LINEAR AND NONLINEAR EXCITATIONS IN MAGNETIC FILMS

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INTRODUCTION
1.1 FUNDAMENTAL MOTIVATION

The phenomenon of magnetism was already known to the ancient Chinese and inspired what is arguably one of the oldest branches of physical research. Early scientific studies on the properties of magnets appeared in 1282 (Peregrinus, *Epistola de magnete*) and 1600 (Gilbert, *De Magnete*). To this day, magnetism is an important sub-field of condensed-matter physics, both for its fundamental interest and its potential for application. Many applications are found in information technology. The use of magnetic media for data storage is well known, but magnetic structures are also increasingly being considered as active elements for data processing.

The strong link between magnetism and information technology is perhaps not surprising. What sets apart the magnetization of a ferromagnet from most other kinds of fields in condensed matter is its inherent nonlinearity. Where the polarization of a dielectric disappears very soon after the electric field is gone, and electric currents in most conductors quickly dissipate away, magnetization always remains. It has no choice but to point in some direction. This simple fact creates a permanent state of frustration, because large magnetic fields are energetically unfavorable. The result is that a magnetized particle may stubbornly refuse to respond to an applied field – until a tipping point is reached, and its condition is changed forever (hysteresis). This kind of behavior is what we need in information systems, where a slight change in the inputs may demand a step change in the response.

The inherent frustration inside the magnet often resolves itself in the creation of intricate structures and patterns in the magnetization field. Magnetic thin films allow these structures to be experimentally observed. A few examples of the structures that may be found in magnetic films are shown in Fig. 1.1. Many samples show a patchwork of domains, each with a different direction of magnetization. We shall see that the boundaries between the domains (domain walls) are intriguing structures in themselves, with a distinctive dynamics.

Like sound waves (phonons), spin waves (magnons) are excitations of the solid state that propagate thorough a material and thus transfer information (see Fig. 1.2). Spin waves exist only in a magnetic material (ferromagnet, antiferromagnet, or ferrimagnet). They are highly sensitive to the orientation of the magnetization field through which they propagate, which makes them easy to switch and manipulate. It is precisely this property that could see spin waves being applied as the building blocks of a new generation of information-processing devices (magnon spintronics).

This thesis asks how structures such as domain walls can be used to manipulate and control the propagation of spin waves. Here, I use the word “spin waves” in a broad sense, also including those types of excitations, linear and nonlinear, that are localized to domain walls and other structures. The theoretical framework that I use, the classical theory of magnetization dynamics, dates back at least to the seminal work of Landau and Lifshitz (1935). Notwith-
Figure 1.1: Some of the magnetic structures in thin ferromagnetic films discussed in Sec. 3.3. (a) In an in-plane magnetized film, the magnetization in each domain aligns itself with the film edges to avoid the creation of magnetic poles (flux closure). A vortex sits at the center of the domain structure. (b) In a film with strong perpendicular magnetocrystalline anisotropy, magnetization points out of the plane and north and south poles exist at the film surfaces. A patchwork of magnetic domains of opposing magnetization directions is formed, which ensure that, over long distances, the fields created by the poles cancel out. (c) On a much smaller scale, certain topologically protected magnetic nanostructures (skyrmions) may occur in the magnetization field of an (ultra-)thin perpendicular-anisotropy film. The Dzyaloshinskii–Moriya interaction (see Sec. 7.A) serves as a stabilization mechanism for such structures. (d) Narrow domain walls separate the magnetic domains, creating a smooth transition from one to the other magnetization direction. Domain walls are mobile and display peculiar dynamical behavior (see Secs. 1.2 [5, 8.3] and Chap. 6).
standing its venerable age, the micromagnetic model has, with some extensions, been able to accommodate and explain many of the more recent developments in the field of magnetism.

1.2 SOME RECENT DEVELOPMENTS

The study of magnetism, both theoretical and experimental, makes up a significant fraction of current research in condensed-matter physics. In this section, we sketch some recent developments in the field. What these topics have in common is that, while their underlying principles have been known, in essence, for a long time, the full potential for application has only relatively recently been recognized, sparking a great deal of renewed interest. The phenomena are all related, in one way or another, to the main results presented in this thesis (see Sec. 1.3).

DOMAIN-WALL DYNAMICS  Domain walls are the boundary surfaces between two magnetic domains with (usually) opposite magnetization directions [see Fig. 1.1(d)]. They may be considered as topological defects carrying a conserved topological charge (winding number – see Sec. 3.6).

It was realized by Döring [2] that domain walls, like particles, show inertia: once set in motion, for example by an applied magnetic field, the domain wall keeps on moving, even after the field is removed, until Gilbert damping or the interaction with another defect causes it to stop. Using some elementary considerations, Döring was even able to put a number (in kg per unit area) on the effective mass that the domain wall can be said to possess. The dipolar interaction plays a crucial role in stabilizing the structure of the domain wall and is normally the main factor determining its effective mass. Unlike particles, however, the kinetic energy a domain wall can store is limited. In strong applied fields, domain walls acquire momentum at a greater rate than can be dissipated through Gilbert damping. As the kinetic energy reaches its limit, the domain wall enters into a regime of irregular motion and its average velocity levels off, a phenomenon known as Walker breakdown [3].

It has more recently emerged that domain walls (and other magnetic nanosstructures) can be propelled not only by applied magnetic fields but also by electric currents [4]. In a ferromagnet, the spins of the current-carrying electrons tend to align themselves with the magnetization direction, like the other electron spins. As they flow from one domain to the other, their orientation is reversed. This process of reversal, forced by the magnetization onto the current-carrying electrons, creates a back-effect (spin-transfer torque), whereby the electric current exerts a torque on the magnetization [5, 6]. Related arguments suggest that a strong flow of spin waves (magnonic current) could have a similar propulsive effect on the domain wall [7].
Current-driven domain-wall motion is being considered as the working principle of a new type of magnetic data-storage device in which magnetic domains, representing bits, are moved up and down for readout inside a strip of magnetic material while the magnetic material itself remains fixed. Such a magnetic “race-track” memory could be a competitive replacement for current random-access memories as it allows the storage of many bits in a single unit of electronic circuitry (a few transistors) on the chip [8].

**Antisymmetric Exchange Interactions** The antisymmetric exchange or Dzyaloshinskii–Moriya interaction (DMI) favors electron spins to be canted with respect to each other, according to a well-defined sense of rotation [9, 10]. At the microscopic level, this canting effect is in direct competition with the ferromagnetic exchange interaction, which favors parallel alignment of spins, and affects the microscopic order of the electron spins. However, at the continuum level, the effects of the DMIs between all magnetic atoms taken together usually cancel out. The DMI is only noticeable in those materials or systems in which inversion symmetry is broken; in other words, if an inversion of all spatial directions at the same time somehow fundamentally changes the physics of the system. As is discussed in more detail in Sec. 7A, this is naturally the case in those very special magnetic materials whose crystal structures lack an inversion center. In more typical materials, the effect of the DMI is felt near surfaces and interfaces, where inversion symmetry is also (locally) broken. The effect is particularly relevant for ultrathin magnetic films (∼1–40 nm), in which a large fraction of the magnetic atoms sits close to one of the two interfaces.

The propensity of the DMI for canting or twisting the magnetization field stabilizes certain magnetic nanostructures that can be seen as tiny circular magnetic domains, with radii on the order of nanometers or tens of nanometers [see Fig. 1.1(c)]. Such “magnetic skyrmions” carry a well-defined topological charge (see Sec. 3.6). The combination of their small size and (in theory) topological stability could make magnetic skyrmions a stable and versatile information carrier that might be applied in a future racetrack-like data-storage technology [11, 12]. In particular, owing to their Thiele dynamics (see Sec. 3.6.1), they tend to go around any lattice defects, following a curve of constant potential energy. At least in the absence of strong damping, this principle should help avoid pinning of moving skyrmions on defects.

At finite temperatures, some materials or surfaces show intriguing magnetic phases in which a regular lattice of skyrmions is visible [13, 14]. In such cases, the skyrmion lattice spontaneously appears as the additional degrees of freedom associated with the skyrmions increase the entropy of the system. Other research focuses on the question of how isolated skyrmions could be inserted, deleted, and moved around within a homogeneous magnetic phase [15, 16].

In domain-wall dynamics, a strong DMI has the effects of stabilizing the domain-wall structure [17, 18], thereby reducing the effective mass and delaying the onset of Walker breakdown, and of enhancing current-driven motion.
Figure 1.2: Like a spinning top, the magnetization in a ferromagnet describes a precessional motion when it is tilted out of its equilibrium. Due to the exchange (and magnetostatic) coupling, the precession of one magnetic moment induces other magnetic moments to follow suit, creating a wave excitation that propagates through the solid (spin wave).

The structural change also plays a key role in Chap. 7, where we study the interaction of spin waves with domain walls in ultrathin films. There is an interesting connection to topological insulators, whose edge electrons couple to the spins in the magnetic layer in a DMI-like fashion [19–22].

Optomagnetic effects have attracted significant attention in recent years [23]. It is well known that the polarization of a laser beam is rotated when it passes through a solid in an applied magnetic field (Faraday effect [24]). Conversely, the inverse effect induces in the solid an effective magnetic field when a circularly polarized laser beam is incident on it [25]. In magnetic materials, this inverse Faraday effect could be used to generate spin waves with a controllable directionality [26]. On ultrashort timescales, the impact of the laser beam can (temporarily) demagnetize and even switch the magnetization of a ferrimagnet [25,27,28].

Magnonics There is a strong interest in applied condensed-matter physics in developing new technologies for information storage and processing that might replace present-day electronic technology, which is based on charge currents. Charge carriers (electrons and holes) are strongly scattered by other charge carriers and by impurities inside the solid. This means, in practice, that the current can only be sustained by applying a voltage difference, resulting in a significant amount of dissipation. Technologies based on spin currents (spintronics) or wave phenomena, such as light waves (photonics) or spin waves (magnonics / magnon spintronics), could reduce the energy consumption and heat generation
in logic circuits as these information carriers can traverse long distances with little scattering or dissipation \[29\].

Two properties of spin waves that make them particularly interesting as information carriers (as compared to light waves or sound waves) are their nonlinear behavior and the strong sensitivity to the magnetization through which they propagate. Spin waves cause a precession of magnetization around its equilibrium orientation (see Fig. 1.2). Already at relatively low spin-wave energies, the deviation angle can measure many degrees and the constraint of constant magnetization magnitude starts to play a significant role \[30\]–\[32\]. This nonlinearity creates an inherent interaction between spin waves, allowing one flow of spin waves to control another – a necessary requirement for any future magnonic information-processing device.

The sensitivity of spin waves to the magnetic texture is the other ingredient creating great flexibility in manipulation and control. It is known that magnetic nanostructures such as domain walls and skyrmions affect the flow of magnons that pass through them, for example by inducing a phase shift \[33\]–\[34\]. Even in uniformly magnetized films, the propagation of spin waves is strongly affected by the orientation of magnetization \[26\]–\[35\]–\[36\]. These aspects of spin-wave propagation form an important theme of this thesis.

**1.3 Main Results**

The design of magnonic circuits and magnonic logic will ultimately depend on the availability of a large “toolbox” of mechanisms and structures that can be used to manipulate and control spin waves. One of the main contributions of this thesis is the realization that the phase of spin waves that pass through a domain wall can be shifted by 180° by switching the domain wall between its two stable equilibrium structures (Chap. 7). Through constructive and destructive interference, this mechanism could turn the domain wall into a spin-wave switch. Interestingly, it is the Dzyaloshinskii–Moriya interaction that plays a key role in bringing about the phase-shift effect.

Magnetic nanostructures do not only scatter and shift incoming spin waves; they also possess excitation modes of their own, which might be considered as “guided” or “localized” spin waves. Such modes are intimately connected to the topology of the magnetic nanostructure and provide useful information about its effective dynamics on longer timescales. Chapter 5 provides a comprehensive overview of such excitations and presents an efficient numerical procedure to calculate them in arbitrary magnetic systems, with a particular focus on the correct treatment of the zero-frequency modes (Goldstone modes) of the magnetic nanostructures.

The tools developed in Chap. 5 provide a theoretical framework for Chap. 6, where we study the effect of lattice discreteness on domain-wall motion and arrive at the interesting result that the nonlinear excitations (kinks) of an extremely
narrow domain wall can cross each other without any significant energy loss. It is known that if domain walls are so narrow (\( \sim 1 \text{ nm} \)) that their width is comparable to the lattice parameter, they begin to “feel” the crystal lattice and respond by forming kink defects. We find that the dynamics of such kinks can be approximately described as equivalent to that of the soliton solutions known from the theory of nonlinear wave equations. Our results lead to the prediction of a new type of localized “breather” excitation that can be relatively long lived.

A particular feature of the dynamics of spin waves, as opposed to sound waves and other excitations, is the important role played by the interaction with the magnetic field. Recent optomagnetic experiments highlighted the fact that spin-wave dispersion is strongly affected both by any externally applied field and by the fields induced by the magnetization of the material and the spin-wave excitation. It is known that these interactions lead to counterintuitive behavior, such as a phase velocity (apparent propagation direction) that is opposite to group velocity (actual propagation direction), as we investigate further in Chap. 8.
OVERVIEW OF METHODS
2.1 THEORETICAL APPROACH

2.1.1 Micromagnetic model

Nearly all results presented in this thesis will be derived in a theoretical framework, micromagnetics, which describes the magnetization inside the magnet as *classical* (no quantization) and *continuous* (smoothly varying in space). Both assumptions may seem mistaken *a priori*: the fundamental interaction creating the net magnetization inside a ferromagnet—an exchange coupling that causes all electron spins to point into the same direction—is a purely quantum-mechanical effect. Moreover, any continuum model would appear to neglect the discreteness of the crystal lattice, which is known to play a significant role in certain magnetic systems (see Chap. 6). The micromagnetic approach is conceptually very similar to that of hydrodynamics or elasticity theory. While those theories describe phenomena which are usually thought of as “purely classical”, let us note that the resistance of liquids and solids to compression or deformation also originates, in the end, from quantum-mechanical effects (e.g., Pauli exclusion). In this light, the micromagnetic approach is not so unusual.

The success of micromagnetic theory (or any other continuum model in condensed-matter physics) ultimately depends on a separation of energy scales. At a microscopic level, the dominant interaction by far is the exchange coupling between electron spins. The exchange interaction, which is perfectly isotropic, determines the existence of a ferromagnetic phase with a net magnetization that has a well-defined magnitude. However, due to the isotropy, it cannot fix the magnetization direction, which remains as an order parameter. In micromagnetics, we study the processes that, in the end, break this rotational symmetry and determine the dynamics of the magnetization direction. The relative weakness of those interactions means that the exchange interaction has plenty of time to create a local thermodynamic equilibrium that is completely described by just this single order parameter. On such time- and lengthscales, any quantum-mechanical or thermal uncertainty in the magnetization direction is also likely to have fizzled out.

The great advantage of the continuum approach is that it reduces the complicated interactions to simple expressions, describing the free energy of the system as a functional of the magnetization field. The surprising fact is that only a few very simple functionals are needed to arrive at an accurate description. For example, we may describe the effect of the exchange interaction as a local functional that depends only on the first derivatives of the magnetization profile. Formally, such functionals could be seen as representing only the first term in an infinite series of terms using higher and higher derivatives. In practice, only the first (and perhaps second) term is relevant, because the characteristic lengthscales of variations in the magnetization profile is considerably larger than the atomic distance. Thus, the microscopic details of the interaction are lost. This makes the
2.1 THEORETICAL APPROACH

micromagnetic approach very powerful and allows us to make accurate quantitative predictions in terms of just a few phenomenological parameters.

2.1.2 Model reduction

Traditionally, the micromagnetic energy functionals are derived as the continuum limit of some classical atomistic spin model. While such a derivation is, of course, helpful in understanding the origin of the interaction and its typical strength, it is important to realize that the continuum functionals thus obtained are, in a sense, the more fundamental objects. Their forms are universal, predetermined by the symmetries of the underlying interactions.

The universality of the continuum formulation can be surprising even to those familiar with micromagnetic theory, as the following example shows. In Ref. [19], a simple expression was recently presented to describe the effective interaction that is felt by the magnetization inside a thin magnetic-insulator layer when it is brought into contact with a topological insulator (TI) in a ferromagnet / TI junction. The effect arises from the edge states of the TI when it is held at a finite chemical potential. It was subsequently reported [21] that this interaction leads to a number of effects that have also been associated with the presence of a DMI (see Sec. 1.2). Many of these effects, such as a significant enhancement of the maximal domain-wall velocity (delay of Walker breakdown), are potentially useful for applications. As it happens, it turns out that the effective interaction [19] is not merely similar but, in fact, mathematically equivalent to the functional describing the interfacial DMI (compare Ref. [19] and, e.g., Sec. 7.A), which makes the results of Ref. [21] look unsurprising. At the same time, ferromagnet / TI junctions remain highly interesting and promising structures, owing to their significant tunability and sensitivity to, e.g., applied electric fields [20,22].

In Chap. 6 we take the model reduction one step further and consider not the magnetization field (3D) but the domain wall (2D) that lives inside this field as the fundamental object of study (see Fig. 2.1). Again, the model reduction is justified by a separation between the energy scales of slow domain-wall dynamics (Winter spin waves [37]) and the comparably fast bulk spin waves. In this two-dimensional continuum model for the domain wall, the translational symmetry is only broken by the (very weak) Peierls potential, which is the effective interaction that the domain wall experiences as a result of the discreteness of the crystal lattice. Thus, we find that it is possible to fit the effect of lattice discreteness into a continuum model. Strikingly, in spite of the enormous variety in crystal structures and microscopic exchange couplings, the effective Peierls potential has again a simple universal form.

The domain wall is also serves as another example of how the reduction of a model can make it more general. In order to accurately describe the magnetization profile of extremely narrow domain walls, we find that higher-order exchange terms (higher derivatives) must be taken into account in the micromag-
Figure 2.1: Effective model of the domain wall (figure partially taken from Fig. 6.2). We pass from a three-dimensional description of the magnetization field to a two-dimensional effective theory (see Chap. 6) describing only the slow dynamics of the domain wall that lives inside it. (The perpendicular dimension, into the page, is not shown in the figure.) Provided that the frequencies considered are well below those of bulk spin waves, the reduced model is, at the same time, more economical and more general than the original micromagnetic model.

2.1.3 Hamiltonian mechanics

The precessional dynamics of the magnetization obeys the laws of Hamiltonian mechanics. However, the constraint that the magnetization magnitude is constant means that the Hamiltonian structure of the equations of motion is greatly less obvious than in most classical systems, where the dynamical variables are neatly divided between canonical coordinates \( q_i \) and canonical momenta \( p_i \). In magnetization dynamics, the pair \( (q_i, p_i) \in \mathbb{R}^2 \) is combined into a single variable (magnetization direction \( m_i \)), which takes values on the unit sphere \( S^2 \) (\( \|m_i\| = 1 \)). This intermixing of momenta and coordinates has consequences not only for the theoretical analysis but also for the practical implementation of numerical calculations (see Sec. 2.2).

We can often restore a more traditional picture of the Hamiltonian mechanics of the nanostructures in the magnetization field by identifying their collective coordinates. An analysis of normal modes (Chap. 5) provides a useful starting point for such a model reduction and results in a separation of momenta and coordinates, at least at the linear level.
Beyond a linear approximation, the nontrivial topology of the dynamical variables again plays an important role. In domain-wall dynamics, it turns out that the internal angle $\theta$ [see Fig. 5.7(b)] acts as the canonical momentum conjugate to the position coordinate $x$. However, unlike a traditional Newtonian momentum $p$, which takes values on the entire real line $\mathbb{R}$, the domain-wall momentum $\theta$ is restricted to the unit circle $S^1$. This fact immediately implies the failure of Newtonian mechanics $F = m\ddot{x}$ when $\theta$ cannot be taken as small (Walker breakdown). It turns out that this transition from Newtonian to non-Newtonian dynamics exactly marks a transition from solitonic to nonsolitonic behavior in the dynamics of kinks in a narrow domain wall (see Chap. 6).

2.1.4 Systematic approximation

The micromagnetic model has been used to describe phenomena on many different lengthscales, ranging from nanometers (a few atomic distances) to hundreds of micrometers. In order to focus on the interactions that are the most relevant, we must carefully consider the characteristic lengthscales of interest. For example, while the exchange interaction is the dominant interaction by far at the atomistic level, on very long lengthscales it may sometimes even be completely neglected (see, e.g., Chap. 8). More background on the origin of the various characteristic lengthscales in micromagnetic theory is given in Chap. 3.

In spite of the enormous simplification effected by micromagnetic theory, its defining equations are usually still too complicated to solve algebraically except in simple and highly symmetric cases. Guided by an analysis of lengthscales, we shall often resort to what might be called the key technique of theoretical physics: expansion in a small parameter. Examples include the expansions in $kL$ or $(kL)^{-1}$, where $k$ is wavenumber and $L$ is film thickness, in the analysis of the dispersion of magnetostatic spin waves (Chap. 8); in $(kl)^{-1}$, where $l$ is the exchange length (see Sec. 3.3), in the analysis of the domain-wall phase shift (Chap. 7); internal angle $\theta$ in the analysis of domain-wall dynamics (see Chap. 6); and $a/l$, where $a$ is a lattice parameter, in the analysis of higher-order exchange (Sec. 6.C).

2.2 Computational approach

In the standard micromagnetic model, the dynamics of the magnetization field is described by a fundamental equation known as the Landau–Lifshitz–Gilbert (LLG) equation (see Sec. 3.5), which plays a similar role in micromagnetic theory as the Navier–Stokes equation in hydrodynamics. The LLG equation consists of a precession term, which describes the conservative dynamics of the magnetization field due to all interactions with itself, and a dissipative term (Gilbert damping), which describes phenomenologically the damping caused by the coupling of the precessional motion to other degrees of freedom of the solid (e.g.,
lattice vibrations). The LLG equation does not, by itself, dictate which interactions should be taken into account; the most appropriate choice depends on the system (see Chap. 3).

Many of the questions that we ask in this thesis can, in the end, be mathematically formulated as high-dimensional time-integration problems, minimization problems, eigenvalue problems, or scattering problems. Since direct solution methods for such problems are usually prohibitively expensive ($N \gtrsim 1000$), we shall rely heavily on a small variety of iterative techniques.

2.2.1 Dipolar interaction

A serious practical complication is that the magnetization field interacts not only locally but also at long range, through the dipolar interaction (see Sec. 3.2). Calculation of the resulting torques in principle requires the evaluation of $O(N^2)$ pair interactions. However, in simple geometries it is possible, owing to translational invariance, to evaluate the dipolar interaction in $O(N \log N)$ time by making use of a fast Fourier transformation (FFT), as discussed in Sec. 7.B.

In more complicated geometries, it is also possible to evaluate the dipolar interaction in an efficient manner, although such methods are somewhat more involved. One usually converts the magnetostatic problem to a Poisson problem (3.8), which is then solved iteratively up to a given tolerance. In naive implementations of the Poisson solver, the number of iterations needed tends to grow strongly with system size. To avoid this issue, a suitable preconditioning scheme is needed (multilevel / multigrid).

Since all systems in this thesis can be modeled on simple regular grids, the FFT approach is, in our cases, the simplest and most efficient choice.

2.2.2 Time integration

The micromagnetic approach idealizes the magnetization field inside a magnetic material as a continuous function of space. In practical numerical computations, it is, however, necessary to discretize the system and describe the fields using a finite number of representative values. Different approaches exist to carry out such a discretization, which may be based on finite differences or finite elements; in either case, the continuum dynamics is reduced to a very large but finite set of $N$ coupled ordinary differential equations (ODEs). Time integration should ideally be performed using a numerical method that conserves the geometric properties of the system.

In most systems, damping can be treated as a small parameter and the precession term, which is energy conserving, is the dominant part of the LLG equation. This fact suggests that it is useful to use a numerical time integration scheme that conserves the Hamiltonian structure of the equations of motion (symplectic integrator). Contrary to typical Hamiltonians, which can be written as the sum of
a potential-energy and a kinetic-energy term, the Hamiltonians governing magnetization dynamics are nonseparable; there is no obvious or natural choice of canonical coordinates and canonical momenta. As a result, the types of symplectic integrators that are standard in the field of molecular dynamics (splitting methods), such as the Verlet method, cannot be used in magnetization dynamics.

A particularly robust technique, which we shall use, is the implicit midpoint method. Here, the change of the configuration between times $t$ and $t + \Delta$, where $\Delta$ is the size of the timestep, is approximated by evaluating the fields and time derivatives at time $t + \frac{1}{2}\Delta$ for a configuration that lies exactly halfway between the configurations at times $t$ and $t + \Delta$. Since we do not know the updated configuration $(t + \Delta)$ when we start, the method is an implicit method; a system of $N$ coupled equations must be solved for each timestep. Fortunately, this can be done efficiently by iterative methods, as discussed in Sec. 4.4. Section 4.5 discusses some alternative integration methods (explicit), which could be appropriate choices in systems where energy conservation is not essential (strong thermal noise or damping).

2.2.3 Relaxation

In the absence of an external driving field, the spin-wave excitations of a magnetic system slowly dampen out as a result of Gilbert damping as the magnetic system approaches an equilibrium. For certain purposes, one is primarily interested in the end result of this process of dissipation: a magnetic nanostructure in its ground state. An analysis of such “relaxed” structures is informative not only to determine their ground-state energy and (meta-)stability, but also to understand phenomena related to hysteresis and thermal activation (see Sec. 3.4).

The coercive field that is needed to flip the magnetization of a certain magnetic element may be obtained by performing successive relaxations of the magnetization at increasing applied fields. The coercive field is defined as the field strength at which the original equilibrium structure becomes unstable and a step change is observed in the magnetic configuration. Similarly, the thermal activation energy corresponding to such a transition, which also determines the rate of spontaneous reversals (superparamagnetic behavior), may be obtained by tracing out the equilibrium configuration as a function of some order parameter, which acts as a constraint in the relaxation process. The activation energy then corresponds to the maximal energy encountered on the path from one to the other value of the order parameter (transition-state theory). We present the results of an example of such a calculation in Sec. 7.2. As well as for such (quasi-)static problems, knowledge of the relaxed configuration is also a prerequisite for the problem of finding normal modes and collective coordinates of a magnetic nanostructure (see Sec. 2.2.4).

The most obvious approach to perform the relaxation is to run an explicit dynamical simulation with the Gilbert damping parameter of the LLG equation set
to a high value. While such an approach is effective in principle and shows linear convergence towards the equilibrium configuration, it is rarely the most efficient or accurate method, especially if a small number of extremely slow modes is present in the system (e.g., translational modes of a domain wall). In such cases, an energy minimization method based on conjugate gradients \cite{38} can bring a significant improvement, especially when used in conjunction with a suitable preconditioning scheme (see Sec. 5.7). The preconditioner reduces the condition number of the optimization problem (ratio between the energies of the slowest and the fastest modes of the system) by smoothing out the shortest-wavelength variations of a trial configuration. Physically, the effectiveness of such a preconditioner reflects the fact that the exchange interaction is the dominant interaction on small length scales.

Since the magnetic system may have many different (meta-)stable equilibrium configurations, it is important, for any of these relaxation methods, to provide an initial configuration that is sufficiently close to the equilibrium configuration of interest. In all cases presented in this thesis, we shall explicitly choose the appropriate initial configuration, putting in any topological defects “by hand”. The spontaneous formation of such structures, as occurs in some magnetic phases under appropriate thermodynamic conditions, is beyond the scope of this thesis. Because some form of thermal randomness is essential to escape local energy minima, such processes should be studied using Metropolis Monte Carlo or stochastic LLG schemes. Moreover, an atomistic model may be needed for the simulation of the thermodynamic stability of phases such as the nanoskyrmion lattice \cite{14}.

2.2.4 Normal-mode analysis

As I argue in Chap. 5, an analysis of spin-wave normal modes is a good starting point for understanding the dynamics of magnetic nanostructures. Conversely, a great deal of the interest in spin waves lies in the fact that their dynamics is highly sensitive to the magnetization structures through which they propagate. In practical terms, this sensitivity is reflected in the fact that we always specify the relevant magnetic ground-state configuration before calculating its normal modes.

Normal modes are defined as solutions of some eigenvalue equation. However, direct matrix-diagonalization methods are prohibitively expensive for systems containing more than a few thousand spins; even relatively simple two- or three-dimensional systems easily exceed this limit. We solve the issue by using iterative schemes that provide the lowest-frequency modes in linear or log-linear time. A stable and efficient formulation of the normal-mode problem should take account of the fact that the dynamics of spin waves is non-Newtonian. A more general Hamiltonian formulation is necessary (see Chap. 5).
The presence of the long-range dipolar interaction means that the interaction matrix, when written out explicitly, is not sparse. This prevents the use of most standard implementations of iterative eigenvalue solvers for sparse matrices. However, in a custom implementation (see Sec. 5.7) we could make use of the fact that the dipolar fields can be evaluated in log-linear time. To this end, we apply an eigenvalue algorithm that uses the action of the interaction matrix only as a “black box” and does not require knowledge of its actual elements (Krylov subspace method). As with relaxation problems, a smoothing preconditioner can be very effective, especially in calculations where a high spatial resolution is required.

2.2.5 Scattering problems

A type of problem somewhat related to the normal-mode problem is the scattering problem, where we ask how the phase and amplitude of an incoming wave is modified as it traverses a magnetic nanostructure. In the types of scattering problems that we will consider, the spin wave approaches the magnetic nanostructure through a uniformly magnetized lead, which we take as infinitely long. Far away from the structure, on the left-hand side, the solution is a linear combination of the incoming wave, propagating towards the right, and a reflected wave, propagating towards the left. On the right-hand side, we only have the transmitted wave (propagating towards the right). The solution of the scattering problem then consists of finding a solution to the normal-mode equation that satisfies these boundary conditions.

We cannot use the eigenvalue algorithm for such a problem, because we are not interested in the lowest eigenvalues; if the leads are infinitely long, there will, in fact, exist a continuum of modes below the scattering state of interest. In the case of a scattering problem, the frequency eigenvalue of the solution is fixed by the frequency of the waves in the leads.

Since the scattering problems we encounter in this thesis are one-dimensional, they can be defined as ODEs. (We must, however, treat the long-range interaction using some self-consistent procedure.) Unfortunately, due to the non-Newtonian structure of the spin-wave normal-mode problem, the resulting ODE is of fourth order and contains spurious exponentially increasing and decreasing solutions. This renders a simple forward integration method (“shooting”) fundamentally unstable. We deal with this issue by dividing the interval into a number of segments and solve the scattering problem by a combination of explicit forward integration (to obtain a transfer matrix describing each segment) and direct diagonalization (to solve the overall scattering problem). Thus, the condition number of each individual transfer matrix remains within reasonable limits. This approach combines speed (the direct diagonalization problem is small) with accuracy (the forward integration can be carried out with an arbitrarily small step size).
Despite its relatively simple theoretical foundations, the classical theory of contin- 
num magnetism can be used to explain a rich variety of phenomena, both 
static and dynamic, covering lengthscales ranging from a few mm down to a 
few nm. The intricate balance between short-range and long-range interactions 
(magnetostatics), the nonlinearity that is inherent in the theory (the constraint of 
constant magnetization magnitude), and the existence of topologically protected 
structures (continuum model) all play a part in bringing about this richness. 
The vast range of applicability is also a source of confusion. Bubble domains 
resemble skyrmionic structures but, in contrast to the latter, may not even have 
a well-defined topological charge. Depending on whom you ask, the disper-
sion relation of spin waves can look completely different. The antisymmetric 
exchange interaction (DMI) has an unequivocal atomistic definition but, when 
describing its effect at the continuum level, qualitatively different expressions 
suddenly appear. 
More often than not, a simple analysis of lengthscales or symmetries resolves 
the paradox. In this chapter, I highlight some of the essential ingredients of 
micromagnetic theory. In particular, I aim to show how the concept of a com-
petition between different interactions can, in many cases, immediately explain 
the characteristic lengthscales that emerge.
3.1 Micromagnetic Model

In the micromagnetic model, we assume that the magnetization of the solid has a constant magnitude $M_S$. The direction of magnetization varies continuously in space and time. It is customary to write

$$\mathbf{M}(t,x,y,z) = M_S \mathbf{m}(t,x,y,z), \quad (3.1)$$

where $\mathbf{m}$ is a unit vector. The saturation magnetization $M_S$ defines the magnetization of the material in a strong applied field (when $\mathbf{m}$ is everywhere perfectly aligned with the field). Notice that $M_S$ is a phenomenological parameter that depends on thermodynamical parameters such as temperature. Above the Curie temperature ($T > T_c$), when the material becomes paramagnetic, $M_S$ vanishes. The assumption that the magnitude of $\mathbf{M}$ is constant may also break down on very short timescales in systems that are strongly out of equilibrium [27]. Such phenomena (longitudinal dynamics) are outside the realm of traditional micromagnetics but might be described phenomenologically by extensions such as the LLB equation [39–41].

The magnetization field shows a rich variety of phases and structures, almost all of which result from the interplay between a few simple interactions. We describe the free energy of the system phenomenologically as the sum of a few simple energy functionals $E[\mathbf{m}(x,y,z)]$. We now discuss the most important of these functionals in some detail. The functionals discussed in the present section are local functionals that derive from short-range interactions in the solid. In the next section, we discuss the long-range dipolar interaction, which results from the interaction of the magnetization with the magnetic field.

The defining interaction of a ferromagnetic material is the exchange energy

$$E_{\text{ex}} = A \iiint \left( \left\| \frac{\partial \mathbf{m}}{\partial x} \right\|^2 + \left\| \frac{\partial \mathbf{m}}{\partial y} \right\|^2 + \left\| \frac{\partial \mathbf{m}}{\partial z} \right\|^2 \right) \, dx \, dy \, dz, \quad (3.2)$$

where $A > 0$ is the exchange stiffness. It can be derived as the continuum limit of a classical Heisenberg model

$$H = -\sum_{i,j} J_{ij} (\mathbf{m}_i \cdot \mathbf{m}_j - 1), \quad (3.3)$$

where the $\mathbf{m}_i$ now represent the directions of individual localized spins and the $J_{ij}$ define the exchange coupling between neighboring spins (we have $J_{ij} > 0$ for ferromagnetic coupling).

The exchange stiffness $A$ in the continuum model is related to the exchange constant as $J \sim A a$, where $a$ is on the order of an atomic distance. Taking typical values $a \sim 0.3 \text{ nm}$ and $A \sim 10^{-11} \text{ J/m}$, we get $J \sim 3 \times 10^{-21} \text{ J} = 0.02 \text{ eV}$, which is indeed the right order of magnitude for exchange interactions at the quantum-mechanical level.
Notice that the functional (3.2) is anisotropic; it is invariant both under rotations of magnetization \( \mathbf{m} \) and under rotations of space \((x, y, z)\). The invariance under spin rotations is a direct result of the same symmetry in the Heisenberg model (3.3). Microscopically, anisotropic exchange interactions also exist but are suppressed by the weakness of the spin-orbit coupling. However, the invariance under spatial rotations is an idealization that, in principle, may fail if the crystal has a non-cubic crystal structure.

The anisotropy of the crystal structure is reflected in an interaction that is modeled in micromagnetic theory by an anisotropy functional. The mathematically simplest form is given by

\[
E_{\text{ani}} = -K \iiint m_z^2 \, dV,
\]

where \( K \) is the anisotropy strength, \( \hat{z} \) is the anisotropy axis, and \( m_z = \hat{z} \cdot \mathbf{m} \) is the component of \( \mathbf{m} \) along this axis. For \( K > 0 \), the anisotropy is of easy-axis type; for \( K < 0 \), of easy-plane type. Of course, the interaction (3.4) might have been written, up to an inconsequential constant term, as

\[
E_{\text{ani}} = K \iiint (m_x^2 + m_y^2) \, dV.
\]

Notice that the anisotropy (3.4) is of second order in the magnetization direction \( \mathbf{m} \). In a cubic crystal structure, the lowest-order terms of the anisotropy energy that are allowed are of forth and sixth order; we have

\[
E_{\text{ani}} = \iiint \left[ K_1 (m_x^2 m_y^2 + m_x^2 m_z^2 + m_y^2 m_z^2) + K_2 m_x^2 m_y^2 m_z^2 \right] \, dV.
\]

In general, the anisotropy parameters are weaker for anisotropies of higher order. For example, we have \( K_1 = 48 \text{ kJ/m}^3 \) for iron while \( K_2 \) is rarely more than a few \( \text{kJ/m}^3 \). If a uniaxial anisotropy (3.4) is present, its strength \( K \) is considerably greater; e.g., we have \( K = 450 \text{ kJ/m}^3 \) for cobalt (hexagonal). The latter value translates to an energy of \( a^3 K \sim 0.1 \text{ meV} \) at the atomistic level, which, due to the smallness of the spin-orbit coupling, is considerably lower than the exchange constant \( J \).

In bulk, the symmetries of the magnetic anisotropy must of course be consistent with the symmetries of the underlying crystal structure. However, magnetic films can have a significant uniaxial anisotropy even if the basic crystal structure is cubic, as in the case of yttrium iron garnet (YIG) films; the film normal then serves as the main anisotropy axis. It is remarkable that the easy-axis anisotropy can be considerable \((K \sim 150 \text{ kJ/m}^3)\) even in films with a thickness \( \sim 10 \mu\text{m} \) (tens of thousands of atomic layers), where one might perhaps expect true interfacial effects to be small. We consider such a system in Chap. 7. It seems that the uniaxial anisotropy in YIG films arises from a combination of magnetostrictive effects (lattice constant mismatch with the substrate) and the growth process (which may affect the organization of the lattice defects) and is considerably enhanced by the addition of impurity atoms.
A final important short-range interaction is the antisymmetric exchange or
Dzyaloshinskii–Moriya interaction (DMI). In contrast to exchange and anisotropy,
it's effect is only noticeable at the continuum level in those special cases where
the symmetry under space inversion \((r \leftrightarrow -r)\) is broken. In bulk materials, this
can happen if the crystal structure itself is noncentrosymmetric (chiral or polar).
A polar axis is also created at the interface of the magnetic layer with another ma-
terial. The interfacial effect can be very strong in ultrathin films (a few nm), but
is inversely proportional to film thickness \([44]\). A typical value for the strength
parameter is \(D \sim 0.5 \text{ mJ/m}^2\) for a typical film thickness \(L \sim 1 \text{ nm}\), translating
to a microscopic strength of \(aDL \sim 1 \text{ meV}\), intermediate between exchange and
anisotropy.

As in the case of the anisotropy interaction, the most appropriate functional
to describe the effect of the DMI at the continuum level depends entirely on
the underlying symmetries of crystal structure and sample geometry. A more
detailed discussion of the distinct continuum forms is provided in Sec. [7.A]. The
DMI plays an essential role in the systems studied in Chap. [7] and Sec. [5.8.5].

### 3.2 Magnetostatic Interactions

In Sec. [3.1], we have defined a number of local effective interactions that origi-
nate from the microscopic physics of the solid. In addition, the magnetization
interacts with the magnetic field. The magnetic field can be external (applied
field) or induced by the magnetization of the sample itself (demagnetizing field).
The energy of the magnetization in an applied field is given by a simple local
functional

\[
E_{\text{Zeeman}} = -\mu_0 \iiint H_{\text{ext}} \cdot M \, dV, \tag{3.6}
\]

known as the Zeeman energy, which favors alignment of magnetization with the
external field \(H_{\text{ext}}\). The demagnetizing field, by contrast, creates a long-range
interaction between the magnetization in different parts of the sample (dipolar
interaction). Like the Zeeman interaction, the dipolar interaction is defined un-
ambiguously by Maxwell’s equations; no phenomenological parameters (other
than \(M_S\)) are needed to calculate it.

Due to its long range, the dipolar interaction is usually the most cumbersome
and expensive interaction in numerical (and analytical) computations. In this
section, we provide the defining equations of the dipolar interaction and solve
them analytically for certain special cases. These analytical solutions also serve
as approximations for the dipolar interaction in relevant limiting regimes.

The electromagnetic fields that mediate the dipolar interaction propagate with
the speed of light \(c\). If the characteristic time scales \(\tau\) of the magnetization dy-
namics are large compared to the length scales \(\lambda\) considered \((\lambda \ll \tau c)\), it is
safe to assume that any change in magnetization almost instantaneously affects
the magnetic field in all space (magnetostatic approximation). In the magne-
tostatic approximation, the fields are calculated quasistatically; in other words,
one neglects the induction terms $\sim \partial \mathbf{E}/\partial t, \partial \mathbf{B}/\partial t$ in Maxwell’s equations. The magnetostatic approximation is almost universally applicable in micromagnetics. As an example, let us consider the long-wavelength regime of the spin-wave dispersion curve of Fig. 8.2. These spin waves have a frequency of about 3 GHz, which translates via $c$ to a characteristic distance of 10 cm. Such distances are much larger than any typical wavelength or sample size. Even for materials with a much stronger magnetization than is considered there ($M_S = 110$ kA/m), the magnetostatic criterion is almost always verified.

In the quasistatic approximation, Maxwell’s equations become

\begin{align}
\nabla \cdot \mathbf{B} &= 0, \\
\nabla \times \mathbf{H} &= \mathbf{J}_{\text{free}} = 0,
\end{align}

where $\mathbf{H} = \frac{1}{\rho_0} \mathbf{B} - \mathbf{M}$ is the auxiliary field. In Eq. (3.7b), we assume that there are no free currents (any applied field $\mathbf{H}_{\text{ext}}$ is generated far away from the region of interest). Notice that, for obvious reasons, we do not assume any constitutive relation $\mathbf{B} = \mu \mathbf{H}$.

It turns out that the magnetostatic equations (3.7) can be reformulated as a Poisson equation. In doing so, we recover the high-school picture of the interaction between magnetic north and south poles as entirely analogous to the attraction between positive and negative electric charges. By Eq. (3.7b), we may write $\mathbf{H} = -\nabla \varphi$ for some function $\varphi$ (magnetostatic scalar potential). By Eq. (3.7a), we have

$$-\nabla^2 \varphi = -\nabla \cdot \mathbf{M} \equiv \rho_M/\mu_0,$$

where $\rho_M$ is known as the magnetostatic charge density (a positive magnetostatic charge $\rho_M$ is a magnetic north pole; a negative charge, a south pole). The total dipolar energy is given by

$$E_d = -\frac{\mu_0}{2} \int \mathbf{H}_{\text{demag}} \cdot \mathbf{M} \, dV = \frac{1}{2} \int \rho_M \varphi \, dV.$$

The factor $\frac{1}{2}$ is a double-counting correction [cf. Eq. (3.6)]. The field $\mathbf{H}_{\text{demag}}$ is often referred to as the demagnetizing field, because it tends to oppose the magnetization that induced it.

We may write the field induced by a magnetization profile $\mathbf{M}(x, y, z)$ as the convolution of $\mathbf{M}(x, y, z)$ with the field induced by a point dipole, which is given by an analytical expression (see Sec. 8.2.1). The field of the point dipole serves as the Green function of the magnetostatic problem. This approach yields an explicit integral expression for the total dipolar energy

$$E_{\text{dip}} = \frac{1}{2} \mu_0 M_S^2 \int \int \int \int \int m_a(r') f_{ab}(r' - r) m_b(r) \, d^3r' \, d^3r,$$

where $a, b$ represent spatial indices $x, y, z$ (summation is implied), and where

$$f_{ab}(r) = -\frac{3r_ar_b - \delta_{ab}r_cr_c}{4\pi r^5}.$$
Notice that the dipolar interaction has an algebraically long range ($\sim r^{-3}$).

In general, the dipolar interaction must be calculated numerically. However, for certain very special geometries we can evaluate the dipolar energy analytically. Examples are given in Secs. 3.2.1–3.2.3. In each of these special cases, we find that the demagnetizing field inside the ferromagnetic element is given by a simple relation

$$H_d = -\hat{N} \cdot M,$$  \hspace{1cm} (3.12)

where $\hat{N}$ is a dimensionless tensor with trace 1. The elements of $\hat{N}$ are known as the demagnetizing factors and are fixed by the geometry. For such systems, the dipolar energy (3.9) is given by

$$E_{dip} = \frac{1}{2} \mu_0 M_s^2 \iiint m \cdot \hat{N} \cdot m \, dV = \frac{1}{2} \mu_0 M_s^2 \iiint (N_{xx} m_x^2 + N_{yy} m_y^2 + N_{zz} m_z^2) \, dV,$$  \hspace{1cm} (3.13)

where in the last line we assume that the cross elements $N_{xy}, N_{yz}, N_{xz}$ vanish by an appropriate choice of the coordinate system. We only need to integrate inside the volume of the magnetic element, where $M \neq 0$. Notice that Eq. (3.13) has the same mathematical form (3.4) as a second-order anisotropy of microscopic origin; unlike crystalline anisotropy, however, its orientation depends in an essential way on the geometry of the magnetic element. For this reason, the effect is often referred to as shape anisotropy.

### 3.2.1 Ellipsoidal geometry

In this section, we calculate the demagnetizing field induced by a uniformly magnetized prolate ellipsoid of revolution (prolate spheroid) and calculate the demagnetizing factors $N_{xx} = N_{yy}$ and $N_{zz}$. While, for simplicity, we consider a cylindrically symmetric shape, the conclusion that the demagnetizing field in the interior of a uniformly magnetized ellipsoidal element is uniform [Eq. (3.12)] even holds if all three axes of the ellipsoid are different. The same principle applies to uniformly magnetized cylinders and films, which might be seen as special cases of ellipsoids where one or two axes are infinitely long.

Let us pass to prolate spheroidal coordinates

$$x = a \sinh \lambda \sin \nu \cos \phi,$$  \hspace{1cm} (3.14a)

$$y = a \sinh \lambda \sin \nu \sin \phi,$$  \hspace{1cm} (3.14b)

$$z = a \cosh \lambda \cos \nu,$$  \hspace{1cm} (3.14c)

where $\lambda, \nu, \phi$ are the three coordinates and $a$ is a length parameter. The three unit vectors $\hat{\lambda}, \hat{\nu}, \hat{\phi}$, where $\hat{\lambda} = h_{\lambda} \nabla \lambda$ and analogously for $\hat{\nu}$ and $\hat{\phi}$, are orthogonal at each point ($h_{\lambda}, h_{\nu}, h_{\phi}$ are the scaling factors). As in the spherical coordinate system, the angle $\phi$ runs from 0 to $2\pi$ and defines the azimuth, while $\nu$ ($0 \leq \nu \leq \pi$) plays a similar role as the polar angle $\theta$. The coordinate $\lambda \geq 0$ is special. Its level surfaces $\lambda = \lambda_0$ define prolate spheroids whose focal points are separated
by a distance \(2a\). The level surface \(\lambda = \lambda_0\) corresponds to a prolate spheroid of length \(L\) and width \(W < L\) if we choose

\[
a = \sqrt{\frac{L^2 - W^2}{2}},
\]

\[
\lambda_0 = \text{arctanh} \frac{W}{L}.
\]  

Let us assume that the magnetization inside the spheroid makes an angle \(\theta\) with the spheroid axis \(\hat{z}\). We have

\[
\mathbf{M} = \begin{cases} 
M_S(\hat{z}\cos \theta + \hat{x}\sin \theta) & \text{for } \lambda < \lambda_0 \\
0 & \text{for } \lambda > \lambda_0 
\end{cases}.
\]

The magnetostatic charge density \(-\mu_0 \nabla \cdot \mathbf{M}\) vanishes in the interior and exterior of the spheroid, but on the boundary we find a magnetostatic surface charge

\[
\sigma_M(\nu, \phi) = \mu_0 \lim_{\lambda \uparrow \lambda_0} \hat{\lambda} \cdot \mathbf{M} = \frac{\mu_0 a M_S}{h_\lambda} [\cosh \lambda_0 g_0^X(\nu, \phi) + \sinh \lambda_0 g_0^Z(\nu, \phi)],
\]

where \(g_0^X(\nu, \phi) = \sin \theta \sin \nu \cos \phi\) and \(g_0^Z(\nu, \phi) = \cos \theta \cos \nu\). Solution of the Poisson problem \(3.18\) gives

\[
\varphi(\lambda, \nu, \phi) = \begin{cases} 
a M_S D \frac{1}{2} f_X(\lambda_0) \sinh \lambda_0 \frac{\sin \phi}{\sinh \lambda_0} g_0^X(\nu, \phi) - f^Z(\lambda_0) \frac{\cosh \lambda_0}{\cosh \lambda_0} g_0^Z(\nu, \phi) & \text{for } \lambda < \lambda_0 \\
a M_S D \frac{1}{2} f_X(\lambda) g_0^X(\nu, \phi) - f^Z(\lambda) g_0^Z(\nu, \phi) & \text{for } \lambda > \lambda_0 
\end{cases}
\]

where \(f_X(\lambda) = \sinh \lambda \log \tanh \frac{\lambda}{2} + \coth \lambda\), \(f^Z(\lambda) = \cosh \lambda \log \tanh \frac{\lambda}{2} + 1\), and \(D = \cosh \lambda_0 \sinh^2 \lambda_0\). Inside the spheroid, the solution might be written in Cartesian coordinates as

\[
\varphi(x, y, z) = M_S (N_{xx} x \sin \theta + N_{zz} z \cos \theta) \quad \text{for } \lambda < \lambda_0,
\]

so that we have a uniform demagnetizing field of the form \(3.12\). The demagnetizing factors can be written as

\[
N_{zz} = \frac{W^2}{L^2 - W^2} \left( \frac{L}{\sqrt{L^2 - W^2}} \arccosh \frac{L}{W} - 1 \right),
\]

\[
N_{xx} = N_{yy} = \frac{1}{2} (1 - N_{zz}).
\]  

We verify that \(N_{xx} + N_{yy} + N_{zz} = 1\).

Notice that, in the limit \(W = L\) (sphere), we obtain \(N_{xx} = N_{yy} = N_{zz} = 1/3\). For \(W \ll L\), we have \(N_{xx} \to 1/2\) and \(N_{zz} \to 0\). Notice that shape anisotropy \(3.13\) favors magnetization to align with the long axis of the spheroid. This is an example of the general phenomenon that the dipolar interaction favors alignment of magnetization parallel to the surfaces, avoiding the creation of magnetostatic surface charges.
3.2.2 Film geometry

Large parts of this thesis are concerned with the magnetization dynamics in magnetic films of a finite thickness \( L \). We take \( z \) as the direction of the film normal and shall often assume that the film extends (more or less) infinitely in the \( x,y \) directions.

Let us consider the case of a uniformly magnetized film of thickness \( L \), so that we have \( \mathbf{M}(x,y,z) = M_S \mathbf{m} \) for \( 0 < z < L \) and \( \mathbf{M}(x,y,z) = 0 \) otherwise. A magnetostatic surface charge \( \sigma = \mu_0 M_S m_z \) exists on the plane \( z = L \) and \( \sigma = -\mu_0 M_S m_z \) on the plane \( z = 0 \). It is easy to see that this configuration of charges leads to a uniform demagnetizing field \( \mathbf{H}_d = -M_S m_z \). Again, we find that the dipolar interaction favors an orientation of \( \mathbf{M} \) that is parallel to the surfaces. The demagnetizing factors are given by \( N_{xx} = N_{yy} = 0 \) and \( N_{zz} = 1 \). The resulting shape anisotropy \([3.13]\) opposes any crystalline easy-axis anisotropy \([3.4]\).

We can extend the expressions for the demagnetization factors by considering the case that the magnetization is still uniform in \( z \) but is periodically modulated in the \( x \) and \( y \) directions, \( \mathbf{M}(x,y) \sim \mathbf{M}_0 e^{i(k_x x + k_y y)} \). (We allow the magnetization to take complex values as a mathematical device.) We obtain wavevector-dependent demagnetizing factors

\[
N_k = \frac{1 - e^{-kL}}{kL},
\]

where \( k = \sqrt{k_x^2 + k_y^2} \) and \( L \) is film thickness (see Sec. 8.2.2). These generalized demagnetizing factors are useful in the analysis of the dynamics of magnetostatic (long-wavelength) spin waves (see Sec. 3.7). Expressions for the demagnetizing factors of magnetization profiles that have a sinusoidal profile instead of a uniform profile in the \( z \) direction also exist and are given in Sec. 8.6.

3.2.3 Planar geometry

As a final (and very important) idealized example, let us consider any magnetization distribution \( \mathbf{M}(x) \) that depends only on a single coordinate \( x \) and extends infinitely in \( y \) and \( z \). We have

\[
\rho_M = -\mu_0 \nabla \cdot \mathbf{M} = -\mu_0 \frac{dM_x}{dx},
\]

giving a demagnetizing field of the form \([3.12]\) with \( N_{xx} = 1 \) and \( N_{yy} = N_{zz} = 0 \). Thus, the dipolar interaction effectively results in a local anisotropy of strength \( \frac{1}{2} \mu_0 M_S \) that penalizes magnetization in the \( \pm x \) directions.

This effectively local description of the dipolar interaction is an appropriate model for a domain wall (oriented normally to the \( \hat{x} \) direction) that has a characteristic width much smaller than the film thickness \( L \). We take this approach, for example, in the analysis of domain-wall dynamics in Chap. 6 and Sec. 5.8.3.
3.3 MAGNETIC TEXTURE OF THIN FILMS

In this section, we briefly review the magnetization textures that occur in large magnetic films.

The shape anisotropy of the film strongly favors an in-plane orientation of magnetization (see Sec. 3.2.2). However, a crystalline perpendicular easy-axis anisotropy (3.4) opposes the dipolar effect. Depending on which of the two anisotropies is stronger, the magnetization is oriented in the plane or out of the plane of the film. While in-plane magnetization is the most typical case, we obtain perpendicular magnetization if the crystalline easy-axis anisotropy $K$ satisfies the condition

$$K > \frac{1}{2}\mu_0 M_S^2.$$  \hspace{1cm} (3.23)

The magnetic textures found in perpendicular-anisotropy films are quite different from those in easy-plane films. Perpendicular-anisotropy films (albeit polycrystalline ones) are of significant practical relevance as they allow for a high data density in magnetic hard drives.

3.3.1 Domain structures in films with in-plane magnetization

The strong easy-plane shape anisotropy leaves one degree of freedom (the in-plane orientation) undetermined. The in-plane orientation may be fixed by an in-plane applied field, as in the system considered in Chap. 8. In the absence of an applied field, the magnetization structure depends very sensitively on the exact two-dimensional shape and size of the film. Unlike in the case of perpendicular anisotropy, the magnetostatic charges created at the film edges are important and it is inappropriate to model the film as effectively infinite in $x$ and $y$. In particular, in larger films, the magnetization structure tends to break apart into distinct domains each of which is aligned with a film boundary [flux closure domains, see Fig. 1.1(a)]. This alignment comes at the price of the creation of a vortex. The magnetization in the vortex core must point out of the film (energetically unfavorable) to ensure continuity of the magnetization field.

3.3.2 Domain structures in films with perpendicular magnetization

In perpendicular-anisotropy films, the overall dipolar energy of the system is much larger due to the magnetostatic charges created at the film surfaces. Unless the lateral dimensions of the film are so small that they are comparable to film thickness $L$, the film edges play only a modest role. In order to reduce the dipolar energy, the dipolar interaction creates alternating areas with magnetization pointing up or down that, on large lengthscales, compensate each other, resulting in a stripe-domain pattern [see Fig. 1.1(b)]. In the presence of a perpendicular applied field, one of the two directions is more favorable than the other. The magnetic texture responds by covering a larger area of the film.
with domains pointing along the field at the expense of domains in the opposing direction. This interrupts the opposing stripes, leading, in more extreme cases, to a pattern of small “islands” of opposing magnetization in a “sea” that is magnetized along the field. Such small islands are known as bubble domains.

A simple analysis gives an estimate of the characteristic width of the stripes in a stripe-domain pattern. More accurate formulas are derived in Ref. [46]. The typical stripe width arises from the competition between the dipolar interaction, which favors narrower stripes, and the energetic cost of the domain walls, which is obviously minimized by having as few domain walls as possible (wide stripes). For simplicity, we shall consider only the regime where film thickness is much larger than the exchange length \( L \gg l \); in other words, when the finite thickness of the domain walls can be neglected.

First, we calculate the cost of the domain walls. The structure of a domain wall in the film is determined predominantly by the competition between exchange \( A \) and crystalline anisotropy \( K \). It can be calculated, by substitution of the equilibrium profile (7.29) into the energy functionals for exchange and anisotropy, that the energy of a domain wall per unit area is given by \( \varepsilon = 4\sqrt{AK} \) (in the absence of a DMI, which modifies the domain-wall energy [47]). In fact, \( \sqrt{AK} \) is the only combination of those parameters that has units of energy per area. If we assume that the domain walls are separated by a distance of \( W \), we find that all domain walls in the film, taken together, cost an average energy of

\[
E_{DW} = \varepsilon/W = 4\sqrt{AK}/W
\]  

per unit volume of film. As for the dipolar interaction, notice that the stripe magnetization pattern can roughly be described as a periodic rectangle function with a period of \( 2W \). We may expand this pattern into a Fourier series and make the (somewhat rough) approximation that we neglect all but the lowest Fourier component, which has wavenumber \( k = \pi/W \). Using the demagnetizing factor (3.21), we obtain an energy density of

\[
E_{dipolar} = \frac{1}{2}\mu_0 M_S^2 N_{zz}(kL) \approx \frac{1}{2}\mu_0 M_S^2/(kL),
\]  

where we have approximated \( N_{zz}(kL) \) in the large-\( k \) limit, which is correct up to an error that is exponentially small in \( kL \). The competition between \( E_{DW} \) and \( E_{dipolar} \) defines a characteristic lengthscale

\[
l_c = \frac{1}{\pi} \frac{\varepsilon}{\frac{1}{2}\mu_0 M_S^2},
\]  

and we may rewrite the total energy density as

\[
E_{DW} + E_{dipolar} = \frac{1}{2}\mu_0 M_S^2(N_{zz}(kL) + l_ck).
\]  

This function is minimized for \( k = (l_cL)^{-1/2} \) or, equivalently,

\[
W = \pi\sqrt{l_cL} = \sqrt{\frac{2\pi\varepsilon L}{\mu_0 M_S^2}},
\]  

(3.28)
The expression \( (3.28) \) is accurate in the regime \( W \lesssim L \), which is verified for \( L \gtrsim \pi^2 l_c \). If \( L < \pi^2 l_c \), the creation of domain walls is exponentially suppressed and the typical stripe size can be considerably larger \([46]\).

Materials such as (doped) YIG can have a low to extremely low \( M_S \sim 15–150\, \text{kA/m} \), which allows for perpendicular magnetization even in samples with a moderate uniaxial anisotropy \( K \sim 4–150\, \text{kJ/m}^3 \) (see also Sec. 3.1). The saturation magnetization of materials such as YIG is lower than that of most simple magnetic metals because it has a large unit cell containing many atoms, only a few of which have a magnetic moment. We obtain stripe widths in the order of \( W \sim 2–20\, \mu\text{m} \) for \( L \sim 10\, \mu\text{m} \).

### 3.3.3 Structure of magnetic domain walls and skyrmions

In the above analysis, we have treated domain walls as two-dimensional objects, boundary planes without any particular structure. In actual fact, the exchange energy ensures that the transition in the magnetization direction from one domain to the next is a smooth one; any discontinuous change would be highly energetically unfavorable.

The boundary region between two domains – a domain wall – is normally much narrower than the typical sizes of magnetic domains [see Fig. 1.1(d)]. The characteristic width of the domain wall arises from a competition between the exchange interaction, which seeks to align neighboring spins as well as possible, and crystalline or shape anisotropy, which favors orientation of magnetization along a preferential axis (as is satisfied inside the domains). The resulting lengthscale is known as the exchange length. It may be defined as \( \sqrt{A/K} \) or \( \sqrt{2A/(\mu_0 M_S^2)} \), depending on the most relevant type of anisotropy in a given system (crystalline anisotropy or shape anisotropy). The exchange length is typically on the order \( \sim 5–50\, \text{nm} \).

In films with a strong DMI, certain small circular domain-wall structures may be stabilized [see Fig. 1.1(c)]. While the exact equilibrium radius of such “magnetic skyrmions” could, in theory, be given any value through very careful fine-tuning of all three interaction parameters (exchange, DMI, anisotropy / applied field), a typical value follows immediately from the competition between exchange and DMI and is on the order of \( A/D \sim 20\, \text{nm} \). Bubble domains, which instead result from a competition between the dipolar interaction and the domain-wall energy, are usually much larger, comparable to the stripe-domain width \( W \), and less regular in shape and size. Due to their small size, skyrmions have a well-defined topological charge (see Sec. 3.6). In bubble domains, Bloch lines tend to disrupt the topological structure of the domain wall, although stable skyrmionic bubble domains can exist in disk-shaped nanoelements \([48, 49]\). The structure and dynamics of domain walls and skyrmions are discussed in more detail in Secs. 5.8.3–5.8.5. We discuss some elements of their topology in Sec. 3.6.
3.4 Transition States and Hysteresis

It is remarkable how much can already be understood about the phases and structures of magnetic films by considering the statics of the micromagnetic models. Already at this level, micromagnetic theory is the key to understanding properties such as hysteresis of simple ferromagnetic particles (Stoner–Wohlfarth model) and of solids that might be modeled as ensembles of such particles [50].

In general, crystals or elements with a stronger anisotropy have a higher coercivity, as it is harder to flip such an element or crystallite. Even without any crystalline anisotropy $K$, magnetic elements show some hysteresis due to shape anisotropy. Let us consider the simple example of a uniformly magnetized prolate spheroid, where the magnetization is at an angle $\theta$ with respect to the long axis of the spheroid (see Sec. 3.2.1). In the presence of an external field $\mathbf{H}_{\text{ext}} = H_{z}\hat{z}$, the total energy of system is given by

$$E_{\text{tot}} = \frac{\mu_0}{2} M_S^2 (N_{xx} \sin^2 \theta + N_{zz} \cos^2 \theta) - \mu_0 M_S H_{z} \cos \theta. \quad (3.29)$$

Let us assume that the spheroid is magnetized in the positive $z$ direction ($\theta = 0^\circ$) and that a field is applied in the opposite direction ($H_z < 0$). While the configuration $\theta = 180^\circ$ would be the most energetically favorable, the magnetization does not flip because it is stuck in a local energy minimum ($d^2 E / d\theta^2 > 0$). Magnetization does not flip until $-H_z$ exceeds the coercive field $H_c = M_S (N_{xx} - N_{zz})$. This result serves as a toy example of hysteresis in magnetic systems.

In the above argument, we assume that the magnetization is uniform inside the ellipsoidal magnetic element; its configuration is described by a single coordinate $\theta$. We briefly comment on the applicability of this assumption. In general, the magnetization is not necessarily uniform; it adapts itself to the shape of the magnetic element in order to minimize dipolar energy. One should be aware that such an effect might reduce the coercive field $H_c$. However, it is important to note that any distortion of $\mathbf{M}(x, y, z)$ is opposed by the exchange interaction, which favors uniform alignment. The competition between the exchange and dipolar interactions results in a characteristic lengthscale $l_{\text{ex}} = \sqrt{2A / (\mu_0 M_S^2)}$, which is the exchange length (see Sec. 3.3.3). This means that there is a regime in which the toy model (3.29) is exact, namely if the dimensions of the magnetic element are much smaller than $l_{\text{ex}}$.

Even in the absence of an applied field, magnetization can spontaneously flip if the thermal energy fluctuations exceed the activation energy (energy of the transition state). Magnetic elements or crystallites that are small and “magnetically soft” enough to display frequent spontaneous reversals are said to be in the superparamagnetic. An ensemble of such particles behaves qualitatively similar to a paramagnetic solid, in which atoms have permanent magnetic moments but where the exchange energy is not strong enough (as compared to thermal energy) to maintain a magnetic order.
We can make a quick estimate of the typical lengthscale below which superparamagnetic behavior is likely. Typical micromagnetic anisotropy energy densities \( K \) or \( \frac{1}{2}\mu_0 M^2 \) range between 1–500 kJ/m\(^3\). Using this energy density, the value of \( k_B T \) at room temperature \( (4 \times 10^{-21} \text{J}) \) corresponds to the volume of a sphere of diameter 2.5–20 nm. However, in practice we need an activation energy of \( \sim 25k_B T \), which corresponds to a minimal diameter of 7–60 nm, to ensure that, even in large ensembles of particles, the time between spontaneous reversals becomes effectively infinite.

### 3.5 Magnetization Dynamics

In this work we will be concerned not only with equilibrium structures and transition states but also with dynamics. A particle with a nonzero magnetic moment shows a precession motion when it is placed in a magnetic field with which it is not perfectly aligned. This is analogous to the motion of a spinning top, which, unless it is placed exactly upright, precesses in the gravitational field.

The precession frequency depends on angular momentum: the larger the angular momentum that is stored in a particle (the faster it “spins”), the greater the torque that is needed to change its orientation and, in principle, the slower the precession. At the same time, a charged particle that spins fast will have a large magnetic moment. It thus experiences a greater torque when it is placed in a given magnetic field, which, other things being equal, increases the precession frequency. The ratio between angular momentum and magnetic moment is known as the gyromagnetic ratio \( \gamma \). By the above argument, we find that the precession frequency (Larmor frequency) is given by

\[
\omega = \gamma B,
\]

where \( B \) the applied magnetic field. In this thesis, we define \( \omega \) as an angular frequency (in rad/s). For an electron, which is negatively charged, angular momentum and magnetic moment point in opposite directions, and we have (in SI units)

\[
\gamma = -g \frac{\mu_B}{\hbar} = -g \frac{e}{2m_e},
\]

where \( \mu_B \) is the Bohr magneton, \( \hbar \) is the reduced Planck constant, \( e \) is the elementary charge, and \( m_e \) is the electron mass. The dimensionless \( g \)-factor normally takes a value close to 2 (total angular momentum originates mostly from the intrinsic electron spin, with only a small contribution from orbital momentum). Experimental data tables often report the value of \( \gamma/(2\pi) \) (in Hz/T) instead of \( \gamma \) (in rad s\(^{-1}\)T\(^{-1}\)). For \( g = g_e \approx 2 \), we evaluate \( |\gamma|/(2\pi) = 28 \text{GHz/T} \) (absolute value; the minus sign is customarily omitted).

In a solid, the precession frequency of the magnetic moments is determined not only by the applied field but also by interactions among the magnetic mo-
ments. These interactions are said to create an “effective magnetic field”, which depends on the present magnetic configuration. Equation (3.30) generalizes to

$$\frac{\partial \mathbf{M}}{\partial t} = -|\gamma| \mu_0 \mathbf{M} \times \mathbf{H}_{\text{eff}},$$

(3.32)

where \( \mathbf{M}(t, x, y, z) \) is magnetization (i.e., magnetic-moment density), \( \mu_0 \) is the permeability of vacuum (\( \mu_0 = 4\pi \times 10^{-7} \text{Tm}^{-1} \text{A}^{-1} \)). The effective field \( \mathbf{H}_{\text{eff}} \) is formally defined as a functional derivative

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0} \frac{\delta E_{\text{tot}}}{\delta \mathbf{M}(x, y, z)},$$

(3.33)

where \( E_{\text{tot}}[\mathbf{M}(x, y, z)] \) is the free-energy functional describing all magnetic interactions (exchange, anisotropy, magnetostatic, ...). Notice that Eq. (3.32) keeps the magnitude \( \| \mathbf{M}(x, y, z) \| = M_S \) constant in time (micromagnetic approximation).

In practice, the precession does not go on forever, because there is a coupling between the magnetization dynamics and other degrees of freedom of the solid. This effect is taken into account phenomenologically by including a dissipative term (Gilbert damping). We obtain the Landau–Lifshitz–Gilbert (LLG) equation

$$\frac{\partial \mathbf{M}}{\partial t} = -|\gamma| \mu_0 \mathbf{M} \times \left( \mathbf{H}_{\text{eff}} - \eta \frac{\partial \mathbf{M}}{\partial t} \right),$$

(3.34)

or

$$\frac{\partial \mathbf{m}}{\partial t} = -|\gamma| \mu_0 \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t},$$

(3.35)

where \( \alpha = \eta |\gamma|M_S \) is the dimensionless Gilbert damping parameter, and where we define unit vector \( \mathbf{m} \) according to Eq. (3.1).

The value of \( \alpha \) varies widely and depends not only on the material but also on its form and the production process; \( \alpha \) can range from \( \sim 0.5 \) for ultrathin layers (a few atoms thick) of metals or alloys to less than \( 10^{-5} \) for pure yttrium iron garnet (YIG) in bulk [51].

The fluctuation–dissipation theorem dictates that Gilbert damping (dissipation) is always accompanied by random fields (fluctuation). Together, these terms ensure that the temperature of the magnetic subsystem converges to the temperature of the other degrees of freedom of the solid in a process of equilibration. A natural extension of the LLG equation (stochastic LLG equation) includes this thermal noise. Thermal noise is especially important on small length and energy scales (especially in simulations at the level of atomistic spin dynamics [52]). On larger lengthscales and energy scales, thermal fluctuations may be neglected, in the same way that we neglect Brownian motion in the mechanics of macroscopic objects even when air resistance must be taken into account.

Several further extensions of the LLG have been developed, for example to model the effect on magnetization dynamics of a spin-polarized electric current (spin-transfer torque, Slonczewski term [47–61]) or to describe a transient deviation
of the magnetization *magnitude* (longitudinal dynamics, Landau–Lifshitz–Bloch equation [39–41]).

### 3.6 Topological Invariants and Dynamics

In the micromagnetic model, magnetization is a continuous unit-vector field. The requirement of continuity implies that certain magnetic nanostructures cannot be created or destroyed except at boundaries, where continuity is broken. Such topological defects carry with them a topological charge that takes only (half-)integral values. In this section, we consider two types of topological charge, *winding number* and *skyrmion number*, which are relevant in many magnetic systems. Conservation and integrity of topological charges are always a consequence of (some version of) the fundamental theorem of calculus. Moreover, in the case of skyrmion number, there exists a direct link between the long-time dynamics of a given topological defect and its topological charge.

Let us consider a continuous field which assigns to each point on the real line a value on the unit circle $S^1$. Many micromagnetic systems could be (approximately) described in this way. For example, many magnetic films strongly favor in-plane magnetization (shape anisotropy). This fact effectively removes one of the two degrees of the magnetization, which now only takes values in in-plane directions $\mathbf{m} \perp \mathbf{z}$, where we take $\mathbf{z}$ as the film normal. If, moreover, the system $\mathbf{m}(x)$ can be described as approximately one-dimensional [e.g., magnetization in a long rectangular strip], we find that *winding number*

$$Z = \frac{1}{2\pi} \int \mathbf{z} \cdot (\mathbf{m} \times \partial_x \mathbf{m}) \, dx$$

(3.36)

constitutes a conserved topological charge. This is easy to see if we define $\mathbf{m}(x) = \hat{x} \cos \phi(x) + \hat{y} \sin \phi(x)$, in which case

$$Z = \frac{1}{2\pi} \int \frac{d\phi}{dx} \, dx = \frac{1}{2\pi} [\phi(\infty) - \phi(-\infty)].$$

(3.37)

The only way in which topological charge can flow into or out of the system is through its boundaries, which here we put at $x = \pm \infty$. If we assume that, at the boundaries, $\mathbf{m}$ always points along the $x$-axis due to in-plane anisotropy, so that $\mathbf{m}(-\infty) = \pm \hat{x}$ and $\mathbf{m}(\infty) = \pm \hat{x}$, we see that $Z$ takes integral (or half-integral) values: when we travel from $x = -\infty$ to $x = \infty$, magnetization $\mathbf{m}(x)$ goes around the unit circle ($2\pi$ rad) an integer (or half-integer) number of times.

Other topological defects of the “winding number” type include domain-wall kinks (see Chap. 6) and the boundary lines where a Bloch domain wall in a stripe- or bubble-domain pattern (in a perpendicular-anisotropy film) changes from one to the other chirality (as defined in Chap. 7).

Let us now consider a two-dimensional system, such as a vortex or a skyrmion in a thin film; we also lift the restriction that magnetization $\mathbf{m}$ must stay in the $x,y$ plane. Mathematically, magnetization direction $\mathbf{m}(x,y)$ is now a function
that maps Euclidean two-space $\mathbb{R}^2$ to the unit sphere $S^2$. An infinitesimal rectangular area element $dx \, dy$ in the plane maps to an infinitesimal parallelogram on the unit sphere covering a (signed) area of
\[ m \cdot (\partial_x m \times \partial_y m). \] (3.38)
This means that the full function $m(x, y)$ covers on the unit sphere a (net) solid angle of
\[ \int \int m \cdot \left( \frac{\partial m}{\partial x} \times \frac{\partial m}{\partial y} \right) \, dx \, dy. \] (3.39)
Let us now assume that the magnetic configuration is such that magnetization $m(x, y)$ always converges to the same constant value (say $\hat{z}$) as we move far away from the origin in any direction. Such a configuration is said to be “continuous at infinity”. For such a configuration, the function $m(x, y)$ covers the unit sphere $(4\pi \text{ sr})$ an integer number of times. We thus find that the skyrmion number
\[ N = \frac{1}{4\pi} \int \int m \cdot \left( \frac{\partial m}{\partial x} \times \frac{\partial m}{\partial y} \right) \, dx \, dy \] (3.40)
is a topologically conserved quantity.

As long as the magnetization remains continuous (and also satisfies the condition of continuity at infinity), skyrmion number remains a conserved topological charge. A magnetic skyrmion [see Fig. 1.1(c)] is a structure carrying a skyrmion charge $N = \pm 1$. There are only two ways in which it, and its charge, can be destroyed: either the core of the magnetic skyrmion becomes so small that its size is comparable to the atomistic length, in which case the assumption of continuity breaks down; or the structure grows so large or is displaced so far that it meets the film edges, in which case skyrmion charge leaves the system through its boundaries.

Like winding number, the skyrmion number can also take half-integral values. This is the case for vortices in in-plane magnetized films, where $m(x, y)$ at infinity does not converge to a single value but instead goes through all in-plane directions.

### 3.6.1 Skyrmion number and dynamics

The slow dynamics of a magnetic vortex or skyrmion is directly related to its skyrmion number, as we now derive.

Let us consider any localized structure in a two-dimensional system (thin film) with a Hamiltonian that is (approximately) translationally invariant. The equilibrium configurations of the structure are given by $m(x, y) = m_0(x - X, y - Y)$, where $m_0(x, y)$ is some fixed profile and $X$ and $Y$ are two collective coordinates defining its position. The effect of an infinitesimal change of the collective coordinates $X, Y$ on the magnetization field $m(x, y)$ is given by
\[ \delta m = - \left( \frac{\partial m}{\partial x} \right) dX - \left( \frac{\partial m}{\partial y} \right) dY + \ldots, \] (3.41)
where the dots represent the contributions of all other collective coordinates. Using the symplectic structure that underlies magnetization dynamics (see Chap. 5), it is possible to provide an adjoint definition of the collective coordinates; in other words, to provide an expression for the effect of an infinitesimal change of the magnetization field \( \mathbf{m}(x, y) \) on the collective coordinates \( X, Y \). By Eq. (5.11), we obtain

\[
\frac{dX}{dt} = -\frac{1}{4\pi N} \iint \left( \frac{\partial \mathbf{m}}{\partial y} \right) \cdot (\mathbf{m} \times \delta \mathbf{m}) \, dx \, dy, \tag{3.42a}
\]

\[
\frac{dY}{dt} = \frac{1}{4\pi N} \iint \left( \frac{\partial \mathbf{m}}{\partial x} \right) \cdot (\mathbf{m} \times \delta \mathbf{m}) \, dx \, dy, \tag{3.42b}
\]

where \( N \) is a normalization factor that we immediately identify as the skyrmion number (3.40).

As we discuss in more detail in Sec. 4.1, magnetization dynamics (without Gilbert damping) fits in the framework of Hamiltonian mechanics. Given any Hamiltonian function, the equations of motion are dictated by the symplectic structure (4.3), which defines which coordinates and momenta are canonically conjugate. For the collective coordinates \( X, Y \) (3.42), we obtain a Poisson bracket

\[
\{ X, Y \} = \frac{4\pi N|\gamma|}{M_S L}, \tag{3.43}
\]

where \( L \) represents film thickness; we verify that \( XY/(\gamma M_S^{-1} L^{-1}) \) has units of energy times time. For \( N \neq 0 \), \( X \) and \( Y \) are, up to a scaling factor, canonically conjugate variables, independent from all other collective coordinates.

Let us now assume that the invariance of the Hamiltonian \( \mathcal{H} \) under translations of the skyrmion structure is broken by a weak perturbation \( V(X, Y) \). We assume that the fields and interactions that break translational invariance are very smooth as compared to the size of the skyrmion and are so weak that the dynamics they induce is considerably slower than the lowest-frequency internal excitations of the skyrmion. Hamilton’s equations give

\[
\frac{dX}{dt} = \{ X, \mathcal{H} \} = -\left( \frac{4\pi N|\gamma|}{M_S L} \right) \frac{\partial V}{\partial Y}, \tag{3.44a}
\]

\[
\frac{dY}{dt} = \{ Y, \mathcal{H} \} = \left( \frac{4\pi N|\gamma|}{M_S L} \right) \frac{\partial V}{\partial X}, \tag{3.44b}
\]

which we may write more succinctly as

\[
\frac{dR}{dt} = -\frac{|\gamma|}{M_S L} \mathbf{G} \times \mathbf{F}, \tag{3.45}
\]

where we define the gyrocoupling vector \( \mathbf{G} = (0, 0, 4\pi N) \), \( \mathbf{R} = (X, Y, 0) \), and \( \mathbf{F} = -\nabla_R V \). Equation (3.45) is known as Thiele’s equation of motion without damping [53]. Notice the crucial role of the skyrmion number \( N \) in \( \mathbf{G} \) in Eq. (3.45).
Thiele’s equation (3.45) is very useful in the analysis of the dynamics of vortices and skyrmions under an applied magnetic field gradient or in confined geometries, where the film edges exert some weak repulsive force on the topological defect due to magnetostatic interactions. In the absence of such perturbations, the \((X,Y)\) degree of freedom constitutes a special zero mode in the sense of Chap. 5. In practice, it is seen that many skyrmions and skyrmionic magnetic bubbles, even in translationally invariant systems, show some kind of inertial behavior, which Thiele’s equation does not account for. This paradox is discussed and resolved in Ref. [49] (see also Sec. 5.8.5).

3.7 SPIN WAVES

When the local orientation of magnetization deviates from its equilibrium direction, the magnetization starts to describe a precession (see Sec. 3.5). In turn, the precession of magnetization in one area of the solid, due to the exchange coupling and other interactions, causes neighboring magnetization to precess with it. The result is a wave excitation that propagates through the material (see Fig. 1.2). In a classical context, such propagating excitations are known as spin waves.

The dispersion relation of spin waves can look very different on different lengthscales. The shortest allowable wavelengths that exist are determined by the lattice parameter \(\sim 0.3–1.5\,\text{nm}\): these spin waves have wavevectors \(\mathbf{k}\) that lie on the edge of the first Brillouin zone of the reciprocal crystal lattice. On this atomistic lengthscale, the dispersion relation is periodic with a periodicity defined by the reciprocal lattice.

In micromagnetic calculations (continuum approximation), we consider only spin waves with a wavelength that is much larger than the lattice parameter; in other words, we consider only a relatively small region of reciprocal space near \(\mathbf{k} = 0\) (wavelengths \(\sim 10–100\,\text{nm}\)). In this regime, the exchange interaction as described by the lowest-order exchange functional (3.2) is dominant; higher-order exchange terms (see Sec. 6.C) may be neglected. Taking into account only exchange, we obtain a simple dispersion relation

\[
\omega = Ak^2. \tag{3.46}
\]

In practice, this dispersion relation is shifted up by a constant term resulting from crystalline anisotropy or an applied magnetic field, as derived in Sec. 5.8.1.

For long-wavelength spin waves (similar to film thickness or larger), the magnetostatic interactions represent another important mode of coupling of the precessional motion of different spins, in addition to the exchange coupling [54]. In fact, if we consider very large wavelengths \(\gg 10\,\mu\text{m}\), the contribution becomes increasingly irrelevant \((k\) very small); indeed, in this regime we can often

\footnote{In this thesis, we shall avoid the word “magnon”, which is the name for the corresponding quantized elementary excitation.}
completely neglect exchange, and spin-wave dispersion is dominated by magnetostatic effects (magnetostatic spin waves). In this regime, spin-wave dispersion depends very strongly on the angle between wavevector $\mathbf{k}$ and equilibrium magnetization direction $\mathbf{m}$, as discussed in detail in Chap. 8. Another unusual feature of magnetostatic spin waves is the cusp (singularity in first derivative) in the dispersion relation at $k = 0$, which is a direct consequence of the long-range nature of the dipolar interaction.

The concept of a dispersion relation is only meaningful, strictly speaking, if the system is translationally invariant. In the above discussion, we tacitly assumed that the equilibrium magnetization is homogeneous; in other words, that the system does not contain any topological defects or other structures that break translational invariance. In the presence of such structures, the dynamics of the spin-wave modes becomes even richer, as we discuss in detail in Chap. 5. Not only do structures such as domain walls and skyrmions scatter or shift the phase of the spin waves (see, for example, the results of Chap. 7), they also create certain localized modes that describe the long-time dynamics of these structures. For example, a special type of low-energy excitation (Winter spin wave $^{37}$) propagates along the surface of a domain wall (see Sec. 5.8.4).
NUMERICAL INTEGRATION OF THE LANDAU–LIFSHITZ–GILBERT EQUATION

In this chapter, we review various schemes for numerical time-integration of the Landau–Lifshitz–Gilbert equation. We also discuss how these schemes may be efficiently implemented in a computer code. We shall assume that the system can be modeled as a finite collection \( m_1, m_2, \ldots, m_n \) of classical spins, since, in numerical computations, the continuous fields reduce to this form after spatial discretization.
4.1 CLASSICAL SPIN SYSTEMS

For simplicity, we shall write the LLG equation \( m_i \in \mathbb{R}^3 \) without damping as

\[
\dot{m}_i = \tilde{\gamma} m_i \times \nabla m_i \mathcal{H}, \tag{4.1}
\]

where \( m_i \in \mathbb{R}^3 \) is a unit vector representing the direction of the magnetic moment at a given site \( i \) and \( \mathcal{H}(m_1, \ldots, m_n) \) is the Hamiltonian (sum of all interaction energies). The dot denotes a time derivative. We call a dynamical system of this form a conservative (no damping) classical spin system. The quantity \( \tilde{\gamma} \) is equal to \( \tilde{\gamma} = |r|/m_S \), where \( r \) is the gyromagnetic ratio (assumed to be negative) and \( m_S \) is the magnitude of the magnetic moment on site \( i \) (in a continuum simulation, \( m_S = M_S V \) with \( V \) the effective cell volume).

Equation (4.1) is equivalent to the generalized form of Hamilton’s equations

\[
\dot{m}_i = \{m_i, \mathcal{H}\} \tag{4.2}
\]

for a Poisson bracket \( \{\cdot, \cdot\} \) that is given by

\[
\{m_{ia}, m_{jb}\} = \begin{cases} \tilde{\gamma} \epsilon_{abc} m_{ic} & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}, \tag{4.3}
\]

where \( a, b, c \) index the spatial coordinates \( x, y, z \) and \( \epsilon_{abc} \) is the Levi-Civita symbol (Einstein summation is implied). The Levi-Civita symbol in the Poisson bracket (4.3) is the origin of the cross product in Eq. (4.1). We verify that Eq. (4.3) satisfies the properties of a Poisson algebra \[55\]. As such, the conservative spin system constitutes a Hamiltonian system, even though its symplectic structure is not immediately apparent (there exists no natural choice of canonical coordinates and momenta). The Poisson bracket (4.3) is the classical analog of the quantum-mechanical commutation relations \( [\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \) etc. between spin operators \( \hat{S}_a \).

With Gilbert damping \[56\], Eq. (4.1) becomes

\[
\dot{m}_i = -\tilde{\gamma} m_i \times \left( -\nabla m_i \mathcal{H} - \frac{\alpha}{\tilde{\gamma}} m_i \right), \tag{4.4}
\]

where \( \alpha > 0 \) is the dimensionless Gilbert damping parameter. The effect of Gilbert damping is to add a term \( -\dot{m}_i \) that opposes spin motion to the effective field \( -\nabla m_i \mathcal{H} \). Equation (4.4) is sometimes written in the explicit form

\[
\dot{m}_i = -\tilde{\gamma}' m_i \times \left( -\nabla m_i \mathcal{H} \right) - \lambda m_i \times \left[ m_i \times \left( -\nabla m_i \mathcal{H} \right) \right], \tag{4.5}
\]

which is the original formulation of the LL equation \[1\]. It is equivalent to Eq. (4.4) if we take \[56\]

\[
\tilde{\gamma}' = \frac{1}{1 + \alpha^2} \tilde{\gamma}, \tag{4.6a}
\]

\[
\lambda = \frac{\alpha}{1 + \alpha^2} \tilde{\gamma}. \tag{4.6b}
\]
Throughout this work, we define the dimensionless damping parameter $\alpha$ as it appears in the LLG equation \((4.4)\) and not as the dimensionless parameter $\lambda/\tilde{\gamma}$ that appears in Eq. \((4.5)\). The distinction may be relevant for high $\alpha$.

For simulations at finite temperature $T$, we may further add a random white noise term to the effective field, yielding the stochastic LLG equation \([52 \, 57]\). In atomistic simulations, the variance of the noise field is directly related to thermal energy $k_B T$ and damping $\alpha$ through the fluctuation–dissipation theorem \([57]\).

### 4.2 Failure of Standard Geometric Integration Schemes

When simulating conservative ($\alpha = 0$) spin systems for any sizable time interval (as compared to the periods of the fastest spin-wave modes in the system), it is essential to utilize a numerical integration scheme that conserves the Hamiltonian dynamics (symplectic integrator) to avoid a large energy drift \([58 \, 59]\). Even in the case of strong damping and noise, it is found that the accuracy of the thermal averages calculated benefits greatly from using geometric integration schemes, allowing the use of larger timesteps $\Delta$ \([57 \, 60]\). In this section, we compare the formal structure of the spin system to more typical Hamiltonian systems such as systems of Newtonian particles. We explain why symplectic integration schemes, which are the norm in the field of molecular dynamics, are harder to implement for spin systems.

The equations of motion of a Newtonian system of particles are generated by a Hamiltonian of the form

$$
\mathcal{H} = T(p_1, \ldots, p_n) + V(q_1, \ldots, q_n), \tag {4.7}
$$

where the $q_i$ and $p_i$ represent a system of canonical coordinates and momenta, which satisfy $\{q_i, p_j\} = \delta_{ij}$ and $\{q_i, q_j\} = \{p_i, p_j\} = 0$. Notice that the Hamiltonian \((4.7)\) is the sum of a kinetic-energy term $T$, which depends only on the momenta $p_i$\(^1\) and a potential-energy term $V$, which depends only on the coordinates $q_i$. Such a Hamiltonian is called separable \([55 \, 59]\) and has the crucial advantage that

$$
\dot{p}_i = -\frac{\partial V}{\partial q_i} \equiv f(q_1, \ldots, q_n), \tag {4.8}
$$

$$
\dot{q}_i = \frac{\partial T}{\partial p_i} \equiv g(p_1, \ldots, p_n); \tag {4.9}
$$

in words, the time derivative of the momenta is a function of the coordinates only while the time derivative of the coordinates is a function only of the momenta. For such systems, it is relatively easy to construct symplectic integrators: these splitting methods update the coordinates and the momenta alternately and can

\(^1\)In the special case of Newtonian dynamics, we have, moreover, that $T = \sum_i p_i^2/(2m_i)$ is quadratic and positive definite.
guarantee that each partial update is a symplectic transformation. The best-known example is the Verlet method, which is standard in molecular dynamics.

For the spin system, it is not obvious even how to define coordinates and momenta; all we have is the unit vectors $\mathbf{m}_i$. It is, in fact, possible to construct a canonical system, but the result is not very elegant: we may choose

$$\tilde{\gamma}^{1/2} q_i = 2 \sin(\theta_i/2) \cos(\phi_i) = \sqrt{\frac{2}{1 + m_{iz}}} m_x,$$  \hspace{1cm} (4.10a)

$$\tilde{\gamma}^{1/2} p_i = 2 \sin(\theta_i/2) \sin(\phi_i) = \sqrt{\frac{2}{1 + m_{iz}}} m_y,$$  \hspace{1cm} (4.10b)

where $\theta_i, \phi_i$ represent the unit vectors $\mathbf{m}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$ in spherical coordinates. We verify that $\{q_i, p_i\} = 1$.

While it is possible, in principle, to express $\mathcal{H}$ in terms of the canonical coordinates (4.10), we find that it usually contains cross terms $p_i q_i$ etc. and is thus not of the separable form (4.7); see also Sec. 5.4.2. An additional complication is that the coordinate system (4.10) is discontinuous (it has a singularity for $\mathbf{m}_i = -\hat{z}$). This discontinuity is essential because the spin system is defined on $(S^2)^n$ while a canonical system is always $\mathbb{R}^{2n}$.

The numerical-integration scheme discussed in Sec. 4.3 can deal with both the issues of the nonseparable Hamiltonian and the nonstandard topology of state space. It comes at the price of being an implicit method: a system of equations must be solved for each timestep.

### 4.3 IMPLICIT MIDPOINT SCHEME (IMP)

If we define $\mathbf{m}_i = \mathbf{m}_i(t)$ (no prime) as the spin vectors at a given time $t$ and $\mathbf{m}_i'(t + \Delta)$ (with prime) as the updated spin vectors at time $t + \Delta$, where $\Delta$ is the size of the timestep, then, starting from Eq. (4.4), the implicit midpoint scheme (IMP) \[58, 60\] for the spin system is given by

$$\frac{\mathbf{m}_i' - \mathbf{m}_i}{\Delta} = \tilde{\gamma} \mathbf{m}_i^{\text{MP}} \times \nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\}) - \alpha \mathbf{m}_i^{\text{MP}} \times \frac{\mathbf{m}_i' - \mathbf{m}_i}{\Delta},$$  \hspace{1cm} (4.11)

where we use $\mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\})$ as a shorthand for $\mathcal{H}(\mathbf{m}_1^{\text{MP}}, \ldots, \mathbf{m}_n^{\text{MP}})$, and where we define

$$\mathbf{m}_i^{\text{MP}} = \frac{\mathbf{m}_i' + \mathbf{m}_i}{2}$$  \hspace{1cm} (4.12)

as the midpoint (MP) between the present and the updated configuration.

The integration scheme (4.11) is called implicit because the value of $\mathbf{m}_i'$ is needed to evaluate the factors $\mathbf{m}_i^{\text{MP}}$ and $-\nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\})$ (effective field for $\mathbf{m}_i^{\text{MP}}$) on the right-hand side of Eq. (4.11). This implicitness means that, for each timestep, a system of $n$ equations (4.11) must be solved. The equations are all coupled, because the value of the effective field $-\nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\})$ on a
given site $i$ depends, in principle, on the orientation of all other spins $\mathbf{m}_{MP}^j$. The implementation of an efficient solver for this system is discussed in Sec. 4.4.

The scheme (4.11) is derived from the formulation (4.4) of the LLG equation. An alternative formulation of the IMP scheme for spin systems is obtained if we start instead from the formulation (4.5). We obtain

$$\frac{\mathbf{m}_i' - \mathbf{m}_i}{\Delta} = \gamma' \mathbf{m}_{MP}^i \times \nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_{MP}^j\}) + \lambda \mathbf{m}_{MP}^i \times \nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_{MP}^j\}),$$

which is the version of the IMP scheme discussed in Ref. [57]. The two schemes (4.11) and (4.13) are identical for $\alpha = 0$ (no damping) but are slightly different for $\alpha > 0$. The properties of the IMP scheme discussed in the sequel apply equally to both formulations; there is, however, some difference in the implementation of the implicitness solver (see Sec. 4.4).

4.3.1 Advantages

First, the IMP scheme is, for $\alpha = 0$, a “nearly symplectic” scheme: it conserves the symplectic structure of the spin system up to an error of $\mathcal{O}(\Delta^3)$ (see Ref. [60] and below).

Second, the LLG equation conserves the magnitude $\|\mathbf{m}_i\| = 1$ of the magnetic moments. The IMP scheme preserves this conservation property exactly; indeed, we have [57]

$$\|\mathbf{m}_i'\|^2 - \|\mathbf{m}_i\|^2 = (\mathbf{m}_i' + \mathbf{m}_i) \cdot (\mathbf{m}_i' - \mathbf{m}_i) = 2\Delta \mathbf{m}_{MP}^i \cdot \frac{(\mathbf{m}_i' - \mathbf{m}_i)}{\Delta} = 0. \quad \text{(4.14)}$$

Third, despite the fact that the IMP scheme for spin systems is not, strictly speaking, a symplectic integrator, it has the useful property that it exactly conserves total energy exactly for a certain very common type of Hamiltonian. Many spin systems have a Hamiltonian that is quadratic in the $\mathbf{m}_i$, so that we can write

$$\mathcal{H} = \sum_{i,j,a,b} C_{iajb} m_{ia} m_{jb} + \sum_{i,a} B_{ia} m_{ia} \quad \text{(4.15)}$$

for certain coefficients $C_{iajb}$ and $B_{ia}$ with $C_{iajb} = C_{jbia}$. Indeed, all spin systems considered in this work are of this form; it includes the exchange, dipolar, and uni- and biaxial anisotropy interactions [for cubic anisotropies (3.5) we must go to fourth or sixth order]. For Hamiltonians of type (4.15) and $\alpha = 0$, the IMP scheme conserves energy exactly. Defining $\mathcal{H}' = \mathcal{H}(\{\mathbf{m}_{MP}^j\})$ and $\mathcal{H} = \mathcal{H}(\{\mathbf{m}_j\})$, we have

$$\mathcal{H}' - \mathcal{H} = (m_{ia}' - m_{ia}) [2C_{iajb} m_{jb} + B_{ia}] = (\mathbf{m}_i' - \mathbf{m}_i) \cdot \nabla_{\mathbf{m}_i} \mathcal{H}(\{\mathbf{m}_{MP}^j\}) = 0. \quad \text{(4.16)}$$

In other words, the total energy at times $t$ and $t + \Delta$ is exactly the same.
4.3.2 Spherical IMP scheme

A recent publication [59] suggested an elegant modification to the IMP scheme that could be useful if the Hamiltonian is not of the form (4.15). For reasons of simplicity and efficiency of implementation (see Sec. 4.4), we shall not use this modification: for quadratic Hamiltonians, as occur in this work, the modification is not essential to avoid energy drift. We discuss it here for completeness.

It may seem surprising that the implicit midpoint method, which is known as a symplectic method, leads to a method that is only approximately symplectic when applied to the spin system. The reason is the Poisson bracket (4.3) between the coordinates \( m_{id} \) is not constant but depends on the present value of the coordinates [60]. As a result, the IMP schemes formulated above may show some energy drift in the \( \alpha = 0 \) case for Hamiltonians more general than Eq. (4.15).

In fact, on closer examination, the schemes (4.11) and (4.13) are somewhat ill defined, as they evaluate the effective field \(-\nabla m H\) at a point where, strictly speaking, the Hamiltonian \( H \) is undefined: the midpoints \( m_{MP} \) do not, in general, lie on the unit spheres \( \| m_{MP} \| = 1 \). Only if we assume that the Hamiltonian is of the special form (4.15) do we have a natural extension of the Hamiltonian function to the interiors of the unit spheres.

A recent publication [59] showed that substitution of the normalized midpoint vectors

\[
\tilde{m}_{MP}^i = \frac{m_i' + m_i}{\| m_i' + m_i \|} = \frac{m_{MP}^i}{\| m_{MP}^i \|}
\]

for \( m_{MP}^i \) into Eq. (4.11) resolves the ambiguity and, at the same time, yields a method that is truly symplectic. It shows no energy drift even for nonquadratic Hamiltonians; energy is conserved (for \( \alpha = 0 \)) to within a finite bandwidth that vanishes in the \( \Delta \to 0 \) limit. Of course, the special property of Eqs. (4.11) and (4.13) that quadratic Hamiltonians are exactly conserved in each timestep is lost if one uses Eq. (4.17).

4.4 IMPLEMENTATION OF THE IMP SCHEME

The stability and conservation properties of the IMP schemes come at a price: we need to solve a set of \( 3n \) coupled equations to find the midpoints \( m_{MP}^i \). Fortunately, we can solve for the \( m_{MP}^i \) using a relatively simple fixed-point iteration (FPI). Fixed-point iteration is the mathematical term for what in electronic-structure calculations is usually called a “self-consistent procedure” or a “mixing scheme” (with a mixing parameter of 100%). The idea is to substitute an initial guess \( m_{i,0} \) for the midpoint into the right-hand side of Eq. (4.11) or Eq. (4.13). This gives, on the left-hand side, an updated value of \( m_i' \) and thus an updated
guess \( \mathbf{m}_{i,0}^{\text{MP}} \) for the midpoint, which we substitute again on the right-hand side, and so on, yielding a sequence

\[
\mathbf{m}_{i,0}^{\text{MP}} \to \mathbf{m}_{i,1}^{\text{MP}} \to \mathbf{m}_{i,2}^{\text{MP}} \to \mathbf{m}_{i,3}^{\text{MP}} \to \ldots \to \mathbf{m}_i^{\text{MP}},
\]

(4.18)

which converges to the solution \( \mathbf{m}_i^{\text{MP}} \) of Eq. (4.13). It can be shown that even this simple formulation of the FPI converges linearly if the timestep \( \Delta \) and the damping parameter \( \alpha \) are not too large.

We terminate the iteration (4.18) once the differences

\[
\sqrt{\sum_i \| \mathbf{m}_{i,(k+1)}^{\text{MP}} - \mathbf{m}_{i,k}^{\text{MP}} \|^2}
\]

become smaller than a certain set tolerance. We may then update the spins from time \( t \) to \( t + \Delta \) using

\[
\mathbf{m}_i' = 2\mathbf{m}_i^{\text{MP}} - \mathbf{m}_i.
\]

(4.19)

As the initial guess for the midpoint, we shall simply use

\[
\mathbf{m}_{i,0}^{\text{MP}} = \mathbf{m}_i,
\]

(4.20)

which is the original configuration of the spins at time \( t \).

In the remainder of this section, we discuss two implementations of the FPI that also show linear convergence towards the true \( \mathbf{m}_i^{\text{MP}} \) but with a significantly improved convergence rate and a larger allowed timestep \( \Delta \). The first of the two formulations (Sec. 4.4.1) is exactly equivalent to the scheme that was proposed (among other results, see Sec. 4.5 in Ref. [57]). The second formulation (Sec. 4.4.2) is discussed here because it is somewhat easier to analyze in terms of the rate of convergence of the FPI (see Sec. 4.4.3) and might provide some small additional improvement of the FPI rate of convergence for high damping \( \alpha \).

### 4.4.1 FPI for IMP scheme

In Ref. [57], it was noted that, of all the factors in Eq. (4.13), only the effective field \( \mathbf{h}_i = -\nabla \mathbf{m}_i \mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\}) \) depends on the orientation of the spins on other sites \( j \neq i \). If one assumed that the effective field \( \mathbf{h}_i \) remains fixed, Eq. (4.13) would turn from a set of \( 3n \) coupled equations into \( n \) independent sets of \( 3 \) equations (3 because each vector \( \mathbf{m}_i^{\text{MP}} \) contains three elements). Each of these sets of \( 3 \) equations could be solved explicitly in constant time, which would make the IMP scheme effectively explicit. We use this idea to construct a more efficient FPI scheme for the real IMP method.

In actual fact, of course, the effective field \( \mathbf{h}_i \) is not independent of orientation of the other spins \( \mathbf{m}_j^{\text{MP}} \), and we must perform a FPI to ensure that \( \mathbf{h}_i \) is consistent with \( \mathbf{m}_i^{\text{MP}} \). Thus, we fix \( \mathbf{h}_{i,k} = -\nabla \mathbf{m}_i \mathcal{H}(\{\mathbf{m}_j^{\text{MP}}\}) \) as the value of the effective field for the \( k \)th iterate \( \mathbf{m}_{i,k}^{\text{MP}} \) and then solve the equation

\[
\frac{2}{\Delta} (\mathbf{m}_{i,(k+1)}^{\text{MP}} - \mathbf{m}_i) = -\tilde{\gamma}' \mathbf{m}_{i,(k+1)}^{\text{MP}} \times \mathbf{h}_{i,k} - \lambda \mathbf{m}_{i,(k+1)}^{\text{MP}} \times [\mathbf{m}_{i,k}^{\text{MP}} \times \mathbf{h}_{i,k}]
\]

(4.21)
to obtain the next iterate \( m_{i,(k+1)}^{MP} \). We may write (4.21) as

\[
\mathbf{m}_{i,(k+1)}^{MP} - \mathbf{m}_i = -\mathbf{m}_{i,(k+1)}^{MP} \times \mathbf{b}_{i,k},
\]  
(4.22)

where we define \( \mathbf{b}_{i,k} = \frac{\Delta}{2} (\gamma' \mathbf{h}_{i,k} + \lambda \mathbf{m}_{i,(k+1)}^{MP} \times \mathbf{h}_{i,k}) \). Schematically, the iteration might be represented as

\[
\mathbf{m}_{i,0}^{MP} \rightarrow \mathbf{b}_{i,0} \rightarrow \mathbf{m}_{i,1}^{MP} \rightarrow \mathbf{b}_{i,1} \rightarrow \mathbf{m}_{i,2}^{MP} \rightarrow \mathbf{b}_{i,2} \rightarrow \mathbf{m}_{i,3}^{MP} \rightarrow \ldots \rightarrow \mathbf{m}_i^{MP}.
\]  
(4.23)

It may seem that we have not gained very much with respect to the naive FPI scheme, because an iterative approach is needed in both cases. However, the iteration scheme (4.23) converges faster than the naive FPI scheme (4.18) because Eq. (4.21) is solved explicitly and the only remaining error is in the fields \( \mathbf{b}_i \).

The FPI scheme (4.21) might be called “semi-implicit” [57] because it requires the solution of \( n \) systems of \( 3 \) coupled equations instead of one big system of \( 3n \) equations. Since the equations are coupled in groups of \( 3 \), they can be solved sequentially for each spin and are effectively explicit [57]. By examining Eq. (4.22), I noticed that it is possible to derive a simple closed-form expression for the iterate \( \mathbf{m}_{i,(k+1)}^{MP} \) given the fields \( \mathbf{b}_{i,k} \). We have

\[
\mathbf{m}_{i,(k+1)}^{MP} = \frac{\mathbf{m}_i - \mathbf{m}_i \times \mathbf{b}_{i,k} + (\mathbf{b}_{i,k} \cdot \mathbf{m}_i) \mathbf{b}_{i,k}}{1 + \|\mathbf{b}_{i,k}\|^2}.
\]  
(4.24)

Thus, given \( \mathbf{b}_{i,k} \), the \( \mathbf{m}_{i,(k+1)}^{MP} \) can be evaluated without invoking any linear-solver routine, resolving the semi-implicitness of the FPI scheme (4.21).

### 4.4.2 FPI for IMP scheme (4.11)

We mentioned in Sec. 4.3 that two formulations (4.11) and (4.13) of the IMP scheme exist that treat Gilbert damping in a somewhat different way. Equation (4.21) defines an FPI that resolves the midpoint for the IMP formulation (4.13). We now derive the analogous iteration scheme for the alternative IMP formulation (4.11).

As above, we shall, for each iteration, evaluate the effective field \( \mathbf{h}_{i,k} = -\nabla \mathcal{H}(\{\mathbf{m}_{i,k}^{MP}\}) \) for the \( k \)th iterate \( \mathbf{m}_{i,k}^{MP} \) of the midpoint and then solve the semi-implicit equation, which assumes that the effective field is fixed, to obtain the next iterate \( \mathbf{m}_{i,(k+1)}^{MP} \), yielding a sequence

\[
\mathbf{m}_{i,0}^{MP} \rightarrow \mathbf{h}_{i,0} \rightarrow \mathbf{m}_{i,1}^{MP} \rightarrow \mathbf{h}_{i,1} \rightarrow \mathbf{m}_{i,2}^{MP} \rightarrow \mathbf{h}_{i,2} \rightarrow \mathbf{m}_{i,3}^{MP} \rightarrow \ldots \rightarrow \mathbf{m}_i^{MP}.
\]  
(4.25)

From Eq. (4.11), we derive the definition of \( \mathbf{m}_{i,(k+1)}^{MP} \) as the solution of

\[
\frac{2}{\Delta} (\mathbf{m}_{i,(k+1)}^{MP} - \mathbf{m}_i) = -\gamma \mathbf{m}_{i,(k+1)}^{MP} \times \mathbf{h}_{i,k} - \frac{2\alpha}{\Delta} \mathbf{m}_{i,(k+1)}^{MP} \times (\mathbf{m}_{i,(k+1)}^{MP} - \mathbf{m}_i),
\]  
(4.26)
which might be rewritten as
\[ \mathbf{m}_{i,(k+1)}^{MP} - \mathbf{m}_i = -\mathbf{m}_{i,(k+1)}^{MP} \times \mathbf{c}_{i,k}, \] (4.27)
where we define \( \mathbf{c}_{i,k} = \frac{\Delta \gamma}{2} \mathbf{h}_{i,k} - \alpha \mathbf{m}_i \). The solution is given by
\[ \mathbf{m}_{i,(k+1)}^{MP} = \frac{\mathbf{m}_i - \mathbf{m}_i \times \mathbf{c}_{i,k} + (\mathbf{c}_{i,k} \cdot \mathbf{m}_i) \mathbf{c}_{i,k}}{1 + \| \mathbf{c}_{i,k} \|^2}. \] (4.28)

4.4.3 Rate of convergence

Let us assume that the \( k \)th iterate \( \mathbf{m}_{i,k}^{MP} \) is already so close to the true midpoint \( \mathbf{m}_i^{MP} \) that we may linearize our analysis of the convergence of the FPI. If we define \( \mathbf{h}_i = -\nabla \mathbf{m}_i \mathcal{H}(\{ \mathbf{m}_j^{MP} \}) \) as the effective field for the true midpoint configuration \( \mathbf{m}_i^{MP} \), we have
\[ \mathbf{h}_{ia,k} - \mathbf{h}_{ia} \approx \frac{\partial^2 \mathcal{H}}{\partial m_{ia} \partial m_{jb}} (m_{jb,k}^{MP} - m_{jb}^{MP}) \] (4.29)
(summation implied), where \( \partial^2 \mathcal{H}/\partial m_{ia} \partial m_{jb} \) is the Hessian matrix of the Hamiltonian evaluated for the true midpoint \( \mathbf{m}_i^{MP} \), so that
\[ \| \mathbf{h}_k - \mathbf{h} \| \lesssim \| \frac{\partial^2 \mathcal{H}}{\partial m \partial m} \| \| m_k^{MP} - m^{MP} \|, \] (4.30)
where \( \| \cdot \| \) represents a vector norm or its induced matrix norm. In other words, the transformation \( \mathbf{m}_{i,k}^{MP} \rightarrow \mathbf{h}_{i,k} \) has a norm of not more than \( \| \partial^2 \mathcal{H}/\partial m \partial m \| \).

Similarly, we find that the transformations \( \mathbf{b}_{i,k} \rightarrow \mathbf{m}_{i,(k+1)}^{MP} \) [Eq. (4.24)] or \( \mathbf{c}_{i,k} \rightarrow \mathbf{m}_{i,(k+1)}^{MP} \) [Eq. (4.28)] each have norms of not more than 1.

The only remaining factor in the rate of convergence arises from the transformation \( \mathbf{h}_{i,k} \rightarrow \mathbf{b}_{i,k} \) (for the scheme of Sec. 4.4.1) or \( \mathbf{h}_{i,k} \rightarrow \mathbf{c}_{i,k} \) (for the scheme of Sec. 4.4.2). This factor is somewhat different for the two schemes for \( \alpha \neq 0 \); we evaluate it here for the second FPI scheme (Sec. 4.4.2). We find
\[ \| \mathbf{c}_k - \mathbf{c} \| \leq \frac{\Delta \gamma}{2} \| \mathbf{h}_k - \mathbf{h} \|, \] (4.31)
Together with the above results, this gives
\[ \| \mathbf{m}_{(k+1)}^{MP} - \mathbf{m}^{MP} \| \lesssim \frac{\Delta}{2 \tau} \| \mathbf{m}_k^{MP} - \mathbf{m}^{MP} \| \] (4.32)
where
\[ \frac{1}{\tau} = \tilde{\gamma} \| \frac{\partial^2 \mathcal{H}}{\partial m \partial m} \|. \] (4.33)
defines a characteristic timescale $\tau$ of the fastest spin-wave modes that exist in the spin system. Thus, we conclude that the FPI converges linearly, with a rate of convergence given by

$$
\mu = \frac{\|m_{MP}^{(k+1)} - m_{MP}\|}{\|m_{MP}^k - m_{MP}\|} = \frac{\Delta}{2\tau}.
$$

(4.34)

It follows that the FPI converges smoothly to the true midpoint $m_{MP}$ unless the timestep $\Delta$ is unphysically large, and that, if implemented in this way, the IMP method is not prohibitively expensive.

4.4.4 Optimal size of the timestep

To estimate the typical value of $\tau$, let us assume that we have discretized a one-dimensional spin system on a regular grid with a cell size of $a$. For $a \ll l$, where $l$ is the exchange length, exchange will be the dominant interaction. Neglecting all other interactions, the norm of the Hessian matrix is bounded by $2A k_{\text{max}}^2$, where $k_{\text{max}} = \pi / a$ is the wavenumber corresponding to the shortest wavelength that can be represented on the grid (Nyquist wavenumber), giving a rate of convergence $\mu = \pi^2 \tilde{\gamma} A / a^2$.

To obtain a smooth convergence, it is advisable to choose the timestep $\Delta$ in such a way that $\mu$ does not exceed about $1/e = 0.37$; otherwise, the loss in computational efficiency from the larger number of FPI iterations needed per timestep (slower convergence) is likely to outweigh the benefit from the reduction in the number of timesteps.

4.4.5 Further optimizations

In many spin systems, especially those that represent continuum systems discretized with a high spatial resolution, the exchange interaction is the dominant interaction determining the frequency of the fastest spin-wave modes. At the same time, the evaluation of the effective fields associated with the exchange interaction is usually relatively cheap, especially if a simple finite-difference discretization has been used; the most computationally expensive part of the effective field is normally the long-range dipolar interaction. These facts suggest a preconditioning scheme for the FPI in which standard iterations, taking into account all interactions, are combined with preconditioning iterations, which require only evaluation of exchange and (possibly) other local interactions. In this way, the total number of iterations needed (standard iterations and preconditioning iterations) remains roughly the same while the average computational cost per iteration is significantly reduced. A somewhat similar preconditioning scheme was proposed in Ref. [60]; however, in that work the midpoint solver was based on the generalized minimal residual method (GMRES) instead of a simple FPI.
Certain numerical methods for magnetization dynamics require the iterative solution of some large linear system for each timestep, in addition to the FPI that would be needed to solve the midpoint. Examples include the overlap matrix in finite-element simulations or the Poisson problem that must be solved to evaluate the dipolar interactions in nonrectangular meshes. The solution of the linear system could then be combined with the FPI of the IMP method in such a way that they converge together at approximately the same rate; in that case, the additional cost of IMP over explicit time-integration schemes would be minimal.

4.5 Semi-Implicit Midpoint Schemes

Many iterations (5–40, depending on $\Delta/\tau$) are typically needed to converge the midpoint $m_i^\text{MP}$ in the IMP scheme to machine accuracy, although the number of iterations could be reduced (see Sec. 4.4.5). The main result of Ref. [57] is that useful integration schemes are already obtained if one truncates the FPI (see Sec. 4.4.1) after one or two iterations. The obvious advantage is that only one or two evaluations of the effective field $-\nabla\mathcal{H}$ are necessary per timestep, reducing the computational cost. These schemes might be called “semi-implicit” (SI) midpoint methods, because for each spin, only a simple system of 3 equations needs to be solved (once or twice) instead of a system of $3n$ coupled equations as in the full IMP method. This makes the SI schemes effectively explicit [57]; see also the discussion around Eqs. (4.24) and (4.28).

Reference [57] defines two semi-implicit schemes, SIA (one iteration) and SIB (two iterations). The updated spin configurations are given by

$$m_{i,SIA} = 2m_{i,1}^\text{MP} - m_i,$$  \hspace{1cm} (4.35a)

$$m_{i,SIB} = 2m_{i,2}^\text{MP} - m_i,$$  \hspace{1cm} (4.35b)

respectively [compare Eq. (4.19), which defines the IMP update $m_{i,IMP}$].

We now compare the configuration $m_{i,SIA/SIB}$ after one timestep of the SIA and SIB schemes to the same for the fully converged IMP scheme. For not too large timesteps, where the initial guess $m_{i,0}^\text{MP}$ is not too far from $m_i^\text{MP}$ and we may assume that the iterations converge approximately at the asymptotic rate $\mu$ given by Eq. (4.34), we have that

$$\|m_{i,SIA} - m_{i,IMP}^\prime\| = O(\mu^2\Delta/\tau) = O(\tau^{-3}\Delta^3),$$  \hspace{1cm} (4.36a)

$$\|m_{i,SIB} - m_{i,IMP}^\prime\| = O(\mu^2\Delta/\tau) = O(\tau^{-3}\Delta^3).$$  \hspace{1cm} (4.36b)

Here we use that the distance $\|m_{i,0}^\text{MP} - m_i^\text{MP}\|$ between the initial guess $m_{i,0}^\text{MP} = m_i$ (4.20) and the fully converged value of the midpoint scales as $\mathcal{O}(\Delta/\tau)$. In a simulation with thermal noise, the amplitude of the random fields scales as $\sqrt{\Delta/\nu}$, where $\nu^{-1} \sim \alpha \tilde{\gamma} k_B T$ (see, e.g., Ref. [57]). Due to the square root, the noise
becomes relatively stronger for shorter timesteps, and the initial guess $m_{i,0}^{MP}$ will be further off the true midpoint. In this case, we obtain

$$
\|m_{i,SIA} - m_{i,IMP}\| = \mathcal{O}(\mu[\Delta^{-1} + \Delta^{1/2}\nu^{-1/2}]) = \mathcal{O}(\Delta^{-1}[\Delta^{-1} + \Delta^{1/2}\nu^{-1/2}]),
$$

$$
\|m_{i,SIB} - m_{i,IMP}\| = \mathcal{O}(\mu^2[\Delta^{-1} + \Delta^{1/2}\nu^{-1/2}]) = \mathcal{O}(\Delta^{-2}\tau^{-2}[\Delta^{-1} + \Delta^{1/2}\nu^{-1/2}])
$$

(4.37a) (4.37b)

In both cases (with and without noise), the above calculations suggest that the SIB scheme approaches the IMP scheme in the limit of small timesteps $\Delta$; moreover, the larger the number of iterations, the faster is the convergence.

One would expect that the accuracy of the consecutive semi-implicit schemes SIA, SIB, ... monotonically increases with the number of iterations at which the FPI is truncated (one, two, ...) and is maximal for the fully converged IMP scheme. Intriguingly, it was reported in Ref. [57] that, at least for some particular benchmark simulation with thermal noise, the SIB scheme has not only a lower computational cost but also a significantly higher accuracy than IMP for any given timestep $\Delta$. This would suggest that there is some finite “magic number” of iterations that is optimal.

We have repeated the numerical experiments of Ref. [57]; our results are shown in Fig. 4.1. We find that the accuracy of the IMP scheme is, in actual fact, significantly higher than SIB, as might be expected of a more computationally expensive scheme. It appears that, in the code that was used for the IMP

Figure 4.1: Accuracy of the SIA, SIB, and IMP schemes for the stochastic two-spin benchmark system defined in Ref. [57] (compare Fig. 5 of that reference). We plot the systematic error in the average energy $\langle E \rangle$ versus timestep size $h (\sim \Delta)$. Solid trend lines indicate the asymptotic behavior of the SIB and IMP schemes (error scales as $h^2$). We reproduce the systematic errors in $\langle E \rangle$ for the SIA and SIB schemes reported in Ref. [57], but find considerably lower systematic errors for IMP. This conclusion holds for both IMP schemes (4.11) and (4.13).
simulation in Ref. [57], but not in the SIA and SIB codes used for the same paper, the random fields of the thermal noise were erroneously capped in such a way that the simulations were performed, in effect, at a different temperature than was set [62]. This observation allows us to explain and predict the difference between the systematic errors of IMP reported in Ref. [57] and Fig. 4.1.

Due to its stability and comparatively low computational cost, the semi-implicit SIB scheme is an appropriate choice if the spin system is nonconservative (it has a nonzero Gilbert damping $\alpha$ and possibly thermal noise) and if a very great accuracy is not needed. Due to the problem of energy drift, the semi-implicit schemes cannot be used if conservative Hamiltonian dynamics is required ($\alpha = 0$ or $\alpha$ very small). For conservative dynamics, implicit schemes such as IMP are, to our knowledge, the only option for spin systems, unless the Hamiltonian has some special structure. Moreover, even with a dissipative system, the IMP scheme has a significantly higher accuracy than SIB (for a given size of the timestep), at least in the simple benchmark of Fig. 4.1 at a computational cost that is more or less commensurate with the increase in accuracy.

In the simulations in the remainder of this work, we shall err on the side of caution and use the standard IMP method for all systems, conservative ($\alpha = 0$) and dissipative ($\alpha > 0$).
The presence of topological defects in magnetic media often leads to normal modes with zero frequency (zero modes). Such modes are crucial for long-time behavior, describing, for example, the motion of a domain wall as a whole. Conventional numerical methods to calculate the spin-wave spectrum in magnetic media are either inefficient or they fail for systems with zero modes. We present a new efficient computational scheme that reduces the magnetic normal-mode problem to a generalized Hermitian eigenvalue problem also in the presence of zero modes. We apply our scheme to several examples, including two-dimensional domain walls and skyrmions, and show how the effective masses that determine the dynamics can be calculated directly. These systems highlight the fundamental distinction between the two types of zero modes that can occur in spin systems, which we call special and inertial zero modes. Whereas the inertial modes are generic Goldstone modes related to a broken continuous symmetry, the special modes arise naturally when two broken continuous symmetries coexist. Our method is suitable for both conservative and dissipative systems. For the latter case, we present a perturbative scheme to take into account damping, which can also be used to calculate dynamical susceptibilities.

This chapter has been published as
5.1 INTRODUCTION

Many properties of magnetic systems can be understood at the classical level by studying their magnetic structure and behavior on the sub-micron lengthscale (micromagnetics \[\text{63–65}\]) or atomistically (atomistic spin dynamics \[\text{52, 66}\]). In these approaches, the dynamics of the microscopic magnetic moments is described by the Landau–Lifshitz–Gilbert (LLG) equation \[\text{1, 56}\]. The various competing interactions (exchange, anisotropy, dipolar, Zeeman, …) in micromagnetic models often result in a rich energy landscape with multiple local energy minima and hysteresis \[\text{50, 63}\]. Nontrivial magnetic configurations may be very stable, for instance if they contain topological defects such as domain walls or magnetic skyrmion bubbles \[\text{50, 67}\].

It is often useful to study the dynamics of small-amplitude deviations from a given magnetic equilibrium configuration (linearization). The eigenmodes of the linearized LLG equation are known as magnetic normal modes. In homogeneous systems, the magnetic normal modes are spin waves, which propagate through the material \[\text{68, 69}\]. The presence of inhomogeneities, whether intrinsic (lattice defects, boundaries) or configurational (domain walls, skyrmions), changes this picture. Such defects do not only affect the dynamics of the spin waves; they also often give rise to special low-energy normal modes that are localized near the defect \[\text{34, 49, 70}\]. The modes localized on configurational defects are particularly interesting. They provide valuable insight into the dynamics of domain walls \[\text{4}\] and other topological defects \[\text{71}\], a sound understanding of which will be important for the development of novel magnetic-storage technologies such as racetrack memory \[\text{8}\]. The low-energy modes also provide a channel for dissipation \[\text{72, 73}\]. Microscopic magnetic elements, such as ferromagnetic rings, are another class of systems with potential for technological application \[\text{74}\]. The spin-wave mode spectrum of these elements can be determined experimentally using magnetic-response measurements or Brillouin light scattering, providing a very direct test of micromagnetic models \[\text{74–77}\].

Zero-frequency modes (zero modes) arise naturally in the presence of broken continuous symmetries. We shall see that for spin systems, such modes require special consideration both from a theoretical and a numerical point of view. This work will introduce a general classification, based on the theory of linear Hamiltonian systems \[\text{55}\], of the normal modes in spin systems, which we shall call positive modes, special zero modes and inertial zero modes. We shall see that the inertial zero modes correspond to a broken continuous symmetry, while special zero modes may arise when two broken continuous symmetries coexist. Both types of zero modes can be associated with a (quasi)continuous spectrum of low-energy excitations in extended systems (Goldstone’s theorem). It turns out that the qualitative shape of the dispersion relation of the Goldstone mode depends on whether the zero mode is special or inertial.

While exact or approximate analytical solutions of the magnetic normal-mode problem do exist in certain special cases \[\text{34, 70, 74}\], in general it can be solved
only numerically. In some cases, the magnetic normal modes can be obtained by a “brute-force” method: numerically integrating the LLG equation over a certain time interval and performing a fast Fourier transformation (FFT) in the time domain \[49, 74, 78, 79\]. While in principle effective, this approach is limited to relatively small systems by the large amounts of CPU power and memory storage it requires, especially if a good frequency resolution is to be achieved (long simulation times). Moreover, it requires some manual tuning (reasonable settings for the initial amplitudes and sampling frequencies) and it fails to detect zero-frequency and degenerate modes. In addition to the theoretical analysis, this work presents a direct numerical procedure that can be used to find the magnetic normal modes of any spin system near any given equilibrium configuration (more precisely, near any local energy minimum). It can deal efficiently and scalably with any type of interaction, including long-range interactions, and does not assume that the material is homogeneous or that the equilibrium configuration is collinear \[80\].

An efficient numerical approach should somehow be based on a direct calculation of the eigenvectors and eigenvalues of the dynamical matrix that results from linearization of the LLG equation \[81\]. However, we shall see that this dynamical matrix is not necessarily diagonalizable, so that eigenvectors in the usual sense may not even exist. Diagonalizability can only be guaranteed if no zero modes are present. To the best of our knowledge, this fact has been overlooked in all previous works describing general methods for the magnetic normal-mode problem \[80–84\]. While there certainly are many cases in which this issue does not occur \[75, 76, 81, 83, 85–91\], or occurs for a very special choice of parameters \[92–94\], we shall see that zero modes appear in many relevant physical systems. Of course, finite-size effects and magnetostatic interactions mean that the Hamiltonian is usually only approximately invariant under the relevant continuous symmetry. However, we shall argue that even in those cases it is useful first to calculate the modes of the topological defect in a system with perfect translational (or other) symmetry in order to investigate the equations of motion and the dynamical parameters. In such situations, zero modes are an essential part of the analysis. Indeed, precisely the zero modes are often the most important for the dynamics of topological defects. For example, we shall see that it is the zero modes that determine whether the dynamics of a topological defect is inertial, and if so, with what effective mass.

Our method has a firm basis in the general theory of Hamiltonian systems \[55\]. We shall show that the normal-mode problem of an arbitrary (conservative) Hamiltonian system at a local energy minimum can be cast in the form of a Hermitian definite generalized eigenvalue problem (HDGEP) \[95\], \[Dx = \lambda Sx\], where the matrices \(D\) and \(S\) are Hermitian and \(S\) is positive definite, which can be solved particularly efficiently. The most popular methods for large eigenvalue problems (Lanczos, conjugate-gradient nonlinear optimization, …) require the problem to be of this form. Important features of these methods are that they operate in an incremental fashion (the lowest modes are calculated first) and that
they can be implemented in a matrix-free manner (they are Krylov-subspace methods). These features make the HDGEP methods considerably scalable. First, the low modes of a very large system, which are often the most physically relevant, may be obtained without solving the full eigenvalue problem for all eigenvectors, which would obviously take at least \( O(N^2) \) time. Second, it is not necessary to store the interaction matrix in explicit form, which will contain \( O(N^2) \) nonzero values if the long-range dipolar interactions are taken into account. It is sufficient to provide a routine that evaluates the forces or torques for any given specific configuration. When implemented using FFT or multigrid techniques, such a routine can run in \( O(N \log N) \) instead of \( O(N^2) \) time.

We obtain a solution method for the normal-mode problem of the conservative (zero damping) spin system as an immediate special case of our method for general Hamiltonian systems. A similar reduction of the conservative magnetic normal-mode problem to the HDGEP was proposed in Refs. [84] and [98] by assuming that the Hessian matrix of the Hamiltonian is positive definite at a local minimum, which is not always the case. Reference [98] raised this issue explicitly but did not provide a solution. We now solve this problem and introduce a systematic classification and a numerical method that also work if the Hessian matrix of the Hamiltonian at the equilibrium configuration is not positive definite but merely positive semidefinite (also called nonnegative definite), as it is in the presence of zero modes. An additional advantage of our method is that it may be used directly in Cartesian coordinates, in which the micromagnetic Hamiltonians normally take a very simple form (often quadratic). We do not need to go over to spherical coordinates, which are more computationally expensive and have singularities at certain points.

For the spin system with damping, we derive explicit expressions for the normal modes by treating the damping term of the LLG equation as a perturbation. In this way we can obtain the damped modes and decay rates to a good approximation without the need for solving non-Hermitian eigenvalue problems.

This paper is organized as follows. In Sec. 5.2, we state some general properties of the normal modes of linearized Hamiltonian systems that are essential for what follows. Here we introduce the nomenclature of special and inertial zero modes and specify their distinct dynamics. A more detailed discussion is provided in Sec. 5.A. In Sec. 5.3, we make the definitions of Sec. 5.2 explicit for the conservative spin system. Section 5.4 then shows how the normal-mode problem of a Hamiltonian system, such as the conservative spin system, near a local energy minimum can be reduced to the HDGEP. We specifically show how to deal with zero modes in a robust way. We present perturbative expressions for the spin system with damping in Sec. 5.5. These expressions can be used to calculate dynamical susceptibility functions (Sec. 5.6). Section 5.7 explains how the method can be efficiently implemented in a computer code. Section 5.8 provides examples of magnetic normal modes in various spin systems, highlighting some key features of magnetic normal modes. Normal modes provide a very convenient starting point for a collective-coordinate analysis of the dynamics.
of topological defects. In Sec. 5.8.2 we focus on the two qualitatively different types of effective dynamical behavior (inertial and noninertial) that may be found when a magnetic equilibrium configuration containing some (topological) defect is perturbed by an external force. We show how a normal-mode analysis that includes zero modes immediately provides the equations of motion and effective masses of such magnetic structures. In Sec. 5.8.3 we discuss in detail the relation between the Goldstone zero modes (special and inertial) and the corresponding branches of low-energy excitations. We apply our framework to the excitations of an extended domain wall and draw an analogy to phonons in two-dimensional crystals such as graphene. Section 5.9 summarizes our results.

5.2 Normal Modes of Hamiltonian Systems

This section states some results from the theory of Hamiltonian systems that are essential for the following sections. In particular, we introduce our nomenclature for the three types of normal modes (positive, special zero, inertial zero) that may appear in systems with a positive semidefinite Hamiltonian. A more thorough discussion with explanations and references is provided in Sec. 5.3.

Let us consider a time-invariant dynamical system near an equilibrium point, which we take to lie at \( x = 0 \). Its equation of motion is given by

\[
\dot{x} = M^j_i x^j + \mathcal{O}(|x|^2),
\]

where \( x^1, \ldots, x^m \) represent a nonsingular system of coordinates and the dot denotes the time derivative. Our goal is to find the eigenvalues and eigenvectors of \( M \). This cannot normally be accomplished by a diagonalization of \( M \), because a) in general, \( M \) is very large but not symmetric, so that the efficient iterative methods for the HDGEP cannot be used; and b) \( M \) might not be diagonalizable at all (it may be defective). However, if the dynamical system (5.1) is a linear or nonlinear Hamiltonian system, we shall see that we can bypass these problems by introducing a certain antisymmetric matrix \( \Omega \). The elements of \( \Omega \) are given by

\[
\Omega^{ij} = -\{x^j, x^i\}|_{x=0} = \{x^i, x^j\}|_{x=0},
\]

the value at the equilibrium point of the Poisson bracket between the coordinates \( x^j \) and \( x^i \). It can be shown (see Sec. 5.3) that for a Hamiltonian system, the matrix \( M \) is such that \( M \Omega \) is symmetric.

For certain physical systems, Hamiltonian dynamics takes place only on a subspace of the space where the coordinates are defined. An example is the spin system: while a magnetic moment \( m \) is defined on \( \mathbb{R}^3 \), its dynamics is restricted to a subset of the form \( \{ m \in \mathbb{R}^3 : ||m|| = c \} \) for some \( c \geq 0 \). The dimension of this “accessible subspace” (symplectic leaf [99]) is always even. For a system of \( n \) spins in Cartesian coordinates, we have \( m = 3n \), while the dimension of the symplectic leaf is only \( 2n \). We remind the reader that the image space of a matrix \( A \) consists of all vectors \( x \) that can be written as \( x = Ay \) for some vector.
the dimension of this linear subspace is denoted by rank $A$. The image space of $\Omega$, which has dimension $2n = \text{rank } \Omega$, is identical to the tangent space of the symplectic leaf at $x = 0$. Vectors that are not contained in the image space of $\Omega$ correspond to an infinitesimal displacement of the system out of the symplectic leaf and are unphysical. We may thus restrict the matrices $\Omega$ and $M\Omega$ to the image space of $\Omega$. We shall denote these restricted matrices by $\langle \Omega \rangle$ and $\langle M\Omega \rangle$; that is, we define

$$\langle \Omega \rangle \equiv F^T \Omega F \quad \text{and} \quad \langle M\Omega \rangle \equiv F^T M\Omega F,$$

where $F$ is an $m \times 2n$ matrix whose columns form an orthonormal basis of the image space of $\Omega$. Since the image space of $M\Omega$ is contained in the image space of $\Omega$, these restrictions are well defined and without loss. Notice that the matrix $\langle \Omega \rangle$ is invertible by definition. In this paper, we shall implicitly convert between vectors in $\mathbb{R}^{2n}$ and vectors in the image space of $\Omega$ without writing $F$. It is unnecessary to explicitly construct $F$ in a computer code (see Sec. 5.7).

It can be shown (see Sec. 5.A) that the $2n \times 2n$ matrix $\langle M\Omega \rangle$ is the Hessian matrix (the matrix of second-order partial derivatives) at $x = 0$ of the restriction of the Hamiltonian $H$ to the symplectic leaf (for a certain parametrization of the symplectic leaf). Therefore, if $x = 0$ is a constrained local minimum of $H$ on the symplectic leaf, the Hessian matrix $\langle M\Omega \rangle$ is guaranteed to be positive semidefinite. However, it may not be assumed (compare Ref. [84]) that $\langle M\Omega \rangle$ is also positive definite. To see this, consider the following simple counterexamples with $m = 2n = 2$: $H(p, q) = 0$, $H(p, q) = p^2$ and $H(p, q) = p^4 + q^4$ all have minima at $p = q = 0$ but not positive-definite Hessians at that point.

If $\langle M\Omega \rangle$ is positive semidefinite, the normal modes of $M$ may be of three distinct types (see Sec. 5.A). We introduce the following names for these three types of modes.

1. A **positive normal mode** of $M$ is a pair $(u_1, u_2)$ of vectors in the image space of $\Omega$ that satisfy

$$\begin{align*}
Mu_1 &= \omega u_2 \\
Mu_2 &= -\omega u_1
\end{align*}$$

for some $\omega > 0$. The corresponding fundamental solutions of the linearization of Eq. (5.1) are [see Fig. 5.1(a)]

$$\begin{align*}
x_1(t) &= \cos(\omega t)u_1 + \sin(\omega t)u_2, \\
x_2(t) &= -\sin(\omega t)u_1 + \cos(\omega t)u_2.
\end{align*}$$

Each positive normal mode corresponds to a pair of eigenvectors of $M$. The eigenvectors are $u_1 - iu_2$ (eigenvalue $i\omega$) and $u_1 + iu_2$ (eigenvalue $-i\omega$).

2. A **special zero normal mode** is a pair $(u_1, u_2)$ of vectors in the image space of $\Omega$ that satisfy

$$\begin{align*}
Mu_1 &= 0 \\
Mu_2 &= 0
\end{align*}$$

y; the dimension of this linear subspace is denoted by rank $A$. The image space of $\Omega$, which has dimension $2n = \text{rank } \Omega$, is identical to the tangent space of the symplectic leaf at $x = 0$. Vectors that are not contained in the image space of $\Omega$ correspond to an infinitesimal displacement of the system out of the symplectic leaf and are unphysical. We may thus restrict the matrices $\Omega$ and $M\Omega$ to the image space of $\Omega$. We shall denote these restricted matrices by $\langle \Omega \rangle$ and $\langle M\Omega \rangle$; that is, we define

$$\langle \Omega \rangle \equiv F^T \Omega F \quad \text{and} \quad \langle M\Omega \rangle \equiv F^T M\Omega F,$$

where $F$ is an $m \times 2n$ matrix whose columns form an orthonormal basis of the image space of $\Omega$. Since the image space of $M\Omega$ is contained in the image space of $\Omega$, these restrictions are well defined and without loss. Notice that the matrix $\langle \Omega \rangle$ is invertible by definition. In this paper, we shall implicitly convert between vectors in $\mathbb{R}^{2n}$ and vectors in the image space of $\Omega$ without writing $F$. It is unnecessary to explicitly construct $F$ in a computer code (see Sec. 5.7).

It can be shown (see Sec. 5.A) that the $2n \times 2n$ matrix $\langle M\Omega \rangle$ is the Hessian matrix (the matrix of second-order partial derivatives) at $x = 0$ of the restriction of the Hamiltonian $H$ to the symplectic leaf (for a certain parametrization of the symplectic leaf). Therefore, if $x = 0$ is a constrained local minimum of $H$ on the symplectic leaf, the Hessian matrix $\langle M\Omega \rangle$ is guaranteed to be positive semidefinite. However, it may not be assumed (compare Ref. [84]) that $\langle M\Omega \rangle$ is also positive definite. To see this, consider the following simple counterexamples with $m = 2n = 2$: $H(p, q) = 0$, $H(p, q) = p^2$ and $H(p, q) = p^4 + q^4$ all have minima at $p = q = 0$ but not positive-definite Hessians at that point.

If $\langle M\Omega \rangle$ is positive semidefinite, the normal modes of $M$ may be of three distinct types (see Sec. 5.A). We introduce the following names for these three types of modes.

1. A **positive normal mode** of $M$ is a pair $(u_1, u_2)$ of vectors in the image space of $\Omega$ that satisfy

$$\begin{align*}
Mu_1 &= \omega u_2 \\
Mu_2 &= -\omega u_1
\end{align*}$$

for some $\omega > 0$. The corresponding fundamental solutions of the linearization of Eq. (5.1) are [see Fig. 5.1(a)]

$$\begin{align*}
x_1(t) &= \cos(\omega t)u_1 + \sin(\omega t)u_2, \\
x_2(t) &= -\sin(\omega t)u_1 + \cos(\omega t)u_2.
\end{align*}$$

Each positive normal mode corresponds to a pair of eigenvectors of $M$. The eigenvectors are $u_1 - iu_2$ (eigenvalue $i\omega$) and $u_1 + iu_2$ (eigenvalue $-i\omega$).

2. A **special zero normal mode** is a pair $(u_1, u_2)$ of vectors in the image space of $\Omega$ that satisfy

$$\begin{align*}
Mu_1 &= 0 \\
Mu_2 &= 0
\end{align*}$$
Figure 5.1: Fundamental solutions $x_1$ and $x_2$ of the linearized equation of motion (5.1) corresponding to the three types of normal modes of a Hamiltonian system: (a) positive (5.3), (b) special zero (5.5) and (c) inertial zero (5.7) modes. The dynamical variables $p$ and $q$ are the amplitudes of the vectors $u_1$ and $u_2$ respectively, as defined in Eq. (5.12). Dashed lines: effect of damping with the indicated decay time $\xi^{-1}$ (see Sec. 5.5).
The corresponding fundamental solutions are [see Fig. 5.1(b)]

\[
\begin{align*}
x_1(t) &= u_1, \\
x_2(t) &= u_2
\end{align*}
\] (constant functions). A special zero normal mode also corresponds to a pair of linearly independent eigenvectors of \( M(u_1 \text{ and } u_2) \).

3. An **inertial zero normal mode** is a pair \((u_1, u_2)\) of vectors in the image space of \( \Omega \) that satisfy

\[
\begin{align*}
Mu_1 &= u_2 \\
Mu_2 &= 0
\end{align*}
\]

The corresponding fundamental solutions are [see Fig. 5.1(c)]

\[
\begin{align*}
x_1(t) &= u_1 + tu_2, \\
x_2(t) &= u_2
\end{align*}
\]

This type of mode results from a nondiagonalizable (defective) matrix \( M \). Technically, an inertial zero normal mode corresponds to a Jordan block of size 2 in the Jordan normal form of \( M \).

The nomenclature chosen for the three types of modes (positive, special and inertial) is explained below. Notice that different types of modes may have different units: for an inertial zero normal mode \( \|u_1\|/\|u_2\| \) has units of time, while for a positive normal mode \( \|u_1\|/\|u_2\| \) is dimensionless. Since each mode contains two vectors, the total number of independent modes \( n \) is one half of the dimension of the symplectic leaf. If \( \langle M\Omega \rangle \) is positive definite, all normal modes are positive normal modes.

We may write the vectors that make up a normal mode as

\[
\begin{align*}
u_1 &= \Omega w_1 \\
u_2 &= \Omega w_2
\end{align*}
\]

for certain vectors \( w_1 \) and \( w_2 \) in the image space of \( \Omega \). Section 5.4 presents an efficient procedure by which suitable vector pairs \( w_1, w_2 \) may be found. All normal modes can and should be chosen to satisfy the relations

\[
\begin{align*}
w_{1k}^T \Omega w_{2l} &= \delta_{kl} \\
w_{1k}^T \Omega w_{1l} &= w_{2k}^T \Omega w_{2l} = 0
\end{align*}
\]

where \( k, l = 1, \ldots, n \) index the modes. As a result, we may decompose an arbitrary vector \( x \) in the image space of \( \Omega \) in terms of the normal modes as

\[
x = \sum_{k=1}^{n} \left[ -(w_{2k}^T x) u_{1k} + (w_{1k}^T x) u_{2k} \right].
\]
Using the fundamental solutions (5.4), (5.6) and (5.8), such a decomposition immediately yields a solution of the initial-value problem for Eq. (5.1) in the linear approximation.

Given a state vector

\[
x = \sum_{k=1}^{n} (p_k u_{1k} + q_k u_{2k}) + \mathcal{O}(p_k^2 + q_k^2),
\]

the quadratic part of the Hamiltonian is given by

\[
\mathcal{H} = \sum_{k \text{ pos.}} \frac{1}{2} \omega_k (p_k^2 + q_k^2) + \sum_{k \text{ in.}} \frac{1}{2} p_k^2,
\]

where the first sum is taken over the positive normal modes and the second sum over the inertial zero normal modes. Special zero modes do not contribute to Eq. (5.13). The variables \( p_k \) and \( q_k \) in Eq. (5.12) are canonically conjugate momenta and coordinates (see Sec. 5.A). Notice that for a given configuration \( m = m_0 + x \), the values of these momenta and coordinates can be determined, to first order, using Eq. (5.11). We find, in the linear limit, that for a special zero normal mode

\[
\begin{align*}
\dot{p}_k &= -\frac{\partial \mathcal{H}}{\partial q_k} = 0 \\
\dot{q}_k &= \frac{\partial \mathcal{H}}{\partial p_k} = 0,
\end{align*}
\]

while for an inertial zero normal mode

\[
\begin{align*}
\dot{p}_k &= -\frac{\partial \mathcal{H}}{\partial q_k} = 0 \\
\dot{q}_k &= \frac{\partial \mathcal{H}}{\partial p_k} = p_k.
\end{align*}
\]

The latter type of dynamics (5.15) corresponds (after a suitable scaling of \( p_k \) and \( q_k \)) to the dynamics of a free massive particle, which explains our choice of the name “inertial zero normal mode”. The former type of dynamics (5.14) does not occur in conventional Newtonian systems such as systems of coupled oscillators (see Sec. 5.A), whence the name “special zero normal mode”.

In practice, zero modes typically originate from a broken continuous symmetry and can thus be seen as Goldstone modes. For example, \( q_k \) might represent the position of some topological defect; if the system is translationally invariant, the Hamiltonian must be independent of \( q_k \). The main difference between the two types of zero modes is the number of broken continuous symmetries from which they arise. For an inertial zero mode \( k \), the Hamiltonian (5.13) is, to second order, independent of \( q_k \) (but not of \( p_k \)). This suggests (but of course does not guarantee) that the system is invariant under arbitrary changes of \( q_k \). A special zero mode \( k \) is special in the sense that the Hamiltonian is to second order independent of both \( q_k \) and \( p_k \). This normally means that two broken continuous symmetries coexist. The relation between the type of zero mode, the number of broken continuous symmetries, and the dispersion relation of soft modes is discussed in more detail in Sec. 5.8.4.
5.3 CONSERVATIVE SPIN SYSTEMS

The conservative dynamics of a spin system is described by the LLG equation without damping,

\[ \dot{m}_i = \tilde{\gamma} m_i \times \nabla m_i \mathcal{H}, \tag{5.16} \]

where \( m_i \in \mathbb{R}^3 \) represents the magnetic moment with position index \( i = 1, \ldots, n \), \( \mathcal{H} \) is the Hamiltonian, and \( \tilde{\gamma} \) is a physical constant. Notice that the magnitude \( \| m_i \| \) of each magnetic moment is constant in time. These magnitudes are fixed by the physics of the system. Equation \( (5.16) \) is equivalent to

\[ \dot{m}_{ia} = \{ m_{ia}, \mathcal{H} \}, \tag{5.17} \]

the generalized form of Hamilton’s equations applied to the (time-invariant) variables \( m_{ia} \), for the Poisson bracket

\[ \{ m_{ia}, m_{jb} \} = \begin{cases} -\tilde{\gamma} \varepsilon_{a\beta\gamma} m_{i\gamma} & \text{for } i = j, \\ 0 & \text{for } i \neq j, \end{cases} \tag{5.18} \]

where Greek indices represent Cartesian coordinates \( x, y, z \) and \( \varepsilon_{a\beta\gamma} \) is the Levi-Civita symbol. Thus, the dynamics of the conservative spin system is Hamiltonian.

For convenience, we shall write Eq. \( (5.16) \) as

\[ \dot{m} = \tilde{\gamma} [m, \nabla \mathcal{H}]. \tag{5.19} \]

The variable \( m \in \mathbb{R}^{3n} \) can be seen as a compound vector that assigns to every position \( i = 1, \ldots, n \) a vector \( m_i \in \mathbb{R}^3 \). The square brackets in Eq. \( (5.19) \) denote an elementwise cross product: given \( x, y \in \mathbb{R}^{3n} \), we define \( z_i = x_i \times y_i \) for each position \( i \). In other words, it is just the ordinary cross product (vector product) performed \( n \) times. For small deviations \( x = m - m_0 \in \mathbb{R}^{3n} \) from some fixed configuration \( m_0 \), Eq. \( (5.19) \) becomes

\[ \dot{x} = -\tilde{\gamma} [m_0, h] + Mx + O(\|x\|^2), \tag{5.20} \]

where \( h_{(ia)} = -\partial \mathcal{H} / \partial m_{ia} |_{m=m_0} \) is the effective field at \( m_0 \). The matrix \( M \) is given by

\[ Mx = \tilde{\gamma} [m_0, Ax] + \tilde{\gamma} [h, x], \tag{5.21} \]

where \( A_{(ia)(jb)} = \partial^2 \mathcal{H} / (\partial m_{ia} \partial m_{jb}) |_{m=m_0} \) is the \( 3n \times 3n \) Hessian matrix of \( \mathcal{H} \) at \( m_0 \). To be explicit, let us mention that the elements of \( M \) are given by

\[ M_{(ia)(jb)} = \begin{cases} \tilde{\gamma} \varepsilon_{a\gamma\delta}(m_0)_{i\gamma} A_{(i\delta)(j\beta)} + \tilde{\gamma} \varepsilon_{a\gamma\beta} h_{i\gamma} & \text{for } i = j, \\ \tilde{\gamma} \varepsilon_{a\gamma\delta}(m_0)_{i\gamma} A_{(i\delta)(j\beta)} & \text{for } i \neq j. \end{cases} \tag{5.22} \]

(Summation is implied for repeated Greek indices but not for repeated Roman indices.) Since we work in Cartesian coordinates, \( A \) is typically of a relatively
simple form. Indeed, many micromagnetic models use a Hamiltonian that is quadratic in the Cartesian coordinates, in which case $A$ does not depend on $m_0$.

We assume that $m_0$ is an equilibrium configuration, $[m_0, h] = 0$. As a result, Eq. (5.20) is of the form (5.1). The matrix $\Omega$ (5.2) is given by

$$\Omega_{(ia)(\beta j)} = -\{m_{ia}, m_{\beta j}\}|_{m = m_0}$$

or equivalently,

$$\Omega x = -\tilde{\gamma}[m_0, x].$$

The $2n$-dimensional image space of $\Omega$ consists of vectors $x \in \mathbb{R}^{3n}$ for which the displacement $x_i \in \mathbb{R}^3$ is orthogonal at each position $i$ to the equilibrium direction $m_0$. Notice also that the equilibrium effective field $h_i$ must be parallel at each position $i$ to the equilibrium direction $m_0$. Combining Eqs. (5.21) and (5.24), the matrix $M\Omega$, which is symmetric (see Sec. 5.2), is given by

$$M\Omega x = -\tilde{\gamma}^2 \left( [m_0, A[m_0, x]] + [h, [m_0, x]] \right)$$

or

$$= \left( \Omega^T A \Omega + \tilde{\gamma} [h, \cdot \Omega] \right) x.$$ 

The second term, which contains $h$, originates from the fact that the Hessian matrix $A$ is calculated in Cartesian coordinates, while the symplectic leaf (a product of $n$ spheres) is curved.

5.4 Reduction to the HDGEP

In this section, we present a method for the solution of the normal-mode problem of a general Hamiltonian system near a local minimum of the Hamiltonian. This includes the normal-mode problem of the conservative spin system as a special case. We show that the normal-mode problem can be reduced to the HDGEP, in which form it can be efficiently solved (see Sec. 5.7). Our method calculates both the positive modes and any zero modes of the system. If zero modes are present, the method detects these and automatically determines their types (special or inertial).

The conservative spin system differs from an important subclass of Hamiltonian systems, which includes systems of coupled point masses, for which the normal-mode problem can be written as a symmetric definite generalized eigenvalue problem (SDGEP) in an obvious way (see Sec. 5.4). Such Hamiltonian systems are defined on a natural set of canonical momenta and coordinates. In terms of these, the Hamiltonian is of the form $H(\{p_i\}, \{q_i\}) = T(\{p_i\}) + V(\{q_i\})$, where the potential-energy term $V$ depends only on the coordinates $q_i$, while the kinetic-energy term $T$ is a positive-definite quadratic function depending only on the
momenta \( p_i \) (typically, \( \mathcal{T} = \sum_i p_i^2 / (2m_i) \)). The spin system is not of this special form. All that is given is the Poisson bracket (5.18) and the Hamiltonian \( \mathcal{H}(\{\mathbf{m}_i\}) \) as a function of the magnetic moments \( \mathbf{m}_i \). Even though it is possible to construct canonical momenta and coordinates \[61\] for this system, an \textit{a priori} separation of kinetic energy and potential energy is not normally known.

We shall first consider the case that \( \langle M\Omega \rangle \) is positive definite (no zero modes). Later in this section, we treat the general case where \( \langle M\Omega \rangle \) is positive semidefinite. This generalization is essential for spin systems such as those discussed in Secs. 5.8.2–5.8.5.

We remind the reader that an HDGEP has the general form

\[ Dx = \lambda Sx, \tag{5.26} \]

where \( D \) is Hermitian and \( S \) is Hermitian and positive definite, which requirements guarantee that all eigenvalues \( \lambda_i \) are real. The usual Hermitian eigenvalue problem is a special case of the HDGEP (set \( S = I \)). If \( D \) and \( S \) are real matrices, so that \( D \) and \( S \) are symmetric, we use the abbreviation SDGEP. The eigenvectors \( x_i \) of a HDGEP may be chosen to satisfy \( x_i^\dagger S x_j = \delta_{ij} \), a generalized orthonormality relation. Alternatively, we may choose to normalize the eigenvectors \( x_i \) in such a way that

\[ x_i^\dagger D x_j = \pm \delta_{ij}, \tag{5.27} \]

provided that \( D \) is invertible, in which case the eigenvalues \( \lambda_i \) are nonzero.

Let us represent a positive normal mode (5.3) as a single vector

\[ w = w_1 + iw_2 \in \mathbb{C}^{2n}, \tag{5.28} \]

where \( w_1 \) and \( w_2 \) are such that

\[ u_1 = \langle \Omega \rangle w_1 \quad \text{and} \quad u_2 = \langle \Omega \rangle w_2. \]

It is easy to see that in this notation, a solution of the generalized eigenvalue problem

\[ \langle M\Omega \rangle w = -\imath \omega \langle \Omega \rangle w \tag{5.29} \]

with \( \omega > 0 \) is also a solution of Eq. (5.3) (after conversion of the vectors in \( \mathbb{R}^{2n} \) to vectors in the image space of \( \Omega \)): take real and imaginary parts. If we \textit{assume} that \( \langle M\Omega \rangle \) is positive definite, Eq. (5.29) is a HDGEP (5.26) with \( D = -\imath \langle \Omega \rangle \), \( S = \langle M\Omega \rangle \) and \( \lambda = \omega^{-1} \), since \( \Omega \) is antisymmetric and \( M\Omega \) is symmetric (see Sec. 5.2). The HDGEP form (5.29) makes the problem suitable for efficient numerical computation. Notice that \( \lambda \neq 0 \), since \( \langle \Omega \rangle \) is invertible. Notice also that each positive normal mode gives rise to two independent solutions of Eq. (5.29): if \( w = w_1 + iw_2 \) is an eigenvector with eigenvalue \( \omega > 0 \), then \( w^* = w_1 - iw_2 \) is an eigenvector with eigenvalue \( -\omega \). By Eq. (5.27), we may normalize the eigenvectors so that they satisfy

\[ (w_1 + iw_2)^\dagger (-\imath \langle \Omega \rangle) (w_1 + iw_2) = 2\delta_{kl} \tag{5.30a} \]

\[ (w_1 - iw_2)^\dagger (-\imath \langle \Omega \rangle) (w_1 + iw_2) = 0, \tag{5.30b} \]
which equations together are equivalent to Eqs. (5.10a) and (5.10b).

Equation (5.29) can be seen as a generalization of Eqs. 27–30 in Ref. [84], which were given for the normal-mode problem of the conservative spin system, to a general Hamiltonian system. Our formulation has the additional advantage that it does not require the use of spherical coordinates. By itself, the method only works if \( \langle M \Omega \rangle \) is positive definite. If \( \langle M \Omega \rangle \) is merely positive semidefinite, Eq. (5.29) is no longer a HDGEP. Zero normal modes may appear and the matrix \( M \) is not even guaranteed to be diagonalizable. These zero modes have important consequences for the dynamics of, for example, domain walls or skyrmions in magnetic systems (see Secs. 5.8.2, 5.8.5). We present here a robust scheme that also works in this more general case. Thus, our method can solve the normal-mode problem of any Hamiltonian system linearized at a local minimum of the Hamiltonian.

The main idea of our approach is that we first find the special and inertial zero normal modes and then exclude them from the problem. The algorithm consists of the steps outlined below. The only two “large” (2\( n \)-dimensional) problems in this procedure are steps 1 and 4. In step 1 we need to find the lowest eigenvalues and corresponding eigenvectors of a symmetric matrix. In step 4 we need to solve a symmetric linear system. Both sub-problems can be efficiently solved using iterative methods. How this may be done is discussed in more detail in Sec. 5.7. The diagonalizations in steps 2 and 5 concern small matrices and can be performed using standard routines.

1. Sequentially find the eigenvectors \( y_1, y_2, \ldots \in \mathbb{R}^{2n} \) of \( \langle M \Omega \rangle \) that correspond to the lowest eigenvalues (see Sec. 5.7). Stop when an eigenvector appears with an eigenvalue that is larger than zero (by a certain small tolerance). Notice that this is an ordinary (nongeneralized) symmetric eigenvalue problem, so that the fact that \( \langle M \Omega \rangle \) is not necessarily positive definite is not a problem. By positive semidefiniteness of \( \langle M \Omega \rangle \), all eigenvalues are greater than or equal to zero. Suppose that there are \( s \) eigenvectors with eigenvalue zero. Then \( y_1, \ldots, y_s \) form a basis of the null space of \( \langle M \Omega \rangle \). In most cases, \( s \) will be a small number. Remember that thanks to the restriction of \( M \Omega \) to \( \langle M \Omega \rangle \), we have already excluded all null vectors of \( M \Omega \) that are also null vectors of \( \Omega \) and thus correspond to a displacement of the system out of the symplectic leaf.

2. Define the \( s \times s \) matrix \( [\Omega]_{ij} = y_i^T \langle \Omega \rangle y_j \). Since \( [\Omega]_{ij} \) is antisymmetric, \( i[\Omega]_{ij} \) is Hermitian and can be diagonalized by a standard routine for Hermitian matrices, which guarantees that the eigenvectors are orthonormal. Let \( s_d \) be the number of independent eigenvectors \( B_{i(k)} \) of \( [\Omega]_{ij} \) with eigenvalue zero (up to a small tolerance). We have \( \sum_{j=1}^{s} [\Omega]_{ij} B_{j(k)} = 0 \) for \( k = 1, \ldots, s_d \). We may take these eigenvectors \( B_{i(k)} \) to be real. The remaining nonnull eigenvectors come in \( s_0 \) pairs. Let \( C_{i(l)} + iD_{i(l)} \) be an eigenvector of \( [\Omega]_{ij} \) with eigenvalue \( i\lambda_{(l)} \), where \( \lambda_{(l)} > 0 \) and \( C_{i(l)} \) and \( D_{i(l)} \) are real. We have \( \sum_{j=1}^{s} [\Omega]_{ij} (C_{j(l)} + iD_{j(l)}) = i\lambda_{(l)} (C_{i(l)} + iD_{i(l)}) \) for \( l = 1, \ldots, s_0 \). Then
$C_{i(l)} - iD_{i(l)}$ is an eigenvector with eigenvalue $-i\lambda_{(l)}$. The total number of eigenvectors is $s = s_d + 2s_o$.

3. Construct the vectors $c_l = \sum_{i=1}^{s} C_{i(l)} y_i$ and $d_l = \sum_{i=1}^{s} D_{i(l)} y_i$ for $l = 1, \ldots, s_o$ and $\bar{b}_k = \sum_{i=1}^{s} B_{i(k)} y_i$ for $k = 1, \ldots, s_d$. Notice that we have $c_l^T \langle \Omega \rangle d_{l'} = 0$ for $l \neq l'$ and $c_l^T \langle \Omega \rangle d_{l} > 0$. Moreover, for all $l, l', k, k'$ we have $c_l^T \langle \Omega \rangle c_{l'} = d_l^T \langle \Omega \rangle d_{l'} = 0$, $c_l^T \langle \Omega \rangle \bar{b}_k = d_l^T \langle \Omega \rangle \bar{b}_k = 0$ and $\bar{b}_k^T \langle \Omega \rangle \bar{b}_{k'} = 0$.

4. For each $k = 1, \ldots, s_d$, find a vector $\tilde{a}_k$ such that $\langle M\Omega \rangle \tilde{a}_k = \langle \Omega \rangle \bar{b}_k$ (see Sec. 5.7). We know that such a vector exists, since by construction $\langle \Omega \rangle \bar{b}_k$ lies in the orthogonal complement of the null space of $\langle M\Omega \rangle$, a symmetric matrix, and hence in the image space of $\langle M\Omega \rangle$. Although this vector $\tilde{a}_k$ is not uniquely defined, there is a unique solution $\bar{a}_k$ that lies in the image space of $\langle M\Omega \rangle$, which is the solution that is obtained by the method given in Sec. 5.7.

5. Define the symmetric $s_d \times s_d$ matrix $[M\Omega]_{kk'} = \tilde{a}_k^T \langle M\Omega \rangle \tilde{a}_{k'}$ and diagonalize it using a standard routine for symmetric matrices. Let the orthonormal eigenvectors be $G_{i(k)}$. We have $\sum_{i=1}^{s_d} [M\Omega]_{ii} G_{j(k)} = \mu(k) G_{i(k)}$ with $\mu(k) > 0$ for $k = 1, \ldots, s_d$. The eigenvalues $\mu(k)$ are positive, since $\langle M\Omega \rangle$ is positive semidefinite and the vectors $\tilde{a}_k$ are independent vectors in the image space of $\langle M\Omega \rangle$.

6. Construct the vectors $b_k = \sum_{i=1}^{s_d} G_{i(k)} \bar{b}_i$ and $\bar{a}_k = \sum_{i=1}^{s_d} G_{i(k)} \tilde{a}_i$ for $k = 1, \ldots, s_d$. Since $\tilde{a}_k^T \langle \Omega \rangle b_{k'} = \tilde{a}_k^T \langle M\Omega \rangle \tilde{a}_{k'}$, we have $\tilde{a}_k^T \langle \Omega \rangle b_{k'} = 0$ for $k \neq k'$ and $\tilde{a}_k^T \langle \Omega \rangle b_k > 0$.

7. Redefine $\bar{a}_k$ as $\bar{a}_k / \sqrt{\bar{a}_k}$, $b_k$ as $b_k / \sqrt{\bar{a}_k}$, $c_l$ as $c_l / \sqrt{\bar{a}_k}$ and $d_l$ as $d_l / \sqrt{\bar{a}_k}$, where $\bar{a}_k = \tilde{a}_k^T \langle \Omega \rangle b_k = \mu(k)$ and $\beta_l = c_l^T \langle \Omega \rangle d_{l} = \lambda_{(l)}/2$. This normalizes the modes so that $\tilde{a}_k^T \langle \Omega \rangle b_k = 1$ for each $k$ and $c_l^T \langle \Omega \rangle d_{l} = 1$ for each $l$.

8. Set $\hat{a}_k = \tilde{a}_k - \sum_{l=1}^{s_o} (c_l^T \langle \Omega \rangle \tilde{a}_k) d_l + \sum_{l=1}^{s_o} (d_l^T \langle \Omega \rangle \tilde{a}_k) c_l$. We have $c_l^T \langle \Omega \rangle \hat{a}_k = d_l^T \langle \Omega \rangle \tilde{a}_k = 0$ for all $l, k$.

9. Set $a_k = \hat{a}_k - \sum_{k'=1}^{s_d} \frac{1}{2}(\hat{a}_k^T \langle \Omega \rangle \hat{a}_k) b_{k'}$. We have $a_k^T \langle \Omega \rangle a_{k'} = 0$ for all $k, k'$.

10. The pairs $(u_1, u_2) = (\Omega a_k, \Omega b_k)$ are the inertial zero normal modes (5.7). The pairs $(u_1, u_2) = (\Omega c_l, \Omega d_l)$ are the special zero normal modes (5.5). All zero normal modes now satisfy the relations (5.10a) and (5.10b).

Let us define the zero normal modes, of which there are $s_d + s_o$, as the first modes in the list of all modes: set $w_{li} = a_i$, $w_{2i} = b_i$ for $i = 1, \ldots, s_d$ and $w_{1(s_d+i)} = c_i$, $w_{2(s_d+i)} = d_i$ for $i = 1, \ldots, s_o$. All normal modes must satisfy the relations (5.30a) and (5.30b), which are equivalent to Eqs. (5.10a) and (5.10b).
Once the zero normal modes have been obtained, we may thus restrict the generalized eigenvalue problem (5.29) to trial vectors \( w \) that satisfy

\[
(w_{1i} + iw_{2i})^\dagger (\Omega) w = 0
\]

for all zero normal modes \( i = 1, \ldots, s_d + s_0 \). These constraints can be implemented in the iterative HDGEP solver in a very natural way (see Sec. 5.7). On this subspace, Eq. (5.29) constitutes an HDGEP, so we can efficiently find the remaining modes \( i = s_d + s_o + 1, \ldots, n \).

5.5 DAMPED SPIN SYSTEMS

We have seen that the magnetic normal modes of a conservative spin system, which is Hamiltonian, can be obtained by solving a HDGEP. However, typical magnetic systems can be modeled more realistically using the LLG equation \[56\] with a nonzero damping parameter \( \eta > 0 \),

\[
\dot{\mathbf{m}}_i = -\tilde{\gamma} \mathbf{m}_i \times (-\nabla_{\mathbf{m}} \mathcal{H} - \eta \mathbf{m}_i)
\] (5.32)

[compare Eq. (5.16)]. Note that some texts write the LLG equation with damping (5.32) in a somewhat different, explicit form \[11,56\]. The damping term affects the magnetic normal modes and the eigenfrequencies \( \omega \), which now acquire an imaginary part \[100,101\]. Our method for the magnetic normal-mode problem can be used even in this nonconservative case if we treat the damping term of the LLG equation as a perturbation. We are justified in doing so, since \( \eta \) is often small (\( \eta \ll 1/\tilde{\gamma} m_S \), where \( m_S \) is the typical magnitude \( \| \mathbf{m}_i \| \) of the spins). In this way, we avoid the need for the solution of non-Hermitian eigenvalue problems \[102\] and describe the effect of damping directly in terms of the conservative normal modes, which correspond to canonical coordinates.

In this section, we derive expressions for the damped modes in first-order perturbation theory. In particular, we obtain very simple and elegant first-order expressions (5.40) and (5.43) for the decay rate of the amplitude of a mode under damping. Decay rates of modes are especially important as they determine the widths of the corresponding peaks in dynamic magnetic susceptibility functions (see Fig. 5.6), which can be measured. In contrast to previous applications of the perturbative method \[103\], our expressions provide first-order corrections to the mode vectors \( u_1, u_2 \) (even for degenerate normal modes) and also cover systems with special or inertial zero normal modes.

Again considering the deviation \( \mathbf{x} = \mathbf{m} - m_0 \in \mathbb{R}^{3n} \) from a fixed equilibrium configuration \( m_0 \) in Cartesian coordinates (see Sec. 5.3), the LLG equation with damping (5.32) becomes, using that \( \dot{\mathbf{x}} = \mathcal{O}(\| \mathbf{x} \|) \),

\[
\dot{\mathbf{x}} = \mathbf{M} \mathbf{x} - \eta \Omega \dot{\mathbf{x}} + \mathcal{O}(\| \mathbf{x} \|^2),
\] (5.33)
with $M$ and $\Omega$ as defined in Eqs. (5.21) and (5.24). We can write this in explicit form as $\dot{x} = M'x + O(\|x\|^2)$, where

$$M' = (I_{3n} + \eta \Omega)^{-1} M = \left( I_{3n} + \eta^2 \Omega^T \Omega \right)^{-1} (M - \eta \Omega M).$$

(5.34)

We see that to first order in $\eta$, the matrix $M'\Omega$ results from perturbation of $M\Omega$ by a term $-\eta \Omega M\Omega$. Since the LLG equation with damping (5.32) respects the constraint that the magnitude $\|m_i\|$ of each magnetic moment be constant, we may still assume that the physically relevant vectors $x \in \mathbb{R}^{3n}$ lie in the $2n$-dimensional image space of $\Omega$.

The presence of (a not too large amount of) damping modifies the three types of normal modes as follows. We use primes for the modes of the damped system.

1. A positive normal mode (5.3) becomes a damped mode of the form

$$\begin{align*}
M'u'_1 &= \omega'u'_2 - \xi'u'_1, \\
M'u'_2 &= -\omega'u'_1 - \xi'u'_2.
\end{align*}$$

(5.35)

The fundamental solutions that correspond to a damped positive mode (5.35) are

$$\begin{align*}
x_1(t) &= e^{-\xi't} \left[ \cos(\omega't)u'_1 + \sin(\omega't)u'_2 \right], \\
x_2(t) &= e^{-\xi't} \left[ -\sin(\omega't)u'_1 + \cos(\omega't)u'_2 \right].
\end{align*}$$

(5.36)

2. A special zero normal mode (5.5) remains unchanged in the presence of damping.

3. An inertial zero normal mode (5.7) becomes a damped mode of the form

$$\begin{align*}
M'u'_1 &= u_2 - \xi'u'_1, \\
M'u'_2 &= 0.
\end{align*}$$

(5.37)

The corresponding fundamental solutions are

$$\begin{align*}
x_1(t) &= e^{-\xi't}u'_1 + [(1 - e^{-\xi't})/\xi']u_2, \\
x_2(t) &= u_2.
\end{align*}$$

(5.38)

Notice that the $u_2$ part of an inertial normal mode remains unchanged in the presence of damping.

Equation (5.35) is equivalent to Eq. (5.29) if we replace $M$ in Eq. (5.29) with $M'$ and $\omega$ with $\omega' - i\xi'$; it is in this sense that the frequency of a damped positive mode acquires an imaginary part. Notice that with damping, Eq. (5.29) is no longer a HDGEP. As a result, the damped modes do not necessarily satisfy the relations (5.10a) and (5.10b).
In first-order perturbation theory, we write a damped positive mode (5.35) as
\[
\omega'_k = \omega_k + \mathcal{O}(\eta^2) \tag{5.39a}
\]
\[
\xi'_k = \eta \xi_k^{(1)} + \mathcal{O}(\eta^2) \tag{5.39b}
\]
\[
u'_1 = u_{1k} + \eta u_{1k}^{(1)} + \mathcal{O}(\eta^2) \tag{5.39c}
\]
\[
u'_2 = u_{2k} + \eta u_{2k}^{(1)} + \mathcal{O}(\eta^2) \tag{5.39d}
\]
where \(k\) is the mode index and \(u_{1k}, u_{2k}\) and \(\omega_k\) is the unperturbed normal mode and frequency. We assume that the vectors \(w_1, w_2\) of all unperturbed normal modes (5.9) satisfy the relations (5.10a) and (5.10b). Moreover, we assume that if any of the unperturbed normal modes are degenerate, they satisfy certain additional conditions (stated below). Using these assumptions and the definitions (5.3), (5.5) and (5.7), it can be derived, by a rather lengthy calculation, that the first-order corrections to a positive mode \(k\) are given by
\[
\xi_k^{(1)} = \frac{1}{2} \omega_k \left( u_{1k}^T u_{1k} + u_{2k}^T u_{2k} \right) = \frac{1}{2} \omega_k \left( \|u_{1k}\|^2 + \|u_{2k}\|^2 \right) \tag{5.40}
\]
where the first sum in Eq. (5.41a) or (5.41b) is over any modes \(l\) that are degenerate with the positive normal mode \(k\), plus \(k\) itself; the second sum is over all other
positive normal modes; the third sum is over the special zero normal modes; and
the fourth sum is over the inertial zero normal modes. For the damped inertial
zero mode (5.37), we have

\[
\xi' = \eta \xi_k^{(1)} + \mathcal{O}(\eta^2) \quad \text{(5.42a)}
\]

\[
u'_{1k} = u_{1k} + \eta u_{1k}^{(1)} + \mathcal{O}(\eta^2) \quad \text{(5.42b)}
\]

The first-order corrections are given by

\[
\xi_k^{(1)} = u_{2k}^T u_{2k} = \|u_{2k}\|^2 \quad \text{(5.43)}
\]

\[
u_{1k}^{(1)} = \sum_{l \in \text{pos.}} -\omega_l^{-1} \left[ (u_l^T u_{2k}) u_{1l} + (u_{2l}^T u_{2k}) u_{2l} \right] + \sum_{l \in \text{in.}} -(u_{1l}^T u_{2k}) u_{1l}, \quad \text{(5.44)}
\]

where the first sum in Eq. (5.44) is over all positive normal modes and the second
sum is over all inertial zero normal modes. We see that in both cases (5.40)
and (5.43), \(\xi^{(1)}\) is guaranteed to be positive: for a positive damping parameter \(\eta\), amplitudes of modes decrease in time. Notice that the frequency \(\omega'\) of a
damped positive mode is constant to first order in \(\eta\); however, there will be a
second-order correction (normally negative).

If all magnetic moments in the equilibrium configuration \(m_0\) have the same
magnitude \(\|m_0\| = m_S\), we have \(\langle \Omega^T \Omega \rangle = \tilde{\gamma}^2 m_S^2 I_{2n}\), and Eq. (5.34) becomes

\[
M' \Omega = \frac{1}{1 + (\eta \tilde{\gamma} m_S)^2} (M \Omega - \eta \Omega M \Omega) \quad \text{(5.45)}
\]

We can then often further reduce the residual error in the damped positive
modes, which is of second order in \(\eta\), simply by dividing the \(\omega'\) and \(\xi'\) as
obtained to first order by \(1 + (\eta \tilde{\gamma} m_S)^2\). For a damped inertial zero mode, divide
the value \(\xi'\) by \(1 + (\eta \tilde{\gamma} m_S)^2\) and multiply the vector \(u_1'\) by the same factor. These
corrections do not eliminate the error of second order completely, but are very
easy to implement.

If there are several distinct positive normal modes with the same frequency \(\omega\), or if the dimension \(s\) of the null space of \(\langle M \Omega \rangle\) is larger than one, the normal-
mode problem is degenerate. The damping perturbation may lift this degeneracy.
For the correctness of the expressions for the first-order corrections it is essen-
tial to choose the degenerate unperturbed normal modes in such a way that the
perturbation does not mix them. We amend the procedure of Sec. 5.4 as fol-
lows. Given any symmetric and positive-definite matrix \(A\), we may choose the
null-space vectors \(y_1, \ldots, y_s\) in step 1 of Sec. 5.4 in such a way that they satisfy
\(y_i^T A y_j = \delta_{ij}\). For the spin system with damping, we must use \(A = \langle \Omega^T \Omega \rangle\). The
rest of the algorithm then automatically ensures that the vectors \( b_k, c_l \) and \( d_l \) (see step 10) of the zero normal modes satisfy

\[
\begin{align}
b_k^T A b_{k'} &= 0 \quad \text{(for } k \neq k') \quad (5.46a) \\
c_l^T A c_{l'} &= d_l^T A d_{l'} = 0 \quad \text{(for } l \neq l') \quad (5.46b) \\
b_k^T A c_l &= b_k^T A d_l = 0 \quad \text{(for all } k,l) \quad (5.46c) \\
c_l^T A d_{l'} &= 0 \quad \text{(for all } l,l') \quad (5.46d)
\end{align}
\]

where \( k,k' \) index the inertial zero normal modes and \( l,l' \) index the special zero normal modes. For example, Eq. (5.46d) is equivalent to the condition that \( u_{1l}^T u_{2l'} = 0 \) for all pairs of special zero normal modes \( l,l' \). As for the positive normal modes, if we have a block of \( r \) degenerate modes at frequency \( \omega > 0 \), we can, without breaking the conditions (5.10a) and (5.10b), choose them in such a way that the Hermitian \( r \times r \) matrix \( [A]_{ij} = (w_1 i + i w_2) A (w_1 j + i w_2) \) is diagonal. Here \( i,j \) index those modes that are part of the degenerate block. Again, we must use \( A = \langle \Omega^T \Omega \rangle \). As a result, the components \( w_1 \) and \( w_2 \) satisfy

\[
\begin{align}
w_1^T A w_{1j} + w_2^T A w_{2j} &= 0 \quad \text{(for } i \neq j) \quad (5.47a) \\
w_1^T A w_{2j} - w_2^T A w_{1j} &= 0 \quad \text{(for all } i,j) \quad (5.47b)
\end{align}
\]

For example, Eq. (5.47b) is equivalent to the condition that \( u_{1i}^T u_{2j} - u_{2i}^T u_{1j} = 0 \) for all pairs of positive normal modes \( i,j \) that are part of the degenerate block.

### 5.6 Dynamic Magnetic Susceptibility

Response functions, such as dynamical magnetic susceptibilities, allow comparison of calculated spectra to experimental observables (see, for example, Ref. [74]). The dynamic susceptibility \( \chi(\omega) \) is defined as the complex amplitude of the magnetization that results in linear response from some applied field, divided by the complex amplitude of this applied field. Here \( \omega \) is the driving frequency. Dynamical magnetic susceptibility functions can be related directly to the eigen-modes of the dynamical matrix in the presence of damping [82][104]. Using the expressions in Sec. 5.5, our scheme allows one to calculate dynamical susceptibility functions in a way that is usually much less computationally expensive than with spin-dynamics simulations. We do not make any further assumptions on the system (in particular, we do not assume that \( M \) and \( \Omega \) commute), and we (optionally) take into account the corrections to the mode vectors \( u'_{1k} \) and \( u'_{2k} \). Our expressions include the contributions from special and inertial zero modes as well as positive modes.

If we introduce a time-dependent external field \( f_i(t) \) into Eq. (5.32), we get

\[
\dot{m}_i = -\gamma m_i \times (-\nabla m_i \mathcal{H} + f_i(t) - \eta m_i).
\]

Linearization of this equation near the equilibrium configuration \( m_0 \) gives

\[
\dot{x} = Mx + \Omega f(t) - \eta \Omega \dot{x},
\]
with \( M, \Omega, \) and \( x \) defined as in Eq. (5.33). We can rewrite this as
\[ \dot{x} - M'x = g(t), \] (5.50)
with \( M' \) as defined in Eq. (5.34) and
\[ g(t) = (I_{3n} + \eta \Omega)^{-1}\Omega f(t). \] (5.51)

Now let us write
\[ x(t) = \sum_k (x_{1k}(t) u'_{1k} + x_{2k}(t) u'_{2k}), \] (5.52a)
\[ g(t) = \sum_k (g_{2k}(t) u'_{1k} - g_{1k}(t) u'_{2k}). \] (5.52b)

Notice that we express \( x(t) \) and \( f(t) \) in terms of the mode vectors \( u'_{1k}, u'_{2k} \) that are corrected for damping, which means that \( x_{1k}, x_{2k} \) are not identical to the canonical variables \( p_k, q_k \). However, for small damping we have
\[ \begin{cases} 
    x_{1k}(t) = p_k(t) + \mathcal{O}(\eta) = -w^T_{2k}x(t) + \mathcal{O}(\eta) \\
    x_{2k}(t) = q_k(t) + \mathcal{O}(\eta) = w^T_{1k}x(t) + \mathcal{O}(\eta),
\end{cases} \] (5.53a)
\[ \begin{cases} 
    g_{1k}(t) = u^T_{1k}f(t) + \mathcal{O}(\eta) \\
    g_{2k}(t) = u^T_{2k}f(t) + \mathcal{O}(\eta),
\end{cases} \] (5.53b)

where \( u_{1k}, u_{2k} \) are the unperturbed mode vectors and \( p_k, q_k \) are the corresponding coefficients (5.12). If the error of \( \mathcal{O}(\eta) \) is unacceptable, one could use Eqs. (5.39) and (5.42) to calculate the corrected \( u'_{1k}, u'_{1k} \) to an error of only \( \mathcal{O}(\eta^2) \) and then use Eq. (5.52).

In terms of the coefficients, Eq. (5.49) separates into pairs of coupled equations of motion, one pair for each mode. For a positive mode \( k \), we have
\[ \begin{cases} 
    \dot{x}_{1k} + \xi_k x_{1k} + \omega_k' x_{2k} = \varepsilon_{2k} \\
    \dot{x}_{2k} - \omega_k' x_{1k} + \xi_k x_{2k} = -\varepsilon_{1k},
\end{cases} \] (5.54)
for a special zero mode \( k \), we have
\[ \begin{cases} 
    \dot{x}_{1k} = \varepsilon_{2k} \\
    \dot{x}_{2k} = -\varepsilon_{1k},
\end{cases} \] (5.55)
and for an inertial zero mode \( k \), we have
\[ \begin{cases} 
    \dot{x}_{1k} + \xi_k x_{1k} = \varepsilon_{2k} \\
    \dot{x}_{2k} - x_{1k} = -\varepsilon_{1k}.
\end{cases} \] (5.56)

If we now assume that the system is driven with a driving frequency \( \omega \), so that \( g_{1k}(t) = g_{1k}e^{i\omega t} \) and similarly for \( g_{2k}(t) \) and \( x_{1k}(t), x_{2k}(t) \) (particular part of the solution), we find
\[ \begin{cases} 
    x_{1k} = \chi_{11k}g_{1k} + \chi_{12k}g_{2k} \\
    x_{2k} = \chi_{21k}g_{1k} + \chi_{22k}g_{2k},
\end{cases} \] (5.57)
where, if $k$ is a positive mode,

\[
\begin{align*}
\chi_{11k} &= \frac{\omega'_k}{(\xi'_k + i\tilde{\omega})^2 + (\omega'_k)^2}, \\
\chi_{21k} &= \frac{-(\xi'_k + i\tilde{\omega})}{(\xi'_k + i\tilde{\omega})^2 + (\omega'_k)^2}, \\
\chi_{12k} &= \frac{\xi'_k + i\tilde{\omega}}{(\xi'_k + i\tilde{\omega})^2 + (\omega'_k)^2}, \\
\chi_{22k} &= \frac{\xi'_k + i\tilde{\omega}}{(\xi'_k + i\tilde{\omega})^2 + (\omega'_k)^2},
\end{align*}
\]

(5.58a) (5.58b)

if $k$ is a special zero mode,

\[
\begin{align*}
\chi_{11k} &= 0, \\
\chi_{21k} &= i/\tilde{\omega}, \\
\chi_{12k} &= -i/\tilde{\omega}, \\
\chi_{22k} &= 0;
\end{align*}
\]

(5.59a) (5.59b)

and if $k$ is an inertial zero mode,

\[
\begin{align*}
\chi_{11k} &= 0, \\
\chi_{21k} &= i/\tilde{\omega}, \\
\chi_{12k} &= \frac{1}{\tilde{\omega}^2 - i\xi'_k\tilde{\omega}}, \\
\chi_{22k} &= -\frac{1}{\tilde{\omega}^2 - i\xi'_k\tilde{\omega}}.
\end{align*}
\]

(5.60a) (5.60b)

Suppose that we apply to the system a driving force with a fixed spatial profile $f \in \mathbb{R}^{3n}$ and driving frequency $\tilde{\omega}$ and that we are interested in the response of the variable $r = v^T x$, where $v \in \mathbb{R}^{3n}$ is a fixed vector. For example, if we are interested in the response of total magnetization in the $\hat{x}$-direction to a uniform external field, also in the $\hat{x}$-direction, we have $f_i = \hat{x}$ and $v_i = \hat{x}$ for all sites $i$.

The total dynamical susceptibility is given by

\[
\chi_{vf} = \sum_k \left[ c_{vf11k}\chi_{11k} + c_{vf12k}\chi_{12k} + c_{vf21k}\chi_{21k} + c_{vf22k}\chi_{22k} \right],
\]

(5.61)

where the amplitudes $c_{vf11k}, c_{vf12k}, c_{vf21k}, c_{vf22k}$ can be derived from Eqs. (5.51) and (5.52). For small damping, Eqs. (5.52a) and (5.53b) give

\[
c_{vf12k} = (u_{1k}^T v)(u_{2k}^T f) + \mathcal{O}(\eta),
\]

(5.62)

and analogously for $c_{vf11k}, c_{vf21k}$ and $c_{vf22k}$.

### 5.7 Implementation

The procedure for finding the magnetic normal modes can be summarized as follows.

A. Find a configuration $m = m_0$ that is a local minimum of the Hamiltonian $H$, under the constraint that $\|m_i\| = \text{constant}$ for each position $i$.

B. If necessary, follow the procedure in Sec. 5.4 to detect and compute any zero normal modes.
C. Solve the HDGEP of Eq. (5.29) to find the (low-energy) positive normal modes.

D. If a damping parameter $\eta > 0$ is used, correct the normal modes using the expressions in Sec. 5.5.

All important steps can be efficiently implemented using iterative methods for large Hermitian problems. For concreteness, we shall discuss the iterative methods based on conjugate gradients in a bit more detail. Alternative approaches, such as matrix-free versions of the Lanczos eigenvalue algorithm \[96\], have similar properties.

Let us first remark that our scheme can also be used to find the magnetic normal modes near a local energy minimum of some continuum model. One discretizes the system using, for example, the finite-difference method or a geometric finite-element method \[105\], which give effective systems that are mathematically equivalent to a finite system \[58\]. It is important to use a mesh that is smooth enough, to avoid effects such as an artificial Peierls pinning of domain walls \[42, 106\]. (This effect decreases exponentially in the inverse lattice constant \[106\], so there is no fundamental problem.)

For completeness, we repeat here the essential properties of the conjugate-gradient methods. In its simplest form, the conjugate-gradient method \[38\] is an iterative method for solving systems of linear equations, $Ax = b$, where $A$ is a symmetric or Hermitian $N \times N$ matrix and $x$ and $b$ are vectors in $\mathbb{R}^N$ or $\mathbb{C}^N$. $A$ and $b$ are given; $x$ is asked. The linear system is considered solved when the norm of the residual vector $r = b - Ax$ is less than a certain (very small) tolerance. In each iteration $i = 1, 2, \ldots$, the trial solution $x_i$ is updated; its new value $x_{i+1}$ is a certain linear combination of $x_i$ and the previous residual vectors $r_i, r_{i-1}, r_{i-2}, \ldots$. The method is designed in such a way that only two vectors need to be kept in memory at any given iteration. A more detailed discussion of the algorithm can be found in most textbooks on numerical methods \[38\]. What is relevant here is the following. a) We do not need to store the $N^2$ elements of $A$. All we need is a routine that can evaluate $Ax$ for any given $x$ (the action $x \mapsto Ax$ of $A$). The conjugate-gradient algorithms use this routine as a “black box”. b) Every trial solution $x_i$ is a linear combination of $b, Ab, A^2b, \ldots, A^{i-1}b$; the conjugate-gradient method is a Krylov-subspace method. A variant of the conjugate-gradient method can be used to solve nonlinear optimization problems \[38\], where a local minimum of a multivariate function $f(x)$ is asked. Here the gradient $\nabla f$ plays the role of the residual vector. This method is also suitable for minimization problems under constraints $g_1(x) = \ldots = g_k(x) = 0$. In that case, one should project the residual vector $r$ onto the tangent space of the allowable hypersurface in the spirit of the method of Lagrange multipliers.

The conjugate-gradient eigenvalue algorithm \[107\] can be seen as a special case of constrained nonlinear optimization. If we minimize the function

$$f(x) = x^\dagger Dx$$

(5.63)
under the constraint
\[ g_1(x) = x^\dagger Sx = 1 \quad \text{(normalization),} \] (5.64)

where \( D \) and \( S \) are Hermitian matrices, we obtain the lowest eigenvalue \( \lambda_1 \) and the corresponding eigenvector \( x_1 \) of the HDGEP \( Dx = \lambda Sx \). (The SDGEP case, where \( D, S \) and \( x \) are real, is entirely analogous.) \( S \) must be positive definite to guarantee that a minimum exists. Once we have the first eigenvector \( x_1 \), we can obtain the next eigenvector by repeating the minimization under an additional constraint:
\[ g_2(x) = x_1^\dagger Sx = 0 \quad \text{(orthogonality).} \] (5.65)

For \( \lambda \neq 0 \), this is equivalent to the constraint
\[ g'_2(x) = \lambda_1 x_1^\dagger Sx = x_1^\dagger Dx = 0. \] (5.66)

Once we have found the second eigenvector, we move on to the third, and so on, applying constraints of the form (5.66) for all previously obtained eigenvectors. We continue until we have found as many eigenvectors \( x_1, x_2, \ldots \) with eigenvalues \( \lambda_1 < \lambda_2 < \ldots \) as we need.

The fact that we do not need to explicitly store the matrices in memory is a crucial advantage. For simplicity, let us first consider a one-dimensional \( n \)-spin chain with only exchange and uniaxial anisotropy energy,
\[ \mathcal{H} = E_{\text{ex}} + E_{\text{ani}} = \sum_{i=1}^{n-1} -2J \mathbf{m}_i \cdot \mathbf{m}_{i+1} - \sum_{i=1}^{n} K m_i^2. \] (5.67)

The Hessian matrix \( A \) (see Sec. [5.3]) is given by
\[
A_{(ia)(j\beta)} = \begin{cases} 
-2K & \text{if } i = j \text{ and } \alpha = \beta = z \\
-2J & \text{if } i = j - 1, j + 1 \text{ and } \alpha = \beta \\
0 & \text{otherwise}
\end{cases}
\] (5.68)
equivalently, it may be defined by its action \( x \mapsto Ax \),
\[
(Ax)_{ia} = \begin{cases} 
-2J(x_{i-1}\alpha + x_{i+1}\alpha) & \text{if } \alpha = x, y \\
-2J(x_{i-1}\alpha + x_{i+1}\alpha) - 2Kx_{ia} & \text{if } \alpha = z
\end{cases}
\] (5.69)

where we take \( x_{ia} = 0 \) for \( i = 0 \) and \( i = n + 1 \). We see that the evaluation of the action of \( A \) on an arbitrary vector \( x \) takes only \( \mathcal{O}(N) \) time, while any manipulation with or decomposition of the \( 3n \times 3n \) matrix \( A \) obviously takes at least \( \mathcal{O}(N^2) \) time if it is explicitly stored in memory in full. That is why Krylov-subspace methods are a popular choice for linear equations or eigenvalue problems of sparse matrices [97]. If long-range interactions are taken into consideration, the matrix \( A \) is dense. Nevertheless, the action of \( A \) can still be evaluated in much less than \( \mathcal{O}(N^2) \) time, as follows. For nearly all physical systems, \( A \) can be separated into a short-ranged part \( A_s \) such as Eq. (5.68), which is sparse, and
a long-ranged part $A_l$, which is invariant under spatial translations (it is a convolution \[82\]). To perform the action on a given vector $x$, we separately evaluate the contributions $A_s x$ and $A_l x$ and then add them up to obtain $A x = A_s x + A_l x$. In typical magnetic systems, the relevant long-range interaction is the dipolar interaction. We can evaluate $A_l x$ by performing the convolution in the Fourier representation of $x$, where it becomes a simple elementwise multiplication. The two Fourier transformations that are necessary take $O(N \log N)$ time \[108\]. A similar mixed real-space–reciprocal-space approach is taken in most plane-wave electronic-structure codes \[109\]. Even if the system is not perfectly translationally invariant, for instance because it has some nonrectangular finite geometry, we can efficiently evaluate $A_l x$ by reducing the dipolar problem to the Poisson problem \[65\] and solving it using multigrid methods \[97\]. The complexity analysis is similar. It is thus possible to implement a routine that can evaluate $A x$, and hence $M \Omega x$ (5.25), for any given $x$ in $O(N \log N)$ rather than $O(N^2)$ time.

In the remainder of this section, we discuss the specific implementation of each of the four stages listed above.

**Stage A** A minimum-energy configuration $m_0$ can be found using, for example, the nonlinear conjugate-gradient optimization method, which is implemented in existing micromagnetics codes. Note that many magnetic systems have multiple local energy minima. In this article, we regard one particular $m_0$ as given.

**Stage B – Step 1** In step 1 of Sec. 5.4, we need to calculate the null vectors $y_1, \ldots, y_s$ of $\langle M \Omega \rangle$. This is in fact a symmetric eigenvalue problem. It might be solved as a particular case of the conjugate-gradient SDGEP algorithm (set $D = \langle M \Omega \rangle$ and $S = I$). The sequential nature of this method means that we can efficiently obtain the lowest few eigenvectors. We stop once we find the first positive eigenvalue. The eigenvectors with eigenvalue zero constitute a basis of the null space of $\langle M \Omega \rangle$. In our definition of the restricted matrix $\langle M \Omega \rangle$, we formally require construction of a basis of the image space of $\Omega$. In practice, we do not normally need to construct the basis explicitly. We may simply set $D = M \Omega$, provided our initial guess $x_0$ is in the image space of $\Omega$ (that is, we set $x_0 = \Omega y_0$, where $y_0$ is a random vector). Since $x_0, M \Omega x_0, \Omega x_0, (M \Omega)^2 x_0, \text{etc.}$ all lie in the image space of $\Omega$, the minimization will automatically be restricted to trial solutions in this space. We remark that for numerical stability, it may be necessary occasionally to project the trial vector $x_i$ back onto the image space of $\Omega$.

**Stage B – Step 4** In step 4 of Sec. 5.4, we need to solve the linear system $\langle M \Omega \rangle x = g$, where $g = \langle \Omega \rangle b_k$. This problem may seem ill posed, since $\langle M \Omega \rangle$ is not invertible (even with the angular brackets). However, we know that a solution exists ($g$ lies in the image space of $\langle M \Omega \rangle$). Since the solution-vector iterates are always linear combinations of $g, \langle M \Omega \rangle g, (\langle M \Omega \rangle)^2 g, \ldots$, we in effect
restrict our search to trial solutions \( x \) in the image space of \( \langle M\Omega \rangle \). In this linear subspace, the solution \( x \) is unique.

In practice, \( g \) will not lie in the image space of \( \langle M\Omega \rangle \) numerically exactly, but only up to a small tolerance, so that the solver may fail once the magnitude of the residual vector becomes on the order of this tolerance. We may remedy this as follows. Project \( g \) onto the orthogonal complement of \( y_1, \ldots, y_s \), and do the same for \( \langle M\Omega \rangle x \) in each iteration. Effectively, we now find a solution of \( P\langle M\Omega \rangle P = Ph \), where \( P \) (symmetric) performs the projection.

For the sake of completeness, we remark that again, we may use \( M\Omega \) instead of \( \langle M\Omega \rangle \), as the image space of \( M\Omega \) is contained in the image space of \( \Omega \).

**Stage C** The problem (5.29) can be solved using the conjugate-gradient HDGEP scheme, where in Eq. (5.26) we set

\[
D = -i\langle \Omega \rangle, \\
S = \langle M\Omega \rangle, \\
\lambda = \omega^{-1}.
\]  

(5.70)

Notice that we only need the (action of the) matrices \( \Omega \) and \( M\Omega \), which have simple forms (5.24) and (5.25). Again, we do not need to implement the restrictions \( \langle \cdot \rangle \) explicitly, provided that our initial guess is in the image space of \( \Omega \). For each positive normal mode (5.3), there are two solutions of Eq. (5.26): one with \( \lambda = \omega^{-1} \) and one with \( \lambda = -\omega^{-1} \). We obviously need to find only one of the two. If we find a negative-\( \lambda \) solution \( x \), we must take the complex conjugate of \( x \) to obtain the positive-\( \lambda \) solution. Notice that the eigenvalue \( \lambda \) that the HDGEP algorithm finds is the reciprocal of the angular frequency \( \omega \). The HDGEP algorithm normalizes the solutions \( x \) so that \( x^\dagger S x_j = x_i^\dagger \langle M\Omega \rangle x_j = \delta_{ij} \). To obtain the correct normalization (5.30a), we must divide each (positive-\( \lambda \)) solution \( x_i \) by \( \sqrt{\lambda_i/2} \); we have

\[
w_{1i} + iw_{2i} = \sqrt{2/\lambda_i} x_i,
\]  

(5.71)

where \( w_{1i} \) and \( w_{2i} \) are the real vectors defined in Eq. (5.9).

The eigenvalues \( \lambda \) at the extremes of the spectrum are \( \lambda = -\omega_0^{-1} \) and \( \lambda = \omega_0^{-1} \), where \( \omega_0 \) is the angular frequency of the lowest-frequency positive normal mode. HDGEP algorithms such as the conjugate-gradient scheme find the solutions of Eq. (5.26) with either the lowest or the highest eigenvalues \( \lambda \). We see that it does not matter if we let the algorithm minimize \( \lambda \) (as we do above) or maximize \( \lambda \); in either case, we obtain the lowest-frequency normal modes first. If we minimize the eigenvalue \( \lambda \), we find the negative-\( \lambda \) solutions and we must apply to the trial solution \( x \) a constraint \((w_{1k} - iw_{2k})^\dagger (-i\langle \Omega \rangle) x = 0 \) for each previously obtained positive normal mode \( k \) [see Eq. (5.66)]. If we choose to maximize the eigenvalue \( \lambda \), we must apply a constraint \((w_{1k} + iw_{2k})^\dagger (-i\langle \Omega \rangle) x = 0 \) for each previously obtained positive normal mode \( k \). If any zero normal modes were found in stage B, we need to eliminate those from the problem to ensure that \( S = \langle M\Omega \rangle \) is positive definite on the space of trial solutions. The constraints (5.31a) and (5.31b)
that accomplish this are of exactly the same form as the constraints for previously obtained positive normal modes.

The simple conjugate-gradient HDGEP scheme outlined above may be improved in several ways. It is well known that matrix-free eigenvalue methods require good preconditioning to be efficient [96, 97, 109, 110]. Indeed, we find that preconditioning as described below greatly improves performance, especially if the exchange constant between adjacent sites is large as compared to the anisotropy constant. This is the case in most atomistic simulations and in continuum systems discretized with a reasonably high spatial resolution. (Only for relatively modest systems, say \( n \sim 1000 \), preconditioning is unnecessary; methods that use explicit matrix decompositions [95] are likely to be more efficient.)

How a preconditioner can be incorporated into the conjugate-gradient HDGEP scheme is described in many texts [96, 97, 109, 110]. In addition, efficiency may be improved by using a simultaneous conjugate-gradient scheme [96, 109], especially if some of the eigenvalues are closely spaced.

We use a preconditioner that is based on an inversion of the spin-wave dispersion relation (5.77) in reciprocal space, similar to the preconditioners used to solve the Schrödinger equation in electronic-structure calculations [109]. In other words, the preconditioner approximates the spectrum of the system with the spin-wave spectrum of a homogeneous system and uses this to speed up convergence of the trial solution. Note that since a typical spin-wave dispersion relation has no zeros (see Fig. 5.4), the preconditioner acts in real space as a convolution with some kernel that decays exponentially, with a characteristic decay distance on the order of the domain-wall width. Thus, we could in principle even implement the preconditioner in \( O(N) \) rather than \( O(N \log N) \) time. If the explicit restrictions \( \langle \cdot \rangle \) of \( M \Omega \) and \( \Omega \) are not used, it is of course important to ensure that the preconditioned reciprocal vector is projected back onto the image space of \( \Omega \) in order to ensure that the trial solution \( x \) does not move out of the image space of \( \Omega \). Preconditioning can also greatly speed up convergence for steps 1 and 4 of stage B.

Stage D In principle, the full set of unperturbed magnetic normal modes needs to be available to calculate the correction due to damping for any given mode. This could be a problem, since we usually know only the normal modes near the bottom of the spectrum. This forces us to truncate the sums in Eqs. (5.41a), (5.41b) and (5.44). We verify in Sec. 5.8.6 that this approximation is justified. In practice, the high-wavenumber spin-wave modes are increasingly oscillatory and have an overlap with the lower, smoother modes that decreases exponentially in wavenumber.

Notice that the damped modes do not, in general, satisfy the relations (5.10a) and (5.10b). To carry out a mode analysis of some configuration near \( m_0 \), first obtain the amplitudes \( p_k, q_k \) of the unperturbed modes using Eq. (5.11) and then use Eqs. (5.41a), (5.41b) and (5.44) to convert these into the amplitudes of the damped modes.
In this section, we study some key examples that are illustrative of the general properties of magnetic normal modes and make evident the fundamental distinction between inertial and special zero normal modes. We also discuss how to calculate effective masses for the inertial zero normal modes. Figure 5.2 provides an overview of the spectra of all systems we consider here.

We begin by studying the one-dimensional (1D) spin chain, possibly with a defect, in Sec. 5.8.1. We specifically look at the effect of damping, and we demonstrate how the expressions in Secs. 5.5 and 5.6 can be used to calculate dynamical magnetic susceptibilities. In Sec. 5.8.2, we discuss how the fundamentally different types of dynamics of magnetic structures can be related to the two types of zero modes (special and inertial). In particular, we show how to calculate effective masses. We focus on the properties of zero modes in spin systems with a 1D or 2D domain wall or a skyrmion (Secs. 5.8.3–5.8.5), and we investigate a general relation between zero modes and the dispersion relations of extended systems.
Section 5.8.4 evaluates the accuracy of our perturbative treatment of damping.

The 2D systems are of a size (40,000 spins) for which we begin to appreciate the scalability of the iterative HDGEP methods (see Sec. 5.7). With our code, we are able to find the 20 or 30 lowest modes of these systems in a matter of minutes on just a single CPU core. (We remark that the calculation time could be reduced further by parallelization. Matrix-free iterative methods such as the conjugate-gradient HDGEP scheme, especially the simultaneous versions, are known for being highly parallelizable [96, 97].) While for the sake of simplicity the examples only take short-range interactions into account, they could be extended to include magnetostatic (dipolar) and other interactions. This may be done in an efficient manner without any fundamental change to the method (see Sec. 5.7). Inclusion of magnetostatic interactions in rectangular systems of a similar size would not lead to much longer calculation times, since for the purpose of preconditioning our present code already performs a full FFT of the trial solution in each iteration.

In addition to normal-mode analysis using the method described in Sec. 5.4, we perform some explicit spin-dynamics simulations for comparison. The simulations referred to in this section are carried out by numerically integrating the LLG equation (5.32) using a self-written C++ code based on the implicit midpoint timestepping scheme [57, 58] (without the stochastic term). We always check convergence of our results in the size of the timestep $\Delta t$.

### 5.8.1 Spin waves in 1D spin chains

We first consider a finite, $n$-atom spin chain without defects. We set $\|m_i\| = m_S$ for all spins. The Hamiltonian $\mathcal{H} = E_{\text{ex}} + E_{\text{ani}}$ consists of nearest-neighbor exchange coupling

$$E_{\text{ex}} = \sum_{i=1}^{n-1} -2Jm_i \cdot m_{i+1}$$

(5.72)

with an exchange constant $J > 0$ (ferromagnetic) and uniaxial anisotropy

$$E_{\text{ani}} = \sum_{i=1}^{n} -K(m_i \cdot \hat{z})^2$$

(5.73)

with $K > 0$ (easy-axis type). We number the spins as $i = 1, \ldots, n$. There is no external magnetic field. We linearize around the uniform, collinear equilibrium configuration $m_{0i} = m_S \hat{z}$, shown in Fig. 5.3, which is one of the two ground-state configurations ($m_{0i} = -m_S \hat{z}$ is the other). Our truncation of the exchange couplings (5.72) at the ends of the chain results in Neumann boundary conditions for the spin waves.

The magnetic normal modes of a 1D spin chain are well known, but we reproduce them here for comparison [see Figs. 5.2(a), 5.3(a), 5.4, and 5.5(a)]. By taking
a general linear combination of the fundamental solutions \((5.4)\), we see that the dynamics of any positive normal mode \((5.3)\) is given by

\[ x_i(t) = A \cos(\omega t + \phi) u_{1i} + A \sin(\omega t + \phi) u_{2i} + O(A^2), \quad (5.74) \]

where \(A\) is the amplitude and \(\phi\) is the phase of the mode. The variable \(x_i = m_i - m_{0i}\) is the deviation of the magnetic moment at site \(i\) from its equilibrium position. For the 1D collinear spin chain with Neumann-type boundary conditions, we have spin-wave modes \((5.74)\) with

\[ u_{1i} = f(i) \hat{x} \quad \text{and} \quad u_{2i} = f(i) \hat{y}, \quad (5.75) \]

where

\[ f(i) = \cos \left[ a k_l \left( i - \frac{1}{2} \right) \right] \quad (5.76) \]

(standing waves). The dispersion relation is given by

\[ \omega(k) = 2\tilde{\gamma} m_S [K + 2J(1 - \cos ak)], \quad (5.77) \]

where \(k\) is the wavenumber and \(a\) is the spacing between lattice sites. The bottom of the spin wave continuum is thus at \(\omega = 2\tilde{\gamma} m_S K\). The wavenumber of the mode with index \(l = 1, \ldots, n\) is given by \(k_l = \pi(l - 1)/an\). Our code finds the
Figure 5.4: Dispersion $\omega(k)$ of the perfect 1D spin chain. The wavenumber $k$ is given in units of $a^{-1}$. The angular frequency $\omega$ is given in units of $\gamma m g$. The solid line is the analytical dispersion relation (5.77) and the dots show the spectrum of a 50-spin chain. The Hamiltonian consists of exchange (5.72) and uniaxial anisotropy (5.73) with $K = 0.45J$. The area in the rectangle is expanded in Fig. 5.2(a). The colored dots correspond to Fig. 5.5(a).

Figure 5.5: Amplitude profiles $f(i)$ (5.75) for some low-energy normal modes of a 1D 50-spin chain, (a) without and (b) with a defect. The spin chain with defect is different from the perfect spin chain only at a single site $i = 26$, where $K = 0.09J$ instead of 0.45J. Notice that the defect gives rise to a localized mode [see also Figs. 5.2(b) and 5.3(b)].
right frequencies $\omega(k_i)$ (see Fig. 5.4) and the right form of the spin waves [see Fig. 5.5(a)].

We now consider the effect of a defect, modeled by reducing the anisotropy constant $K$ at a single site. The normal modes are still of the form (5.75), but have different profiles $f(i)$ [see Fig. 5.5(b)]. The lowest mode is localized at the defect site and decays exponentially away from it [evanescent spin wave; see also Fig. 5.3(b)]; its frequency is just below the spin wave continuum [see Fig. 5.2(b)]. The other $n - 1$ modes are spin-wave modes. They are perturbed with respect to the normal modes of the perfect spin chain. Since in the example of Fig. 5.5(b) we place the defect almost in the middle ($i = 26$) of a chain of $n = 50$ spins, the odd-numbered spin-wave modes have a “kink” at the defect site while the even-numbered spin-wave modes are almost identical to those of the perfect spin chain.

In Fig. 5.6, we plot the absolute value of the dynamical susceptibility $\chi(\omega)$ of the 50-spin system with defect for several values of the damping parameter $\eta$. Here we consider the response of the magnetization in the $\hat{x}$-direction (perpendicular to the equilibrium magnetization, which is in the $\hat{z}$-direction) to an oscillating external magnetic field, also in the $\hat{x}$-direction. We have obtained $\chi(\omega)$ numerically from spin-dynamics simulations, where we integrate the LLG equation (5.48) with some small time-dependent driving force. We compare these numerical results to the analytical expression (5.61) based on the calculated normal modes, taking damping into account to first order. We find an excellent agreement. Higher-order corrections to the eigenfrequencies $\omega'_k$ under damping probably explain why the actual dynamical susceptibility function for $\eta = 0.050 \tilde{\gamma}^{-1}m_S^{-1}$ is very slightly shifted to the left (see also Sec. 5.5). Each peak in the dynamical susceptibility function corresponds to some mode $l$, and its width is proportional to the decay rate $\xi'_l$ (5.35), which we can estimate using Eq. (5.40). We highlight in Fig. 5.6 the peaks of the most relevant modes of our example system.

5.8.2 Inertial versus noninertial behavior of topological defects

The fundamental distinction between inertial and special zero normal modes described in Sec. 5.2 is further clarified by examining the effect of a magnetic field on the dynamics of a topological defect. The general considerations we present here are applied to specific systems in Secs. 5.8.3–5.8.5.

Zero modes typically appear as a consequence of a broken continuous symmetry of the system. For example, the energy of a system with a domain wall (see Secs. 5.8.3 and 5.8.4) or a skyrmion (see Sec. 5.8.5) in a homogeneous material is invariant under translation of the topological defect. Since no microscopic energy scale is associated with changes of the system that respect the symmetry, weak external perturbations of the Hamiltonian that couple to such changes can have a significant effect over time. By studying the response of the system to
Figure 5.6: Absolute value of the magnetic susceptibility function $\chi(\omega)$ (driving field perpendicular to equilibrium magnetization) of the 1D 50-spin chain with a defect ($K = 0.09J$ at site $i = 26$; $K = 0.45J$ everywhere else), for three different values of the damping parameter $\eta$. The driving frequency $\omega$ is given in units of $\tilde{\gamma} m_s$, $\chi$ in $J^{-1}$ and $\eta$ in $(\tilde{\gamma} m_s)^{-1}$. We compare the overall magnetic susceptibility function as obtained in “brute-force” spin-dynamics simulations to the analytical expression (5.61), which uses the calculated normal modes. We find excellent agreement. In the first plot, we also show the absolute value of the contribution of each individual mode. For our particular example, only the modes 1, 3 and 5 contribute significantly to the dynamical susceptibility. Other modes generate a magnetization that is negligible when integrated over the whole length of the chain [see, for example, mode 2 in Fig. 5.5(b)].
such external forces, we establish its effective (that is, low-energy or long-time) dynamics. For example, an effective force on a topological defect may result from an external magnetic field or from dipolar interactions within the system.

Our method establishes a direct link between the normal modes and the most relevant collective coordinates of a topological defect. Even in those systems which are only approximately translationally invariant, such as most systems in which long-range magnetostatic interactions are important, an analysis of the zero and positive normal modes in the absence of magnetostatic interactions is a useful starting point for a collective-coordinate analysis of the dynamical behavior in a weak magnetic field, which can be taken into account as an effective force acting on the defect. We shall demonstrate this approach in the examples of Secs. 5.8.3–5.8.5

We consider the dynamics of just a single degree of freedom, corresponding to a zero normal mode \((u_1, u_2)\). The deviation \(x = m - m_0\) of the system from its equilibrium configuration is given by [see Eq. (5.12)]

\[
x = p_q u_1 + q u_2 + \mathcal{O}(p_q^2 + q^2).
\] (5.78)

We write \(p_q\) instead of just \(p\) to emphasize that this variable is canonically conjugate to \(q\). Let us for concreteness assume that the vector \(u_2\) generates an infinitesimal translation of a topological defect. Thus we have, for a certain constant \(\alpha\),

\[
s = \alpha q,
\] (5.79)

where \(s\) is the position of the center of the defect, in units of length. Using Eq. (5.78), it is straightforward to obtain the coefficient \(\alpha\) from the calculated normal mode. The variable canonically conjugate to \(s\) is

\[
p_s = \alpha^{-1} p_q.
\] (5.80)

Let us first consider the case that the zero normal mode is inertial. The unperturbed Hamiltonian is then given, to second order, by [see Eq. (5.13)]

\[
\mathcal{H}^{\text{iner}} = \frac{1}{2} p_q^2 = \frac{1}{2} \alpha^2 p_s^2 = p_s^2 / (2m_{\text{eff}}),
\] (5.81)

where we have

\[
m_{\text{eff}} = \alpha^{-2},
\] (5.82)

the effective mass of the degree of freedom. Suppose that the Hamiltonian (5.81) is perturbed by an external potential \(V(s)\) which depends only on the position of the defect, so that we have \(\mathcal{H} = \mathcal{H}^{\text{iner}} + V(s)\). We get

\[
\ddot{s} = \frac{d}{dt} \frac{\partial \mathcal{H}}{\partial p_s} = \frac{1}{m_{\text{eff}}} \dot{p}_s = -\frac{1}{m_{\text{eff}}} \frac{\partial \mathcal{H}}{\partial s} = -\frac{1}{m_{\text{eff}}} \frac{dV}{ds},
\] (5.83)

which is Newton’s equation of motion.
For a special zero normal mode, the picture is different. The unperturbed Hamiltonian is then given, to second order, by [see Eq. (5.13)]

\[ \mathcal{H}^{\text{spec}} = 0, \]  

which implies, in a sense, an infinite effective mass. Since for the special zero mode no energy term is associated with \( p_s \), an effective force in the \( s \)-direction does not, by itself, cause an acceleration in the \( s \)-direction. It does generate a motion in the canonically conjugate variable; however, here the first, not second, time derivative is proportional to the force. Let us consider a case where \( p_q \) and \( q \) correspond to orthogonal displacements of a 2D magnetic defect, such as a skyrmion (see Sec. 5.8.5). We have, for certain constants \( \alpha \) and \( \beta \),

\[
\begin{align*}
    s_x &= \alpha q \\
    s_y &= \beta p_q,
\end{align*}
\]

where \( s_x \) and \( s_y \) respectively represent the \( x \)- and \( y \)-coordinate of the position of the defect. Again, we can straightforwardly obtain \( \alpha \) and \( \beta \) from the calculated normal mode using Eq. (5.78). If the Hamiltonian (5.84) is perturbed by an external potential \( V(s_x, s_y) \), we get

\[
\begin{align*}
    \dot{s}_x &= \alpha \beta \left( \partial V / \partial s_y \right) \\
    \dot{s}_y &= -\alpha \beta \left( \partial V / \partial s_x \right).
\end{align*}
\]

Notice that the velocity (not acceleration!) in the \( s_y \)-direction is proportional to the force in the positive \( s_x \)-direction, while the velocity in the \( s_x \) direction is proportional to the force in the negative \( s_y \)-direction with the same constant of proportionality. We see that we can interpret effective dynamical behavior described by Thiele’s equation of motion \(^{49, 53}\) as a direct consequence of the existence of a special zero mode.

### 5.8.3 1D domain wall

Even if the Hamiltonian as such is translationally invariant (the material properties are homogeneous), translational symmetry may be broken by the equilibrium configuration \( m_0 \), for instance if \( m_0 \) contains a domain wall. We consider a 1D spin chain with a domain wall like the one in Fig. 5.7. We ensure that the equilibrium width of the domain wall is large enough to make the system effectively continuous (Peierls pinning \(^{42, 106}\) is negligible). The 1D domain wall is the simplest case where the two types of zero modes arise. As in the previous examples, the Hamiltonian consists of exchange and anisotropy terms, which are taken the same for all spins in the system. We will consider, however, two types of anisotropy that yield one or the other type of zero mode. We shall see that the inertial dynamics of many domain walls \(^{2, 4}\) can be interpreted as a consequence of the existence of an inertial zero mode.
Figure 5.7: Spin chain with domain wall. The domain wall separates two domains, magnetized in either the positive or the negative $\hat{z}$-direction. We set $K_1 = 0.04J$, giving the domain wall a characteristic width of $\delta \propto \sqrt{J/Ka} = 5.0a$. The spin chain (200 spins, Neumann boundary conditions) may be considered as effectively continuous and effectively infinite. (Only a part of the chain is shown in the picture. We show one in every three spins of this part of the chain.) The big arrows show the equilibrium configuration $m_0$. The vectors $u_1$ and $u_2$ of the zero mode of the domain wall are indicated in (a) with red ($u_1$) and gray ($u_2$) arrows. The actual magnitudes of $u_1$ and $u_2$ depend on the type of mode (special or inertial) and the effective mass. (b) Top view of the domain wall. The position $x_{DW}$ of the domain wall and the angle $\theta_{DW}$ are indicated. (c) Spin-wave mode with $k = 0.37a^{-1}$ for $K_2 = 0.004J$. 
Figure 5.8: Time evolution of $x_{\text{DW}}$ and $\theta_{\text{DW}}$ in the presence of an external magnetic field $\mathbf{h} = 0.005m_S\hat{\mathbf{z}}$, for $K_1 = 0.04J$. Due to the external field, the domain wall experiences an effective external potential (5.89). The position $x_{\text{DW}}$ is given in units of $a$, angle $\theta_{\text{DW}}$ in radians and time $t$ in units of $\tau = (\tilde{\gamma}m_S)^{-1}$. The plots have been obtained in spin-dynamics simulations. (a) Behavior of a domain wall with a special zero mode for $K_2 = 0$. (b) Behavior of a domain wall with an inertial zero mode for $K_2 = 0.016J$. The dotted line is a quadratic fit to the behavior of $x_{\text{DW}}$, which satisfies Newton’s law (5.83) in the limit of small $\theta_{\text{DW}}$. The shaded area indicates where deviations occur (see text).

For a 1D domain wall, we find below the spin-wave continuum only a single zero mode [see Fig. 5.2(c)]. If the Hamiltonian is the form considered up to now, with exchange and uniaxial anisotropy, this mode is a special zero mode. In Fig. 5.7(a) we show the two components $u_1$ and $u_2$ of the zero mode. The component $u_2$ generates an infinitesimal increase of the position $x_{\text{DW}}$ of the domain wall whereas $u_1$ generates an infinitesimal increase of the angle $\theta_{\text{DW}}$ [see Fig. 5.7(b)]. An angle $\theta_{\text{DW}} = 0$ or $\theta_{\text{DW}} = \pi$ corresponds to a Bloch domain wall, whereas $\theta_{\text{DW}} = \pm \pi/2$ corresponds to a Néel domain wall [4]. The coordinate $x_{\text{DW}}$ is canonically conjugate [4] to

$$p_{\text{DW}} = \frac{2m_S}{a\tilde{\gamma}}\theta_{\text{DW}}.$$  

If we apply an external magnetic field in the $\hat{\mathbf{z}}$-direction, which adds to the Hamiltonian a contribution (Zeeman energy) of the form

$$E_{\text{Zeeman}} = \sum_{i=1}^{n} -h \cdot \mathbf{m}_i = \sum_{i=1}^{n} -h_z(\mathbf{m}_i \cdot \hat{\mathbf{z}}),$$  

the domain wall experiences an effective force that acts on the $x_{\text{DW}}$ coordinate. In fact, a displacement of the domain wall by one site (distance $a$) leads to one more spin aligned along the field and one fewer spin antialigned. This results in an effective external potential

$$V(x_{\text{DW}}) = -2h_zm_Sx_{\text{DW}}/a.$$
Nevertheless, the domain wall position $x_{\text{DW}}$ remains constant, as shown in Fig. 5.8(a). The conjugated $\theta_{\text{DW}}$ increases linearly (the spins near the center of the domain wall rotate around the $\hat{z}$ axis). This is in line with the general dynamical behavior predicted for systems with a special zero mode (see Sec. 5.8.2).

Motion of the domain wall in an external magnetic field along $\hat{z}$ occurs if we add to the Hamiltonian a term that breaks the symmetry under rotation of the magnetic moments around $\hat{z}$. In many magnetic systems, magnetostatic interactions favor Bloch domain walls, where the magnetization is in the plane of the domain wall. We model this effect by introducing a second term to the anisotropy energy (5.73). We use [70, 72]

$$E_{\text{ani}} = \sum_i [-K_1(m_i \cdot \hat{z})^2 + K_2(m_i \cdot \hat{x})^2]$$

(5.90)

with $K_1, K_2 > 0$. In this case, we find an inertial zero mode, with the components $u_1$ and $u_2$ again as in Fig. 5.7(a) but with a different dynamics. Even in the absence of an external field, a small deviation of $\theta_{\text{DW}}$ from its equilibrium value $\theta_{\text{DW}} = 0$ now causes a linear motion of the domain wall, $\dot{x}_{\text{DW}} = \text{constant}$. In the presence of an external magnetic field in the $\hat{z}$-direction, which creates a constant effective force $-\partial V / \partial x_{\text{DW}} = 2E_{\text{ani}}/a$ (5.86), we find that $x_{\text{DW}}$ initially increases quadratically in time [see Fig. 5.8(b)], in perfect agreement with the general dynamical behavior (5.83) predicted for inertial zero modes.

In Fig. 5.9 we show how the presence of nonuniaxial anisotropy leads to a finite effective mass, transforming a special zero mode ($K_2 = 0$) into an inertial zero mode ($K_2 > 0$). The notion of the effective mass of a domain wall was first introduced by Döring [2]. The deviations from quadratic behavior calculated at large times [shaded area in Fig. 5.8(b)] are beyond the linearized approach. In principle, the effective mass, defined as the inverse of the second derivative

Figure 5.9: Inverse Döring effective mass $m_{\text{eff}}^{-1}$ of a domain wall as a function of $K_2$, for $K_1 = 0.04 J$. We determine the effective masses from the calculated zero modes using Eq. (5.82). $K_2$ is given in units of $J$, $m_{\text{eff}}^{-1}$ in units of $a^2 \gamma^2 J$. 
Figure 5.10: Spin-wave modes in a 1D uniaxial ($K_1 = 0.04J$, $K_2 = 0$) 200-spin chain with a domain wall at the center. We compare the numerical results (thick solid lines) to the analytical form \[34\] for the continuum model (thin dashed lines). Away from the domain wall, in the shaded area, the spin-wave modes resemble those of a perfect chain and can be characterized by a wavevector $k$. In addition to the spin-wave modes, the system has a localized special zero normal mode [not shown here; see Fig. 5.7(a)].

of the Hamiltonian $H$ with respect to the momentum $p_{DW}$ conjugate to $x_{DW}$, depends on $\theta_{DW}$. Eventually, in a conservative system the domain wall starts reverting to its original position when $\theta_{DW}$ reaches $\pi/2$. This type of motion of the domain wall, which occurs when damping is absent or small as compared to the effective force, is responsible for the phenomenon called Walker breakdown \[3\].

In addition to the zero mode, we have a spin-wave continuum [see Fig. 5.2(c)]. In general, it is hard to find analytical solutions of the magnetic normal-mode problem for systems such as these, where the magnetic moments in the equilibrium configuration are not all parallel. However, in this simple case, an analytical solution for the spin-wave modes has been found \[34\], which we can use to verify the numerical results. In Fig. 5.10, we compare the calculated spin-wave modes successfully to this analytical solution. It is convenient to express the analytical solution in the coordinate system \[34\]

\[
\begin{align*}
m_{jx} &= (\cosh \zeta_j)^{-1} \cos \phi_j \\
m_{jy} &= (\cosh \zeta_j)^{-1} \sin \phi_j \\
m_{jz} &= -\tanh \zeta_j
\end{align*}
\] (5.91)

In this system the equilibrium configuration $m_0$ of the domain wall is given by the linear functions $\zeta_j = (aj - x_{DW})/\delta$ and $\phi_j = \text{constant}$, where $j$ is the index of the spin, $x_{DW}$ is the position of the center of the domain wall and $\delta = \sqrt{J/K_a}$ is the characteristic domain-wall length. We convert the Cartesian deviations from the equilibrium orientations, $x_j = m_j - m_{0j}$, into values $d\zeta_j, d\phi_j$ in the coordinate
Figure 5.11: Sketches of the lowest modes of (a) the 2D domain wall and (b) the skyrmion. The modes are shown in order of increasing frequency. In both cases, the lowest mode is a zero mode that corresponds to an infinitesimal translation of the defect. For our choice of parameters (see text), the four lowest modes of the skyrmion are 1) $m = 1$, 2) $m = 2$, 3) $m = 0$, and 4) $m = 3$ [see Fig. 5.2(e)].

system (5.91). For any given mode $l$, both functions $d\zeta_j, d\phi_j$ and both parts $u_1, u_2$ of the normal mode (5.3) all have a common shape $f_j^{(l)}$, though the amplitudes may be different. We plot $\psi_j^{(l)} = f_j^{(l)} / \cosh(\zeta_j)$. The fundamental solutions are given by $\psi_j = [-ik + \tanh(\zeta_j)]e^{ik\zeta_j}$ [34], where $k \in \mathbb{R}$ is the wavenumber of the spin wave away from the domain wall, in units of $\delta^{-1}$. In our finite system, the spin-wave spectrum is discretized. We calculate the right $k$-values for the analytical solutions from the numerically obtained values of $\omega$ via Eq. (5.77). A linear combination of the solutions for $k$ and $-k$ is taken in such a way that a real solution is obtained with a vanishing derivative at the boundaries of the chain.

5.8.4 2D domain wall and Goldstone modes

If a domain wall is extended to two dimensions, the zero mode of the 1D domain wall turns into a continuum of low-frequency modes [37, 70]. These modes correspond to bending of the domain wall, as sketched in Fig. 5.11(a); in other words, they represent small spatial variations of the position $x_{\text{DW}}$ of the domain wall. The domain-wall modes, which form a one-dimensional continuum with a vanishing frequency in the low-$k$ limit, exist alongside the two-dimensional continuum of spin-wave modes [see Fig. 5.2(d)]. A domain-wall mode can only exist if its frequency is below the bottom of the spin-wave continuum, which puts a maximum on its wavenumber. The dispersion relation of the domain-wall modes in a system with arbitrary (possibly nonuniaxial) anisotropy was derived in Ref. [71]. Here we show, using very general arguments, that the
Figure 5.12: A domain-wall mode. Only one spin is shown for each block of $5 \times 5$ spins; the system ($100 \times 400$ spins) may be considered as effectively continuous. Here we show the 16th domain-wall mode, with wavenumber $k = 15\pi/(400a)$. Notice that the motion of the spins is in phase, since the boundary conditions used result in standing waves. When the deviation of the spins at the center of the domain wall from their equilibrium orientations is vertical, the domain wall is bent in a way similar to what is shown in Fig. 5.11(a). When it is horizontal, the domain wall is not bent; at this point, the energy of the mode is stored as a spatial variation of $\theta_{\text{DW}}$ rather than of $x_{\text{DW}}$.

Qualitative features of this dispersion relation follow immediately from the type of zero mode present in the system.

The domain-wall modes are a good example of physically interesting low-energy excitations of large systems, which can be found very efficiently using our method. The domain-wall mode in Fig. 5.12 was calculated in a system of $100 \times 400$ spins (square lattice) with exchange and uniaxial anisotropy ($K = 0.04J$). As in Sec. 5.8.1 our truncation of the expression for the exchange energy results in Neumann boundary conditions. We find that the lowest 26 modes (including the zero mode) of this system are domain-wall modes [see Fig. 5.2(d)].

The distinction between special and inertial zero modes has important consequences for the dispersion relations of the Goldstone modes that correspond to them, as we show in the following. For the case with uniaxial anisotropy, shown in Fig. 5.2(d), we see that the zero mode of the domain wall, which is a special zero mode, turns into a continuum with quadratic dispersion. In Fig. 5.13 we compare this case to a similar system with nonuniaxial anisotropy. For $K_2 > 0$, where the domain wall has an inertial zero mode, the dispersion relation $\omega(k)$ is linear in $k$ in the limit of low wavenumber $k$. This suggests that long-wavelength
waves in a system with an inertial zero mode propagate with a finite group velocity. Indeed, a finite group velocity is also observed for acoustic waves in crystals, which agrees with the fact that zero modes of systems of coupled point masses are always inertial (see Sec. 5.8.3).

It is easy to understand the link between the type of zero mode and the low-$k$ behavior of the dispersion relation. Suppose we have a system with a zero mode, such as the 1D spin chain with a domain wall. We describe the relevant dynamics of this system with just two variables, the canonical momentum $p$ and coordinate $q$ corresponding to the zero mode. In the case of the domain wall, $p$ and $q$ are proportional to $x_{\text{DW}}$ and $\theta_{\text{DW}}$ respectively (see Sec. 5.8.3). We now extend the system to a higher dimension. The variables $p$ and $q$ become functions of position: we have $p(r)$ and $q(r)$. (In the case of the 2D domain wall, $r \in \mathbb{R}^1$ represents a position along the length of the domain wall.) It is reasonable to assume that for functions $p(r)$ and $q(r)$ that vary very smoothly in $r$ and for short-range interactions, the Hamiltonian of the system can be approximated by the functional

$$H = \int \left[ f(p,q) + \frac{1}{2} \rho \| \nabla p \|^2 + \frac{1}{2} \sigma \| \nabla q \|^2 \right] dr$$

for certain constants $\rho, \sigma > 0$. In the limit of small $p$ and $q$ we have that $f(p,q) = 0$ for a special zero mode, $f(p,q) = \frac{1}{2} p^2$ for an inertial zero mode and $f(p,q) = $
\( \frac{1}{2} \omega (p^2 + q^2) \) for a positive mode [see Eq. (5.13)]. After Fourier transformation in \( r \), spatial variations with different wavevectors \( k \) decouple and we get

\[
H^\text{spec}_k = \frac{1}{2} \rho k^2 p_k^2 + \frac{1}{2} \sigma k^2 q_k^2
\]

(5.93)

for the system with a special zero mode and

\[
H^\text{iner}_k = \frac{1}{2} p_k^2 + \frac{1}{2} \rho k^2 p_k^2 + \frac{1}{2} \sigma k^2 q_k^2
\]

(5.94)

for the system with an inertial zero mode, where we define \( k = \| k \| \). It follows immediately from Hamilton’s equations that for \( H^\text{spec}_k \), we get

\[
\begin{align*}
\dot{p}_k &= -\frac{\partial H}{\partial q_k} = -\sigma k^2 q_k \\
\dot{q}_k &= \frac{\partial H}{\partial p_k} = \rho k^2 p_k
\end{align*}
\]

(5.95)

while for \( H^\text{iner}_k \), we get

\[
\begin{align*}
\dot{p}_k &= -\sigma k^2 q_k \\
\dot{q}_k &= p_k + \rho k^2 p_k
\end{align*}
\]

(5.96)

The momenta \( p_k \) can be eliminated from both systems of equations, yielding equations of motion of the form

\[
\ddot{q}_k = -\omega (k)^2 q_k.
\]

(5.97)

For the special zero mode we get a quadratic dispersion relation

\[
\omega (k) = \sqrt{\rho \sigma \| k \|^2},
\]

(5.98)

whereas for the inertial zero mode we get a linear dispersion relation

\[
\omega (k) = \left[ (1 + \rho \| k \|^2) \sigma \right]^{1/2} \| k \| = \sqrt{\sigma} \| k \| + O(\| k \|^2).
\]

(5.99)

As discussed in Sec. 5.2, a special zero mode naturally arises from a pair of broken continuous symmetries. The above derivation explains why a special zero mode corresponds to a Goldstone mode with a quadratic dispersion relation. The situation is reminiscent of the out-of-plane lattice vibrations (flexural modes) of 2D crystals such as graphene embedded in 3D space \([111, 112]\), which we briefly discuss here. Their quadratic dispersion has been related to a pair of broken continuous symmetries, namely translation and rotation of the graphene sheet in 3D space \([113]\). (The latter freedom does not exist for 3D crystals embedded in 3D space, whence the linear dispersion relation for traditional acoustic lattice vibrations.) We can model the transversal phonons in 2D crystals using the Hamiltonian

\[
H = \int \left[ \frac{1}{2m} p^2_h + \frac{1}{2} \kappa \left( \frac{\partial^2 h}{\partial x^2} \right)^2 \right] dx,
\]

(5.100)
where $m$ and $\kappa$ are constants, $x$ represents the position along the length of the sheet (for simplicity, we consider variations in one spatial direction only), $h(x)$ displacement in the direction perpendicular to the sheet, and $p_h(x)$ linear momentum in the $h$-direction. Paradoxically, a direct application of our method would indicate that this Hamiltonian, like all systems of coupled point masses (see Sec. 5.1A), has an inertial zero mode, which would suggest a linear dispersion relation. The reason that this is not the case is of course that the energetical penalty on spatial variations is proportional to $(\partial^2 h/\partial x^2)^2$ rather than $(\partial h/\partial x)^2$.

However, if we write this system in terms of the new variables

$$p_q(x) = \int -\frac{1}{2} \text{sign}(x - x') p_h(x') \, dx', \quad \text{(5.101)}$$

$$q(x) = \frac{\partial h}{\partial x'} |_{x' = x},$$

which can again be shown to be canonically conjugate, the Hamiltonian takes the form

$$\mathcal{H} = \int \left[ \frac{1}{2m} \left( \frac{\partial p_q}{\partial x} \right)^2 + \frac{1}{2} \kappa \left( \frac{\partial q}{\partial x} \right)^2 \right] \, dx. \quad \text{(5.102)}$$

Since now the Hamiltonian depends only on the spatial derivatives of $p_q$ and $q$ and not on $p_q$ or $q$ itself, we are back in the situation (5.93) with a special zero mode.

### 5.8.5 Skyrmion

Magnetic bubbles and skyrmions can be seen as circular domain walls (see Fig. 5.14). The dynamics of a skyrmion in an effective potential can be understood very well in terms of its normal modes (gyrotropic modes) [49, 98, 114–116]. We shall see that our algorithm for normal-mode analysis provides a direct way to calculate the effective mass $M$ and gyrocoupling constant $G$ of any skyrmion-like structure, regardless of the details of the interactions present in the system. This is another example of how a normal-mode analysis that includes the zero modes gives the effective equation of motion of some magnetic structure almost immediately.

Skyrmion structures can be stabilized by magnetostatic interactions [67] or by the Dzyaloshinskii–Moriya interaction (DMI) [117]. In the latter case, which we shall consider here, the equilibrium radius is fixed by the material parameters. In the example shown in Fig. 5.14, we consider a system of $200 \times 200$ spins (square lattice) with only the exchange interaction, uniaxial anisotropy ($K = 0.04$J) and the DMI (no external field). We write the DMI as [79]

$$E_{DM} = \sum_x -D m_x \cdot \left( \sum_{\hat{r}} \hat{r} \times m_{x + a\hat{r}} \right), \quad \text{(5.103)}$$

where $m_x$ is the magnetic moment at the lattice site $x$, $\hat{r}$ sums over the directions of the nearest neighbors in the square lattice ($\hat{r} = \hat{x}, \hat{y}, -\hat{x}, -\hat{y}$), $a$ is the lattice
Figure 5.14: A skyrmion shown with (a) the $m = 1$ special zero mode and (b) the $m = -1$ positive mode. Only one spin is shown for each block of $5 \times 5$ spins; the system may be considered as effectively continuous. For our choice of parameters (see text), the $m = -1$ mode is the 7th-lowest mode of the spectrum ($\omega = 0.0293 \tilde{\gamma} m_5$).
constant and $D$ is the interaction strength. Here, we set $D = 0.125 J$. We use periodic boundary conditions. We construct a skyrmion configuration and relax it. For the given parameters, we get an equilibrium radius of $\sim 27 \, a$. We find 10 normal modes below the spin-wave continuum (edge modes $[49]$), as shown in Fig. 5.2(e). We may interpret these modes as domain-wall modes traveling around the skyrmion [see Fig. 5.14(b)]. The edge modes can be identified by the number of periods $m$ seen when going around the skyrmion once. We use a positive or negative value of $m$ to indicate the direction in which the wave travels around the skyrmion $[49]$. As pointed out in Ref. $[49]$, the edge-mode spectrum is chiral: it is not symmetric for positive and negative $m$ [see Fig. 5.2(e)].

The system has translational symmetry in two spatial directions. This symmetry gives rise to a special zero mode ($m = 1$). The vector $u_1$ of this mode generates an infinitesimal translation in the $\hat{y}$-direction and the vector $u_2$ generates an infinitesimal translation in the $\hat{x}$-direction [see Fig. 5.14(a)]. The existence of this special zero mode suggests that the dynamical behavior of the position of the skyrmion in an external potential is described by the noninertial equation of motion (5.86), which is equivalent to Thiele’s equation $[53]$ without damping. It has recently been observed that the actual behavior of the skyrmion position is more accurately described by an equation which has an additional inertial term $[48, 49]$, a result which seems to contradict our statement that the skyrmion possesses a special zero mode and has noninertial character. It is therefore important to make a detailed comparison with the interesting findings of Ref. $[49]$, as we do in the following. An analysis of the normal modes indicates that the inertial term results in this case from the positive mode $m = -1$ $[49]$. Despite its finite frequency, this mode gives rise to a displacement of the skyrmion similar to that of the $m = 1$ zero mode, albeit with a concomitant change of the skyrmion configuration [see Fig. 5.14(b)]. A derivation of the equation of motion of the skyrmion was given in the Lagrangian formalism in Ref. $[49]$. Here we reproduce this result in the Hamiltonian formalism and show how the parameters $G$ and $M$ of the equation of motion can be obtained immediately from the normal-mode calculation.

The crucial observation, which also underlies the derivation in Ref. $[49]$, is that if we define the position of the skyrmion as

$$
X = \frac{\int (m_z(\mathbf{r}) - m_S) x \, d\mathbf{r}}{\int (m_z(\mathbf{r}) - m_S) \, d\mathbf{r}}, \quad Y = \frac{\int (m_z(\mathbf{r}) - m_S) y \, d\mathbf{r}}{\int (m_z(\mathbf{r}) - m_S) \, d\mathbf{r}},
$$

as was done in Ref. $[48]$, then not only the $m = 1$ zero mode [see Fig. 5.14(a)] but also the $m = -1$ mode [see Fig. 5.14(b)], which is a positive mode, generates a change in position. In fact, we find from our normal-mode calculation that

$$
\begin{align*}
X - X_0 &= \alpha p_+ + \alpha q_-, \\
Y - Y_0 &= \alpha p_- + \alpha q_+,
\end{align*}
$$

where $p_+, q_+$ are the canonical momentum and coordinate corresponding to the special zero mode $m = 1$, $p_-, q_-$ correspond to the positive mode $m = -1$,
(X₀, Y₀) is the position of the skyrmion in the equilibrium configuration and α is a constant that can be obtained easily from the calculated normal modes. In our calculation, we find α = 0.282 aγ₁/₂ m⁻¹/₂. Since the system is rotationally invariant, the normal modes output by the computer code may be oriented in any direction but we can always rotate them to satisfy Eq. (5.105). Since we consider only the modes m = ±1 that couple to position, the unperturbed Hamiltonian is given, to second order, by [see Eq. (5.13)]

\[ H = \frac{1}{2} \omega (p_+^2 + q_-^2), \]  \tag{5.106}

where \( \omega \) is the angular frequency of the positive mode \( m = -1 \) (in our example, \( \omega = 0.0293 a \gamma_1/2 m J \)). There is no energy term associated with the special zero mode \( m = 1 \). If we introduce an external potential that depends only on the position \( (X, Y) \), Eq. (5.106) becomes

\[ H = \frac{1}{2} \omega (p_+^2 + q_-^2) + V(X, Y). \]  \tag{5.107}

Using Hamilton’s equations, Eq. (5.107) gives

\[
\begin{align*}
\dot{p}_+ &= -\partial H / \partial q_+ = -\alpha \partial V / \partial Y \\
\dot{q}_+ &= \partial H / \partial p_+ = \alpha \partial V / \partial X \\
\dot{p}_- &= -\partial H / \partial q_- = -\omega q_- - \alpha \partial V / \partial X \\
\dot{q}_- &= \partial H / \partial p_- = \omega p_- + \alpha \partial V / \partial Y
\end{align*}
\] \tag{5.108}

from which it follows that

\[
\begin{align*}
\dot{X} &= \alpha \dot{p}_+ + \alpha \dot{q}_- = \alpha \omega q_- \\
\dot{Y} &= \alpha \dot{p}_- + \alpha \dot{q}_+ = -\alpha \omega q_-.
\end{align*}
\]  \tag{5.109}

Again taking the time derivative and applying Hamilton’s equations, this becomes

\[
\begin{align*}
\dot{\dot{X}} &= \omega \dot{Y} - \alpha^2 \omega \partial V / \partial X \\
\dot{\dot{Y}} &= -\omega \dot{X} - \alpha^2 \omega \partial V / \partial Y
\end{align*}
\] \tag{5.110}

These equations of motion are equivalent to Eq. 3 in Ref. [49] if we set

\[
\begin{align*}
\mathcal{M} &= 1 / (\alpha^2 \omega), \\
\mathcal{G} &= -1 / \alpha^2.
\end{align*}
\] \tag{5.111, 5.112}

The equations of motion \( (5.110) \) consist of a “gyrocoupling” term, which is also present in Thiele’s equation, and an additional inertial term, which gives a contribution to the acceleration proportional to the force. For the parameters used in our example, we find \( \mathcal{M} = 4.29 \times 10^2 a^{-2} \gamma^{-2} J^{-1} \) and \( \mathcal{G} = -12.6 a^{-2} \gamma^{-1} m_s \approx -4 \pi a^{-2} \gamma^{-1} m_s \). For \( \mathcal{G} \), an analytical expression was given in Refs. [49] and [53], with which our calculated value is in excellent agreement. From Eqs. (5.111) and (5.112) we also recover \( \omega = -\mathcal{G} / \mathcal{M} \), which is indeed the frequency of the
5.8.6 Accuracy of the corrections to the modes due to damping

If we introduce damping ($\eta > 0$), this has an effect not only on the amplitudes of the modes, which now decay in time, but also on the mode vectors $u_1, u_2$ (see Sec. 5.5). Since for large systems we can usually only calculate a number of the lowest modes of the system, which are of the greatest interest, we are forced to truncate the perturbative expressions (5.41a, 5.41b) and (5.44) for these corrections to those modes that are available. In principle, this approximation is uncontrolled. However, we may argue that modes with very different frequencies also have very different characteristic wavelengths and hence have a very small overlap, so that the contribution of high-frequency modes to the damping correction of the low-frequency modes that we are interested in is likely to be negligible. Here, we test the accuracy of the damping correction by comparing the actual time evolution of a skyrmion system to the linearized solutions (5.36) obtained from normal-mode analysis. This also serves as a test of the expressions (5.40), (5.41a) and (5.41b).

We consider the time evolution of an initial configuration $m = m_0 + Au_{1k}$, where mode $k$ is given an initial amplitude $A$. The details of the simulated system are specified below. In Fig. 5.15 we plot the difference between the results of a numerical time integration of the LLG equation (5.32) and the linearized solution (5.4) or (5.36). Since the error in the numerical solution can be made very small, we may use this difference to evaluate the accuracy of the normal modes. The error stems from two sources. First, the linearization of the LLG equation necessary for normal-mode analysis results in an error of second order
Figure 5.15: Accuracy of the linearized solution of an initial-value problem for the LLG equation (see text). (a) Error as a function of the amplitude $A$ for zero damping. (b) Error as a function of the damping parameter $\eta$ for a very small, fixed initial amplitude $A = 1 \times 10^{-4} m_S^{1/2} \tilde{\gamma}^{-1/2}$. We consider three different levels of correction for damping in the linearized solution. Red circles: damping is not taken into account at all. Green diamonds: the decay rate $\xi'$ from first-order perturbation theory is taken into account, but the zerodamping modes $(u_1, u_2)$ are used. Blue squares: both the modes $(u'_1, u'_2)$ and the decay rate $\xi'$ are corrected to first order of perturbation theory. For a fair comparison between different values of $\eta$, we have scaled the errors by the decay factor between the initial and final amplitudes, as indicated by the upper horizontal curve. The lower horizontal line indicates the accuracy of the numerical timestepping solution.
in the amplitude $A$. Second, the fact that the modes of a damped system are calculated in perturbation theory gives an additional error that depends on the damping parameter $\eta$.

Figure 5.15(a) shows the error as a function of the amplitude $A$ for a conservative spin system ($\eta = 0$). We find a quadratic dependence, as expected (5.1). Figure 5.15(b) shows the error as a function of $\eta$, for an amplitude $A$ that is chosen so small that the error from nonlinearity is smaller than the error in the numerical solution. The error that we see in the plot is thus due to the error in the perturbative solution of the damped modes. We see that if we do not take damping into account at all (5.4), the error in the solution is of first order in $\eta$, as expected. If we take damping into account by using the calculated decay rate $\xi'$ (5.36), but without correcting the modes $(u_1, u_2)$, the error is much smaller, but it is still of first order in $\eta$. If we also correct the modes $(u'_1, u'_2)$, so that we use the full first-order perturbation theory, we get an error of second order in $\eta$. Notice that we get this order of accuracy even though we use only the contributions of the lowest modes to the perturbative correction. We conclude that, at least in this case, any first-order error due to this truncation is so small as to be insignificant.

The results in Fig. 5.15 are obtained in a system of $86 \times 86$ spins (square lattice) with uniaxial anisotropy ($K = 0.12J$) and the DMI (5.103) ($D = 0.20J$). We use an equilibrium configuration $m_0$ containing a single skyrmion. After relaxation, the skyrmion is similar to the one in Fig. 5.14 but has a different radius (owing to the different interaction parameters used). We construct a configuration $m = m_0 + Au_{1k}$ in which the second mode ($\omega = 3.56 \times 10^{-2} \tilde{\gamma}m_S J$, $\tilde{\zeta}^{(1)} = 1.18 \times 10^{-1} \tilde{\gamma}m_S J$) is given a finite initial amplitude $A$. The magnitudes of the magnetic moments are normalized to $m_S$. We then numerically integrate the LLG equation (5.32) starting from this initial configuration with $\Delta t = 0.1\tau$ where $\tau = (\tilde{\gamma}m_S J)^{-1}$. The simulated time is $300\tau$.

The above results suggest that it is useful to take into account damping in a calculation of the normal modes. Using the expressions in Sec. 5.5 this can be done relatively easily and at a low computational cost. It is already very useful to take into account the decay rate $\tilde{\zeta}'$ calculated to first order. An even better accuracy can be achieved by also using the first-order corrections to the modes $(u'_1, u'_2)$. We find that in practice, we get an error of second order in $\eta$ in the time evolution of a low-frequency mode even when only a relatively small set of other low-frequency modes were used to calculate the correction. The results also suggest that it is unnecessary to go beyond first-order perturbation theory for damping unless $\eta$ is unusually large.

5.9 Concluding Remarks

Using explicitly the symplectic structure of the dynamical spin system, we have developed a method that allows us to solve the magnetic normal-mode problem in a very general situation, with the only assumption that the equilibrium
magnetic structure corresponds to a local minimum of the Hamiltonian. The examples we have considered (1D and 2D domain walls, skyrmions) clearly demonstrate that zero modes are an essential part of this normal-mode analysis and can be very useful for understanding dynamics.

Systems with zero modes were difficult to treat within the framework of previous approaches for the magnetic normal-mode problem. To our knowledge, all previous approaches assume that the dynamical matrix of the spin system is diagonalizable. This is not the case when inertial zero modes are present, which may occur even for the 1D domain wall. Our approach allows one to calculate, in an efficient and scalable manner, all magnetic normal modes, including the spin-wave modes and those modes that are related, for example, to the motion of localized or extended defects (domain walls, skyrmions, ...). For the latter case, we give a clear and computationally efficient procedure to calculate the parameters that determine the motion under external forces, such as effective masses. Last but not least, we have developed an efficient perturbation scheme to take into account dissipation effects and calculate dynamical magnetic susceptibilities.

We believe that this approach can be useful in many further problems of spin dynamics, especially those dealing with the motion of skyrmions and other defects in the magnetic configuration under an external field, their collision (momentum transfer), pinning, dissipation, and so on.

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Appendix

5. THE NORMAL-MODE PROBLEM OF HAMILTONIAN SYSTEMS

In this Appendix, we investigate the general properties of linear and nonlinear Hamiltonian systems and their normal modes. An advantage of our general approach is that it explains why it is possible to reduce the magnetic normal-mode problem to the HDGEP: this is a natural consequence of the symplectic structure of the conservative spin system. Moreover, it means that the same method may be reused for other kinds of Hamiltonian systems.

The best-known example of a linear Hamiltonian system is a set of point masses coupled by harmonic springs. For this system the normal-mode problem can be reduced to the symmetric definite generalized eigenvalue problem (SDGEP) in an obvious way (see Sec. 5.A.2). However, the general normal-mode problem of linear Hamiltonian systems is much richer [55]. We consider here the normal-mode problem of a linear Hamiltonian system with a positive semidefinite Hamiltonian, as results from the linearization of a general Hamiltonian system near an energy minimum.

This Appendix is organized as follows. In Sec. 5.A.1 we reproduce the definition of a linear Hamiltonian system and consider the types of normal modes that it may have. We also explain how the Hamiltonian structure can be used to efficiently perform mode analysis on a given state vector once the normal modes of the system have been calculated. For comparison, we discuss the well-known special case of a system of coupled point masses in Sec. 5.A.2. In Sec. 5.A.3 we generalize the results to a nonlinear Hamiltonian system, possibly defined on a Poisson manifold rather than a symplectic manifold. We show that the linearization of a general Hamiltonian system near a local energy minimum results in a linear Hamiltonian system with a positive-semidefinite matrix $\langle M\Omega \rangle$ (defined in Sec. 5.2).

5.A.1 Linear Hamiltonian systems

Let us first reproduce the definition of a linear Hamiltonian system on the vector space $\mathbb{R}^{2n}$. Fix some arbitrary basis set $e_1, \ldots, e_{2n}$, and let $x^1, \ldots, x^{2n}$ represent the coefficients of a vector $x$ in this basis. Let the matrix $\Omega$ be antisymmetric ($\Omega^{ij} = -\Omega^{ji}$) and invertible. (We will relax the latter condition in Sec. 5.A.3.) Then the symplectic form

$$\omega(e_i, e_j) = (\Omega^{-1})_{ij}$$  \hspace{1cm} (5.113)

defines a symplectic structure on $\mathbb{R}^{2n}$. Since symplectic forms are bilinear, Eq. (5.113) fixes the value of the form for any pair of vectors. The symplectic structure induces a Poisson bracket

$$\{x^i, x^j\} = -\Omega^{ij}$$  \hspace{1cm} (5.114)
between the variables \( x_i, x_j \); more generally, for any two functions \( f, g \),

\[
\{ f, g \} = -\frac{\partial f}{\partial x^i} \Omega^{ij} \frac{\partial g}{\partial x^j}.
\]  

(5.115)

The condition that \( \Omega \) be invertible ensures that the symplectic form on \( \mathbb{R}^{2n} \) is nondegenerate. In the special case that the \( x^i \) with \( 1 \leq i \leq n \) represent canonical momenta and the \( x^i \) with \( n + 1 \leq i \leq 2n \) represent the corresponding canonical coordinates, \( \Omega \) takes the familiar form

\[
\Omega = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix},
\]  

(5.116)

where \( I_n \) is the identity matrix, and in particular, \( \Omega \) is orthogonal (\( \bar{\Omega} = \Omega \), where we define \( \bar{\Omega} = \Omega^{-T} \)); but we shall not make this assumption in this paper.

It is always possible in principle to construct a system of canonical momenta and coordinates of a symplectic vector space. Let us write our momenta and coordinates as linear combinations

\[
p_{(k)} = -w_{2(k)} x^i,
\]

(5.117)

\[
q_{(k)} = w_{1(k)} x^i
\]

(5.118)

of the variables \( x^i \) for certain vectors \( w_{1(k)} \) and \( w_{2(k)} \). By definition, we must have \( \{ q_{(k)}, p_{(l)} \} = \delta_{kl} \) and \( \{ p_{(k)}, p_{(l)} \} = \{ q_{(k)}, q_{(l)} \} = 0 \) for all \( k, l \). Using Eq. (5.114), this can be rewritten as

\[
w_{1(k),i} \Omega^{ij} w_{2(l),j} = \delta_{kl}
\]

(5.119a)

\[
w_{1(k),i} \Omega^{ij} w_{2(l),j} = w_{2(k),i} \Omega^{ij} w_{2(l),j} = 0
\]

(5.119b)

[see Eqs. (5.10a) and (5.10b)]. As a result, we may decompose an arbitrary state vector \( x \) as

\[
x^i = \sum_{k=1}^{n} \left[ -(w_{2(k),i} x^h) \Omega^{ij} w_{1(k),j} + (w_{1(k),i} x^h) \Omega^{ij} w_{2(k),j} \right]
\]

(5.120a)

\[
= \sum_{k=1}^{n} \left( p_{(k)} \Omega^{ij} w_{1(k),j} + q_{(k)} \Omega^{ij} w_{2(k),j} \right)
\]

(5.120b)

[see Eqs. (5.11) and (5.12)]. The vectors \( e_{p_{(k)}} = \Omega^{ij} w_{1(k),j} e_i \) and \( e_{q_{(k)}} = \Omega^{ij} w_{2(k),j} e_i \) form a symplectic basis of the symplectic vector space.

Let us return to the original system of variables \( x^1, \ldots, x^{2n} \) (not necessarily canonical) of our symplectic vector space. We define a (time-invariant) Hamiltonian function

\[
\mathcal{H} = \frac{1}{2} x^i H_{ij} x^j,
\]

(5.121)

where \( H \) is symmetric. Using the generalized form of Hamilton’s equations and the properties of Poisson brackets, we now derive the equation of motion

\[
x^i = \{ x^i, \mathcal{H} \} = -\Omega^{ij} H_{jk} x^k,
\]

(5.122)
where the dot denotes the time derivative. We may rewrite Eq. (5.122) as
\[ \dot{x}^i = M^i_j x^j, \tag{5.123} \]
with
\[ M = -\Omega H. \tag{5.124} \]

We see that for a linear Hamiltonian system, \( M\Omega = \Omega^T H\Omega \) is symmetric. Conversely, if a given matrix \( M \) is such that \( M\Omega \) is symmetric (or equivalently, if \( \Omega M + M^T \Omega = 0 \)), it is is called a Hamiltonian matrix \[118]. The dynamical system (5.123) is then a linear Hamiltonian system on the symplectic vector space defined by \( \Omega \). In Sec. 5.A.3 we generalize the result that \( M\Omega \) is symmetric to Hamiltonian systems that are nonlinear or for which \( \Omega \) is not necessarily invertible.

The matrix \( M \) describes the dynamical behavior (5.123) of the linear Hamiltonian system. This matrix is not necessarily diagonalizable \[55\]; its Jordan normal form may contain Jordan blocks of high order. Moreover, the eigenvalues of these blocks, which often but not always appear in pairs or quadruples, may be zero, real, imaginary or complex. Linear Hamiltonian systems may thus display a wide variety of inequivalent types of motion. An exhaustive list of possibilities is given in Ref. \[55\]. In this paper, we restrict ourselves to systems where \( M\Omega \) is positive semidefinite. Even though this condition considerably limits the forms the normal modes may take, we shall see that three inequivalent types still need to be distinguished.

It can be shown that any linear Hamiltonian system admits a special symplectic basis in which the Hamiltonian takes its normal form \[55 \, 119\]. In terms of the momenta \( p_{(k)} \) and coordinates \( q_{(k)} \) that correspond to this special symplectic basis, the Hamiltonian is a direct sum of simple terms, each of which belongs to one of the families listed in Ref. \[55\]. Note that many of those types of irreducible terms depend on not just one but two or more pairs of canonical momenta and coordinates. Here we consider Hamiltonians that are positive semidefinite, for which the possibilities are more limited. Indeed, we have verified that for all but three types, the irreducible term cannot be positive semidefinite by finding a counterexample where the term takes a negative value. The only three exceptions, which are positive semidefinite, are
\[ H^\text{pos}_k(p_{(k)}, q_{(k)}) = \frac{1}{2} \omega_k (p^2_{(k)} + q^2_{(k)}) \tag{5.125a} \]
\[ H^\text{spec}_k(p_{(k)}, q_{(k)}) = 0 \tag{5.125b} \]
\[ H^\text{iner}_k(p_{(k)}, q_{(k)}) = \frac{1}{2} p^2_{(k)}, \tag{5.125c} \]
where in Eq. (5.125a), \( \omega_k > 0; \) a term of this type is in fact positive definite. We introduce the names positive, special zero and inertial zero respectively for the three types of terms that may appear in the normal form of a positive-semidefinite Hamiltonian.
By Hamilton’s equations, \( \dot{p}(k) = -\partial H / \partial q(k) \) and \( \dot{q}(k) = \partial H / \partial p(k) \), the three types of terms correspond to the following types of motion:

positive: \[
\begin{align*}
\dot{p}(k) &= -\omega_k q(k) \\
\dot{q}(k) &= \omega_k p(k)
\end{align*}
\]

special zero: \[
\begin{align*}
\dot{p}(k) &= 0 \\
\dot{q}(k) &= 0
\end{align*}
\]

inertial zero: \[
\begin{align*}
\dot{p}(k) &= 0 \\
\dot{q}(k) &= p(k)
\end{align*}
\]

It follows immediately from Eqs. (5.120b) and (5.123) that Eq. (5.126a) corresponds to a positive normal mode (5.3) with \( \omega = \omega_k \), that Eq. (5.126b) corresponds to a special zero normal mode (5.5) and that Eq. (5.126c) corresponds to an inertial zero normal mode (5.7), as defined in Sec. 5.2 if we set \( (\tilde{u}_1', \tilde{u}_2') = (\Omega^{ij} w_{1(k)j}, \Omega^{ij} w_{2(k)j}) \). An important practical consequence of the fact that the normal modes of a Hamiltonian system form a symplectic basis is that we have a direct expression (5.120a) for the decomposition of an arbitrary state vector into a linear combination of the normal modes.

While the special zero normal mode (5.5) can be interpreted as the \( \omega \rightarrow 0 \) limit of the positive normal mode (5.3), the inertial zero normal mode (5.7) is fundamentally different. One might interpret it as the \( \omega \rightarrow 0 \) limit of

\[
\begin{align*}
M\tilde{u}_1 = & \tilde{u}_2 \\
M\tilde{u}_2 = & -\omega^2 \tilde{u}_1,
\end{align*}
\]

which for \( \omega > 0 \) is equivalent to Eq. (5.3) if one sets \( \tilde{u}_1 = u_1 / \sqrt{\omega} \) and \( \tilde{u}_2 = \sqrt{\omega} u_2 \).

Notice that even if the original dynamical variables \( x^i \) represent canonical momenta and coordinates (which is not necessary), the special canonical momenta \( p(k) \) and canonical coordinates \( q(k) \) of the normal form are still, in principle, linear combinations of all of the \( x^i \). There is thus no guarantee that \( p(k) \) is a linear combination of the original momenta, or that \( q(k) \) is a linear combination of the original coordinates, unless the system is of the special form discussed in Sec. 5.A.2.

5.A.2 Harmonically coupled point masses

The variety in the types of dynamics that linear Hamiltonian systems display (see Sec. 5.A.1 and Ref. [55]) may seem surprising. Such variety is not seen in the archetypal example of a linear Hamiltonian system, a collection of point masses coupled by harmonic springs, for which it is obvious how the normal-mode problem can be cast in the form of a SDGEP. We shall see that this type of system is considerably simplified by the special structure of its Hamiltonian, which is not present in all linear Hamiltonian systems. We discuss the system of
coupled oscillators here to show how it is special and to explain why the most common method for solving the normal-mode problem cannot be used in the more general case discussed in Sec. 5.2 and Sec. 5.A.1.

The Hamiltonian of a system of harmonically coupled point masses is given by \( H = \sum_{i,j} \frac{1}{2} p_i (S^{-1})_{ij} p_j + \sum_i \frac{1}{2} q_i D_{ii} q_i \), where \( D \) is the force-constant matrix and \( S \) is the mass matrix. The matrix \( S \) is positive definite; both matrices are symmetric. In the simplest case, we have \( S = m I_n \), where \( m \) is the mass of a single particle. The variables \( p_i \) and \( q_i \) represent the momentum and the displacement of particle \( i = 1, \ldots, n \). (In multidimensional systems, we let \( i \) represent the spatial direction as well as the particle index; this does not affect the mathematical structure.) If we write the state of the system as a single vector

\[
x = \begin{bmatrix} p \\ q \end{bmatrix} \in \mathbb{R}^{2n},
\]

(5.128)

the matrix \( \Omega \) takes its standard form (5.116), since the variables \( p_i \) and \( q_i \) form a canonical system. The Hamiltonian takes the form (5.121) if we set

\[
H = \begin{bmatrix} S^{-1} & 0 \\ 0 & D \end{bmatrix}.
\]

(5.129)

Notice that \( H \) is block diagonal: the Hamiltonian does not contain any terms that couple coordinates to momenta. The equation of motion is given by

\[
\begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = M \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} 0 & -D \\ S^{-1} & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix},
\]

(5.130)

where we have used Eq. (5.124). The structure of Eq. (5.130) is such that we can derive equations of motion for the momenta and for the coordinates separately. For the coordinates, we have

\[
\ddot{q} = S^{-1} \dot{p} = -S^{-1} D q.
\]

(5.131)

The fundamental solutions of this equation may be found by calculating the eigenvectors \( q^* \), which satisfy \( S^{-1} D q^* = \lambda q^* \). This equation is equivalent to the SDGEP

\[
D q^* = \lambda S q^*.
\]

(5.132)

If we assume that the Hamiltonian is positive semidefinite, so that the the classification of Sec. 5.A.1 is applicable, then \( D \) must also be positive semidefinite. We have that \( \lambda \geq 0 \), and the vector pair

\[
(\tilde{u}_1, \tilde{u}_2) = \left( \begin{bmatrix} S q^* \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ q^* \end{bmatrix} \right)
\]

(5.133)

satisfies Eq. (5.127) with \( \omega = \sqrt{\lambda} \). If \( \omega > 0 \), this is a positive normal mode (5.3); if \( \omega = 0 \), it is an inertial zero normal mode (5.7). Notice that special zero normal modes (5.5) do not occur in a system of coupled point masses.
We see that the normal-mode problem of a system of coupled point masses can be reduced to the SDGEP, as is well known. The same is true for the normal-mode problems of the wave equation or in elasticity theory, which have a similar mathematical structure (and are in a sense continuum analogues of systems of harmonically coupled masses). However, the same reduction cannot be applied to arbitrary linear Hamiltonian systems. What makes the system of coupled point masses special is that (a) there is a natural system of canonical variables (the momenta and displacements of the individual masses); (b) in this canonical system, the Hamiltonian is the sum of a kinetic-energy term, which depends only on the momenta, and a potential-energy term, which depends only on the coordinates; and (c) the kinetic-energy term is positive definite. As for the spin system, while it is not hard to construct a system of canonical momenta and coordinates (condition a; see Ref. [61]), in this system the Hamiltonian generally does not separate into a kinetic-energy and a potential-energy part (condition b), especially if the equilibrium configuration is not collinear. One might remark that if the Hamiltonian is positive semidefinite a system of momenta and coordinates that satisfies condition b must exist: such a system is a by-product of the solution of the normal-mode problem (see Sec. 5.A.1). The issue, of course, is that we do not know this system when we start. Moreover, the kinetic-energy term is not guaranteed to be positive definite (condition c) unless the Hamiltonian is positive definite. Section 5.4 presents a way in which the normal-mode problem of any linear Hamiltonian system can be reduced to the HDGEP, provided that its Hamiltonian is positive semidefinite.

5.A.3 General Hamiltonian systems

In this section, we generalize the approach of Sec. 5.A.1 in two ways. First, we allow the Hamiltonian system to be nonlinear. Second, we no longer require that the matrix $\Omega$ defining the Poisson bracket at $x = 0$ is invertible. In the language of symplectic geometry, the latter generalization means that the Hamiltonian system may be defined on a Poisson manifold rather than a symplectic manifold. While any symplectic manifold is also a Poisson manifold, the converse is not true. The spin system in Cartesian coordinates (see Sec. 5.3) is an important example. We shall show that even under these relaxed conditions, linearization of the equation of motion of a general Hamiltonian system near an equilibrium point $x^i = 0$ results in a linear Hamiltonian system. In particular, we shall show that the matrix $M\Omega$ (see Sec. 5.2) is symmetric. Moreover, we show that $\langle M\Omega \rangle$ can be interpreted as the Hessian matrix at the equilibrium point of the restriction of the Hamiltonian function to the symplectic leaf that contains $x = 0$. This implies that $\langle M\Omega \rangle$ is indeed guaranteed to be positive semidefinite, as we require, provided that we linearize at a constrained local minimum of the Hamiltonian.
We fix a nonsingular local system of variables $x^1, \ldots, x^m$ in such a way that $x^i = 0$ is an equilibrium point. In this system of variables, we expand the Hamiltonian $H$ to second order in $x$ as

$$H(x) = H_0 - h_i x^i + \frac{1}{2} x^i A_{ij} x^j + \mathcal{O}(\|x\|^3), \quad (5.134)$$

for a constant scalar $H_0 = H(0)$, vector $h_i = -\partial H / \partial x^i|_{x=0}$, and symmetric matrix $A_{ij} = \partial^2 H / (\partial x^i \partial x^j)|_{x=0}$. We expand the Poisson bracket to first order as

$$\{x^i, x^j\} = -\Omega^{ij} + K_{ij} x^k + \mathcal{O}(\|x\|^2). \quad (5.135)$$

The properties of the Poisson bracket (antisymmetry, Jacobi identity) give the following conditions on the coefficients of this expansion: $\Omega^{ij}$ must be antisymmetric ($\Omega^{ij} = -\Omega^{ji}$); $K_{ij}$ must be antisymmetric in the first two indices ($K_{ij} = -K_{ji}$); and we must have

$$K_{ij} \Omega^{ik} + K_{ik} \Omega^{ij} + K_{ji} \Omega^{ki} = 0. \quad (5.136)$$

The last condition follows from the Jacobi identity,

$$\{x_i, \{x_j, x_k\}\} + \{x_j, \{x_k, x_i\}\} + \{x_k, \{x_i, x_j\}\} = 0, \quad (5.137)$$

which holds for any Poisson bracket $\{\cdot, \cdot\}$. From Eq. (5.135), we get

$$\{x_i, \{x_j, x_k\}\} = -\Omega^{ik} \{x^i, 1\} + K^{ik} \{x^i, x^j\} + \{x^i, \mathcal{O}(\|x\|^2)\} = K^{ik} \Omega^{ij} + \mathcal{O}(\|x\|). \quad (5.138)$$

Since this expression holds at any point $x$, we obtain Eq. (5.136) by collecting the constant parts of the three cyclic permutations of it that appear in Eq. (5.137).

Using Eqs. (5.134) and (5.135) and the general properties of Poisson brackets, we derive the equation of motion to first order from the generalized Hamilton equations,

$$\dot{x}^i = \{x^i, H\} = \Omega^{ij} h_j + M^i_j x^j + \mathcal{O}(\|x\|^2), \quad (5.139)$$

where

$$M^i_j = -\Omega^{ik} A_{kj} - K^{ik} h_k. \quad (5.140)$$

Equation (5.140) may be considered as the equivalent of Eq. (5.21) for a general Hamiltonian system. Since $\dot{x}^i = 0$ at $x^i = 0$, we must have $\Omega^{ij} h_j = 0$. From this fact and Eq. (5.136), we can derive that $M \Omega$ is symmetric, as follows. We may write $(M \Omega)^{ij} = F^{ij} + G^{ij}$, where $F^{ij}$ is given by

$$F^{ij} = -\Omega^{ik} A_{kl} \Omega^{lj} = \Omega^{kl} A_{kl} \Omega^{lj}, \quad (5.141)$$

and $G^{ij}$ is given by

$$G^{ij} = -K^{ik} h_k \Omega^{lj} = K^{ki} h_k \Omega^{lj}. \quad (5.142)$$
\[ F^{ij} \] is obviously symmetric (\( A_{ij} \) is symmetric). We can see that \( G^{ij} \) is symmetric by rewriting it as

\[
G^{ij} = \frac{1}{2} \left( K^{ki} \Omega^{lj} - K^{lk} \Omega^{ij} - K^{ij} \Omega^{lk} \right) h_k
\]

\[
= \frac{1}{2} K^{ki} \Omega^{lj} h_k + \frac{1}{2} K^{lk} \Omega^{ij} h_k - \frac{1}{2} K^{ij} \Omega^{lk} h_k,
\]  

where we have used Eq. (5.136). If \( x = 0 \) is an equilibrium position, Eq. (5.139) implies \( \Omega^{ij} h_j = 0 \) and the last term vanishes. The other two terms together are explicitly symmetric under \( i \leftrightarrow j \).

Except for the fact that \( \Omega \) is not necessarily invertible, we could conclude from the symmetry of \( M \Omega \) that the linearization \( \dot{x}^i = M^i_j x^j \) of a general Hamiltonian system near an equilibrium point is a linear Hamiltonian system in the sense of Sec. 5.A.1. To be explicit, the matrix \( \Omega \) of this linear Hamiltonian system is defined, according to Eq. (5.135), by

\[
\Omega^{ij} = -\{x^i, x^j\}_x = \{x^i, x^j\}_{x=0},
\]  

which is the value of the Poisson bracket between \( x^i \) and \( x^j \) at \( x = 0 \), while the symmetric matrix \( M \Omega \) is given by

\[
(M \Omega)^{ij} = -\Omega^{ik} A_{kl} \Omega^{lj} - K^{ik} h_l \Omega^{lj}.
\]  

Since \( \Omega \) is antisymmetric, its rank is always even. We write \( \text{rank}(\Omega) = 2n \). If \( m > 2n \) (\( \Omega \) is not invertible), we can make \( \Omega \) invertible by interpreting the matrices \( \Omega \) and \( M \Omega \) as restricted to the \( 2n \)-dimensional image space of \( \Omega \). In the notation of Sec. 5.2, we get \( \langle \Omega \rangle \) and \( \langle M \Omega \rangle \). We may do this because the image space of \( M \Omega \) is contained in the image space of \( \Omega \). Thus, the matrices \( \langle M \Omega \rangle \) and \( \langle \Omega \rangle \) together define a proper linear Hamiltonian system.

Our method for the normal-mode problem requires that \( \langle M \Omega \rangle \) be positive semidefinite (see Sec. 5.4). We can show that it is if \( x = 0 \) is a (constrained) local minimum of the Hamiltonian \( \mathcal{H} \). For simplicity, we first consider the case \( m = 2n \) (\( \Omega \) is invertible). If \( \Omega \) is invertible, we have \( h = 0 \), so that \( M \Omega = -\Omega A \Omega = \Omega^T A \Omega \). Evidently, \( M \Omega \) is positive (semi-)definite if and only if \( A \), the Hessian matrix of \( \mathcal{H} \), is positive (semi-)definite. Consequently, if \( x = 0 \) is a local minimum of \( \mathcal{H} \), then \( M \Omega \) is positive semidefinite.

For \( m > 2n \), the dynamical matrix (5.140) is no longer determined only by the Hessian matrix \( A \) of \( \mathcal{H} \); there is an additional \( h \)-dependent term, which is essential. We shall see that the matrix \( \langle M \Omega \rangle \) can be interpreted as the Hessian matrix of the restriction of the Hamiltonian function \( \mathcal{H} \) to a certain \( 2n \)-dimensional submanifold containing \( x = 0 \). For example, while the Hamiltonian \( \mathcal{H} = -m \cdot \dot{z} \) has no local minimum on \( \mathbb{R}^3 \), it has a constrained minimum at \( m = \dot{z} \) on the set \( S^2_{c=1} = \{m \in \mathbb{R}^3 : \|m\| = 1\} \). For positive semidefinite of \( \langle M \Omega \rangle \) we do not require that \( x = 0 \) be an actual local minimum of \( \mathcal{H} \); it is sufficient that \( x = 0 \) be a constrained local minimum on this submanifold. To define the relevant
submanifold in a general setting, it is necessary to use some elements from
the theory of symplectic structures and Poisson structures [99].

In a symplectic manifold, any point (that is, any state of the system) may be
reached from any other point by following the trajectory generated by a suit-
ably chosen Hamiltonian function $H$, or a finite sequence of such trajectories.
In a Poisson manifold, this is not necessarily the case. However, by the splitting
theorem on Poisson manifolds [99], a Poisson manifold can be divided into 
equivalence classes of points for which this is possible. These equivalence classes are
symplectic submanifolds of the Poisson manifold and are called symplectic leaves.
Two points of a Poisson manifold are in the same symplectic leaf if one can get
from one point to the other through a finite sequence of trajectories induced by
Hamiltonian functions. For example, consider a conservative spin system (see
Sec. 5.3) with a single spin $m \in \mathbb{R}^3$, which is governed by the equation of mo-
tion $\dot{m} = m \times \nabla H$. Since this equation conserves $\|m\|$, a spin in position $m = \hat{z}$
will never end up in position $m = \frac{1}{2} \hat{z}$, regardless of the choice of $H$. However,
it may at some point in time reach $m = \hat{y}$, for instance if the Hamiltonian is
given by $H = m \cdot \hat{x}$. Thus, the Poisson manifold of the conservative single-spin
system (that is, $\mathbb{R}^3$ equipped with the spin Poisson bracket; see Sec. 5.3) splits
into symplectic leaves of the form $S^2_c = \{m \in \mathbb{R}^3 : \|m\| = c\}$ for $c \geq 0$.

It can be shown that the $2n$-dimensional symplectic leaf containing the equi-
librium point $x = 0$ can locally be parametrized by a vector $v_i$, which we require
to lie in the image space of $\Omega_{ij}$, as

$$x^i = -\Omega^i_j v_j - \frac{1}{2} K_{ijkl} v_k v_l + O(\|v\|^3) \quad (5.146)$$

if we assume that the Poisson bracket of the Poisson manifold is of the form
(5.135). By substitution of this expression into (5.134), we find that in terms of $v,$
the Hamiltonian becomes

$$\mathcal{H}(v) = H_0 + h_i \Omega^{ij} v_j + \frac{1}{2} \left( -\Omega^{ik} A_{kl} \Omega^{lj} - K^{ikj} h_k \Omega^{lj} \right) v_i v_j + O(\|v\|^3). \quad (5.147)$$

Here we have used that $v = O(\|x\|):$ the fact that $v$ lies in the image space of
$\Omega$ guarantees $\Omega^{ij} v_j \neq 0$ in Eq. (5.146). If $x = 0$ is an equilibrium point, the
linear term in Eq. (5.147) vanishes ($\Omega^{ij} h_j = 0$). The matrix of the quadratic term
in Eq. (5.147), which is identical to the Hessian matrix of the Hamiltonian $\mathcal{H}$
restricted to the symplectic leaf, is identical to $\langle M \Omega \rangle$ (5.145). (We must write the
angular brackets $\langle \cdot \rangle$ here because $v$ was assumed to lie in the image space of $\Omega$.)
Thus, if $x = 0$ is a local minimum of $\mathcal{H}$ on the symplectic leaf that contains the
point $x = 0$, the matrix $\langle M \Omega \rangle$ is positive semidefinite and the method presented
in Sec. 5.4 can be used.
We study the dynamics of magnetic domain walls in the Peierls potential due to the discreteness of the crystal lattice. The propagation of a narrow domain wall (comparable to the lattice parameter) under the effect of a magnetic field proceeds through the formation of kinks in its profile. We predict that, despite the discreteness of the system, such kinks can behave like sine-Gordon solitons in thin films of materials such as yttrium iron garnets, and we derive general conditions for other materials. In our simulations we also observe long-lived breathers. We provide analytical expressions for the effective mass and limiting velocity of the kink in excellent agreement with our numerical results.

This chapter has been published as
6.1 INTRODUCTION

The statics and dynamics of magnetic domain walls have been studied intensively because they determine the most important technical characteristics of magnetic materials, such as magnetization curves and hysteresis [64]. Recently, there has been a revival of interest in this field due to the development of new techniques to manipulate magnetization, such as current-induced spin transfer torque [5,6] and optical control [23]. These developments open new perspectives for magnetic data storage [8] and call for a deeper understanding of the elementary processes associated with domain-wall motion. Traditionally, magnetization profiles are described using continuum models (micromagnetics) [63]. However, it is increasingly being recognized that the discrete nature of the crystal lattice can play an important role in both the statics and the dynamics of magnetic topological defects including domain walls [42], (nano-)skyrmions [14], and Bloch points [121].

It has been predicted [122–124] that if the characteristic width of a domain wall is comparable to the lattice parameter, it may become trapped in a favorable position between two crystallographic planes, as shown in Fig. 6.1. The energy of the domain wall as a function of the position \( x \) of its center shows a pattern of peaks and valleys with a periodicity \( a \) determined by the lattice. The analogous effect for dislocations is known in the field of crystal plasticity as the Peierls potential or Peierls relief [125]. Novoselov et al. [42] confirmed the existence of the magnetic Peierls potential in thin films of yttrium iron garnet (YIG) that combine the very large unit cell (80 atoms) with relatively strong perpendicular anisotropy. Jumps of a domain wall between valleys of the Peierls potential were detected as a very fine and regular staircase pattern in the hysteresis curve. Reference [42] shows that, while the domain wall is only a few nanometers wide, parts of it can be approximately straight over many micrometers in a demagnetized sample at low temperatures (\( \sim 5 \) K). The observation of Peierls jumps implies that the domain wall is straight to within a single Peierls valley at least within the range of the 1.5 \( \mu \)m Hall probe.

If the domain wall is at a small angle with respect to the crystallographic plane, it becomes favorable to maximize the areas which lie in Peierls valleys at the cost of creating kinks, as shown in Fig. 6.1(a). Such kinks can slide freely along the domain wall, effectively moving it in steps of distance \( a \). Dislocations in crystals are known to move in a similar way [125,126]. Measurements of AC magnetic susceptibility provide evidence for kinks in domain walls (DW-kinks) in YIG thin films [42].

If the Peierls potential is significant, the motion of a domain wall is determined by the dynamics of DW-kinks. A crucial question is what happens when two kinks of opposite sign collide: either they pass through each other, like sine-Gordon solitons [127], or they annihilate. In the former case, a domain wall can jump to another Peierls valley and propagates more efficiently. While many authors have discussed the dynamics of kinks in dislocations [126,128,129],
Figure 6.1: (a) A Bloch domain wall with a kink in a thin film with perpendicular anisotropy. The center of the domain wall is indicated as a translucent strip. The segments of domain wall on either side of the kink lie in different valleys of the Peierls potential (top). (b,c) Side views of the domain wall corresponding to horizontal lines in (a), where the domain wall is at a minimum [(b), solid lines in (a)] or a maximum [(c), dashed line in (a)] of energy. While the continuum magnetization profile is the same for (b) and (c), the atomistic configuration is subtly different, which is the microscopic origin of the Peierls potential.
we point out that DW-kinks are different in essential respects (see Sec. 6.A). In this Letter, we show that DW-kinks can display solitonic behavior. We derive necessary conditions in terms of the characteristic length scales of the system, and we predict the existence of long-lived breathers (bound kink-antikink pairs \[127\]) in thin films of materials such as YIG. We also find that DW-kinks possess inertia, somewhat analogous to the Döring effective mass \[2\], and we derive an expression for the DW-kink mass valid for both solitonic and nonsolitonic cases, in excellent agreement with numerical simulations.

6.2 Model

We consider a domain wall in a thin film of thickness \(L\) with perpendicular anisotropy, assuming for simplicity a simple cubic lattice. We argue that for our purposes the film may be considered as effectively two-dimensional if \(L \ll w\), where \(w\) is the characteristic width of the DW-kink (determined below). In the direction normal to the domain wall, while the magnetization profile varies on the much shorter scale of the exchange length, the domain wall is blocked in a valley of the Peierls potential.

We model the dynamics of the localized magnetic moments, described by unit vectors \(m_{ij}\), using the Landau–Lifshitz–Gilbert (LLG) equation \[64\],

\[
\frac{d m_{ij}}{d t} = \frac{|\gamma|}{a^2 M_S} m_{ij} \times \nabla m_{ij} \mathcal{H} + \alpha m_{ij} \times \frac{d m_{ij}}{d t},
\]  

(6.1)

where \(\gamma\) is the gyromagnetic ratio, \(M_S\) is the saturation magnetization and \(\alpha\) is the dimensionless Gilbert damping parameter. The lattice sites are located at \((x, y) = ((i + \frac{1}{2})a, (j + \frac{1}{2})a), i, j \in \mathbb{Z}\), where \(a\) is the lattice parameter. The Hamiltonian \(\mathcal{H}\) is given by

\[
\mathcal{H} = \sum_{ij} a^2 \left( -\frac{2A}{a^2} \left[ m_{ij} \cdot m_{(i+1)j} + m_{ij} \cdot m_{i(j+1)} \right] - K_1 (m_{ij} \cdot \hat{z})^2 + K_2 (m_{ij} \cdot \hat{x})^2 - M_S H_{\text{app}} \cdot m_{ij} \right). 
\]  

(6.2)

Here \(A\) represents the exchange parameter, \(K_1 > 0\) the anisotropy for the easy axis \(\hat{z}\), \(K_2\) the in-plane anisotropy, and \(H_{\text{app}}\) the applied field. The corresponding continuum model gives an exchange length \(l_1 = \sqrt{A/K_1}\), a Bloch domain-wall width of \(\pi l_1\), and a Bloch domain-wall energy of \(\epsilon_1 = 4\sqrt{AK_1}\) per unit area.

We choose the \(x\)-axis to be normal to the domain wall, as in Fig. 6.1(a). The effect of dipolar interactions is taken into account through the second anisotropy parameter \(K_2 = 2\pi M_S^2\), which penalizes magnetization in the \(x\)-direction. This approximation, exact for planar magnetization profiles \(m(x)\) \[64, 127\], has been used in other contexts where the domain wall is only approximately flat \[70\]. It can be justified here because we assume \(l_1 \ll L\) and \(l_1 \ll w\).
6.3 Statics

Minimizing the atomistic Hamiltonian \( H \) under the constraint of a fixed domain-wall center \( x \) gives a Peierls potential of the form

\[
V(x) = V_0 (1 - \cos 2 \pi x / a).
\]

This sinusoidal shape is known to be insensitive to the crystal structure up to exponentially small corrections [123, 128]. The strength \( V_0 \) depends very sensitively on the ratio between the domain-wall width \( \pi l_1 \) and the distance \( a \) between equivalent crystallographic planes; we have \( V_0 \sim e^{-\pi^2 l_1 / a} \) [123]. Noticeable effects require \( l_1 \lesssim 2.5a \).

Static configurations of domain walls with kinks and the thermally activated formation of kink loops were studied theoretically in Ref. [130]. Let us describe the profile of the domain-wall center, shown as a strip in Fig. 6.1(a), as a function \( x(y) \), which we define via the average magnetization \( m_z \) on a line of constant \( y \).

The equilibrium profile of a single kink is given by

\[
x(y) = \frac{2a}{\pi} \arctan \left[ \exp \left( \pi \frac{y - y_0}{w} \right) \right],
\]

where \( y_0 \) is the center of the kink and \( w = \frac{1}{2} a \sqrt{\epsilon_1 / V_0} \) is its characteristic width, which arises from a competition between the Peierls potential and the exchange energy. (For clarity, Fig. 6.1(a) shows an antikink.) The kink energy per unit length is \( \lambda \approx 4a \sqrt{\epsilon_1 V_0 / \pi} \) [130].

We express the kink width in the experimentally accessible quantity \( H_c \), the coercive field of the Peierls barrier:

\[
w = \sqrt{\frac{\pi a \epsilon_1}{4M_5 H_c}}.
\]

Taking experimental parameters from Ref. [42], we find \( l_1 = 3.6 \text{ nm} = 2.0a, \epsilon_1 = 2.0 \text{ erg cm}^{-2}, \lambda = 2.5 \times 10^{-10} \text{ erg cm}^{-1} = 7 \times 10^{-4} a \epsilon_1, \) and \( w = 1.6 \mu \text{m} \approx 900a. \)

6.4 Dynamics

We express the Hamiltonian (6.2) in terms of the collective coordinates \( x(y), \vartheta(y) \) of the domain wall. The angle \( \vartheta \), canonically conjugate to \( x \), represents the in-plane orientation of the magnetization near the center of the domain wall [4]. We define \( \vartheta = 0, \pi \) for a Bloch domain wall and \( \vartheta = \pm \pi / 2 \) for a Néel domain wall. For \( H_{\text{app}} = 0 \) and in the limit of small \( \vartheta \), we get

\[
H \approx \int \left[ \frac{\epsilon_1 K_2}{2 K_1} \vartheta^2 + \frac{\epsilon_1}{2} \left( \frac{\partial x}{\partial y} \right)^2 + V(x) + \frac{\epsilon_1 l_1^2}{2} \left( \frac{\partial \vartheta}{\partial y} \right)^2 \right] dy.
\]

We assume \( w \gg a \), so that the system is effectively continuous in \( y \). Since \( l_1 \sim a \), higher-order terms of the exchange energy may give corrections to Eq. (6.6), but we find that such corrections are relatively small (see Sec. 6.C).
The Poisson brackets for \( x(y), \vartheta(y) \) are given by \( \{ x(y), \vartheta(y') \} = |\gamma|/(2M_S) \delta(y - y') \) and \( \{ x(y), x(y') \} = \{ \vartheta(y), \vartheta(y') \} = 0 \). Taking into account Gilbert damping in the small-\( \vartheta \) limit, we get equations of motion

\[
\dot{x}(y) = \frac{|\gamma|}{2M_S} \frac{\delta H}{\delta \vartheta(y)} + a_1 \dot{\vartheta}(y), \tag{6.7a}
\]
\[
\dot{\vartheta}(y) = -\frac{|\gamma|}{2M_S} \frac{\delta H}{\delta x(y)} - \frac{\alpha}{l_1} \dot{x}(y), \tag{6.7b}
\]

where a dot denotes the time derivative.

### 6.5 Solitonic Behavior

Let us define a second “exchange length” \( l_2 = \sqrt{A/K_2} \). Neglecting the term in \( \partial \vartheta/\partial y \) in Eq. (6.6), Eq. (6.7) with \( \alpha = 0 \) reduces to the sine-Gordon equation,

\[
T^2 \frac{\partial^2 \varphi}{\partial t^2} - Y^2 \frac{\partial^2 \varphi}{\partial y^2} + \sin \varphi = 0, \tag{6.8}
\]

where we define \( \varphi = 2\pi x/a, Y = w/\pi, \) and

\[
T = \frac{a^2}{2\pi^2 E} \frac{M_S l_2}{|\gamma| l_1}, \tag{6.9}
\]

with \( E = \lambda/8 \) (characteristic energy scale). The sine-Gordon equation is one of the very few mathematical models that allow for truly solitonic behavior [127]. This means that DW-kinks behave like solitons only to the extent that Eq. (6.8) is a good approximation. We now investigate under which conditions this is the case.

First, \( \vartheta \) must remain small at all times. For \( w \gg l_2 \) and \( \alpha = 0 \), we have that \( T \partial \varphi/\partial t \approx 2l_1 w/(al_2) \dot{\vartheta} \). A two-kink breather solution of Eq. (6.8), similar to Fig. 6.3(d), is given by [127]

\[
\varphi(y, t) = 4 \arctan \left[ \frac{\sqrt{1 - \omega^2 Y}}{\omega} \text{sech} \left( \frac{\sqrt{1 - \omega^2 y}}{Y} \right) \cos \left( \frac{\omega t}{T} \right) \right], \tag{6.10}
\]

where \( \omega \in (0, 1) \) is a parameter. Notice that \( |\partial \varphi/\partial t| \) attains a maximum at \( y = 0, t = \pi/(2\omega) T \), where the two kinks collide. In the limit \( \omega \to 0 \), the breather (6.10) is equivalent to the collision of two nearly free kinks of opposite signs with negligible initial velocities. We find \( T|\partial \varphi/\partial t|_{\text{max}} = 4 \) and \( \vartheta_{\text{max}} = 2a_2/(l_1 w) \). Since typically \( 2a/l_1 \sim 1 \), we conclude that the small-\( \vartheta \) approximation is valid for

\[
w \gg l_2. \tag{6.11}
\]

This condition must also be assumed to neglect the term in \( \partial \vartheta/\partial y \) in Eq. (6.6).
Second, Gilbert damping must not be too strong. We estimate the energy dissipated in a collision, treating Gilbert damping as a perturbation. For \( \alpha > 0 \), Eq. (6.8) becomes

\[
T^2 \frac{\partial^2 \varphi}{\partial t^2} - Y^2 \frac{\partial^2 \varphi}{\partial y^2} + \sin \varphi = -\xi T \frac{\partial \varphi}{\partial t},
\]

where \( \xi = \alpha w / (\pi l_2) \) is a dimensionless damping rate. The energy dissipated in half a period of the breather (one collision) is given by

\[
\Delta H = -\xi ET \frac{\pi T}{2} \int_{-\infty}^{\infty} \left( \frac{\partial \varphi}{\partial t} \right)^2 dy dt.
\]

Substituting the original solution (6.10), which has an energy of \( 16E\sqrt{1 - \omega^2} \), we find that \( \Delta H = -16\xi Er(\omega)/\sqrt{1 - \omega^2} \), where \( r(\omega) \) is a monotonic function with \( r(0) = \pi^2/2 \) and \( r(1) = \pi \). The relative energy loss for \( \omega \to 0 \) is thus given by \( D = \pi \alpha w / (2l_2) \), and Gilbert damping may be considered small if

\[
\alpha w \ll l_2.
\]

This condition is consistent with Eq. (6.11) only in materials with a very low Gilbert damping parameter \( \alpha \).

For comparison, we perform atomistic spin-dynamics simulations, where we generate an initial configuration containing a domain wall with a two-kink profile, as shown in Fig. 6.2(a), and numerically integrate the LLG equation (6.1) for the Hamiltonian (6.2). We use the C++ code we developed with the implicit midpoint integration scheme, verifying convergence of our results. We extract the domain-wall profiles \( x(y) \), shown in Fig. 6.2(b-d), from the evolving atomistic spin configurations. These results confirm that kinks may display solitonic behavior if the conditions (6.11) and (6.14) are satisfied. Figure 6.3 shows that long-lived breathers can be observed under the same conditions.

For a crystal with uniaxial, perpendicular anisotropy (\( K_2 \) purely magneto-static), we have \( l_2 = M_2^{-1} \sqrt{A/(2\pi)} \). With parameter values from Ref. [42], we get \( l_2 = 0.11 \mu m \approx 61a \) and \( w/l_2 \approx 15 \), so that Eq. (6.11) is satisfied. We remark that, while uniaxial anisotropy is dominant in thin films of bismuth- and gallium-substituted YIG [42, 43], there will be an additional contribution to \( K_2 \) from in-plane crystalline anisotropy. The extremely low Gilbert damping in pure YIG [51] suggests that Eq. (6.14) may also be satisfied and that breathers could survive for many periods.

### 6.6 Equations of Motion

A sine-Gordon soliton possesses inertia; its rest mass is given by \( 8ET^2 / Y^2 \) [127]. For DW-kinks, this evaluates to a mass of

\[
m_{\text{sol}} = \frac{2a^2 M_2^2}{\pi \gamma^2 K_2 l_1 w}
\]
Figure 6.2: Simulations of kink–antikink collisions with initial velocities of $\pm 0.2Y/T$ ($\alpha = 0.0004$, $l_1 = 1.58a$, $w \approx 79a$). (a) Initial configuration. We extract the domain-wall profile $x(y)$ (strip) from the atomistic simulations. Not all magnetic moments are shown. (b) For $w \lesssim l_2$, colliding kinks annihilate under emission of Winter spin waves [37]. (c) If conditions (6.11) and (6.14) are both satisfied, colliding kinks pass through each other. A segment of the domain wall makes a jump of distance $2a$ into another Peierls valley, and propagation continues. (d) For $\alpha w \gtrsim l_2$, colliding kinks lose energy through Gilbert damping. Like in (b), they become trapped in a breather and eventually annihilate.
Figure 6.3: Domain-wall profiles \(x(y,t)\) extracted from atomistic simulations of a breather \((w \approx 79a, \omega = 0.25)\). (a) If \(w \sim l_2\), the sine-Gordon picture of DW-kinks is inapplicable. The breather loses energy through spin-wave emission. (b,c) Spin-wave emission is virtually absent for \(w \gg l_2\). However, for high \(w/l_2\) the breather is more susceptible to Gilbert damping \((\alpha = 0.0004)\), resulting in a faster-decreasing amplitude and period. (d) Solitonic limit \((w \gg l_2\) and no Gilbert damping). A video of the atomistic simulation is available (see Sec. 6.B).
per unit length. We now derive nonrelativistic equations of motion valid for solitonic and nonsolitonic DW-kinks. We linearize the Hamiltonian (6.6) near a single kink at rest, for which we take \( \vartheta(y) = 0 \) and \( x(y) \) as in Eq. (6.4) with \( y_0 = 0 \). An inertial zero-frequency normal mode (see Chap. 5) is associated with the collective coordinate \( y_0 \). We have \( \partial x(y)/\partial y_0 = -(a/w) \text{sech}(\pi y/w) \) and \( \partial \vartheta(y)/\partial y_0 = 0 \). We introduce a momentum \( p \) and require that \( p \) and \( y_0 \) decouple to second order from the other degrees of freedom. From \( \dot{y}_0 = p/m_{\text{eff}} \), we derive \( \partial x(y)/\partial p = 0 \) and

\[
m_{\text{eff}} \frac{\partial \vartheta(y)}{\partial p} = -\frac{a M_S}{2|\gamma| K_2 l_1 w} \left( 1 - l_2^2 \frac{d^2}{dy^2} \right)^{-1} \text{sech} \frac{\pi y}{w}.
\]

The effective mass \( m_{\text{eff}} \) is fixed by the requirement that \( y_0 \) and \( p \) be canonically conjugate, \( \{y_0, p\} = 1 \):

\[
m_{\text{eff}} = f(w/l_2) m_{\text{sol}},
\]

where we define

\[
f(\eta) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\text{sech}^2 x}{1 + 4x^2/\eta^2} \, dx.
\]

For \( \eta \gg 1 \), \( f(\eta) = 1 - \pi^2/(3\eta^2) + O(\eta^{-4}) \). In Fig. 6.4(a), we compare Eq. (6.17) to the effective kink masses obtained for the atomistic model (6.2) using the numerical method described in Chap. 5. We find a very good agreement.

We introduce a characteristic angle \( \vartheta_0 \) related to the kink momentum \( p \) via \( \vartheta_0 = \pi|\gamma|/(4a M_S) p \). We derive from Eq. (6.7) the linearized equations of motion for the collective coordinates \( \vartheta_0 \) and \( y_0 \),

\[
\vartheta_0 = -\frac{\pi}{2} |\gamma| H_z - \frac{\alpha}{R} y_0,
\]

\[
y_0 = \left| \frac{\gamma R}{f(\eta)} \right| \left[ \left( \frac{2K_2}{M_S} - \frac{\pi H_y}{2g(\eta)} \right) \vartheta_0 + \frac{\pi^2}{4} H_x + \frac{\alpha}{|\gamma| g(\eta)} \vartheta_0 \right],
\]

where \( \mathbf{H}_{\text{app}} = H_x \mathbf{x} + H_y \mathbf{y} + H_z \mathbf{z} \) is the applied field, \( \eta = w/l_2 \), \( R = l_1 w/a \), and \( g(\eta) = 2f(\eta)/\left[\int_{-\infty}^{\infty} (1 + 4x^2/\eta^2)^{-2} \text{sech}^2 x \, dx \right] \). We have \( \dot{\vartheta}(y_0) = -h(\eta) \vartheta_0 \), where \( h(0) = 2/\pi \) and \( h(\infty) = 1 \). The condition \( \dot{\vartheta}_0 = 0 \) results in a final velocity

\[
v_{\text{final}} = -\frac{\pi}{\alpha} \left( \frac{l_1}{2a} \right) |\gamma| H_z w.
\]

Our simulations, shown in Fig. 6.4(b), confirm this expression in the regime that \( \vartheta_0 \ll 1 \) and \( v_{\text{final}} \ll Y/T \).

### 6.7 Conclusion and Outlook

We have derived explicit conditions for solitonic behavior of DW-kinks, in terms of Gilbert damping \( \alpha \) and the lengths \( w \) and \( l_2 \): \( 1 \ll w/l_2 \ll 1/\alpha \). For certain YIG films these conditions appear to be satisfied. In the solitonic regime, long-lived
Figure 6.4: (a) Our analytical expression (6.17) for the kink effective mass $m_{\text{eff}}$ is in very good agreement with the numerical values for the atomistic model. Small corrections result from higher-order exchange terms (see Sec. 6.C). For $w \lesssim l_2$, $m_{\text{eff}}$ is reduced with respect to the sine-Gordon value $m_{\text{sol}}$. (b) Final velocity $v_{\text{final}}$ for $\alpha = 0.02$ and $\alpha = 0.04$ and for three values of $w/l_2$ ($w \approx 79a$). In the regime $v_{\text{final}} \ll Y/T$, $v_{\text{final}}$ follows Eq. (6.20) (solid lines) and is independent of $w/l_2$. Deviations occur when $v_{\text{final}}$ becomes comparable to $Y/T$ (horizontal lines). Unlike in the sine-Gordon model, the kink velocity can exceed $Y/T$. 
breathers can exist, as confirmed by our atomistic spin-dynamics simulations. The sharp peak in the dynamical magnetic susceptibility observed in Ref. [42], which survives for some time when the applied field is switched off, might be related to the existence of such breathers [131], although more experimental investigations are needed. We have found expressions for the main dynamical characteristics of kinks, including effective rest mass, Eq. (6.17), and limiting velocity, Eq. (6.20), which apply both in the solitonic regime and beyond. By combining a number of Hall probes [42], one might be able to track the motion of individual DW-kinks. Given the size of DW-kinks (~ 1 µm), it is conceivable that optomagnetical stimuli could be used to create kink pairs. Such techniques would open the way to manipulation of magnetic domain walls with atomistic precision.

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6.A KINKS IN DOMAIN WALLS VERSUS KINKS IN DISLOCATIONS

We show that under certain conditions, DW-kinks may display solitonic behavior. It is interesting to compare the dynamics of DW-kinks to kinks in dislocations in the crystal lattice. Reference \cite{126} found that solitonic behavior can be observed for dislocation kinks in a two-dimensional rigid-substrate model of the slip plane. However, Kosevich argues that the sine-Gordon equation cannot be a satisfactory model for the dynamics of a free dislocation because dislocation motion couples in an essential way to lattice vibrations \cite{128}. Moreover, it seems that ballistic effects (let alone solitonic behavior) play no role of significance in practical simulations of kink or dislocation dynamics \cite{129}. It is important to note that a real dislocation is a line defect in three-dimensional space; its spatial profile depends in an essential way on the perpendicular coordinate. A domain wall, by contrast, is a planar defect. This justifies our approximation of a magnetic thin film containing a domain wall as effectively two-dimensional.

6.B ATOMISTIC SIMULATION OF A BREATHER (MOVIE)

A movie file with an atomistic simulation of a breather has been made available as Supplemental Material at \url{http://dx.doi.org/10.1103/PhysRevLett.113.217202} (see Fig. 6.5). It shows a single period of a breather with $\omega = 0.1$ for $l_1 = l_2 = 1.58a$, $w \approx 79a$, and no Gilbert damping ($\alpha = 0$). The simulation box contains $40 \times 960$ magnetic moments. The translucent yellow strip indicates the evolution of the domain-wall profile according to the analytical breather solution of the sine-Gordon equation.

![Atomistic simulation](image)

Figure 6.5: Atomistic simulation (movie snapshot).
6. C  HIGHER-ORDER EXCHANGE

6. C. 1  Continuum model

For magnetization profiles smooth on the scale of the lattice constant \( a \), the atomistic Hamiltonian (see Sec. 6.2) is equivalent to the sum of the continuum energy functionals

\[
E_{\text{ex}}[\mathbf{m}(x,y)] = \int A \left[ \left\| \frac{\partial \mathbf{m}}{\partial x} \right\|^2 + \left\| \frac{\partial \mathbf{m}}{\partial y} \right\|^2 \right] dx \, dy, \quad (6.21a)
\]

\[
E_{\text{ani}}[\mathbf{m}(x,y)] = \int \left[ -K_1 (\mathbf{m} \cdot \mathbf{\hat{z}})^2 + K_2 (\mathbf{m} \cdot \mathbf{\hat{x}})^2 \right] dx \, dy, \quad (6.21b)
\]

\[
E_{\text{Zee}}[\mathbf{m}(x,y)] = \int -M \mathbf{S} \mathbf{H}_{\text{ext}} \cdot \mathbf{m} \, dx \, dy, \quad (6.21c)
\]

where \( \mathbf{m} \) represents as before the reduced magnetization (\( \| \mathbf{m}(x,y) \| = 1 \)). If the characteristic length scale of the magnetization profile, set by the exchange length \( l_1 \), becomes comparable to \( a \), the continuum energy functionals (6.21) are no longer a good representation of the atomistic Hamiltonian and correction terms are needed. For our purposes, the most important correction is the Peierls potential, which breaks translational symmetry. The Peierls potential vanishes exponentially fast in \( l_1 / a \). However, there are also corrections to \( E_{\text{ex}} \) that are algebraically small. These can be expressed in terms of the higher-order spatial derivatives of \( \mathbf{m}(x,y) \). The dominant correction is

\[
E_{\text{ex}4}[\mathbf{m}(x,y)] = \int B \left[ \left\| \frac{\partial^2 \mathbf{m}}{\partial x^2} \right\|^2 + \left\| \frac{\partial^2 \mathbf{m}}{\partial y^2} \right\|^2 \right] dx \, dy. \quad (6.22)
\]

While the usual exchange parameter \( A \) is proportional to the second moment of the atomistic exchange kernel, the parameter \( B \) is proportional to the fourth moment. For nearest-neighbor exchange in a square lattice, we derive

\[
B = -a^2 A / 12. \quad (6.23)
\]

Energy terms such as Eq. (6.22) do not affect the qualitative features of domain-wall kinks, but they do give certain corrections to kink parameters. Since \( l_1 \sim a \), we may not assume that such corrections can be neglected. Notice that Eq. (6.23) is specific to systems with only nearest-neighbor exchange; crystals with wider exchange kernels are likely to have a larger parameter \( B / A \), so that the corrections derived here may be more significant.

6. C. 2  Derivation of the domain-wall Hamiltonian

We now write the Hamiltonian in terms of the collective coordinates \( x_0(y), \theta(y) \) of the domain wall. We aim to derive the effective Hamiltonian of the domain...
wall from the atomistic Hamiltonian in a systematic way, and we apply the approximation that \( \theta \) is small only as a final step. In this section, we write \( x_0 \) for the position of the center of the domain wall to distinguish it from the spatial coordinate \( x \).

Let us express the reduced magnetization \( \mathbf{m}(x, y) \) in spherical coordinates,

\[
\mathbf{m} = \sin(\theta) \cos(\phi) \mathbf{i} + \sin(\theta) \sin(\phi) \mathbf{j} + \cos(\theta) \mathbf{k}.
\]  

(6.24)

Notice that we use \( \theta \) to denote the collective coordinate of the domain wall, while we use \( \phi \) for the polar angle of the magnetization \( \mathbf{m} \) at a given point in space. We assume that \( \phi(x, y) = \theta(y) - \pi/2 \); the azimuthal angle \( \phi \) is constant in \( x \) and depends only on \( \theta(y) \). As a result, a domain wall with \( \theta \neq 0 \) is equivalent to a Bloch domain wall (\( \theta = 0 \)) but with a modified anisotropy. The effective anisotropy \( K \) that the domain wall experiences is given by

\[
K = K_1 + K_2 \sin^2 \theta,
\]

(6.25)

and we can define an effective “exchange length”

\[
I(\theta) = \sqrt{\frac{A}{K_1 + K_2 \sin^2 \theta}} = \frac{l_1}{\sqrt{1 + (K_2/K_1) \sin^2 \theta}}.
\]

(6.26)

We may now write the Hamiltonian of the domain wall, very generally, as

\[
\mathcal{H}[x_0(y), \theta(y)] = \int \frac{4A}{I(\theta)} \left[ s_0(x_0, I(\theta)) + \frac{1}{2} s_x(x_0, I(\theta)) \left( \frac{\partial x_0}{\partial y} \right)^2 \right. \\
+ \left. \frac{l(\theta)^2}{2} s_\theta(x_0, I(\theta)) \left( \frac{\partial \theta}{\partial y} \right)^2 + \frac{\pi^2}{24} s_l(x_0, I(\theta)) \left( \frac{\partial l(\theta)}{\partial y} \right)^2 \right] dy.
\]

(6.27)

Here \( s_0, s_x, s_\theta, \) and \( s_l \) are dimensionless functions of \( x_0/a \) and \( l/a \) that remain to be determined. The characteristic length scale on which the domain-wall variables \( x_0(y), \theta(y) \) vary in \( y \) is \( w \). Since we do not take into account higher-order derivatives in \( y \), the Hamiltonian (6.27) is valid up to corrections of \( O((w/a)^{-2}) \). This is acceptable because \( w \gg a \) while the dominant energy scale \( \lambda \) is of \( O((w/a)^{-1}) \). For all four functions \( s_0, s_x, s_\theta, \) and \( s_l \), the dependence on \( x_0 \) vanishes as \( \sim e^{-\pi^2 l/a} \sim O(w/a)^{-2} \). As the factors \((\partial \cdot /\partial y)^2 \) are already of order \( O(w/a)^{-2} \), we may neglect the \( x_0 \)-dependence of \( s_x, s_\theta, \) and \( s_l \). For \( s_0 \), we write

\[
s_0(x_0, l) = s_0(l) - v(l) \cos \frac{2\pi x_0}{a},
\]

(6.28)

which defines the Peierls potential. Higher Fourier components may be neglected (see Sec. 6.3). In conclusion, we get

\[
\mathcal{H}[x_0(y), \theta(y)] = \int \frac{4A}{I(\theta)} \left[ s_0(l(\theta)) + \frac{1}{2} s_x(l(\theta)) \left( \frac{\partial x_0}{\partial y} \right)^2 - v(l(\theta)) \cos \frac{2\pi x_0}{a} \right. \\
+ \left. \frac{l(\theta)^2}{2} s_\theta(l(\theta)) \left( \frac{\partial \theta}{\partial y} \right)^2 + \frac{\pi^2}{24} s_l(l(\theta)) \left( \frac{\partial l(\theta)}{\partial y} \right)^2 \right] dy.
\]

(6.29)
If we expand to second order in $\vartheta$ and neglect any corrections of $\mathcal{O}((w/a)^{-2})$, Eq. (6.29) becomes

$$
\mathcal{H} \approx \frac{4A}{l_1} \int \left[ s_0(l_1) + \frac{1}{2} \frac{K_2}{K_1} (s_0(l_1) - l_1 s'_0(l_1)) \vartheta^2 + \frac{1}{2} s_x(l_1) \left( \frac{\partial x_0}{\partial y} \right)^2 \right.
$$

$$
- v(l_1) \cos \frac{2\pi x_0}{a} + \frac{l_1^2}{2} s_\vartheta(l_1) \left( \frac{\partial \vartheta}{\partial y} \right)^2 \right] \, dy. \quad (6.30)
$$

Equation (6.30) is equivalent to the domain-wall Hamiltonian given in Sec. 6.4 except for the correction factors $(s_0(l_1) - l_1 s'_0(l_1))$, $s_x(l_1)$, and $s_\vartheta(l_1)$. By definition, $V_0 = \epsilon_1 v(l_1)$.

6.3.3 Perturbative calculation of the functions $s_0(l)$, $s_x(l)$, $s_\vartheta(l)$, and $s_l(l)$

Let us consider a planar domain wall with collective coordinates $x_0$, $\vartheta$ and effective exchange length $l$. As is well known, in spherical coordinates (6.24), its equilibrium magnetization profile $m(x)$, taking into account only the continuum energy functionals (6.21), is given by

$$
\theta(x) = 2 \arctan \left[ \exp \left( \frac{x - x_0}{l} \right) \right], \quad (6.31a)
$$

$$
\phi(x) = \vartheta - \pi/2. \quad (6.31b)
$$

We derive the effect of the fourth-order exchange term (6.22) on the equilibrium magnetization profile in first-order perturbation theory. In spherical coordinates (6.24) and under the assumption that $\phi$ is constant, we have the identities $\|m'\|^2 = (\theta')^2$ and $\|m''\|^2 = (\theta')^4 + (\theta'')^2$, where the prime denotes the derivative in $x$. (For constant $\theta$, we have $\|m'\|^2 = (\phi')^2 \sin^2 \theta$.) For a planar profile, the continuum energy terms (6.21) become

$$
E_{\text{ex}} = \int A (\theta')^2 \, dx, \quad (6.32a)
$$

$$
E_{\text{ani}} = \int K \sin^2 \theta \, dx, \quad (6.32b)
$$

while the fourth-order exchange term (6.22) becomes

$$
E_{\text{ex}4} = \int B[(\theta')^4 + (\theta'')^2] \, dx. \quad (6.33)
$$

We find that, to first order in $B$, the equilibrium configuration is given by

$$
\theta(x) = 2 \arctan \left[ \exp \left( \frac{x - x_0}{l} \right) \right] + \frac{B}{Al^2} \theta_1 \left( \frac{x - x_0}{l} \right), \quad (6.34)
$$

where

$$
\theta_1(\zeta) = -3 \tanh \zeta \sech \zeta + \frac{1}{2} \zeta \sech \zeta. \quad (6.35)
$$
We calculate the coefficients in Eq. (6.30) from the (perturbed) magnetization profile of the planar domain wall. Notice that the functions $s_0(l)$, $s_x(l)$, $s_\theta(l)$, and $s_l(l)$ are normalized in such a way that they approach 1 in the continuum limit $B/(Al^2) \rightarrow 0$. We have

\begin{align}
  s_0 &= \frac{1}{4A} \int \left( A(\theta')^2 + K\sin^2 \theta + B[(\theta')^4 + (\theta'')^2] \right) dx, \\
  s_x &= \frac{1}{2} \int \left( \frac{\partial m}{\partial x_0} \right)^2 dx = \frac{1}{2} \int (\theta')^2 dx, \\
  s_\theta &= \frac{1}{2l} \int \left( \frac{\partial m}{\partial \theta} \right)^2 dx = \frac{1}{2l} \int \sin^2 \theta dx, \\
  s_l &= \frac{6l}{\pi^2} \int \left( \frac{\partial m}{\partial l} \right)^2 dx = \frac{6}{\pi^2 l} \int (x-x_0)^2 (\theta')^2 dx,
\end{align}

where we treat $l$ as a constant when taking the derivative in $\theta$. We get

\begin{align}
  s_0(l) &= 1 + \frac{1}{2}(B/A)l^{-2} + O((l/a)^{-4}), \\
  s_x(l) &= 1 - \frac{3}{2}(B/A)l^{-2} + O((l/a)^{-4}), \\
  s_\theta(l) &= 1 + \frac{3}{2}(B/A)l^{-2} + O((l/a)^{-4}), \\
  s_l(l) &= 1 - (24/\pi^2 + \frac{1}{2})(B/A)l^{-2} + O((l/a)^{-4}).
\end{align}

### 6.3.4 Corrections to kink parameters

For convenience, let us define

\begin{align}
  S_0 &= s_0(l_1) - l_1 s_0'(l_1) = 1 + \frac{3}{2}(B/A)l_1^{-2} + O(l_1/a)^{-4}, \\
  S_x &= s_x(l_1) = 1 - \frac{3}{2}(B/A)l_1^{-2} + O(l_1/a)^{-4}, \\
  S_\theta &= s_\theta(l_1) = 1 + \frac{3}{2}(B/A)l_1^{-2} + O(l_1/a)^{-4}, \\
  S_l &= s_l(l_1) = 1 - (24/\pi^2 + \frac{1}{2})(B/A)l_1^{-2} + O((l_1/a)^{-4}),
\end{align}

which are the correction factors that appear in Eq. (6.30). Equation (6.23) gives $S_0 \approx 1 - \frac{1}{8}(l_1/a)^{-2}$, $S_x \approx 1 + \frac{1}{8}(l_1/a)^{-2}$, and $S_\theta \approx 1 - \frac{1}{8}(l_1/a)^{-2}$ for a square lattice with nearest-neighbor exchange.

As for the statical kink parameters, the Hamiltonian (6.30) gives us a sine-Gordon kink solution (see Sec. 6.3) with

\begin{equation}
  w = \frac{a}{2} \sqrt{\frac{S_x}{v(l_1)}} = S_x^{1/2} w_{\text{cont}},
\end{equation}

where the subscript $\text{cont}$ denotes the value in the continuum model with only second-order exchange, as used in Secs. 6.1 - 6.7. The kink energy is given by

\begin{equation}
  \lambda = \frac{4a}{\pi} \epsilon_1 \sqrt{S_x v(l_1)} = S_x^{1/2} \lambda_{\text{cont}}.
\end{equation}
Figure 6.6: The analytical expression \((6.41)\) for the effective mass \(m_{\text{eff}}\) corrected for the effect of fourth-order exchange (solid black lines) is in almost perfect agreement with the numerical results for the atomistic model (symbols). The dotted lines show the uncorrected analytical expression given in Sec. 6.6, which differs by \(\sim 5\%\). The dashed line shows the effective mass in the solitonic limit. We find that the (corrected) analytical expression deviates from the numerically calculated values only in the regime \(w \lesssim 10a\) (not shown). This is not surprising because all our calculations assume \(w \gg a\), as is always verified unless the Peierls potential is extremely strong.

As for the dynamical kink parameters, we find

\[
wm_{\text{eff}} = \frac{2a^2 M_s^2 f(w/l_2)}{\pi \gamma^2 K_1 l_1 S_0} = \frac{f(w/l_2)}{f((w/l_2)_{\text{cont}})} S_0^{-1} (wm_{\text{eff}})_{\text{cont}},
\]

where

\[
l_2 = l_1 \sqrt{\frac{K_1}{K_2}} \sqrt{\frac{S_{\theta}}{S_0}} = S_0^{-1/2} S_{\theta}^{1/2} l_{2,\text{cont}}.
\]

Figure 6.6 shows that this correction to the effective mass \(m_{\text{eff}}\) is small but significant. With the corrections, the agreement of our analytical expression to our numerical results is almost perfect. The characteristic time scale of the approximate sine-Gordon description is given by

\[
T = \frac{a M_s}{\pi |\gamma| \epsilon_l} \sqrt{\frac{K_1}{v(l_1) K_2 S_0}} = S_0^{-1/2} T_{\text{cont}}.
\]

The final velocity (in the linear regime, where \(\theta_0 \ll 1\) and \(v_{\text{final}} \ll Y/T\)) is given by

\[
\frac{v_{\text{final}}}{w} = S_x^{-1} \left( \frac{v_{\text{final}}}{w} \right)_{\text{cont}}.
\]
6.4 Strength of the Peierls Potential

The kink width $w$ depends on the strength $V_0$ of the Peierls potential, which in turn depends on the ratio between the domain-wall width and the lattice periodicity $a$. For the biaxial type of anisotropy defined in Sec. 6.2, the equilibrium domain-wall width for a fixed value of $\theta$ is given by $\pi \sqrt{A/(K_1 + 2K_2 \sin^2 \theta)}$. For a Bloch domain wall ($\theta = 0$), this becomes $\pi l_1 = \pi \sqrt{A/K_1}$ [123]. Since we derive all analytical results in the limit of small $\theta$, $V_0$ can be taken as constant (see also Sec. 6.C.2). It must be some dimensionless function of $l_1/a$ times the Bloch domain-wall energy $\epsilon_1 = 4\sqrt{AK_1}$.

For a line of fixed $y = (j + 1/2)a$, we define the center $x$ of the domain wall as

$$x = \frac{a}{2} \sum_i (m_{ij} \cdot \hat{z}), \quad (6.45)$$

which defines a position relative to the middle of the sample. The magnetic Peierls potential $V(x)$ can be obtained by minimizing the atomistic Hamiltonian of some configuration with a domain wall under the constraint of a fixed value of $x$. We find, in agreement with previous considerations [122, 123],

$$V(x) = V_0 \left[ 1 - \cos \frac{2\pi x}{a} \right], \quad (6.46)$$

where $V$ is an energy per unit area. We have $V_0 \sim \epsilon_1 e^{-\pi^2 l_1/a}$ [123]. For a noticeable Peierls relief, we must have $l_1 \lesssim 2.5a$. Higher Fourier components of $V(x)$ decrease even faster in $l_1/a$ [128], so that Eq. (6.46) is expected to describe the Peierls potential almost perfectly unless $l_1 \lesssim 1.2a$. It is easy to see that an external field $H_{\text{app}} = H_z \hat{z}$ results in an additional potential $V_H(x) = -2M_S H_z x$. Combining these two expressions gives a coercive field $H_c = \pi V_0 / (M_S a)$ [130]. This provides an alternative way to determine numerically the strength $V_0$ of the Peierls potential for a given atomistic model.

For a domain wall in a \{100\} plane of the simple cubic lattice with nearest-neighbor exchange, we find that $V_0$ depends on the domain-wall width $l_1$ as

$$V_0 = (P \frac{l_1}{a} + Q) \epsilon_1 e^{-\pi^2 l_1/a}. \quad (6.47)$$

A fit of the coercive fields gives $P \approx 181$ and $Q \approx -36$. Our expression (6.47) is equivalent to previous results [122, 123] if we set $Q = 0$ and $P = C/(4\pi)$. We find that the refinement $Q \neq 0$ is significant and makes the fit to the numerical results almost perfect. If we consider a system with nearest-neighbor and next-nearest-neighbor exchange, Eq. (6.47) remains valid but $P$ and $Q$ take different values. The Peierls relief might thus be useful as a probe for the strength and type of the exchange interaction on the atomic scale.

Given $V_0$, we can calculate the kink width $w$ using the relation [130]

$$w = \frac{1}{2} a \sqrt{\epsilon_1 / V_0}. \quad (6.48)$$
Figure 6.7: Kink width $w$ versus exchange length $l_1$. Symbols: Obtained by numerical minimization of the atomistic Hamiltonian (specified in Sec. 6.2) starting from a spin configuration containing a domain wall with a single kink. The kink width is extracted from the domain-wall profile $x(y)$ in the final, relaxed configuration. Curves: Calculated from Eq. (6.47) using Eq. (6.48), where the parameters $P$ and $Q$ are independently obtained from a fit to the coercive field. Notice that here the corrections to Eq. (6.48) that result from higher-order terms of the exchange energy (see Sec. 6.5) are tiny.

Figure 6.7 shows that the kink widths calculated from Eq. (6.47) agree with the results found by numerical relaxation of a domain wall with a kink.

6.6 Adjoint forms of the kink collective coordinates

In Sec. 6.6 it is derived that the collective coordinates $y_0, p$ of the kink are given by

$$\frac{\partial x(y)}{\partial y_0} = -\frac{a}{w} \frac{\pi y}{w}, \quad (6.49a)$$

$$\frac{\partial \theta(y)}{\partial y_0} = 0, \quad (6.49b)$$

$$\frac{\partial x(y)}{\partial p} = 0, \quad (6.49c)$$

$$\frac{\partial \theta(y)}{\partial p} = -\frac{a M_s}{2|\gamma|K_2l_1m_{eff}w} \left(1 - l_2^2 \frac{d^2}{dy^2} \right)^{-1} \frac{\pi y}{w}. \quad (6.49d)$$
For completeness, we mention that, owing to the symplectic structure (see Chap. 5 on the domain-wall coordinates $x(y), \vartheta(y)$, these expressions immediately imply a “direct” definition of $y_0$ and $p$, namely

$$y_0 = -\frac{\pi}{2af(w/l_2)} \int_0^{\Delta x(y)} \left(1 - \frac{l_2^2 d^2}{dy^2}\right)^{-1} \operatorname{sech} \frac{\pi y}{w} dy,$$

(6.50a)

$$p = \frac{2aM_S}{|\gamma|w} \int \vartheta(y) \operatorname{sech} \frac{\pi y}{w} dy.$$  

(6.50b)

This definition is valid up to first order in the deviations $\Delta x(y), \vartheta(y)$ from the equilibrium kink configuration (for which $\vartheta(y) = 0$ identically). We have

$$\Delta x(y) = x(y) - \left(2a/\pi\right) \arctan \left[\exp \left(\frac{\pi y}{w}\right)\right].$$

(6.51)

6.F SPECIAL FUNCTIONS

Sections 6.5 and 6.6 introduce the special functions $r(\omega), f(\eta), g(\eta),$ and $h(\eta)$. For completeness, we summarize their definitions and limiting behavior here. The functions are plotted in Figs. 6.8 and 6.9. We have

$$r(\omega) = \frac{2\pi}{16\sqrt{1-\omega^2}} \int_0^{\pi/\omega} \int_{-\infty}^{\infty} \left(\frac{\partial \varphi}{\partial t}\right)^2 dy dt,$$

(6.52)

where

$$\varphi(y, t) = 4 \arctan \left[\frac{\sqrt{1-\omega^2}}{\omega} \operatorname{sech} \left(\sqrt{1-\omega^2}y\right) \cos (\omega t)\right].$$

(6.53)

is a breather solution of the sine-Gordon equation, with parameter $\omega \in (0, 1)$. We have made all variables dimensionless. The solution (6.53) is periodic in $t$ with a period of $2\pi/\omega$. Equation (6.52) can be evaluated as

$$r(\omega) = \frac{2\pi}{\sqrt{1-\omega^2}} \arctan \sqrt{\frac{1-\omega}{1+\omega}}.$$  

(6.54)

It is easy to see that $r(\omega)$ is a bounded function with

$$r(\omega \downarrow 0) = \pi^2/2 \approx 4.935,$$

(6.55a)

$$r(\omega \uparrow 1) = \pi \approx 3.142.$$  

(6.55b)

For $\eta > 0$ we define

$$f(\eta) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\operatorname{sech}^2 x}{1 + 4x^2/\eta^2} dx,$$

(6.56)
Figure 6.8: Special function $r(\omega)$, with limiting values.

Figure 6.9: Special functions $f(\eta)$, $g(\eta)$, and $h(\eta)$, with limiting behavior.
which has the following limiting behavior:

\[ f(\eta) = \frac{1}{4} \pi |\eta| + O(\eta^2) \text{ for } \eta \ll 1, \tag{6.57a} \]
\[ f(\eta) = 1 - \frac{1}{3} \pi^2 / \eta^2 + O(\eta^{-4}) \text{ for } \eta \gg 1. \tag{6.57b} \]

We also define two related functions

\[ g(\eta) = 2 f(\eta) \left[ \int_{-\infty}^{\infty} \frac{\text{sech}^2 x}{\left(1 + 4x^2 / \eta^2\right)^2} dx \right]^{-1}, \tag{6.58} \]
\[ h(\eta) = \frac{1}{\pi f(\eta)} \int_{-\infty}^{\infty} \frac{\text{sech} x}{1 + 4x^2 / \eta^2} dx, \tag{6.59} \]

for which we have

\[ g(\eta \downarrow 0) = 2, \tag{6.60a} \]
\[ g(\eta) = 1 + \frac{1}{3} \pi^2 / \eta^2 + O(\eta^{-4}) \text{ for } \eta \gg 1, \tag{6.60b} \]
\[ h(\eta \downarrow 0) = 2 / \pi \approx 0.6366, \tag{6.61a} \]
\[ h(\eta) = 1 - \frac{2}{3} \pi^2 / \eta^2 + O(\eta^{-4}) \text{ for } \eta \gg 1. \tag{6.61b} \]

Notice that \( f(\eta), g(\eta), \) and \( h(\eta) \) are defined in such a way that they approach 1 for large \( \eta \) (solitonic limit).
Spin-wave technology (magnonics) has the potential to further reduce the size and energy consumption of information processing devices. In the submicrometer regime (exchange spin waves), topological defects such as domain walls may constitute active elements to manipulate spin waves and perform logic operations. We predict that spin waves that pass through a domain wall in an ultrathin perpendicular-anisotropy film experience a phase shift that depends on the orientation of the domain wall (chirality). The effect, which is absent in bulk materials, originates from the interfacial Dzyaloshinskii–Moriya interaction and can be interpreted as a geometric phase. We demonstrate analytically and by means of micromagnetic simulations that the phase shift is strong enough to switch between constructive and destructive interference. The two chirality states of the domain wall may serve as a memory bit or spin-wave switch in magnonic devices.

This chapter has been published as
7.1 INTRODUCTION

Motivated by the aim to reduce energy dissipation in electronic devices, spin waves are considered as an alternative information carrier in the field of magnon spintronics [29]. A spin wave acquires a phase shift when it passes through a magnetic domain wall (DW) [33]. In this Letter, we show that the Dzyaloshinskii–Moriya interaction (DMI) in ultrathin ferromagnetic films makes the phase shift dependent on the DW chirality, leading to constructive/destructive interference in a two-branch interferometer. The mechanism we identify raises the prospect of magnonic devices in which DW chirality acts as a spin-wave switch.

It is by now clear that the DMI plays a crucial role in the magnetization dynamics of ultrathin films [17,18,47,132], due to the broken inversion symmetry at the interfaces. The interfacial DMI favors, in a perpendicular-anisotropy film, Néel DWs with a fixed chirality [Fig. 7.1(d)] [17,133], in competition with the dipolar interaction, which tends to favor Bloch DWs [Fig. 7.1(b)]. The most interesting regime is when the two interactions have a comparable strength, yielding a DW intermediate between Bloch and Néel [133,134] with two stable minimum-energy configurations (chirality states) whose in-plane orientations differ by $\sim 90^\circ$, as shown in Fig. 7.1(c).

Recent experiments demonstrated that DWs can be brought into the intermediate regime, and that the DMI strength can be fine-tuned by modifying the thicknesses of the adjacent nonmagnetic layers [135]. The internal orientation might be also tuned by an adjacent layer of a topological insulator; its surface states induce in the magnetic layer an interfacial-DMI-like effect that depends on chemical potential and applied electric field [19–22].

7.2 MAIN RESULTS

Our main result is summarized in Fig. 7.2 where we consider an interferometer in which incoming spin waves are divided between two identical waveguides, each containing a DW. The two DWs are identical in every respect except possibly their chirality. When the spin waves rejoin, they are transmitted or reflected depending on the phase difference. While it is obvious that spin waves interfere constructively if the two DWs have the same chirality [Fig. 7.2(a)], we ask if it is possible to achieve destructive interference (spin wave blocked) by reversing the chirality of one DW [Fig. 7.2(b)]. Without DMI, the two chirality states of the Bloch DW induce identical phase shifts, leading to constructive interference [Fig. 7.2(c)]. For strong DMI, the DW has a single stable (Néel) configuration and the phase shifts are obviously also identical [Fig. 7.2(e)]. However, for intermediate DMI, the two equilibrium orientations induce geometric phase shifts differing by as much as $180^\circ$ [Fig. 7.2(d)]. In this regime, the interferometer can switch between constructive and destructive interference – transmission or reflection – depending on whether the chiralities are identical or opposite.
Figure 7.1: Effect of the interfacial DMI on the magnetization profile $m(x)$ of a DW in a thin film with perpendicular anisotropy. (a) Away from the DW, magnetization points out of the film ($\hat{z}$ or $-\hat{z}$). Near the DW, the DMI creates an effective field $H_{\text{DMI}}$ in the $-\hat{x}$ direction. Depending on the competition between the dipolar and DMI interactions, the equilibrium configurations $\bigcirc$, $\bigcirc'$, $\bigstar$, $\bigstar'$, and $\Box$, shown in (b)–(d), are possible. (b) Without DMI, the minimum-energy configurations (flux closure) are two equivalent Bloch DWs ($\bigcirc$, in dark colors, and $\bigcirc'$, in light colors), whose in-plane orientations differ by $180^\circ$. (c) For intermediate DMI, the minimum-energy configurations are intermediate between Bloch and Néel. There are two equivalent minimum-energy states ($\bigstar$ and $\bigstar'$), whose in-plane orientations differ by approx. $90^\circ$ for an appropriately tuned DMI strength $D$. (d) For strong DMI, a single minimum-energy configuration $\Box$ exists: a Néel DW with magnetization in the center pointing in the $-\hat{x}$ direction.
Figure 7.2: Interferometer setup in a thin film with perpendicular anisotropy. The two DWs may have (a) identical or (b) opposite chiralities. Spin waves enter the device from the left. If the chiralities are identical, constructive interference is always obtained on the right-hand side. For opposite chiralities, the phase difference depends on the DMI strength, as shown in (c)–(e). (c) Without DMI, spin waves interfere constructively even if the chiralities are opposite (○, ○'). (d) For intermediate DMI, we find a phase difference $\Delta \varphi$ of up to $180^\circ$ (destructive interference) for opposite chirality states ★, ★'. (e) For strong DMI, the configurations in both branches are the same (□), trivially resulting in constructive interference. In (c)–(e), large arrows represent the equilibrium magnetization direction $m(x)$. On the left, spin-wave basis vectors $\hat{a}, \hat{b}$ are defined identically for all configurations ○, ○', ★, ★', □. Their orientation after parallel transportation, shown on the right, depends on the DW configuration. In (d), notice that the transported basis vectors for ★ and ★' are rotated by $180^\circ$. This geometric phase difference $\Delta \varphi_{geom}$ is the dominant contribution to $\Delta \varphi$. 
The two chirality states are separated by an energy barrier $\Delta E$ (an unfavorable Néel configuration). If $\Delta E$ is high enough, spontaneous reversals of chirality due to thermal fluctuations are very rare (for the system in Fig. 7.3, we obtain $\Delta E = 2.5 \times 10^{-12}$ erg $= 61 k_B T_{\text{room}}$). We could consider the intermediate-DMI interferometer as a two-state memory device where the transmission of spin waves serves as readout mechanism (“open” or “closed”).

Switching does not require modifications of the material parameters, nor to insert or remove DWs [33], but only to reverse the chirality of one DW, for instance by a field pulse normal to the plane of the film. (The “field pulse” might alternatively be generated through optomagnetic effects [23], provided the light can be focused onto a single branch.) The field causes the DW magnetization to precess as shown in Fig. 7.4 until, when it is switched off, the DW relaxes to the nearest chirality state.

### 7.3 Micromagnetic Model

We have tested the results of Fig. 7.2 which we derive analytically below, by means of explicit micromagnetic simulations. The total energy $E$ is given by the sum of the usual micromagnetic energy functionals for exchange $E_{\text{ex}} = A \int \left( \| \partial_x m \|^2 + \| \partial_y m \|^2 \right) \, dx \, dy$, uniaxial anisotropy $E_{\text{ani}} = -K \int m_z^2 \, dx \, dy$, and dipolar energy (see Sec. 7.B), plus a functional

$$E_{\text{DMI}} = -2D \int \int m \cdot \left( \nabla m_z \right) \, dx \, dy$$

(7.1)

describing the DMI induced near the interfaces of the ultrathin film [17]. The DMI strength $D$ can be positive or negative (we take $D > 0$ in Figs. 7.1 and 7.2). We treat the film as effectively two-dimensional (magnetization is a function of $x$ and $y$ only), but we do consider the finite film thickness $L$ in the $z$ direction for the dipolar interactions (see Sec. 7.B). Here we consider a waveguide made of a long strip of ultrathin film with perpendicular magnetization ($K > 2\pi M_S^2$, where $M_S$ is saturation magnetization). The waveguide width $W$ is at least so large that the dipolar interactions, in the absence of DMI, favor a Bloch DW.

The interfacial DMI is qualitatively different from a DMI $\propto \int \int \int m \cdot (\nabla \times m) \, dV$ present in isotropic bulk materials with a chiral crystal structure (see Sec. 7.A). The effect of a bulk DMI on the interaction of spin waves with DWs was considered in Refs. [7] and [136]. Since a bulk DMI favors the Bloch DW (⊙ in Figs. 7.1 and 7.2), it does not, in the geometry considered here, provide the competition with dipolar interactions that is essential to obtain the intermediate DW with two equivalent minimum-energy orientations ⭐, ⭐′ differing by approximately 90°.

Figure 7.3 shows how spin waves, generated on the left-hand side of the strip, pass through a DW. We solve the Landau–Lifshitz–Gilbert (LLG) equation, for relaxed initial states, on a square grid $(0.33l \times 0.33l$ cells) using a self-developed C++ code (see Chap. 5) with implicit midpoint time integration [58].
Figure 7.3: Micromagnetic simulations of the propagation of spin waves in a ferromagnetic thin-film waveguide with perpendicular magnetization \((2\pi M_S^2 = 0.907 K, L = 3 l, \text{where } l = \sqrt{A/K})\) through DWs of the indicated chiralities (○′, ⋆′ vs. ○, ⋆). (a) Without DMI \((D = 0)\), spin waves experience the same phase shift regardless of DW chirality, leading to constructive interference (avg = average). (b) For intermediate DMI \((D = 0.06 A/l)\), there is a phase difference of almost 180° between spin waves that passed through DWs of different chirality, leading to destructive interference. We remark that the attenuation on the right-hand side is not the result of Gilbert damping (we take \(\alpha = 0.0030\)), but merely represents the present location of the wavefront \([t = 89.6 M_S/(|\gamma|K)]\).
Spin waves are generated by a space-local, time-periodic in-plane applied field \( \omega = 1.70 \gamma K / M_s \), switched on at \( t = 0 \). Each waveguide strip \((267l \times 10l)\) is simulated in a vacuum-padded periodic box \((333l \times 27l)\). We calculate the difference \( \Delta \varphi = \varphi' - \varphi \) in phase shift between the two chiralities at the right-hand side of the interferometer, comparing intermediate DMI to the case without DMI. A phase difference of up to \( 180^\circ \) (destructive interference) is obtained for intermediate DMI.

Fixing \( 4\pi M_s = 3.8 \) kG and \( A = 10^{-6} \) erg/cm \[^{132}\], the other parameters of Fig. 7.3 become \( f = 9.9 \) GHz (frequency), \( W = 127 \) nm (waveguide width \( \approx \) wavelength), \( D = 0.047 \) erg/cm\(^2\), and \( L = 38 \) nm, assuming the free-electron gyromagnetic ratio. Spin waves of such frequencies and wavelengths can be experimentally generated, observed, and visualized \[^{137} -^{139}\]. Since the DMI is an interfacial effect, \( D \) is inversely proportional to film thickness \( L \) \[^{44}\]. Extrapolation of the values in Ref. \[^{132}\] \((D = 0.5 \) erg/cm\(^2\), \( L = 3 \) nm\) suggests that \( D \sim 0.04 \) erg/cm\(^2\) is realistic for \( L \sim 38 \) nm.

### 7.4 Derivation as a Geometric Phase

The phase difference \( \Delta \varphi \) between spin waves traveling along the two paths (★ and ★') has a geometric \[^{140}\] origin. It is convenient to define \( \varphi = \varphi_{\text{geom}} + \varphi_{\text{rel}} \). A spin wave causes magnetization to precess around its local equilibrium direction \( \mathbf{m}(x) \).\[^{1}\] In the limit of exchange spin waves \((k_x \to \infty)\), the dynamics induced by the wave is given by the real part of

\[
\mathbf{m}(x) + \epsilon e^{i(\omega t + k_x x + k_y y + \varphi_{\text{rel}}(x))} [\hat{a}(x) - i\hat{b}(x)],
\]

\(^{1}\) In our (semi-)analytical calculations, we assume an infinite waveguide in the \( y \) direction. In the \( z \) direction, we consider a finite \( L \) in the calculation of the dipolar interactions but neglect the \( z \) dependence of the magnetization inside the film, making the magnetization a function of \( x \) only. The two-dimensional simulations of Fig. 7.3 show that the essence of our analytical results carries over to waveguides of finite width \( W \).
where $\epsilon > 0$ is the infinitesimal amplitude of the spin wave (linear regime). The orthonormal basis vectors $\hat{a}(x), \hat{b}(x)$ must be perpendicular to $m(x)$ for all $x$, so that their orientation continually changes across the DW. A natural choice is to define $\hat{a}(x), \hat{b}(x)$ according to parallel transport, $\frac{d\hat{a}}{dx} = - (\hat{a} \cdot \frac{dm}{dx}) m$, by which the basis vectors, at any given point $x$, match their orientation in an infinitesimal neighborhood of $x$ as closely as possible.

The function $\varphi_{\text{rel}}(x)$ in Eq. (7.2) determines the phase of the spin wave relative to the basis $\hat{a}, \hat{b}$. However, the orientation of the basis $\hat{a}, \hat{b}$ after parallel transport across the DW strongly depends on the DW configuration ($\bigcirc, \bigcirc', \bigstar, \bigstar'$, or $\square$), as shown in Fig. 7.2(c)–(e). This reorientation of $\hat{a}, \hat{b}$ implies an additional phase shift $\varphi_{\text{geom}}$, which is purely geometric in nature.

It is apparent from Fig. 7.2(c)–(e) that the geometric contribution is approximately given by

$$\Delta \varphi_{\text{geom}} \approx 4 \vartheta,$$  

(7.3)

where $\vartheta$ is the in-plane angle of the magnetization at the DW center, as shown in Fig. 7.2(d). For example, we have a geometric phase difference $\Delta \varphi_{\text{geom}} \approx 180^\circ$ for intermediate DWs with $\vartheta = 45^\circ$. The value of $\vartheta$ is determined by the competition between the DMI and the dipolar interaction, as shown in Fig. 7.3(a)–(c).

While in principle $\Delta \varphi_{\text{geom}}$ depends on the exact shape of the equilibrium profile $m(x)$, we find that the deviation from Eq. (7.3) is at most a few degrees (see Sec. 7.C).

We derive (see Sec. 7.C) the relative contribution $\Delta \varphi_{\text{rel}}$ for $k_x \to \infty$, up to a correction of order $|k_x|^{-1}$, as

$$\Delta \varphi_{\text{rel}} = \frac{D}{2A} \int_{-\infty}^{\infty} m'_y(x) \, dx - \frac{D}{2A} \int_{-\infty}^{\infty} m_y(x) \, dx,$$  

(7.4)

where $m'_y$ and $m_y$ are the magnetization profiles $\bigstar', \bigstar$ calculated numerically, taking into account DMI and dipolar interactions. Notice that the exchange interaction does not contribute directly to Eq. (7.4) because the basis $\hat{a}(x), \hat{b}(x)$ (parallel transport) absorbs such a contribution into $\Delta \varphi_{\text{geom}}$.

Equation (7.4) gives, approximately,

$$\Delta \varphi_{\text{rel}} = \varphi'_{\text{rel}} - \varphi_{\text{rel}} \approx \frac{D}{A} w_0 \cos \vartheta,$$  

(7.5)

where $w_0$ is a characteristic DW width ($w_0 \approx \pi l$ for $2\pi M_s^2 \ll K$). Notice that $\Delta \varphi_{\text{rel}}$ vanishes for $D = 0$ ($\bigcirc, \bigcirc'$) and for large $D$ ($\square$), where $\vartheta = \pi/2$ (Néel wall). As shown in Fig. 7.3(b), the contribution of $\Delta \varphi_{\text{rel}}$ enhances the effect of $\Delta \varphi_{\text{geom}}$ and merely shifts the critical internal angle $\vartheta$ for perfect destructive interference ($\Delta \varphi = 180^\circ$) to a somewhat lower value (more Bloch-like DW). Therefore the concept of the interferometer spin-wave switch is robust: we can always find

\footnote{Notice that the DMI strength $D$ used in Fig. 7.3(b) is significantly lower than the value suggested by the plot of Fig. 7.5(b) for $\vartheta \approx 45^\circ$. The data in Fig. 7.5 assume that the waveguide is infinite in the $y$ direction.}
Figure 7.5: (a) DW angle $\theta$ as a function of the ratio of DMI strength $D$ and dipolar interaction, for three film thicknesses $L$, taking $\sqrt{2\pi M_S^2/K} = 0.8$. The angle $\theta$ determines whether intermediate DWs (⋆′, ⋆) are closer to a Bloch or a Néel configuration. More “Néel-like” DWs (larger $\theta$) are obtained for stronger $D$. Conversely, the dipolar interaction penalizes the Néel configuration (this effect is weaker in thinner films). (b) Phase difference $\Delta \varphi$ between spin waves passing through DWs of opposite chiralities (⋆′ vs. ⋆), as a function of $\theta$, in the $k_x \to \infty$ limit, for two values of $\sqrt{2\pi M_S^2/K}$, taking $L = 3.0l$. The dominant contribution $\Delta \varphi_{\text{geom}}$ is separated out. The remaining contribution $\Delta \varphi_{\text{rel}}$ lowers the value of $\theta$ needed for destructive interference ($\Delta \varphi = 180^\circ$). For $\sqrt{2\pi M_S^2/K} = 0.9$, $\Delta \varphi_{\text{rel}}$ is larger than for 0.5 because a relatively strong DMI $D/(Aw_0^{-1})$ is then needed to obtain a given $\theta$. 
a DW angle $0^\circ < \vartheta < 90^\circ$ such that the phase difference $\Delta \varphi$ between opposite chiralities is exactly $180^\circ$. The desired value $\vartheta$ could then be realized by fine-tuning the DMI strength $D$ [Fig. 7.5(a)].

While Eq. (7.4) is derived in the short-wavelength limit, we have numerically solved the spin-wave normal-mode problem (see Chap. 5) for incoming waves of arbitrary wavenumber $k_x$. The phase shifts $\varphi'$, $\varphi$ depend significantly on $k_x$, as in the case without DMI ($\varphi = 2 \arctan (k_x l)^{-1}$ [141]), but the difference $\Delta \varphi = \varphi' - \varphi$ between the two chiralities, which is the relevant quantity in our interferometer, is weakly wavelength dependent for wavelengths comparable to (or shorter than) the DW width. The weak dependence of $\Delta \varphi$ on $k_x$ can, under certain approximations, also be derived analytically (see Sec. 7.D). This observation justifies our approach $k_x \to \infty$.

7.5 CONCLUSION AND OUTLOOK

In summary, we have shown that the interfacial Dzyaloshinskii–Moriya interaction in ultrathin magnetic films provides a new way of manipulation of spin waves. With this interaction, spin waves experience a different phase shift when passing through DWs of different chiralities, leading to either constructive or destructive interference in a two-branch interferometer. One can open or close the transmission of spin waves through the device by changing the DW chirality in one of the two branches. This opens the possibility of developing a memory element or transistor based on the manipulation of magnonic currents without charge transport.

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Appendix

7. A SYMMETRIES AND THE DZYALOSHINSKII–MORIYA INTERACTION

This section provides some background on the distinct forms of the Dzyaloshinskii–Moriya interaction (DMI) referred to in Sec. 7.3.

7. A. 1 Bulk versus interfacial DMI

For the DMI to be noticeable at the continuum level, it is necessary that the central inversion symmetry of the system is broken. This may be the case because the crystal structure itself is noncentrosymmetric (chiral or polar) or because the geometry of the system breaks the inversion symmetry, for instance near a surface or interface. A variety of continuum models for the DMI exist, which all arise from the same microscopic definition. The difference lies in the orientation of the Dzyaloshinskii–Moriya vectors $D_{ij}$ that define the interaction between atoms $i, j$.

We consider two high-symmetry special cases of the DMI. The continuum form $E_{DMI} = D \int m \cdot (\nabla \times m) \, dV$ describes a DMI that is chiral (it changes sign under any reflection) but which is otherwise completely isotropic. An alternative form $E_{DMI} = -2D \int m \cdot \nabla (\hat{n} \cdot m) \, dA$ pertains to a system that is polar: the inversion symmetry is broken by a director $\hat{n}$, which changes sign under central reflection; however, the system is achiral in that it remains invariant under any reflections that leave $\hat{n}$ intact. The system is isotropic only in the plane normal to $\hat{n}$.

The interface of a magnetic layer with another material defines a polar axis $\hat{n}$ (the interface normal), which gives rise to a DMI of the polar form (if we neglect any in-plane anisotropies). For this reason, the polar form is usually referred to as the interfacial DMI. The chiral but isotropic form of the DMI is usually referred to as the bulk DMI, since it is the simplest expression that models the DMI in a chiral crystal in bulk (again neglecting any anisotropies). A crystal structure is chiral if it cannot be superimposed onto its mirror image in any way. We remark, for completeness, that a bulk crystal may also show an “interfacial” DMI effect if it has a polar crystal structure [142].

The distinct effects of the bulk DMI and the interfacial DMI are well known from the theory of magnetic skyrmions, where it is found that the “bulk” model predicts Bloch skyrmions while the “interfacial” model predicts Néel skyrmions [143]. Similarly, it is found that a strong interfacial DMI tends to push a domain wall into a Néel configuration with a well-defined chirality, while a strong bulk DMI stabilizes one particular chirality of the Bloch domain wall.

In Sec. 7. A. 2, we link the cases of bulk DMI and interfacial DMI to atomistic toy models. In Sec. 7. A. 3, we explain that the preference of each type of DMI for
Figure 7.6: Directions of the Dzyaloshinskii–Moriya vectors $D_{ij}$ and the lattice displacement vectors $r_{ij}$ between atoms $i,j$. (a) For a bulk DMI, the $D_{ij}$ roughly point into the direction of $r_{ij}$. The $D_{ij}$ “diverge away from” (or “converge to”) a given atom $i$. (b) For an interfacial DMI, the $D_{ij}$ “curl around” a given atom $i$, with a sense determined by the normal $\hat{n}$.

one or the other type of domain wall (Bloch vs. Néel) is a direct consequence of its symmetries.

7.4.2 Atomistic and continuum models

This section shows how the continuum energy functionals for bulk (7.9) and interfacial (7.12) DMI can be derived from the atomistic definition Eq. (7.6), given appropriate choices for the Dzyaloshinskii–Moriya vectors $D_{ij}$.

At the level of individual magnetic moments, the DMI is by definition any interaction that can be written as

$$E_{DMI} = \sum_{ij} D_{ij} \cdot (m_i \times m_j),$$  

(7.6)

where $m_i$ is the microscopic magnetic moment on site $i$ and $D_{ij}$ is the Dzyaloshinskii–Moriya interaction vector between sites $i$ and $j$, which without loss of generality satisfies $D_{ij} = -D_{ji}$. For simplicity, let us assume that the magnetic atoms of the crystal are arranged as a Bravais lattice, where we use the symbol $\mathbf{z}_{ij} = r_j - r_i$ to represent any given (near-neighbor) lattice vector. (Notice that, for obvious reasons, the overall crystal structure of a noncentrosymmetric crystal must be more complicated than just a single Bravais lattice.)

By translation invariance in the bulk, the magnitude and direction of $D_{ij}$ must be a function of $\mathbf{z}_{ij}$ only. For simplicity, we shall assume that only nearest-neighbor interactions are important and that $\mathbf{z}_{ij}$ represents a nearest-neighbor lattice vector. If the material is isotropic, the only reasonable choice for the Dzyaloshinskii–Moriya vector is $D_{ij} = D \mathbf{z}_{ij}$, where $D$ is a (positive or negative) interaction strength. The Dzyaloshinskii–Moriya vectors $D_{ij}$ seem to “diverge” from any given site $i$, as shown schematically in Fig. 7.6(a).

Near a surface or interface, by contrast, the interface normal $\hat{n}$ introduces a preferential direction, which we could give a definite sense be defining it to
point from material $A$ into material $B$. By symmetry arguments, it is found that the $D_{ij}$ vectors “curl around” a given site $i$ with a well-defined sense induced by the direction of $\mathbf{n}$, as shown schematically in Fig. 7.6(b). Considering only the highest layer of magnetic atoms below the interface and only their nearest-neighbor interactions, the only natural choice in the absence of in-plane anisotropy is $D_{ij} = D \mathbf{n} \times \mathbf{z}_{ij}$, since $D_{ij}$ must be a vector-valued function linear both in $\mathbf{z}_{ij}$ (because of the rule $D_{ij} = -D_{ji}$) and in $\mathbf{n}$ (because the polar axis $\mathbf{n}$ is the only element that breaks inversion symmetry).

Passing to a continuum theory, Eq. (7.6) becomes

$$E_{\text{DMI}} = \int \sum \mathbf{D}(\mathbf{z}) \cdot [\mathbf{m} \times (\mathbf{z} \cdot \nabla) \mathbf{m}] \Omega^{-1} d^3 r,$$

(7.7)

where $\Omega$ represents a unit-cell volume and the sum is over all relevant near-neighbor lattice vectors. In the case of isotropic bulk DMI with only nearest-neighbor interactions, we substitute $\mathbf{D}(\mathbf{z}) = D \mathbf{z}$. Equation (7.7) becomes, in tensor notation,

$$E_{\text{DMI}} = \int \sum \epsilon_{abc} \epsilon_{ade} m_b \partial_d m_c \Omega^{-1} d^3 r,$$

(7.8)

where $\epsilon_{ab} = \sum \mathbf{z}_a \mathbf{z}_b$. Assuming $\epsilon_{ab} = \alpha \delta_{ab}$ for some scalar $\alpha > 0$ (isotropy), we get

$$E_{\text{DMI}} = -\alpha D \int m_b \epsilon_{bac} \partial_d m_c = -\alpha D \int \mathbf{m} \cdot (\nabla \times \mathbf{m}).$$

(7.9)

For the interfacial DMI, on the other hand, we have $D_{ij} = D \mathbf{n} \times \mathbf{z}_{ij}$, where $\mathbf{n}$ is the interface normal. For simplicity, we take $\mathbf{n} = \mathbf{z}$. We get

$$E_{\text{DMI}} = \sum \int (\mathbf{D}\epsilon_{abc} \mathbf{z}_b \mathbf{z}_c) \mathbf{D}\epsilon_{ade} m_d \mathbf{z}_f \partial_d m_e \Omega^{-1} d^3 r$$

(7.10a)

$$= \int \sum \epsilon_{abc} \epsilon_{ade} \mathbf{z}_b m_d \mathbf{z}_f \partial_d m_e \Omega^{-1} d^3 r$$

(7.10b)

$$= \int \sum \epsilon_{abc} \epsilon_{ade} \mathbf{z}_b m_d \mathbf{z}_f \partial_d m_e \Omega^{-1} d^3 r.$$  

(7.10c)

Notice that we now integrate over the interface plane only and assume that $\mathbf{m}$ does not depend on the perpendicular coordinate $z$ (here $\Omega$ represents a unit area). Assuming $\epsilon_{ab} = \alpha \delta_{ab}$, we get

$$E_{\text{DMI}} = \alpha D \int (z_b m_d \partial_c m_e - z_b m_e \partial_c m_d) \Omega^{-1} d^2 r$$

(7.11a)

$$= \alpha D \int [(\mathbf{z} \cdot \mathbf{m})(\nabla \cdot \mathbf{m}) - \mathbf{m} \cdot (\mathbf{z} \cdot \mathbf{m})] \Omega^{-1} d^2 r.$$  

(7.11b)

Using the divergence theorem, we get

$$E_{\text{DMI}} = -\frac{2 \alpha D}{\Omega} \int_U \mathbf{m} \cdot (\nabla m_z) \, d^2 r + \frac{\alpha D}{\Omega} \int_{\partial U} (m_z \mathbf{m}) \cdot d\mathbf{z}_{\partial U},$$

(7.12)

where $m_z(r) = \mathbf{z} \cdot \mathbf{m}(r)$. The boundary term is irrelevant if we integrate over all space ($U = \mathbb{R}^2$).
150 Chirality-dependent transmission of spin waves through domain walls

(a) Bloch walls

⊙ ⊗ ⊙ ⊗

reflection

x

y

z

(b) Néel walls

⊙ ⊗ ⊙ ⊗

180° rotation

n

Figure 7.7: Symmetries of the two types of domain wall. (a) The two distinct states of the Bloch wall are related by a reflection that leaves the surface normal \( \hat{n} \) invariant. The bulk DMI selects one Bloch state as the most favorable and the other Bloch state as the least favorable orientation. The interfacial DMI does not discriminate between the two. (b) The two distinct states of the Néel wall are related by 180° rotation that reverses the surface normal \( \hat{n} \). The interfacial DMI selects one Néel state as the most favorable and the other Néel state as the least favorable orientation. The bulk DMI does not discriminate between the two.

7.4.3 Effect on domain-wall energy

While the bulk DMI is chiral but isotropic, the interfacial DMI is polar but achiral (and isotropic under rotations around the \( \hat{z} \) axis). The two forms considered here are the only possibilities that satisfy these respective constraints, regardless of the details of the microscopic model. The same symmetry considerations determine how the two forms of the DMI respond to Bloch or Néel domain walls in a thin film with perpendicular anisotropy. In Fig. 7.7 we compare the two chirality states that exist of either type of wall. The bulk DMI selects one of the two chiralities of the Bloch wall as its most favorable orientation (energy minimum), and the other Bloch chirality as the least favorable orientation (energy maximum). On the other hand, the interfacial DMI selects one of the two chiralities of the Néel wall as its most favorable orientation, and the other Néel chirality as the least favorable orientation.

We can interpret this behavior as follows. The two chirality states of the Bloch wall are related by a reflection in the \( xz \) plane. Since such a reflection leaves
the \( z \)-director unchanged, it follows that the interfacial DMI cannot discriminate between the two chiralities of the Bloch wall. The bulk DMI can, because the bulk DMI is not invariant under any spatial reflections. The two chiralities of the Néel wall, on the other hand, are related by a 180° rotation around the \( y \) axis. Such a rotation is a symmetry of the bulk DMI (isotropy) but not of the interfacial DMI (reversal of \( \hat{n} \)). As a consequence, only the interfacial DMI discriminates between the two chiralities of the Néel wall.

The orientation of a Bloch domain wall will not be affected by a small bulk DMI, as both chiralities represent extrema of the bulk DMI. A small interfacial DMI, by contrast, causes a change in orientation of the Bloch domain wall, reorienting it slightly towards the favorable Néel state.

### 7.7 Dipolar Interaction

This section specifies the energy functionals used to describe the dipolar (magnetostatic) interaction in our micromagnetic simulations and numerical calculations.

Throughout this work, we assume that the magnetization is homogeneous in \( z \) inside the ferromagnetic film (uniform-mode approximation). In other words, we assume that the magnetization may be written as \( \mathbf{M}(x, y, z) = M_S \mathbf{m}(x, y, z) = M_S \Pi(z/L) \mathbf{m}(x, y) \), where \( L \) is the film thickness and where \( \Pi(\xi) = 1 \) for \( |\xi| < \frac{1}{2} \) and \( \Pi(\xi) = 0 \) otherwise. This simplification can be justified in the regime that \( L \lesssim l \), where \( l \) is the exchange length.

It can be derived (see, for example, Chap. [8]) that the total dipolar energy (defined per unit thickness) is given, in reciprocal space, by

\[
E_{\text{dip}} = 2\pi M_S^2 \int \tilde{m}_a^* (\mathbf{k}) \tilde{g}_{ab} (\mathbf{k}) \tilde{m}_b (\mathbf{k}) \frac{d^2 k}{(2\pi)^2} \tag{7.13}
\]

with

\[
\tilde{g}_{uv}(k_x, k_y) = (1 - N_k) \frac{k_uk_v}{k^2}, \quad (7.14a)
\]

\[
\tilde{g}_{uz}(k_x, k_y) = 0, \quad (7.14b)
\]

\[
\tilde{g}_{zz}(k_x, k_y) = N_k, \quad (7.14c)
\]

where \( k = \sqrt{k_x^2 + k_y^2} \) and where the indices \( u, v \) represent the in-plane coordinates \( x, y \). The function \( m_a(r) \) describes the \( a \) component of the normalized magnetization field. Its Fourier transform \( \tilde{m}_a (\mathbf{k}) \) is defined as

\[
\tilde{m}_a (\mathbf{k}) = \int \int m_a(r) e^{-i\mathbf{k}\cdot r} \, d^2 r. \tag{7.15}
\]

The demagnetizing factor \( N_k \) is given by

\[
N_k = \frac{1 - e^{-kL}}{kL}. \tag{7.16}
\]
We define $N_{k=0} = 1$ by continuity. Notice that $N_{k \to \infty} = 0$. We have omitted from Eq. (7.13) some contributions of the form $\int \int \| \mathbf{m}(k) \|^2 \, d^2k = (2\pi)^2 \int \int \| \mathbf{m}(r) \|^2 \, d^2r$, which are constant.

For a system with periodic boundary conditions that is defined on a rectangular grid, we evaluate the dipolar interaction in $O(n \log n)$ time using a fast Fourier transform (FFT). Finite magnetic elements, such as a waveguides with a finite width, might also, somewhat approximately, be simulated in this way, provided that sufficient zero padding is inserted around the object to minimize the influence of the other periodic copies.

For a one-dimensional magnetization profile $m(x)$, assumed to extend infinitely and uniformly in the $y$ direction ($k_y = 0$), we may write the dipolar energy in real space as

$$E_{\text{dip}} = 2\pi M_S^2 \int \int m_a(x') g_{ab}(x' - x) m_b(x) \, dx \, dx' \quad (7.17)$$

where

$$g_{xx}(x) = \delta(x) - \frac{1}{2\pi L} \log \left( 1 + \frac{L^2}{x^2} \right), \quad (7.18a)$$

$$g_{zz}(x) = \frac{1}{2\pi L} \log \left( 1 + \frac{L^2}{x^2} \right), \quad (7.18b)$$

$$g_{xy}(x) = g_{yy}(x) = g_{xz}(x) = g_{yz}(x) = 0. \quad (7.18c)$$

These expressions can be useful when evaluating the dipolar interaction for a system that is not periodic in $x$, such as a domain wall, where we have $m(-\infty) = \hat{z}$ while $m(\infty) = -\hat{z}$. We remark that an efficient numerical implementation of Eq. (7.17) might still evaluate the convolution through an FFT, but special care must be taken to correctly take into account the asymptotic behavior of $m(x)$ for $x \to -\infty$ and $x \to \infty$.

7.C PHASE SHIFT IN THE WKB APPROXIMATION ($k \to \infty$)

In this section, we provide a derivation of our expression for the relative part $\varphi_{\text{rel}}$ of the phase shift in the $k \to \infty$ limit, presented as Eq. (7.4). In Fig. 7.8, we evaluate the geometric phase shift $\varphi_{\text{geom}}$ and the expression (7.4) for $\varphi_{\text{rel}}$ for numerically calculated equilibrium domain-wall profiles $m(x)$, confirming the accuracy of Eqs. (7.3) and (7.5).

An equilibrium magnetization profile $m(x)$ is found by minimization of total energy $E$ under the constraint that $\| m(x) \| = 1$ for all $x$. It satisfies

$$\frac{\delta E}{\delta m(x)} = -h(x) m(x), \quad (7.19)$$

where the expression on the left-hand size denotes a functional derivative. The scalar-valued function $h(x)$ is a Lagrange multiplier. The equilibrium profile
\( \mathbf{m}(x) \) suffices to calculate the geometric phase induced by parallel transport of the basis vectors. However, to determine the relative phase we must solve the normal-mode equation, which can be expressed in coordinate-free form [23] as
\[
\int \frac{\delta^2 E}{\delta \mathbf{m}(x) \delta \mathbf{m}(x')} \cdot \mathbf{u}(x') \, dx' + h(x) \mathbf{u}(x) = - \frac{M_s}{|\gamma|} i \omega [\mathbf{m}(x) \times \mathbf{u}(x)] = \lambda(x) \mathbf{m}(x),
\] (7.20)
where \( \gamma \) is the gyromagnetic ratio, \( h(x) \) is fixed by Eq. (7.19), and where \( \lambda(x) \) is a Lagrange multiplier, under the constraint that \( \mathbf{m}(x) \cdot \mathbf{u}(x) = 0 \) at all \( x \). The frequency \( \omega \) is fixed by the wavenumber \( k_x \) of the spin wave far away from the domain wall.

Equation (7.20), when written out explicitly in terms of \( \mathbf{u}(x) = a(x) \hat{\mathbf{a}}(x) + b(x) \hat{\mathbf{b}}(x) \), becomes a complicated integro-differential equation. (Nonlocality arises from the dipolar interaction.) Here we find an approximate solution using the Wentzel–Kramers–Brillouin (WKB) approximation, which is exact in the short-wavelength limit. We assume that the solution \( \sim e^{i \int k'(x') \, dx' \phi} \) locally resembles a plane wave and replace any differential operator \( \partial_x \) with \( ik'_x \) (analogously for convolution operators) in order to solve for \( k'_x \) independently for each \( x \). For the interactions specified in Sec. 7.3 including interfacial DMI, we get
\[
\left( \begin{array}{c} A(k'_x)^2 \\
-\frac{M_s \omega}{2|\gamma|} i - Dm_y i k'_x \\
A(k'_x)^2 \\
M_s \omega i + Dm_y i k'_x \end{array} \right) \left( \begin{array}{c} a \\
b \end{array} \right) = 0,
\] (7.21)
where, anticipating the limit \( |k_x| \to \infty \), we have written only terms that are of at least first order in \( k'_x \) or \( k_x \). The exchange interaction acts as a scalar \( A(k'_x)^2 \) because we define the basis \( \hat{\mathbf{a}}(x), \hat{\mathbf{b}}(x) \) according to parallel transport. We substitute the dispersion relation far away from the domain wall, \( \omega \approx (2|\gamma|A/M_s)k^2_x \), again up to corrections of constant order. The characteristic equation of the matrix in Eq. (7.21) has four solutions. We are interested in the solution \( k'_x \) closest to \( k_x \), which is given by
\[
k'_x(x) = k_x + \frac{D}{2A} m_y(x) + \mathcal{O}(|k_x|^{-1}).
\] (7.22)
The phase induced by the domain wall on top of the phase factor \( e^{ik'_x x} \) is now given in the WKB approximation by \( \phi = \int_{-\infty}^{\infty} [k'_x(x) - k_x] \, dx \). We find
\[
\phi_{\text{rel}} = \frac{D}{2A} \int_{-\infty}^{\infty} m_y(x) \, dx,
\] (7.23)
up to a correction of order \( |k_x|^{-1} \).

Figure 7.8 shows a numerical evaluation of the two contributions \( \Delta \phi_{\text{geom}} \) and \( \Delta \phi_{\text{rel}} \) to the phase-shift difference \( \Delta \phi = \phi' - \phi \) between domain walls of opposite chirality (e.g., \( \star' \) and \( \star \)). To describe the behavior of \( \Delta \phi_{\text{rel}} \), we introduce
Figure 7.8: Phase-shift contributions $\Delta \varphi_{\text{geom}}$ and $\Delta \varphi_{\text{rel}}$ (for $k_x \to \infty$) obtained from the minimum-energy domain-wall profiles, which are numerically calculated as a function of the parameters $A$, $K$, $M_S$, $L$, and $D$ taking the dipolar interaction (7.17) into account. The variables $\theta$ and $w_0$ are also evaluated. (a) The geometric part $\Delta \varphi_{\text{geom}}$ follows Eq. (7.3) (solid line), with a deviation of at most a few degrees even in extreme cases (dashed line, $\sqrt{2 \pi M_S^2 / K} = 0.98$). (b) The relative part $\Delta \varphi_{\text{rel}}$ depends on the DMI strength $D$ (as compared to exchange) and on the domain-wall angle $\theta$; it follows approximately Eq. (7.5). For given $Dw_0/A$ and $\theta$, the dependence on the third dimensionless parameter is negligible. The dashed line indicates the relation between $D$ and $\theta$ if we fix $\sqrt{2 \pi M_S^2 / K} = 0.90$ and $L = 3.0l$. 
the characteristic domain-wall width \( w = \int \sqrt{m_x^2 + m_y^2} \, dx \), which we evaluate from the equilibrium profile \( m(x) \). The variable \( w_0 \) is then the value of \( w \) for an equivalent domain wall with \( D = 0 \) and the other parameters \((A, K, M_S, \text{ and } L)\) the same.

For completeness, we derive that the equivalent of Eq. (7.23) for a bulk DMI is \( \varphi_{\text{rel}} = -\left[D/(2A)\right] \int_{-\infty}^{\infty} m_x(x) \, dx \). Notice that the latter expression vanishes for any Bloch domain wall.

### 7.D Phase Shift in a Localized Model

In this section, we derive analytically, under certain approximations, the effect of an interfacial DMI on the equilibrium profile and phase shift of a Bloch domain wall. In particular, we present a closed-form expression (7.41) for the phase shift that is valid for arbitrary wavenumber \( k_x \). The expression suggests that the difference in phase shift between the two chiralities is almost independent of the wavelength of the spin wave.

Our analytical treatment complements the WKB approach of Sec. 7.C in two ways. First, it allows one to obtain a semianalytical expression for the equilibrium domain-wall profile, which in the WKB approach is taken as given (i.e., calculated numerically). Second, it provides an expression for the phase shift for arbitrary \( k_x \), where the WKB approach considers only the \( k_x \to \infty \) limit. The two approximations made are that we take into account the main effect of the dipolar interaction as an effective local interaction, and that we treat the effect of the DMI perturbatively (small \( D \)). The results presented here are consistent with the WKB expression (Sec. 7.C) if we substitute into (7.23) the equilibrium profile \( m(x) \) calculated for the approximated dipolar interaction [but notice that we need to add the geometric part \( \varphi_{\text{geom}} \) to Eq. (7.23) to obtain the total phase shift].

#### 7.D.1 Simplified treatment of dipolar interaction

In our analytical treatment, we follow Ref. [145] in including the dipolar effects (shape anisotropy) into a local anisotropy energy. We argue that, on scales much smaller than the film thickness \( L \), only the \( \delta \)-function part of Eq. (7.18a) is important and the effect of the dipolar interaction (7.17) reduces to a local anisotropy \( \int K_\perp m_x(x)^2 \, dx \) with \( K_\perp = 2\pi M_S^2 \). Notice that, even though the dipolar interaction is isotropic, the \( x \) coordinate plays a special role because we assume that \( \hat{x} \) is the domain-wall normal (magnetization is a function of \( x \) only). The total anisotropy energy is now given by

\[
E_{\text{ani}} = \int \left( -K m_x^2 + K_\perp m_x^2 \right) \, dx,
\]  

where \( K, K_\perp \) are positive constants. The in-plane anisotropy \( K_\perp \) models the dipolar interaction in introducing a preference for Bloch domain walls (flux closure).
This localized approximation is formally valid in the limit that the magnetization profile $m$ depends only on $x$ and extends infinitely not only in the $y$ but also in the $z$ direction. In practice, this means that we assume normal incidence of spin waves and a wavelength and exchange length much shorter than film thickness $L$. While these assumptions are unrealistic in most practical cases, they allow us to obtain some analytical results that are qualitatively correct.

In addition to the easy-axis and in-plane anisotropies, we take into account the interfacial DMI

$$ E_{\text{DMI}} = -2D \int m_x(x)m'_z(x) \, dx $$

and the usual exchange term $E_{\text{ex}} = A \int \|m'(x)\|^2 \, dx$, where a prime denotes a derivative with respect to $x$.

### 7.D.2 Equilibrium profile

In a one-dimensional system, the magnetization profile may be described by two functions $\theta(x), \phi(x)$, defined by

$$ m(x) = \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}. $$
The equilibrium magnetization profile of the domain wall is a solution of

\[
\frac{\delta E}{\delta \theta(x)} = -2A\theta'' + A(\phi')^2 \sin 2\theta + (K + K_\perp \cos^2 \phi) \sin 2\theta - 2D \sin^2 \theta \sin \phi \phi' = 0,
\]

\[
(7.27a)
\]

\[
\frac{\delta E}{\delta \phi(x)} = 2A \sin \phi'' + 4A \cos \theta' \phi' + 2K_\perp \sin \theta \sin \phi \cos \phi - 2D \sin \theta \sin \phi \phi' = 0,
\]

\[
(7.27b)
\]

where the expressions on the left-hand side are functional derivatives of total energy.

For a system with only exchange \(A\) and uniaxial anisotropy \(K\) \((D = K_\perp = 0)\), it is well known that the equilibrium profile, assuming \(m(-\infty) = \hat{z}\) and \(m(\infty) = -\hat{z}\), is given by

\[
\theta_0(x) = 2 \arctan[\exp(x/l)],
\]

\[
(7.28a)
\]

\[
\phi_0(x) = \pm \pi/2.
\]

\[
(7.29a)
\]

The sign \((\pm)\) defines the chirality of the domain wall. Both chiralities represent equivalent stable energy minima. The positive sign corresponds to the configuration \(\bigcirc'\); the negative sign to \(\bigcirc\).

As a result of the competition with \(K_\perp\), the interfacial DMI \(7.25\) modifies the domain-wall profile, as calculated numerically in Ref. \[134\]. Here, we treat the DMI as a small perturbation \((|D| \ll K_\perp l)\). It can be derived that we get, to first order in \(D\), a minimum-energy configuration

\[
\theta_0(x) = 2 \arctan[\exp(x/l)],
\]

\[
(7.30a)
\]

\[
\phi_0(x) = \pm \pi/2 \pm \frac{D}{K_\perp l} q\left(\frac{x}{l}; s\right),
\]

\[
(7.30b)
\]

where \(s = \sqrt{K/K_\perp}\). Perpendicular magnetization implies \(s > 1\). The function \(q(\zeta;s)\), shown in Fig. 7.9, is uniquely defined as the solution of

\[
\left(-s^2 \cosh^2 \zeta \frac{d}{d \zeta} \operatorname{sech}^2 \zeta \frac{d}{d \zeta} + 1\right) q = \operatorname{sech} \zeta
\]

\[
(7.31)
\]

that is even and vanishes at infinity (particular part).

It is useful to compare Eq. \(7.30\) to the equilibrium profile that is obtained if a bulk DMI instead of the interfacial DMI is present. In that case, we obtain the same equilibrium profile as in Eq. \(7.29\); in other words, the bulk DMI has no effect on the profile of the Bloch domain wall. The reason is that, given any Bloch profile, where \(\phi(x) = \pm \pi/2\) and \(\theta(x)\) is arbitrary, the functional derivatives \(\delta E_{\text{DMI}}/\delta \theta(x)\) and \(\delta E_{\text{DMI}}/\delta \phi(x)\) of the bulk DMI energy \(E_{\text{DMI}} = D \int m \cdot (\nabla \times m) \, dx = -2D \int m_y m_z' \, dx\) with respect to the profile functions \(\theta(x), \phi(x)\) vanish.
7.D.3  Linearized dynamics

The dynamics is described by the Landau–Lifshitz–Gilbert (LLG) equation without damping

\[ -\frac{M_S}{|\gamma|} \frac{\partial \mathbf{m}}{\partial t} = \mathbf{m} \times \left( -\frac{\delta E}{\delta \mathbf{m}(x, y)} \right), \]  

(7.32)

where \( M_S \) is the saturation magnetization, \( \gamma \) is the gyromagnetic ratio, and \( E = E_{\text{ex}} + E_{\text{ani}} + E_{\text{DMI}} \) is the total interaction energy. Let us consider small variations \( \delta \theta = \theta(t, x, y) - \theta_0(x) \) and \( \delta \phi = \phi(t, x, y) - \phi_0(x) \) around Eq. (7.30). We get a linearized equation of motion

\[
\begin{pmatrix}
-A\left(\partial_x^2 + \partial_y^2\right) + K(1 - 2 \text{sech}^2 x/l) & -[M_S/(2|\gamma|)]\partial_t \mp (2D/l)\hat{F} \\
[M_S/(2|\gamma|)]\partial_t \mp (2D/l)\hat{F}^\dagger & -A\left(\partial_x^2 + \partial_y^2\right) + K(1 - 2 \text{sech}^2 x/l) + K_\perp
\end{pmatrix} \times \begin{pmatrix}
\delta \theta \\
\text{sech}(x/l)\delta \phi
\end{pmatrix} = 0
\]  

(7.33)

where

\[ \hat{F} = (l/2) \text{sech}(x/l)h(x/l; s)\partial_x \cosh(x/l) + q(x/l; s) \tanh(x/l) \]  

(7.34)

with \( h = s^2q'' - q \) is the perturbation caused by the DM interaction, to first order in \( D \). Notice that \( \hat{F} \) is odd in \( x \) and breaks reflection symmetry. (The system remains invariant under a simultaneous reflection and change in polarity, which is equivalent to a rotation around \( \hat{z} \).)

7.D.4  Transmission phase shift

We assume that the solutions are periodic in \( t \) and \( y \). Equation (7.33) becomes a Hamiltonian normal-mode problem (see Chap. 5). Away from the domain wall \((|x| \gg l)\), the spin waves take the form

\[ \begin{pmatrix}
\delta \theta \\
\text{sech}(x/l)\delta \phi
\end{pmatrix} = \begin{pmatrix}
-i\sqrt{\frac{1}{K+Ak^2}} \\
-i\sqrt{\frac{1}{K+K_\perp+Ak^2}}
\end{pmatrix} e^{i(\omega t+k_xx+k_yy)}, \]  

(7.35)

with \( \omega = (2|\gamma|/M_S)\sqrt{(K+Ak^2)(K+K_\perp+Ak^2)} \), where \( k = \sqrt{k_x^2+k_y^2} \).

We now calculate the reflection (\( r \)) and transmission (\( t \)) amplitudes of an incoming spin wave with wavenumber \( k_x \) that propagates in the positive-\( x \) direction. The amplitudes \( r', t' \) refer to an incoming spin wave wave that propagates in the negative-\( x \) direction (wavenumber \( -k_x \)) and approaches the domain wall from the other side. Equation (7.35) defines the scattering states.

For \( D = 0 \), the analytic solutions of Eq. (7.33) are well known [34]. The propagating-wave solutions take the form

\[ f(x) e^{i(\omega t+k_xx+k_yy)}, \]  

(7.36)
where \[ f(x) = -ik_xl + \tanh(x/l). \] 

It follows immediately that

\[
\begin{pmatrix}
  r' \\
  t'
\end{pmatrix} =
\begin{pmatrix}
  0 & e^{i\varphi_0} \\
  e^{i\varphi_0} & 0
\end{pmatrix}
\begin{pmatrix}
  r \\
  t
\end{pmatrix},
\] \tag{7.38}

where

\[
\varphi_0 = \arg \left( \frac{ik_xl - 1}{ik_xl + 1} \right) = 2 \arctan \frac{1}{k_xl}.
\] \tag{7.39}

Notice that the domain wall shows total transmission in the localized model\[3\]

We now calculate the effect of the interfacial DMI on the transmission phase and amplitude. As above, we take into account the DMI to first order in the interaction strength \(D\). With some algebraic work, we obtain

\[
\begin{pmatrix}
  r' \\
  t'
\end{pmatrix} =
\begin{pmatrix}
  0 & e^{i(\varphi_0 - \varphi_1)} \\
  e^{i(\varphi_0 + \varphi_1)} & 0
\end{pmatrix}
\begin{pmatrix}
  r \\
  t
\end{pmatrix},
\] \tag{7.40}

where \(\varphi_0\) is again given by Eq. (7.39), and where

\[
\varphi_1 = \mp \pi \left( \frac{D}{Kl} + \frac{D}{K_{\perp}l} \right) \frac{\sqrt{(K + Ak^2)(K + K_{\perp} + Ak^2)}}{2K + K_{\perp} + 2Ak^2}.
\] \tag{7.41}

Notice that only \(\varphi_1\) depends on chirality \(\pm\). Since (7.33) defines the scattering problem relative to the basis vectors \(\hat{\theta}, \hat{\phi}\), which have a fixed orientation at \(x = -\infty\) and at \(x = \infty\), the expression (7.41) includes both the geometric and relative parts of the phase shift.

Unlike \(\varphi_0\), the chirality-dependent part \(\varphi_1\) depends only very weakly on wavenumber \(k\); it is, in fact, almost constant in \(k\), as shown in Fig. 7.10. We find numerically that this conclusion even holds if \(D\) is not small or if the full dipolar interaction (7.17) is taken into account in the scattering problem, at least in the regime where the wavelength is comparable to the domain-wall width or shorter. This justifies our approach of taking the \(k_x \to \infty\) limit in the calculation of \(\varphi_{\text{rel}}\) in Sec. 7.C (the geometric part \(\varphi_{\text{geom}}\) is independent of \(k_x\) by definition).

\[3\] However, if the full dipolar interaction is taken into account, we find a nonzero reflection for long-wavelength spin waves (see also, for example, [141]).
Figure 7.10: Dependence of the phase shifts $\phi_0$ [given by Eq. (7.39)] and $\phi_1$ [given by Eq. (7.41)] on wavenumber $k$. For a spin wave propagating in the positive-$x$ direction, the total phase shift induced by the domain wall is the sum $\phi_0 + \phi_1$. Notice that $\phi_1$ is almost constant in $k$. Since only the part $\phi_1$ depends on domain-wall chirality ($\pm$), the difference in phase shift between the two chiralities – in other words, the phase difference obtained on the right-hand side of the interferometer shown in Fig. 7.2(d) – is also almost independent of $k$. 
The dipolar (magnetostatic) interaction dominates the behavior of spin waves in magnetic films in the long-wavelength regime. In an in-plane magnetized film, volume modes exist with a negative group velocity (backward volume magnetostatic spin waves), in addition to the forward surface-localized mode (Damon–Eshbach). Inside the film of finite thickness $L$, the volume modes have a non-trivial spatial dependence, and their two-dimensional dispersion relations $\omega(k)$ can be calculated only numerically. We present explicit perturbative expressions for the profiles and frequencies of the volume modes, taking into account an in-plane applied field and uniaxial anisotropy, for the regimes $\|kL\| \gg 1$ and $\|kL\| \ll 1$, which together provide a good indication of the behavior of the modes for arbitrary wavevector $k$. Moreover, we derive a very accurate semianalytical expression for the dispersion relation $\omega(k)$ of the lowest-frequency mode that is straightforward to evaluate using standard numerical routines. Our results are useful to quickly interpret and control the excitation and propagation of spin waves in (opto-)magnetic experiments.

This chapter has been submitted as
8.1 Introduction

The dipolar interaction endows magnetostatic (long-wavelength) spin waves with a very peculiar dynamics. In an in-plane magnetized ferromagnetic film, their dispersion shows a strong anisotropy originating from the magnetization vector \( \mathbf{M} \). Spin waves propagating through the volume of the film appear to move backwards as their group velocity is opposite to their phase velocity (backward volume magnetostatic spin-wave modes, BVMSW) [24]. Conversely, spin waves with a wavevector \( \mathbf{k} \perp \mathbf{M} \) tend to localize near the surface of the film in Damon–Eshbach (DE) modes [35], which are forward modes. The surface localization of DE modes is exponential, with a decay length inversely proportional to the perpendicular component of \( \mathbf{k} \) [54].

While the backward volume propagation of parallel spin waves \( \mathbf{k} \parallel \mathbf{M} \) is well known, in the case of perpendicular propagation \( \mathbf{k} \perp \mathbf{M} \) usually only the DE modes are considered [54, 138, 147]. The DE modes are the most likely to be excited by a microstrip antenna in the Damon–Eshbach geometry [148] and show unusual features such as nonreciprocal propagation [149]. However, in a film of finite thickness, BVMSWs are not restricted to the case \( \mathbf{k} \parallel \mathbf{M} \) and can exist with any (in-plane) wavevector \( \mathbf{k} \); in particular, perpendicularly propagating volume modes also exist and have frequencies below the DE branch [146, 150]. The BVMSW modes are, in fact, the dominant modes in optomagnetic [23, 25] experiments as in Ref. [26], where the two-dimensional profile of the initial excitation (almost homogeneous in the film thickness) can be shaped and the subsequent dynamics observed with spatial and temporal resolution.

The propagation of spin waves can only be understood if their dispersion relation is known. For exchange spin waves (wavelength small compared to the exchange length \( l \)), as well as for spin waves propagating in an ultrathin film (thin compared to \( l \)), the dispersion relations are given by fairly simple analytical expressions [147]. On micrometer lengthscales, however, exchange interactions are negligible and the film thickness \( L \) remains as the only characteristic lengthscale of the system. In this regime, the film can never be considered as effectively two-dimensional, and the perpendicular profile of the volume spin-wave modes, as shown in Fig. 8.1, is essential for an accurate description.

Because of the nontrivial profile of the mode, the true dispersion relation of the volume modes can in principle be found only numerically [26, 146]. To our knowledge, the closed-form expressions that have been derived, while useful, rely on either an effectively two-dimensional approach [151–154] or on an artificial decoupling of Fourier components [155]. References [36] and [148], on the other hand, provide an analytical treatment that is in principle exact but which in practice requires the numerical solution of a set of coupled transcendental equations.

In this article, we study the dispersion and depth profile of BVMSW modes, with a particular focus on the case that \( \mathbf{k} \parallel \mathbf{M} \). The profiles of such modes show an interesting asymmetry in the perpendicular coordinate \( z \), reminiscent of the
Figure 8.1: Spin-wave modes in ferromagnetic films with a thickness $L$ larger than the exchange length $l$ have a nontrivial perpendicular profile $\delta y(z), \delta z(z)$ inside the film ($0 < z < L$). We take $\hat{z}$ as the film normal and $\hat{x}$ as the direction of magnetization $M$, which is in the plane of the film. In the uniform-mode approximation, we assume that $\delta y(z)$ and $\delta z(z)$ are constant functions.

We derive explicit expressions for the mode profiles $\delta y(z), \delta z(z)$, up to first order in $kL$ or $(kL)^{-1}$. Such expressions allow one, for example, to estimate to what extent the various spin-wave modes couple to an excitation homogeneous in $z$ [26]. We also present, in Table 8.1, simple analytical expressions describing the asymptotic behavior of the dispersion relations of the BVMSW modes.

In addition, we present a practical and very accurate semianalytical approximation to the dispersion relation of the lowest-frequency BVMSW mode, valid on the entire $k$ plane. Our expression (8.62) retains the mathematical structure of an eigenvalue equation and is equivalent to the solution of a quartic polynomial equation. It can be evaluated simply and cheaply using standard numerical routines. We believe that our results are useful for a quick interpretation of experiments and for the development of new applications of directional control of optomagnetic spin-wave excitation [26, 32].

This article is organized as follows. In Sec. 8.2, we derive, as a first step, the spin-wave dispersion relation in the uniform-mode (effectively two-dimensional) approximation valid for ultrathin films. In Sec. 8.3, we formulate the normal-mode problem for films of arbitrary thickness. In Sec. 8.4, we describe the typical behavior of the mode profiles and the dispersion relations. We successfully compare the numerical solutions to our perturbative results, which we present in detail in Sec. 8.5. In Sec. 8.6, we present our semianalytical expression for the dispersion relation. Section 8.7 provides a summary of our main conclusions.

8.2 uniform-mode analysis

In this section, we review the derivation of the dispersion relation of spin waves in a film in the uniform-mode approximation, where we assume that the precession amplitudes $\delta y(z), \delta z(z)$ of the magnetization inside the film do not depend
on the perpendicular coordinate \( z \). Formally, this approximation is valid only in the limit of ultrathin films \( (L \ll l) \). While there are some important qualitative differences between the uniform-mode expression and the dispersion relation for large film thickness \( L \), it provides a useful first indication of the dispersion behavior of the BVMSW modes.

Specifically, taking \( \hat{z} \) as the film normal, we assume

\[
\mathbf{M}(t, x, y, z) = M_S \mathbf{m}(t, x, y) \Pi^*(\frac{z}{L}),
\]

where \( M_S \) is saturation magnetization, unit vector \( \mathbf{m}(t, x, y) \) is the magnetization direction, and \( \Pi^*(z/L) \) is the rectangular function

\[
\Pi^*(z/L) = \begin{cases} 
1 & \text{for } 0 < z/L < 1 \\
0 & \text{for } z/L < 0 \text{ or } z/L > 1 
\end{cases}.
\]

In view of Sec. 8.5.4, it is convenient to define \( \Pi^*(0) = \Pi^*(1) = \frac{1}{2} \).

### 8.2.1 Magnetostatic energy: General case

It is well known that the interaction between two magnetic point dipoles \( \mathbf{v}_i, \mathbf{v}_j \) located at \( \mathbf{r}_i, \mathbf{r}_j \) is given by

\[
E_{\text{dip}} = -\frac{\mu_0}{4\pi} \frac{3(\mathbf{v}_i \cdot \mathbf{e}_{ij})(\mathbf{v}_j \cdot \mathbf{e}_{ij}) - \mathbf{v}_i \cdot \mathbf{v}_j}{r_{ij}^3},
\]

where \( r_{ij} = \mathbf{r}_j - \mathbf{r}_i, r_{ij} = ||\mathbf{r}_{ij}||, \) and \( \mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij} \). For a continuous magnetization distribution \( \mathbf{M}(\mathbf{r}) = M_S \mathbf{m}(\mathbf{r}) \), total energy becomes, in tensor notation,

\[
E_{\text{dip}} = \frac{1}{2} \mu_0 M_S^2 \int \int m_a(\mathbf{r}') f_{ab}(\mathbf{r}' - \mathbf{r}) m_b(\mathbf{r}) \, d^3r' \, d^3r
\]

\[
= \frac{1}{2} \mu_0 M_S^2 \int \tilde{m}_a^*(\mathbf{k}) f_{ab}(\mathbf{k}) \tilde{m}_b(\mathbf{k}) \frac{d^3k}{(2\pi)^3},
\]

where \( a, b \) represent the spatial directions \( x, y, z \); \( \tilde{m}_a(\mathbf{k}) \) is the Fourier transform of \( m_a(\mathbf{r}) \); and where we define

\[
f_{ab}(\mathbf{r}) = -\frac{A_{ab}^{(2)}(\mathbf{r})}{4\pi r^5}.
\]

The factor 1/2 is a double-counting correction. The functions \( A_{ab}^{(2)}(\mathbf{r}) \) are the second-order spherical polynomials

\[
A_{ab}^{(2)}(\mathbf{r}) = 3r_a r_b - \delta_{ab} r_c r_c
\]
We use the nonunitary definition of the Fourier transform $\tilde{f}(k) = \int f(x)e^{-ik\cdot x}\,dx^n$, where $n$ is the dimension of space. The inverse transform is given by $f(x) = (2\pi)^{-n}\int\tilde{f}(k)e^{ik\cdot x}\,dk^n$. We use the result that, for a spherical polynomial $A^{(m)}(r)$ of order $m$, the Fourier transform of a function of the form $f(r) = f_0(r)A^{(m)}(r)$ is given by $\tilde{f}(k) = f_0(k)A^{(m)}(k)$, where $f_0(k) = \frac{1}{(2\pi)^{n/2}\Gamma(-n-2m)}\int f_0(r)r^{-n-2m-2}\,f_{n+2m-2}(kr)\,dr$ with $I_k(z)$ a Bessel function of the first kind.

$A^{(2)}_{xx}(r) = 3x^2 - r^2$. The Fourier transform of Eq. 8.5 is given by

$$\tilde{f}_{ab}(k) = \frac{A_{ab}^{(2)}(k)}{3k^2}. \quad (8.7)$$

### 8.2.2 Magnetostatic energy: Uniform mode

For a magnetization profile (8.1) that is homogeneous in $z$ inside the film, we have

$$E_{\text{dip}} = \frac{1}{2}\mu_0 M^2_S \int m_a(r')g_{ab}(r' - r)m_b(r)\,d^2r'\,d^2r$$

$$= \frac{1}{2}\mu_0 M^2_S L \int \tilde{m}_a(k)\tilde{g}_{ab}(k)\tilde{m}_b(k)\frac{d^2k}{(2\pi)^2}, \quad (8.8)$$

where

$$\tilde{g}_{ab}(x,y) = \frac{1}{L} \int \int \Pi^*(\frac{z'}{L})f_{ab}(x,y,z' - z)\Pi^*(\frac{z}{L})\,dz'\,dz. \quad (8.9)$$

By the convolution theorem,

$$\tilde{g}_{ab}(k_x,k_y) = L \int_{-\infty}^{\infty} \tilde{f}_{ab}(k_x,k_y,k_z) \operatorname{sinc}^2 \frac{k_zL}{2} \frac{dk_z}{2\pi}, \quad (8.10)$$

where we have used the Fourier transform $\tilde{\Pi}^*(kL) = e^{-ikL/2} \operatorname{sinc}(kL/2)$ with $\operatorname{sinc} \phi = (\sin \phi)/\phi$. We evaluate

$$\tilde{g}_{uv}(k_x,k_y) = (1 - N_k) \frac{k_xk_y}{k^2} - \frac{1}{3} \delta_{uv}, \quad (8.11a)$$

$$\tilde{g}_{uz}(k_x,k_y) = 0, \quad (8.11b)$$

$$\tilde{g}_{zz}(k_x,k_y) = N_k - \frac{1}{3}, \quad (8.11c)$$

where $u,v$ represent the in-plane coordinates $x,y$. The demagnetizing factor $N_k$ is given by

$$N_k = \frac{1 - e^{-kL}}{kL}. \quad (8.12)$$

We define $N_{k=0} = 1$ (continuity); notice that $N_{k\to\infty} = 0$.

Notice that, if we assume that the magnetization of the film is completely homogeneous ($k = 0$), we get $E_{\text{dip}} = \frac{1}{2}\mu_0 M^2_S V\left(-\frac{1}{3}m_x^2 - \frac{1}{3}m_y^2 + \frac{2}{3}m_z^2\right)$, where $V$ is...
the total film volume. Due to the constraint $|\mathbf{m}| = 1$, this is effectively a hard-axis anisotropy of strength $\frac{1}{2} \mu_0 M_S^2$, where $\mathbf{z}$ is the hard axis. This confirms that the dipolar interaction favors in-plane magnetization, and gives the well-known condition $K > \frac{1}{2} \mu_0 M_S^2$ for perpendicular (out-of-plane) magnetization due to an intrinsic perpendicular anisotropy $K$ in the absence of an applied field. As a second limiting case, let us consider a system where $\mathbf{m}(x, y)$ depends only on $x$ ($k_y = 0$) and where $L$ is very large (thick film, $L \gg |k_x|^{-1}$). For a fixed $k_x \neq 0$, we get, in the limit $L \to \infty$, an effective local hard-axis anisotropy of strength $\frac{1}{2} \mu_0 M_S^2$, where the hard axis is $\mathbf{x}$.

8.2.3 Linearization

In addition to the dipolar interaction, we take into account the usual micromagnetic energy functionals for exchange $E_{ex} = AL \int (|\mathbf{d} \times \mathbf{m}|^2 + |\mathbf{d} \cdot \mathbf{m}|^2) \, d^2r$, intrinsic easy-axis anisotropy $E_{ani} = -KL \int m_z^2 \, d^2r$, and Zeeman energy $E_H = -\mu_0 M_S H_x L \int m_x \, d^2r$. The applied field $H_x$ fixes the equilibrium magnetization along $\mathbf{x}$.


$$\frac{\partial \mathbf{m}}{\partial t} = \frac{|\gamma|}{M_S L} \mathbf{m} \times \frac{\delta E}{\delta \mathbf{m}(r)}$$

around the equilibrium $\mathbf{m}(r) = \mathbf{x}$ gives, very generally (see Chap. 5),

$$\left( \begin{array}{c} \frac{\partial t}{\partial x} \\ -\frac{M_S L}{|\gamma|} \frac{\partial t}{\partial y} \\ -\frac{\partial t}{\partial z} \\ \frac{\delta E}{\delta x} \\ \frac{\delta E}{\delta y} \\ \frac{\delta E}{\delta z} \end{array} \right) \left( \begin{array}{c} \delta y \\ \delta x \\ \delta z \end{array} \right) + \int \left( \begin{array}{ccc} \frac{\delta^2 E}{\delta y^2} & \frac{\delta^2 E}{\delta y \delta z} \\ \frac{\delta^2 E}{\delta z \delta y} & \frac{\delta^2 E}{\delta z^2} \end{array} \right) \left( \begin{array}{c} \delta y' \\ \delta z' \end{array} \right) \, d^2r' = 0,$$

where $\gamma$ is the gyromagnetic ratio and where the functional derivatives of $E$ are to be evaluated for the equilibrium configuration $\mathbf{m}(r) = \mathbf{x}$. For brevity, we write $\delta y$ for $\delta m_y(t, r)$ and $\delta y'$ for $\delta m_y(t, r')$. The functions $\delta y, \delta z$ represent the infinitesimal deviation of magnetization $\mathbf{m}$ from its equilibrium direction.

Substituting $E = E_{ex} + E_{ani} + E_H + E_{dip}$ and passing to Fourier space, Eq. (8.14) becomes

$$\left( \begin{array}{c} \frac{H_x}{M_S} + \frac{2Ak^2}{\mu_0 M_S} + (1 - N_k) \frac{k_y^2}{k^2} \\ \frac{1}{\mu_0 |\gamma| M_S} i \omega \\ \frac{1}{\mu_0 |\gamma| M_S} i \omega \end{array} \right) \cdot \left( \begin{array}{c} \tilde{\delta y} \\ \tilde{\delta x} \\ \tilde{\delta z} \end{array} \right) = 0,$$

(8.15)

The positive solution for $\omega$ in the characteristic equation gives the dispersion relation (cf. Refs. [147], [138], [156], [157])

$$\omega = |\gamma| \mu_0 \sqrt{\left[ \frac{2Ak^2 - 2K}{\mu_0 M_S} + H_x + M_S N_k \right] \left[ \frac{2Ak^2}{\mu_0 M_S} + H_x + M_S (1 - N_k) \sin^2 \theta \right]},$$

(8.16)
8.2 Uniform-mode analysis

Figure 8.2: Dispersion relation of BVMSWs in the uniform-mode approximation, for $H_x = 80 \text{kA/m}$, $K = 3.5 \text{kJ/m}^3$, $L = 100 \text{μm}$, and $M_S = 110 \text{kA/m}$. We neglect exchange $A$, assuming that wavenumber $k$ is much smaller than the inverse exchange length $1/l = \sqrt{\mu_0 M_S^2/(2A)}$. Notice that, in the magnetostatic regime, $\omega$ (mostly) decreases in $k_x$, giving the spin waves a backward-propagating character. We define $\theta$ as the polar angle of the wavevector $\mathbf{k} = (k_x, k_y) = (k \cos \theta, k \sin \theta)$. 
where $\vartheta$ is the polar angle of wavevector $k$, as shown in Fig. 8.2.

Figure 8.2 shows an example of the dispersion relation (8.16) for typical parameters. Notice that the dispersion relation has a cusp at the origin $k = 0$. With the exception of a small area right above and below the point $k = 0$, the frequency decreases with increasing $k$. This implies that the spin waves have a group velocity that is opposite to their wavevector $k$ (backward modes).

### 8.3 General Formulation

We now turn to the general case that film thickness $L$ is not small as compared to exchange length $l$, and the dependence of the modes on the perpendicular coordinate $z$ cannot be neglected. For simplicity, we shall, in fact, assume that both film thickness $L$ and wavelength $2\pi/k$ are much greater than exchange length $l$. This allows us to neglect the exchange energy $E_{ex}$. In the following, whenever we refer to the short-wavelength limit $k \to \infty$, we mean the regime where the wavelength is much less than film thickness ($kL \gg 1$) but still well above the exchange length $l$ (magnetostatic spin waves, $kl \ll 1$).

Fixing wavenumber $k = (k_x, k_y)$, we allow the spin-wave mode to have an arbitrary profile $\delta y(z), \delta z(z)$ inside the film. Analogously to Eq. (8.15), we obtain an eigenvalue equation

\[
\begin{pmatrix}
H_x \hat{S} + M_S \hat{D}^{yy} \\
M_S \hat{D}^{yz}
\end{pmatrix}
\begin{pmatrix}
\delta y \\
\delta z
\end{pmatrix}
= \frac{\omega}{\mu_0|\gamma|} \begin{pmatrix}
0 & i\hat{S} \\
- i\hat{S} & 0
\end{pmatrix}
\begin{pmatrix}
\delta y \\
\delta z
\end{pmatrix},
\]  

(8.17)

where $\delta y(z), \delta z(z)$ are now functions of $z$, supported on the interval $0 \leq z \leq L$. Here $\hat{S}$ represents the identity operator. The operators $\hat{D}^{ab}$ may be represented in Fourier space as

\[
\hat{D}^{ab}(k_x, k_y) = \frac{k_x k_y}{k_x^2 + k_y^2 + k_z^2},
\]  

(8.18)

where $k_x, k_y$ should be treated as numerical constants (parameters of $\hat{D}^{ab}$) but $k_z$ as an operator $\hat{k}_z = -i\partial_z$ acting on the functions $\delta y(z), \delta z(z)$.

The functions $\delta y(z), \delta z(z)$ vanish outside the interval $0 < z < L$. The finite film thickness $L$ quantizes the modes that can be excited for any given $k_y, k_z$. We label the modes as $n = 1, 2, \ldots$ in order of increasing $\omega > 0$.

It is convenient to normalize the solutions $\Psi_+$ to satisfy

\[
\Psi_+^\dagger \hat{Q} \Psi_+ = \frac{1}{\mu_0|\gamma|} \begin{pmatrix}
\delta y \\
\delta z
\end{pmatrix}^\dagger \begin{pmatrix}
0 & i\hat{S} \\
- i\hat{S} & 0
\end{pmatrix}
\begin{pmatrix}
\delta y \\
\delta z
\end{pmatrix}
= \frac{2}{\mu_0|\gamma|} \text{Im} \int_0^L \delta y(z) \delta z^*(z) \, dz = 1,
\]

(8.19)
where the asterisk denotes complex conjugation. Because the cross elements $M_S \hat{D}^{yz}$ in Eq. (8.17) are Hermitian, we may assume without loss of generality that $\delta y(z)$ is purely real and $\delta z(z)$ is purely imaginary. Notice that if $\Psi_+$ is a solution of Eq. (8.17) with eigenvalue $\omega$, its complex conjugate $\Psi_-$ is a solution with eigenvalue $-\omega$ (and norm $\Psi_+^\dagger \hat{Q} \Psi_- = -1$). The fact that solutions occur in conjugate pairs is a result of the Hamiltonianness of the normal-mode problem (see Chap. 5). The negative-$\omega$ solution $\Psi_-$ is redundant.

8.3.1 Asymptotic frequencies

Fixing the polar angle $\vartheta$, we now turn to the behavior of Eq. (8.17) in the limits $k \to 0$ and $k \to \infty$ along a radial half-line $(k_x, k_y) = (k \cos \vartheta, k \sin \vartheta)$. For $k \to \infty$, the operator $\hat{D}^{yy}$ reduces to

$$\hat{D}^{yy} = \frac{k_y^2}{k_x^2 + k_y^2 + k_z^2} \to \left( \sin^2 \vartheta \right) \hat{S},$$

(8.20)

which is a simple scalar operator; analogously, we find

$$\begin{pmatrix} \hat{D}^{yy} & \hat{D}^{yz} \\ \hat{D}^{yz} & \hat{D}^{zz} \end{pmatrix} \to \begin{pmatrix} (\sin^2 \vartheta) \hat{S} & 0 \\ 0 & 0 \end{pmatrix}.$$ (8.21)

We conclude that all modes $n$ are degenerate in the limit $k \to \infty$, since now only the identity operator $\hat{S}$ acts on $\delta y(z), \delta z(z)$ in Eq. (8.17). In particular, it follows that the uniform-mode expression (8.16) for $\omega$ is exact in this limit, and we have

$$\omega_{k \to \infty} = |\gamma| \mu_0 \sqrt{H_x - \frac{2K}{\mu_0 M_S}} \left( H_x + M_S \sin^2 \vartheta \right).$$ (8.22)

In the opposite limit $k \to 0$ (uniform precession), we find

$$\begin{pmatrix} \hat{D}^{yy} & \hat{D}^{yz} \\ \hat{D}^{yz} & \hat{D}^{zz} \end{pmatrix} \to \begin{pmatrix} 0 & 0 \\ 0 & \hat{S} \end{pmatrix},$$

(8.23)

and again all modes $n$ are degenerate; the precession frequency is given by

$$\omega_{k=0} = |\gamma| \mu_0 \sqrt{\left( H_x + M_S - \frac{2K}{\mu_0 M_S} \right) H_x},$$ (8.24)

in agreement with the uniform-mode expression (8.16).

8.3.2 Asymptotic profiles

In the limits $k \to 0$ and $k \to \infty$, the only operator acting on the profiles $\delta y(z), \delta z(z)$ is the identity operator $\hat{S}$. The matrices of operators in Eq. (8.17)
reduce to simple $2 \times 2$ scalar matrices. As a result, we can solve Eq. (8.17) analytically and multiply the solution vector by an arbitrary function. We obtain solutions $\Psi_+$ of the form

$$\Psi_0 = \begin{pmatrix} \delta y(z) \\ \delta z(z) \end{pmatrix} = \sqrt{\frac{\mu_0|\gamma|}{2ab}} \begin{pmatrix} a \psi_0(z) \\ -ib \psi_0(z) \end{pmatrix}, \quad (8.25)$$

where $\psi_0(z)$ is a real-valued function supported on the interval $0 \leq z \leq L$. Notice that $\delta y(z), \delta z(z)$ differ only by a scalar factor. For the regime $k \to 0$, the values of $a, b$ are given by

$$a = \sqrt{H_x + M_S - \frac{2K}{\mu_0 M_S}}, \quad (8.26a)$$

$$b = \sqrt{H_x}; \quad (8.26b)$$

for the regime $k \to \infty$, we have

$$a = \sqrt{H_x - \frac{2K}{\mu_0 M_S}}, \quad (8.27a)$$

$$b = \sqrt{H_x + M_S \sin^2 \theta}. \quad (8.27b)$$

The profile $\psi_0(z)$ must satisfy the normalization condition $\int_0^L \psi_0(z)^2 \, dz = 1$, but is otherwise arbitrary.

In Sec. 8.5, we find that the degeneracy of the modes $n$ is lifted and $\psi_0(z)$ fixed by the higher-order terms in the expansion of Eq. (8.17) in $k$ or $k^{-1}$. For $k \to 0$, the profile $\psi_0(z)$ depends on the angle of approach $\theta$ [36].

### 8.4 Mode Profiles and Dispersion

Figure 8.3(a) shows the dispersion relations obtained from a numerical solution of the eigenvalue equation (8.17). We find a sequence of modes $n = 1, 2, \ldots$ that can be identified as the BVMSW modes [36, 150]. Their frequencies monotonically decrease in any direction $\theta$ as we move away from the origin $k = 0$. In addition, we find, for wavevectors $\mathbf{k}$ pointing predominantly along the $k_y$ axis (perpendicular to magnetization), a single special branch, which we identify as the DE surface mode [35]. Its frequency increases in $k$ before leveling off to a constant value.

At $k = 0$, all modes have the same frequency $\omega_{k=0}$, given by Eq. (8.24). The behavior of $\omega(\mathbf{k})$ in the opposite limit $k \to \infty$ is somewhat more involved. Any given volume mode $n$ eventually converges to the same frequency $\omega_{k=\infty}$, given by Eq. (8.22), as we take $k \to \infty$. However, for any fixed wavevector $\mathbf{k}$, the frequency in the limit $n \to \infty$ converges to $\omega_{k=0}$. As a consequence, there is a quasicontinuum of high-$n$ volume modes just below the line $\omega = \omega_{k=0}$.

Figure 8.4 shows the mode profiles $\delta y(z), \delta z(z)$ of the two lowest volume modes $n = 1, 2$ for a range of wavevectors $\mathbf{k} = (k_x, k_y) = (k \cos \theta, k \sin \theta)$. While
Figure 8.3: (a) Numerical dispersion relations of the volume modes \( n = 1, 2, \ldots \) and the DE surface mode, along the \( k_y \) axis (\( \theta = 90^\circ \)), the \( k_x \) axis (\( \theta = 0^\circ \)), and a circular arc (\( k = 10 L^{-1} \)), taking \( H_x = 0.73 M_S \) and \( 2K = 0.46 \mu_0 M_S^2 \). For \( k = 0 \), all modes are degenerate, with \( \omega = \omega_{k=0} \) given by Eq. (8.24). Taking the \( k \to \infty \) limit in a fixed direction \( \theta \), each volume mode \( n \) eventually approaches the frequency \( \omega_{k=\infty} \) (short dotted lines), given by Eq. (8.22). (b) Numerical dispersion relations of the \( n = 1 \) and DE modes, compared to the uniform-mode expression (8.16). Along the \( k_x \) axis, Eq. (8.16) is fairly accurate, predicting the correct group velocity \( d\omega/dk \) of the \( n = 1 \) mode for \( k \to 0 \). Along the \( k_y \) axis, there is a significant deviation. The correct asymptotic behavior of the \( n = 1 \) mode (thin solid lines) is given in Table 8.1 (c) For small \( k \), the crossover between the \( n = 1 \) and DE modes might be seen as an avoided band crossing. The behavior of the \( n = 1 \) mode below \( \theta_{cr} = 49^\circ \) is similar to that of the DE mode above \( \theta_{cr} \), but the two modes are not continuously connected; the DE mode instead emerges from the quasicontinuum of high-\( n \) volume modes.
Figure 8.4: Profiles $\delta y(z)$ (solid lines) and $-i\delta z(z)$ (dashed lines), with $0 \leq z \leq L$, of the lowest-frequency volume modes $n = 1, 2$, for a range of wavevectors $\mathbf{k} = (k \cos \vartheta, k \sin \vartheta)$, taking $H_x = 0.73 M_S$ and $2K = 0.46 \mu_0 M_S^2$. The modes are invariant under a reflection of $\mathbf{k}$ with respect to the $k_y$ axis ($\vartheta \leftrightarrow 180^\circ - \vartheta$). Notice that the limiting profile for $k = 0$ depends on the direction $\vartheta$ from which we approach the singularity at $\mathbf{k} = 0$ [56]. The critical angle $\vartheta_{cr} = 49^\circ$ defines the boundary between regions A (uniform limiting profile for $n = 1$) and B (sinusoidal limiting profile), as shown schematically in Fig. 8.5.
Figure 8.4 (continued)

For \( k = 1 \ L^{-1} \) and \( k = 12 \ L^{-1} \), we compare the numerical solutions (black lines) of the normal-mode problem (8.17) to the first-order approximations (gray lines) given by Eqs. (8.29), (8.31), (8.32), and Table 8.2. Our first-order expressions provide a good indication of the numerical mode profiles, not only in the \( k \to 0 \) or \( k \to \infty \) limits but also for finite \( k \).
we find that the profiles do not depend in any way on the sign of $k_x$, notice that the cases $k_y > 0$ and $k_y < 0$ are inequivalent [36]. In particular, the antinode (amplitude maximum) of the $n = 1$ mode tends to move towards one or the other surface of the film ($z = 0$ or $z = L$) depending on the sign of $k_y$. A similar nonreciprocity is seen in the DE modes, which exponentially localize near either of the two film surfaces [35]. The explicit perturbative expressions for the mode profiles, which we present in Sec. 8.5, can be used to quantify the asymmetric behavior.

### 8.4.1 Relation to uniform-mode analysis

It is interesting to compare the numerical dispersion relation of the $n = 1$ volume mode to the dispersion relation (8.16) obtained in the uniform-mode approximation. As shown in Fig. 8.3(b), we find that Eq. (8.16) predicts the correct group velocity $d\omega/dk$ in the $k \to 0$ limit when approaching the point $k = 0$ along the $k_x$ axis ($\theta = 0^\circ$ or $\theta = 180^\circ$). Along the $k_y$ axis ($\theta = \pm 90^\circ$), however, the numerical dispersion relation differs very significantly from the uniform-mode expression. In particular, the slope $d\omega/dk$ predicted for $k \to 0$ is incorrect: we have $d\omega/dk \to 0$ for the volume modes, but Eq. (8.16) predicts a positive group velocity. A qualitative explanation for the discrepancy may be found in Fig. 8.4 Approaching $k = 0$ along the $k_x$ axis ($\theta = 0^\circ$), it is found [36] that the limiting profile $\psi_0(z)$ of the $n = 1$ mode is indeed a constant function on the interval $0 \leq z \leq L$, as was assumed in the uniform-mode approach. Along the $k_y$ axis ($\theta = 90^\circ$), by contrast, we have that $\psi_0(z)$, for $0 \leq z \leq L$, is a cosine function with wavenumber $\pi/L$, and as a result, the uniform-mode analysis is inaccurate even for small $k$. Regardless of $\theta$, the uniform-mode analysis is also inaccurate in the large-$k$ regime (limiting profile for $k \to \infty$ is a sine function). However, the limiting frequency (8.22) is reproduced correctly.

Along the $k_y$ axis, the uniform-mode dispersion relation (8.1) coincides, in the small-$k$ regime, with the DE curve. The DE mode, which is exponentially localized to the surface with a decay rate proportional to $k_y$ [35], assumes a uniform profile in the limit $k \to 0$. In other words, the uniform profile, which corresponds to the lowest-frequency mode ($n = 1$) for $\theta = 0^\circ$, becomes the highest-frequency mode (DE) for $\theta = 90^\circ$. At the same time, the profile of the $n = 1$ volume mode goes from uniform ($\theta = 0^\circ$) to sinusoidal ($\theta = 90^\circ$). We might interpret the transition as an avoided band crossing, as shown in Fig. 8.3(c). The reason for the dependence of the limiting profile $\psi_0(z)$ on $\theta$ is given in more formal terms in Sec. 8.5.

### 8.5 Limiting behavior

In this section, we present explicit analytical expressions for the frequency $\omega$ and profiles $\delta y(z), \delta z(z)$ of the volume modes $n$ in the small-$k$ and large-$k$ regimes.
While the limiting profiles for $k \to 0$ and $k \to \infty$ (zeroth order) are well known \[36\], our expressions, which are accurate up to first order in $k$ or $1/k$, give a good impression of the behavior of the modes even for finite $k$, as shown in Fig. 8.4. They can be used to estimate how strongly each volume mode $n$ couples to an external field pulse with a given depth profile, or to predict the contribution of the mode to net magnetization $\delta z(t, x, y) = \int \delta z(t, x, y, z) \, dz$ as measured using Faraday rotation \[26\]. They also describe quantitatively the asymmetry in the profiles obtained for $k_y \neq 0$. Moreover, we use the perturbation theory derived here to construct an accurate semianalytical expression for the dispersion relation of the $n = 1$ volume mode in Sec. 8.6.

The limiting behavior for $k \to 0$ depends essentially on the polar angle $\vartheta$. It is useful to introduce the quantity

$$H = H_x \cos^2 \vartheta - \left( M_S - \frac{2K}{\mu_0 M_S} \right) \sin^2 \vartheta. \tag{8.28}$$

The boundary lines $H = 0$ separate the small-$k$ domain into four sectors, as shown in Fig. 8.5. We distinguish between region A, where $H > 0$, and region B, where $H < 0$. Regions A and B meet at the critical angle $\vartheta_{ct} = \arctan \left( H_x / (M_S - \frac{2K}{\mu_0 M_S}) \right) \[36\]. The large-$k$ domain is designated as region C.

It is convenient to write the mode profiles as

$$\Psi_+ = \left( \begin{array}{c} \delta y \\ \delta z \end{array} \right) = \sqrt{\frac{\mu_0 |\gamma|}{2ab}} \left( a \left[ \psi(z) - \phi(z) \right] - ib \left[ \psi(z) + \phi(z) \right] \right), \tag{8.29}$$
where \( \psi(z), \phi(z) \) are real-valued functions supported on the interval \( 0 \leq z \leq L \). The constants \( a, b > 0 \) are defined by Eq. (8.26) for small \( k \) (regions A and B) and by Eq. (8.27) for large \( k \) (region C). The normalization condition (8.19) becomes

\[
\Psi^+_+ \hat{Q} \Psi_+ = \int_0^L [\psi(z)^2 - \phi(z)^2] \, dz = 1. \tag{8.30}
\]

In the small-\( k \) regime (regions A and B), we expand the wavefunctions and eigenfrequencies as

\[
\begin{align*}
\omega &= \omega_0 + k\omega_1 + k^2\omega_2 + \ldots, \tag{8.31a} \\
\psi(z) &= \psi_0(z) + k\psi_1(z) + \mathcal{O}(k^2), \tag{8.31b} \\
\phi(z) &= k\phi_1(z) + \mathcal{O}(k^2); \tag{8.31c}
\end{align*}
\]

in the large-\( k \) regime (region C), we define

\[
\begin{align*}
\omega &= \omega_0 + k^{-1}\omega_1 + k^{-2}\omega_2 + \ldots, \tag{8.32a} \\
\psi(z) &= \psi_0(z) + k^{-1}\psi_1(z) + \mathcal{O}(k^{-2}), \tag{8.32b} \\
\phi(z) &= k^{-1}\phi_1(z) + \mathcal{O}(k^{-2}). \tag{8.32c}
\end{align*}
\]

In all three regions, only the \( \psi(z) \) component of the wavefunction contributes at zeroth order (\( k = 0 \) or \( k = \infty \)); the function \( \phi(z) \) vanishes in those limits [see Eq. (8.25)].

The main results of this section are summarized in Tables 8.1 and 8.2, which list explicit perturbative expressions for frequency (up to second order) and profiles (up to first order) of the volume modes \( n \), for each of the regions. For brevity, we introduce the quantities

\[
\begin{align*}
A &= (H_x + M_S - \frac{2K}{\mu_0 M_S}) \sin^2 \theta + H_x, \tag{8.33a} \\
G &= H_x \cos^2 \theta - \frac{2K}{\mu_0 M_S} \sin^2 \theta, \tag{8.33b} \\
J &= H_x \cos^2 \theta + (\frac{2K}{\mu_0 M_S} + M_S) \sin^2 \theta. \tag{8.33c}
\end{align*}
\]

The asymptotic behavior of the dispersion relations, given by the expressions in Table 8.1 is shown for \( n = 1 \) in Fig. 8.3(b). In Fig. 8.4, we successfully compare our first-order mode profiles, given by the expressions in Table 8.2 to the numerical results.

In the remainder of this section, we present in more detail the derivations for each of the regions A (Sec. 8.5.1), B (Sec. 8.5.2), and C (Sec. 8.5.4). The boundary between regions A and B, where \( |\theta| = \theta_{cr} \) or \( |\theta| = 180^\circ - \theta_{cr} \), requires special consideration (Sec. 8.5.3). In the interest of readability, we focus on the limiting profiles \( \psi_0(z) \) of the \( n = 1 \) mode and on the asymptotic behavior of its dispersion relation. A more mathematical derivation of the perturbation theory used to obtain all results in Tables 8.1 and 8.2 is given in Appendix 8.B.
8.5.1 Region A

The operators \( \hat{D}^{ab}(k_x, k_y) \), defined in Eq. (8.18), are the only nontrivial operators appearing in the eigenvalue equation (8.17). We expand \( \hat{D}^{ab}(k \cos \theta, k \sin \theta) \) in the parameter \( k \) (for fixed \( \theta \)). Using Appendix 8.A we obtain

\[
\begin{pmatrix}
\hat{D}_{yy} & \hat{D}_{yz} \\
\hat{D}_{yz} & \hat{D}_{zz}
\end{pmatrix} = \hat{D}_0 + k \hat{D}_1 + k^2 \hat{D}_2 + k^3 \hat{D}_3 + \ldots
\]

\[
= \begin{pmatrix} 0 & 0 \\ 0 & \hat{S} \end{pmatrix} + k \begin{pmatrix} \frac{\pi (\sin^2 \theta) \delta(\hat{k}_z)}{(\sin \theta) \hat{k}_z^{-1}} & (\sin \theta) \hat{k}_z^{-1} \\ (\sin \theta) \hat{k}_z^{-1} & -\pi \delta(\hat{k}_z) \end{pmatrix} + k^2 \begin{pmatrix} (\sin \theta) \hat{k}_z^{-2} & (\sin \theta) \delta'(\hat{k}_z) \\ (\sin \theta) \delta'(\hat{k}_z) & -\hat{k}_z^{-2} \end{pmatrix} + k^3 \begin{pmatrix} -\frac{1}{2} \pi (\sin \theta) \delta''(\hat{k}_z) & -(\sin \theta) \hat{k}_z^{-3} \\ -(\sin \theta) \hat{k}_z^{-3} & \frac{1}{2} \pi \delta''(\hat{k}_z) \end{pmatrix} + \mathcal{O}(k^4), \quad (8.34)
\]

where \( \delta \) represents the Dirac delta distribution. The expressions containing \( \hat{k}_z \) represent (in real space) convolution operators acting on the profiles \( \delta y(z), \delta z(z) \); for example, the action of \( \hat{D}_1 \) may be expressed as

\[
\hat{D}_1 \begin{pmatrix} \delta y(z) \\ \delta z(z) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \int [\sin^2 \theta \delta y(z') + i \sin \theta \text{sign}(z-z') \delta z(z')] \, dz' \\ \int [i \sin \theta \text{sign}(z-z') \delta y(z') - \delta z(z')] \, dz' \end{pmatrix}, \quad (8.35)
\]

where we have used the Fourier transforms \( f(z) = 1 \leftrightarrow \tilde{f}(k_z) = 2\pi \delta(k_z) \) and \( f(z) = \text{sign}(z) \leftrightarrow \tilde{f}(k_z) = -2i/k_z \).

All modes \( n \) are degenerate for \( k = 0 \), with \( \omega_0 = |\gamma|\mu_0ab \). The first- and second-order terms of the expansion of \( \hat{D}^{ab} \) in \( k \) lift this degeneracy and fix the spatial profile \( \psi_0(z) \) in Eq. (8.25). We obtain the profile of the lowest mode \( n = 1 \) by minimizing

\[
\omega_1 = \Psi_0^+ (M_S \hat{D}_1) \Psi_0
\]

\[
= -\frac{|\gamma|\mu_0 M_S}{4ab} [H_x \cos^2 \theta - (M_S - \frac{2K}{\mu_0 M_S}) \sin^2 \theta] \left( \int_0^L \psi_0(z) \, dz \right)^2 \quad (8.36)
\]

under the constraint \( \int_0^L \psi_0(z)^2 \, dz = 1 \) [Eq. (8.88a)].

We identify the prefactor between square brackets in Eq. (8.36) as the quantity \( H \). In region A \( (H > 0) \), minimization of \( \omega_1 \) is equivalent to maximization of \( (\int_0^L \psi_0(z) \, dz)^2 \), yielding the uniform profile

\[
\psi_0(z) = \frac{1}{\sqrt{L}} \Pi^* \left( \frac{z}{L} \right). \quad (8.37)
\]

By definition, \( \omega_1 = \lim_{k \to 0} d\omega / dk \) is the group velocity for \( k = 0 \). We obtain

\[
\frac{d\omega}{dk} = -\frac{\mu_0 |\gamma| M_S L}{4ab} H + \mathcal{O}(k), \quad (8.38)
\]
Table 8.1: Asymptotic behavior of the dispersion relations of the volume modes \( n \) in each of the long-wavelength regions A, B, and the A–B boundary line and in the short-wavelength region C (see Fig. 8.5). The \( \vartheta \)-dependent quantities \( H, J, G \) are defined in Eqs. (8.28) and (8.33). The profiles \( \psi_0, \psi_1, \phi_1 \) (see Table 8.2) are shown for \( n = 1 \) (black lines) and \( n = 2 \) (gray lines).

<table>
<thead>
<tr>
<th>Region</th>
<th>Profiles</th>
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<tbody>
<tr>
<td>A</td>
<td>( \psi_0(\vartheta) )</td>
<td>[ \omega = ab ]</td>
</tr>
<tr>
<td>B</td>
<td>( \psi_1(\vartheta), \phi_1(\vartheta) )</td>
<td>[ \omega = ab + \ldots ]</td>
</tr>
<tr>
<td>C</td>
<td>( \psi_0(\vartheta) )</td>
<td>[ \omega = ab ]</td>
</tr>
</tbody>
</table>

where

\[
\begin{align*}
\psi_0(\vartheta) &= \sqrt{Hx - 2K\mu_0 M_S} \\
\psi_1(\vartheta) &= \sqrt{Hx + M_S} \\
\phi_1(\vartheta) &= \frac{\vartheta}{\sin 2\vartheta}
\end{align*}
\]

and \( \vartheta = \pi = 2 \) (gray lines).
Table 8.2: Mode profiles and first-order corrections. All functions to be multiplied by $\Pi^*(z/L)$. See Eqs. (8.29), (8.31), (8.32).

**Region A ($n = 1$)**

| $\psi_0(z)$ | $1/\sqrt{L}$ |
| $\psi_1(z)$ | $-1/H\sqrt{L}$ |
| $\times \left[ \frac{AM_S \sin \vartheta \, 2z - L}{2ab} + \frac{3(2z - L)^2 - L^2}{12L} \right] $ |
| $\phi_1(z)$ | $\frac{1}{\sqrt{L} \, 2ab} \left( \frac{AL}{4ab} + \sin \vartheta \frac{2z - L}{2} \right)$ |

**Region A ($n > 1$)**

| $\psi_0(z)$ | $\sqrt{2} \cos \left( \frac{(n-1)\pi z}{L} \right)$ |
| $\psi_1(z)$ | $-\sqrt{2} \, \frac{1}{L} \frac{1}{H \, (n-1)\pi} \left( \frac{AM_S \sin \vartheta \, 2z - L}{2ab} \sin \left( \frac{(n-1)\pi z}{L} \right) \right.$ |
| $\times \left. + \frac{G \left( \frac{2z - L}{L} \sin \left( \frac{(n-1)\pi z}{L} \right) \right) + \frac{1}{(n-1)\pi} \cos \left( \frac{(n-1)\pi z}{L} \right) \right)$ |
| $\phi_1(z)$ | $\sqrt{2} \, \frac{M_S \sin \vartheta \, L}{2ab \, (n-1)\pi} \sin \left( \frac{(n-1)\pi z}{L} \right)$ |

**Boundary A–B (for $\eta = 0$ and $k_y > 0$)**

| $\psi_0(z)$ | $\sqrt{2} \cos \left( \frac{(2n-1)\pi z}{2L} \right)$ |
| $\psi_1(z)$ | $-\sqrt{2} \, \frac{2L}{L \, (2n-1)\pi} \left[ \frac{z-L}{L} \sin \left( \frac{(2n-1)\pi z}{2L} \right) \right.$ |
| $\times \left. + \frac{1}{(2n-1)\pi} \cos \left( \frac{(2n-1)\pi z}{2L} \right) \right]$ |
| $\phi_1(z)$ | $\sqrt{2} \, \frac{M_S \sin \vartheta \, L}{2ab^2 \, (2n-1)\pi} \sin \left( \frac{(2n-1)\pi z}{2L} \right)$ |

\(^a\) For $k_y < 0$, take $\psi_0(z) \leftarrow (-1)^{n-1} \psi_0(L - z)$ for $\psi_0, \psi_1, \phi_1$. 

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8.5 Limiting Behavior
Table 8.2 (continued)

Region B\textsuperscript{b}

\begin{align*}
\psi_0(z) &= \pm \sqrt{\frac{2}{L}} \cos \left( \frac{n\pi z}{L} \right) \\
\psi_1(z) &= \mp \sqrt{\frac{2}{L}} \frac{1}{H} \int_{-\infty}^{\infty} \frac{AM_s \sin \vartheta}{2ab} \sin \left( \frac{n\pi z}{L} \right) \\
&\quad + G \left[ \frac{2z - L}{L} \sin \left( \frac{n\pi z}{L} \right) + \frac{1}{n\pi} \cos \left( \frac{n\pi z}{L} \right) \right] \\
\phi_1(z) &= \sqrt{\frac{2}{L}} M_s |\sin \vartheta| \left( \frac{2}{n\pi} \right) \sin \left( \frac{n\pi z}{L} \right) \\
\text{For } k_y > 0 \text{ (upper signs) and } k_y < 0 \text{ (lower signs).}
\end{align*}

Region C

\begin{align*}
\psi_0(z) &= \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi z}{L} \right) \\
\psi_1(z) &= \sqrt{\frac{2}{L}} \frac{1}{n\pi} \int_{-\infty}^{\infty} \frac{AM_s \sin \vartheta}{2ab} \cos \left( \frac{n\pi z}{L} \right) \\
&\quad - G \left[ \frac{2z - L}{L} \cos \left( \frac{n\pi z}{L} \right) + \frac{1}{n\pi} \sin \left( \frac{n\pi z}{L} \right) \right] \\
\phi_1(z) &= -\sqrt{\frac{2}{L}} M_s \sin \vartheta \frac{n\pi}{2ab} \cos \left( \frac{n\pi z}{L} \right)
\end{align*}
as in the uniform-mode approach [see Fig. 8.3(b)].

Now that the $k = 0$ profile $\psi_0(z)$ of the $n = 1$ mode is known, the part $\phi_1(z)$ of the first-order correction is given by Eq. (8.90), which condition results from minimization of $\omega_2$. However, the other part $\psi_1(z)$ does not affect the value of $\omega_2$, given by Eq. (8.87c), if the constraint $\int_0^L \psi_0(z) \psi_1(z) \, dz = 0$ is satisfied, and hence $\psi_1(z)$ cannot be determined by minimization of $\omega_2$. This indeterminacy is a consequence of the degeneracy of the $\psi(z)$ component of the modes at zeroth order of perturbation theory. We turn to minimization of $\omega_3$ to fix $\psi_1(z)$, yielding the condition (8.94). The resulting profiles are listed in Table 8.2.

### 8.5.2 Region B

In region B, where $H < 0$, minimization of Eq. (8.36) is equivalent to minimization of $(\int_0^L \psi_0(z) \, dz)^2$. The minimum value

$$\omega_1 = \lim_{k \to 0} \frac{d\omega}{dk} = 0 \tag{8.39}$$

is obtained for any profile $\psi_0(z)$ for which $\int_0^L \psi_0(z) \, dz = 0$. In other words, the zeroth-order profile $\psi_0(z)$ is indeterminate even in first-order perturbation theory. The degeneracy is lifted by the second-order term of Eq. (8.34). By Eq. (8.91), the profile $\psi_0(z)$ minimizes

$$\omega_2 = -\frac{|\gamma| \mu_0 M_S}{2ab} [H_x \cos^2 \theta + \frac{2k}{\mu_0 M_S} \sin^2 \theta] \int_0^L \psi_0 k_z^{-2} \psi_0 \, dz. \tag{8.40}$$

The operator $k_z^{-2}$ represents, as usual, a convolution in real space. Using the Fourier transform $\hat{f}(k) = k^{-n} \leftrightarrow f(x) = i(x)^{n-1} \text{sign}(x) / [2(n-1)!]$, we have

$$\int_0^L \psi_0 \hat{k}_z^{-2} \psi_0 \, dz = -\frac{1}{2} \int_0^L \psi_0(z) \int_0^L |z - z'| \psi(z') \, dz' \, dz. \tag{8.41}$$

Minimization of $\omega_2$ gives

$$\psi_0(z) = \sqrt{\frac{2}{L}} \cos \left( \frac{\pi z}{L} \right) \Pi^* \left( \frac{z}{L} \right), \tag{8.42}$$

and we evaluate

$$\omega_2 = \lim_{k \to 0} \frac{d\omega}{dk} = \lim_{k \to 0} \frac{1}{2k} \frac{d\omega}{dk} = -\frac{\mu_0 |\gamma| M_S L^2}{2\pi^2 ab} \left[ H_x \cos^2 \theta + \frac{2k}{\mu_0 M_S} \sin^2 \theta \right]. \tag{8.43}$$

As in region A, minimization of $\omega_2$ immediately fixes $\phi_1(z)$ according to Eq. (8.90). However, the third-order expression (8.93) for $\psi_1(z)$ is indeterminate in region B. We need to minimize the fourth-order functional $\omega_4$, given by Eq. (8.96), to determine $\psi_1(z)$. The resulting expressions are listed in Table 8.2.
8.5.3 Boundary line A–B

The boundary line between regions A and B requires special consideration, as neither the perturbation theory of region A nor of region B is valid on this line. We find that the boundary line in some sense interpolates between the profiles in the interiors of regions A and B.

On the boundary, where \( H = 0 \), we have that \( \omega_1 \) as given by Eq. (8.36) is identically zero. This means that, as in region B, the profile \( \psi_0(z) \) is fixed by minimization of \( \omega_2 \). In contrast to region B, however, there is no constraint \( \int_0^L \psi_0(z) \, dz = 0 \) from minimization of \( \omega_1 \). By Eq. (8.91), \( \psi_0(z) \) minimizes

\[
\omega_2 = -\frac{1}{2\omega_0} \int_0^L |(\hat{Y}_1^+ \psi_0)|^2 \, dz,
\]

where

\[
(\hat{Y}_1^+ \psi_0)(z) = -C \int_0^z \psi_0(z') \, dz' \quad \text{for} \quad k_y > 0, \tag{8.45a}
\]

\[
(\hat{Y}_1^+ \psi_0)(z) = C \int_z^L \psi_0(z') \, dz' \quad \text{for} \quad k_y < 0, \tag{8.45b}
\]

with \( C = \mu_0 |\gamma| M_S \sin \vartheta \). Minimization gives

\[
\psi_0(z) = \sqrt{\frac{2}{L}} \cos \left( \frac{\pi z}{2L} \right) \Pi^*(\frac{z}{L}) \quad \text{for} \quad k_y > 0, \tag{8.46a}
\]

\[
\psi_0(z) = \sqrt{\frac{2}{L}} \sin \left( \frac{\pi z}{2L} \right) \Pi^*(\frac{z}{L}) \quad \text{for} \quad k_y < 0, \tag{8.46b}
\]

and we evaluate

\[
\omega_2 = \lim_{k \to 0} \frac{1}{2} \left( \frac{\partial^2 \omega}{\partial k^2} \right)_{H=0} = -|\gamma| \mu_0 \frac{4L^2}{\pi^2} \frac{M_S G_0}{2ab}, \tag{8.47}
\]

where

\[
G_0 = G|_{\vartheta=\vartheta_{cr}} = \frac{b^2 M_S}{a^2}. \tag{8.48}
\]

Minimization of \( \omega_2 \) also fixes \( \phi_1(z) \) by Eq. (8.90). The other first-order component \( \psi_1(z) \) is again determined only at fourth order of perturbation theory.

In the above expressions, we assume that we approach the point \( k = 0 \) along a line \( H = 0 \); in other words, we fix \( \vartheta = \pm \vartheta_{cr} \). We can generalize Eq. (8.47) by carrying out the expansion along a curve of constant \( \eta \), as shown in Fig. 8.6, where we define

\[
\eta = \left( \frac{a^2}{2b^2 M_S L} \right) \frac{H}{k}. \tag{8.49}
\]

We obtain, for the lowest mode \( n = 1 \),

\[
\omega_2 = \lim_{k \to 0} \frac{1}{2} \left( \frac{\partial^2 \omega}{\partial k^2} \right)_{\eta} = -|\gamma| \mu_0 \frac{4L^2}{\pi^2} \frac{M_S G_0}{2ab} q_1(\eta). \tag{8.50}
\]
Notice that Eq. (8.47) corresponds to \( \eta = 0 \). The generalization \( \eta \neq 0 \) interpolates between regions A \( (\eta \to \infty) \) and B \( (\eta \to -\infty) \) and allows one, in principle, to construct a second-order approximation of \( \omega \) around \( k = 0 \) uniform in \( \vartheta \).

Table 8.1 gives \( \omega_2 \) for arbitrary mode index \( n \). While we are unaware of a closed-form expression for the functions \( q_n(\eta) \), we have a small-\( \eta \) expansion

\[
q_n(\eta) = \frac{\pi^2}{12}(1 + 3\eta) + \mathcal{O}(\eta^{-1}) \quad \text{for } \eta > 0, n = 1, \tag{8.51}
\]

and large-\( \eta \) expansions

\[
q_n(\eta) = \left( \frac{n - 1}{n} \right)^2 + \mathcal{O}(\eta^{-1}) \quad \text{for } \eta > 0, n > 1, \tag{8.52a}
\]

\[
q_n(\eta) = \left( \frac{n - 1}{n} \right)^2 + \mathcal{O}(\eta^{-1}) \quad \text{for } \eta < 0. \tag{8.52c}
\]

A very good approximation for \( q_1(\eta) \), with a maximal absolute error of 0.00363, is given by

\[
q_1(\eta) \approx \frac{1}{24} \left[ 3 + \pi^2(1 + 3\eta) + \sqrt{[3 + \pi^2(1 + 3\eta)]^2 - 12\pi^2(1 + 3\eta + 3) + 432} \right]. \tag{8.53}
\]
8.5.4 Region C

For large $k$, we have the expansion [cf. Eq. (8.34)]

$$
\begin{pmatrix}
\hat{D}_{yy} \\
\hat{D}_{yz} \\
\hat{D}_{zy} \\
\hat{D}_{zz}
\end{pmatrix}
= \hat{D}_{-0} + k^{-1}\hat{D}_{-1} + k^{-2}\hat{D}_{-2} + \ldots
$$

$$
= \sin^2 \theta \left( \begin{pmatrix}
\hat{\sigma} & 0 \\
0 & 0 
\end{pmatrix} + \frac{\sin \theta}{k} \begin{pmatrix}
0 & \hat{k}_z \\
\hat{k}_z & 0 
\end{pmatrix} + \frac{1}{k^2} \left( -\left(\sin^2 \theta\right)\hat{k}_z^2 & 0 \\
0 & \hat{k}_z^2 
\right) 
\right) 
\left( \begin{pmatrix}
0 & \hat{k}_z \\
\hat{k}_z & 0 
\end{pmatrix} - \frac{1}{k^4} \left( -(\sin^2 \theta)\hat{k}_z^4 & 0 \\
0 & \hat{k}_z^4 
\right) + O(k^{-5}).
\right)
$$

(8.54)

All modes $n$ are degenerate at zeroth order. In the $k \to \infty$ limit, the mode profiles are of the form (8.25) with $a, b$ given by Eq. (8.27). Notice that, for region C, the value of $b$ depends on $\theta$. The second-order term $\hat{D}_{-2}$ in Eq. (8.54) lifts the degeneracy and fixes the spatial profile $\psi_0(z)$.

Regardless of $k_y$, we have

$$
\lim_{k \to \infty} -k^2 \frac{d\omega}{dk} = \omega_1 = \Psi_0^\dagger(M_S \hat{D}_{-1}) \Psi_0 = 0.
$$

(8.55)

For $k_y = 0$, the first-order term $\hat{D}_{-1}$ in Eq. (8.54) even vanishes identically. In this case, we may somewhat simplify our calculations by treating $\omega_2$ as the first-order term of a perturbation series in $k^2$. We find the limiting profile $\psi_0(z)$ of the $n = 1$ mode by minimization of

$$
\omega_2 = \Psi_0^\dagger(M_S \hat{D}_{-2}) \Psi_0 = \frac{\mu_0|\gamma|M_S}{2ab} H_x \int_0^L \left( \frac{d\psi_0}{dz} \right)^2 dz,
$$

(8.56)

under the constraint (8.88a). We obtain

$$
\psi_0(z) = \sqrt{\frac{2}{L}} \sin \left( \frac{\pi z}{L} \right) \Pi^+ \left( \frac{z}{L} \right)
$$

(8.57)

and

$$
\lim_{k \to \infty} - \frac{k^3}{2} \frac{d\omega}{dk} = \omega_2 = \mu_0|\gamma|M_S \frac{\pi^2 H_x}{2ab}.
$$

(8.58)

Notice that $\psi_0(z)$ satisfies Dirichlet boundary conditions $\psi_0(0) = \psi_0(L) = 0$. Such conditions are necessary to give Eq. (8.56) a finite value, since $\psi_0(z)$ must vanish outside the interval $0 \leq z \leq L$. However, higher-order terms $\phi_1(z), \psi_1(z)$ of the expansion can have finite values for $z = 0$ or $z = L$.

In the general case $k_y \neq 0$, the profile $\psi_0(z)$ is still a sine function (8.57). Using Eq. (8.91), we evaluate

$$
\omega_2 = \frac{\mu_0|\gamma|M_S G}{2ab} \int_0^L \left( \frac{d\psi}{dz} \right)^2 dz = \mu_0|\gamma|M_S \frac{\pi^2 L^2 G}{2ab}.
$$

(8.59)
The profile $\phi_1(z)$ is fixed by Eq. (8.90). The other first-order profile $\psi_1(z)$ is determined, again, only by minimization of the fourth-order functional $\omega_4$ [Eq. (8.96)]. Table 8.2 lists the resulting expressions.

When performing the derivation of the profile $\psi_1(z)$, we take into account the following. Writing out Eqs. (8.92) and (8.96) for region C, we find that the functionals $\omega_3$ and $\omega_4$ contain terms such as $i \int \psi_1 k_z \phi_1 \, dz = \int \psi_1 \partial_z \phi_1 \, dz$ or $\int \psi_0 k_z^2 \psi_0 \, dz = \int \psi_0 \partial_z^2 \psi_0 \, dz$, which must be regularized; indeed, the profiles $\phi_0(z), \psi_0(z)$ have discontinuities at $z = 0$ and $z = L$, while $\psi_0(z)$ has discontinuities in its first derivative. The functionals $\omega_3, \omega_4$ can each be written as a sum of regular integral terms plus boundary terms of the forms (a) $\lim_{\Delta \to 0^+} \int_{-\Delta}^{\Delta} \Theta(z) \delta(z) \, dz$ and (b) $\lim_{\Delta \to 0^+} \int_{-\Delta}^{\Delta} \Theta(z) \delta'(z) \, dz$, where $\Theta(z)$ is the Heaviside step function. It is natural to assign the value $\frac{1}{2}$ to (a). As for terms (b), which diverge, we must require that the sum of their prefactors vanishes, yielding a boundary condition that acts as a constraint in the minimization of $\omega_4$.

8.6 SEMIANALYTICAL SOLUTION

In this section, we present a semianalytical expression for the dispersion relation of the $n = 1$ BVMSW mode that can be evaluated in constant time using standard numerical routines. The expression is accurate up to an error that is negligible for any practical purpose (well below 0.01% in the example of Fig. 8.8). It takes a given wavevector $(k_x, k_y)$ as input; evaluation does not require an initial guess for $\omega$.

Figure 8.7 shows that typical profiles $\delta y(z), \delta z(z)$ of the $n = 1$ mode can be written, to a very reasonable approximation, as a linear combination of only four basis functions

\[ u_0(z) = \Pi^* \left( \frac{z}{L} \right), \]
\[ u_1(z) = \left( \frac{z}{L} - \frac{1}{2} \right) \Pi^* \left( \frac{z}{L} \right), \]
\[ u_2(z) = \sin \left( \frac{\pi z}{L} \right) \Pi^* \left( \frac{z}{L} \right), \]
\[ u_3(z) = -\cos \left( \frac{\pi z}{L} \right) \Pi^* \left( \frac{z}{L} \right). \]

For our semianalytical approximation, we restrict the profiles to such linear combinations

\[ \delta y(z) = c_0 u_0(z) + c_1 u_1(z) + c_2 u_2(z) + c_3 u_3(z), \]
\[ \delta z(z) = d_0 u_0(z) + d_1 u_1(z) + d_2 u_2(z) + d_3 u_3(z). \]

On this basis set, the operators $\dot{S}, \dot{D}^{yy}, \dot{D}^{yz}, \dot{D}^{zz}$ reduce to simple $4 \times 4$ matrix blocks, given below, and Eq. (8.17) becomes an $8 \times 8$ eigenvalue problem

\[ \begin{bmatrix} H_x S + M_S D^{yy} & M_S D^{yz} \\ M_S D^{yz} & (H_x - \frac{2K}{\mu_0 M_S}) S + M_S D^{zz} \end{bmatrix} \begin{bmatrix} 0 \\ iS \end{bmatrix} = \begin{bmatrix} \omega \\ -iS \end{bmatrix}, \]
where square brackets indicate block matrices and \( v = (c_0, c_1, c_2, c_3, d_0, d_1, d_2, d_3)^T \) represents the eigenvector. The approximate frequency of the \( n = 1 \) mode is given by the lowest positive eigenvalue \( \omega \).

Equation (8.62) takes the form of an \( 8 \times 8 \) generalized Hermitian eigenvalue problem, the solutions \( \omega \) of which can be found numerically using standard routines. While not all linear-algebra computer packages may support the generalized format \( Hv = \omega Qv \), it can always be rewritten as \( Q^{-1}Hv = \omega v \) and solved as an ordinary non-Hermitian eigenvalue problem.

Explicit analytical expressions exist for all matrix elements in Eq. (8.62). The identity operator \( \hat{S} \) becomes the overlap matrix

\[
S = L \begin{pmatrix}
1 & 0 & \frac{2}{\pi} & 0 \\
0 & \frac{1}{12} & 0 & \frac{2}{\pi^2} \\
\frac{2}{\pi} & 0 & \frac{1}{2} & 0 \\
0 & \frac{2}{\pi^2} & 0 & \frac{1}{2}
\end{pmatrix},
\] (8.63)

where the matrix elements are defined by \( S_{ij} = \int u_i(z)u_j(z)dz \). The elements of the \( D^{ab} \) matrix blocks can be evaluated in Fourier space as

\[
D_{ij}^{yy}(k_x, k_y) = \frac{1}{2\pi} \int \tilde{u}_i^*(k_z) \frac{k_yk_y}{k_x^2 + k_y^2 + k_z^2} \tilde{u}_j(k_z)dk_z,
\] (8.64)
and analogously for $D_{ij}^{yz}$ and $D_{ij}^{zz}$, where $\tilde{u}_i(k_z)$ is the Fourier transform of the basis function $u_i(z)$. We obtain

$$D_{yy} = L \frac{k_y^2}{k^2} \times \begin{pmatrix} 1 - N_{00} & 0 & \frac{2}{\pi} (1 - N_{02}) & 0 \\ 0 & \frac{1}{12} (1 - N_{11}) & 0 & \frac{2}{\pi^2} (1 - N_{13}) \\ \frac{2}{\pi} (1 - N_{02}) & 0 & \frac{1}{2} (1 - N_{22}) & 0 \\ 0 & \frac{2}{\pi^2} (1 - N_{13}) & 0 & \frac{1}{2} (1 - N_{33}) \end{pmatrix},$$

and

$$D_{zz} = L \begin{pmatrix} N_{00} & 0 & \frac{2}{\pi} N_{02} & 0 \\ 0 & \frac{1}{12} N_{11} & 0 & \frac{2}{\pi^2} N_{13} \\ \frac{2}{\pi} N_{02} & 0 & \frac{1}{2} N_{22} & 0 \\ 0 & \frac{2}{\pi^2} N_{13} & 0 & \frac{1}{2} N_{33} \end{pmatrix},$$

where

$$N_{00} = \frac{1 - e^{-kL}}{kL},$$

$$N_{11} = 12 \left[ 1 + e^{-kL} \frac{1 + e^{-kL} - 1}{4kL} + \frac{(1 + kL)e^{-kL} - 1}{k^3 L^3} \right],$$

$$N_{22} = \frac{\pi^2}{k^2 L^2 + \pi^2} - \frac{2\pi^2 kL(1 + e^{-kL})}{(2kL^2 + \pi^2)^2},$$

$$N_{33} = \frac{\pi^2}{k^2 L^2 + \pi^2} + \frac{2k^3 L^3 (1 + e^{-kL})}{(2kL^2 + \pi^2)^2},$$

$$N_{02} = \frac{\pi^2}{k^2 L^2 + \pi^2} \frac{1 + e^{-kL}}{2},$$

$$N_{13} = \frac{\pi^2}{k^2 L^2 + \pi^2} \frac{(1 + e^{-kL})(2 + kL)}{4},$$

are the so-called demagnetizing factors; and we obtain

$$D_{yz} = \frac{k_y L^2}{2\pi i} \begin{pmatrix} 0 & \frac{\pi}{6} Z_{01} & 0 & \frac{2}{\pi} Z_{03} \\ -\frac{\pi}{6} Z_{01} & 0 & -\frac{4}{\pi^2} Z_{21} & 0 \\ 0 & \frac{4}{\pi^2} Z_{21} & 0 & Z_{23} \\ -\frac{2}{\pi} Z_{03} & 0 & -Z_{23} & 0 \end{pmatrix},$$
Figure 8.8: Relative error $\Delta \omega/\omega$ of the semianalytical expression (8.62) for the dispersion relation $\omega(k \cos \theta, k \sin \theta)$, along three radials $\theta = 0^\circ$ (region A), $\theta = 90^\circ$ (region B), and $\theta = \theta_{\text{cr}} = 49^\circ$ (A–B boundary), as compared to converged solutions of the full eigenvalue problem (8.17) for $H_x = 0.73 M_S$ and $2K = 0.46 \mu_0 M_S^2$. In the interior of region A, we have second-order accuracy in $k [\Delta \omega = O(k^3)]$; for region B, third-order accuracy $[\Delta \omega = O(k^4)]$; in region C, third-order accuracy in $k^{-1} [\Delta \omega = O(k^{-4})]$. On the A–B boundary line, we have only first-order accuracy $[\Delta \omega = O(k^2)]$. However, the relative error remains very small on the entire domain (well below $10^{-4}$).

where

$$Z_{01} = \frac{e^{-kL} + 1 - 2N_{00}}{k^2 L^2},$$  \hspace{1cm} (8.69a) \\
$$Z_{03} = N_{02},$$  \hspace{1cm} (8.69b) \\
$$Z_{21} = \frac{\pi^2}{k^2 L^2 + \pi^2} \left(1 - \frac{\pi}{4} Z_{01} kL\right),$$  \hspace{1cm} (8.69c) \\
$$Z_{23} = N_{22}. $$  \hspace{1cm} (8.69d)

Notice that the basis set (8.60) has been chosen in such a way that it can represent exactly the profiles $\psi_0(z), \phi_1(z)$ of the $n = 1$ mode in each of the regions A, B, and C (see Table 8.2). As a result, we have at least second-order accuracy of $\omega$ in $k$ or $1/k$ in those regions, as shown in Fig. 8.8. Since the mode profile $\psi_1(z)$ is fixed only at third (or, in regions B and C, fourth) order of perturbation theory (see Sec. 8.5), it does not need to be included in the basis set to obtain second-order accuracy.
On the boundary line between regions A and B ($\theta = \theta_{cr}$), we have only first-order accuracy, because the corresponding profiles $\psi_0(z), \phi_1(z)$ are not represented in the basis set. Figure 8.8 shows that the error $\Delta \omega$ nonetheless remains very small. The exact small-$k$ behavior of $\omega$ on the A–B boundary is given in Sec. 8.5.3

We comment on our claim that the approximate expression for $\omega(k_x, k_y)$ can be evaluated in constant time. In general, the solution of an eigenvalue problem for matrices of size $5 \times 5$ or larger requires the use of iterative methods, the convergence rate of which may depend on system parameters. In our case, the characteristic equation $\text{Det}(H - \omega Q) = 0$ of the eigenvalue problem (8.62) contains only even powers of $\omega$, since all eigenvalues appear in conjugate pairs (Hamiltonian problem; see Chap. 5). We could therefore write the characteristic equation, a polynomial of eighth degree in $\omega$, as a quartic polynomial in $\omega^2$, which can be explicitly solved by radicals. This guarantees the existence of an analytical expression for $\omega$ in principle.

8.7 conclusions

BVMSWs in magnetic films display unusual and highly nontrivial dispersion behavior. Their strongly anisotropic and nonreciprocal propagation means that they can be excited and manipulated with a great deal of flexibility and control [26]. Their specific dispersion characteristics are an important ingredient in the analysis of all-optical excitation [159, 160] and nonlinear effects [30–32].

Since the defining equations of the BVMSW modes can be solved only numerically, we believe that it is useful to have some approximate analytical results describing their essential features. In Table 8.1 we summarize the simple analytical expressions that we have derived for the mode frequencies in the short-wavelength and long-wavelength regimes, including the behavior for wavevectors $\mathbf{k}$ pointing in a direction close to the critical angle $\theta_{cr}$. We have also obtained explicit first-order expressions for the depth profiles $\delta y(z), \delta z(z)$ of the modes, given by Eqs. (8.29), (8.31), (8.32), and Table 8.2. These expressions highlight and quantify the asymmetry in $z$ found for $k_y \neq 0$ (nonreciprocal behavior).

In addition to the perturbative results, we provide a semianalytical expression for the dispersion relation of the lowest mode $n = 1$ valid for arbitrary wavevector $(k_x, k_y)$. While this expression is, strictly speaking, an approximation, we find that the error is so small as to be negligible for practical purposes. The semianalytical expression is straightforward to implement using standard numerical routines.
8. Distributional limits

This appendix provides some elementary results needed to carry out the small-$k$ expansion (8.34). If we set $(k_x, k_y) = (k \cos \vartheta, k \sin \vartheta)$, the operators $\hat{D}^{yy}, \hat{D}^{yz}, \hat{D}^{zz}$, defined by Eq. (8.18), become

\[
\hat{D}^{yy} = \frac{k^2}{k^2 + \hat{k}_z^2} \sin^2 \vartheta, \quad (8.70a)
\]

\[
\hat{D}^{yz} = \frac{k \hat{k}_z}{k^2 + \hat{k}_z^2} \sin \vartheta, \quad (8.70b)
\]

\[
\hat{D}^{zz} = \frac{\hat{k}_z^2}{k^2 + \hat{k}_z^2} = \hat{S} - \frac{k^2}{k^2 + \hat{k}_z^2}. \quad (8.70c)
\]

Equation (8.34) is obtained by expanding the operators $k^2 / (k^2 + \hat{k}_z^2)$ and $k \hat{k}_z / (k^2 + \hat{k}_z^2)$ as a Taylor series in the parameter $k > 0$. In the following, $\hat{k}_z$ may be substituted for $x$ and $k$ for $\varepsilon$.

We consider the expressions $\varepsilon^2 / (x^2 + \varepsilon^2)$ and $\varepsilon x / (x^2 + \varepsilon^2)$ as functions of $x$ and calculate derivatives with respect to the parameter $\varepsilon$ in the limit $\varepsilon \to 0^+$. Most of these limits can only be defined if we turn to generalized functions (distributions) of $x$. We obtain

\[
\lim_{\varepsilon \to 0^+} \frac{\varepsilon^2}{x^2 + \varepsilon^2} = 0, \quad (8.71a)
\]

\[
\lim_{\varepsilon \to 0^+} \frac{\varepsilon x}{x^2 + \varepsilon^2} = 0; \quad (8.71b)
\]

\[
\lim_{\varepsilon \to 0^+} \frac{\partial}{\partial \varepsilon} \frac{\varepsilon^2}{x^2 + \varepsilon^2} = \pi \delta(x), \quad (8.72a)
\]

\[
\lim_{\varepsilon \to 0^+} \frac{\partial}{\partial \varepsilon} \frac{\varepsilon x}{x^2 + \varepsilon^2} = \frac{1}{x'}, \quad (8.72b)
\]

where $\delta(x)$ is the Dirac delta distribution;

\[
\lim_{\varepsilon \to 0^+} \frac{\partial^2}{\partial \varepsilon^2} \frac{\varepsilon^2}{x^2 + \varepsilon^2} = \frac{2}{x^2'}, \quad (8.73a)
\]

\[
\lim_{\varepsilon \to 0^+} \frac{\partial^2}{\partial \varepsilon^2} \frac{\varepsilon x}{x^2 + \varepsilon^2} = 2\pi \delta'(x); \quad (8.73b)
\]
and
\[
\lim_{\varepsilon \to 0^+} \frac{\partial^3}{\partial \varepsilon^3} \frac{\varepsilon^2}{x^2 + \varepsilon^2} = -3\pi \delta''(x), \quad (8.74a)
\]
\[
\lim_{\varepsilon \to 0^+} \frac{\partial^3}{\partial \varepsilon^3} \frac{\varepsilon x}{x^2 + \varepsilon^2} = -\frac{6}{x^3}. \quad (8.74b)
\]
Expressions of the form \(1/x^n\) are formally defined as distributional derivatives
\[
\frac{(-1)^{n-1}}{(n-1)!} \frac{d^n}{dx^n} \log |x|.
\]

8.8 Perturbation theory

The generalized Hermitian eigenvalue problem
\[
H \Psi = \omega Q \Psi, \quad (8.75)
\]
where \(H\) and \(Q\) are Hermitian operators one of which is positive definite, can be cast as a problem of minimization of the functional
\[
\omega = \Psi^\dagger H \Psi \quad (8.76)
\]
under the constraint
\[
\Psi^\dagger Q \Psi = 1. \quad (8.77)
\]
We suppose that \(H\) depends on a parameter \(k\) and expand the solution \(\Psi\) around \(k = 0\). Equations (8.76) and (8.77) become
\[
(\omega_0 + k\omega_1 + \ldots) = (\Psi_0 + k\Psi_1 + \ldots)^\dagger (H_0 + kH_1 + \ldots)(\Psi_0 + k\Psi_1 + \ldots) \quad (8.78)
\]
and
\[
(\Psi_0 + k\Psi_1 + \ldots)^\dagger Q(\Psi_0 + k\Psi_1 + \ldots) = 1. \quad (8.79)
\]
Collecting like powers of \(k\), we obtain
\[
\omega_0 = \Psi_0 H_0 \Psi_0, \quad (8.80a)
\]
\[
\omega_1 = 2\Psi_0^\dagger H_0 \Psi_1 + \Psi_0^\dagger H_1 \Psi_0, \quad (8.80b)
\]
\[
\omega_2 = 2\Psi_0^\dagger H_0 \Psi_2 + \Psi_1^\dagger H_0 \Psi_1 + 2\Psi_0^\dagger H_1 \Psi_1 + \Psi_0^\dagger H_2 \Psi_0, \quad (8.80c)
\]
\[
\omega_3 = 2\Psi_0^\dagger H_0 \Psi_3 + 2\Psi_1^\dagger H_0 \Psi_2 + 2\Psi_2^\dagger H_1 \Psi_1 + 2\Psi_0^\dagger H_1 \Psi_2 + \Psi_1^\dagger H_1 \Psi_1 + \Psi_0^\dagger H_2 \Psi_0 + \Psi_0^\dagger H_3 \Psi_0, \quad (8.80d)
\]
\[
\omega_4 = 2\Psi_0^\dagger H_0 \Psi_4 + 2\Psi_1^\dagger H_0 \Psi_3 + \Psi_2^\dagger H_0 \Psi_2 + 2\Psi_1^\dagger H_1 \Psi_3 + 2\Psi_2^\dagger H_1 \Psi_2 + 2\Psi_0^\dagger H_2 \Psi_2 + \Psi_1^\dagger H_1 \Psi_1 + 2\Psi_0^\dagger H_3 \Psi_1 + \Psi_0^\dagger H_4 \Psi_0 \quad (8.80e)
\]
and

\[ 1 = \Psi_0^\dagger Q \Psi_0, \]  
\[ 0 = 2 \Psi_0^\dagger Q \Psi_1, \]  
\[ 0 = 2 \Psi_0^\dagger Q \Psi_2 + \Psi_1^\dagger Q \Psi_1, \]  
\[ 0 = 2 \Psi_0^\dagger Q \Psi_3 + 2 \Psi_1^\dagger Q \Psi_2, \]  
\[ 0 = 2 \Psi_0^\dagger Q \Psi_4 + 2 \Psi_1^\dagger Q \Psi_3 + \Psi_2^\dagger Q \Psi_2, \]

(8.81a)-(8.81e)

where we assume that all terms \( \Psi_A^\dagger H \Psi_B \) and \( \Psi_A^\dagger Q \Psi_B \) are real. To obtain the expansion \( \Psi_0 + k \Psi_1 + k^2 \Psi_2 + \ldots \) of the eigenfunction \( n = 1 \) with the lowest eigenvalue \( \omega \), we sequentially minimize the functionals \( \omega_0, \omega_1, \omega_2, \ldots \) under the constraints (8.81).

In the following, we assume that the eigenvectors \( \Psi \) are written in the form (8.29), and we assume that \( Q \) and \( H_0 \) are given by

\[ \Psi_A^\dagger Q \Psi_B = \psi_A \psi_B - \phi_A \phi_B, \]  
\[ \Psi_A^\dagger H_0 \Psi_B = \mu_0 |\gamma| ab (\psi_A \psi_B + \phi_A \phi_B). \]

(8.82) \hspace{1cm} (8.83)

The positive-\( \omega \) solutions of the zeroth-order eigenvalue equation \( H_0 \Psi_0 = \omega_0 Q \Psi_0 \) have \( \phi_0 = 0 \) and \( \psi_0 \) arbitrary (provided \( \psi_0^2 = 1 \)). We further assume that the \( H_i \) for \( i \geq 1 \) are of the form

\[ H_i = \left( \begin{array}{cc} \hat{A}_i & \hat{C}_i \\ \hat{C}_i & \hat{B}_i \end{array} \right), \]

(8.84)

where \( \hat{C} \) is Hermitian. We have

\[ \Psi_A^\dagger H_i \Psi_B = \psi_A \hat{X}_i \psi_B + \phi_A \hat{Y}_i \phi_B + \psi_A \hat{Y}_i^\dagger \phi_B + \phi_A \hat{X}_i^\dagger \psi_B \]

(8.85)

with

\[ \hat{X}_i = \frac{\mu_0 |\gamma|}{2ab} (a^2 \hat{A}_i + b^2 \hat{B}_i), \]  
\[ \hat{Y}_i = \frac{\mu_0 |\gamma|}{2ab} (-a^2 \hat{A}_i + b^2 \hat{B}_i - 2iab \hat{C}_i). \]

(8.86a) \hspace{1cm} (8.86b)
The functionals (8.80) become

\[
\begin{align*}
\omega_0 &= \mu_0 |\gamma| ab, \\
\omega_1 &= \psi_0 \dot{X}_1 \psi_0, \\
\omega_2 &= 2\omega_0 \phi_1^0 + 2\psi_0 \dot{X}_1 \psi_1 + 2\psi_0 \dot{Y}_1 \psi_1 + \psi_0 \dot{X}_2 \psi_0, \\
\omega_3 &= 4\omega_0 \phi_1 \phi_2 + 2\psi_0 \dot{Y}_1 \phi_2 \\
&\quad + \psi_1 \dot{X}_1 \psi_1 + \phi_1 \dot{X}_1 \phi_1 + 2\psi_1 \dot{Y}_1 \phi_1 \\
&\quad + 2\psi_0 \dot{X}_1 \psi_2 + 2\psi_0 \dot{X}_2 \psi_1 + 2\psi_0 \dot{Y}_2 \phi_1 \\
&\quad + \psi_0 \dot{X}_3 \psi_0, \\
\omega_4 &= 4\omega_0 \phi_1 \phi_3 + 2\omega_0 \phi_2^0 \\
&\quad + 2\psi_0 \dot{X}_1 \psi_3 + 2\psi_0 \dot{Y}_1 \phi_3 + 2\phi_1 \dot{X}_1 \phi_3 + 2\psi_1 \dot{X}_1 \phi_2 \\
&\quad + 2\phi_1 \dot{Y}_1 \phi_2 + 2\phi_1 \dot{Y}_1^\dagger \psi_2 \\
&\quad + 2\psi_0 \dot{X}_2 \psi_2 + 2\psi_0 \dot{Y}_2 \phi_2 \\
&\quad + \psi_1 \dot{X}_2 \phi_1 + \phi_1 \dot{X}_2 \phi_1 + 2\phi_1 \dot{Y}_2 \phi_1 \\
&\quad + 2\psi_0 \dot{X}_3 \phi_1 + 2\psi_0 \dot{X}_3 \phi_1 + \psi_0 \dot{X}_4 \psi_0,
\end{align*}
\]

(8.87a - 8.87e)

where we have substituted constraint (8.81b) into Eq. (8.80b) and so on. The constraints (8.81) become

\[
\begin{align*}
1 &= \phi_0^0, \\
0 &= 2\psi_0 \psi_1, \\
0 &= 2\psi_0 \psi_2 + \phi_1^0 - \phi_1^2, \\
0 &= 2\psi_0 \psi_3 + 2\phi_1 \psi_2 - 2\phi_1 \phi_2.
\end{align*}
\]

(8.88a - 8.88d)

If we wish to obtain the higher modes \( n = 2, 3, \ldots, \) we carry out the minimization of the functionals \( \omega_i \) under additional constraints \( \phi_0^{(m)} \phi_0^{(m)} = 0, \phi_0^{(m)} \phi_1^{(m)} + \phi_0^{(n)} \phi_1^{(n)} = 0, \) etc. for all \( m < n. \)

The function \( \psi_0 \) is found by minimization of \( \omega_1 \) (8.87b), lifting the degeneracy at zeroth order. It satisfies

\[
\dot{X}_1 \psi_0 = \omega_1 \psi_0.
\]

(8.89)

Together with Eqs. (8.88b) and (8.88c), this implies \( \psi_0 \dot{X}_1 \psi_0 = 0 \) and \( 2\psi_0 \dot{X}_1 \psi_2 = -\omega_1 [\phi_1^2 - \phi_1^2]. \) Given \( \psi_0, \) minimization of \( \omega_2 \) (8.87c) then yields

\[
\phi_1 = -\frac{1}{2\omega_0} \dot{Y}_1^\dagger \psi_0.
\]

(8.90)

If \( \psi_0 \) is not yet (completely) determined by minimization of \( \omega_1, \) it may be obtained by minimization of

\[
\omega_2 = \psi_0 \dot{X}_2 \psi_0 - \frac{1}{2\omega_0} \psi_0 \dot{Y}_1 \dot{Y}_1^\dagger \psi_0,
\]

(8.91)
where we have substituted Eq. (8.90) into Eq. (8.87c).

Notice that, owing to the degeneracy of the modes at zeroth order, the other first-order component $\psi_1$ is not fixed by minimization of $\omega_2$. We minimize

$$\omega_3 = \psi_1(\hat{X}_1 - \omega_1)\psi_1 + \phi_1(\hat{X}_1 + \omega_1)\phi_1 + 2\psi_1\hat{Y}_1\psi_1 + 2\phi_0\hat{X}_2\psi_1 + 2\phi_0\hat{Y}_2\phi_1 + \phi_0\hat{X}_3\phi_0,$$

yielding the condition

$$(\hat{X}_1 - \omega_1)\psi_1 = -\hat{Y}_1\phi_1 - \hat{X}_2\psi_0 + \lambda\psi_0,$$

where $\lambda$ is chosen such that the equation has a solution. The solution $\psi_1$ is now defined up to a term $\propto \psi_0$, which is fixed by the constraint (8.88b).

If $\hat{X}_1 - \omega_1$ has null vectors other than $\psi_0$, the profile $\psi_1$ is not yet (completely) fixed by the condition (8.93). We then consider

$$\omega_4 = 2\omega_0\phi_2^2 + 2[(\hat{X}_1 + \omega_1)\phi_1 + \hat{Y}_1^\dagger\psi_1 + \hat{Y}_2^\dagger\phi_0]^\dagger\phi_2 + \psi_1(\hat{X}_2 - \lambda)\psi_1 + \phi_1(\hat{X}_2 + \lambda)\phi_1 + 2\psi_1\hat{Y}_2\phi_1 + 2\phi_0\hat{X}_3\psi_1 + 2\phi_0\hat{Y}_3\phi_1 + \phi_0\hat{X}_4\phi_0,$$

where $\lambda = \psi_0\hat{Y}_1\phi_1 + \psi_0\hat{X}_2\psi_0$. Minimization gives

$$\phi_2 = -\frac{1}{2\omega_0}[(\hat{X}_1 + \omega_1)\phi_1 + \hat{Y}_1^\dagger\psi_1 + \hat{Y}_2^\dagger\phi_0].$$

Eliminating $\phi_2$, we obtain

$$\omega_4 = -\frac{1}{2\omega_0}\|[(\hat{X}_1 + \omega_1)\phi_1 + \hat{Y}_1^\dagger\psi_1 + \hat{Y}_2^\dagger\phi_0]\|^2 + \psi_1(\hat{X}_2 - \lambda)\psi_1 + \phi_1(\hat{X}_2 + \lambda)\phi_1 + 2\psi_1\hat{Y}_2\phi_1 + 2\phi_0\hat{X}_3\phi_1 + 2\phi_0\hat{Y}_3\phi_1 + \phi_0\hat{X}_4\phi_0,$$

which functional should be minimized treating Eq. (8.93) as an additional constraint.


[62] By inspection of the MATLAB (IMP) and FORTRAN (SIA, SIB) codes provided by J. H. Mentink (private communication).


[131] K. S. Novoselov, Private communication.


Small pressure variations inside a material create a propagating excitation we all know as a sound wave. A somewhat similar phenomenon is seen when slight spatial variations exist in the magnetization field of a magnetic solid. In this case, the resulting propagating excitation is known as a spin wave. Spin waves, like sound waves and light waves, play an important role in the physics of the solid state. Increasingly, spin waves are also being considered for their potential for application as the basis of a future energy-efficient information-processing technology. They might, one day, be utilized as a means to encode, transfer, and process information within a logic circuit.

From the theoretical point of view, two properties make spin waves particularly interesting as an information carrier. First, the behavior of spin waves becomes nonlinear even at low energies, which means that one spin-wave packet could be used to control the propagation of the other. Second, spin waves are very sensitive to the local orientation of the magnetization field through which they propagate, creating useful interactions with the many different magnetic textures that can be identified in ferromagnetic media. Magnetic thin films tend to form patchworks of domains with alternating magnetization directions. The boundaries between such domains (domain walls) are intriguing structures in themselves, with a particular dynamics. Topological defects such as domain walls may constitute active elements to manipulate submicrometer spin waves and perform logic operations.

Modern research of magnetism has developed a rich set of theoretical approaches and covers an enormous variety of phenomena. At the same time, it is surprising how much of it can already be understood at the level of classical theory [Chap. 3]. In 1935, L. D. Landau and E. M. Lifshitz formulated an elegant equation that describes the dynamics of the magnetization field inside a ferromagnetic medium. With the contributions of T. L. Gilbert (1955), their equation is now known as the Landau–Lifshitz–Gilbert (LLG) equation. Stripped to its essence, the equation simply describes how the magnetic dipoles inside the solid precess in an applied magnetic field. But by taking into account spatial variations in the magnetization of the solid, it also predicts the existence of spin waves. The LLG equation captures the dynamics of topological defects in the magnetization field, such as domain walls, and their interaction with the spin waves, in a unified model.

Translating the LLG equation into concrete predictions for the behavior of spin waves in nontrivial geometries (magnetic nanoelements) or nontrivial magnetic textures requires the solution of large eigenvalue problems, optimization problems, scattering problems, and time-integration problems [Sec. 2.2], which must normally be solved numerically. The non-Newtonian dynamics of mag-
Summary

Magnetization and its long-range interactions create specific requirements for the numerical techniques to be used. In the first part of this thesis, we develop the necessary numerical algorithms and theoretical tools. In Chap. 4, we critically review and analyze various schemes for numerical time-integration of the LLG equation. We also discuss how these schemes may be efficiently implemented in a computer code, deriving quantitative results on their convergence. In Chap. 5, we present a computational scheme that can solve the problem of finding the spin-wave eigenmodes (magnetic normal-mode problem) in a numerically stable and efficient way even if zero-frequency modes (zero modes) are present. We provide a large number of example calculations, which focus on the relation between magnetic normal modes and topologically protected magnetic structures. As we argue, the zero modes are crucial for understanding the long-time behavior of topological defects in magnetic media, describing, for example, the motion of a domain wall or a magnetic skyrmion structure as a whole. We highlight a fundamental distinction between two types of zero modes that can occur in magnetic systems.

Throughout this thesis, we seek to match our numerical results with simplified analytical models that capture the essence of the physical behavior and create a deeper understanding of what is going on (Sec. 2.1). An important example of this approach is given by Chap. 6. In this case, the analytical model is a nonlinear wave equation known as the sine-Gordon equation. The fundamental solutions of the sine-Gordon equation have certain counterintuitive (solitonic) properties which set it apart from most other nonlinear partial differential equations. By identifying the key parameters of the magnetic system under study, we are able to justify approximations that allow us to map the magnetic system onto the sine-Gordon equation. Thus, we are able to predict and explain, in mathematically simple terms, the intriguing results we observe in a much more involved micromagnetic model based on the LLG equation.

The main question we try to answer in Chap. 6 is how the discreteness of the crystal lattice of the solid affects the dynamics of domain walls. While many models of domain walls represent the magnetization field as a continuum, it has been established, both theoretically and experimentally, that lattice discreteness causes a weak residual effect, which is known as the Peierls potential. As a consequence of this effect, the propagation of a very narrow domain wall, at low temperatures, proceeds through the formation of kinks in its profile. Our analytical description and numerical simulations establish a link between the dynamics of these domain-wall kinks and kinks in the sine-Gordon model. This connection leads to the surprising results that, in a certain well-defined regime of material parameters, domain-wall kinks can pass through each other without any significant energy dissipation and can bond together to form a special type of localized nonlinear excitation (breather).

In Chap. 7, we focus on the effect of a domain wall on spin waves that pass through it. We consider the case of a domain wall in an ultrathin magnetic film with perpendicular magnetic anisotropy. A domain wall in this system
may exist in two equivalent but distinct equilibrium states, which have opposite orientations of the magnetization inside the domain wall. Our main contribution in this chapter is the realization that the phase of the transmitted spin waves may be shifted by up to $180^\circ$ by switching the domain wall between its two stable equilibrium states. Thus, the domain wall could act as a spin-wave switch by inducing either constructive or destructive interference depending on its internal state.

The origin of the state-dependent phase-shift effect, which is absent in most bulk materials, is an antisymmetric exchange interaction that is present at the thin-film interface (interfacial Dzyaloshinskii–Moriya interaction). The effect depends essentially on the specific broken symmetries associated with this interaction. We demonstrate, by a combination of analytical theory, semianalytical numerical calculations, and explicit micromagnetic simulations, that the difference in phase shift between the two domain-wall states is large enough to switch between constructive and destructive interference, creating the possibility of a domain-wall-based spin-wave switch or memory element. Our analytical model allows us to understand the phase shift in topological terms. It demonstrates that the phase shift is not the result of a fortuitous choice of simulation parameters but corresponds to an essential geometric phase.

The final chapter of this thesis (Chap. 8) considers the behavior of spin waves on a very different lengthscale. In the long-wavelength regime (tens to hundreds of micrometers), the behavior of spin waves in magnetic films is determined by the dipolar (magnetostatic) interaction, while the exchange interactions, which dominate the behavior of nanometer spin waves, are broadly negligible. This reversal leads to a number of well-established but highly counterintuitive effects. For example, in an in-plane magnetized film, spin-wave modes exist which have a negative group velocity, meaning that their actual propagation is opposite to their apparent direction of propagation. Such effects can be observed in opto-magnetic experiments, in which spin waves are excited and detected using light pulses. We derive new explicit analytical expressions for the behavior of the volume spin-wave modes in two asymptotic regimes. These results are combined to obtain a very accurate semianalytical expression for the dispersion relation of the lowest-frequency volume mode that is straightforward to evaluate using standard numerical routines.
SAMENVATTING

Een geluidsgolf wordt gevormd door kleine variaties in de druk in een materiaal. Het is een voorbeeld van een zich voortplantende excitatie waarmee wij allemaal bekend zijn. Een enigszins vergelijkbaar fenomeen doet zich voor als er kleine variaties bestaan in het magnetisatieveld van een magnetische vaste stof. De overeenkomende lopende excitatie staat in dat geval bekend als een spingolf. Spingolven spelen, evenzeer als geluidsgolven en lichtgolven, een grote rol in de fysica van de vaste stof. In toenemende mate worden spingolven bovendien gezien als de mogelijke basis voor de energiezuinige informatietechnologie van de toekomst. Ze zouden kunnen worden toegepast als een middel om informatie te coderen, over te dragen en te verwerken binnen een logisch circuit.

Uit theoretisch oogpunt maken twee eigenschappen spingolven in het bijzonder interessant als drager van informatie. Ten eerste vertonen spingolven al bij lage energieën niet-lineair gedrag. Dit betekent dat het ene spingolfpakketje kan worden gebruikt om het andere te schakelen. Ten tweede zijn spingolven zeer gevoelig voor de plaatselijke oriëntatie van het magnetisatieveld waardoor ze zich voortplanten. Hierdoor ontstaan bruikbare wisselwerkingen tussen de spingolven en de talloze magnetische structuren die in ferromagnetische materialen te vinden zijn. In veel dunne magnetische films vormt zich een lappendeken van domeinen met steeds een andere magnetisatie-richting. De grenslijnen tussen die domeinen (domeinwanden) zijn interessante structuren op zich, met een geheel eigen dynamica. Topologische defecten zoals domeinwanden kunnen fungeren als actieve schakelelementen voor korte spingolven en zo logische bewerkingen uitvoeren.


Om de LLG-vergelijking te vertalen naar concrete voorspellingen voor het gedrag van spingolven in niet-triviale geometrieën (zoals nano-elementen) of
Samenvatting

niet-triviale magnetische structuren is het vaak nodig om grote eigenwaardeproblemen, optimalisatieproblemen, verstrooingsproblemen of tijdsintegratieproblemen numeriek op te lossen (par. 2.2). De niet-newtoniaanse dynamica en verdragende wisselwerkingen van het magnetisatielveld leggen bijzondere voorwaarden op aan de numerieke methoden die kunnen worden gebruikt. In het eerste deel van dit proefschrift ontwikkelen we de benodigde numerieke algoritmen en het theoretische gereedschap. In hs. 4 geven we een kritische beschouwing en analyseren we enkele methoden voor numerieke tijdsintegratie van de LLG-vergelijking. We bespreken ook hoe deze methoden efficiënt kunnen worden geïmplementeerd in computercode, waarbij we enkele kwantitatieve convergentie-eigenschappen afleiden. In hs. 5 presenteren we een rekenmethode om de spingolf-eigenmodi te vinden (het magnetisch normaalmodusprobleem) die numeriek stabiel en efficiënt is, zelfs als er één of meerdere normaalmodi aanwezig zijn met een frequentie van nul (nulmodi). We laten een groot aantal voorbeeldberekeningen zien, die in het bijzonder de relatie verduidelijken tussen de normaalmodi en topologisch beschermde magnetische structuren. Wij betogen dat de nulmodi essentieel zijn om het gedrag van magnetische topologische defecten op een langere tijdsschaal te begrijpen. Zo beschrijven ze de translatiebeweging van een domeinwand of magnetische skyrmionstructuur als geheel. We belichten een fundamenteel onderscheid tussen twee typen nulmodi die in magnetische systemen voorkomen.

In dit proefschrift probeer ik steeds om het numerieke resultaat te koppelen aan een vereenvoudigd analytisch model dat de kern van het waargenomen gedrag op een zo eenvoudig mogelijke manier verklaart (par. 2.1). Een belangrijk voorbeeld van deze aanpak is te vinden in hs. 6. Hier is het gebruikte analytische model een niet-lineaire golfvergelijking die bekend staat als de sine-Gordonvergelijking. De elementaire oplossingen van de sine-Gordonvergelijking hebben een aantal tegenintuitive eigenschappen (solitonisch gedrag) die haar onderscheiden van de meeste andere partiële differentiaalvergelijkingen. Door te identificeren wat de belangrijkste parameters van het betreffende magnetische systeem zijn, kunnen we het systeem benaderen op een manier die het mogelijk maakt om een vertaalslag te maken naar de sine-Gordonvergelijking. Op deze manier zijn we in staat om de intrigerende resultaten die we waarnemen in het ingewikkelde micromagnetische model van de LLG-vergelijking te voorspellen en te verklaren in wiskundig eenvoudige termen.

De hoofdvraag die we beantwoorden in hs. 6 is hoe het feit dat een vaste stof bestaat uit een discreet kristalrooster van invloed is op de dynamica van domeinwanden. Hoewel veel modellen voor domeinwanden het magnetisatieveld als continuïm behandelen, is uit theorie en experiment gebleken dat de discreetheid van het kristalrooster zich wel degelijk openbaart, namelijk als een zwak restverschijnsel dat bekend staat als de Peierlspotential. Als gevolg van dit effect verloopt, bij lage temperatuur, de beweging van een zeer smalle domeinwand via de vorming van kinks in het profiel van de domeinwand. Onze analytische beschrijving en numerieke resultaten leggen een verband tussen de
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Dynamica van deze domeinwandkinks en de kinks in het sine-Gordonmodel. Deze link leidt tot het interessante resultaat dat, binnen een zeker welgedefinieerd bereik van materiaalconstanten, de domeinwandkinks bij benadering zijn op te vatten als solitonen die elkaar kruisen zonder wezenlijk energieverlies. We voorspellen daarmee tevens een nieuw type gelokaliseerde niet-lineaire excitatie van de smalle domeinwand (breather).

In hs. onderzochten we wat er gebeurt met spingolven die door een domeinwand gaan. We beschouwden het geval van een domeinwand in een ultradunne magnetische film met een magnetische anisotropieas die loodrecht op het vlak van de film staat. Een domeinwand in dit systeem heeft twee gelijkwaardige maar verschillende evenwichtstoestanden met een tegengestelde magnetisatierichting binnen de domeinwand. De belangrijkste bijdrage van dit hoofdstuk is dat de fase van de doorgelaten spingolven die een domeinwand passeren met ° kan worden verschoven door de domeinwand om te zetten van de ene naar de andere stabiele evenwichtsstructuur. Dat maakt de domeinwand tot een schakelaar: de spingolven vertonen constructieve of destructieve interferentie al naar gelang de interne toestand van de domeinwand.

De oorsprong van dit toestandsafhankelijke faseverschuivingseffect, dat niet bestaat voor domeinwanden in de meeste materialen in bulk, is een antisymmetrische uitwisselingswisselwerking die ontstaat aan de grensvlakken van de film (grenslaag-Dzyaloshinskii-Moriyawisselwerking). Het effect hangt op een essentiële manier af van de symmetriën die worden gebroken door deze wisselwerking. Door middel van een combinatie van analytische theorie, semianalytische numerieke berekeningen en expliciete micromagnetische simulaties laten we zien dat het verschil in faseverschuiving geïnduceerd door de twee verschillende toestanden van de domeinwand groot genoeg is om het verschil te maken tussen constructieve en destructieve interferentie. Dit opent de mogelijkheid van de domeinwand als schakelaar voor spingolven of als geheugenelement. Ons analytische model verklaart de faseverschuiving in topologische termen. Het laat zien dat de faseverschuiving niet het gevolg is van gelukkig gekozen simulatieparameters, maar een geometrische fase vertegenwoordigt die een essentiële onderdeel is van het systeem.

Het laatste hoofdstuk van dit proefschrift (hs. beschouwde het gedrag van spingolven op een heel andere lengteschaal. Voor lange golflengten (enkele tientallen tot honderden micrometer) bepaalt de dipoolwisselwerking (magnetostatische wisselwerking) het gedrag van spingolven. In dit regime is de uitwisselingswisselwerking, die dominant is voor het gedrag van nanometerspingolven, grotendeels verwaarloosbaar. Deze omkering heeft een aantal gevolgen die welbekend maar sterk tegenintuïtief zijn. Zo bestaan er, voor een film waarvan de magnetisatierichting in het vlak ligt, spingolfmodi met een negatieve groepssnelheid. Dat betekent dat de feitelijke voortplantingsrichting van de spingolven tegengesteld is aan de schijnbare voortplantingsrichting. Dergelijke verschijnselen zijn goed waar te nemen in optomagnetische experimenten, waarin de spingolven worden geëxciteerd en gedetecteerd door middel van lichtpulsen. Wij lei-
den nieuwe analytische uitdrukkingen af voor het gedrag van de volumemodi van de spingolven in twee asymptotische regimes. We combineren deze resultaten tot een nauwkeurige semianalytische uitdrukking voor de dispersierelatie van de laagstfrequente volumemodus die gemakkelijk kan worden geëvalueerd met numerieke standaardalgoritmes.
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LIST OF PUBLICATIONS


Frank Buijnsters was born in Nijmegen, the Netherlands, on 21 February 1988. He received his BSc degrees in Physics (cum laude) and Mathematics (cum laude) from Radboud University, Nijmegen in 2010, and received his MSc degree in Theory and Simulation of Materials (with distinction) from Imperial College, London in 2011. From January 2012, he started working towards a PhD degree in the Theory of Condensed Matter group at Radboud University. Frank’s research interests include the theory of magnetization dynamics, spin waves, molecular simulation, and numerical methods and algorithms.