Numerical studies of transition states for magnetization reversal in
ferromagnetic nanostructures

by

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Dedication

A mis papás, Carol y Jairo; y a mi esposa Ivonne.
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Abstract

My PhD dissertation research focuses on transition states for thermally activated magnetization reversal in ferromagnetic nanostructures. Problems of this type can be classified by whether the torques on the magnetization can be written in terms of the gradient of a potential energy or not, i.e. whether the forces are conservative or non-conservative. Gradient driven dynamics can be studied using Kramer’s reaction rates theory in which the rate $\nu$ can be written in Arrhenius form $\nu = \nu_0 e^{-\frac{\Delta E}{kT}}$ where $\Delta E$ is the activation energy to escape from a basin of attraction, and $\nu_0$ is determined by the linearized dynamics close to critical points. For gradient systems, I used a numerical bisection method to verify an analytical theory of transition between the circumferential states of ferromagnetic nanorings. This required use of micromagnetic simulations because the transition states are non uniformly magnetized. The theory predicts how thin and narrow rings reverse from clockwise to counterclockwise magnetization configurations. I found that the analytical theory works very well for rings with annular width much greater than the one predicted in the model. In addition, transition states between higher energy metastable states that con-
sist of trapped $2\pi$ domain walls were found using the String Method, which is a technique that finds the minimal energy barrier between two basins of attraction. I found that the transition for annihilation and creation of $2\pi$ domain walls correspond to propagation of a topological defect across the sample. The String Method was also used in a new structure made of a ferromagnetic materials with perpendicular anisotropy and the energy barriers were found to be smaller than the predictions of uniformly magnetized models. However the String Method can not be used in non-gradient systems which are also of importance e.g. spin-transfer torque driven magnetization dynamics. In this case, the gMAM method may be used to find the most probable transition paths between two states. We have applied the gMAM method to the case of a uniformly magnetized particle subject to a spin-transfer torque and found that it changes the transition paths and reversal rates.
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Chapter 1

Introduction

The magnetization of a ferromagnetic nanostructure depends on its magnetic past: for the same applied magnetic field the nanostructure can have two or more distinct magnetizations. This suggests that for the same external conditions there must be more than one internal state in which the particle’s free energy is a minimum. Given enough time the magnetization would be in a state that is a global minimum of the energy. So this hysteresis is an out-of-equilibrium phenomena. It is a memory effect, that is at the heart of the modern magnetic information storage devices as magnetic states are used to encode digital information (such as magnetic hard drives and MRAM).

Unfortunately this memory is not eternal. The approach to equilibrium is inevitable and the nanostructure would eventually find its way to the global free energy minimum and as a consequence information will eventually be lost. For technological purposes, it is critical that this relaxation occurs on a timescale
that is longer than the timescale desired to retain the data. The important physical quantity is the relaxation rate from a local to the global energy minimum. We can determine this quantity using an appropriate theory of reaction rates [1, 2] in conjunction with a theory of the underlying physics of the magnetic interactions. We do this in a conceptual framework known as Micromagnetism which is explained in chapter 2. The key concepts of reaction rates needed to understand the approach towards thermal equilibrium in magnetic structures are introduced in Chapter 3.

The simplest model of magnetization relaxation assumes that the object is uniformly magnetized during the process of transition between two well defined magnetization directions (See Fig. 1.1). It is commonly known as the Néel-Brown [3, 4] or macrospin model; the relaxation process is usually described as “magnetization reversal”. The Néel-Brown model correctly describes the magnetization relaxation rate observed in very small magnetic particles as a
function of temperature [5]. In this model the magnetization $M$ of a particle is described by a three dimensional vector with constant magnitude in a potential energy landscape with two distinct energy minima. The relaxation rate is determined by the probability of the system overcoming the barrier and escaping from the basin of attraction of one energy minimum into the other. This model is discussed in detail in chapter 4.

Small particles can be considered to have uniform magnetization because the ferromagnetic exchange interaction is very strong at short distances and dominates over all other magnetic interactions, such as magnetic dipole interactions. However, it decays very quickly: its magnitude is negligible beyond next to nearest neighbor distances; for larger distances other interactions become dominant which don’t necessarily favour uniform magnetization (e.g. dipole-dipole interaction). As consequence, large magnetic objects will present nonuniform magnetizations and reversal should occur by different mechanism of that of the Néel-Brown model.

In a series of papers [6, 7, 8, 9] Braun pioneered the study of non uniform magnetization reversal. He focused on very long cylinders of constant cross-section for which the magnetization is best described as a field $M(x)$ where $x$ is the position along the axis of the magnet. In long cylinders, the magnetostatic energy is minimized by orientations of the magnetization collinear with the cylinder axis.

Braun’s main prediction is that the transition between two collinear states, magnetization up and down, occurs either through uniform magnetization re-
versal (as in the Néel-Brown model) or through a so-called instanton saddle state. The instanton saddle state corresponds to a nucleus of critical size (see Fig. 1.2 c); fluctuations smaller than the critical nucleus size relax back to the original state and fluctuations larger than the critical nucleus size stow into the opposite magnetization state.

Braun’s results were criticized by Aharoni who argued that only curling or uniform magnetization rotation are possible mechanisms of magnetization reversal in ferromagnetic cylinders [10] (see Fig 1.2). Most of Aharoni’s comments concerned the validity of certain approximations to the magnetostatic energy used by Braun. Later on, the issues raised by Aharoni were addressed by Braun in subsequent work. I give a brief description of this discussion in
Figure 1.3: Geometry of the Martens et al. model for thin ferromagnetic nanorings. The magnetization is favored for circumferential directions, is constrained to the plane and is independent of the radial coordinate. A current flowing through the ring’s axis produces a counterclockwise magnetic field.

Martens et al. built upon Braun’s analytical results by reformulating his theory of non uniform magnetization reversal and applying it to thin ferromagnetic nanorings [11] (see Fig. 1.3). The rings do not have end caps which play an important role in magnetization reversal of long cylinders. From a technological point of view, the ring geometry is attractive because in the ground state the magnetization is never perpendicular to the material surface and there are no stray fields flowing out of the magnet. As the density of magnetic storage devices increases stray fields may induce unwanted reversal of the magnetization in neighboring memory units; the circular geometry avoids this problem.

In the work of Martens et al. [11] the rings were considered to be narrow enough for the magnetization to be independent of the radial coordinate, so
that the magnetization was a function only of the azimuthal coordinate; moreover the ring width is considered much larger than its thickness so that the magnetization is constrained to remain in plane and its fully described by the deflection from the tangential direction. A critical assumption is that the most important contribution to the magnetostatic energy occurs at the narrow sides of the ring while the bulk contribution is but negligible. This assumption is justified analytically in the thin film limit which is described at the end of chapter 2.

The analysis of Martens et. al predicted that thin ferromagnetic nanorings also have instanton and constant saddle transition states for magnetization reversal. The bulk of this dissertation focuses on the numerical calculation of the energy barriers to verify these analytical predictions. The relevant features of the Martens et al. model are discussed in chapter 5. My contribution to the understanding of the thermal properties of thin ferromagnetic nanorings starts in chapter 5 after the introduction of the Martens et al. model.

I verified numerically that the predicted transition states are in fact critical points of the magnetization dynamics. For these calculations I used the publicly available package for micromagnetic analysis OOMMF. The simulations are obtained without using the assumptions of the Martens et al model; i.e. in the simulations the magnetization is represented by a three dimensional vector in a two dimensional mesh which varies in the radial as well as the circumferential direction.

I studied a variety of rings and verified that the instanton saddle is preferred
to the uniform magnetization reversal. Moreover, I simulated rings of increasing annular width and observed that the Martens et al. model assumptions are valid even for wide rings where one should expect that bulk contributions to the magnetostatic energy would overcome the contribution from the edges.

Numerical simulations also allowed me to study rings of increasing radius. I observed that rings with very large radius present a multiplicity of metastable configurations which had not been considered in previous work of thermal excitations of nanorings or cylinders. It raised the question of what mechanism allows thermal agitation to switch the magnetization configuration between these newly found magnetization states. Since I lacked an analytical theory for the transition states, the transition states and energy barriers had to be found numerically. I used a numerical technique developed by Eric Vanden-Eijnden, Weiqing Ren and Weinan E known as the “String Method for the Study of Rare Events” which finds the transition states for physical systems with a well defined potential energy. The implementation of the String Method using OOMMF is summarized in chapter 6 and the manual for its use is provided in the Appendix.

The study of magnetization reversal in thin rings in chapters 5 and 6 presumes that a current flowing through the axis of the ring produces a counterclockwise magnetic field that lifts the degeneracy between the clockwise and counterclockwise magnetization. In reality it is experimentally challenging to produce an electrical current that does not permeate the magnetic region. Electrons flowing through magnetic materials tend to align their spins with that
of the magnetic layers. This interaction is known as Spin Transfer Torque (STT) and results from conservation of angular momentum. In the presence of STT there is no longer a well defined potential energy – spin transfer torques are nonconservative torques in the magnetization.

The theory of reversal rates presented in chapters 3 and 4 breaks down in these systems. However, the transition state and most probable paths can be studied using action minimization methods. The transition states provide information on the reversal rates. We found transition states and most probable reversal paths for Néel-Brown particles in the presence of spin polarized currents with a technique developed by Eric Vanden-Eijnden and Matthias Heynmann named “the geometrical Minimum Action Method (gMAM)”. The theory and techniques are described in chapter 8. The results are consistent with previous work on thermally activated reversal in the presence of STT. The results indicate that STT shifts the transition state out of the film’s plane, which will result in a large contribution to the magnetostatic energy and increases the height of the energy barrier. More importantly, the results of chapter 8 should motivate the magnetism community to shift from the Néel-Brown model of magnetization reversal to a more general theory of transition states.

The String Method can be used to study a large variety of magnetic systems and I applied it to find the transition states and energy barriers of thin films where the crystalline anisotropy favors out of plane magnetizations. In similarity with Braun’s theory, small samples reverse in a uniform mode while large sample reverse by a localized fluctuation of the magnetization. The en-
ergy barrier calculations present behavior analogous to those of the Martens et al. model. This work is presented in chapter 7. This work forms part of an ongoing project at NYU to characterize the switching of the magnetization of small systems with perpendicular magnetic anisotropy experimentally.

In the last section of this work, I will summarize these results and provide ideas for subsequent research.
Chapter 2

Micromagnetism

Micromagnetism describes the behavior of the magnetic systems on a length scale greater than the atomic scale in which a continuum description is adequate. The state of the system is described by a continuous magnetization field $M(r)$ which measure the local magnetic moment density per unit volume. A magnetic object of arbitrary shape can be divided into volume elements $d\tau$ with each element having a total magnetic moment $M(r)d\tau$. The volume $d\tau$ is considered much larger than the materials unit cell, but small enough to maintain a constant magnetization magnitude $|M| = M_s$.

To understand how the magnetization in a volume element reacts to the presence of external fields it is convenient to consider its simple analog in classical electrodynamics: a coil of current with the same magnetic moment. A coil carrying an electric current and with an infinitesimal area but finite magnetic moment equal to $Md\tau$. A magnetic field $H_{\text{eff}}$ produces a torque which
changes the orientation of the angular momentum by \( \vec{\tau} = \frac{dL}{dt} = M d\vec{r} \times \mu_0 \mathbf{H}_{\text{eff}}. \)

The angular momentum is linked to the magnetic moment by the gyromagnetic ratio \( \gamma: \gamma L = -\mu_0 M d\vec{r} \) \( (\gamma = 2.21 \times 10^5 \text{ m} / \text{As}) \) and as a result, the magnetization evolves according to:

\[
\frac{dM}{dt} = -\gamma M \times \mathbf{H}_{\text{eff}}. \tag{2.1}
\]

This expression predicts the magnetization precesses indefinitely around the field \( \mathbf{H} \). Experimentally, precessions of the magnetization decay in time towards an energy minimum \( (M \parallel \mathbf{H}_{\text{eff}}) \) and a damping term needs to be added to Eq. 2.1. The damping term results from complex interactions between the magnetic moment and the crystal lattice and cannot be obtained rigorously from basic principles; for this reason it is added as a phenomenological term. It was first proposed by Gilbert who added a term to the equation of motion:

\[
\frac{dM}{dt} = -\gamma M \times \mathbf{H}_{\text{eff}} - \frac{\alpha}{M_s} (M \times \frac{dM}{dt}). \tag{2.2}
\]

The effect of both terms in the magnetization vector is shown in Fig. 2.1 where the direction of each component is represented.

The effective field \( \mathbf{H}_{\text{eff}} \) results from interactions with the environment and between the different volume elements that compose the object; it determines the magnetization dynamics and the energy landscape, \( \mathbf{H}_{\text{eff}} \) is defined as: \( \mathbf{H}_{\text{eff}} = -\nabla M E \), where \( E \), the micromagnetic energy density, depends on the specific system being considered. Most experiments are successfully ex-
plained using four energy terms which are known as exchange, magnetostatic, Zeeman, and magnetocrystalline.

\section*{2.0.1 Exchange energy}

It is well known from quantum mechanics that two charged fermions with overlapping wavefunctions interact there is a contribution to the energy known as the exchange interaction. The total energy can be expressed as the Heisenberg hamiltonian:

\[ E_{\text{ex}} = - \sum_i^N \sum_{j \in \text{nn}(i)} J_{ij} S_i \cdot S_j \] (2.3)
where the sum over \( j \) considers only the nearest neighbors of \( i \) and the value of \( J \) determines the strength of the interaction as well as whether it is ferromagnetic (\( J > 0 \)) or antiferromagnetic (\( J < 0 \)). In micromagnetics the expression is rewritten in what is known as the “continuum approximation”. This is done by changing the spins \( S_i \) to the continuous variable \( m = M/M_s \). And expanding the dot product as \( M_{r(i)} \cdot M_{r(i)+\Delta r} \approx M_s^2 (1 - \frac{1}{2} \theta_{ij}^2) \) where \( \theta_{ij} \) is the angle between neighboring volume elements and is approximated by \( \theta_{ij} \approx (\nabla m) \cdot \Delta r \).

After dropping the constant term the sum in the continuous limit become:

\[
E_{ex} = A \int (\nabla m)^2 \, dV \tag{2.4}
\]

where the constant \( A \) represents the strength of the exchange interaction. For the ferromagnetic case, the exchange energy is minimized when all moments are aligned in the same direction. Since it is very strong at small distances, magnetic elements of very small size can be considered as having uniform magnetization. Small systems are commonly known as the single spin or macrospin models.

### 2.0.2 Zeeman energy

The magnetic energy due to the external magnetic field is simply

\[
E_Z = - \int \mu_0 H_{ex} \cdot M \, dV \tag{2.5}
\]
where $H_{\text{ex}}$ is the external field applied to the magnetic object.

### 2.0.3 Magnetocrystalline energy

Although in the continuum limit the magnetization is considered to be isotropic; the spin-orbit interaction results in certain directions of the magnetization being favored. The electron spins tend to align along well defined crystallographic axes. The direction of space in which the magnetization is energetically favored is called ‘easy axis’; the direction of space in which hard to magnetize the sample is named ‘hard axis’.

The specific expression for the magnetocrystalline depends on the crystal structure of the magnet and can be described by a linear combination of spherical harmonics on $m$. However, higher order terms are usually averaged out because of thermal agitation; only at low temperatures do higher order terms become important. As a result, most magnetic materials are well described by two kinds of anisotropy associated with hexagonal and cubic lattices.

The magnetocrystalline energy of a volume elements depends solely on its internal magnetic state (i.e. it is a local contribution to the micromagnetic energy). In this work we will express this energy in a variety of ways chosen so that it reflects previous uses in the available literature. A simple case would be an anisotropy of the form

$$E_{\text{anis}} = -K_1 m_x^2 + K_2 m_z^2$$

(2.6)
with $K_1, K_2 > 0$. Here, $\hat{x}$ is the easy axis direction and $\hat{z}$ is the hard axis direction. In the absence of an external field the magnetization would be along $+\hat{x}$ or $-\hat{x}$, $m_x = \pm 1$. It is convenient to associate an “anisotropy field" to the easy axis $h = \frac{2K_1}{\mu_0 M_s}$ which measures the minimum field required to switch the magnetization at zero temperature.

2.0.4 Magnetostatic energy

The last energy term to consider results from the long-range dipolar interaction between the magnetic moments of all volume element of the magnetic object. It is better treated starting from the magnetostatic Maxwell’s equations in the absence of free currents and charges:

$$\nabla \cdot B = 0 \quad (2.7)$$

$$\nabla \times H = 0 \quad (2.8)$$

and the material’s law of magnetic materials

$$B = \mu_0 (M + H). \quad (2.9)$$

Eq. 2.8 is satisfied if we write $H$ as the gradient of a magnetostatic potential
\( \mathbf{H} = -\nabla U; \) which substituting into Eq. 2.9 and Eq. 2.7 implies that

\[
\nabla \cdot \mathbf{B} = 0 = \mu_0 \nabla \cdot (\mathbf{M} + \mathbf{H}) = \mu_0 \nabla \cdot (\mathbf{M} + \nabla U) \tag{2.10}
\]

and

\[
\nabla^2 U = \nabla \cdot \mathbf{M}. \tag{2.11}
\]

For a given magnetization configuration \( \mathbf{M}(\mathbf{r}) \) the magnetostatic potential needs to be calculated to obtain the magnetostatic field. This is a Poisson equation for \( U \) in which the bulk sources are given by \( \nabla \cdot \mathbf{M} \) and boundary sourced by \( \mathbf{M} \cdot \hat{n} \) where \( \hat{n} \) is the normal to the surface. At the boundaries of the magnetic object the discontinuity of \( \mathbf{M} \) produces “magnetic charges” that produce an energy penalty for magnetizations that are perpendicular to the surface and favour magnetizations parallel to the surface \( (\mathbf{M} \perp \hat{n}) \).

From this point of view, magnetic objects behave as dielectrics in which \( \mathbf{M} \) serves the role of polarization and \( \mathbf{H}_{\text{dip}} = \nabla U \) that of the electric field produced by polarization; the magnetostatic energy can be written as:

\[
E_{ms} = -\frac{\mu_0}{2} \int_{\Omega} \mathbf{M}(\mathbf{r}) \cdot \mathbf{H}_{\text{dip}} d^3 \mathbf{r} \tag{2.12}
\]

where \( \Omega \) is the space occupied by the magnetic material and the dipole field \( \mathbf{H}_{\text{dip}} \) at position \( \mathbf{r} \) is the leading order multipole expansion

\[
\mathbf{H}_{\text{dip}}(\mathbf{r}) = \frac{1}{4\pi} \int_{\Omega} \frac{3(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^5}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{M} - \frac{\mathbf{M}}{|\mathbf{r} - \mathbf{r}'|^3} d^3 \mathbf{r}'. \tag{2.13}
\]
It is convenient to define a ‘magnetostatic tensor’ $\vec{N}(r, r')$ given by

$$
\vec{N}(r - r') = \frac{3(r - r')}{4\pi|r - r'|^5}(r - r') - \frac{1}{4\pi|r - r'|^3}, \tag{2.14}
$$

which allows to write the magnetostatic energy as

$$
E_{\text{dip}} = \frac{\mu_0}{2} \int \int_{\Omega} \mathbf{M}(r) \cdot \vec{N}(r - r') \cdot \mathbf{M}(r') d^3r' d^3r. \tag{2.15}
$$

If the object in uniformly magnetized a further simplification is possible

$$
E_{\text{dip}} = \frac{\mu_0}{2} \mathbf{M} \cdot \vec{N} \cdot \mathbf{M}. \tag{2.16}
$$

the trace of $\vec{N}$ equals 1. If the magnetic material is in the form of an infinite plane in the $xy$ plane it becomes $N_{zz} = 1$ and zero in all other terms leaving a simple expression for the magnetostatic of a uniformly magnetized film

$$
E_{\text{dip}} = \frac{\mu_0 M^2}{2}, \text{ (uniformly magnetized plane)} \tag{2.17}
$$

The magnetostatic term is long range and causes the formation of magnetic domains (separate regions of the ferromagnet magnetized in different directions).
2.0.5 Summary of magnetic interactions

For the systems considered here, the full micromagnetic has four contributions:

\[ E_{\text{tot}} = E_{\text{anis}} + E_{\text{ex}} + E_{\text{Z}} + E_{\text{ms}} \] (2.18)

and the magnetization dynamics tends to drive the system towards energy minima. In most cases the interactions compete against each other and the minimization is achieved for nontrivial magnetization configurations. Moreover, there could be many states which are local energy minima. Thermal agitation may push the system out of a global minimum and into the boundary of attraction of another minimum. In the following chapter I explain the earlier theories of how this transition occurs in magnetism.

At this point we can introduce the exchange length \( l_{\text{ex}} = 2A/(\mu_0 M_s^2) \) as the ratio between the exchange and magnetostatic energy densities. It is the length at which the exchange length is overcomed by the magnetostatic energy and represent the width of the interface between regions of opposite magnetization. The values of the stiffness constant \( A \) and \( l_{\text{ex}} \) are known for commonly used materials.
2.1 Thin film analytical micromagnetism, classification of thin film regimes

In studies of micromagnetism, the magnetostatic term is the most difficult to treat analytically and numerically. Recent analytical studies of micromagnetics provide a classification of thin films for which a variety of simplifications of the magnetostatic term can be used [12]. Depending on the dimensions of the system, a thin ferromagnet is classified in any of the four categories of table 2.1. The full micromagnetic energy reduces to expressions that are easier to treat.

In these systems the film is considered to have a disk shape of lateral dimension $R$, thickness $t$ and exchange length $l_{ex} = \sqrt{2A/\mu_0 M_s}$. The scaling regime is determined by the relative values between the aspect ratio $k = \frac{t}{R}$, and normalized exchange length $L = \frac{l_{ex}}{R}$. If both $k$ and $L$ are small the magnetostatic energy is the sum of three terms with energies that scale very differently

$$E_{dip} = E_{\text{trans}} + E_{\text{bdry}} + E_{\text{bulk}}. \quad (2.19)$$

Where

$$E_{\text{trans}} = R^3 L k \int_\omega m_z^2 \quad (2.20)$$

$$E_{\text{bdry}} = \frac{1}{2\pi} R^3 k^2 |\log k| \int_{\partial \omega} (\mathbf{m} \cdot \hat{n}) \quad (2.21)$$
Table 2.1: Relative importance of the energy terms. Element size increases from left to right.

\[
E_{\text{bulk}} = \frac{1}{2} R^3 k^2 \int_\omega (\nabla U)^2. \tag{2.22}
\]

Here, \(\omega\) and \(\partial \omega\) are the surface area and edge respectively.

Early rigorous results were obtained by Gioia and James [13] and Carbou [14] in the limit of very small films. As the size of the film increases while keeping the aspect ratio \(k\) fixed, the role of the energy terms changes from being negligible, to becoming part of the variational problem, to become constraints. Kohn and Slatiskov have indicated [15] which is the appropriate expression for a given element size.

The smallest elements \((L\ fixed, k \to 0)\) obey the description of Gioia and James and Carbou [13, 14]. They overlap the Kohn-Slatiskov regime for small particles \((L^2 \gg k |\log k|, \text{“Stoner-Wohlfarth” regime})\). The terms \(E_{\text{ex}}, E_{\text{trans}}\) are treated as constraints, \(E_{\text{bulk}}\) is negligible and \(E_{\text{bdry}}\) is the leading order term.

This regime can be identified with the model of ferromagnetic rings used in the following chapters. As the size of the element increases \((L^2 \sim k |\log k|, \text{“Boundary penalty”})\) the magnetization is no longer constant and the exchange
energy becomes a new leading order $E_{\text{ex}}$ interacting with $E_{\text{bdry}}$.

A key issue is that $E_{\text{bulk}}$ and $E_{\text{bdry}}$ scale very differently and cannot be leading order terms simultaneously. Larger systems ($k \sim L^2$, “boundary vortex”) will have $E_{\text{bdry}}$ as constraints and $E_{\text{ex}}$ and $E_{\text{bulk}}$ interact in the variational optimization problem. The constraints forced by $E_{\text{bdry}}$ cannot be satisfied without sharp changes in the magnetization. The system develops boundary vortices. This regime is covered on the work of Moser and Kurzke [16].

The last regime occurs for extremely large samples where $E_{\text{ex}}$ becomes negligible ($L^2 \ll k |\log k|$, “Magnetostatic”). Both $E_{\text{bdry}}$ and $E_{\text{trans}}$ are constraints. The optimization problem reduces to minimizing $E_{\text{bulk}}$. This regime is studied in the work of DeSimone et al [17].

This classification of thin film regimes becomes useful for the study of reaction rates by simplifying the micromagnetic terms that must be optimized to find the metastable and transition states for a given geometry. It is also potentially useful to accelerate micromagnetic simulations of extended films.

In the context of this work, we study the magnetization reversal of ferromagnetic nanorings in the three smallest regimes. I confirm in full three dimensional micromagnetic simulations the validity of a theory for ring shaped ferromagnets based on the Braun’s model. Smallest rings are dominated by the exchange interaction and follow a constant saddle reversal. As rings get larger one enters the “boundary penalty” regime; it is confirmed numerically that in this regime the bulk term is in fact negligible and the magnetization reversal occurs through an instanton saddle state. For even larger rings we
enter the “boundary vortex” regime, we report the existence of a multiplicity of metastable state with energies equally spaced. The stability of these states is explained by the interaction between boundary vortices.
Chapter 3

Theory of Reaction Rates

3.1 The approach towards equilibrium

Let’s consider the abstract potential in Fig. 3.1 to represent a magnetic system. There are two stable configuration separated by some intermediate state. The temperature introduces random fluctuations that allow the system to cross the transition state which is associated to an energy barrier [4, 3]. Due to the probabilistic nature of these thermal fluctuations it is necessary to consider ensembles of systems.

The total population \( n \) is the sum of the populations at the basin of attraction of each stable state, \( n_+, n_- \); the average magnetization is equal to the difference between populations \( \langle m \rangle = n_+ - n_- \). The net rate of change of the populations is: \( n_\pm = k_{(\pm \rightarrow \mp)} n_\pm - k_{(\mp \rightarrow \pm)} n_\mp \) where \( k_{(\pm \rightarrow \mp)} \) is known as the single particle rate of escape from each basin of attraction. In equilibrium the
rate of change equals zero so that we obtain the detailed balance equation:

\[ k_{(+\to-)} \bar{n}_+ = k_{(-\to+)} \bar{n}_- \]  \hspace{1cm} (3.1)

The relaxation of the average magnetization towards its equilibrium value is obtained by noting that the total number of particles stays constant so that at any moment \( n_\pm = \frac{n_\pm \langle m \rangle}{2} \) and \( \dot{n}_\pm = \pm \frac{\dot{\langle m \rangle}}{2} \). The net magnetization changes as

\[ \langle \dot{m} \rangle = -2n_- = -2k_{+-}n_+ + 2k_{-+}n_- \]  \hspace{1cm} (3.2)

\[ = -2k_{+-} \frac{n + \langle m \rangle}{2} + 2k_{-+} \frac{n - \langle m \rangle}{2} \]  \hspace{1cm} (3.3)

\[ = (k_{-+} - k_{+-})n - (k_{-+} + k_{+-})\langle m \rangle. \]  \hspace{1cm} (3.4)

The first term is independent of time and can be written with the values at
equilibrium

\[(k_{---} - k_{---})n = k_{---}(2\bar{n} + \langle \bar{m} \rangle) - k_{---}(2\bar{n} - \langle \bar{m} \rangle)\]  

\[= (k_{---} + k_{---})\langle \bar{m} \rangle.\]  

(3.5)

We then have:

\[\langle \dot{m} \rangle = -(k_{---} + k_{---})(\langle m \rangle - \langle \bar{m} \rangle)\]  

(3.6)

which has a solution of the form

\[\Delta m(t) \equiv \langle m \rangle - \langle \bar{m} \rangle = \Delta m(0)e^{-(k_{---} + k_{---})t}\]  

(3.7)

where \(\Delta m(0)\) is the initial deviation from equilibrium. This expression describes the time dependence of the remanent magnetization; the key feature is the exponential decay of the fluctuations. The total relaxation rate is then \(k = k_{---} + k_{---}\). Notice that these results are independent of the underlying dynamics that influence the particle in either locus of attraction: all the information is contained in \(k_{---}\). The fundamental problem in the theory of reaction rates is to accurately obtain \(k_{---}\).
3.2 Stochastic Calculus

We start from the equation of motion of an arbitrary system:

$$\frac{dX}{dt} = b(X)$$  \hspace{1cm} (3.9)

in which the variable $X$ represents the slowest varying degrees of freedom. Thermal effects are associated to the rapid degrees of freedom and incorporated as a random perturbation $\dot{W}$ with a gaussian profile:

$$\frac{dX}{dt} = b(X) + \sqrt{\epsilon \sigma(X)} \dot{W};$$  \hspace{1cm} (3.10)

$$\langle \dot{W} \rangle_t = 0, \langle \dot{W}(t) \dot{W}(t') \rangle = \delta(t - t')$$  \hspace{1cm} (3.11)

the value of $\epsilon$ determines the strength of the thermal fluctuations. Equations such as 3.10 that include both deterministic and random terms are called equations of the Langevin type. The value of $\epsilon$ in terms of temperature is obtained from the fluctuation-dissipation theorem to reflect that the system and the bath are in thermal equilibrium. The diffusion matrix $\sigma(X)$ indicates how the system reacts to the thermal fluctuation.

We can calculate the change of $X$ by integrating over a short time interval:

$$dX = \int_t^{t+dt} b(X) dt' + \int_t^{t+dt} \sqrt{\epsilon \sigma(X)} \dot{W} dt'.$$  \hspace{1cm} (3.12)
while the first integral is simply \( b(X)dt \). The second integral is ambiguous because of the presence of \( \delta(t - t') \): should it be taking in the beginning, the middle or the end of the integration integral? The answer to this results in different interpretations of the Langevin equation. A properly defined stochastic problem therefore should explicitly state the interpretation being used. The most commonly used interpretations are the Itô, Stratonovich and kinetic interpretation which correspond to evaluation the integrals in the beginning, middle and end of the interval.

The change \( \Delta X = X(t + \Delta t) - X(t) \) for each interpretation, is then:

\[
\Delta X = b(X(t))\Delta t + \sqrt{\epsilon \sigma(X)} \int_t^{t+\Delta t} \dot{W} dt \quad \text{Itô (3.13)}
\]
\[
\Delta X = b(X(t))\Delta t + \sqrt{\epsilon \sigma(X(t)) + \sigma(X(t + \Delta t))} \int_t^{t+\Delta t} \dot{W} dt \quad \text{Stratonovich (3.14)}
\]
\[
\Delta X = b(X(t))\Delta t + \sqrt{\epsilon \sigma(X(t + \Delta t))} \int_t^{t+\Delta t} \dot{W} dt \quad \text{kinetic. (3.15)}
\]

This technical detail has profound implications for the subsequent statistical analysis of physical systems. Of particular importance is how the choice of interpretation determines the form of the Fokker-Planck equation.

An equation of the Fokker-Planck type describes how the probability distribution function of a system changes in time. In what follows I will provide a derivation of the Fokker Planck equation. Let's \( P(X, t) \) be the probability distribution function of the variable which evolves according to 3.10. We start
from the following identity:

\[ P(X, t + dt) = \int T(X, t + dt|X - \Delta X, t) P(X - \Delta X, t) d(X - \Delta X) \] (3.16)

where \( T(X, t + dt|X - \Delta X, t) \) is the transition probability for small \( dt \). The integrand can be expanded in powers of \( \Delta X \) as:

\[
T(X - \Delta X + \Delta X, t + dt|X - \Delta X, t)P(X - \Delta X, t) = \\
\sum_{n=0}^{\infty} \frac{(-\Delta X)^n}{n!} \cdot \nabla_X^n (T(X + \Delta X, t + dt|X, t)P(X, t))
\] (3.17)

so that the integral can be done in \( \Delta X \)

\[ P(X, t + dt) = \int \sum_{n=0}^{\infty} \frac{(-\Delta X)^n}{n!} \cdot \nabla_X^n (T(X + \Delta X, t + dt|X, t)P(X, t)) d(\Delta X). \] (3.18)

After separating the first term of the expansion

\[
= \int \sum_{n=0}^{\infty} \frac{(-\Delta X)^n}{n!} \cdot \nabla_X^n T(X + \Delta X, t + dt|X, t)P(X, t) d(\Delta X) \\
+ \int T(X + \Delta X, t + dt|X, t)P(X, t) d(\Delta X)
\] (3.19)

realizing that the second factor on the last term is independent of the variable
of integration

\[ dP(X, t) = \int \sum_{n=1}^{\infty} \frac{(-\Delta X)^n}{n!} \cdot \nabla^n_X T(X + \Delta X, t + dt|X, t) P(X, t) d(\Delta X) \]

(3.20)

and that the remaining integral is simply unity we obtain:

\[ dP(X, t) = \int \sum_{n=1}^{\infty} \frac{(-\Delta X)^n}{n!} \cdot \nabla^n_X T(X + \Delta X, t + dt|X, t) P(X, t) d(\Delta X). \]  (3.21)

We now switch the order of the sum and the integral to get

\[ dP(X, t) = \sum_{n=1}^{\infty} \frac{(-1)^n \nabla^n_X}{n!} \left( P(X, t) \int (-\Delta X)^n T(X + \Delta X, t + dt|X, t) d(\Delta X) \right) \]

(3.22)

using only the terms up to second order we end up with

\[ dP(X, t) = -\nabla_X (P(X, t) M_1) + \frac{1}{2} \nabla^2_X (P(X, t) M_2) \]  (3.23)

where

\[ M_n = \int (\Delta X)^n T(X + \Delta X, t + dt|X, t) d(\Delta X) = \langle (\Delta X)^n \rangle \]  (3.24)

are the moments of \( T \). The Taylor expansion of \( M_n \) to first order in \( dt \) is

\[ M_n \approx \frac{dM_n}{dt} dt \] because at \( dt = 0 \) the system is known to be at \( X \) and \( \Delta X = 0 \).
We then have the Fokker-Planck equation:

\[
\frac{dP(X,t)}{dt} = -\nabla_X (P(X,t) \frac{d\langle (\Delta X)^1 \rangle}{dt}) + \frac{1}{2} \nabla^2_X (P(X,t) \frac{d\langle (\Delta X)^2 \rangle}{dt}). \quad (3.25)
\]

The values for \(\frac{d\langle (\Delta X)^n \rangle}{dt}\) differ in the Itô and Stratonovich representations. We express both results indexing the components of \(X\) and \(\sigma\)

\[
\begin{align*}
\frac{dP}{dt} = & -\frac{\partial}{\partial x_i} [b_i P] + \sum_{ij} \frac{\partial^2}{\partial X_i \partial X_j} [\frac{\xi}{2} \sigma_{ik} \sigma_{jk} P] \quad \text{(I)} \quad (3.26) \\
\frac{dP}{dt} = & -\frac{\partial}{\partial x_i} \left[ (b_i + \frac{\xi}{2} \sigma_{jk} \frac{\partial \sigma_{ik}}{\partial x_j}) P \right] + \sum_{ij} \frac{\partial^2}{\partial X_i \partial X_j} \left[ \frac{\xi}{2} \sigma_{ik} \sigma_{jk} P \right] \quad \text{(S).} \quad (3.27)
\end{align*}
\]

### 3.3 Macrospin magnetization dynamics in the presence of thermal noise.

The magnetization dynamics is described by the Landau-Lifshitz equation:

\[
\frac{d\mathbf{m}}{dt} = \frac{\gamma}{1 + \alpha^2} \mathbf{m} \times \nabla E + \frac{\gamma \alpha}{1 + \alpha^2} \mathbf{m} \times (\mathbf{m} \times \nabla E) \quad (3.28)
\]

We add a white noise random field \(\mathbf{h} = \sqrt{\tau} \mathbf{W}\) to the effective field \((\mathbf{H}_{\text{eff}} = \frac{\nabla E}{\mu_0})\) and the result is an equation of the Langevin type. We write it in tensor notation

\[
\partial_t m_\rho = \frac{\gamma}{1 + \alpha^2} (\epsilon_{\mu \rho} m_\mu \left( \frac{\partial E}{\mu_0} + \sqrt{\tau} W_\nu \right) + \alpha (\delta_{\mu \rho} - m_\mu m_\rho) \left( \frac{\partial E}{\mu_0} + \sqrt{\tau} W_\nu \right)). \quad (3.29)
\]
There is controversy about the appropriate interpretation to be used. One should note that in the Stratonovich representation the magnetization norm is automatically conserved. It was pointed out in Ref. [18] that in cartesian coordinates (CC) the Gibbs distribution is a solution of the Fokker-Planck corresponding equation to eq. 3.29 only in the Stratonovich representation; on the other hand, Berkov indicates that the Itô drift term is irrelevant since it is discarded when considering that the magnetization’s magnitude must remain constant [19]. According to Berkov, the practical realizations of systems trajectories will change but the average system properties will be the same regardless of the stochastic interpretation. In spherical coordinates (SC) the noise is additive so the two interpretations are equivalent [20]; however, the metric in spherical coordinates contains singularities in the poles which make CC more appealing for numerical work; the following work does not assume SC. We interpret eq. 3.29 in the Stratonovich sense:

\[
\partial_t m_\rho = \frac{\gamma}{1+\alpha^2} (\epsilon \epsilon_{\mu\nu\rho} m_\mu \left( \frac{\partial E_\mu}{\mu_0} + \sqrt{\epsilon} W_\nu \right) - \alpha \left( \delta_{\rho\nu} - m_\rho m_\nu \right) \left( \frac{\partial E_\mu}{\mu_0} + \sqrt{\epsilon} W_\nu \right) ) \text{ (Itô)}. \tag{3.30}
\]

We can rewrite this equation as:

\[
\partial_t m_\rho = -K_{\rho\nu} \frac{\partial E}{\mu_0} - \epsilon \frac{\gamma^2}{1+\alpha^2} m_\rho + \sqrt{\epsilon} \sigma_{\rho\nu} \dot{W}_\nu \tag{3.31}
\]

where the symmetric \( K^S \) antysimmetric \( K^A \) drift matrices and the diffusion
matrix $\sigma$ are defined as:

\[
K^S_{\rho\nu} = \frac{\alpha \gamma}{1 + \alpha^2} (m^2 \delta_{\rho\nu} - m_\rho m_\nu)
\]

\[
K^A_{\rho\nu} = \frac{\gamma}{1 + \alpha^2} \epsilon_{\mu\nu\rho} m_\mu
\]

\[
\sigma_{\rho\nu} = \frac{\gamma}{1 + \alpha^2} (\epsilon_{\mu\nu\rho} m_\mu - \alpha (m^2 \delta_{\rho\nu} - m_\rho m_\nu)) \sqrt{\epsilon}.
\]

The Fokker-Planck equation for a Langevin equation in the Itô representation is written as [18]:

\[
\partial_t P = \partial_\rho (b_\rho P) + \partial_\rho \partial_\nu (\epsilon \sigma_{\rho\mu} \sigma_{\nu\mu} P)
\]

(3.33)

where $b_\rho = -K_{\rho\mu} \partial_\mu E - \epsilon \frac{\gamma^2}{1 + \alpha^2} m_\rho$ is the deterministic drift vector.

### 3.3.1 The stationary distribution function of the Stochastic Landau Lifshitz equation is the Gibbs distribution

It is a known fact from elementary statistical mechanics that physical systems governed by a Hamiltonian set of equation of motion obey the Gibbs probability distribution. However, one would be misled to believe that this result could be applied directly to a probabilistic study of ensembles governed by the Landau Lifshitz Equation.

First, we point out that the LLG equations do not form a Hamiltonian system. Hamiltonian system are described by a parameter $X(q, p)$ which contains information on both the spatial coordinates and momenta and satisfy the Hamiltonian equations of motion: $\dot{X} = \{q, p, H\}$, $\dot{p} = -\nabla_q H$ where $H$ is
the Hamiltonian. This is clearly not the structure of the Landau-Lifshitz-Gilbert equation. To name only one aspect, in a Hamiltonian system the momenta account for the inertial energy of the system and the coordinates are associated with the position of the system and the potential energy. In the LLG equations the magnetization serves the dual role of being the angular momentum and the orientation of the system.

Nevertheless, the LLG system of equations do share algebraic features with Hamiltonian systems which, remarkably, guarantee that the Gibbs distribution is the equilibrium distribution of the LLG equation. Namely, a Hamiltonian system can be expressed as \( \{q, p\} = A_{q,p} \nabla H(q, p) \) where \( A_{q,p} \) is an antisymmetric matrix. Substituting this expression into the Fokker-Planck equation one proves that the distribution \( P = e^{-E/k_B T}/Z \) satisfies \( \partial_t P = 0 \).

In what follows, we apply this procedure to the magnetism case in which the dynamical system is more complex and reads: \( \dot{M} = A_M \nabla E + S_M \nabla E \) where \( A, S \) are symmetric and antisymmetric matrices.

We need to prove that the Gibbs distribution function is a stationary solution \( (\partial_t P = 0) \) of eq. 3.33 and that the noise level is related to the temperature by the fluctuation dissipation principle: \( \epsilon = \frac{2k_B T \alpha}{\mu_0 M_s \gamma v} \).

We first note that \( a_{\rho \nu} \equiv \sigma_{\rho \mu} \sigma_{\nu \mu} = \frac{2^2}{1+\alpha^2} (m^2 \delta_{\rho \nu} - m_\rho m_\nu) = -\frac{2}{\alpha} K_s^{\rho \nu} \) and rewrite the FP equation as:

\[
\partial_t P = \partial_\rho (b_\rho P + \partial_\nu (\epsilon a_{\rho \nu} P)).
\] (3.34)
After substitution the parenthesis on the right hand side becomes:

\[
(-K_{\rho\nu}\frac{\partial_{\nu}E}{\mu_0} - 2\epsilon\frac{\gamma^2}{1 + \alpha^2}m_{\rho})P + \partial_{\nu}(-\frac{\gamma}{\alpha}K_{\rho\nu}^S\epsilon P) \tag{3.35}
\]

\[
= -(K^A_{\rho\nu} + K^S_{\rho\nu})P\frac{\partial_{\nu}E}{\mu_0} - 2\epsilon\frac{\gamma^2}{1 + \alpha^2}m_{\rho}P
- \frac{2\alpha}{\alpha}(P\partial_{\nu}K^S_{\rho\nu} - \frac{1}{k_B T}PK^S_{\rho\nu}\partial_{\nu}E) \tag{3.36}
\]

The second and last term cancel so Eq. 3.34 becomes

\[
\partial_t P = -K^A_{\rho\nu}\frac{\partial_{\nu}E}{\mu_0} P = \epsilon_{\mu\nu\rho}\frac{k_BT\gamma m_{\mu}}{\mu_0(1 + \alpha^2)}\partial_{\nu}P \tag{3.37}
\]

where we have used
\[
-\frac{2\alpha}{\alpha}\epsilon\partial_{\nu}K^S_{\rho\nu} = \frac{\gamma^2}{1 + \alpha^2}\epsilon\partial_{\nu}(m_{\mu}m_{\mu}\delta_{\rho\nu} - m_{\rho}m_{\nu}) = -2\epsilon\frac{\gamma^2}{1 + \alpha^2}m_{\rho}.
\]

The remaining term is divergenceless since:

\[
\partial_{\rho}(\epsilon_{\mu\nu\rho}m_{\mu}\partial_{\nu}P) = \epsilon_{\mu\nu\rho}\delta_{\rho\nu}\partial_{\nu}P + \epsilon_{\mu\nu\rho}m_{\mu}\partial_{\rho}\partial_{\nu}P = 0. \tag{3.38}
\]

The first term contains an index repetition of an antisymmetric vector. The second is null because it contains the curl of a gradient. We conclude that the Gibbs distribution is a statistical steady state distribution of the stochastic Landau-Lifshitz equation. Although we derived this result for the case of a single macrospin it also applies for cases with multiple particles (e.g. a system of interacting dipoles) or nonuniform magnetizations (e.g. multidomain magnetic system).
Chapter 4

Néel-Brown Models for magnetization reversal of single domain particles.

4.1 Néel’s approach

Néel proposed the earliest theoretical model of relaxation of ferromagnetic particles [3] in an attempt to explain remanent magnetization data taken by Tellier, Roquet and Nagata. They studied the remanent magnetization behavior of baked clay and lava and found that clay aged for a long time at room temperature ($10^2$ years, 300K) had the same remanent magnetization of similar samples exposed to high temperatures for short times (5 minutes, 650K). Néel’s results provide an expression for the magnetization relaxation rates based on
the magnetoelastic properties of the particles. Néel’s work was done without considering the underlying dynamics of the magnetization (i.e. Landau-Lifshitz-Gilbert equation); instead he considered that thermal agitation close to the energy barrier was derived from the vibrational modes of the crystal lattice. Temperature is not defined by use of the Fokker-Planck equation but by equating the vibrational energy of the lattice to $k_B T$. Then, thermal equilibrium is the result of balancing fluctuations of the magnetization and vibrations of the lattice.

In Néel’s work, the magnetization $M$ was constant in magnitude $M_s$ and the particle had small volume $v$ and uniaxial anisotropy of magnitude $K$ along the $z$ axis. This is known as the macrospin or Stoner-Wohlfarth model [21]. A field $H_{\text{ext}}$ is applied along the anisotropy axis. Using normalized magnetization components (e.g. $m_z = \frac{M_z}{M_s}$), the energy of the particle as a function of its magnetization along $z$ can be written as:

$$E = -K m_z^2 - \mu_0 H_{\text{ext}} M_s m_z. \quad (4.1)$$

The key features of this system’s hysteresis loop at zero temperature are captured in Fig.4.1 which present the magnetic energy as a function of the scaled field $h \equiv \frac{\mu_0 H_{\text{ext}} M_s}{2K}$. The value of $m_z$ corresponding to the energy minima are $\pm 1$. The energy barrier is $\Delta E = K(|h| - 1)^2$ for fields between $h = \pm 1$ with maxima at $m_z = -h$. The coercive field corresponds to the dissapearance of the energy barrier.
In thermal equilibrium, the Boltzmann probability distribution reads $P(m_z)dm_z = Z^{-1}e^{-\frac{E(m_z)}{k_B T}} dm_z$ where $Z$ is the partition function $Z = \int_{-1}^{1} e^{-\frac{E(m_z)}{k_B T}} dm_z$ (using $\int_{0}^{\pi} f(\theta) \sin \theta d\theta = \int_{-1}^{1} f(m_z) dm_z$). Néel assumes an out of equilibrium configuration in which all particles are initially oriented opposite to the magnetic field $(n_+ = 0, n_- = n)$, but inside the metastable potential well the ensemble is at equilibrium. The probability distribution function for this system will be:

$$P^*(m_z) = \frac{g^*(m_z)dm_z}{Z^*} = \frac{e^{-\frac{E(m_z)}{k_B T}}}{\int_{-h/2}^{h/2} e^{-\frac{E(m_z)}{k_B T}} dm_z} \approx 2K \frac{e^{-\frac{\Delta E(m_z)}{k_B T}}}{k_B T} dm_z,$$

(4.2)
where we have assumed that the barrier is high enough for the integral to be dominated by the bottom of the well. The number of particles that escapes the potential barrier in a time interval $dt$ is $n_- k_{+\rightarrow} dt$. This matches the number of particles moving towards the barrier with a speed $|\frac{dm_z}{dt}|$ provided by a random bath. The region between $|\frac{dm_z}{dt}| dt$ of the energy maximum at $m_z = -\hbar/2$ is populated by $n_- g^*(m_z) |\frac{dm_z}{dt}| dt$. Therefore:

$$n_- k_{+\rightarrow} dt = \frac{1}{2} n_- g^*(m_z) |\frac{dm_z}{dt}| dt.$$  \hspace{1cm} (4.4)

And the rate is obtained from

$$k_{+\rightarrow} = \frac{1}{2} g^*(m_z) |\frac{dm_z}{dt}| \approx \frac{K e^{-\frac{\Delta E(m_z)}{k_B T}}}{k_B T} \left|\frac{dm_z}{dt}\right|.$$  \hspace{1cm} (4.5)

The value of $|\frac{dm_z}{dt}|$ is obtained by Néel from the oscillation modes of the crystal lattice and is proportional to $\sqrt{\frac{kT}{\pi}}$. So that

$$k_{+\rightarrow} \approx \frac{C K}{\sqrt{\pi k_B T}} e^{-\frac{\Delta E(m_z)}{k_B T}} = f_0(T) e^{-\frac{\Delta E}{k_B T}}$$  \hspace{1cm} (4.6)

where $C$ measures the lattice response to thermal fluctuations.

Eqs. 4.6 and 3.8 summarize the essential features of magnetization reversal processes. The approach towards equilibrium is an exponential decay with a rate equal to the sum of forward and backward reversal rate. It easily explains the relation of aging and temperature of magnetic nanoparticles. However, the proximity to the energy maximum is not clearly defined. It also
ignores the dynamics close to the transition point, and is not valid in system without axial symmetry.

4.2 Macrospin Model - Brown’s approach

Brown applied Kramer’s theory of reaction rates to the study of themally assisted magnetization reversal. As opposed to Néel he took into account the Landau-Lifshitz-Gilbert equation to obtain the prefactors. Close the critical points \( \mathbf{m}^\ast \) the total magnetic energy can be approximated as a quadratic function

\[
E(\mathbf{m}^\ast) \approx E(\mathbf{m}^\ast) + \frac{1}{2}(m_\mu - m_\mu^\ast)(m_\nu - m_\nu^\ast)\partial_\mu \partial_\nu E(\mathbf{m}^\ast) \tag{22}.
\]

The term includes the Hessian Matrix \( \partial_\mu \partial_\nu E(\mathbf{m}^\ast) \) and can be written in the basis which diagonalizes it

\[
E(\mathbf{m}^\ast) \approx E(\mathbf{m}^\ast) + \frac{1}{2} \lambda_\mu \eta_\mu^2
\]

where \( \eta_\mu = (m_\mu - m_\mu^\ast) \) and \( \lambda_\mu \) are the eigenvectors and eigenvalues of the energy functional close to the critical points.

In the previous section we demonstrated that in equilibrium the magnetization follows a Gibbs distribution. Brown assumes that the populations close to each energy minima have achieved thermal equilibrium so that two independent probability distribution functions can be defined

\[
P^\pm(\mathbf{m})\delta(1-m^2)d^3\mathbf{m} = \frac{e^{-\frac{E(\mathbf{m})}{k_B T}} \delta(1-m^2)d^3\mathbf{m}}{Z^\pm}\approx \frac{e^{-\frac{E(\mathbf{m}^\pm)}{k_B T}}e^{-\frac{\lambda_\nu \eta_\nu^2}{2k_B T}} \delta(1-m^2)d^3\mathbf{m}}{Z^\pm}
\]

where

\[
Z^\pm = \int_{\Omega^\pm} e^{-\frac{E(\mathbf{m}^\pm)}{k_B T}}e^{-\frac{\lambda_\nu \eta_\nu^2}{2k_B T}} \delta(1-m^2)d^3\mathbf{m}
\]

are the independent partition

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functions in each basin of attraction $\Omega_\pm$. The probability of finding the system in any of the basins of attraction is: $P(\mathbf{m} \in \Omega_\pm) = \frac{Z_\pm}{Z_\pm}$. The probability of escape is proportional to the rms velocity of particles in a very small region to the saddle point $\mathbf{m}_s$, which can be written approximately as proportional to the eigenvalue on the unstable direction $\lambda^i_s$. We account for these particles in this small region using the probability density in the proximity of the saddle state $n_s = \frac{1}{Z_\pm} \int \sqrt{\lambda^i_1} \delta(\eta_1) e^{-\frac{E(\mathbf{m}_s) - \frac{1}{2} \lambda^i_1 \eta_1^2}{k_B T}} \delta(1 - \mathbf{m}^2) d^3\mathbf{m}$, where $\eta_1$ identify the single unstable direction. The rate is then

$$k_{\rightarrow\leftarrow} = \frac{\lambda^i_s}{2\pi} e^{-\frac{E(\mathbf{m}_s)}{k_B T}} \int e^{-\frac{1}{2} \lambda^i_1 \eta_1^2}{k_B T} \delta(1 - \mathbf{m}^2) d^3\mathbf{m} = \frac{\lambda^i_s}{2\pi} \sqrt{\frac{\Pi_1^\pm \lambda^i_1}{\Pi_2^\pm \lambda^i_1}} e^{-\frac{\Delta E}{k_B T}}.$$

This is a general result of transition state theory [1]: the escape rate from a basin of attraction is the product of an exponential of the activation energy and a prefactor that depends on the local dynamics around the minima and the saddle point. This summarizes the Néel-Brown model. The $T^{1/2}$ temperature dependence of the prefactor of the Néel-Brown model may not be detected experimentally due to the long extrapolation of the Arrhenius plot required to estimate the prefactor [23].

Another approach to study reversal rate is by use of telegraph noise measurements in which the observable quantity exhibit fast switching between two well defined values: the dwell times are recorded and then the probability of the system reversing between a certain interval $dt$ around a time $t$ are obtained.
[24]. The relaxation time $\tau$ is obtained by fitting the data to $P(\tau) = 1 - e^{-\frac{t}{\tau}}$. In addition, reversal studies allow us to estimate the activation energy and prefactor for thermal induced reversal. An exhaustive numerical study of magnetic properties for the stochastic Landau-Lifshitz equation on the Néel-Brown model summarizes key aspects of numerical integration for the model [18].

### 4.3 Non uniform magnetization reversal

While the Transition Rate Theory still applies, the energy function is no longer as simple as Eq.4.1. One should now rewrite and incorporate further terms in the micromagnetic energy. Most magnetic systems are well described by four micromagnetic energy terms introduced in [25]. Since the local Langevin equation does not change in structure, the Gibbs distribution can be used in conjunction with Kramers' theory of reaction rates to characterize magnetization reversal in ferromagnetic nanostructures.

#### 4.3.1 Braun’s study of elongated magnetic particles

The transition states can be found by finding the critical points of the energy defined by Eq. 2.18. We can rewrite the energy function (Eq. 2.18) as

$$E = \int_{\Omega} (A(\nabla m)^2 + \xi(M))dV.$$  \hspace{1cm} (4.9)
with $\xi(M)$ is an abstract function that depends solely on $M$ and is independent of its derivatives. The Euler-Lagrange equation states that critical points should satisfy

$$2A\nabla^2 m - \nabla_M \xi = 0.$$ \hfill (4.10)

A localized fluctuation of the magnetization results in a positive exchange energy which can be out balanced by a combined net decrease due to the remaining energy terms. The Néel-Brown transition state ($\nabla m = 0$), is a possible transition state of all ferromagnetic systems. However, it is obvious from Eq. 4.9 that the energy barrier will become arbitrarily large with increasing volume. It had been already observed that reversal by nucleation and propagation of domain walls present much smaller activation energies than those predicted by the Néel-Brown model. All solutions of Eq. 4.10 correspond to stationary points of Eq. 3.29. The same argument used for the Néel-Brown model can be used in this continuum model to conclude that the reversal rate is of the form given by Eq. 4.8.

Braun focused in an elongated systems where the magnetization only depends in the axial coordinate (labeled $x$). The emphasis was on geometries where the external fields was applied along the easy magnetization axis and the combined crystalline and shape anisotropies resulted in a high cost for fluctuations out of the easy plane. In such cases, the magnetization is constrained to the easy plane and the configuration is captured in the dependence of the
angle $\phi$ that the magnetization makes with the easy axis. Hence Eq. 4.10 becomes

$$2A \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial \xi}{\partial \phi} = 0. \tag{4.11}$$

Multiplying by $\frac{\partial \phi}{\partial x}$ and integrating on $x$ an “energy conservation equation” can be obtained [26]

$$A \left( \frac{\partial \phi}{\partial x} \right)^2 - \xi(\phi) = C \tag{4.12}$$

in which the coordinate $x$ serves the role of the time $t$ and the angle $\phi$ represents the position of an imaginary particle on a reversed potential $-\xi(\phi)$.

The analogy is represented in Figure 4.2. The constant of integration $C$ is analog to the total energy and is drawn as horizontal lines. Non uniform configurations are represented by the oscillations of the particle between two points. The instanton saddle configuration starts from $\phi = \pi$ passes through the position occupied by the constant saddle and bounces back after reaching the opposite side of the energy well. Precisely at the value of $C$ that matches the value of the reversed potential the ‘velocity’ approaches zero as the metastable state is reached. The information is converted to the real representation of angle as a function of position in Fig. 4.2 b. The slope of the curve is zero at the amplitude given by the metastable state and at the return point, and maximum at the constant saddle magnitude.

Pushing the analogy further allows to find the minimum length of a particle to permit reversal through the instanton saddle. The uniform saddle, $\frac{\partial \phi}{\partial x} = 0$ is obtained at the value of $\phi$ for which $-\xi$ is a minimum. The period of oscillation
Figure 4.2: a) Reversed potential where the minimum value corresponds to the transition state and the two maxima represents the two attractive configurations. The constant of integration $C$ in Eq. 4.2 is analog to the total energy of a particle moving in the reversed potential. The blue lines indicate the maximum amplitude of the instanton saddle.
around a parabolic potential is mostly dominated by the restoring forces at the bottom of the potential. By the same reasoning, the magnetization fluctuates around this angle with a wavelength which is at least \[ L = 2\pi \sqrt{A \frac{\partial^2 \xi}{\partial \phi^2}} |_{\phi_{\text{min}}}^{-1} \]. This proves that nonuniform transition states can only exist for sample lengths larger than \[ 2\pi \sqrt{A \frac{\partial^2 \xi}{\partial \phi^2}} |_{\phi_{\text{min}}}^{-1} \]; for smaller samples reversals can only through the constant saddle.

An important consequence of nonuniform magnetization reversal in infinite cylinders is that the nucleation can occur anywhere in the sample. This introduces a degeneracy of the reversal which results in a zero energy excitation mode (Goldstone mode) around the instanton saddle configuration [9]; the eigenvalue must be removed from rate calculations by use of a regularization procedure. This changes the prefactor behavior dramatically: while in the Néel-Brown case the prefactor has a mild dependence on external fields smaller than the coercive field [27], for the instanton case the prefactor changes by almost three orders of magnitude as the external field varies by the same amount [6].

### 4.3.2 Criticism by Aharoni to Brauns model of non uniform magnetization reversal

Aharoni disagreed with the approximations used by Braun in the development of the instanton model [28]. Aharoni argued that soft ferromagnetic cylinder reverse its magnetization via the “curling mode” proposed by Frei et. al [29].
In particular, Aharoni mentioned criticised Braun’s work in three aspects. First, Braun postulated his model to be exact for cases on which the magnetostatic can be neglected and if crystalline anisotropies dominate; this does not occur for typical materials. Second, the model could apply when the magnetization varies slowly compared to the particle diameter so that all anisotropy constants are related to the components of the demagnetizing tensor. For Aharoni, no variation of the magnetization was slow enough in Braun’s model because all configurations described resulted in large magnetostatic charges [30]. In the third approach, the magnetostatic energy was included in a renormalized value of the crystalline anisotropy, Aharoni disagreed with this approach on two grounds: that the renormalization was field dependent and reversal through solitons would take much longer than curling mode nucleation for all relevant fields, and that Braun implicitly assumed that demagnetization and crystalline anisotropy axis were parallel which does not occur in general.

4.3.3 Numerical evidence against Braun’s model for non-uniform magnetization reversal.

The intrinsic danger of simplifications on the energy functional can be avoided by the use of numerical techniques for the study of magnetization reversal. Numerical investigation of long elongated particle have indicated that end caps of the cylinder play an important role on the magnetization reversal Brown et al. [31], E et al. [32]. The remanent magnetization at the end caps is not collinear
with applied fields, so that the reversal occurs by propagation of domain walls starting at the sample ends and not at an arbitrary position along the sample as would happen for infinite samples. Neither the metastable states, nor the saddle configurations are dependent solely on the axial coordinate.

4.3.4 Refinements to the original Braun’s model

Despite these caveats, progress in fabrication and measurement of magnetic properties of nanowires proved that the instanton fluctuation was an accurate description of reality. Experimental measurements in ferromagnetic nanowires proved that wires of small diameter actually present activation energies consistent with Braun’s model [33, 34]. The analytical issues were later addressed by separating the magnetostatic energy into a local and nonlocal terms so that, to a good approximation, all anisotropy terms can be absorbed into a local demagnetizing tensor. Similarly, a refinement of the model incorporated the effect of the end caps giving an energy barrier of about half the original Braun’s model. Furthermore, Braun indicated that the curling mode requires wire diameters much larger than the exchange length and there is a high topological energy barrier that prevents passage through the curling mode in small diameters. Lastly, Braun indicated that Aharoni’s objection resulted from a misinterpretation of the parameters involved and showed that Aharoni’s exact calculation of the magnetostatic energy was identical to the results obtained using only Braun’s local approximation.

The discussion of the validity of Braun’s model for magnetization reversal
in long cylinders is also relevant for the model of magnetization reversal of ferromagnetic nanorings. In the next chapter, we present numerical evidence in agreement with the Martens et al. model.
Chapter 5

Thermally induced reversal in ferromagnetic nanorings

In this chapter, numerical micromagnetics are used to test the predictions of the analytical theory of Martens et al. [11] for thermally induced transitions between states of opposite chirality in a 1D approximation to the ring. The simulations were made for a variety of mean radii, annular widths and magnetic fields.

The geometry under study and accompanying relevant parameters are represented in Fig. 5.1. The magnetic material is in the shape of an annulus of mean radius $R$, annular width $\Delta R$ and (in the third dimension) thickness $t$. A current $I$ running along the axis of the ring produces a circumferential external field $H(r) = (I/2\pi r)\hat{\theta}$. The ring is composed of a soft isotropic ferromagnet (e.g., permalloy) with saturation magnetization $M_s$ and exchange length $l_{ex}$. 
In all of the geometries considered, the aspect ratio $k = t/R \ll 1$, giving rise to magnetostatic forces that constrain the magnetization to lie in the plane of the ring ($M_z = 0$) [11]. A magnetization configuration can therefore be completely described by $\phi(\theta, r)$, the angle the magnetization at a given radius makes with the unit vector lying along the tangent to the circle with that radius: 

$$M(\theta, r) = (M_x, M_y, M_z) = M_s(\sin(\phi - \theta), \cos(\phi - \theta), 0).$$
5.1 Model

Our starting point is the Landau-Lifshitz-Gilbert (LLG) equation [35, 36]

\[ \frac{dM}{dt} = -|\gamma|M \times H_{\text{eff}} - |\gamma|\alpha M \times (M \times H_{\text{eff}}), \]  

(5.1)

where \( \gamma \) is the gyromagnetic ratio and \( \alpha \) is the (phenomenological) damping constant. The effective magnetic field, \( H_{\text{eff}} = -\nabla M E \), contains all (external and internal) fields and is the variational derivative of the total micromagnetic energy

\[ E[M(r)] = \mu_0 l_{ex}^2 \int_{\Omega} d^3r |\nabla M|^2 \]

(5.2)

\[ + \frac{\mu_0}{2} \int_{R^3} d^3r |\nabla U|^2 - \mu_0 \int_{\Omega} d^3r \mathbf{H}_e \cdot \mathbf{M}. \]

The three terms above correspond respectively to the exchange energy, demagnetization (or magnetostatic) energy, and Zeeman energy, with the (small) magneto-crystalline anisotropy term neglected. (The last of these can be easily included, but for the materials and geometries considered here, it is typically overwhelmed by the much larger shape anisotropy arising from the demagnetization term.) Here \( \Omega \) is the volume of the ring, \( l_{ex} = \sqrt{2A/(\mu_0 M_s^2)} \) is the exchange length (where \( M_s \), the magnitude of the magnetization, is assumed to be the same everywhere, and \( A \) is the exchange constant), \( \mathbf{H}_e \) is the applied external magnetic field, and \( |\nabla M|^2 \equiv |\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2 \).

The “magnetostatic potential” \( U \), arising from long-range dipole-dipole interactions within the magnetic material, satisfies \( \nabla^2 U = \nabla \cdot \mathbf{M} \) (and suitable
boundary conditions in the interfaces between media), which can be derived through Maxwell’s equations. Our simulations involve numerical integration of the above set of equations.

The extremal states of a quasi-1D ferromagnetic ring (i.e., $\Delta R \ll R$ so that the external magnetic field does not vary significantly with distance from the center of the ring) in a circumferential magnetic field have been analytically obtained [11]. The solutions found there apply in the thin-ring limit: $k = t/R \ll 1$ and $(l_{ex}/R)^2 \sim (t/R)|\ln(t/R)|$. Under these conditions the second term on the RHS of (5.2) separates into three main terms (and a number of smaller ones): a term which extracts a large energy cost when the magnetization does not lie completely within the plane of the annulus; a local surface term (the shape anisotropy, which favors alignment of the magnetization with the tangential direction at the inner and outer ring radius); and a nonlocal bulk contribution. Analysis of these terms finds that the bulk term is small compared to the surface term and can therefore be neglected [11]. In Sec. 5.3 we test these conclusions for more realistic geometries by computing numerically the total demagnetization energy and comparing it to the (analytically computable) local surface (i.e., shape anisotropy) term.

In the 1D approximation the total energy reduces to

$$E = 2\mu_0 M_0^2 \left(\frac{t}{\pi}\right)^2 \frac{t}{R} \Delta R \times l_{ex}^2 \int_0^{\pi} \left[\left(\frac{2h}{\ell} \frac{\partial \phi}{\partial \theta}\right)^2 + \sin^2 \phi - 2h \cos \phi\right] d\theta,$$

(5.3)
where the parameters $\ell$ and $h$ are the scaled circumference and field:

$$
\ell = \frac{R}{l_e} \sqrt{2\pi \left( \frac{\ell}{\Delta R} \right) \left| \ln \left( \frac{\ell}{R} \right) \right|}
$$

$$
h = \frac{H_e}{H_c} = \frac{\mu_0 M_s}{\pi} \frac{H_e}{\left| \ln \left( \frac{\ell}{R} \right) \right|},
$$

(5.4)

and $H_c$ is defined below. The first term in the integrand is the exchange energy, the second the shape anisotropy (i.e., the surface term arising from the demagnetization energy), and the last is the Zeeman term.

Given an external magnetic field that is circumferential and points everywhere in the counterclockwise direction, there are two states that are local minima of the energy: a stable magnetization configuration (ground state), which is everywhere aligned with the external field, and a metastable state that is everywhere antiparallel to the field (i.e., circumferential and pointing everywhere in the clockwise direction). $H_c$ corresponds in eq. 5.4 to the magnetic field at which the metastable configuration becomes unstable.

There are also two relevant unstable stationary configurations (i.e. saddle states). These are defined by the angle $\phi$ that the magnetization direction makes with the circumferential direction at each point in the annulus; i.e., $\phi$ is a function of the angle $\theta$ (as shown in Fig. 5.1), $\phi_{h,\ell}(\theta)$ or $\phi_h(\theta)$. In the limit of low noise, reversal of the magnetization occurs through the lower energy saddle state. One of these corresponds to a global rotation of the magnetization in which $\phi$ is independent of $\theta$; we therefore label it the “constant saddle”, and is denoted $\phi_h$. The constant saddle favors the exchange and Zeeman energies.
at the expense of the demagnetization energy. The second saddle state is a localized fluctuation of the magnetization and we therefore refer to it as the “instanton saddle”, and denote it by $\phi_{h,\ell}(\theta)$ (denoted as instanton saddle in [11]). This state favors the demagnetization energy at the expense of the exchange and Zeeman energies.

Which of these two saddles is energetically favored depends on the applied field and the ring size. When the scaled field $h$ is smaller than $\sqrt{1 - \left(\frac{2\pi}{\ell}\right)^2}$ the instanton saddle has a lower energy than the constant saddle; otherwise, the constant saddle is lower in energy. Fig. 2 of [11] shows the phase boundary between the two activation regimes as a function of $h$ and $\ell$.

We simulated the dynamics using the analytical solutions as our initial configurations for the two saddle states:

$$\phi_h = \cos^{-1}(-h) \quad (5.5)$$

for the constant saddle, and

$$\phi_{h,\ell} = 2\cot^{-1}\left(\vartheta \, \text{dn}\left(\frac{\theta K(m)}{\pi} | m \right)\right) \quad (5.6)$$

for the instanton saddle. Here $\text{dn}(\cdot|m)$ is the Jacobi elliptic function with $0 \leq m \leq 1$, and $K(m)$ is the complete elliptic integral of the first kind[37]. The
parameter \( m \) satisfies,

\[
\frac{\ell}{2K(m)} = \frac{m}{\sqrt{2 - m - \sqrt{m^2h^2 + 4(1-m)}}}
\]  

(5.7)

and \( \vartheta \) is defined by,

\[
\vartheta = \sqrt{\frac{2 - mh - \sqrt{m^2h^2 + 4(1-m)}}{2m - 2 + mh + \sqrt{m^2h^2 + 4(1-m)}}}
\]  

(5.8)

For sufficiently small rings (\( \ell \leq 2\pi \)), the instanton saddle does not exist (essentially, the variation of the magnetization, which is of order the exchange length, cannot “fit” onto the ring). In this limit \( m \to 0 \) and the instanton solution reduces to the constant saddle. As the ring becomes larger the parameter \( m \) increases from 0 to 1 monotonically with \( \ell \). For \( \ell \gg 2\pi \) the \( m \) becomes numerically indistinguishable from 1. In this limit the instanton saddle configuration is given by:

\[
\phi_{h,\ell} = 2 \tan^{-1} \left( \sqrt{\frac{h}{1-h}} \cosh \left( \frac{\theta \ell}{2\pi} \sqrt{1-h} \right) \right).
\]  

(5.9)

We classify rings according to their \( \ell \) values as small (\( \ell \leq 2\pi \)), medium (\( \ell \gtrsim 2\pi \)), and large (\( \ell \gg 2\pi \)). Physically, \( \ell \) characterizes the ratio of the magnetostatic to exchange energies. A medium ring (\( \ell \gtrsim 2\pi \)) has a scaled circumference close in size to a domain wall in the material. The saddle configurations of each regime are shown in Fig. 5.2.

The activation energies within the 1D analytical model can be calculated
Figure 5.2: Saddle configurations computed analytically from the 1D model of Martens et al. for small, medium and large ring sizes. a) For small rings the magnetization reversal goes through the constant saddle state; b) when $\ell > 2\pi$ the transition is via the instanton saddle; c) as the relative size of the ring increases the fluctuation in the instanton saddle occupies a smaller fraction of the ring.
using 5.3(cf. [11]). For the constant saddle they can be analytically computed:

$$\Delta E = \mu_0 M_0^2 t^2 R | \ln(t/R) | (1 - h)^2.$$ 

### 5.2 Method

#### 5.2.1 Micromagnetic Simulations

We studied thin nanorings by running simulations on the model of Sect. 5.1 using the publicly available packages OOMFF and Nmag [38, 39]. These packages effectively simulate the dynamics specified by (5.1) and (5.2) at zero temperature; i.e., all runs start from an initial configuration and run downhill in energy.

Our initial states were the instanton and constant saddles described by (5.5) and (5.6), which provided starting points that were guessed to be relatively close to the actual saddles. The system subsequently relaxed to the actual saddle states, which turned out to be remarkably close to analytical solutions. We describe below how this was determined.

Depending on the starting state, the system will evolve to one or the other (meta)stable state, i.e., either the clockwise or the counterclockwise magnetization configuration. In order to find the actual 2D saddle numerically (recall that the magnetization is forced by the magnetostatic energy term to lie in the plane of the ring), we introduce a new field value, denoted $h_t$, an “effective field” for which the state $\phi_{h,t}$ behaves as a saddle state. In determining $h_t$,
two criteria are used. First, $\phi_{h,t}$ must be as nearly a stationary state as the numerics allow, i.e., the initial time derivative of the total micromagnetic energy should be close to zero ($\lim_{h \to h_t} \frac{\delta E}{\delta t} |_{t=0} \to 0$). Second, the state $\phi_{h,t}$ should mark the boundary between the basins of attraction of each (meta) stable state (i.e., for $h < h_t$ the system evolves to a clockwise state, while for $h > h_t$, it evolves to the counterclockwise state). In the following sections, we show that these criteria are satisfied in a variety of rings with different exchange lengths and annular widths. We also show how the model eventually breaks down when the width of the ring becomes very large.

The procedure can be summarized as follows. For a given initial $\phi_{h,t}$ we find the appropriate $h_t$ by a bracket and bisection iterative process. We set the initial configuration $\phi_{h,t}$, fix the external magnetic field at the value $h_e$ and allow the system to relax. If the final state is the metastable (clockwise) configuration we increase $h_e$ by an amount $\delta h_e$; if the final state is the stable (counterclockwise) configuration we decrease $h_e$ by $\delta h_e$. We then start a new run and reduce $\delta h_e$ by a factor of 2. As $\delta h_e$ decreases, the total relaxation time increases due to the slow dynamics at the start of the simulation, providing evidence that the initial configurations are approaching the true saddle states. We iterate until we reach a numerical uncertainty of $\delta h = 6 \times 10^{-3}$.

The Nmag simulations were run using a mesh consisting of 20963 volume elements, 15154 surface elements, and 7594 points with an edge length of average 3.89 nm and standard deviation of 0.7. (The quality distribution of the mesh was 1.66% below 0.6; 9.11% between 0.6 and 0.7, 57.28% between 0.7
and 0.8, 32.05% between 0.8 and 0.9, and 0.01% above 0.9.) The simulations in OOMMF were run in the three different regimes in the following way: values of \( \ell \) for a given geometry were set by changing the exchange constant \( A \) (cf. below (5.2)) and keeping the ring dimensions constant. This changes \( l_{ex} \) and therefore \( \ell \). This permits side by side comparisons of rings with the same size and aspect ratio in the different regimes. The cell size in the OOMMF simulations were selected to be about \( l_{ex} \) for all regimes. For the cases where \( l_{ex} \) is large, this change reduces the simulation time considerably.

### 5.2.2 String Method in Rare Events

The String Method [40] is a recently introduced numerical procedure for calculating transition energies and paths within the context of large fluctuations and rare events. It is useful to find the path connecting two stable configurations \( M_A \) and \( M_B \), through a curve \( \xi \) with minimum energy. The obtained path corresponds to the reversal trajectory in the limit where the precession term of (5.1) is negligible compared to the damping term. This curve \( \xi \) satisfies

\[
\nabla M E^\perp(\xi) = \nabla M E(\xi) - [\nabla M E(\xi) \cdot \hat{t}] \hat{t} = 0
\]

(5.10)

where \( \hat{t} \) is the unit tangent of the curve \( \xi \). The curve \( \xi \) is found by guessing a parametrized path \( \xi(0) = \{M(\alpha) \in [0, 1], M(0) = M_A, M(1) = M_B\} \) and evolving it in “time” according to:
\[ \partial_t \mathbf{M}(\alpha) = - \nabla_{\mathbf{M}} E^\perp(\mathbf{M}(\alpha)) + l_{ex} \hat{t}. \] (5.11)

The second term is added to enforce a particular parametrization; it does not alter the actual evolution of the curve. It is convenient to rewrite this equation as:

\[ \partial_t \mathbf{M}(\alpha) = H_{\text{eff}}^\perp(\mathbf{M}(\alpha)) + l_{ex} \hat{t} \] (5.12)

For numerical purposes the path \( \xi \) is discretized with \( N + 1 \) points between \( \mathbf{M}_A \) and \( \mathbf{M}_B \). After each iteration of (5.12) with an Euler forward algorithm the magnetization vectors are renormalized to \( \mathbf{M}_s \). In Sect. 5.5 we use this method to find the barrier between two states connected through a transition state.

### 5.3 Medium Size Narrow Ring

We consider a narrow ring of medium reduced circumference \( \ell \) (i.e., the parameter \( m \) not close to 1) with \( l_{ex}/R \ll 1 \), \( t/R \ll 1 \) and \( (l_{ex}/R)^2 \sim (t/R)|\ln(t/R)| \)

\( \ell = 3.2 \times 10^{-10} \text{ J/m}, \Delta R = 40 \text{ nm}, R = 200 \text{ nm}, t = 2 \text{ nm}, M_s = 8 \times 10^5 \text{ A/m}. \)

With these values, \( \ell \) and \( H_c \) are 12 and 73.9 mT, respectively. We first test numerically whether the surface, or shape anisotropy, term is in fact the main contributor to the magnetostatic energy, as required for the validity of the analytic solutions to hold [11]. Using OOMMF and Nmag the total demagnetization energy were obtained for different values of \( \ell \) and compared to the values of
the surface term (second term in the integrand of (5.3)). The results of this comparison are presented in Fig. 5.3, which shows that the numerical computation of the total demagnetization energy gives a dependence on $h$ close to the contribution from the shape anisotropy alone: the agreement is within 5% for the instanton saddle and 10% for the constant saddle. This provides numerical support for the approximations used to arrive at the $1D$ analytical solutions of [11] and confirms that the bulk magnetostatic term, neglected in the analytic model, is indeed not important.

We also compare the total demagnetization energies computed using OOMMF for different cell sizes in Fig. 5.3b. Three suitable methods to calculate the demag energy are available in the OOMMF package; ConstMag, 3dSlab, 3dCharge. Constmag calculates the average demagnetization field assuming the magnetization is constant in each cell; 3dSlab uses a demag field obtained from blocks of constant charge; and 3dCharge uses constant magnetization to calculate the in-plane component of the magnetic field, and constant charges to calculate the out of plane demagnetizing field. As seen in the figure, the consistency between different methods of calculation improves as cell size is reduced; and the numerical results approach that of the $1D$ model.

Once $h_t$ is obtained following the method described in Sect. 5.2, the saddle state is numerically obtained and the activation energy is thereby determined from the difference between each saddle state and the metastable state. Fig. 5.4 displays curves at $h_t = 0.21$ for each of the two saddle states used as initial configurations.
Figure 5.3: Total demagnetization energies, using different calculation methods, compared to analytical results for the shape anisotropy term alone ($A = 3.2 \times 10^{-10} \text{ J/m}$, $R = 200 \text{ nm}$, $t = 2 \text{ nm}$ and $\Delta R = 40 \text{ nm}$). a) Comparison of OOMMF using the ConstMag method at cell size 1 nm and Nmag with theoretical predictions vs. $h$. b) Demagnetization energy vs. cell size using three different methods for computing this energy in OOMMF, all for $h = 0.2$. The solid line is the analytical computation of the shape anisotropy term alone.
Figure 5.4: Evolution of the total micromagnetic energy with time. Arrows show activation energy of each saddle. The configurations shown bifurcates at the field given ($h_t = 0.21$) and have an initial slow evolution. The two criteria used to determine a saddle state are clearly seen.
As can be seen in the figure, after a very short transient the system arrives at a configuration in which the energy stays almost constant for an extended period; this indicates that the initial 1D analytical solution is close in both energy and its geometrical configuration to the true 2D saddle. Eventually, the saddle state decays into one of the two stable configurations. The activation energy is easily computed this way (as seen in Fig. 5.4), and a glance at the figure confirms that for the applied field \( h_t = 0.21 \) the instanton configuration has a lower activation energy than the constant saddle, as predicted theoretically [11].

The method described in Sect. 5.2 was repeated to obtain the behavior of \( \Delta E \) as a function of \( h_t \). Using this approach one can calculate \( h_t \approx \frac{h_t^+ + h_t^-}{2} \) and \( \Delta E = \frac{E[\phi_{h_t^+}, h_t^+]}{2} + \frac{E[\phi_{h_t^-}, h_t^-]}{2} - E[\phi = \pi, h_t] \) for each of the two saddle configurations. Here, \( E[\phi, h_e] \) represents the numerical energy of a configuration \( \phi \) under an applied field of magnitude \( h_e \). The results are summarized in Fig. 5.5 together with the analytical predictions.

Figs. 5.5a and 5.5b show \( \Delta E(h_t) \) for the instanton saddle and constant saddle, respectively. From bottom to top the curves represent calculations in OOMMF for two different cell sizes, an Nmag calculation and the analytical prediction.

The Nmag results are closer to the analytical predictions than the OOMMF calculations. This is due to the fact that the curvature is more faithfully represented by a mesh of tetrahedrons in Nmag, whereas OOMMF represents the ring with a square grid. The edges of the tetrahedrons can be arranged

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Figure 5.5: Comparison of the activation energies for the (a) instanton and (b) constant saddles. Data points represent steps of 0.1 in $\hbar$. As the numerics are refined both by using Nmag and by reducing the cell size in OOMMF simulations the results approach the theoretical predictions. (c) Comparison for Nmag for the middle size, narrow ring ($\ell=12$, $\Delta R=40$ nm) of the corresponding curves shown in (a) and (b).
to follow closely the curvature of the ring, whereas the square cells edges will in most cases make a finite angle with the ring tangent. This results in a much larger error contribution to the demagnetization energy in square grids in OOMMF than in Nmag. This is expected because the cells in the OOMMF calculations are larger in volume than the tetrahedrons used in Nmag.

Fig. 5.5c presents the Nmag simulation results for the activation energy. As predicted in Ref. [11], the instanton saddle configuration has a lower activation energy at lower fields. For a fixed $\ell$ the activation energy curves are predicted to merge at $h_c(\ell) = \sqrt{1 - (2\pi/\ell)^2}$ because the instanton saddle reduces to the constant saddle when $m \to 0$. For higher fields, the constant configuration is the sole saddle state (this is in contrast to the low-field side, where both solutions exist but the constant saddle has higher energy). Numerically, the field at which the saddles merge is somewhat lower than that predicted. This discrepancy arises because the theoretical model applies to a strictly $1D$ ring, whereas the simulations run using higher-dimensional rings (2D in OOMMF and 3D in Nmag).

### 5.4 large size narrow ring

We now investigate an annular film with the same dimensions but different $l_{ex}$ (e.g., permalloy with $A = 1.3 \times 10^{-11}$ J/m); the rest of the dimensions are kept the same as above. Such a ring belongs to the large ring regime ($\ell = 60, m \approx 1$). As before, we can obtain a qualitative understanding of the
reversal process by following the time evolution of the micromagnetic energy; this is presented in Figs. 5.6, 5.7. Using the fact that an instanton is a superposition of two domain walls with opposite chirality (Fig. 5.10b)[6], the features observed in Figs. 5.6, 5.7 can be explained and an intuitive idea of the reversal mechanism developed.

We begin by discussing the evolution of energy with time as shown in Fig. 5.6a. For $h_e < h_t$ the instanton decays into the metastable state with a rapid decrease in energy (seen to the left of $t = 0$). This corresponds to the annihilation of two transverse domains walls. The field in this case is not sufficient to separate the two transverse walls. When $h_e > h_t$ (right side) the energy of the system decays linearly with time towards the stable state and then sharply decreases. The linear time decay corresponds to movement of the transverse domain walls in opposite directions (due to the external field) at approximately constant speed as can be seen in Fig. 5.6. The final, sharp decrease in energy results from the collision and annihilation of the walls. Note that the magnetostatic and exchange energies remain almost constant while the walls are propagating (roughly) independently of each other. The annihilation energies of the domain walls (indicated by the arrows in Fig. 5.6a) are roughly the same magnitude.

The slope of the $E(t)$ curve during the propagation phase provides a measure of how fast the reversal proceeds. For the particular damping parameter used, the last term of (5.3) relates the slope of the energy curve to the speed of the wall by $v = \frac{1}{4n\mu_0 M_0^2} \left( \frac{2\pi}{\ell} \right)^2 \frac{R^2}{R_e \Delta R} \left( \frac{dE}{dt} \right)$, where $n$ is the number of domain wall
Figure 5.6: Evolution of the total energy with time for the instanton saddle, with energies measured with respect to that of the stable state. The decay to the metastable state is shown as proceeding to the left of $t = 0$, and to the stable state to the right of $t = 0$. The ring dimensions are $\Delta R = 40$ nm, $\ell = 60$. When $h_e < h_\ell$ the instanton saddle (II close to $t=0$) decays quickly into the metastable configuration (I at $t=0.7$ ns); domain walls are annihilated. When $h_e > h_\ell$ the two domain walls of the instanton saddle (III close to $t=0$) separate (IV, $t=1.5$ ns), move to the opposite side of the ring (V, $t=5.4$ ns) and annihilate (VI, $t=5.7$ ns).
Figure 5.7: Evolution of the total energy with time for the constant saddle, with energies measured with respect to that of the stable state. The decay to the metastable state is shown as proceeding to the left of $t = 0$, and to the stable state to the right of $t = 0$. The ring dimensions are $\Delta R = 40$ nm, $\ell = 60$. When $h_e < h_t$ the constant saddle (II at $t = 0.15$ ns) starts to decay into the metastable configuration (I at $t = 0.28$ ns), it is possible to see that this decay is not uniform in all the ring, and some regions decay faster than others. When $h_e > h_t$ the constant saddle quickly develops domains (III at $t = 0.51$ ns). Counterclockwise domains expand at the expense of clockwise domains (IV, $t = 0.83$ ns), with annihilation that produce a sudden decrease in energy (V, $t = 1.03$ ns) leaving a single domain wall pair which continues moving (VI, $t = 2.52$ ns) until eventual annihilation; the slope during the last stage is very close in magnitude to the slope of Fig. 5.6 during domain wall propagation, the discrepancy is due to the difference of applied fields.
pairs present in the ring. Direct observation of the micromagnetic configurations gives an average wall speed of \( v = 108.5 \) m/s while the calculation from the energy graph equals \( v = 108.1 \) m/s. In deriving this expression \( \phi = 0, \pi \) for each domain and domain wall widths are assumed to remain constant during propagation. A comparison to medium-sized rings shows that at fixed \( h \) the reversal time increases as \( l_{ex} \) decreases for two reasons: the domain wall width is comparatively smaller and the effective scaled circumference \( \ell \) is comparatively larger (cf. Figs. 5.4 and 5.6).

The time dependence of the energy for the constant saddle case, Fig. 5.7, is seen to proceed in several steps where the energy decrease is gradual, punctuated by large changes in the slope \( dE/dt \). These features can be explained as follows. Fig. 5.8 shows that the activation energy of the constant saddle at \( h \approx 0.17 \) is several times larger than the activation energy of the instanton saddle at the same field. With such a large activation energy, it
is relatively easy to create several domain wall pairs along different (randomly placed) parts of the ring, each of them with an energy cost roughly equal to the activation energy of the instanton. In the simulations, this process is modified by the discretization of the ring, and in an experimental setup it is possible that impurities and edge roughness might play a similar role. The abrupt changes in slope are due, as before, to the annihilation of domain wall pairs and hint at a richer variety of states that are stationary in the energy when the scaled circumference is large compared to the exchange length.

5.4.1 Multiple Wall Pair Energies

We have also gone beyond the work of Martens et al. by finding numerically new stable states consisting of multiple domain wall pairs. When present, these states influence the time evolution of the system in a manner similar to that just described. In this section we discuss these new states and present a model to incorporate their effects on magnetization reversal.

Fig. 5.10d shows one of these locally stable double pair states. They can be described as a combination of topological defects, in particular edge defects and domain walls, which we will now describe (cf. Fig. 5.9). Bulk topological defects are vortex and antivortex singularities of the magnetization configurations with a net contribution to the exchange energy[41]. They are characterized by their winding number which is conserved over any continuous transformation of the magnetization. Close to an edge of the material the singularities become half-vortices with winding number $\pm 1/2$[42]. Since
Figure 5.9: Topological defects of the XY model in the bulk (a,b) and in the presence of an edge (c,d), with winding numbers of $1,-1,+1/2,-1/2$ respectively.

$\ell \to \infty$ for the limit $m \to 1$, we can consider any small segment of the ring as a strip: the outer edge of the ring maps into the lower part of the strip.

A transverse domain wall can be described as a composite of two edge defects of opposite sign[42] at opposite sides of a ferromagnetic strip (see Fig. 5.10a). In the ring, it is convenient to label such a domain wall using the sign of the topological defect on the inner side of the ring. The topological defects experience a “Coulomb-like” attraction or repulsion. Walls where the magnetization points in opposite directions (equal signs for same side edge defects as in Fig. 5.10c) experience repulsive interactions. The origin of repulsion arises from the magnetostatic and exchange energies in the region between walls. Walls which are parallel to each other (with opposite signs in the same side edge defects, as in Fig. 5.10b) experience attractive interactions.

Any small thermal fluctuation of the magnetization initially parallel to the ring (strip) edges would be a precursor to a double wall of this last type (Fig. 5.10b)
Figure 5.10: a) Transverse domain wall composed of two edge defects of opposite sign. b) Magnetic configuration equivalent to the instanton state in a stripe. c) A trapped domain between two antiparallel walls. d) Low energy metastable state configuration. The topological defect sign at the inner boundary determines if the domain wall pairs are stable with respect to the external magnetic field. With respect to the ground state (counterclockwise), this state has a winding number of zero, as do the instanton saddle, constant saddle and clockwise configurations.
as illustrated by the profile of such configurations. The radial component of the magnetization in the ring (transversal component in the strip) edges could have any sign: the fluctuation will have the same energy whether the magnetization tilts towards the inside or the outside of the ring (up or down in a strip). A reversal can be produced by a fluctuation with equal probability for any of these two orientations.

The domain between two walls will expand under the influence of an external magnetic field parallel to the domain’s magnetization (producing a repulsive pressure on the walls), and contract under an antiparallel magnetic field (producing an attractive pressure on the walls). The balance between the interdefect interaction and the field determines whether a configuration is in stable or unstable equilibrium. For example, an instanton saddle configuration is equivalent to two domain walls with opposite signs on their innermost defects which enclose a domain parallel to the field (cf. signs in Fig. 5.10 b). The field pushes the domain walls away from each other while their mutual interaction tends to bring them together. These opposing tendencies produce the unstable equilibrium which makes this configuration a saddle state.

The opposite situation, in which edge defects repel and the enclosed domain is antiparallel to the field, produces a metastable state. The enclosed magnetic domain does not vanish because the half vortices experience an effective repulsion: it is energetically costly to unwind the topological defects. As a result this configuration is stable, with an energy intermediate between the clockwise and counterclockwise configurations.
Figure 5.11: Two possible evolutions of a fluctuation with two instantons in different parts of the ring. (A) The magnetization relaxes to the metastable state only if the radial magnetization components are parallel. (B) Otherwise, two trapped domains (360 degree walls) appear.
We can now explain how the metastable state evolves into the state represented in Fig. 5.10d. If the ring is sufficiently large, two instantons (one domain wall pair each) are produced (Fig. 5.11). If both instantons point in the same radial direction the system evolves into the counterclockwise state (Fig. 5.11 A). However, if the instanton fluctuations point in opposite radial directions (Fig. 5.11 B) the system evolves to the state shown with 4 domain walls.

The domain wall pairs need not be at opposite sides of the ring for this configuration to be stable, as confirmed by displacing one of the wall pairs by several angles and waiting for the system to relax.

It is interesting to summarize the new possible configurations and their total energies in the large ring case. The lowest state is the stable configuration, and there exists a series of metastable states separated from each other by the energy of a double wall trapped domain (Fig. 5.12)
With the exception of the single wall pair, all configurations shown have a total winding number difference from the counterclockwise state of zero for a path that completely encloses the central hole of the ring. The single wall pair configuration has this winding number difference equal to one. While reversing the field will make the double wall system decay into the stable state; the single wall pair configuration cannot decay into the counterclockwise configuration. A trapped domain configuration using a single pair of domain walls has already been proposed for an MRAM device [43]. These 360 degree walls were also found to form and to be stable in simulations conducted using Nmag. These structures have been also observed in experiments. [44]

5.5 Wide rings

Having verified numerically the conclusions and predictions of the analytical model of Martens et al.[11] for narrow rings, we now proceed to test the limits of its applicability with increasing annular width. Given the $1D$ nature of the analytical model, we expect that at some width the model should break down and its conclusions no longer apply. Surprisingly, this breakdown finally occurs at a larger width than initially expected.

Increasing the ring width introduces two new effects that cause the analytical model to break down. First, it allows the external field to vary in magnitude appreciably as one moves along a radial direction. Second, it increases the relative magnitude of the (previously neglected) nonlocal bulk term of the mag-
Figure 5.13: Activation energies for $R = 200$ nm, $\ell = 12$ and a) $\Delta R = 40$ nm, b) 100 nm, c) 200 nm.

netostatic energy with respect to that of the local surface term.

In our simulations, $\Delta R$ is set to the values 100 nm ($H_c = 29.5$ mT), 200 nm ($H_c = 14.7$ mT) and 380 nm ($H_c = 7.8$ mT). The central hole of the annulus is a few exchange lengths in diameter in the latter case. For this reason vortex-like “singularities” remain in the gap.

Fig. 5.13 summarizes the activation energies for the widths considered. It should be noticed that as $\Delta R$ increases for fixed $l_{ex}$, $\ell$ decreases and the annulus shifts away from the large ring ($m \approx 1$) approximation. We consequently discuss only middle size rings where $\ell \approx 12$. Fig. 5.13 a,b,c shows that the main predictions of the model hold even for very wide rings: the configura-
tions $\phi_h$ are saddles for certain $h_t$, and for fields below $h_c$ the instanton saddle configuration is preferred to the constant saddle configuration.

We have found that the annular width must be increased to the extreme wide-ring limit $\Delta R \approx 2R$ in order for the model to fail. Its breakdown can be observed in the $E(t)$ curve of Fig. 5.14a. In this regime, there are still fields $h_t$ for which the dynamics bifurcates to either the stable or metastable state on either side of $h_t$, but at such fields it is clear from Fig. 5.14a that

$$\left(\lim_{h \to h_t} \frac{\delta E}{\delta t}\bigg|_{t=0} \neq 0^-\right).$$

This indicates that the initial configurations chosen from the 1D analytical solutions are no longer close to the true saddles. Instead of a long initial period of little change, we find instead relaxation to a state in which the central region of the ring is magnetized circumferentially and the outer edge of the ring retains some memory of the starting configuration. This appears to be a new type of saddle configuration, which we call the \textit{relaxed state}, and is shown in Fig. 5.14.

For simulations starting from the instanton saddle with parameters $h = 0.1, ..., 0.4$ the system evolves to the relaxed state. At higher values of $h$ ($h = 0.5, ..., 0.8$ for the instanton, and $h = 0.7, ..., 1.0$ for constant saddle configurations) the relaxed state does not satisfy the stationarity condition, but the bifurcation condition can still be satisfied with a particular $h_t$. The absence of a plateau in the $E$ vs. $t$ curves makes the definition of the activation energy somewhat more problematic, but it can still be defined by using as the energy of the saddle state the point at which the curves $E[\phi_h, h_c^-]$ and $E[\phi_h, h_c^+]$ separate. In this way approximate activation energies can be determined, and the
Figure 5.14: a) Time evolution of the total energy, for both initial saddle configurations. At a given $h_t$, the dynamics do not slow arbitrarily as $t \to 0$. b) Energies of the approximate activation energies (measured close to the bifurcation in time, not at $t = 0$). c) The new metastable state of Fig. 5.15 is found at lower energies than either saddle. The 1D saddle configurations (instanton center-up, constant center-down) and their corresponding relaxed states at $t=0.8$ ns for ($h_+^+$ right, $h_-^-$ left); inside the ring the strong field aligns the magnetization clockwise.
results are shown in Fig. 5.14b.

For values of $h$ that correspond to the constant saddle $(0.2, \ldots, 0.6)$ another feature of the breakdown of the $1D$ model can be seen. The system relaxes to neither of the stable states considered so far (see Fig. 5.15). It evolves to a radially dependent state with counterclockwise orientation at the inner edge of the ring and clockwise orientation at the outer edge. This configuration is stabilized by the large inhomogeneity in the magnitude of the magnetic field as one moves outward along a radial direction. It is important to note that the energy of this state is lower than the energies of either initial configuration used (the $1D$ analytical saddle solutions), but is higher than either the clockwise or counterclockwise state.

There exists a low barrier that prevents this configuration from relaxing into either of the counterclockwise configurations in the limiting fields of Fig. 5.14. We obtain an estimate of this energy by using the String Method without reparametrization[40] as described in Sect. 5.2. We start with sequences of 50 equally spaced configurations that connect each of the circumferencial configurations to this newly found metastable state along an straight line. The result of the relaxations are shown in Fig. 5.16. Fig. 5.16 (a) shows the total energy of the string points after relaxation; the inset shows a very shallow energy barrier that prevents decay to the two lowest stable configurations. It is interesting to observe that this barrier almost disappears on the left at $h_e = 0.22500$ and on the right at $h_e = 0.25625$ explaining why this state is stable only for a very narrow band of field values.
The physical origin of the two barriers is clear if the three components are studied separately (Fig. 5.16 b, c,d). For all graphs the origin corresponds to the state represented in Fig. 5.15, and the clockwise oriented magnetization is 50 steps to the left of zero, the counterclockwise configuration is located 50 steps to the right of zero.

The Zeeman energy (Fig. 5.16d) prevents the system from moving towards the clockwise configuration for all states along the string. It is maximum for the clockwise configuration and decreases monotonically along the path. Any point of the trajectory is pushed to the right of the graph by the external field.

Fig. 5.16b shows the demagnetization energy with a sharp barrier that prevents the magnetization from pointing perpendicular to the ring edges. At this barrier, the magnetization at the surface points radially outward (as in Fig. 5.14$h_0^+$ for the constant saddle). This produces a sharp barrier at this step of the path. At this point, the magnetostatic energy is the only energy term acting against the reversal of the magnetization from clockwise to counterclockwise orientations; other terms favors the reversal. The net effect of the demagnetization energy barrier is to favor configurations away from this barrier. Fig. 5.16c represents the exchange energy. The exchange energy is minimal in the two circumferential states.

When these three interactions are considered together the stability of this state is understood: at lower fields the exchange and magnetostatic energy are balanced by the Zeeman energy. At large fields Zeeman and exchange favor a magnetization out of the ring’s surface, when the shape anisotropy
barrier is overcome, the system reverses suddenly into the counterclockwise configuration.

The analytical model presumed the field to be constant in the radial direction as in the narrow ring case. Although the field inhomogeneity eventually renders this assumption invalid, the $1D$ model is surprisingly robust and breaks down only in the extreme case just considered.

### 5.6 Conclusion

The $1D$ analytical model of Martens et al. [11] has been tested and confirmed using numerical simulations for a variety of ring sizes and external magnetic fields that more closely approximate realistic laboratory situations. Although it was initially expected that the analytical model would apply only to narrow annuli, our simulations show that it is surprisingly robust, eventually
Figure 5.16: Energies of the configurations along the string after 100 iterations at two different applied fields. The center of the figure represents the magnetization configuration of Fig. 5.15. The clockwise configuration is at -50, and the counterclockwise is located at +50. Energies are a) total b) demagnetization c) exchange d) Zeeman. The inset on (a) shows the energy on a finer scale, illustrating the existence of an energy barrier.
breaking down only in the extreme two-dimensional limit.

By studying a large portion of the relevant parameter space, \((l_{\text{ex}}, \Delta R)\), we have also found new saddle and stable states. These findings enrich our understanding of the energy landscape of ferromagnetic rings.

Two limits present particularly interesting features: the large-\(R\) narrow ring \((\Delta R \ll R)\) and the extremely wide ring. The large narrow ring allows for the appearance of multiple instantons at energies below the constant saddle configuration; their relative orientations and positions determine the final magnetization configuration. We provide a topological analysis of these new configurations and predict a hierarchy of such states differing by the number of domain wall pairs in each. The interaction between these domain walls can be characterized and understood through “edge defects” that compose them. Moreover, by following the evolution of the downhill energy run from one of these states to the stable configuration, one can infer the propagation of domain wall pairs in the ring: sudden changes in energy indicate annihilation of domain wall pairs, while linear decrease of energy occurs during domain wall propagation.

The 1D model predicts well the activation energy for magnetization reversal even for wide rings. Eventually, though, in the extremely wide regime limit, the 2D nature of the magnetic field becomes important and the 1D approximation breaks down. In this regime, a new stable state arises in which the magnetization is radially dependent but independent of the angle. The String Method [40] has been used to verify the existence of a barrier between this
state and other stable states with lower energy, and is used to clarify the physical origin of this barrier, in terms of the various contributions to the energy from exchange, magnetostatic, and external field sources.
Recent observations [45, 46, 44] in thin ferromagnetic stripes show magnetization configurations in which the magnetization makes a full $2\pi$ turn in a localized region of the stripe, while the rest of the stripe is magnetized parallel to the edges of the stripe. These structures are stable against small applied external magnetic fields which makes them potentially useful for information storage devices[47]. The same phenomenon has been observed in thin ferromagnetic annuli[45, 47], which then results in the existence of a hierarchy of equally spaced metastable states[48].
of magnetic nanodevices[49, 50]. Here we explore the stability of $2\pi$ domain walls in ferromagnetic nanoring using the string method [32, 51, 40]. We find the energy barrier $\Delta E$ separating two metastable configurations. This barrier determines the escape rate from a metastable state through the Arrhenius law, to leading order $e^{-\frac{\Delta E}{k_B T}}$ [1]. The string method also gives the minimum energy path and transition state.

We distinguish two types of domain walls by their winding number in the global (local) coordinate system $\omega$ ($\Omega$). We compare the energy barriers that separates each type of wall from the ground state to the activation energy that separates the two vortex configurations [11, 48]. A current flowing along the axis of the ring produces a circumferential field. The application of this field has two effects. First, the degeneracy of the two vortex states is lifted. Second, the field determines the width of the domain wall; in its absence the $2\pi$ walls could dissociate into two independent $\pi$ transverse walls.

6.1 Method

Following previous work [11, 48], we study a permalloy ring with the following dimensions and material properties: outer radius $R_2 = 220$ nm; inner radius $R_1 = 180$ nm, thickness $t = 2$ nm, magnetization saturation $M_s = 8 \times 10^5 A/m$, and exchange length given by $l_{ex} = \sqrt{\frac{2A}{\mu_0 M_s^2}} = 5.6$ nm. A current flowing along the axis of the ring produces a field $\mathbf{H}(r) = (hH_c(R_1 + R_2)/2r)\hat{\theta}$ A/m. Here $h = H/H_c$ and the characteristic field strength at midradius is $\mu_0 H_c = 73.9$ mT.
(for $H > H_c$, the clockwise vortex state is no longer stable). The calculations were performed at $h=0.1$.

Precessional effects do not modify the location of the critical points in the energy landscape: the exponential factor in the Arrhenius formula is unaltered if we ignore them. We consider the overdamped case so that the escape trajectory follows the negative gradient of the energy. This is done by integrating only the damping term of the Landau-Lifshitz-Gilbert equation

$$\frac{d\mathbf{M}}{dt} = -\frac{|\gamma| \alpha}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}). \quad (6.1)$$

Here $\alpha = 1$ is the damping coefficient, $\gamma$ is the gyromagnetic constant, and $\mathbf{H}_{\text{eff}} = -\nabla_{\mathbf{M}} E/\mu_0$ is the effective magnetic field. The total micromagnetic energy $E$ is the sum of the exchange $E_{\text{ex}}$, Zeeman $E_Z$ and magnetostatic terms $E_{\text{mag}}$.

The string method is necessary to calculate the minimum energy path between two stable states ($\mathbf{M}_A, \mathbf{M}_B$) when there is no a-priori knowledge of the transition state. In practice, the path is discretized in $N+1$ images between $\mathbf{M}_A$ and $\mathbf{M}_B$ denoted as $\mathbf{M}_i(t) \equiv \mathbf{M}_i(r, t)$ with $i = 0, ..., N$. The images are updated using a two-step iteration procedure as follows: First, each image evolves using the publicly available micromagnetic code OOMMF[39] until the time reaches some interval $\Delta t$ which we have selected to be 10 ps. This gives
a sequence of configurations:

\[ M'_i \equiv M'_i(r) = M_i(t) + \int_t^{t+\Delta t} \frac{dM_i(t')}{dt} dt' \quad (6.2) \]

Once all the \( M'_i(r) \) have been obtained, the second step in the string method is a reparametrization step used to keep these images equidistant. First the complete arc \( s_N \) length of the trajectory is calculated by

\[ s_0 = 0, \quad s_i = s_{i-1} + |M'_i - M'_{i-1}|. \quad (6.3) \]

The arc lengths are renormalized using \( \alpha'_i = s_i/s_N \). Finally we do a simple linear interpolation for all \( i \) along the trajectory so that

\[ M_i(t + \Delta t) = M'_{j(i)} + \frac{M'_{j(i)+1} - M'_{j(i)}}{\alpha'_{j(i)+1} - \alpha'_{j(i)}}(\frac{i}{N} - \alpha'_{j(i)}) \quad (6.4) \]

where \( j(i) \) is the index of the string where \( \alpha'_{j+1} \geq i/N \geq \alpha'_{j(i)} \). During each step we observe the magnetic energy \( E_i(t) = E_{ex}(M_i(r, t)) + E_Z(M_i(r, t)) + E_{mag}(M_i(r, t)) \) as indicator of how far from convergence the current step is. The iteration process is stopped when there is no visible change in the function \( E_i(t) \).
6.1.1 Preliminary example, magnetization reversal of a nanoring.

The original String Method has been applied previously to obtain the energy landscape of ferromagnetic nanoelements[32]. We show now results of applying the Simplified and Improved String Method for the reversal of nanorings. We show that our implementation of the string Method gives results consistent with previous work on nanoring reversals, and illustrates some features of the evolution of the string which are of relevance in the thermally activated dynamics of thin nanostructures.

We start with an initial string formed by a sequence of configurations in which the magnetization vector is deflected a constant angle from the tangential direction \( \phi_{i,n=0}(\theta) = \frac{i\pi}{100} \). The evolution of the total and demagnetization energies are shown in figures 6.1 and 6.2, for comparison we show in figure 6.3 the initial guessed string, the string at 80 iterations and the final string (440 iterations). The color code in this and subsequent plots of magnetization is as follows: blue for counterclockwise magnetizations, white for radially outward, red for clockwise and green for radially inwards magnetizations.

The evolution of the energy with the number of iteration proceed very quickly initially since we are in highly excited states. The highly excited states decay quickly into configurations which contain regions of counterclockwise and clockwise configurations separated by single transverse walls. Adjacent points in the string simply reflect the motion of these walls as the domain ex-
Figure 6.1: Evolution of the total energy of the string as successive iterations. The energy curve converges after about 440 iterations. The transition state is the maximum of the relaxed energy curve.
Figure 6.2: Magnetostatic energy of the string states at different iteration states. The plateaus are present where a constant number of domain walls are propagating along the ring. The energy is almost independent of the distance between domain wall pair indicating that dipolar interaction is negligible.
Figure 6.3: Transition paths connecting the two vortex configurations, n=0 corresponds to the initial guessed path using a global rotation of the magnetization; n=80 iteration after that show formation of domains and transverse wall; n=440 reached final minimum energy path.

...and under the influence of the external magnetic field. This is seen clearly in the plot of demagnetization energy vs. point in the string where several plateaus are formed as indicators of the propagation of domain walls: once a domain wall is created the magnetostatic point is independent of its position in the ring.

The string evolves very slowly once it reaches points close to stationarity. There are bottlenecks in the evolution of the string at points in which two walls collide: since these are “duplicate” copies of the true transition state of the ring. These are seen in the total energy curve of the string as maxima. However, the string finally converges and its energy curve has a single maximum: the transition state. The profile of the saddle state ($\phi(\theta)$) obtained in this manner is shown in figure ... and compared to the analytical saddle state from the 1D model of Martens et al. The state is degenerate with respect to rotations, so horizontal position of the soliton is nonrelevant. This results indicates a
good agreement between the analytical prediction and the implementation of the String Method. In addition, it is further evidence that in the regime where the exchange length $l_{ex}$ is much smaller than the scaled circumference, the dynamics of the magnetization is dominated by the dynamics of domain walls propagating in the circumferencial direction without considerable dipolar interaction between the walls.

### 6.1.2 Magnetization decay of a clockwise configuration into a pair of transverse wall with equal winding.

The degeneracy between the two vortex configurations (clockwise and counterclockwise) is lifted by the presence of the counterclockwise field. And the previous section confirms that when the magnetization is independent of the radial direction the instanton saddle is the preferred transition configuration between these two. However the energy landscape of nanorings presents several local minima separated by the presence of $2\pi$ domain walls. We now find the activation energy required to produce two transverse wall having the same direction of torsion. Once these two transverse walls are created they will propagate along the ring to meet again approximately at the opposite side.

We use the Improved String Method for the Study of Rare Events to obtain the preferred transition path between a clockwise configuration and a $2\pi$ wall. Under the influence of the counterclockwise configuration the $2\pi$ wall is not stable, and the enclosed domain expands breaking the configuration into two
separate transverse walls. As a result, one end of the string is not stationary and continues to evolve towards a far located minimum. Once the string finds the local saddle state the height of the energy barrier does not change, but the number of configurations between the clockwise configuration and the saddle is reduced (because the opposite end of the string represents two transverse walls getting farther apart). We stop the iterative process once it is clear that energy maximum is not decreasing, only moving sideways.

We have observed the need for a further refinement for this question. It is necessary to consider the sign of the winding of the $2\pi$ domain wall with respect to the local coordinate. We have to separately evolve two strings, corresponding to each type of wall labeled by its winding number with respect to the local direction $\Omega = \pm 1$. Figure 6.4 shows the total energy of the final string versus coordinate $i$ in the string. The companion figure (Fig. 6.5) shows the preferred path between the states considered. To produce a $\Omega = +1, 2\pi$ wall, a vortex crosses the annular stripe inward, resulting in a total winding $\omega = 2$ for the annular structure; to produce a $\Omega = -1, 2\pi$ wall a vortex crosses the annular stripe outward. The energy barriers are slightly different the majority of which comes from exchange energy.

Finally both energies are around twice the activation energy of the instanton saddle for nanorings. As can be seen by comparing figures 6.1 and 6.4. This is expected, the presence of a vortex increases the exchange energy dramatically. A purely 2D topological defect would have infinite exchange energy at the core, in ferromagnetic nanoelements this is avoided by allowing the
Figure 6.4: Total energy of the relaxed string for the two possible $2\pi$ domain wall to escape from the clockwise magnetization state.

Figure 6.5: Minimum energy path for the creation of a $2\pi$ domain wall from the clockwise configuration.
6.2 Annihilation of $2\pi$ domain wall.

We now present the results of the string method to find the minimum energy path for destruction of a $2\pi$ wall for the two types of $2\pi$ domain wall, $\Omega = \pm 1$. Fig. 6.6 and Fig. 6.7 present the string energies and configurations after relaxation of the string. The $\Omega = +1$, $2\pi$ wall decays into the counterclockwise configuration by the expulsion of a vortex from the inner hole. On the other
hand, the $\Omega = -1$, $2\pi$ wall decays into the counterclockwise configuration by the expulsion of an antivortex. This observation shows a correspondence between a topological defect crossing the stripe and the signature of the $2\pi$ walls being annihilated. For comparison purposes we provide magnitudes of the energy landscape of ferromagnetic nanorings obtained with the string method. The lowest energy barrier between the counterclockwise and the clockwise vortex configurations passes through a configuration denoted as the instanton saddle [11](with $\Omega = 0$); the activation energy of this event is $3.0 \times 10^{-19}$ J. This is consistent with our previous work on nanorings [48]. For a $2\pi$ wall with $\Omega = 1$ the decay into the ground state has an energy barrier equal to $1.9 \times 10^{-19}$ J. The annihilation of a $2\pi$ wall with index $\Omega = -1$ has an energy barrier equal to $2.8 \times 10^{-19}$ J. This shows the energy barrier to annihilate a $2\pi$ domain wall by the expulsion of a topological defect is comparable to that of reversal between vortex states by a instanton fluctuation.

### 6.3 Discussion

For annuli with the dimensions being considered the magnetization is constrained to lie in the plane of the ring; for the stable states the magnetization can be considered to be independent of the radial coordinate. The exchange energy $E_{\text{ex}}$ of a stable state is given by [11]:

$$E_{\text{ex}} = \frac{\mu_0 M_s^2 \mu_0}{2} \ln \left( \frac{R_2}{R_1} \right) \left[ 2\pi (1 + 2\Omega) + \int_0^{2\pi} \left( \frac{\partial \phi}{\partial \theta} \right)^2 d\theta \right] (6.5)$$
Figure 6.7: Segment of the ring encompassing each $2\pi$ domain wall. Minimum energy path for the annihilation of $2\pi$ domain walls in consideration. (Above) $2\pi$ wall with topological index $\Omega = -1$, (below) $2\pi$ wall with topological index $\Omega = +1$. The configurations shown correspond to the following images in the string (left) $i=0$, (center) $i=50$, (right) $i=100$. 
where \( \phi(\theta) \) is the angle that the magnetization makes with the tangent of the ring at a given angle \( \theta \); \( \Omega \) is the “winding number” of the magnetization with respect to the local coordinate system.

The difference in winding numbers (\( \Delta \Omega \)) of the \( 2\pi \) walls considered results in an exchange energy difference \( \Delta E_{\Omega} \) between these two states. Using Eq. (6.5) the difference can been shown to be approximately:

\[
\Delta E_{\Omega}[M(r)] \approx 2\pi \mu_0 M_s t_{ex}^2 \ln \left( \frac{R_2}{R_1} \right) \Delta \Omega = 1.298 \times 10^{-19} \text{ J.} \tag{6.6}
\]

The total exchange energy difference between these \( 2\pi \) walls (\( \Omega = \pm 1 \)) obtained from the micromagnetic simulation results is \( 1.357 \times 10^{-19} \text{ J} \). Here we have ignored a contribution to this difference of terms of the form \( \int \left( \frac{\partial \phi}{\partial \theta} \right)^2 d\theta \) since it is not a topological term. This shows a very good agreement between an estimate obtained from the 1D model and the full numerical simulation. The exchange energy term is the biggest contributor to the difference between the total energies of the two domain walls: the numerical values from the demagnetization and Zeeman energy are 10 times smaller. The main point is that most of the energy difference between these two types of \( 2\pi \) domain wall is the result of their respective topological windings. It is worth noting that this is a curvature effect as can be seen from Eq. (6.6): the energy difference tends to zero in the limit when the radii approaches infinity –i.e. in the limit of a straight ferromagnetic strip.
We now consider the question of how to experimentally produce these two types of $2\pi$ walls. We use the information contained in their global topological number $\omega$ and compare it to other known states of nanorings. In particular, the well-known "onion" state has $\omega = 0$. Since the onion is the remanent magnetization after saturation by an in-plane uniform field, one can produce the $\Omega = -1$ wall by applying a strong field in-plane followed by a circumferential field. The two walls will approach and form a $2\pi, \Omega = -1$ wall. Changing the direction of either the in-plane field or the circumferential field will only change the final position of the $2\pi$ wall, not its topological index.

The $2\pi, \omega = 2$ domain wall cannot be produced using only uniform and circumferential fields. However, we propose the following technique to produce that configuration in nanorings: apply a strong dipolar field ($\omega = 2$) in the interior of the ring. This could be produced by a small current loop with its axis coplanar to the structure, or by bringing a magnetic tip close to the device. If this dipolar field is strong enough, two transverse walls would be produced at opposite sides of the ring; the magnetization vector at the centers of the wall will point in the opposite direction of the overall magnetization of the ring. Activating the circumferential field as the dipole strength is decreased will result in the desired configuration.

One final question is whether resistance measurements can distinguish the difference between the two types of $2\pi$ structures reported in this work. For instance, one could attempt to use anisotropic magnetoresistance effect to read the overall winding number of the configuration. An estimate of this
effect can be obtained by integrating $\mathbf{J} \cdot \mathbf{M}$ along a certain segment of the ring that spans the whole $2\pi$ domain wall. Since $\mathbf{J}$ runs along $\hat{\theta}$ the AMR would be proportional to $\langle M_\theta / M_s \rangle$ which can be directly calculated from the $2\pi$ domain structure. For two electrodes located at the top and bottom of the segment shown in Fig. 6.7 these values are 0.042 and 0.016 for the $\Omega = +1$ and $\Omega = -1$ walls respectively. It therefore should be possible to apply a current to probe the winding number of the $2\pi$ domain.

6.4 Conclusion

We have presented results on the thermal annihilation of $2\pi$ domain walls. We differentiated between two types of $2\pi$ walls through their winding number in curved nanowires. We have observed a simple arithmetical relation between the topological index of the different configurations and the processes by which each structure decays into the ground state. The fact that the energy difference between the two states is dominated by the exchange energy allows to identify the states through their winding number. The transition path requires the motion of a singularity through the bulk: an antivortex destroys $\Omega = -1$ walls, and a vortex annihilates $\Omega = +1$ walls. Similar behavior is expected to work in linear stripes. Topological defects are known to play a role in certain types of phase transitions; here we have determined the mechanism by which they destroy $2\pi$ wall structures.

The two types of $2\pi$ domain wall correspond to distinct metastable states:
the greatest contribution to the energy difference comes from the exchange energy difference. The energy can be directly associated with the topological signature of the magnetization configuration. The stability of these two states is comparable to the stability of the clockwise configuration. We suggest to use AMR noise measurements as a way to verify the presence of the two types of wall in magnetic nanowires and study their stability. Thermal fluctuations should generate both types of wall which could be recognized as two separate values of the AMR.

Further micromagnetic exploration of the $2\pi$ wall annihilation problem presented here can be done moving away from the overdamped regime by using a nonzero precessional term. The results presented here will be interesting to compare to this case. While we have presented results on a 2nm thick ring, we expect the observed transition states in thicker rings. The key parameter is the ratio of the thickness to the mean radius which should be less than approximately 0.1 [11]. We plan to explore the energy barriers and transition states as a function of thickness and ring radii.
Chapter 7

Transition states of perpendicular anisotropy materials

The spin-transfer switching of nanomagnets with perpendicular anisotropy has received intense attention in recent years [52]. Perpendicular anisotropy elements are good candidates for magnetic random-access memory applications (ST-MRAM)[53]. A key figure of merit for thermal stability is the ratio of the spin polarized current to the energy barrier for thermal reversal. Experiments on objects with uniform magnetization (Macrospin model) indicate that these elements are thermally stable[54] in agreement with analytical predictions[55].

For samples larger than the exchange length the uniform magnetization assumption breaks down and the energy barrier needs to be recalculated. Due to the multiscale character of micromagnetism, analytical calculations are complicated and transition states have been calculated only for a handful of
physical systems [56, 2]. Numerical calculations become necessary for the majority of systems. In this work, we use the String Method [32] to find the transition states and activation energies in perpendicular anisotropy elements without the assumption of uniform magnetization.

We studied thin layers of thickness \( t = 1.6 \) nm, with saturation magnetization \( M_s = 713 \times 10^3 \) A/m, exchange constant \( A = 8.3 \times 10^{-12} \) J/m, and anisotropy constant \( K = 403 \times 10^3 \) J/m\(^3\). A constant field perpendicular to the film \( B_z \) is applied with a maximum magnitude equal to the coercive field \( B_c = \left( 2K - \mu_0 M_s^2 \right) / M_s = 0.245 \) T, this breaks the degeneracy between the two lowest lying magnetization states. We investigate the transition from the metastable state (downward magnetization) to the ground state (upward magnetization) and compare to the macrospin model.

We describe the micromagnetic energy of this system by:

\[
E = t \int_\Omega \left[ A |\nabla \mathbf{m}|^2 + \frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{N} \cdot \mathbf{M} - Km_z^2 - B_z M_z \right] d\Omega \quad (7.1)
\]

where \( \mathbf{N} \) is the spatially dependent demagnetizing tensor, and \( \mathbf{m} \) is the normalized magnetization vector. In the macrospin approximation \( A \to \infty \), this first term becomes a constraint and the energy reduces to:

\[
E_{\text{macrospin}} = t \Omega \left[ \frac{\mu_0 M_z^2}{2} - Km_z^2 - B_z M_z \right] \quad (7.2)
\]

where \( \Omega \) is the inplane cross-sectional area of the film. The magnetization dynamics is governed by the Landau-Lifshitz-Gilbert equation which we write
where $\gamma' = \gamma/(1+\alpha^2)$ is the gyromagnetic ratio and $\alpha$ is the damping constant.

Transition state theory indicates that reversal occurs through the critical points of the magnetization dynamics (i.e. $\frac{dm}{dt} = 0$) which in this system coincide with the stationary configurations of the energy surface ($\nabla M E = 0$). The probability for thermal induced magnetization reversal follows the Arrhenius law $e^{-\Delta E/k_B T}$ where $\Delta E$ is the energy difference between the transition state and the metastable configuration[1].

We implemented the String Method in conjunction with OOMMF [39] to find the transition states by integrating only the non conservative term of Eq. 7.3 (the magnetization evolves parallel to $-\nabla M E$). We use 100 images between the two energy minima and reparametrize the string every 40 ps. Our initial guess path passed through a fully randomized magnetization configuration and was allowed to evolve according to the String Method prescription to its minimal energy path, details are presented elsewhere[40, 51, 57]. A typical result is presented in Fig. 7.1 where the reversal can be seen to occur by propagation of a Bloch across the sample.

The field dependence of the activation energy is shown in Fig. 7.2 for the large samples the activation energy is clearly lower than the prediction of the
Figure 7.1: Images of the minimum energy path. Images number are at locations 0, 20, 40, 60, 80, 100. Red and blue colors represent downward and upward magnetization respectively. Reversal occurs by nucleation of a domain on one corner, and propagation of a domain wall across the material. The transition state is located close to image 20.

Figure 7.2: Field dependence of thermal activation energy for elements with two different sizes. It can be seen that the activation energy is lower than the predicted by the macrospin model.
macrospin model which from eq. 7.2 can be derived to be

\[ \Delta E_{\text{macrospin}} = t\Omega \left( \frac{M_s B_z^2}{2B_c} + \frac{B_c M_s}{2} - B_z M_s \right) \]  \hspace{1cm} (7.4)

with the transition state at \( m_z = -B_z / B_c \). As expected, the activation energy decreases as the field approaches the coercive field.

Two points needs to be made regarding the change of size in Fig 7.2. First, the activation energy barrier is independent of the cell size used in the numerical integration once the cells become smaller than the exchange length; which is the standard requirement of numerical micromagnetics. This is then a real physical effect and not a numerical artifact of changing the relative scales of the system. Second, an effective size reduction can be achieved by increasing the exchange constant to a very large value \( (10^2 \times A) \). In this limit our result should approach the macrospin model. The results are shown in Fig. and indicate that merely increasing \( A \) is not sufficient to match the macrospin model and the String Method. However, a refinement of the magnetostatic energy term in which the film is not considered an infinite plane, but the actual demagnetization tensor is calculated with the formulae by Newell [58] result in a perfect match. Considering the extremely small aspect ratio of the samples this is an important result: it warns that finite size effects are important even for very thin geometries.

Size effects of the activation energy in square geometries are summarized in Fig. 7.4 where two regimes can clearly be identified. For small samples,
Figure 7.3: Comparison of two versions of the macrospin model: $N_{zz} = 1$ correspond to the commonly used infinite film limit, $N_{zz} = 0.95$ is a wide film with finite aspect ratio, blue circles are calculated with the string method for a very large exchange constant.

Figure 7.4: Activation energy for square samples (blue) and circular samples (red).
the activation energy increases with the size of the element, this regime corresponds to the macrospin model. Beyond a certain size (∼50 nm) the activation energy becomes a constant. For large elements, the radius of the reversed nucleus is independent of the element size. For all size considered, the reverse domain resembles a circular region with domain walls making right angles with the sample’s edge (see second image at Fig. 7.1). At the given configuration eq. 7.1 can be approximated as the sum of three dominant terms:

- A switched domain with area $\Omega_1 = (\pi R^2/4)$ with energy density per unit area $\xi_1$ approximate to $t \left( \frac{\mu_0 M_s^2}{2} - K - B_z M_s \right)$;
- An unswitched domain with downward magnetization of area $\Omega_2 = \Omega - \Omega_1 = \Omega - \pi R^2/4$ and surface energy density $\xi_2 \approx t \left( \frac{\mu_0 M_s^2}{2} - K + B_z M_s \right)$; and
- The domain wall of length $s_3 = 2\pi R/4$ with a linear energy density per unit length $\lambda_3 \approx 4\sqrt{AK}$[59]. Here, $K'$ is an effective crystalline anisotropy constant $K' = (K - \frac{\mu_0 M_s^2}{2})$. The total energy $\xi_1\Omega_1 + \xi_2\Omega_2 + s_3\lambda_3$ is a maximum for $R = 38$ nm with an activation energy of $\Delta E \approx 16 \times 10^{-20}$ J which is a good approximation to the energy plateau presented in figure 7.4.

Fig. 7.4 also presents the obtained activation energies for circular samples ad a function of inplane diameter. The absence of corners prevents the circular shape of reaching a plateau on the activation energy. As a result circular samples become more thermally stable for increasing size.

In conclusion, using the String Method we have calculated activation energies for thermally induced magnetization reversal and compared the results to a uniform magnetization model. Our results indicate that finite size effects
on the macrospin model are important even for very thin samples. In addi-
tion, the activation energy for square samples as a function of size present
a transition from linear dependence to a constant value. This result mimics
previous prediction of activation energies for elongated particles and circular
nanorings[11, 8].
Chapter 8

Minimum Action Paths for Spin-Torque Driven Thermally Induced Magnetization Reversal

There is considerable interest in controlling the magnetization in thin film magnetic elements using spin-polarized currents. The interaction between a spin-current and background magnetization, known as Spin Transfer Torque (STT) [60, 61, 62], holds promise as a means of information storage and retrieval without the use of moving parts. A critical issue in designing STT devices is thermal stability: thermal fluctuations can cause spontaneous reversal of a desired magnetization state. What makes the analysis of these thermally-induced reversals challenging is that STT introduces a non-gradient term in the magnetization dynamics, which implies that the reversals are non-equilibrium
transition events and the standard reaction rate theory of Kramers [1] cannot be used to describe them. Early work on these reversals was carried out by Li and Zhang [24] as well as Apalkov and Visscher [63]. Here we calculate relaxation rates of STT systems using the geometrical Minimum Action Method (gMAM) [64, 65] to obtain the most probable transition paths and transition states of a single domain nanomagnet. Our result are consistent with the numerical simulations of Li and Zhang [24], and suggest the possibility of using the gMAM technique to study more complex problems involving nonequilibrium transitions.

We begin by distinguishing in which way nonequilibrium transitions differ from equilibrium ones. When the zero-noise dynamics is derivable from a potential $V$, the thermally-induced transitions occur at equilibrium and the
Kramers theory predicts that the transition paths are minimum energy paths (MEPs) and that the transition rates $k$ (formally the inverse of the mean first passage time) are given by Arrhenius formula: $k = k_0 \exp\left(-\frac{\Delta V}{k_B T}\right)$ where $T$ is the temperature and $k_B$ is Boltzmann’s constant. In this formula, the leading-order asymptotics are governed by $\Delta V$, the potential energy difference to the transition state. The prefactor (or subdominant term) $k_0$ depends on the curvature of the potential at the local minimum and at the saddle along the MEP. Kramers formula is asymptotically correct in the limit $T \to 0$; in practical problems, it is usually sufficient that $k_B T / \Delta V$ be small. Numerical methods to calculate the MEPs and estimate $\Delta V$ include the Nudged Elastic Band Method [66], and the String Method [40].

In the presence of STT, there is not a well defined potential and the magnetization reversals are nonequilibrium transitions. In particular, the transition paths are no longer MEPs and the transition rates cannot be derived from Kramers theory. The appropriate formalism to calculate the transition paths and rates for these non-gradient systems is the theory of large deviations [67]. This theory gives an action whose minimizers are the most probable reaction pathways and expresses the reaction rate in terms of an Arrhenius-like formula in which the energy barrier is replaced by the minimum of the action. Large deviation theory has been previously used in field-driven magnetization reversal of macrospins [68] and micromagnetics [69]. It is also implicit in the work by Serpico et al. [70]. The geometrical Minimum Action Method [64, 65] is based on large deviation theory: it can be used to minimize the action func-
tional and obtain the most probable transition paths and transition states of a
single domain nanomagnet.

Here we focus on magnetic systems of the type studied by Li and Zhang [24],
i.e., thin film nanomagnets of volume $v$, saturation magnetization $M_s$, and an
in-plane anisotropy field $H_K$ directed along the $\hat{x}$-axis (the film is taken to lie
in the $xy$ plane). We wish to find the most probable path $m(t)$ connecting two
magnetization states $m_i$ and $m_f$, which are dynamic attractors of the system
in the absence of noise. If a spin-polarized current flows in the direction per-
pendicular to the film plane, then the dynamics are governed by the stochas-
tic Landau-Lifshitz-Gilbert equation, which in the Stratonovich interpretation
reads

$$\dot{m} = -\gamma' m \times H_{\text{eff}} + \gamma' m \times (m \times (a_J \hat{P} - \alpha H_{\text{eff}})).$$  \hspace{1cm} (8.1)

Here $\gamma' = \gamma/(1 + \alpha^2)$, $\gamma$ is the gyromagnetic ratio, $\alpha$ is the damping constant
and $\hat{P}$ is the current polarization vector oriented along $m_x = +1$. The strength
of the spin torque effect is determined by $a_J$. The effective field contains de-
terministic and stochastic components

$$H_{\text{eff}} = -\nabla_m \frac{E(m)}{\mu_0 M_s} + \sqrt{\epsilon} \dot{W},$$  \hspace{1cm} (8.2)

where $\dot{W}$ is a Gaussian white noise process, $\epsilon = 2\alpha k_B T/\mu_0 \gamma v M_s$ measures
the noise amplitude and $E$ is the micromagnetic energy density which, in the
presence of an external field $H_{\text{ext}}$, reads

$$E(m) = -\mu_0 M_s H_{\text{ext}} \cdot m - \frac{\mu_0 H K M_s}{2} m_z^2 + \frac{\mu_0 M^2}{2} m_z$$ (8.3)

Note that the presence of the spin torque interaction term in (8.1) makes the dynamics non-gradient.

Eq (8.1) can be written as the following stochastic differential equation:

$$\dot{m} = b + \sqrt{\epsilon} \sigma(m) \dot{W}$$ (8.4)

where

$$b \equiv -\mathbf{K}_A \left( \frac{\gamma' \nabla m E}{\mu_0 M_s} \right) - \alpha \mathbf{K}_S \left( \frac{\gamma' \nabla m E}{\mu_0 M_s} - \frac{a J_P}{\alpha} \right)$$ (8.5)

is the deterministic drift vector and

$$\sigma(m) \equiv -\gamma' (\mathbf{K}_A + \alpha \mathbf{K}_S)$$ (8.6)

is the diffusion matrix. Here $\mathbf{K}_S$ and $\mathbf{K}_A$ are symmetric and antisymmetric matrices with components

$$K_{s_{\mu\nu}} = (\delta_{\mu\nu} - m_\mu m_\nu); K_{A_{\mu\nu}} = \epsilon_{\rho\mu\nu} m_\rho.$$ (8.7)

The presence of noise allows the system to deviate from the deterministic flow lines given by $\dot{m} - b = 0$. From (8.4), the system’s response to an
instantaneous thermal fluctuation is

$$\dot{W} = \frac{1}{\sqrt{\epsilon}} \sigma^{-1}(\dot{m} - b). \quad (8.8)$$

Since the probability of these fluctuations on the interval between times $t_0$ and $t_f$ is proportional to $\exp\left(-\frac{1}{2} \int_{t_0}^{t_f} |\dot{W}|^2 dt\right)$, a given trajectory occurs with probability proportional to $\exp(-\epsilon^{-1} S)$ where the action $S$ is defined as

$$S = \frac{1}{2} \int_{t_0}^{t_f} |\sigma^{-1}(\dot{m} - b)|^2 dt. \quad (8.9)$$

Hence, the most probable path is the trajectory that minimizes this action. The gMAM algorithm permits to numerically obtain this trajectory. Furthermore, the value of the minimum action between $m_i$ and $m_f$ defines a pseudopotential $V$, which provides information of the system statistical properties. In particular, the transition rates between states follow an Arrhenius-like formula

$$k_{1,2} \sim \exp(-\epsilon^{-1} V(m_1, m_2)).$$

To proceed further the action functional is rewritten as the following dot product $\mathcal{L} \equiv \frac{1}{2} \langle (\dot{m}' - b)|a^{-1}(m' - b) \rangle$ where $a \equiv \sigma \sigma^T$ is the diffusion tensor. The prime subscript is the derivative of the parametrized curve $m' \equiv \frac{dm}{ds}$ where $s$ is the curve length measured from $m_i$. The tensor $a$ is clearly symmetric since $a^T = (\sigma \sigma^T)^T = \sigma \sigma^T = a$. From the action functional we can obtain a generalized momentum $\Theta_\mu = \frac{\partial \mathcal{L}}{\partial (m'_{\mu})} = a_{\mu\nu}^{-1}(m'_{\nu} - b_{\nu})$ and a corresponding hamiltonian $\mathcal{H}(\Theta, m) \equiv \Theta_\mu m'_{\mu} - \mathcal{L} = \Theta_\mu (a_{\mu\nu} \Theta_{\nu} + b_{\mu}) - \frac{1}{2}(\Theta_\mu a_{\mu\rho} a_{\rho\sigma}^{-1} a_{\sigma\nu} \Theta_{\nu}) = \frac{1}{2} \Theta_\mu a_{\mu\nu} \Theta_{\nu} + b_{\mu} \Theta_\mu$. For compactness the hamiltonian may be written in vector
notation as
\[ H = \frac{1}{2} \langle \Theta | a \Theta \rangle + \langle b | \Theta \rangle. \] (8.10)

Heymann and Vanden-Eijnden [65] proved that the minimum action path can be obtained by iteratively evolving each point in the trajectory according to
\[ \dot{m}_\mu = \lambda^2 m''_\mu - \lambda \frac{\partial^2 H}{\partial \Theta_\mu \partial m_\nu} m'_\nu + \frac{\partial^2 H}{\partial \Theta_\mu \partial \Theta_\nu} \frac{\partial H}{\partial m_\nu} + \lambda' m'_\mu \] (8.11)
and reparametrizing the obtained path. Here \( \lambda = \sqrt{\langle b | a^{-1} b \rangle / \langle m' | a^{-1} m' \rangle} \), \( \lambda' = \frac{d\lambda}{ds} \), the derivatives of the Hamiltonian are evaluated at \( \Theta = \vartheta \equiv a^{-1}(\lambda m' - b) \). The right hand side of Eq. 8.11 depends on the metric tensor \( a \), its inverse \( a^{-1} \) and its derivatives \( \frac{da_{\sigma\rho}}{dm_\mu} \) and \( \frac{d^2 a_{\sigma\rho}}{dm_\nu dm_\mu} \). We should describe some relevant mathematical properties of these objects.

The matrices \( \hat{K}_S \) and \( \hat{K}_A \) satisfy
\[ \left( \hat{K}_A \hat{K}_A^T \right)_{\mu\nu} = \left( \delta_{\mu\nu} - m_\mu m_\nu \right) = \left( \hat{K}_S \right)_{\mu\nu}, \] (8.12)
\[ \left( \hat{K}_A \hat{K}_S^T \right)_{\mu\nu} = \epsilon_{\rho\mu\nu} m_\rho = - \left( \hat{K}_A \hat{K}_S^T \right)^T_{\mu\nu} = - \left( \hat{K}_S \hat{K}_A^T \right)_{\mu\nu} \] (8.13)
and
\[ \left( \hat{K}_S \hat{K}_S^T \right)_{\mu\nu} = \hat{K}_S \] (8.14)
so that the diffusion tensor \( a \) can be written as
\[ a = \sigma \sigma^T = \gamma^2 (1 + \alpha^2) \hat{K}_S. \] (8.15)
The matrix $\sigma$ indicates how a given fluctuation of the field $\sqrt{\epsilon} \dot{\mathbf{m}}$ translates into a change in magnetization direction. One of its eigenvalues is zero which reflects the fact that the magnetization has constant magnitude and fields along $\mathbf{m}$ produce no response on the dynamics. The components of the fluctuation perpendicular to the magnetization are transformed with eigenvalues $-\gamma'(\alpha + i)$, the $-i\gamma'$ indicates a rotation of $90^\circ$ in the plane perpendicular to the magnetization and corresponds to the precessional term of the LLG equation while the $-\alpha\gamma'$ reflects the damping component derived from perturbation of the noise.

We can conclude that eigenvalues of $a$ are 0 along $\mathbf{m}$ and $\gamma'^2(1 + \alpha^2)$ for any vector tangential to the unit sphere.

Since one of the eigenvalues of the diffusion tensor $a$ is zero, the inverse does not exist. However, all relevant quantities used in the gMAM algorithm are restricted to the 2D dimensional space enclosed by the unit sphere (for example, $\mathbf{m}'$ and $\mathbf{b}$ belong to the range of $a$). We use instead the following pseudotensors in the calculation of the hamiltonian and its derivatives

\begin{equation}
\tilde{a}_{\phi\mu} = a_{\phi\mu} = \gamma'^2(1 + \alpha^2)(\delta_{\phi\mu} - m_{\phi}m_{\mu})
\end{equation}

and

\begin{equation}
(\tilde{a}^{-1})_{\phi\mu} = \frac{(\delta_{\phi\mu} - m_{\phi}m_{\mu})}{\gamma'^2(1 + \alpha^2)} = \frac{\tilde{K}_S}{\gamma'^2(1 + \alpha^2)}.
\end{equation}

Numerically this procedure has the advantage that avoids the singularities that arise when using non cartesian coordinates. It is convenient to write explicitly
the derivatives of $\hat{K}_S$ and $\hat{K}_A$ with respect to the magnetization coordinates:

$$\begin{align*}
\frac{\partial K_{S\mu\nu}}{\partial m_{\phi}} &= (2\delta_{\mu\nu}m_{\phi} - \delta_{\mu\phi}m_{\nu} - \delta_{\phi\nu}m_{\mu}) \\
\frac{\partial K_{A\mu\nu}}{\partial m_{\phi}} &= \epsilon_{\phi\mu\nu}.
\end{align*}$$

(8.18)

(8.19)

The derivatives of the hamiltonian required for evaluation of the RHS of Eq. 8.11 can be written explicitly as:

$$\begin{align*}
\frac{\partial H}{\partial \Theta_{\mu} \partial \Theta_{\nu}} &= a_{\mu\nu}, \\
\frac{\partial H}{\partial \Theta_{\mu} \partial m_{\nu}} &= \frac{\partial a_{\mu\rho}}{\partial m_{\nu}} \Theta_{\rho} + \frac{\partial b_{\mu}}{\partial m_{\nu}}, \\
\frac{\partial H}{\partial m_{\nu}} &= \frac{1}{2} \Theta_{\mu} \frac{\partial a_{\mu\rho}}{\partial m_{\nu}} \Theta_{\rho} + \frac{\partial b_{\mu}}{\partial m_{\nu}} \Theta_{\mu}.
\end{align*}$$

(8.20)

(8.21)

(8.22)

At these point we can give a detailed description of the gMAM algorithm as described by Heymann and Vanden-Eijnden. To begin, we find the critical attractive points of the deterministic LLG equation (the noise and itô drift term must dropped). There are simple analytical expressions for the stable critical points when the external field is directed along one the main axis. For more general cases the stable points must be found by numerical integration. We label these points as $m_i$ and $m_f$.

We solve Equation 8.11 by discretizing both in time and along $s$. To do this,
an initial sequence \( t = 0 \) of \( N + 1 \) images \( m^i,0 \) is created so that \( m^{0,0} = m_i \) and \( m^{N,0} = m_f \). The images are equally spaced at intervals of arclength \( \frac{s}{N} \).

The iterative loop consists of the following three steps:

1. The quantities \( m'^{i,k}_\mu, b^{i,k}_\mu, \lambda^{i,k}_\mu, \vartheta^{i,k}_\mu, \lambda'^{i,k}_\mu \) are obtained using:

\[
m'^{i,k}_\mu = \frac{N(m^{i+1,k}_\mu - m^{i-1,k}_\mu)}{2}, \quad 0 < i < N \tag{8.23}
\]

\[
b^{i,k}_\mu = \frac{\partial b^{i,k}_\mu}{\partial m^{i,k}_\nu} \quad \text{From Eq. 8.5} \tag{8.24}
\]

\[
\lambda^{i,k} = \sqrt{\frac{b^{i,k}_\mu K_{\mu\nu} b^{i,k}_\nu}{m^{i,k}_\mu K_{\mu\nu} m^{i,k}_\nu}} \quad 0 < i < N \tag{8.25}
\]

\[
\vartheta^{i,k}_\mu = K_{\mu\nu}(\lambda^{i,k}_\mu m'^{i,k}_\nu - b^{i,k}_\nu) \quad 0 < i < N \tag{8.26}
\]

\[
\lambda'^{i,k}_\mu = \frac{N(\lambda^{i+1,k}_\mu - \lambda^{i-1,k}_\mu)}{2} \tag{8.27}
\]

2. Solve the linear system for \( \tilde{m}^{i}_\nu \) that satisfies the discretized version of equation 8.11:

\[
\frac{\tilde{m}^{i}_\nu}{\Delta t} - (\tilde{m}^{i+1}_\nu - 2\tilde{m}^{i}_\nu + \tilde{m}^{i-1}_\nu)(N\lambda^{i,k})^2 = \\
\frac{m^{i-1}_\nu}{\Delta t} + \lambda^{i,k}_\mu \frac{\partial H}{\partial \Theta^{i,k}_\mu} \frac{\partial}{\partial m^{i,k}_\nu} m'^{i,k}_\nu + a_{\mu\nu} \frac{\partial H}{\partial m^{i,k}_\rho} + \lambda^{i,k}_\mu \lambda'^{i,k}_\mu m'^{i,k}_\nu \tag{8.28}
\]

for \( 0 < i < N \) with the derivatives of the hamiltonians evaluated with \( \Theta^{i,k}_\mu = \vartheta^{i,k}_\mu \) and \( m_\mu \). The derivatives are written explicitly in Eqs. 8.20-
8.22. The endpoints of the chain of states are kept fixed so that

\[ \tilde{m}_i^0 = m_{i\nu} \]
\[ \tilde{m}_i^N = m_{f\nu} \]  \hspace{1cm} (8.29)

The resulting linear system is tridiagonal for each dimension and its solution is straightforward.

3. Reparametrize the trajectory described by \( \tilde{m}_i^i \) so that adjacent images are separated by the same arcdistance and all vectors are renormalized \((m_{\nu_i} m_{\nu_f} = 1)\). In this work, this step has been done using simple linear interpolation. The results form the updated sequence of images \( m_{i\nu}^{i+1} \).

These steps are repeated iteratively, the transition time and action can be calculated at the end of each iteration from the following expressions:

\[ S^k = \frac{1}{N} \left( \frac{3}{2} \varphi^{1, k}_{\mu} \varphi_{1, k_{\mu}} \sum_{i=2}^{N-2} \varphi^{i, k}_{\mu} \varphi_{i, k_{\mu}} + \frac{3}{2} \varphi^{N-1, k}_{\mu} \varphi_{N-1, k_{\mu}} \right) \]  \hspace{1cm} (8.30)

and

\[ T^{i, k} = -\frac{1}{2\lambda_{0, k}} + \sum_{j=0}^{i} \frac{1}{\lambda_{j, k}} - \frac{1}{2\lambda_{i, k}}. \]  \hspace{1cm} (8.31)

If the trajectory passes through a critical point the total time should become infinite, numerically this exact condition may be difficult to reach. However, the general tendency is that the transition time \( T \) increases and the total action \( S \) decreases with subsequent iterations. The optimal criterion for stopping the
iteration would be when the change in the action is less than a convenient threshold: \(|S^k - S^{k-1}| < \delta_s\).

The algorithm can be optimized further as described in Ref. [65]. In particular, images very close to critical points (identified by small values of \(\lambda\)) can be isolated and made to evolve towards the transition points. The chain of states is broken into separate pieces and each piece is reparameterized independently.

Figure 8.1 shows typical trajectories obtained using the gMAM algorithm. For comparison purposes the deterministic trajectories are also shown. The basin of attraction of the \(m_x = +1\) contracts with increasing current.

The minimum action paths present kinks at the transition points \((b = 0)\). This is explained as follows: the trajectory from the transition points to the attractive critical points (downstream) follow the deterministic driftlines. The segment running from the attractive critical point to the transition point (upstream) needs to overcome the drift field, but the action is a maximum if the trajectory is antiparallel to the drift fields. The action minimization can be achieved by a trajectory which is not entirely antiparallel to the drift lines. The sharp change of direction at the transition point occurs because the trajectory switches from upstream to downstream.

For finite currents the critical points of Eq. 8.5 no longer coincide with the saddle points of the energy surface. The effect of currents on the minimum action paths is shown in Fig.8.1 It is evident that the transition state now has an out of plane magnetization component. This arises because the coefficient
of $\hat{K}_S$ and $\hat{K}_A$ are not simultaneously zero. A positive current favors $m_x = -1$ and shifts the critical point towards $m_x = +1$ ($\phi = 0$). With this in-plane displacement of the magnetization, the precessional term is no longer zero and needs to be counterbalanced by an upward shift. As the magnetization moves upward, the shape anisotropy field becomes non zero and acts downward on the magnetization. The net effect is that the current produces a leftward and upward shift of the transition magnetization. The critical points have now an out-of-plane magnetization component. This simple result may have important consequences on current understanding of nonuniform magnetization reversal of thin films: while it is known that stationary points in the energy surface of thin films occurs for in plane magnetizations, the effect described here shows that when a spin-torque is presence thermal transitions may have an out-of-plane magnetization component.

In what follows we focus in transitions from $m_{i_x} = -1$ to $m_{f_x} = +1$. To obtain the dependence of the action on the current strength we evaluated the minimum action path in a two step procedure. First, we use gMAM to find an approximate action path that allows us to visually identify the location of the transition point. We discard the downstream section of the path and recalculate the action using gMAM only in the upstream direction. That value is our estimate for the minimum action.

We now present results of the action’s dependence on field and current magnitude in Fig. 8.2.

The action is calculated for trajectories from $m_x = -1$, to $m_x = +1$. In a
Figure 8.2: Dependence of the minimum of the action (left) and of the effective energy barrier in (8.32) (right) on external field $H_{ext}$ and current magnitude $a_j$. Action is calculated for forward reversal (from $m_x = -1$ to $m_x = +1$). Here, $E_0 = 59.02 k_B T$. The critical spin current is $a_c = \alpha (H_{ext} + H_K + M_S/2)$. The expected range of validity of the Zhang-Li theory spans only positive fields.

magnet with $\mu_0 M_s = 1.2 \text{ T}$, $\alpha = 0.05$, $H_K = 0.05$. The action has positive values and approaches zero as the switching field is reached. Positive currents result in larger values for the action.

By calculating the rate of the transition and using it in an Arrhenius-like formula, Li and Zhang [24] describe an effective activation energy which in our
geometry reads:

\[ E_b = E_0 \left( 1 - \frac{H_{\text{ext,x}}}{H_K} \right)^2 \left( 1 + \frac{a_J}{\alpha(H_{\text{ext,x}} + H_K + M_s/2)} \right). \]

where \( E_0 \) is the activation energy at zero current and zero field. This effective energy can be compared directly to the minimum of the action calculated using gMAM. While our results do present a quadratic dependence on the external field, as can be seen in Fig. 8.2, we have found a different dependence of the action on the current magnitude \( a_J \). Our results cover regimes were the energy barrier is high with respect to thermal noise while the numerical approach of Li and Zhang requires applied fields close to the switching fields. With gMAM we are able to explore a wider region of the parameter space.

Summarizing, we have calculated Minimum Action Paths and corresponding Actions for magnetic particle under the influence of spin torque. Our results indicate that the transition state has an out of plane magnetization component, while previously they have been considered to be in-plane magnetizations. The Minimum Action Method promises to be a useful tool for the study of a large variety of magnetic systems.
Chapter 9

Conclusions and prospectives

This work has focused on techniques to find transition states and energy barrier in ferromagnetic elements. The initial stages of this work consisted in numerical verification of the analytical model of Martens et al. [11] by direct numerical simulation using the theoretical saddle points as the initial magnetization configuration. As we numerically explored this geometry we found that the analytical model was in fact applicable to a greater wide of geometries than previously expected.

Similarly, we used the String Method to find the transition states for nanorings. This provided stronger evidence in support of the analytical theory of Martens et al. The advantage of the String Method is the lack of assumptions regarding the profile of the transition state.

In addition, we found that the energy landscape of permalloy rings was feature rich in the sense that there is a multiplicity of metastable states sep-
rated by the energy of $2\pi$ domain walls. Interestingly Permalloy nanorings are well described by one of the regimes characterized by De Simone et al [12]; namely, the magnetostatic limit where magnetization configurations can be described by a collective coordinate description in terms of isolated magnetic charges. The transition states where found to be associated with motions of this charges through the material so that transition between states is described simply by operations on the topological winding numbers of the materials.

One interesting line of inquiry that these results open relates to the collective coordinate description of transition states in nanomagnets. In the collective coordinate description of the magnetostatic limit, the full micromagnetic configuration is described using the coordinates of isolated topological defects. The Landau Lifshitz Gilbert equation rewritten as the combination of a gyrotropic and a damping term, it is well known that the dynamics of the magnetization is well captured by this description. The interesting question to solve would be: How well does the collective coordinate description of magnetization states capture the transition states between different metastable configurations?

We also explored the thermal barriers of ferromagnets with perpendicular anisotropy, which provide a new example of non uniform magnetization reversal in magnetic materials. The transition from uniform to non-uniform magnetization reversal is clearly observed in the dependence of energy barrier vs. element size.

During this investigation it was clear that the fabrication of nanostructures with currents flowing along a filament at the center of the samples would be
a serious design challenge. A way around this problem was to permit current to flow inside the magnetic material. This will in turn, inject spin polarized currents which incorporate non gradient terms in the magnetization dynamics. To advance in this direction, we used the gMAM method to find minimum action paths for magnetization reversal in nanomagnets under the influence of magnetic fields and spin polarized currents. We were able to explore a wide region of the parameter space.

Recently, researchers Katherine Aidala from Mount Holyoke College and Mark Tuominen at MassNano Tech presented a technique for direct injection of currents into the center of a ferromagnetic ring using the tip of a Scanning Probe Microscope. The microscope allows to control the precise location at which the current is applied and could be potentially be used in experimental setups as envisioned in the original Martens et. al model.

It is clear from this work that both non uniform magnetization and spin transfer torque effects will be important on the understanding of the next generation of magnetic storage devices. An important next step in this investigation requires the implementation of the gMAM method for non uniform magnetization samples. In this regard, Fast Fourier Transform techniques can be used to implement the necessary steps of the gMAM algorithm.
Appendix A


The majority of numerical work in this dissertation was used in conjunction with the two dimensional version of the micromagnetic simulation package OOMMF. In addition to OOMMF, the following publicly available packages should also be installed.

- GSL, Gnu Scientific Library [71]. This library is used in the calculations of the Jacobi elliptic function.

- nr.h, This is the famous numerical recipes library of Press, Teukolsky, Vetterling and Flannery [72]. It is used for a variety of purposes.

- Image Magick [73], this is graphic manipulation package used in the code to convert between different graphic file types.

- QT, version 3[74], this compiles the graphic interface.
• gdcOVFfile.h, header library to manipulate vector field files of OOMMF.

A.1 gdcOVFfile.h library

The library gdcOVFfile.h is a utility to manipulate OOMMF vector fields. It contains all of the functions written for the manipulation of OOMMF files with meshes of the “irregular binary 8” type. Many of the algorithms use this class.

The object is defined as:

```cpp
class OVFfile
```

with the following members:

```cpp
friend void INTERPOLATE(OVFfile, OVFfile, int, char *); Connects two configurations by a sequence of steps. Initially the intermediate steps follow a straight line and then the vectors are normalized to one. The output is stored in a file name given by the last parameter.
```

```cpp
public:

OVFfile(); Initializes the value multiplier to one. So far I have not really needed it. And it is required by the compiles.

OVFfile(char *name); Reads the file with name equals to the string. Stores relevant values in the object attributes.

OVFfile(int size, char * name); Creates a new object with a mesh of n points and the name of the files pointed by name.

void OVFfile_save(char *name); Saves the object on a file under the name name. It uses the attribute named filename to clone the appropriate header for the new OOMMF vector file.
```
void OVFFile_load(char *); Reads a vector file with called name and stores the information on the current object. Similar to OVFFile(char *name) but using the old memory.

void getfilename(char *) const; This function is written with the purpose of copying the header of the original files into newly saved files. It returns the string of the file name.

void windingnumbers(); This function goes over the whole mesh calculating the winding numbers around unit cells. When the winding numbers are greater than $\frac{1}{4}$ it rounds to the nearest half integer. And prints in the screen the location of possible topological defects. Not entirely safe. It requires critical comparison with the displayed field.

void multiply (double); multiply the vectors by a double precision floating number.

void subtract (const OVFFile &); subtract an OVFFile (equivalent cells of the mesh) to the current one.

void add (const OVFFile &); add an OVFFile (equivalent cells of the mesh) to the current one.

void conditionaladd (const OVFFile &); adds the mesh of another vector file only if both cells of the magnetization are different from zero. The reason for this behavior is that magnetic field are different from zero outside the material. When the magnetization is zero (outside the material) the field is not added.

void copy (const OVFFile &); Copies a vector object into the current one.

double dotmultiply (const OVFFile & factor); Gets the dot product of one
vector field to the current one.

    long int get_pointcount (void) const; Reads the pointcount attribute. Which
stores the number of points in the mesh.

    long int set_pointcount (long int); Sets the pointcount attribute.

    void derivative(const OVFfile &,const OVFfile &,const OVFfile &); Calculates
the tangential derivative of the string. Using three consecutive points.

    mcell *mesh; POINTS TO THE FIRST CELL OF THE VECTOR FIELD.

    ~OVFfile(); destroys the object.

    void Hfield (double,double,double,double *,double *,double *, double *); Calculates
the magnetostatic field produced by the micromagnetic configuration
at a point in space using formulae by Newell [58].

    private:

    int modeoffield; value is 6 or 3 depending on the number of columns

    double valuemultiplier; Contains the value of the magnetization saturation

    vector.... Permalloy 800000

    double xmax; size of the box, xdirection

    double ymax; size of the box, ydirection

    int normal;

    char filename[255]; Contains the name of a file which will be used to extract
the appropriate header at the moment of saving the object.

    FILE *archivo; necessary to manipulate the object during reading and saving operations.

    long int pointcount; Number of points in the file.
Figure A.1: Mask generator of the ring manager application.
A.2 Ring simulations generator

Chapter 5 presents OOMMF simulations of ferromagnetic nanorings. These simulations require the generation of four independent files. That is the purpose of the QT application “ring manager” included in the supplementary material.

The simulation of ferromagnetic nanorings requires four different files: a bitmap mask that restricts the geometry to the annulus, an SVF file of the external field produced by the current flowing perpendicular to the ring, an OMF describing the initial saddle configuration, and a MIF problem definition file which specifies the properties of the material. The structure of the OMF, SVF and MIF files is described in the OOMMF user manual [39].
The program also serves as calculator of the characteristic physical quantities described in the original Martens et al. model. It should be a helpful tool for the design and characterization of annular structures made of soft ferromagnetic materials.

The main window is shown in Fig. A.1. The entry “Working directory” indicates where the generated files are going to be stored. The first tab queues for the dimensions of the ring and generates the bitmap mask. As values are modified the application updates the derived quantities.

The second tab (Fig. A.2) produces an external circumferential field with a magnitude given by the characteristic field at the center of the ring. Multipliers can be added to the MIF file to vary its magnitude. Three options are given for the radial dependence: “concentric field” produces a field independent of the radial coordinate; “1/r” creates the field produced by a current filament running through the axis of the ring; permeating field represents a field where the current flow uniformly inside the magnetic material (so it is actually proportional
The initial magnetization is set up in the third tab (Fig A.3). The tab provides information on the value of the scaled circumference, when the value of the scaled field is introduced the program determines whether the appropriate saddle is the constant saddle, the instanton saddle for medium sized rings, and the instanton saddle for very large rings. It provides the information on the parameters of the instanton saddle. By clicking the buttons, the user can select which type of initial magnetization file is created for the simulation.

The fourth tab (Fig A.4) allows to define the properties of the material, when the button is clicked the program calculates the appropriate exchange length and creates the MIF problem definition files. By marking the “Do Precess” check box the user can toggle between the underdamped and overdamped dynamics. This allows to simulate anisotropic materials of any saturation magnetization value.
A.3 String Manager

The String Manager application creates a string and relaxes it using the string method using the OOMMF command line tools. The dialog box is shown in Fig. A.5. The user provides the folder in which the string files will be stored, and the basename for all output files. The OOMMF folder input should be modified to point to the local installation of the OOMMF package.

The user can generate an interpolation using two or three files and indicating how many states are going to be used in the string. It is recommended to use three files to create the interpolation because the two metastable states are usually antiparallel to each other and direct vector interpolation may produce null vectors. Doing the interpolation with an intermediate file breaks the axial symmetry and indicates the program in which sense to rotate the magnetic moments in the initial string. The files are generated once the user clicks on the “interpolate” button.

Once the initial interpolation is generated the user should specify the initial iteration step and the final iteration step; and how often should files should be kept in disk. Magnetization files are big and it is recommended not to save very often. The user should try several times to optimize the time step, if the timestep is too large all states in the string will decay into either of the metastable states.

The text area presents a basic MIF file that would appropriately evolve any initial micromagnetic string. However, most features available in the OOMMF
Figure A.5: String Manager Dialog Box
package are incorporated better by loading a separate 'seed' MIF file. It is important that the MIF file does not include the stage epilog. The user should delete the text area before loading the seed MIF file. The String Manager will add the limiting time and overwrite the “Do Precess” option to force the string method into the overdamped regime. Then it will run iteratively each of the states in the string. The progress is shown in the progress bar, but it is updated with more frequency directly as output in the command line.

The string can be monitored frequently and the information on energies of each micromagnetic state from the command line. The algorithm 1 shows an example on how to use OOMMF’s command line to obtain all energies. It is assumed that OOMMF is installed in: /home/users/oommf/oommf.tcl. The output is redirected to files with the extension ‘all’. Which can be accessed afterwards. The program readenergies.c reads these files and stores the energy information of the whole string in files with extension ‘string’.
Algorithm 1 energymeasurement.c: algorithm to measure the energies on all the images of the string.

```c
int main(int argc, char *argv[]){
    FILE *infile;
    FILE *outfile;
    char cadena[500];
    int i=0,j,currentstep,totalsteps,currentpoint,totalpoints,energytype;
    double total, exchange, demag, anisotropy, zeeman, someenergy, maxperpfield=0.0, perpfield=0.0;
    if(argc==4 || argc==5){
        if (argc==4) i=0;
        if (argc==5) sscanf(argv[4],"%d",&i);
        sscanf(argv[2],"%d",&totalsteps);
        sscanf(argv[3],"%d",&totalpoints);
        for(currentstep=i;currentstep<=totalsteps;currentstep++){
            for(currentpoint=0;currentpoint<=totalpoints;currentpoint++){
                printf("%s\n",cadena);
                sprintf(cadena,"tclsh /home/users/oommf/oommf.tcl mag2hfield -component all -data energy %s_%04d_t%04d.mif %s_%04d_t%04d.omf > %s_%04d_t%04d.all\n",argv[1],
                        currentpoint, currentstep, argv[1], 0, 0, argv[1], currentpoint,
                        currentstep);
                system(cadena);
            }
        }
    } else {
        printf("Parameters are: \n1. FILEBASENAME \n2. NUMBEROFITERATIONS \n3. NUMBER OF POINTS IN PATH 4. starting step (optional)\n");
    }
    return 0;
}
```

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