac{V}{KS^2}$) is plotted against the spin value in the z- and x-direction. The potential minima are dependent on S_x and they are no eigenstates of the spin Hamiltonian. Due to parity symmetry we know that the eigenstates are a superposition of the potential minima. The two lowest eigenenergies are not equal. This means that the minimal eigenstates are non-degenerate and thus the spin-instanton has to be taken into account. We used that $\frac{B_x}{K} = -6$ and $S = 5.5$. We look at $\frac{B_x}{K}$ and not at B_x and K individually, as $\frac{B_x}{K}$ is dimensionless and B_x and K come always in pairs in the potential divided by KS^2.*

3.2 The symmetric and antisymmetric state

The spin Hamiltonian is invariant under parity in the z-direction. This means that the ground state and first excited state are given by the symmetric $|S\rangle = \frac{1}{\sqrt{2}}(|l\rangle + |r\rangle)$ and antisymmetric spin eigenstates $|A\rangle = \frac{1}{\sqrt{2}}(|l\rangle - |r\rangle)$ respectively. Here the state $|l\rangle$ and $|r\rangle$

are defined as the spin in a local ground state of a potential minimum of the potential in equation (3.2). The symmetric eigenstate has an eigenenergy which is slightly lower than the energy of a local ground state of the spin. Similarly, the antisymmetric eigenenergy is slightly higher. Due to symmetry we know that the eigenenergies are given by

$$E_0 = E_S = E_{\text{ref}} - \frac{1}{2}\Delta\epsilon, \tag{3.4}$$

and

$$E_1 = E_A = E_{\text{ref}} + \frac{1}{2}\Delta\epsilon. \tag{3.5}$$

The reference energy E_{ref} is the energy for a spin which is not influenced by another local minimum. Fortunately we know this energy as it is the ground-state energy of the easy-axis Hamiltonian.[3] Locally around the extrema, the easy-axis Hamiltonian is a good approximation for the spin Hamiltonian. Therefore, we can use the easy-axis Hamiltonian to find a good approximation of the reference energy.

The ground states of the easy-axis Hamiltonian are given by the spin pointing either in the positive z-direction, $|S, S\rangle$, or in the negative z-direction, $|S, -S\rangle$. In this thesis we denote these states as follows: The spin in the positive z-direction, $|S, S\rangle \coloneqq |\Uparrow\rangle$ and in the negative z-direction, $|S, -S\rangle \coloneqq |\Downarrow\rangle$. The eigenenergies of the ground states are found by

$$E_{\text{ref}} |\Uparrow\rangle \approx \hat{H}_{\text{ea}} |\Uparrow\rangle = -K\hat{S}_z^2 |\Uparrow\rangle . \tag{3.6}$$

From appendix E we know that $\hat{S}_z |\Uparrow\rangle = S |\Uparrow\rangle$. This leads to $E_{\text{ref}} \approx -KS^2$.

Next, we want to find the energy gap $\Delta\epsilon$. As said before, we are going to calculate the energy gap with the spin-instanton. We can already make some educated guesses about the energy gap. It must be dependent on the magnetic field, as at $B_x = 0$, there is no energy gap. For the double-well potential, the energy gap is dependent on the mass. This is because the bigger the mass, the more energy it costs to go from one well to the other. We expect that the energy gap for spin is dependent on the inertia as inertia determines how difficult it is for a particle to go from one place to another. We expect that the bigger the inertia is, the more energy it costs to tunnel from potential minimum. It is interesting to know what the influence of inertia on the ground state is exactly.

3.3 The spin propagator

We have now described the model for a spin. Next, we want to get the ground-state energies of the spin and we want to find the description of the spin-instanton. To find this, we take the same steps as we did for the particle in the double-well potential. We start by

[3] To better understand why we can use the easy-axis Hamiltonian to find the reference energy E_{ref}, we want the reader to be aware of the analog with the double-well potential. For the double-well potential, we found that the reference energy is found by looking at an infinite barrier. Here a particle in one well is not influenced by the other well. The single reference energy is then found by looking at the ground state of a single well (see [14]). Similarly, for the spin system, one minimum spin state is not influenced by another minimum, if there is no magnetic field. We can therefore find the reference energy by looking at the easy-axis Hamiltonian and finding its ground-state energy.

deriving a path integral from the propagator (for a detailed derivation of equation (3.7) see appendix F). In this derivation we use that the spin is not interacting with anything

$$\lim_{\tau\to\infty}\sum_{n\epsilon\{S,A\}}\langle\psi_f|n\rangle\, e^{-E_n\tau}\,\langle n|\psi_i\rangle = \lim_{\tau\to\infty}\langle\psi_f|e^{-\hat{H}\tau}|\psi_i\rangle = c\lim_{\tau\to\infty}\int_{\psi_i}^{\psi_f} Dg\exp(-\mathcal{S}[g]). \tag{3.7}$$

The initial and final states of the propagator are given by $|\psi_i\rangle$ and $|\psi_f\rangle$ respectively. Further, we have that c is a prefactor, which is not important in this thesis.[4] In equation (3.7), $\mathcal{S}[g]$ is the spin action, which depends on the spin coherent states $|g\rangle$. For more information about spin coherent states, see appendix E. To derive equation (3.7), we add unit operators of coherent states and time evolution operators in the propagator.

On the left-hand side of equation (3.7) we take into account the ground state and the first excited state of the spin. We take into account both states as we are interested in the energy gap between the eigenenergies of the ground state and the first excited state. We take the limit of $\tau\to\infty$ to be able to ignore all higher energy levels than the first excited state. We can only ignore the higher energy levels and take into account the first excited state, after taking the limit of $\tau\to\infty$, if

$$\frac{E_1 - E_0}{E_2 - E_0} \ll 1. \tag{3.8}$$

For this limit the ground-state energy E_0 and the energy of the first excited state E_1 are nearly identical.

A part of the results of this thesis is to find the ground-state energy and the energy of the first excited state for the spherical-spin model. We can therefore not give an analytical derivation yet to relate the variables K, B_x and S to see when inequality (3.8) holds. We need this inequality to be able to include both the ground state and first excited state and not the higher order states in our calculation to find a result for E_0 and E_1. However, we can calculate E_0, E_1 and E_2 numerically for a spin with easy-axis anisotropy in a magnetic field as described above (see figure 8). The numerical results do not include a bath, and thus also no spin inertia.

We see in figure 8) that the first excited state and the ground state have eigenenergies are nearly identical compared with higher order eigenenergies of the spin Hamiltonian, if we take $\frac{|B_x|}{K} < S$. This has the consequence that, for $\frac{|B_x|}{K} < S$, we have to take not only the symmetric state into account in equation (3.7), but we also have to take into account the antisymmetric state, which is the first excited state. This is exactly what we wanted, because with the instanton calculus we can find the energy gap between the ground state energy and the first excited state energy. We are therefore looking at a model where $\frac{|B_x|}{K} < S$.

[4] We are not interested in the prefactor c for the same reasons as we are not interested in the prefactor in equation (2.3) for the double-well potential. In this thesis the prefactor is not of importance, as only the dependence in the exponential leads to the energy gap between the ground-state energy and first excited state energy. The prefactor leads to the so-called reference energy, $E_{\text{ref}} = \frac{1}{2}(E_0 + E_1)$. However, there is another way to find this prefactor, so for now we ignore it and say only that the probability amplitude is proportional to the path integral.

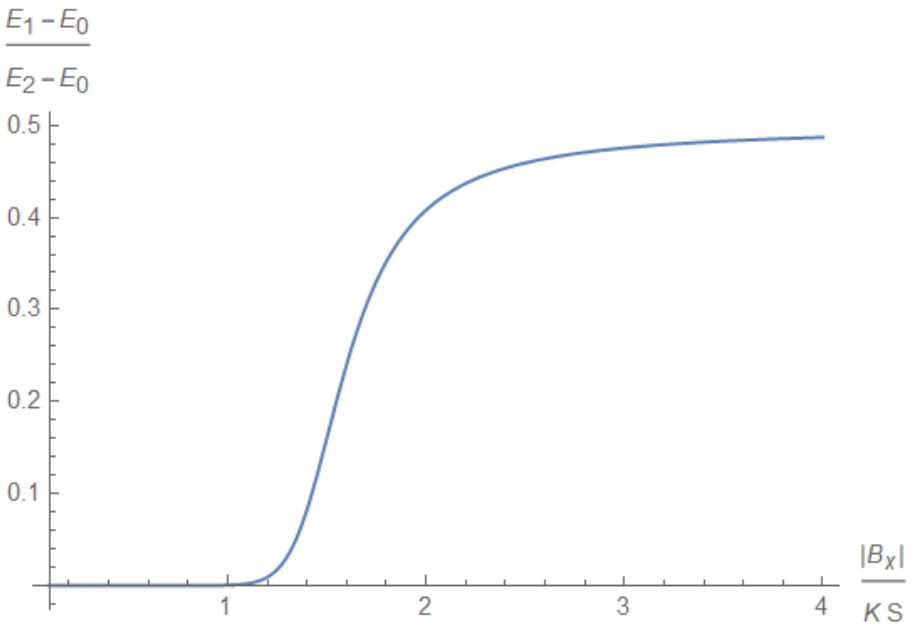

Figure 8: *The difference in energy between the two lowest states $E_1 - E_0$ over the difference in energy between the ground state and second excited state $E_2 - E_0$ are plotted against the magnetic field over the anisotropy parameter multiplied with the total spin. We see that the fraction is very small for $\frac{|B_x|}{K} < S$. This result is found numerically for a spin system with $S = 10$. In the numerical calculation of the energies, we did not include any bath.*

Later in the thesis, we are going to work with a bath of harmonic oscillators. The interaction with a bath changes the energies, but we find later in this thesis that if the spin is interacting with a bath, the energy difference $E_1 - E_0$ becomes smaller (see 4.9). This means that the fraction is only smaller for a larger regime of $\frac{|B_x|}{K} < S$, which coincides with the approximation we made of ignoring higher energy levels in equation (3.7). We see in figure 8 that the fraction in equation (3.8 is very small for $\frac{|B_x|}{K} < S$. We can now include the ground state and first excited state in equation (3.7) and discard all higher energy levels when we take the limit of $\tau \to \infty$.

3.4 The spin action

Next, we have a look at the action corresponding to the spherical-spin model. We identified in appendix F, that the action is given by

$$\mathcal{S}[g] = \int d\tau (i \langle \dot{g}|g\rangle + \langle g|\hat{H}|g\rangle). \tag{3.9}$$

Here $|g\rangle$ are the spin coherent states. The term given by $\langle \dot{g}|g\rangle$, is called the Berry-phase term [17] (see appendix G).

To include spin inertia in the model, we look at a spin in a bath. We do this because we have to take into account conservation of angular moment. This means that if the

spin inertia changes, somewhere else a rotation must change too. This is accomplished by placing the spin in a bath. When the spin interacts with a bath, it can dissipate energy and therefore the spin inertia can be included in the equations of motion of the system. For this thesis we choose a simple bath, namely a bath of harmonic oscillators. Using this bath makes it easy to do integration over position and momenta, as the harmonic oscillators has the consequence that we have to work with Gaussian integrals.

We can split the Hamiltonian of a spin in a bath into three parts

$$\hat{H} = \hat{H}_{\text{spin}} + \hat{H}_{\text{bath}} + \hat{H}_{\text{int}}. \tag{3.10}$$

We already know what is $\hat{H}_{\text{spin}}$ (see equation (3.1)). The Hamiltonian of the bath is given by harmonic oscillators so

$$\hat{H}_{\text{bath}} = \sum_{\alpha} \left(\frac{\hat{\mathbf{p}}_{\alpha}^2}{2m_{\alpha}} + \frac{m_{\alpha}\omega_{\alpha}^2}{2} \hat{\mathbf{q}}_{\alpha}^2 \right). \tag{3.11}$$

Here the index α runs over all harmonic oscillators in the bath and $\mathbf{q}_{\alpha}$ is the position of the harmonic oscillator with index α. The last term, $\hat{H}_{\text{int}}$, describes the interaction between the bath and the spin. For simplicity, we assume linear coupling between the spin and the harmonic oscillators

$$\hat{H}_{\text{int}} = -\sum_{\alpha} \gamma_{\alpha} \hat{\mathbf{S}} \cdot \hat{\mathbf{q}}_{\alpha}. \tag{3.12}$$

Here γ_{α} is a coupling constant.

As the spin is now interacting with a bath, the expression for the propagator changes. We now have to integrate not only over the spin coherent states but also over the positions and momenta of the harmonic oscillators. We then have the following path integral

$$\langle \psi_f | e^{-\hat{H}\tau} | \psi_i \rangle \propto \prod_{\alpha'} \int D\mathbf{p}_{\alpha'} \int D\mathbf{q}_{\alpha'} \int_{\psi_i}^{\psi_f} Dg \exp(i \int d\tau \left(-i \langle \dot{g} | g \rangle + \langle g | \sum_{\alpha} \mathbf{p}_{\alpha} \cdot \dot{\mathbf{q}}_{\alpha} - \hat{H} | g \rangle \right)). \tag{3.13}$$

In this equation we write the Hamiltonian still as an operator, as it is an operator with respect to the spin coherent states. This means that all spin operators are still operators. However, the terms with the momenta and positions of the harmonic oscillators are no operators. This is for the same reasons as we used in section 2.1 in the derivation of the path integral. We can now write the propagator as follows

$$\langle \psi_f | e^{-\hat{H}\tau} | \psi_i \rangle \propto \prod_{\alpha'} \int D\mathbf{p}_{\alpha'} \int D\mathbf{q}_{\alpha'} \int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}'[g, \mathbf{q}_{\alpha}]). \tag{3.14}$$

Here $\mathcal{S}'$ is the action which is given by

$$\mathcal{S}'[g, \mathbf{q}_{\alpha}] = \int d\tau \sum_{\alpha} \left(-i \langle \dot{g} | g \rangle + \langle g | \hat{H}_{\text{spin}} - \gamma_{\alpha} \hat{\mathbf{S}} \cdot \mathbf{q}_{\alpha} + \frac{\mathbf{p}_{\alpha}^2}{2m_{\alpha}} + \frac{m_{\alpha}\omega_{\alpha}^2}{2} \mathbf{q}_{\alpha}^2 + \mathbf{p}_{\alpha} \cdot \dot{\mathbf{q}}_{\alpha} | g \rangle \right). \tag{3.15}$$

This action is long and hard to work with. In the next section we write this action in a more convenient way.

3.5 Retarded and advanced kernel functions

To simplify equation (3.15), we want to get rid of the spin operators. To do so, we use that $\langle g|\hat{\mathbf{S}}|g\rangle = \mathbf{S}$. Then we can write the action as

$$\mathcal{S}'[g,\mathbf{q}_\alpha] = \int d\tau \sum_\alpha \left(-i\langle \dot{g}|g\rangle - KS_z^2 - B_xS_x + \gamma_\alpha \mathbf{S}\cdot\mathbf{q}_\alpha + \frac{\mathbf{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha\omega_\alpha^2}{2}\mathbf{q}_\alpha^2 + \mathbf{p}_\alpha\cdot\dot{\mathbf{q}}_\alpha\right). \quad (3.16)$$

In equation (3.16) the action is quadratic both in the momenta and in the positions of the harmonic oscillators. This means that we can simplify the equation with Gaussian integrals. The Gaussian integral over the momenta of the harmonic oscillators gives us a term of the form $-\frac{m\dot{\mathbf{q}}^2}{2}$.

We can use integration by part to get a term quadratic in the positions of the harmonic oscillators. We can only find this quadratic term if we do a Fourier transformation. Using the Fourier transformation, we find the following action (see appendix H)

$$\mathcal{S}[g] = \int d\tau' \left(-i\langle \dot{g}|g\rangle - KS_z^2 - B_xS_x) + \int d\tau' \int d\tau'' \mathbf{S}(\tau')\alpha^{R/A}(\tau'-\tau'')\mathbf{S}(\tau'')\right). \quad (3.17)$$

In this equation, $\alpha^R(\tau-\tau')$ is the retarded kernel function between the spin at time τ and τ'. The advanced kernel function is $\alpha^A(\tau-\tau')$. The kernel functions are given by

$$\alpha^{R/A}(\tau-\tau') = \int \frac{d\omega}{4\pi}\sum_\alpha e^{-i\omega(\tau-\tau')}\frac{\gamma_\alpha^2}{m_\alpha(\omega_\alpha^2-(\omega\pm i\eta)^2)}. \quad (3.18)$$

This expression is not useful in this form, but we will be working a lot with its Fourier transform. The Fourier transform of the retarded and advanced kernel functions can be approximated to

$$\alpha^{R/A}(\omega) \approx \pm i\alpha_0\omega + \frac{I}{2}\omega^2. \quad (3.19)$$

Here α_0 is the Gilbert damping coefficient and I is the spin inertia. This approximation is discussed in detail in the paper by R. Verstraten *et al.* [18].[5] The Gilbert damping is a damping term, which brings back a spin out of equilibrium to its equilibrium position [20]. The Gilbert damping coefficient and the spin inertia in equation (3.19) are the same quantities as in the ILLG equation (1.2).

We can now Fourier transform the retarded and advanced kernel functions back to find $\alpha^{R/A}(\tau-\tau')$.

$$\alpha^{R/A}(\tau-\tau') = \mp\alpha_0\partial_{\tau'}\delta(\tau-\tau') - \frac{I}{2}\partial_{\tau'}^2\delta(\tau-\tau'). \quad (3.20)$$

[5] In the thesis by M. Gaspar Quarenta [4] and the paper by R. Verstraten *et al.* [18] a similar action is used as our action. The difference is that we are working with normal integrals and they are working with Keldysh integrals. In Keldysh formalism, time is transformed into a contour over infinitely large future and past times [19]. We use normal integrals as this makes it possible to find relatively easy results for instantons. Even though we use different integrals than in Keldysh formalism, we use the same approximation for the retarded kernel function as in the references [4, 18]. We can do this because the kernel functions are identical. In this thesis we do not give a derivation of this approximation. For a full derivation one should have a look at chapter 4 in the thesis by M. Gaspar Quarenta [4].

We use this result of the kernel function, and we get that the action is given by

$$\mathcal{S}[g] = \int d\tau' \left(-i \langle \dot{g}|g \rangle - B_x S_x - K S_z^2 \pm \alpha_0 \mathbf{S} \cdot \dot{\mathbf{S}} + \frac{I}{2} \dot{\mathbf{S}} \cdot \dot{\mathbf{S}} \right). \tag{3.21}$$

The Gilbert damping term vanishes as $\mathbf{S} \cdot \dot{\mathbf{S}} = 0$. One can see this by looking at the definition of the spin vector S and just take the time derivative (see appendix E). As a result we find that the action does not lead to a dependence on the Gilbert damping.[6]

In our kernel function, only the inertia term gives a non-zero result. We are therefore looking at a setup where there is no Gilbert damping. For the rest of this thesis we set the Gilbert damping coefficient to zero, so $\alpha_0 = 0$. Now the kernel functions are both given by

$$\alpha^{R/A}(\tau - \tau') = \delta(\tau - \tau') \partial_{\tau'}^2. \tag{3.22}$$

This is the final approximation we use for the kernel functions.

We can use the approximation of the kernel functions to get a convenient expression for the spin action

$$\mathcal{S}[g] = \int d\tau \left(-i \langle \dot{g}|g \rangle - K S_z^2 - B_x S_x - \frac{I}{2} \mathbf{S} \cdot \ddot{\mathbf{S}} \right). \tag{3.23}$$

Here the minus sign comes from integration by parts. We continue working with the action in equation (3.23) to find the energy gap for the spin. We will determine the equations of motion for this action, but first we look at what this action tells us about the propagator in equation (3.14.

We simplified equation (3.14) by getting rid of the dependence on position and momentum of the harmonic oscillators in the bath. This makes it possible to write the propagator as follows

$$\langle \psi_f | e^{-\hat{H}\tau} | \psi_i \rangle \propto \int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}[g]). \tag{3.24}$$

This equation is the same as the right equality in equation (3.7) without taking the limit of $\tau \to \infty$. However, in equation (3.24) the action is dependent on the spin inertia, as we derived this action from a spin interacting with a bath. In the next section, we determine the main contributions of the action to the integral on the right-hand side of equation (3.24). These are the paths where the action is small. Now one can see why we are looking at a macrospin. For a large spin, the paths in equation (3.24) are exponentially suppressed. Only the paths with a small action will give a relevant contribution. This paths are exactly the paths which correspond to the equations of motion. We look therefore in the next section at the equations of motion of the action.

[6]The Gilbert term is leading to a nonzero term in Keldysh formalism, as here the integral is split in a path going forward with fluctuations, and a path going backward with fluctuations. These paths do not cancel out as for a normal integral, but they add up. I will not work out the result of the Gilbert term in Keldysh formalism in this thesis, as this is not possible if you are working with normal integrals. The instanton is namely not well-known in Keldysh formalism, but it is better understood with normal integrals. There are ideas on how to look at instantons in Keldysh formalism [21], but that goes beyond this thesis. In this thesis, we are be working with a system without a Gilbert term, so we can focus on the spin inertia, which is well-defined with normal integral. By only looking at the spin inertia we find interesting results too.

3.6 Spin equations of motion

To find the equations of motion, we write the spin in spherical coordinates. The spin vector, $\mathbf{S} = \langle g|\hat{\mathbf{S}}|g\rangle$, is in spherical coordinates given by (see appendix E)

$$\mathbf{S} = S\begin{pmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{pmatrix}. \tag{3.25}$$

We find the equations of motion by varying the action. The quasi-classical equations of motion are given by

$$\frac{\delta\mathcal{S}}{\delta\theta} = S\dot{\phi}\sin\theta + \begin{pmatrix}\cos\theta\cos\phi\\ \cos\theta\sin\phi\\ -\sin\theta\end{pmatrix}\cdot\left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right) = 0, \tag{3.26}$$

and

$$\frac{\delta\mathcal{S}}{\delta\phi} = -S\dot{\theta}\sin\theta + \begin{pmatrix}-\sin\theta\sin\phi\\ \sin\theta\cos\phi\\ 0\end{pmatrix}\cdot\left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right) = 0, \tag{3.27}$$

where we introduced the effective magnetic field

$$\mathbf{B}_{\text{eff}} = \begin{pmatrix}-B_x\\ 0\\ -2KS_z\end{pmatrix}. \tag{3.28}$$

Equations (3.26) and (3.27) are equivalent to the following equation (see appendix I)

$$\dot{\mathbf{S}} = \mathbf{S}\times\left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right). \tag{3.29}$$

The best way to derive the equations of motion to the form of equation (3.29), is by writing out the expression for $\dot{S}$ and writing out the cross product. Then one should find terms in $\dot{S}$ which are of the form $\dot{\theta}\sin\theta$ and $\dot{\phi}\sin\theta$ and use equations (3.26) and (3.27) to find the right-hand side of equation (3.28).

Equation (3.29) is the Inertial-Landau–Lifshitz–Gilbert (ILLG) equation (see equation 1.2) without Gilbert damping. For more information about the ILLG equation we refer to the paper by E. Olive *et al.* [3].

We can write not only the action in spherical coordinates, but also the potential. If we combine equations (3.2) and (3.25), we find that the potential in spherical coordinates is given by (see figure 9)

$$V(\theta,\phi) = -KS^2\cos^2\theta - B_xS\sin\theta\cos\phi. \tag{3.30}$$

The two potential minima in spherical coordinates are $\phi = \pi$ and $\theta \in \{b, \pi - b\}$, where b is defined as $b := \arcsin(\frac{-B_x}{2KS})$.

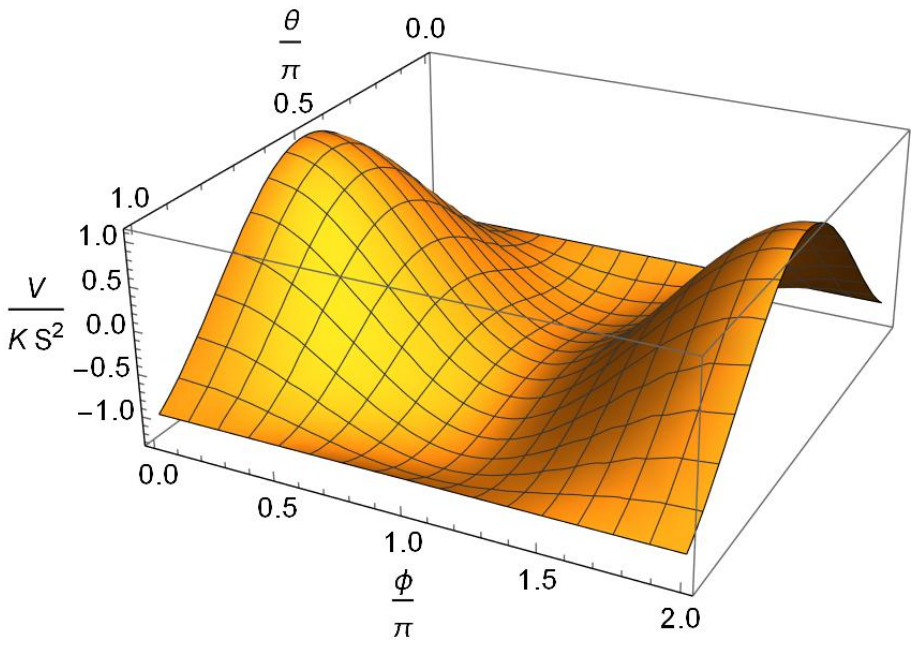

Figure 9: *The potential of the spin in spherical coordinates, corresponding to equation (3.30). We see that there are two potential minima. These are located at* $\phi = \pi$ *and* $\theta \in \{b, \pi - b\}$*, where* b *is defined as* $b := \arcsin(\frac{-B_x}{2KS})$*. The parameters in the plot are again* $\frac{B_x}{K} = -6$ *and* $S = 5.5$*.*

3.7 The lowest energy levels of a spin

To find the lowest energy levels of the spherical-spin model, we take similar steps as is done for the particle in a double-well potential. First we relate the two lowest energy levels with the path integral, as in equation (3.7). Then, as we have an expression for the action, we compute the integral. We have to look at the quantum fluctuations and classical instanton trajectories.

Finding the classical instanton trajectories for the spherical-spin model, however, is not easy. This is because there are infinitely many paths to go from one potential minimum to the other (see figure 7), while the path is still a solution of the equations of motion. This means that there are infinitely many different single instanton trajectories. The derivation of the path integral is a lot more complicated if we have to take into account all these single instanton trajectories. There are infinitely many paths to go from one minimum classically to the other minimum, because we have two degrees of freedom in our action, namely the θ and ϕ dependence, and there is only one restriction on the equations of motion, namely conservation of energy.

To go around this difficulty, we have first a look at a simplification of the spherical-spin model. This is the circular-spin model. In the circular-spin model we only have to deal with one degree of freedom, as in the circular-spin model the ϕ-coordinate is set to a constant. This makes it a lot easier to find the main contributions of the path integral and thus to find the lowest energy levels.

4 The circular-spin model

Before we go further with the spherical-spin model, we look at a simplification: the circular-spin model. The circular-spin model is a spin system where we can describe the model with a single coordinate. The possible spin states spins pointing in the direction of a value on a circle instead of on a sphere. As there is only a single coordinate in the circular-spin model, there is a limited amount of quasi-classical paths between the potential minima. This makes it possible to find the lowest energies of the circular-spin model with the spin-instanton. We derive in this chapter the lowest energies of the circular-spin model and the energy gap between these energies.

4.1 The circular-spin potential

We want the circular-spin model to be such that it has again two classical minima, which are not eigenstates of the Hamiltonian. As with the double-well potential, we want to calculate the instanton, going from one minimum to the other. We choose the circular-spin model as a restriction on the spherical-spin model of chapter 3. The restriction is given by taking $\phi \in \{0, \pi\}$ and $\theta \in [0, \pi]$. This is equivalent to taking $\phi = \pi$ and $\theta \in [0, 2\pi]$, where we do the following transformation. We replace the points on $(\phi, \theta) = (0, \theta)$ for $(\phi, \theta) = (\pi, 2\pi - \theta)$. We choose the circular-spin model as described above, because it tells us something about the spherical-spin model. Further, we choose the ϕ-coordinate such that the potential minima of equation (3.30) are included in the circular-spin model. By defining the circular-spin model in this way, we are able to use many techniques which we used for the double-well potential. This is because both models have one spatial degree of freedom.

We have been mathematically a little inaccurate with the poles of the spin model when we did the transformation. We did not specify well what happens exactly at $\theta = 0$ and $\theta = 2\pi$. This is not needed as it turns out that the problematic points are not part of any relevant path in the path integral, that we use to find the lowest energies of the spin.

By taking $\phi = \pi$ in equation (3.30), we can write the potential of the circular-spin model as

$$V_1(\theta) = -KS^2 \cos^2\theta + B_x S \sin\theta. \tag{4.1}$$

In this potential we are still working with real-time t. We find that the minima of the potential located at $\theta = b$ and $\theta = \pi - b$ with b as before $b := \arcsin(\frac{-B_x}{2KS})$.

For later purposes we shift the potential in a way that the potential minima are zero. We find that at $\theta = b$ and $\theta = \pi - b$, the minima of V_1 are given by

$$V_1(b) = -\frac{B_x^2}{4K} - KS^2. \tag{4.2}$$

After shifting the potential we find a new potential $V(\theta) = V_1(\theta) - V_1(b)$. We find that

$$V(\theta) = -KS^2 \cos^2\theta + B_x S \sin\theta + \frac{B_x^2}{4K} + KS^2. \tag{4.3}$$

This potential is called the circular-spin potential.

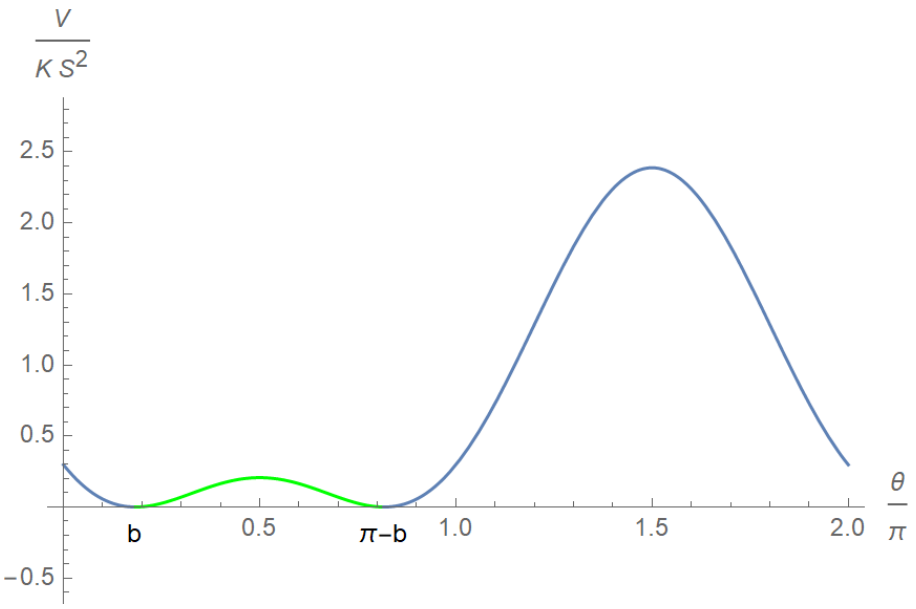

Figure 10: *The circular-spin potential, corresponding to equation (4.3). The shortest path between the two minima is plotted in green. The minima of the potential are located at* $\theta = b$ *and* $\theta = \pi - b$ *with* $b := \arcsin(\frac{-B_x}{2KS})$*. Here the parameters are as follows:* $\frac{B_x}{K} = -6$ *and* $S = 5.5$*.*

4.2 Potential barriers

The calculation of the instanton trajectories is more convenient if we only have to take into account one trajectory between the extrema. If we look at figure 10, we see that the spin can tunnel more easily through the green barrier than through the blue barrier, as this barrier is larger. For now it is unclear when the single instanton trajectory is negligible, for a particle moving through the blue barrier in figure 10 from one extremum to the other. We want to work with a model where one of the potential barriers is much higher than the other, just as is the case in figure 10. This means roughly that

$$\frac{V(\frac{3\pi}{2})}{V(\frac{\pi}{2})} \gg 1, \tag{4.4}$$

as there is a maximum at $\theta = \frac{3\pi}{2}$ and a local maximum at $\theta = \frac{\pi}{2}$. For such a model, we only have to take into account tunneling through the green barrier in figure 10 and we can ignore tunneling through the blue barrier. This means that we only have to take into account one kind of instanton trajectory, namely the instanton trajectory from b to $\pi - b$ corresponding with tunneling through the green barrier.

We want to write the difference in barrier heights in terms of the variables we can change in our system, namely B_x, K and S. We can write the inequality (4.4) in terms of the variables

$$\frac{-B_xKS + \frac{1}{4}B_x^2 + (KS)^2}{B_xKS + \frac{1}{4}B_x^2 + (KS)^2} \gg 1. \tag{4.5}$$

This is the same as

$$\frac{(2KS - B_x)^2}{(2KS + B_x)^2} \gg 1. \tag{4.6}$$

As the magnetic field is always negative in the x-direction, we see that one barrier is a lot higher than the other if $2KS + B_x$ is small compared with $2KS - B_x$ and when $-B_x < 2KS$. However, $-B_x$ cannot be much smaller than $2KS$, otherwise we have to take into account tunneling through the blue barrier too. Notice that for determining the regime, we can only compare the magnetic field with the product of anisotropy parameter K and the total spin S, and not with them separately. If B_x would not be big enough, we would have to take into account the paths via both potential barriers.

In figure 10 we used the following parameters $\frac{B_x}{K} = -6$. For these parameters

$$\frac{(2KS - B_x)^2}{(2KS + B_x)^2} = 16 \gg 1, \tag{4.7}$$

We can conclude that the plots we made coincide with the regime we are working with to find the lowest energy levels. Later we give an accurate regime where we only have to take into account the instanton which corresponds to tunneling through the green barrier and where we can ignore the instanton which corresponds to tunneling through the blue barrier.

4.3 The circular-spin model action

The action for the circular-spin model is given by

$$\mathcal{S}[\theta] = \int dt \mathcal{L}(\theta) = \int dt \left(T(\theta) - V(\theta)\right). \tag{4.8}$$

Here T is the kinetic energy, given by $T(\theta) = -\frac{I}{2}S^2\dot{\theta}^2$. We choose for our model to have this kinetic energy as it coincides with the kinetic energy in the spherical-spin model on the regime of the circular-spin model. Why the kinetic energies coincide for $T(\theta) = -\frac{I}{2}S^2\dot{\theta}^2$ will become clear in a moment. In total we find that the action is given by

$$\mathcal{S}[\theta] = \int dt \Big(KS^2 \cos^2\theta - B_x S \sin\theta - \frac{B_x^2}{4K} - KS^2 - \frac{I}{2}S^2\dot{\theta}^2 \Big). \tag{4.9}$$

Varying the action with respect to θ gives us the equation of motion

$$B_x \cos\theta + 2KS \sin\theta \cos\theta + IS\ddot{\theta} = 0. \tag{4.10}$$

In action and the equations of motion above we see why the spin inertia is the spin equivalent of mass. In the action and the equations of motion the spin inertia has exactly the same role as the mass for a particle in a potential.

For the circular-spin model we use the saddle-point approximation (see appendix J), to calculate the path integral. Before we can use the saddle-point approximation we have to write the action in equation (4.9) in Wick-rotated time

$$\mathcal{S}[\theta] = \int d\tau \Big(KS^2 \cos^2\theta - B_x S \sin\theta - \frac{B_x^2}{4K} - KS^2 + \frac{I}{2}S^2\dot{\theta}^2 \Big). \tag{4.11}$$

From this action we can see why we have the kinetic energy as above. This is because now we find the action for the spherical-spin model (see equation (3.23)), but now for a constant angle ϕ. Taking ϕ constant has the consequence that the Berry phase disappears. The minus sign in front of $\frac{I}{2}S^2\dot{\theta}^2$ is different than in equation (3.23). This is because of integration by parts.

For the next steps, we write the action as follows

$$\mathcal{S}[\theta] = S\, f[\theta], \tag{4.12}$$

where $f[\theta]$ is a smooth functional. We are looking at the action in Wick-rotated time, as the path integral in real-time is an integral over the action multiplied with i. If we work in Wick-rotated time, we can use the saddle-point approximation, as now the integral is of the right form. For the circular-spin model, where the action is only dependent on one variable, the saddle-point approximation is given by

$$\begin{aligned}
&\int_{q_i}^{q_f} D\theta \exp(-S\, f[\theta(\tau)]) \\
&\approx \sum_{\text{minima}} \int_{q_i}^{q_f} D\theta \exp\Big(-S\Big(f[\theta_0(\tau)] + \int d\tau \int d\tau' \frac{1}{2}\Delta\theta(\tau)\frac{\delta^2 f[\theta_0(\tau)]}{\delta\theta(\tau)\delta\theta(\tau')}\Delta\theta(\tau')\Big)\Big) &(4.13)\\
&= \sum_{\text{minima}} \exp\big(-S f[\theta_0(\tau)]\big) I_{qf}, &(4.14)
\end{aligned}$$

where I_{qf} are the quantum fluctuations. First we have to find the trajectories between the classical potential extrema via the equations of motion, the so-called quasi-classical trajectories. We start by looking at a single path from one minimum to the other.

4.4 The quasi-classical trajectories

We continue by finding the quasi-classical trajectories of the spin. The sum over all quasi-classical trajectories is given by

$$\sum_{\text{minima}} \exp\big(-S f[\theta_0(\tau)]\big) = C \sum_n \int_0^{\tau} d\tau_1 \ldots \int_0^{\tau_{n-1}} d\tau_n \left(I_{\text{sins}}\right)^n, \tag{4.15}$$

where I_{sins} is the integral over a single spin-instanton going from one extremum to the other, which is called a single instanton trajectory. Further, the prefactor C contains all prefactor for the individual paths. Equation (4.15) is correct if there is only one kind of single spin-instanton trajectory we have to take into account. This is when we can ignore tunneling through the blue barrier in figure 10.

In equation (4.15) we made the assumption that the instantons do not overlap in time. This is a good assumption if the spin has non-zero inertia, because when the inertia is non-zero, the spin is most of its (Wick-rotated) time in one of the potential minima. Only rarely the spin changes direction and therefore we can assume that the instantons do not overlap in time. However, when the spin has no inertia, it does not take energy for the spin to change from potential minimum. The assumption above does not hold for a spin with

no inertia. We can only do the derivation of the quasi-classical trajectories of the spin if we look at a spin with inertia.

Next, we use that in equation (4.15) all single instanton trajectories can be time ordered. Therefore, the sum over all quasi-classical trajectories is given by

$$\sum_{\text{minima}} \exp\big(-Sf[\theta_0(\tau)]\big) = C\sum_n \frac{1}{n!}\left(\tau I_{\text{sins}}\right)^n. \tag{4.16}$$

To continue simplifying the expression of the sum of the quasi-classical trajectories, we have to focus on the single instanton trajectory.

4.5 The single instanton trajectory

To calculate the classical-instanton trajectories, we flip the potential with a Wick rotation $t \to -i\tau$ around the horizontal axis. This flip is exactly the same as we did for a particle in the double-well potential (see figure 11). In both cases the action is of the form

$$\mathcal{S}[x] = \exp\left(-\int_0^t dt'(V(x) - \frac{C}{2}\dot{x}^2)\right). \tag{4.17}$$

Therefore, the Wick rotation has the same effect on the spin potential as it had on the double-well potential, namely it flips it around the horizontal axis. Now there exists a quasi-classical solution to go via the red trajectory in figure 11 from $\theta = b$ to $\theta = \pi - b$. This solution is the single spin-instanton for the circular-spin model.

The single spin-instanton trajectory is given by the following

$$I_{\text{sins}} \propto \exp(-\mathcal{S}_{\text{sins}}), \tag{4.18}$$

where $\mathcal{S}_{\text{sins}}$ is the single spin-instanton action, which we find after doing a Wick rotation. The single spin-instanton action in Wick-rotated time is given by

$$\mathcal{S}_{\text{sins}}[\theta_{cl}] = \int_0^\tau d\tau'\Big(KS^2\cos^2\theta_{cl} - B_xS\sin\theta_{cl} - \frac{B_x^2}{4K} - KS^2 + \frac{I}{2}S^2\dot{\theta}_{cl}^2\Big). \tag{4.19}$$

Here θ_{cl} is the quasi-classical path.

We can calculate the single instanton trajectory by using conservation of energy. In appendix B we see that the conservation law for total energy $E = V + T$ in Wick-rotated time is given by

$$\frac{d}{d\tau}E = \frac{d}{d\tau}\Big(-KS^2\cos^2\theta_{cl} + B_xS\sin\theta_{cl} + \frac{B_x^2}{4K} + KS^2 - \frac{I}{2}S^2\dot{\theta}_{cl}^2\Big) = 0. \tag{4.20}$$

The minus sign in front of the inertia term comes from the fact that we work in Wick-rotated time. Energy conservation has the consequence that on the path of the instanton, the energy is always the same. We know the total energy E when the spin is in a classical minimum and without motion as this is the same as the potential at $\theta = b$ and $\theta = \pi - b$.

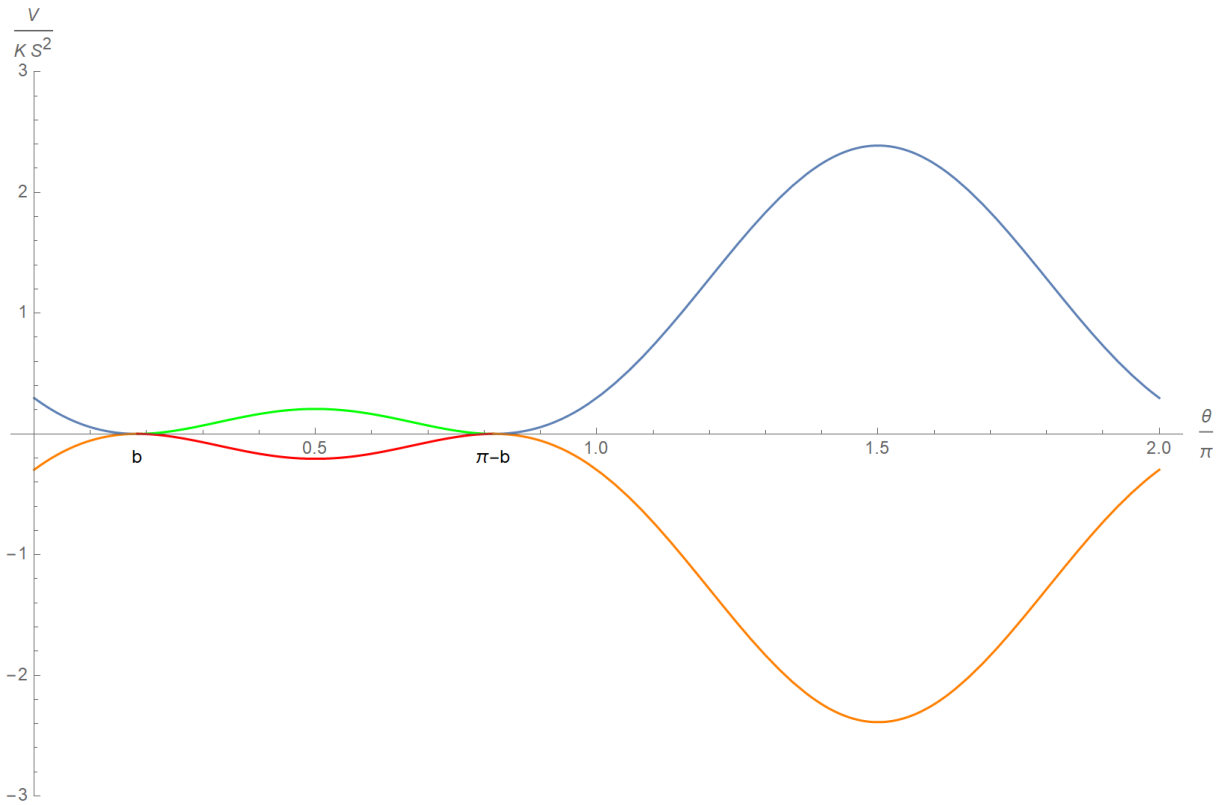

Figure 11: *This is the same plot as in figure 10, but now with the potential after a Wick rotation. A single spin-instanton is exactly a particle going from* $\theta = b$ *to* $\theta = \pi - b$ *over the red trajectory or over the orange trajectory. The parameters are as usual* $\frac{B_x}{K} = -6$ *and* $S = 5.5$.

Therefore, the total energy is zero. This means that we have the following conserved quantity

$$-KS^2\cos^2\theta_{cl} + B_x S\sin\theta_{cl} + \frac{B_x^2}{4K} + KS^2 - \frac{I}{2}S^2\dot{\theta}_{cl}^2 = 0. \tag{4.21}$$

After combining equation (4.21) with equation (4.19), we find that the single spin-instanton action can now be written by the following expression

$$\mathcal{S}_{\text{sins}}[\theta_{cl}] = \int_0^\tau d\tau' I S^2\dot{\theta}_{cl}^2. \tag{4.22}$$

We can simplify this, because the total energy is time-independent and because we can integrate over the angle θ_{cl} instead of time. The single instanton trajectory over the red trajectory in figure 11 the action is given by

$$\mathcal{S}_{\text{sins}}[\theta_{cl}] = \int_b^{\pi-b} d\theta_{cl} I S^2\dot{\theta}_{cl}. \tag{4.23}$$

Now we rewrite equation (4.21) to find an expression for $\dot{\theta}_{cl}$

$$\dot{\theta}_{cl} = \sqrt{\frac{2}{IS^2}\left(-KS^2\cos^2\theta_{cl} + B_x S\sin\theta_{cl} + \frac{B_x^2}{4K} + KS^2\right)}. \tag{4.24}$$

Further, we can integrate over θ instead of θ_{cl}, as the angle became a dummy variable. Now the action of a single instanton is given by

$$\mathcal{S}_{\text{sins}}[\theta] = \sqrt{2IS^2}\int_b^{\pi-b} d\theta\sqrt{-KS^2\cos^2\theta + B_x S\sin + \frac{B_x^2}{4K} + KS^2}. \tag{4.25}$$

We recognize the potential in this equation

$$\mathcal{S}_{\text{sins}}[\theta] = \sqrt{2IS^2}\int_b^{\pi-b} d\theta\sqrt{V(\theta)}. \tag{4.26}$$

Here we note that this integral is well-defined as the potential in real-time is always positive.

Taking the integral over θ gives us the following result

$$\mathcal{S}_{\text{sins}} = \sqrt{2IKS^4}\left(\sqrt{4-\left(\frac{B_x}{KS}\right)^2} - \frac{\pi}{2}\frac{B_x}{KS} + \frac{B_x}{KS}\arcsin\left(\frac{B_x}{2KS}\right)\right). \tag{4.27}$$

In this equation we wrote the expression in terms of $\frac{B_x}{KS}$. This makes it possible to plot the action as a function of $\frac{B_x}{KS}$ (see figure 12). Now we have an expression for the single instanton trajectory by combining equations (4.18) and (4.27). We find that

$$I_{\text{sins}} \propto \exp\left(-\sqrt{2IKS^4}\left(\sqrt{4-\left(\frac{B_x}{KS}\right)^2} - \frac{\pi}{2}\frac{B_x}{KS} + \frac{B_x}{KS}\arcsin\left(\frac{B_x}{2KS}\right)\right)\right). \tag{4.28}$$

4.6 Excluding instanton trajectories

To use the expression in equation (4.15), we have to exclude instanton trajectories over the orange trajectory in figure 11. We found a way to calculate the instanton trajectories. Now we can find in what regime the instanton trajectory over the red trajectory is way larger than the instanton trajectory over the orange trajectory. We remind you that the single spin-instanton trajectory (equation (4.18)) is given by

$$I_{\text{sins}} \propto \exp(-\mathcal{S}_{\text{sins}}). \tag{4.29}$$

We find the wanted regime by looking at

$$\frac{I_{\text{orange}}}{I_{\text{sins}}} \ll 1. \tag{4.30}$$

Here I_{orange} is the single spin-instanton trajectory over the orange trajectory. This is given by

$$\mathcal{S}_{\text{orange}}[\theta] = \sqrt{2IS^2}\int_{\pi-b}^{2\pi+b} d\theta\sqrt{V(\theta)} \tag{4.31}$$

$$= \sqrt{2IKS^4}\left(\sqrt{4-\left(\frac{B_x}{KS}\right)^2} + \frac{\pi}{2}\frac{B_x}{KS} + \frac{B_x}{KS}\arcsin\left(\frac{B_x}{2KS}\right)\right). \tag{4.32}$$

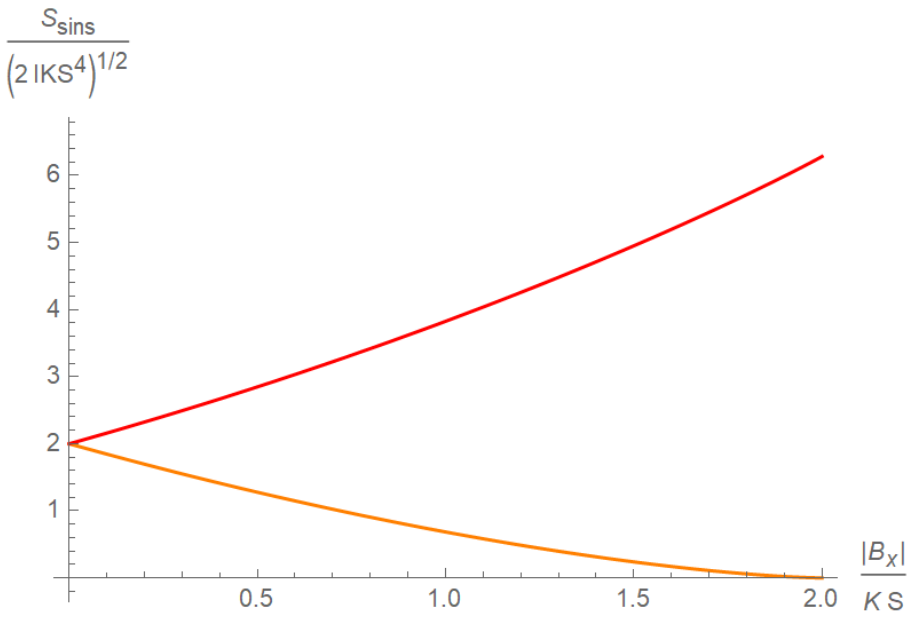

Figure 12: *The actions of a single instanton. In red we see the single spin-instanton action of the red trajectory in figure 11 and in orange we see the single spin-instanton action of the orange trajectory.*

Here we note that this is just a minus sign different from equation (4.27). Now we can find the single spin-instanton trajectory over the orange trajectory by

$$I_{\text{orange}} \propto \exp(-\mathcal{S}_{\text{orange}}). \tag{4.33}$$

In figure 13 we see that the single spin-instanton trajectory over the orange trajectory can be neglected for $\frac{B_x}{KS} > 0.5$ as here it is significantly smaller than the single spin-instanton trajectory over the red trajectory.

4.7 The regime of the magnetic field

Our derivation of the ground-state energies for the spin using instanton calculus uses many approximations. These approximations only work in certain regimes. We find in figure 13 that the magnetic field should be big enough compared with KS in order to only include one single instanton trajectory. We also see in figure 8 that $\frac{B_x}{KS}$ should be small enough in order to have the energies of the two lowest energy levels of nearly the same size. These regimes exclude a big part of the spectrum of magnetic fields for which we can do predictions on the ground-state energies. Fortunately, for $B_x \approx KS$, both approximations can be made and therefore there is a regime in which our model can be tested experimentally.

4.8 Quantum fluctuations

Now we look at the quantum fluctuations. As discussed before, we only have to consider the quantum fluctuations in the classical minima. Also, the fluctuations are the same in

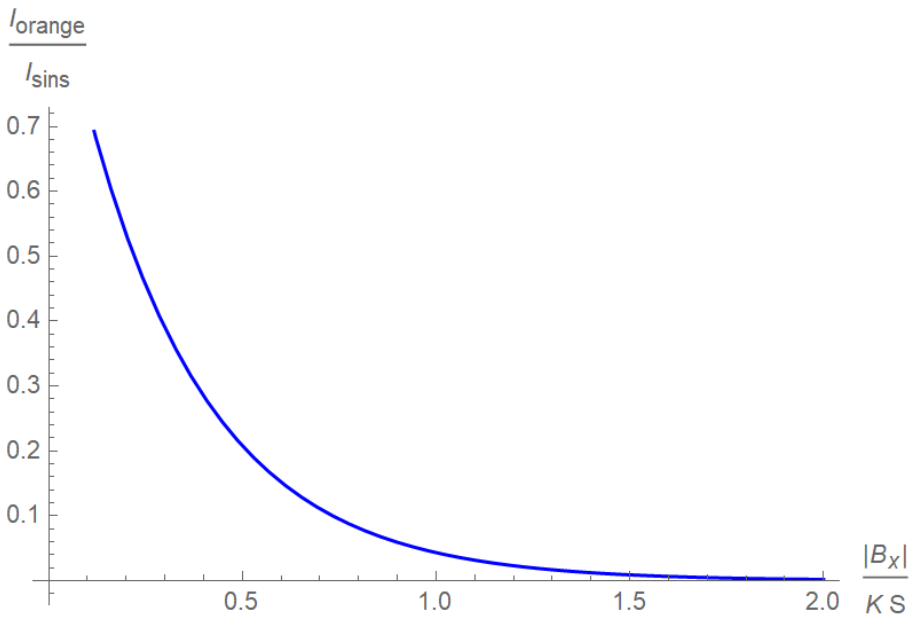

Figure 13: *Here the fraction of single spin-instanton trajectories via the red and orange trajectorys in figure 11 is plotted against the magnetic field over the anisotropy parameter multiplied by the total spin.*

both minima. The fluctuations I_{qf} in a minimum are given by the following expression

$$I_{qf} = \int_{\theta_i}^{\theta_f} D\Delta\theta \exp\Big(-\int d\tau \int d\tau' \frac{1}{2}\Delta\theta(\tau)\left[\frac{\delta^2\mathcal{S}[\theta]}{\delta\theta(\tau)\delta\theta(\tau')}\right]_{\theta=b}\Delta\theta(\tau')\Big). \tag{4.34}$$

Here we used the action from equation (4.11). This we can solve by taking the functional derivatives of the action to $\theta(\tau)$ and $\theta(\tau')$

$$\frac{\delta^2\mathcal{S}[\theta]}{\delta\theta(\tau)\delta\theta(\tau')} = \delta(\tau-\tau')\Big(B_x S\sin\theta(\tau) + 2KS^2\left(\sin^2\theta(\tau) - \cos^2\theta(\tau)\right)\Big) + IS^2\frac{\partial^2}{\partial\tau'^2}\delta(\tau-\tau'). \tag{4.35}$$

Combining this with equation (4.34) leads to

$$I_{qf} = \int_{\theta_i}^{\theta_f} D\Delta\theta \exp\Big(-\frac{1}{2}\int d\tau \Delta\theta(\tau)\left[M(\tau)\right]_{\theta=b}\Delta\theta(\tau)\Big), \tag{4.36}$$

where $M(\tau)$ is an operator, given by

$$M(\tau) = B_x S\sin\theta(\tau) + 2KS^2\left(\sin^2\theta(\tau) - \cos^2\theta(\tau)\right) + IS^2\frac{\partial^2}{\partial\tau'^2}. \tag{4.37}$$

We look at the quantum fluctuations when the spin is in a minimum, so $\theta = b$ or $\theta = \pi - b$. Due to symmetry, the quantum fluctuations of both minima give the same contribution to the path integral. We therefore only calculate the quantum fluctuations for $\theta = b$. This leads to

$$\left[M(\tau)\right]_{\theta=b} = -2KS^2 - \frac{B_x^2}{2K} + IS^2\frac{\partial^2}{\partial\tau^2}. \tag{4.38}$$

We can write the integral of the quantum fluctuations as follows

$$I_{qf} = \int_{\theta_i}^{\theta_f} D\Delta\theta \exp\Big(-\frac{1}{2}\int_0^{\tau'} d\tau \Delta\theta(\tau)\left(-2KS^2 - \frac{B_x^2}{2K} + IS^2\frac{\partial^2}{\partial\tau^2}\right)\Delta\theta(\tau)\Big). \tag{4.39}$$

Here τ' is the time we integrate over to find the quantum fluctuations. In our case this is the Wick-rotated time between two instanton trajectories. The next step is Wick rotating back to real-time

$$I_{qf} = \int_{\theta_i}^{\theta_f} D\Delta\theta \exp\Big(-\frac{i}{2}\int_0^{t'} dt \Delta\theta(t)\left(-2KS^2 - \frac{B_x^2}{2K} - IS^2\frac{\partial^2}{\partial t^2}\right)\Delta\theta(t)\Big). \tag{4.40}$$

Now the integral is exactly of the same form as the quantum fluctuations of the harmonic oscillator. We solved the path integral of the harmonic oscillator in appendix C. As we are working now with quantum fluctuations which are only around the potential minima of the circular-spin model, we can follow exactly the same steps as we did for the harmonic oscillator.

After taking the Gaussian integral over $\Delta\theta$, we find that the quantum fluctuations are given by

$$I_{qf} = A\det\left(KS^2 + \frac{B_x^2}{4K} + \frac{I}{2}S^2\partial_t^2\right)^{-\frac{1}{2}}. \tag{4.41}$$

Here A is a prefactor. We can solve this determinant by looking at a basis of eigenstates of the operator $KS^2 + \frac{B_x^2}{4K} + \frac{I}{2}S^2\partial_t^2$. We use the assumption that at the initial and final time, the spin is at an extremum, so there is no fluctuation. This means that the boundary conditions are $\Delta\theta(t=0) = 0$ and $\Delta\theta(t=t') = 0$. Now the basis of eigenstates is given by $\theta_n(t) = \sin\left(n\pi\frac{t}{t'}\right)$ with eigenenergies $\epsilon_n = KS^2 + \frac{B_x^2}{4K} + \frac{I}{2}S^2\left(\frac{n\pi}{t'}\right)^2$. With this we find that the determinant is as follows

$$I_{qf} = A\det\left(KS^2 + \frac{B_x^2}{4K} + \frac{I}{2}S^2\partial_t^2\right)^{-\frac{1}{2}} = A\prod_{n=1}^{\infty}(\epsilon_n)^{-\frac{1}{2}}. \tag{4.42}$$

This infinite product diverges and we can therefore not find a reasonable result for the quantum fluctuations. However, we can find the quantum fluctuations of a spin in the easy-axis model, which is not influenced by inertia.

The ground-state energies for the easy-axis Hamiltonian are independent of the instanton trajectories. Therefore the ground-state energies are fully determined by the quantum fluctuations. The quantum fluctuations are now given by the exponential of the spin being in the ground state for a time τ

$$I_{ea,qf} = e^{\tau E_0} = e^{-\tau KS^2}, \tag{4.43}$$

where $E_0 = -KS^2$ is the minimal energy of the easy-axis model.

The easy-axis potential and the potential with a magnetic field are locally in their minima nearly identical. The quantum fluctuations are small and local too. We make the educated guess that the quantum fluctuations for the ground states of the easy-axis

Hamiltonian are nearly the same as the quantum fluctuations for the ground-state energies of the system we are looking at. We can therefore neglect the dependence on the magnetic field in the quantum fluctuations. The ground states of the easy-axis Hamiltonian are independent of inertia. However, inertia probably changes the ground-state energy of a spin in a bath of harmonic oscillators but without a magnetic field, even for a spin in an easy-axis potential. This would be a spin described with the Hamiltonian in equation 3.10, but with $B_x = 0$. In this thesis we do not show the change of the ground state of the easy-axis Hamiltonian by the inertia. We assume that this change is small compared with the energy gap. We use the approximation that the quantum fluctuations are given by

$$I_{qf} = e^{\tau E_0} = e^{-\tau K S^2}. \tag{4.44}$$

With this result, we now know that the ground-state energy for the circular-spin model is given by $E_0 = -KS^2 - \frac{1}{2}\Delta\epsilon$ and the first excited state energy is given by $E_1 = -KS^2 + \frac{1}{2}\Delta\epsilon$.

4.9 The energy gap

To find the energy gap, we are going to use equation (3.7)

$$\lim_{\tau\to\infty} \sum_{n\epsilon\{S,A\}} \langle\psi_f|n\rangle\, e^{-E_n\tau}\, \langle n|\psi_i\rangle \propto \lim_{\tau\to\infty} \int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}[g]). \tag{4.45}$$

To find the left-hand side of equation (3.7) we do the same steps as for the double-well potential to relate the eigenenergies with the action (see appendix D). First we look at the spin starting and ending in a potential minimum, $|\psi_i\rangle = |\psi_f\rangle = |l\rangle$. We could also have chosen the starting and ending state to be $|r\rangle$. This leads to the same result due to parity symmetry. The states $|l\rangle$ and $|r\rangle$ are defined by a spin being in a local ground state of a potential minimum. We also used this states for the spherical-spin model. Now these are local ground states of the potential minima of the circular-spin potential (equation (4.3)). For the following steps, we do not write the limit of $\tau \to \infty$ for convenience in writing. We will include the limit later again. With the choices above we find that

$$\begin{aligned} \langle l|S\rangle\, e^{-E_S\tau}\, \langle S|l\rangle + \langle l|A\rangle\, e^{-E_A\tau}\, \langle A|l\rangle &= e^{-(KS^2 - \frac{\Delta\epsilon}{2})\tau} + e^{-(KS^2 + \frac{\Delta\epsilon}{2})\tau} \\ &= e^{-KS^2\tau} \cosh(\Delta\epsilon\tau). \end{aligned} \tag{4.46}$$

The steps in equation (4.46) are straightforward, so we let this as an exercise for the reader to check.

Next, we look at the right-hand side of equation (4.45). With equation (4.13) and equation (4.16) we can write the right-hand side without the limit as follows

$$\int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}[g]) = I_{qf} \sum_n \frac{1}{n!} \left(\tau I_{\text{sins}}\right)^n. \tag{4.47}$$

For the spin starting and ending in the same state, n is even. We then find that

$$\int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}[g]) \propto e^{-KS^2\tau} \sum_{n\, even} \frac{1}{n!} \left(\tau I_{\text{sins}}\right)^n = e^{-KS^2\tau} \cosh\left(\tau I_{\text{sins}}\right). \tag{4.48}$$

Next, we combine the right and left-hand sides of equation (4.45) using equations (4.48) and (4.46). This leads to

$$\lim_{\tau\to\infty} e^{-KS^2\tau}\cosh(\Delta\epsilon\tau) \propto \lim_{\tau\to\infty} e^{-KS^2\tau}\cosh\left(\tau I_{\text{sins}}\right). \tag{4.49}$$

As equation (4.49) holds for all large time τ, we can read off that the energy gap is given by

$$\Delta\epsilon = I_{\text{sins}} \propto \exp\left(-\sqrt{2IKS^4}\left(\sqrt{4-\left(\frac{B_x}{KS}\right)^2}+\frac{\pi}{2}\frac{B_x}{KS}+\frac{B_x}{KS}\arcsin\left(\frac{B_x}{2KS}\right)\right)\right). \tag{4.50}$$

We find that the spin-instanton action is proportional to the square root of the spin inertia, $\sqrt{I}$. However, we found in chapter 2 that the action for a particle in a double-well potential is proportional to the mass, m. The square root over the spin inertia comes from the fact that the circular-spin potential (4.3) has no spin inertia dependence The double-well potential (2.1), however, is dependent on the mass.

We expected the energy gap to be zero when there is no magnetic field. However, if we fill in $B_x = 0$ in equation (4.50), we find a non-zero term for $\Delta\epsilon$. It seems that our result is wrong. However, in the derivation we said that we could only exclude other instanton paths than the minimum path if B_x is not too small (see section 4.6). Therefore, the expression in equation (4.50) is not valid for a small magnetic field. We can only give a result of the energy gap for a magnetic field if $\frac{|B_x|}{K} \approx S$.

In figure 8 we said that the energy gap between the ground state and the first excited state becomes smaller if the spin is interacting with a bath. This is the case because when there the spin is interacting with a bath, the inertia becomes larger. In equation (4.50) we find that the energy gap becomes smaller when we add a non-zero spin inertia or when the spin inertia becomes larger.

5 Back to the spherical-spin model

We found the ground-state energies for the circular-spin model, but we want to find the same for the spherical-spin model. In this chapter we are not going to do the derivation in detail, but we make some educated guesses. We therefore only give the result we expect and do not claim that we found the right result. We use the results we found for the circular-spin model to substantiate our predictions. We leave it as a task for further research to check the educated guesses we make.

5.1 Single spin-instantons

The solutions of the equations of motion are the main contributions of the path integral. To find the main contributions of the path integral, we therefore look at the paths when $\frac{\delta \mathcal{S}[g(\tau)]}{\delta g(\tau)} = 0$. We remind the reader that the potential minima of the spherical-spin model are the same as the potential minima of the circular-spin model. The two potential minima in spherical coordinates are $\phi = \pi$ and $\theta \in \{b, \pi - b\}$, where b is defined as $b := \arcsin(\frac{-B_x}{2KS})$. The green path in the circular-spin model (10) is plotted in figure 14.

There are more solutions to the equations of motion for the spherical-spin model. Many of these solutions are single instanton trajectories of the spherical spin model and therefore contribute to the energy gap between the lowest state energies. We label these single instanton trajectories with an index i. Any trajectory can be determined by a quasi-classical path in spherical coordinates. We call the coordinates of the i^{th} instanton trajectory $\theta_{cl,i}$ and $\phi_{cl,i}$.

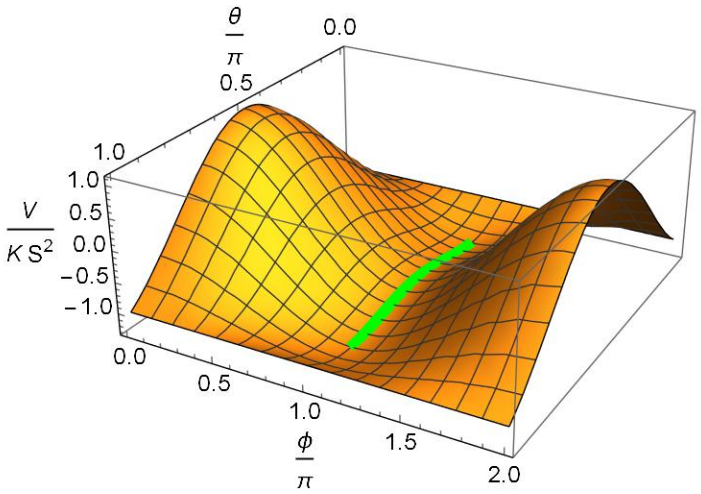

Figure 14: *The potential of the spin model in spherical coordinates, corresponding to equation (3.30). This is the same plot as figure 9, but now with the minimal path of the spherical spin model plotted in green. The parameters are again* $\frac{B_x}{K} = -6$ *and* $S = 5.5$.

Finding the instanton trajectories out of these equations of motion is hard, as we have a path with two degrees of freedom, but only one conserved quantity. This means that there are infinitely many instanton trajectories. The conserved quantity in this system is

the total energy. In general, a system can be analytically solved if there are at least as many conserved quantities as free parameters. Therefore we are not going to find the exact instanton trajectories for all paths.

In the circular-spin model, we only had to consider one trajectory between the potential minima. The other path we could neglect as its contribution was small compared with the minimal path in a certain limit. The spherical-spin model, in contrary to the circular-spin model, has infinitely many quasi-classical paths to go from one minimum to the other. Some paths are just slightly less likely to happen than others as the spin potential (3.2) is smooth. Therefore, these paths have nearly the same contribution to the path integral as the minimal path. We can therefore not exclude all paths but one, as we did for the circular-spin model. It is also hard to find the minimal path between the potential minima. What we can do, is making an educated guess about the instanton trajectories.

We expect that for a single path with index i from one potential minimum to the other the action is given by

$$\mathcal{S}_{\text{sins},i}[\theta_{cl,i},\phi_{cl,i}] = \sqrt{2IS^2}\int_b^{\pi-b} d\theta_{cl,i}\int_0^0 d\phi_{cl,i}\sqrt{V(\theta_{cl,i},\phi_{cl,i})}, \tag{5.1}$$

where we use that any solution to the equation of motion, is fully determined by the coordinates. The equation above is an educated guess as we have not derived this equation. We expect this result, because one can parameterize the trajectories between the minima. The same has been done for the circular-spin model, but there the parametrization was trivial. After the parametrization, one can use energy conservation to get rid of time derivatives. What we are left with is an integral over the square root of the potential and $\sqrt{2IS^2}$ in front of the integral, because of the substitution of the kinetic term. With this substitution we can find with the energy conservation as is done in equation (4.24). We see the parametrization of the instanton trajectories as a good starting point for further research.

5.2 A predicted energy gap

With the actions in equation (5.1) we can find the single instanton trajectories

$$I_{\text{sins},i} \propto \exp(-\mathcal{S}_{\text{sins},i}). \tag{5.2}$$

In our educated guess, the dependence on inertia I is the same for all different single instanton paths. They only differ in the integral over angles θ and ϕ. To find the main contributions of the path integral for the spherical-spin model, we have to include not only the sum over instanton trajectories which are the same, as we did for the circular-spin model, but we should include all trajectories where the spin switches from one minimum to the other first via one path, and then via other paths too (see equation (5.3)). We find that the sum over all full instanton trajectories is given by

$$I_{\text{full}} \propto \sum_{\text{minima}} \exp\left(-Sf[\theta_0(\tau),\phi_0(\tau)]\right) = \sum_n \sum_i \int_0^{\tau} d\tau_1 ... \int_0^{\tau_{n-1}} d\tau_n \left(I_{\text{sins},i}\right)^n. \tag{5.3}$$

The fact that we have different single instanton trajectories makes the derivation of the full instanton trajectory a lot more complicated.

However, we made the educated guess that the dependence on inertia I is the same for all different single instanton paths, so we can take that term out of the summations. We therefore expect that the energy gap between the ground-state energy and the first excited state energy of the spherical-spin model has the same dependence on inertia as the circular-spin model, namely

$$\Delta\epsilon \propto \exp\left(-\sqrt{I}\kappa\right), \tag{5.4}$$

where κ is a parameter that is independent of inertia.

Before we can claim the relation in equation (5.4), we need to argue why the quantum fluctuations do not influence the energy gap. For this we can use the same argument as in the circular-spin model and the particle in the double-well potential. We assume that the spin is most of the time in one of the extrema. Only here the quantum fluctuations are of significant role as, when the spin is on a trajectory from one minimum to the other, the quantum fluctuations are negligible. The quantum fluctuations can therefore be approximated by a spin in a local potential minimum. This does not influence the energy gap, it only determines the reference energy E_{ref}.

We could use the educated guess that the dependence on inertia I is the same for all different single instanton paths would be correct for the circular spin model too. This would have the consequence that for the circular-spin model, we can include not only the red trajectory in figure 11, but also the orange trajectory. If we could include the orange trajectory for finding the energy gap, the theory would be valid for a larger regime of the magnetic field B_x.

6 Conclusion and outlook

The goal of this thesis is to find when and how the ground-state energies of a spin are dependent on the spin inertia. We argued that inertia changes the energy gap between the ground-state energy and the first excited state energy if the lowest energy levels are a superposition of multiple potential minima. This is because a spin is influenced by the spin inertia when it has to cross a barrier. We therefore looked at the spherical-spin model and the circular-spin model.

For the circular-spin model, with a magnetic field which obeys $Bx \approx KS$, we found that the lowest eigenenergies are given by

$$E_0 = -KS^2 - \frac{1}{2}\Delta\epsilon, \tag{6.1}$$

and

$$E_1 = -KS^2 + \frac{1}{2}\Delta\epsilon, \tag{6.2}$$

where the energy gap is given by

$$\Delta\epsilon \propto \exp\left(-\sqrt{2IKS^4}\left(\sqrt{4-\left(\frac{B_x}{KS}\right)^2} + \frac{\pi}{2}\frac{B_x}{KS} + \frac{B_x}{KS}\arcsin\left(\frac{B_x}{2KS}\right)\right)\right). \tag{6.3}$$

This is an interesting result as it relates the lowest energies with the spin inertia.

As we said before, the spin inertia is the spin equivalent of mass. We find it therefore interesting that the energy gap for a particle in a double-well potential is given by

$$\Delta\epsilon \propto \exp\left(-\frac{2}{3}m\omega_0 a^2\right). \tag{6.4}$$

Remarkably, there is no square root for the mass in this equation. To explain this difference in energy gap for the spin and the particle in the double-well potential we have to look at the procedure with which we found the energy gap.

We found that the energy gap is proportional to a single instanton trajectory. Such a single instanton trajectory for the circular-spin model is given by (4.26)

$$I_{\text{sins}} \propto \exp\left(-\sqrt{2IS^2}\int_b^{\pi-b} d\theta\,\sqrt{V(\theta)}\right), \tag{6.5}$$

and for the particle in the double-well potential, the single instanton trajectory is given by (2.9)

$$I_{\text{inst}} \propto \exp\left(-\sqrt{2m}\int_{-a}^{a} dq\sqrt{V(q)}\right). \tag{6.6}$$

The reason that there is no square root in equation (6.4) comes from the fact that the double-well potential is itself dependent on the mass. If the potential would be independent of the mass, the relation between the energy gap and the mass for a particle in a double-well potential would be the same as the relation between the energy gap and the spin inertia for a circular-spin model.

The energy gap in equation (6.3) is maximal when there is no spin inertia. The larger the spin inertia gets, the smaller the energy gap becomes. This is what we expected, because for a large spin inertia, it is more difficult for a spin to switch from one potential minimum to the other. This is not intuitive for a spin, but by considering spin inertia as the spin equivalent of mass, this makes sense as for a particle with a mass it is more difficult to go from one potential minimum to another if the mass becomes larger. This is because the higher the mass the less likely a particle is to tunnel. If the spin inertia is infinitely large, it costs infinitely much energy to go from one potential minimum to the other. In this limit, the regions around the two potential minima are seen as completely independent and then the model has two degenerate ground states.

We made an educated guess for the energy gap between the ground-state energy and the first excited state energy

$$\Delta\epsilon \propto \exp\left(-\sqrt{I}\kappa\right). \tag{6.7}$$

As we have not proven the result of the energy gap for the spherical-spin model, this would be interesting for further research.

Until now, we focused on the spin inertia dependence on the instanton trajectories and not on the quantum fluctuations. However, it is still an open question how the quantum fluctuations depend on spin inertia too. We expect that even without a magnetic field, the energy levels would depend on spin inertia. Looking at the dependence on spin inertia of the quantum fluctuations is something which should be worked out in further research.

We found a result that could be tested experimentally, namely, the dependence of the energy gap between the ground-state energy and the first excited state energy (see equations (6.3)). The energy gap could be found experimentally for different baths, which leads to different values in spin inertia. Further, the magnetic field can be varied easily, so this could be checked experimentally too. An experimental check whether the outcome of the thesis is correct, would be valuable.

In this thesis, we looked at a system without Gilbert damping. In future research, Gilbert damping should be taken into account.

In earlier research, the tunneling rate has been calculated with instantons for potentials, where the potential minima are not the same [7, 22]. For a follow-up of this thesis, it would be interesting to look at the influence of tunneling on the lowest energy levels of a particle in a potential with unequal potential minima. In relation with this thesis, it is especially interested to look at spin systems with this phenomenon.

A From the probability amplitude to a path integral

In this appendix we derive equation (2.3), which relates the path integral with the probability amplitude between q_i and q_f and with the eigenenergies of a Hamiltonian. Equation (2.3) is given by

$$\sum_n \langle q_f|n\rangle\, e^{-E_n\tau}\, \langle n|q_i\rangle = \langle q_f|e^{-\hat{H}\tau}|q_i\rangle \propto \int_{q_i}^{q_f} Dq \exp(-\mathcal{S}[q]). \tag{A.1}$$

We start with the left-hand side. All the eigenstates of the Hamiltonian, $|n\rangle$, form a basis of states. Further, the equation for eigenstates is $\hat{H}\,|n\rangle = E_n\,|n\rangle$. We use the following identities

$$\sum_n |n\rangle\,\langle n| = 1 \tag{A.2}$$

and

$$\langle n|n'\rangle = \delta(n-n'). \tag{A.3}$$

If we sum over all eigenstates of the Hamiltonian we find that

$$\begin{aligned}
\langle q_f|e^{-\hat{H}\tau}|q_i\rangle &= \sum_{n,n'} \langle q_f|n'\rangle\,\langle n'|e^{-\hat{H}\tau}|n\rangle\,\langle n|q_i\rangle && \text{(A.4)}\\
&= \sum_{n,n'} \langle q_f|n'\rangle\,\langle n'|e^{-E_n\tau}|n\rangle\,\langle n|q_i\rangle && \text{(A.5)}\\
&= \sum_{n} \langle q_f|n\rangle\, e^{-E_n\tau}\,\langle n|q_i\rangle\,. && \text{(A.6)}
\end{aligned}$$

Next, we look at the right-hand side of equation (A.1). Again, we do not worry about the limit in the beginning. To find the path integral of the form in equation (A.1) we look first at the Hamiltonian.

For a single particle in a potential we have the following Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}). \tag{A.7}$$

Using the path integral we find

$$\langle q_f|e^{-\hat{H}\tau}|q_i\rangle = \int_{q_i}^{q_f} Dq \int Dp\; e^{\int_0^\tau d\tau'(-H+ip\dot{q})}. \tag{A.8}$$

In the notation of the path integral we have the advantage that there are no longer operators, but all operators are replaced by variables. We can now just fill in $H = \frac{p^2}{2m} + V(q)$ and get

$$\langle q_f|e^{-\hat{H}\tau}|q_i\rangle = \int_{q_i}^{q_f} Dq e^{-\int_0^\tau d\tau' V(q)} \int Dp\; e^{\int_0^\tau d\tau'(-\frac{p^2}{2m}+ip\dot{q})}. \tag{A.9}$$

The next step we take, is completing the square to write the integral such that it becomes Gaussian

$$-\frac{p^2}{2m} + ip\dot{q} = (\frac{ip}{\sqrt{2m}} + \sqrt{\frac{m}{2}}\dot{q})^2 - \frac{m}{2}\dot{q}^2. \tag{A.10}$$

Next, we substitute equation (A.10) in equation (A.9) and we get a Gaussian integral. We can solve this integral, but it gives a prefactor C, which is not interesting for this thesis. We end up with the following equation

$$\langle q_f|e^{-\hat{H}\tau}|q_i\rangle = C\int_{q_i}^{q_f} Dq e^{-\int_0^\tau d\tau'(V(q)+\frac{m}{2}\dot{q}^2)}. \tag{A.11}$$

The term in the exponent is exactly the instanton action. We can see this, because the action is related with the Lagrangian in the following way

$$\mathcal{S}[q] = \int_0^\tau d\tau' L(q,\dot{q}). \tag{A.12}$$

If we now make a Wick rotation back to real-time, we find that the Lagrangian for a particle in a potential is given by

$$L(q,\dot{q}) = -V(q) + \frac{m}{2}\dot{q}^2. \tag{A.13}$$

This is exactly the standard expression for a Lagrangian, and therefore we can conclude that the probability amplitude between q_i and q_f is related with the action in the following way

$$\langle q_f|e^{-\hat{H}\tau}|q_i\rangle = C\int_{q_i}^{q_f} Dq e^{-\mathcal{S}[q]}. \tag{A.14}$$

When we combine equations (A.4) and (A.14), we find the wanted equation (A.1).

We are not interested in the prefactor C. In this thesis the prefactor is not of importance, as only the dependence in the exponential leads to the energy gap between the ground-state energy and first excited state energy. The prefactor leads to the so-called reference energy, $E_{\text{ref}} = \frac{1}{2}(E_0 + E_1)$, however, there is another way to find this prefactor, so for now we ignore it and say only that the probability amplitude is proportional to the path integral.

B Energy conservation in Wick-rotated time

Noethers theorem states that energy conservation is a result of symmetry in time. For the instanton we are not working with real-time, but with Wick-rotated time. If a system is symmetric in time, it has a symmetry in Wick-rotated time too. In this appendix we are going to derive a conserved quantity corresponding to symmetry in Wick-rotated time.

First we look at the conservation of energy in real-time for a Lagrangian $\mathcal{L}[x]$ dependent on position x, with kinetic energy $T = \frac{m\dot{x}^2}{2}$ and potential energy $V = V(x)$

$$\mathcal{L}[x] = \frac{m\dot{x}^2}{2} - V(x). \tag{B.1}$$

The Euler-Lagrange equations are now given by

$$m\ddot{x} = -\partial_x V(x). \tag{B.2}$$

If we multiply both sides with $\dot{x}$, we find

$$m\dot{x}\ddot{x} = -\dot{x}\partial_x V(x) \tag{B.3}$$

$$= \frac{d}{dt}\left(\frac{m\dot{x}^2}{2}\right) = -\frac{d}{dt}V(x). \tag{B.4}$$

We then find the following conservation law

$$\frac{d}{dt}E = \frac{d}{dt}\left(\frac{m\dot{x}^2}{2} + V(x)\right) = 0, \tag{B.5}$$

where $E = T + V = \frac{m\dot{x}^2}{2} + V(x)$ is the conserved energy, which corresponds with Noethers theorem.

In Wick-rotated time we have a similar result. By rotating the time to imaginary time $t \to -i\tau$, we find that the Lagrangian is given by

$$\mathcal{L}[x] = -\frac{m\dot{x}^2}{2} - V(x). \tag{B.6}$$

With exactly the same derivation as for real-time we find that the conservation law in Wick-rotated time is given by

$$\frac{d}{dt}E = \frac{d}{dt}\left(-\frac{m\dot{x}^2}{2} + V(x)\right) = 0. \tag{B.7}$$

Now the conserved energy is given by $E = T + V = -\frac{m\dot{x}^2}{2} + V(x)$, where the kinetic energy is now given by $T = -\frac{m\dot{x}^2}{2}$. This means that we can still talk about conservation of energy in Wick-rotated time.

C The path integral for a harmonic oscillator

The quantum fluctuations of a particle in one of the potential minima of the double-well potential are nearly identical to the quantum fluctuations of a particle in a single well. This is because the potentials are locally nearly identical and because the energies involved with quantum fluctuations are a lot smaller than the energy it costs to go over the potential barrier in the double-well potential. As we can find the quantum fluctuations of a particle in the double-well potential to a good extend with the quantum fluctuations of a particle in a single well, we work out this result in this appendix. To calculate the path integral for a particle in a single well, we use that the single-well potential is of the same form as in section 2.6

$$V_{HO}(x) = \frac{m}{2}\omega_0^2 x^2. \tag{C.1}$$

A particle in the single-well potential above is called an harmonic oscillator.

The quantum fluctuations for a particle being at $x = 0$ after a time τ is given by

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = \int_{x_i}^{x_f} Dx \exp\left(-\int_0^\tau d\tau' (V_{HO}(x) + \frac{m}{2}\dot{x}^2)\right) \tag{C.2}$$

$$= \int_{x_i}^{x_f} Dx \exp\left(-\int_0^\tau d\tau'\, x\frac{m}{2}(\omega_0^2 - \partial_{\tau'}^2)x\right). \tag{C.3}$$

We know how to work with the harmonic oscillator in real-time. We therefore make a transformation from imaginary time to real-time $\tau \to it$. This leads to

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = \int_{x_i}^{x_f} Dx \exp\left(-i \int_0^t dt'\, x \frac{m}{2}(\omega_0^2 + \partial_{t'}^2)x\right). \tag{C.4}$$

This is a Gaussian integral, so [8]

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C \det\left(-\frac{m}{2}(\omega_0^2 + \partial_t^2)\right)^{-\frac{1}{2}}. \tag{C.5}$$

Here C is a prefactor.

We can find the value of this determinant by looking how it acts on the basis of eigenstates of the particle in the single-well potential. This basis consists of the eigenstates of the operator $-\frac{m}{2}(\omega_0^2+\partial_{t'}^2)$. We use the boundary condition that the particle starts and ends at the position $x = 0$, so $x_i = x(t' = 0) = 0$ and $x_f = x(t' = t) = 0$. The basis of eigenstates is given by $x_n(t') = \sin(n\pi \frac{t'}{t})$ and the eigenvalues are $\epsilon_n = \frac{m}{2}((\frac{n\pi}{t})^2 - \omega_0^2)$. Now we can solve equation (C.5)

$$C \det\left(-\frac{m}{2}(\omega_0^2 + \partial_t^2)\right)^{-\frac{1}{2}} = C \prod_{n=1}^{\infty} \left(\frac{m}{2}\left((\frac{n\pi}{t})^2 - \omega_0^2\right)\right)^{-\frac{1}{2}}. \tag{C.6}$$

This is an inconvenient expression as we have an infinite product. Fortunately, we can solve this by comparing this expression with the path integral of a free particle.

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C \prod_{n=1}^{\infty} \left(\frac{m}{2}\left((\frac{n\pi}{t})^2\right)\right)^{-\frac{1}{2}} \prod_{n=1}^{\infty} \left(1 - (\frac{\omega_0 t}{n\pi})^2\right)^{-\frac{1}{2}}. \tag{C.7}$$

Here the path integral of a free particle is given by equation (C.6) with $\omega_0 = 0$ as the potential (C.1) is constant when $\omega_0 = 0$

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{free}[x]) = C \prod_{n=1}^{\infty} \left(\frac{m}{2}\left((\frac{n\pi}{t})^2\right)\right)^{-\frac{1}{2}}. \tag{C.8}$$

We can also calculate the path integral of a free particle differently

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{free}[x]) = \langle x_f | e^{-it\hat{H}_{free}} | x_i \rangle = \langle x_f | e^{-it\frac{\hat{p}^2}{2m}} | x_i \rangle = \langle x_f | e^{-it\frac{\hat{p}^2}{2m}} \int dp\, |p\rangle \langle p| x_i \rangle. \tag{C.9}$$

Here we implemented 1 written as $1 = \int dp\, |p\rangle \langle p|$. We can take the integral in front, as it commutes with the momentum operator. We also use that $\langle p|x_i\rangle = e^{-ipx_i}$. Then

$$\langle x_f | e^{-it\frac{\hat{p}^2}{2m}} \int dp\, |p\rangle \langle p| x_i \rangle = \int dp\, e^{ipx_f} e^{-it\frac{p^2}{2m}} e^{-ipx_i}. \tag{C.10}$$

This is a simple Gaussian integral, so we find that

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{free}[x]) = \sqrt{\frac{2\pi m}{it}} e^{\frac{im}{2t}(x_f - x_i)^2} = \sqrt{\frac{2\pi m}{it}}. \tag{C.11}$$

Here we used again, for the particle in the single well, that $x_i = x_f = 0$. Now we look at the other part of equation (C.7) by using the identity

$$\prod_{n=1}^{\infty}\left(1-(\frac{y}{n\pi})^2\right)^{-1} = \frac{y}{\sin y}. \tag{C.12}$$

Now we can combine the results of equations (C.8) and (C.12) in equation (C.7)

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C\sqrt{\frac{2\pi m}{it}}\sqrt{\frac{t\omega_0}{\sin(t\omega_0)}} = C'\sin(t\omega_0)^{-\frac{1}{2}}. \tag{C.13}$$

We have now calculated the quantum fluctuations for the single well. We now want to go back to complex time, to get a result for equation (C.2). To do so we do again a Wick rotation. We find that for a particle on an extremum after a time τ, its path integral is proportional to the following

$$\int_{x_i}^{x_f} Dx \exp(-\mathcal{S}_{qu}[x]) = C'\sin(-i\omega_0\tau)^{-\frac{1}{2}}, \tag{C.14}$$

where C' is a constant. This are the quantum fluctuations of a particle in a single-well potential.

D The ground state energies and the instanton

To find the energy gap between the ground-state energy and the energy of the first excited state, we use equation (2.21)

$$\lim_{\tau\to\infty}\sum_{n\epsilon\{S,A\}}\langle q_f|n\rangle\, e^{-E_n\tau}\,\langle n|q_i\rangle = \lim_{\tau\to\infty} Ce^{-\frac{\omega_0\tau}{2}}\sum_n \frac{1}{n!}(\tau I_{\text{inst}})^n. \tag{D.1}$$

The lowest energy levels for the double-well potential are the symmetric and antisymmetric states. These are given by $|S\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$ and $|A\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$, and they have eigenenergies $E_S = \frac{1}{2}(\omega_0 - \Delta\epsilon)$ and $E_A = \frac{1}{2}(\omega_0 + \Delta\epsilon)$. As before, $|L\rangle$ and $|R\rangle$ are the local ground states of the left and right well respectively, without taking into account quantum effects.

It is now a useful step to look at two different solutions of the path integral in equation (D.1). The first solution is where the particle starts and ends at the same place. For simplicity we let the particle start and end in the left well, so $q = -a$. Taking $q = a$ gives the same result due to symmetry. The number of instanton contributions to let the particle start and end in the same well has to be even. Now equation (2.21) is, ignoring the limits on both sides, given by

$$\langle -a|S\rangle\, e^{-E_S\tau}\,\langle S|-a\rangle + \langle -a|A\rangle\, e^{-E_A\tau}\,\langle A|-a\rangle \propto e^{-\frac{\omega_0\tau}{2}}\sum_{n\ \text{even}}\frac{1}{n!}\left(\tau I_{\text{inst}}\right)^n. \tag{D.2}$$

The next simplification we can do is by looking at the brackets. We use that $\langle L|a\rangle = 0$ because the single well around $q = -a$ is not influenced by the right well. Similarly we have that $\langle R|-a\rangle = 0$. On the other hand, $\langle R|a\rangle = C_1$, with C_1 a constant and due to symmetry we have the same constant for $\langle L|-a\rangle = C_1$. Now, after filling in the eigenenergies for $|S\rangle$ and $|A\rangle$, the left-hand side of equation (D.2) is written as

$$\begin{aligned}\langle -a|S\rangle\, e^{-E_S\tau}\,\langle S|-a\rangle + \langle -a|A\rangle\, e^{-E_A\tau}\,\langle A|-a\rangle &\propto C_1^2 e^{-(\frac{\omega_0}{2}-\frac{\Delta\epsilon}{2})\tau} + C_1^2 e^{-(\frac{\omega_0}{2}+\frac{\Delta\epsilon}{2})\tau} \\ &\propto C_1^2 e^{-\frac{\omega_0\tau}{2}}\cosh(\Delta\epsilon\tau).\end{aligned} \tag{D.3}$$

Next, we look at the right-hand side of equation (D.2). We see that the sum is the Fourier series of the hyperbolic cosine

$$e^{-\frac{\omega_0\tau}{2}}\sum_{n\ \text{even}}\frac{1}{n!}\left(\tau I_{\text{inst}}\right)^n = e^{-\frac{\omega_0\tau}{2}}\cosh\left(\tau I_{\text{inst}}\right). \tag{D.4}$$

We can now combine equation (D.3) with (D.4)

$$e^{-\frac{\omega_0\tau}{2}}\cosh(\Delta\epsilon\tau) \propto e^{-\frac{\omega_0\tau}{2}}\cosh\left(\tau I_{\text{inst}}\right). \tag{D.5}$$

This equality holds for all time τ. This leads to the following

$$\Delta\epsilon = I_{\text{inst}}. \tag{D.6}$$

We can also start at $q = -a$ and end at $q = a$. Doing the same steps as above, but with the other boundary condition and taking only even values for n, we find that

$$e^{-\frac{\omega_0\tau}{2}}\sinh(\Delta\epsilon\tau) \propto e^{-\frac{\omega_0\tau}{2}}\sinh\left(\tau I_{\text{inst}}\right). \tag{D.7}$$

This gives the same result for $\Delta\epsilon$ as equation (D.6). With this result, we now see why we had to include both the ground state and the first excited state in equation (2.4).

E Spin coherent states

We want to write a path integral over all possible spin states. To do this mathematically efficiently, we introduce spin coherent states. Spin coherent states are defined in a way that they span all possible spin states [8]

$$|g'(\phi,\theta,\psi)\rangle = e^{-i\phi\hat{S}_z}e^{-i\theta\hat{S}_y}e^{-i\psi\hat{S}_z}\,|\Uparrow\rangle\,. \tag{E.1}$$

Here $|\Uparrow\rangle$ is defined as spin pointing in the z-direction, such that $\hat{S}_z\,|\Uparrow\rangle = S\,|\Uparrow\rangle$, where S is the total spin. This coincides with the spin state $|S, m = S\rangle$, where $|S,m\rangle$ is the spin state defined by: $\hat{\mathbf{S}}^2\,|S,m\rangle = S(S+1)\,|S,m\rangle$ and $\hat{S}_z\,|S,m\rangle = m\,|S,m\rangle$. For a spin pointing in the z-direction $|S, m = S\rangle$, we find that $\hat{S}_z\,|S,S\rangle = S\,|S,S\rangle$

Further in equation (E.1), ϕ, θ and ψ are the so-called Euler angles. The angles ϕ, θ determine the direction the spin points at. We call this the direction of the spin. The angle ψ determines how quickly the spin turns around the direction of the spin. We are

not interested in ϕ throughout the whole thesis, as no physical quantity is dependent on it. This means that we have the freedom to choose ψ. We take $\psi = 0$ which leads to a new definition of coherent states

$$|g(\phi,\theta)\rangle = e^{-i\phi\hat{S}_z}e^{-i\theta\hat{S}_y}\,|\Uparrow\rangle\,, \tag{E.2}$$

Now we have a look at some properties of spin coherent states, which also motivate why we have defined these states in this way.

Spin coherent states are such that $\langle g|\hat{\mathbf{S}}|g\rangle = \mathbf{S}$, where the spin vector S

$$\mathbf{S} = S\begin{pmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{pmatrix}. \tag{E.3}$$

This is the spin written in spherical coordinates. Further, the spin coherent states have the property that

$$1 = \int dg\,|g\rangle\,\langle g|\,. \tag{E.4}$$

This property is useful as well for creating the path integral. Also, the spin coherent states are normalized, so $\langle g|g\rangle = 1$.

F The isolated spin path integral

As for the quantum particle, we want to relate the eigenenergies of a spin with the action of an isolated. With an isolated spin we mean a spin which is not interacting with a bath or something else. To find this relation we want to use the following equation

$$\sum_n \langle\psi_f|n\rangle\, e^{-E_n\tau}\,\langle n|\psi_i\rangle = \langle\psi_f|e^{-\hat{H}\tau}|\psi_i\rangle \propto \int_{\psi_i}^{\psi_f} Dg\exp(-\mathcal{S}[g]) \tag{F.1}$$

In this appendix we show that why equation (F.1) holds.

The proof of the left equality in equation (F.1) is exactly the same as the proof for the left equality in equation (A.1) (see appendix A), so we only look at the other equality in the equation. We start by writing the time evolution operator, which is given as follows

$$\hat{U}(\tau,\tau_0) = e^{-i\hat{H}(\tau-\tau_0)}. \tag{F.2}$$

We can also split the time evolution operator in many pieces

$$\hat{U}(\tau,\tau_0) = \hat{U}(\tau,\tau_{N-1})\hat{U}(\tau_{N-1},\tau_{N-2})...\hat{U}(\tau_1,\tau_0). \tag{F.3}$$

Now we add between all small time evolution operators a unit operator, consisting of spin coherent states. We choose $\tau_0 = 0$. Then

$$\hat{U}(\tau,0) = \hat{U}(\tau,\tau_{N-1})1_{N-1}...1_{n+1}\hat{U}(\tau_{n+1},\tau_n)1_n...1_1\hat{U}(\tau_1,0). \tag{F.4}$$

Here the unit operator is defined by

$$1_n = \int dg_n \, |g_n\rangle \langle g_n| \, . \tag{F.5}$$

In this equation n is an index. It is useful to focus on the following expression

$$\langle g_{n+1}|\hat{U}(\tau_{n+1}, \tau_n)|g_n\rangle \, . \tag{F.6}$$

Next, we Taylor expand $\hat{U}(\tau_{n+1}, \tau_n)$ as $\tau_{n+1} - \tau_n = \Delta\tau$ is very small. We get that

$$\langle g_{n+1}|\hat{U}(\tau_{n+1}, \tau_n)|g_n\rangle = \langle g_{n+1}|1 - i\Delta\tau\hat{H}|g_n\rangle = \langle g_{n+1}|g_n\rangle + \langle g_{n+1}| - i\Delta\tau\hat{H}|g_n\rangle \, . \tag{F.7}$$

We use the trick of adding zero written as $\langle g_n|g_n\rangle - \langle g_n|g_n\rangle$ and we remark that the spin coherent states are normalized, so $\langle g_n|g_n\rangle = 1$. We then find that

$$\langle g_{n+1}|\hat{U}(\tau_{n+1}, \tau_n)|g_n\rangle = 1 + i\Delta\tau \left(-i \frac{\langle g_{n+1}|g_n\rangle - \langle g_n|g_n\rangle}{\Delta\tau} - \langle g_{n+1}|\hat{H}|g_n\rangle \right) \tag{F.8}$$

$$= 1 + i\Delta\tau \left(-i \langle \dot{g}_{n+1}|g_n\rangle - \langle g_{n+1}|\hat{H}|g_n\rangle \right) . \tag{F.9}$$

Here $\dot{g}$ is the derivative of g to τ. Now we can write the time evolution operator as an exponential

$$\begin{aligned} &\langle g_N|\hat{U}(\tau_N, \tau_{N-1})1_{N-1}...1_{n+1}\hat{U}(\tau_{n+1}, \tau_n)1_n...1_1\hat{U}(\tau_1, 0)|g_0\rangle = \\ &\sum_{n=0}^{N} (1 + i\Delta\tau \left(-i \langle \dot{g}_{n+1}|g_n\rangle - \langle g_{n+1}|\hat{H}|g_n\rangle \right)). \end{aligned} \tag{F.10}$$

We used in this equation that $|g_N\rangle = |\psi_f\rangle$ and $|g_0\rangle = |\psi_i\rangle$. For small $\Delta\tau$ we can write this as an integral over an exponential. Then the following expression holds

$$\sum_{n=0}^{N} (1 + i\Delta\tau \left(-i \langle \dot{g}_{n+1}|g_n\rangle - \langle g_{n+1}|\hat{H}|g_n\rangle \right)) = \int_{\psi_i}^{\psi_f} Dg e^{i \int d\tau \left(-i\langle \dot{g}|g\rangle - \langle g|\hat{H}|g\rangle \right)} \tag{F.11}$$

$$= \int_{\psi_i}^{\psi_f} Dg e^{-i\mathcal{S}[g]} . \tag{F.12}$$

Here the integral in the exponent is identified as the action $\mathcal{S}[g]$, so

$$\mathcal{S}[g] = \int d\tau \left(i \langle \dot{g}|g\rangle + \langle g|\hat{H}|g\rangle \right) . \tag{F.13}$$

In equation (F.13) the term $\langle \dot{g}|g\rangle$ is called the Berry-phase term (see appendix G).

If we combine the equations above, we find that the right equality in equation (F.1) holds. We found a starting position to calculate the energy levels of an isolated spin with the action.

G Berry-phase term

The Berry-phase term was introduced in 1984 by Michael Berry [17]. Berry found that there is a geometric change in the Hamiltonian under which the ground state of a quantum system does not change. This change in the Hamiltonian means that we can include a phase factor in the Hamiltonian, without changing the lowest energy levels [23]. This phase is called the Berry-phase term.

For our system, the Berry-phase term is given by $\langle \dot{g}|g\rangle$. We want to write the Berry-phase term in polar coordinates, in order to take the path integral over the action. For this, we need the definition of the spin coherent states from equation (E.2). Now we see that

$$\langle \dot{g}|g\rangle = \langle \Uparrow |\partial_t (e^{i\theta \hat{S}_y} e^{i\phi \hat{S}_z}) e^{-i\phi \hat{S}_z} e^{-i\theta \hat{S}_y}| \Uparrow\rangle = \langle \Uparrow |i\dot{\theta}\hat{S}_y| \Uparrow\rangle + \langle \Uparrow |e^{i\theta \hat{S}_y} i\dot{\phi}\hat{S}_z e^{-i\theta \hat{S}_y}| \Uparrow\rangle . \tag{G.1}$$

We use the identity from [8] that for $i \neq j$

$$e^{i\theta \hat{S}_i} \hat{S}_j e^{-i\theta \hat{S}_i} = \hat{S}_j \cos\theta + \epsilon_{ijk} \hat{S}_k \sin\theta, \tag{G.2}$$

and find that

$$\langle \dot{g}|g\rangle = \langle \Uparrow |i\dot{\theta}\hat{S}_y| \Uparrow\rangle + \langle \Uparrow |i\dot{\phi}(\hat{S}_z \cos\theta + \hat{S}_x \sin\theta)| \Uparrow\rangle . \tag{G.3}$$

Now we use that $\langle \Uparrow |\hat{S}_y| \Uparrow\rangle = \langle \Uparrow |\hat{S}_x| \Uparrow\rangle = 0$ and $\langle \Uparrow |\hat{S}_z| \Uparrow\rangle = S$, and we find the convenient expression

$$\langle \dot{g}|g\rangle = iS\dot{\phi}\cos\theta. \tag{G.4}$$

This outcome can be used to calculate the equations of motion for the spin system.[7]

H The Gaussian integrals of the spin action

In this appendix, we simplify the action in equation (3.16). We start with the relation between the propagator and the path integral from equation (3.14)

$$\langle \psi_f|e^{-\hat{H}\tau}|\psi_i\rangle \propto \prod_{\alpha'} \int D\mathbf{p}_{\alpha'} \int D\mathbf{q}_{\alpha'} \int_{\psi_i}^{\psi_f} Dg \exp(-\mathcal{S}'[g, \mathbf{q}_\alpha]), \tag{H.1}$$

where the action is given by (see equation (3.16))

$$\mathcal{S}'[g, \mathbf{q}_\alpha] = \int d\tau \sum_\alpha \left(-i \langle \dot{g}|g\rangle - K S_z^2 - B_x S_x + \gamma_\alpha \mathbf{S}\cdot\mathbf{q}_\alpha + \frac{\mathbf{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2}\mathbf{q}_\alpha^2 + \mathbf{p}_\alpha \cdot \dot{\mathbf{q}}_\alpha \right). \tag{H.2}$$

Notice here that the action is quadratic in both the momenta and the positions of the harmonic oscillators. This means that we can do a Gaussian integral twice. The Gaussian

[7] In many pieces of literature they use a different value for ψ, which leads to $\langle \dot{g}|g\rangle = iS\dot{\phi}(1-\cos\theta)$. However, for this thesis it is fine to work with the expression in equation (G.4) as they both lead to the same result. For the rest of the thesis it is more convenient to work with equation (G.4) so that is why we chose this.

integral over the momenta of the harmonic oscillators gives us a term of the form $-\frac{m\dot{\mathbf{q}}^2}{2}$. Now we can do a Gaussian integral over the positions of the harmonic oscillators. We then get the following

$$\langle\psi_f|e^{-\hat{H}\tau}|\psi_i\rangle \propto \prod_{\alpha'}\int D\mathbf{q}_{\alpha'}\int_{\psi_i}^{\psi_f} Dg\exp\Bigg(-\int d\tau\sum_{\alpha}\Bigg(-i\langle\dot{g}|g\rangle - KS_z^2 - B_xS_x \\ -\gamma_\alpha\mathbf{S}\cdot\mathbf{q}_\alpha + \mathbf{q}_\alpha\frac{m_\alpha(\omega_\alpha^2+\partial_\tau^2)}{2}\mathbf{q}_\alpha\Bigg)\Bigg). \tag{H.3}$$

We want to take the Gaussian integral over all q_α. We cannot do this yet as we cannot take the inverse of the time derivative. We can use the following equation to do the Gaussian integral for a path integral, which has an operator $M(t,t')$ [8].

$$\int Dx(t)\exp\Bigg(-\frac{1}{2}\int dt\int dt'\,x(t)M(t,t')x(t') + \int dtj(t)x(t)\Bigg) \propto \\ \big(\det M\big)^{-\frac{1}{2}}\exp\Bigg(\frac{1}{2}\int dt\int dt' j(t)M^{-1}(t,t')j(t')\Bigg). \tag{H.4}$$

For now, we are only looking at the action of the system. The action is only dependent on the terms which are in the exponent and not on the prefactors. We therefore ignore the determinant, as it only gives a prefactor. This means that we only have to focus on the following part of equation (H.3), which we call Z

$$Z = \prod_{\alpha'}\int D\mathbf{q}_{\alpha'}\exp(-\int d\tau\sum_{\alpha}\Bigg(\gamma_\alpha\mathbf{S}(\tau)\cdot\mathbf{q}_\alpha(\tau) + \int d\tau'\mathbf{q}_\alpha(\tau)\frac{m_\alpha}{2}(\omega_\alpha^2+\partial_\tau^2)\delta(\tau-\tau')\mathbf{q}_\alpha(\tau')\Bigg)). \tag{H.5}$$

Here we added an integral and a delta function. By integrating by parts with respect to τ, we find an operator $A_\alpha(\tau-\tau') = \frac{m_\alpha}{2}(\omega_\alpha^2\delta(\tau-\tau') + \delta''(\tau-\tau'))$. Finding the inverse of this operator is equivalent to finding an operator $A_\alpha^{-1}(\tau-\tau')$ such that

$$\int d\tau' A_\alpha^{-1}(\tau-\tau')A_\alpha(\tau'-\tau'') = \delta(\tau-\tau''). \tag{H.6}$$

To find $A_\alpha^{-1}(\tau-\tau')$, we have to do a Fourier transform. We then find that

$$A_\alpha^{-1}(\omega) = \frac{1}{A_\alpha(\omega)} = \frac{2}{m_\alpha(\omega_\alpha^2-\omega^2)} \tag{H.7}$$

and

$$A_\alpha^{-1}(\tau-\tau') = \int\frac{d\omega}{2\pi}e^{-i\omega(\tau-\tau')}\frac{2}{m_\alpha(\omega_\alpha^2-\omega^2)}. \tag{H.8}$$

This integral is not well-defined, as it diverges at $\omega = \pm\omega_\alpha$, for all ω_α. To solve this we make an infinitesimal shift η into the imaginary plane. We have two choices for the shift $\omega\to\omega\pm i\eta$. When the plus sign is used, the operator is called retarded (R). When the minus sign is used, the operator is called advanced (A). With the retarded/advanced operator we can do a contour integral.

$$(A^{R/A})^{-1}_{\alpha}(\tau-\tau') = \int \frac{d\omega}{2\pi} e^{-i\omega(\tau-\tau')} \frac{2}{m_\alpha(\omega_\alpha^2 - (\omega \pm i\eta)^2)}. \tag{H.9}$$

The added η is infinitesimally small.

Next, we combine equation (H.4) with equation (H.5). We find that

$$Z \propto \exp\left(\frac{1}{4}\int \tau \int \tau' \sum_\alpha \mathbf{S}(\tau)\gamma_\alpha^2 (A^{R/A})^{-1}_{\alpha}(\tau-\tau')\mathbf{S}(\tau')\right). \tag{H.10}$$

Now we define the retarded and advanced kernel functions in the following way

$$\alpha^{R/A}(\tau-\tau') = \frac{1}{4}\sum_\alpha \gamma_\alpha^2 (A^{R/A})^{-1}_{\alpha}(\tau-\tau') = \int \frac{d\omega}{4\pi} \sum_\alpha e^{-i\omega(\tau-\tau')} \frac{\gamma_\alpha^2}{m_\alpha(\omega_\alpha^2 - (\omega \pm i\eta)^2)}. \tag{H.11}$$

This means that the Fourier transform of the kernel functions is

$$\alpha^{R/A}(\omega) = \frac{1}{4}\sum_\alpha \gamma_\alpha^2 (A^{R/A})^{-1}_{\alpha}(\omega) = \frac{1}{2}\sum_\alpha \frac{\gamma_\alpha^2}{m_\alpha(\omega_\alpha^2 - (\omega \pm i\eta)^2)}. \tag{H.12}$$

For now it is unclear when we have to use the retarded or the advanced kernel function. It turns out that they lead to the same action and thus to the same equations of motion. It thus does not matter which kernel function we choose to use. We get that the action is given by

$$\mathcal{S}[g] = \int d\tau \left(-i\langle \dot{g}|g\rangle - KS_z^2 - B_x S_x + \int d\tau \int d\tau' \mathbf{S}(\tau)\alpha^{R/A}(\tau-\tau')\mathbf{S}(\tau')\right). \tag{H.13}$$

In the end we found an expression for the action, which is only dependent on the spin.

I Equations of motion for spin

To find the equations of motion for the spin system corresponding with the action in equation (H.13), we have to vary the action. As has been shown before, we know that the coherent states are dependent on θ and ϕ, which are dependent on the time τ. We therefore vary with respect to $\theta(\tau)$ and $\phi(\tau)$. To not be confused with the imaginary time integrals in the action, we write the action as follows

$$\mathcal{S}[g] = \int d\tau' \left(-i\langle \dot{g}|g\rangle - KS_z^2 - B_x S_x + \int d\tau' \int d\tau'' \mathbf{S}(\tau')\alpha^{R/A}(\tau'-\tau'')\mathbf{S}(\tau'')\right). \tag{I.1}$$

We now vary the action with respect to θ and take the functional derivative

$$\frac{\delta\mathcal{S}[g]}{\delta\theta(t)} = \frac{\delta(-i\langle \dot{g}|g\rangle - KS_z^2 - B_x S_x)}{\delta\theta(t)} + \int d\tau'' \frac{\delta(\mathbf{S}(\tau))}{\delta\theta(\tau)}\alpha^{R/A}(\tau-\tau'')\mathbf{S}(\tau'') \tag{I.2}$$

$$+ \int d\tau' \mathbf{S}(\tau')\alpha^{R/A}(\tau'-\tau)\frac{\delta(\mathbf{S}(\tau))}{\delta\theta(\tau)}. \tag{I.3}$$

For this thesis, we take the same approximation as is done in Keldysh formalism [18]

$$\alpha^{R/A}(\omega) \approx \pm\alpha_0\omega + \frac{I}{2}\omega^2. \tag{I.4}$$

Here α_0 is the Gilbert damping and I is the spin inertia. We can now Fourier transform back to find $\alpha(\tau - \tau')$

$$\alpha^{R/A}(\tau - \tau') = \mp\alpha_0\partial_{\tau'}\delta(\tau - \tau') - \frac{I}{2}\partial^2_{\tau'}\delta(\tau - \tau'). \tag{I.5}$$

We have the following relation between the retarded and advanced kernel function

$$\alpha^R(\tau - \tau') = \alpha^A(\tau' - \tau). \tag{I.6}$$

Further, we note that $\alpha^{R/A}$ and S commute as $\alpha^{R/A}$ is a function and not as an operator. This means that we can write the variation of the action as

$$\frac{\delta\mathcal{S}[g]}{\delta\theta(\tau)} = -i\frac{\delta\langle\dot{g}|g\rangle}{\delta\theta(\tau)} + \frac{\delta\mathbf{S}(\tau)}{\delta\theta(\tau)}\cdot\mathbf{B}_{\text{eff}} + \int d\tau'\mathbf{S}(\tau')(\alpha^R(\tau - \tau') + \alpha^A(\tau - \tau'))\frac{\delta\mathbf{S}(\tau)}{\delta\theta(\tau)}, \tag{I.7}$$

where the effective magnetic field $\mathbf{B}_{\text{eff}}$ is given by

$$\mathbf{B}_{\text{eff}} = \begin{pmatrix} -B_x \\ 0 \\ -2KS_z \end{pmatrix}. \tag{I.8}$$

It does not matter which shift we make into the complex plain. We add either a small frequency η in the positive complex direction or in the negative complex direction. Both the retarded and advanced kernel function lead to the same action and thus the same physics. Now we can fill in the expression for the kernel functions from equation (I.5) into equation (I.7), we find that

$$\frac{\delta\mathcal{S}[g]}{\delta\theta(\tau)} = -i\frac{\delta\langle\dot{g}|g\rangle}{\delta\theta(\tau)} + \frac{\delta\mathbf{S}(\tau)}{\delta\theta(\tau)}\cdot\left(\mathbf{B}_{\text{eff}} - I\int d\tau'\mathbf{S}(\tau')\partial^2_{\tau'}\delta(\tau - \tau')\right) \tag{I.9}$$

$$= -i\frac{\delta\langle\dot{g}|g\rangle}{\delta\theta(\tau)} + \frac{\delta\mathbf{S}(\tau)}{\delta\theta(\tau)}\cdot\left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}(\tau)\right). \tag{I.10}$$

So far, we only varied the action with respect to θ. We have not used any property of θ yet, so we can do exactly the same for ϕ. We then get exactly the same equation, but with ϕ instead of θ.

For finding the equations of motion, we look at $\frac{\delta\mathcal{S}[g]}{\delta\theta(\tau)} = 0$ and $\frac{\delta S}{\delta\phi(\tau)} = 0$. This gives us the following equations

$$\frac{\delta\mathcal{S}[g]}{\delta\theta(\tau)} = S\dot{\phi}\sin\theta + \begin{pmatrix}\cos\theta\cos\phi \\ \cos\theta\sin\phi \\ -\sin\theta\end{pmatrix}\cdot\left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right) = 0, \tag{I.11}$$

and

$$\frac{\delta \mathcal{S}[g]}{\delta \phi(\tau)} = -S\dot{\theta}\sin\theta + \begin{pmatrix} -\sin\theta\sin\phi \\ \sin\theta\cos\phi \\ 0 \end{pmatrix} \cdot \left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right) = 0. \tag{I.12}$$

These expressions are equivalent with

$$\dot{\mathbf{S}} = \mathbf{S} \times \left(\mathbf{B}_{\text{eff}} - I\ddot{\mathbf{S}}\right). \tag{I.13}$$

This equation is the Inertial-Landau–Lifshitz–Gilbert (ILLG) equation (see equation 1.2) without Gilbert damping [4]. One can easily find that equation (I.13) is equivalent to equations (I.11) and (I.12). First one needs to get the expressions for $\dot{\phi}$ and $\dot{\theta}$ out of equations (I.11) and (I.12) respectively. Then one takes the time derivative of S and fills the expressions for $\dot{\phi}$ and $\dot{\theta}$. One can see then that this is equivalent to the right-hand side of equation (I.13). Equation (I.13) consists of three equations and (I.11) and (I.12) are just two equations. In (I.13) we have included that the length of the spin is constant, which we also assume in the equations before.

About this expression, some nice approximations are made in Keldysh formalism [4]

$$\alpha^{R/A}(\omega) = \pm i\alpha_0\omega + \frac{I}{2}\omega^2. \tag{I.14}$$

In this thesis, we use this approximation and we have a look at its consequences.

J The saddle-point approximation

We cannot solve the path integral in equation (3.23) exactly. However, with the saddle-point approximation we can approximate the path integral. For the spin-instanton we are considering, we can use this technique. In this appendix we explain what is the saddle-point approximation.

The saddle-point approximation for a smooth function f of a single variable x, is the following. For $Q \gg 1$, the following integral, is approximated by

$$\int_a^b dx \exp(-Qf(x)) \approx \sum_{\text{minima of f}} \int_a^b dx \exp(-Q(f(x_0) + \frac{f''(x_0)}{2}\Delta x^2)), \tag{J.1}$$

where $\Delta x = x - x_0$ and $f''(x_0)$ is the second derivative of f at the point x_0. This approximation is good for large Q, as in that case the only parts of the function that have a contribution to the integral, are the minima and the vicinities of the minima.

Using the saddle-point approximation is similar to what we have done for the particle in the double-well potential. Here we had that the path that gives the main contribution, is the classical solution. The second-order corrections in equation (J.1) lead to the paths, which are equivalent to the paths in the vicinity of the minimal solution. For the spherical-spin model there are many of such paths, as it is a two dimensional model. Therefore we use the saddle-point approximation for the path integral over the action. Further, the second-order corrections in equation (J.1) include also the quantum corrections.

There is one important difference between the normal saddle-point approximation and the approximation for the path integral we have to take into account, and that is that the action is not a function, but a functional. The idea of the saddle-point approximation is that we look at the main contributions of the path integral. The other contributions are ignored. We can do this as we look at a system where $Q \gg 1$.

For the path integral over the action, see equation (J.2), we have to take into account the paths when the action is very small

$$I_{\text{path}} = \int_{q_i}^{q_f} Dq \exp(-S[q(t)]). \tag{J.2}$$

We find the minima of the action when $\frac{\delta \mathcal{S}[q(t)]}{\delta q(t)} = 0$. We also have to include the paths close to these minima of the action. These close paths we find by fluctuating around the minima. So around a minimum path $q_0(t)$, which goes from q_i to q_f, we can write the action as

$$\mathcal{S}[q(t)] = \mathcal{S}[q_0(t)] + \int dt' \int dt'' \frac{1}{2} \Delta q(t') \frac{\delta^2 \mathcal{S}[q_0(t)]}{\delta q(t') \delta q(t'')} \Delta q(t'') + \mathcal{O}(\Delta q^3). \tag{J.3}$$

The first-order derivative of the functional is zero as we look at a minimal path. The saddle-point approximation says that, if we can write the action as $\mathcal{S}[q(t)] = Sf[q(t)]$, with $S \gg 1$, we find that the path integral is given by

$$I_{\text{path}} \approx \sum_{\text{minima}} \int_{q_i}^{q_f} Dq \exp\left(-S\big(f[q_0(t)] + \int dt' \int dt'' \frac{1}{2} \Delta q(t') \frac{\delta^2 \mathcal{S}[q_0(t)]}{\delta q(t') \delta q(t'')} \Delta q(t'') \big) \right). \tag{J.4}$$

We now integrate over all paths, but we only have to take into account the minimal paths and the paths which are in the vicinity of the minimal paths. All other paths have an irrelevant contribution to the integral, because the constant S is large.

For the spherical-spin model, we have that the action is dependent on two variables θ and ϕ. For the approximation, we now have to take the functional derivatives to both θ and ϕ. Now we have to take also cross-terms into account. The path integral can now be calculated by

$$\begin{aligned}
&\int_{q_i}^{q_f} Dg \exp(-S\, f[\theta(t), \phi(t)]) \approx \\
&\sum_{\text{minima}} \int_{q_i}^{q_f} Dg \exp\Big(-S\big(f[\theta_0(t), \phi_0(t)] + \int dt' \int dt'' \frac{1}{2} \Delta\theta(t') \frac{\delta^2 f[\theta_0(t), \phi_0(t)]}{\delta\theta(t') \delta\theta(t'')} \Delta\theta(t'') \\
&+ \int dt' \int dt'' \Delta\theta(t') \frac{\delta^2 f[\theta_0(t), \phi_0(t)]}{\delta\theta(t') \delta\phi(t'')} \Delta\phi(t'') + \int dt' \int dt'' \frac{1}{2} \Delta\phi(t') \frac{\delta^2 f[\theta_0(t), \phi_0(t)]}{\delta\phi(t') \delta\phi(t'')} \Delta\phi(t'') \big) \Big).
\end{aligned} \tag{J.5}$$

This is the saddle-point approximation for the spherical-spin model.

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