

PRECESSION DAMPING IN ITINERANT FERROMAGNETS

by

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in

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November, 2007

To my parents,

Footsteps left in sand
guidance, encouragement, love
finding my own way.

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ABSTRACT

Precession damping in metallic ferromagnets had been assumed to result from the spin-orbit interaction. While several theories of spin-orbit damping had been postulated, no convincing numerical comparisons to data existed. We selected one promising theory and performed first-principles numerical calculations of damping for bulk iron, cobalt, and nickel. Comparison of minimal calculated and measured damping rates demonstrated a 70 % agreement for nickel, 60 % for iron, and 40 % for cobalt.

We then relaxed the initial constraint of a universal electron-lattice scattering rate by allowing the scattering rate to be spin dependent. The spin dependent lifetime ratio was equated to the ratio of the spin resolved density of states at the Fermi level. This modification improved the agreement to 95 % for nickel, 70 % for iron, and 47 % for cobalt.

With this level of agreement, we next constructed a simple effective field explanation for the damping process. As the magnetization rotates, the energy of the spin system gets pushed out of equilibrium and this excitation is quenched by electron-lattice scattering. The energy of the spin system changes by two mechanism: the energies of the states change and transitions to excited states occur. The first mechanism had previously been described within the effective field picture as producing a breathing of the Fermi surface. As the magnetization precesses, the spin-orbit energy of each state changes leading to expansions and contractions of the Fermi surface that are periodic with the precession. To expand this metaphor, we have dubbed the second effect of transitions to excited states as a bubbling of the Fermi sea. In this picture, individual electrons across the Fermi surface undergo larger excitations.

Finally, we investigated the dependence of the damping rate on the density of states and the spin-orbit coupling parameter. We found that the damping due to the breathing effect was roughly proportional to the density of states while damping from the bubbling terms correlated strongly with the density of states squared. By tuning the spin-orbit parameter we found that the breathing terms were proportional to the spin-orbit parameter cubed while the bubbling terms went as the spin-orbit parameter squared.

CHAPTER 1

TECHNOLOGICAL MOTIVATION

Magnetization dynamics has been an active area of research for nearly 100 years. In addition to traditional applications such as electric transformers, motors, and generators, magnets have become fully ingrained into important and sophisticated technologies such as computer memories and a wide variety of sensors. The critical role played by magnets and magnetization dynamics in modern technology has recently been highlighted by the awarding of the 2007 Nobel Prize in Physics for the discovery of the Giant Magnetoresistance effect, which provided the most recent revolution in computer hard drives.

Magnetic devices are dynamic elements that typically operate at picosecond time scales. What is most critical to many devices is the rate at which the magnetization loses energy, and the mechanism by which this energy is lost. A sore point in the magnetism community has been the lack of a detailed understanding of magnetization dynamics generally and damping in particular. This is most true for itinerant ferromagnets, which are universally used in devices. Therefore, we set out to identify the important loss mechanisms in simple metallic ferromagnets and to quantify the damping rates.

Magnets are useful as information storage devices because they can be made to have two stable configurations which can be easily discerned. An important empirical observation is that it takes less energy to point the magnetization in some directions with respect to the crystal axes than in other directions. This fact is due in part to the shape of the magnet, which affects the dipole self-interaction, and also to the magnetocrystalline anisotropy, which originates in the spin-orbit interaction. A useful result is that it is often easy to point the magnetization of a material either direction along one particular crystal axis, but hard to point the magnetization perpendicular to this easy axis; see Fig. (1.1). Because of the en-

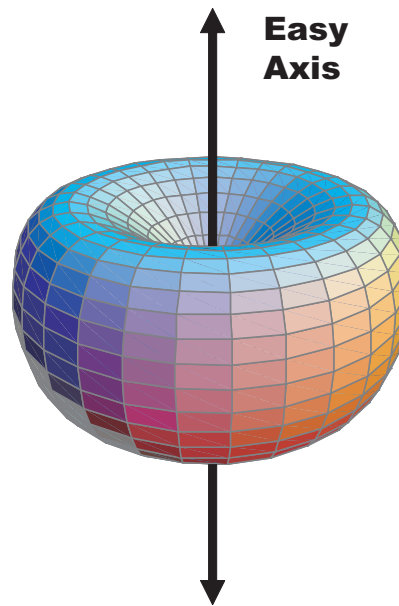


Figure 1.1: Uni-axial magnetocrystalline anisotropy surface. Energy surface for pointing the magnetization in a particular direction with respect to the crystal axes. Uni-axial materials have one low energy axis along which it is easy to point the magnetization. The two directions along the easy axis are separated by an energy barrier in the perpendicular plane.

energy barrier between the two low energy directions these magnetic systems are very stable against decay. Such magnets are useful for storage of binary information.

Storing information also requires reversing bits, that is, rotating the magnetization from one direction along the easy axis, over the energy barrier, and to the opposite direction along the easy axis. This is typically accomplished by applying an external field in the direction opposite to the magnetization. The external field adds a Zeeman energy such that the initial magnetization direction becomes a higher energy state and the final direction a lower energy state. Any misalignment between the magnetization direction and the applied field will result in a torque on the magnetization that causes it to precess about the applied field. This precession will not cause the magnetization to reverse. The fact that the precession dynamics are damped, and the magnetization loses energy to its environment, allows the

magnetization to switch from the high energy direction to the low energy direction.

Magnetization dynamics and damping are fundamentally important to the computer hardware industry. Companies such as Hitachi [1] and Seagate [2] devote considerable resources and effort toward constantly improving the performance of their magnetic media recording devices. In this introductory chapter we will very briefly discuss a few instances in which controlling magnetization dynamics are critical to the performance of memory elements. Additionally, since dissipation and fluctuations are intimately related through the fluctuation-dissipation theorem, understanding the damping of magnetization dynamics is also essential to improving the performance of conventional magnetic sensors.

Hard Disk Devices

Figure (1.2) shows a schematic representation of a typical magnetic hard drive and read/write head. Magnetization dynamics play a critical role in several aspects of the read/write process. The magnetic core of the write-head must be appropriately magnetized (clock-wise or counter-clock-wise) by application of a very short current pulse through the coil set. The bit to be written must undergo a reversal. The magnetically soft (low magnetocrystalline anisotropy) underlayer of the media must respond to the applied field so that the field lines can reconnect at the other pole face of the magnet. The bits underneath the trailing pole face, which are in the field reconnection path, should not undergo a reversal.

The read-head consists of a magnetoresistive (MR) stack. A magnetoresistive element is a material or composite material for which the electrical resistance through the element depends on its magnetic configuration. There are several varieties of magnetoresistance. The anisotropic magnetoresistance (AMR) was one of the earliest MR phenomena discovered. In this case, the resistance of a ferromagnetic material depends on the direction which the current is sent through the ferromagnetic with respect to the magnetization direction.

Later, a much larger effect was discovered, the giant magnetoresistance (GMR). When two ferromagnetic films are separated by a non-magnetic spacer and a current is driven perpendicular to the films the resistance observed depends strongly on the relative orientation of the magnetizations of the two ferromagnetic layers. This effect is strong enough to be used as a room temperature sensor for detecting the magnetization direction of materials, such as hard drive bits. The newest magnetoresistive discovery is tunneling magnetoresistance (TMR). A TMR device is very similar to a GMR device, but the spacer is now a tunnel barrier material. The first popular barrier was amorphous Al_2O_3 for its ubiquity as a capping layer and ease of growth. However, researchers are moving to crystalline MgO for the superior bias in selectively tunneling only certain states.

The read element in a hard drive is a stack of several thin films that collectively form either a GMR or TMR sensor. There are two ferromagnetic layers with uni-axial magnetic anisotropy. The easy axes of the two layers are typically aligned perpendicularly to each other, and in the film planes. Since the aligned and anti-aligned states translate into low and high resistance states, the perpendicular configuration is maximally sensitive to changes in the alignment of the two films. One of the ferromagnetic layers is referred to as the 'free' layer while the other is the 'fixed' layer. The magnetization of the fixed layer does not rotate, its orientation is fixed through exchange bias coupling to an adjacent antiferromagnetic layer. The free layer can be rotated by an external field. As the read-head passes over a magnetic bit in the hard drive, the stray field from the bit acts on the free layer in the GMR/TMR element, causing the free layer to partially align with the bit it is passing over. A current is then driven through the MR stack to measure the MR value. The result of this resistance measurement – high resistance or low resistance – indicates the direction of the magnetization of the bit (its state). All of these processes must presently occur in under one nanosecond.

Conventional recording media consists of granularly deposited soft magnetic material.

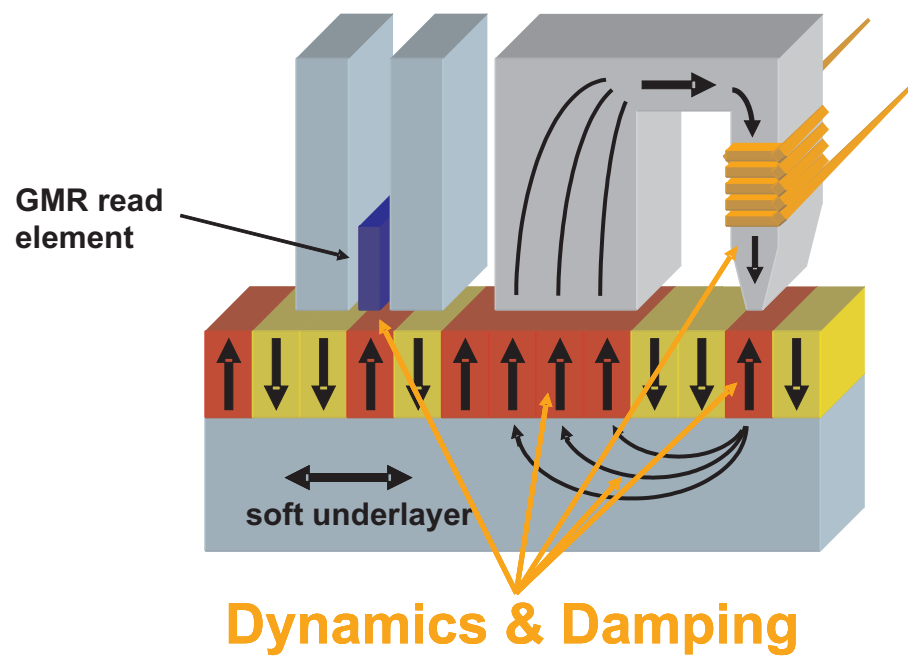


Figure 1.2: Schematic of hard drive read/write head in the perpendicular recording configuration. Arrows indicate some of the many instances of magnetization dynamics occurring during the operation of the read/write head.

Bits consist of a group of granules, roughly 100. Bits consisting of fewer granules become poorly defined and errors ensue. Until a few years ago recording techniques wrote bits in-plane, that is, the magnetization of the bits was in the plane of the media. This method of operation became problematic as bit and granule size was reduced. The granules are not completely stable against thermally induced reversals. In fact, as the size of the granules decreases their stability against thermal reversals decreases rapidly. Thus, companies ran into the problem that as they attempted to reduce bit sizes while maintaining the needed number of granules-to-bit, the granules had to be made so small that they became unstable against thermal reversals, the media became useless. This is known as the superparamagnetic limit problem. To get around this difficulty and continue to reduce aerial density, industry made a fundamental shift, turning the bits out-of-plane and introducing what is known as perpendicular media (shown schematically in Fig. (1.2)) [3, 4]. Perpendicular recording was able to reduce aerial densities while maintaining bit and granule size by turning the bit direction out-of-plane. While a bit still consisted of the same number of grains they took up less surface area of the media. However, this technique too has now reached the superparamagnetic limit.

To continue the trend of increasing bit densities the thermal stability of the bits must be increased. This is typically accomplished by increasing the energy barrier between the two states. There are two options for increasing the energy barrier. First, the superparamagnetic limit may be extended by switching to materials with higher anisotropies. The difficulty with this avenue is that these materials would require larger write fields. To circumvent the larger write fields, industry is investigating the possibility of selectively softening the media very locally and on very short time scales by optical heating [5]. This approach is often referred to as heat assisted magnetic reversal. This technique introduces the very serious challenge of understanding how ultrafast heating (non-equilibrium and non steady-state) affects the damping rate of a material.

The second option is bit-patterned media. In such media, the bits consist of a single patterned grain rather than a collection of randomly formed grains [6]. These grains could, for example, be lithographically patterned either by standard photolithography or the newer nano-imprint lithography technique. The challenge in this case is to make the switching fields of all the bits very uniform. The switching fields of the bits depend sensitively on the damping rates, which can in turn be affected by lithographical imperfections, particularly along the bit edges.

Both of these routes toward increased thermal stability have a host of significant difficulties. One difficulty they share in common is a greatly increased likelihood for write errors. The error rate depends sensitively on variations of the damping rates of the bits. Therefore it is advantageous to understand the damping process in detail.

For completeness, it is worth mentioning that the thermal stability of bits depends not only on the energy barrier between the two states, but also on the damping rate. Bits are unstable because they experience fluctuations and the energy of these fluctuations can be comparable to the energy barrier. The fluctuations are phenomenologically described in terms of a reversal attempt frequency. Using the fluctuation-dissipation theorem, it can be shown that the stability of bits depend exponentially on the attempt frequency and that the attempt frequency is linearly proportional to the damping rate, to lowest order in the damping rate [7–9]. Thus, the stability of bits could be increased by decreasing the damping rate. However, this approach is flawed because fast reversals rely on large damping rates.

Magnetic Random Access Memory

Conventional capacitor based random access memory (RAM) has two drawbacks: it is volatile, and it is inefficient in power consumption. Each memory bit is stored in the charge of a capacitor: an uncharged state represents a "0" while a charged capacitor represents

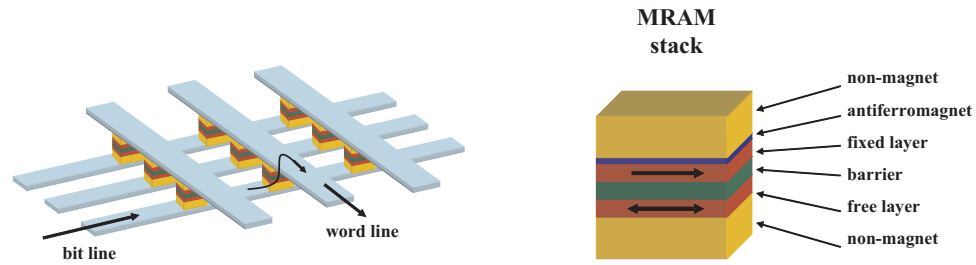


Figure 1.3: Schematic of a MRAM device. The figure on the left shows the lattice architecture. Bits consist of a MR stack – shown at the right – which are placed at each intersection point. Arrows indicate the read-out current path.

a "1". The tiny capacitors used in RAM devices are very leaky and the charge dissipates rapidly when the potential is removed. Therefore, to keep a capacitor in the "1" state requires the constant application of a current, which is wasteful because energy is being consumed but information is not changing. Further, when the computer is shut down and current is removed from all capacitors in the "1" state they rapidly decay to the "0" state and all information stored in RAM is lost.

Magnetic memory is preferable to capacitive memory because it is non-volatile and much more energy efficient. In the conventional hard disk form, magnetic memory is also very inexpensive relative to RAM. The problem with magnetic hard disk memory is that it is slow. For a long time there has been a hope that a fast, dense, and inexpensive magnetic memory system could be developed. There is finally a possibility that this hope may be realized. Magnetic random access memory (MRAM) currently exists, but it is not yet replacing conventional capacitive RAM. A simple MRAM device is depicted in Fig. (1.3). The frame of the device consists of a crossed lattice of metallic wires. A magnetoresistive element is placed at each intersection and serves as a bit.

To read the state of a bit (one stack) a current pulse is sent down the appropriate bit line, travels up through the stack, and then proceeds along the appropriate word line. The resistance, which depends on the magnetic configuration of the stack, is measured. For ex-

ample, the resistance may be low when the magnetizations are aligned and high when they are anti-aligned, but for some systems the opposite will be true. In either case, measuring the resistance of the stack reveals whether it is in the "0" state of the "1" state. For more details on the physics of this process see [10].

Writing the bits is more challenging. Two schemes exist for writing bits. In the first approach, a current pulse is sent down one bit line and one word line. As the current pulses travel down the wires they generate Ampère fields. These magnetic fields are too weak to switch the magnetic layers on their own. However, the pulses are timed to simultaneously reach the bit that is to be written. As the pulses pass each other at the selected bit, their fields add and become strong enough to reverse the magnetic layers. The fixed layer does not switch because its magnetization is pinned by coupling to a neighboring antiferromagnetic layer. The free layer does undergo a reversal.

As difficult as that bit writing process sounds, it has been made to work. There is a significant drawback, though. Increasing the aerial bit density requires scaling down the wire dimensions. As the wire cross section decreases the current density required to produce an adequate switching field rapidly increases. This results in device burn-out. Therefore, a second write technique has been proposed. This technique uses only one current pulse, in the same configuration as the read current (see Fig. (1.3)). The current pulse is sent down a bit line, through the selected stack, and out along the corresponding word line. As the electrons travel through the fixed magnetic layer they become spin polarized. When these spin polarized electrons hit the free magnetic layer they exert a torque on the magnetization. This torque can be sufficient to switch the direction of the free layer, thus reversing the alignment of the bit. To estimate what kinds of current densities are required to achieve switching is necessary to understand how much energy is lost during the reversal process. For more details on the physics of this spin-transfer torque see [11–13].

Magnetic Sensors

Superconducting quantum interference devices (SQUIDs) make extremely sensitive magnetic field detectors. However, they have certain drawbacks. To be effective they must be kept at cryogenic temperatures, which makes them expensive, bulky, and immobile. It is desirable to have the same sensitivity in an inexpensive, small, and mobile device.

The signal-to-noise ratio of a SQUID is about three orders of magnitude better than that of a magnetic sensor made from conventional ferromagnetic materials. There are two ways to increase the signal-to-noise ratio of conventional devices: increase the signal, and decrease the noise. Noise occurs in sensors because the electron spins are not completely decoupled from the electron orbits and the lattice. This coupling of the spin system to the environment allows energy to flow into and out of the system. Therefore, the spins will experience occasional energy fluctuations that appear as noise in a measurement. This coupling to the environment will also bring the spin system into equilibrium with the environment, should the spins be excited to a higher temperature than the lattice. Therefore, the same environmental coupling that is responsible for causing fluctuations (noise) in the magnetization will also dissipate energy from the system. Since noise and damping are two manifestations of environmental coupling we can learn how to reduce noise in the magnetic system by studying how the excitations of the spins are damped.

CHAPTER 2

PROBING MAGNETIZATION DYNAMICS

Magnetization precession damping is a complicated irreversible process that is roughly the angular analog to frictional or viscous damping of linear momentum. Just as damping of linear momentum is typically described by some phenomenological damping term, several phenomenological expressions have been postulated to describe magnetization dynamics. These expressions all take the form

$$\dot{\mathbf{M}} = -|\gamma|(\mathbf{M} \times \mathbf{H}) + \mathbf{D}. \quad (2.1)$$

Each equation has the term $-|\gamma|(\mathbf{M} \times \mathbf{H})$ which describes the undamped precession of the magnetization $\mathbf{M}$ about the effective field $\mathbf{H}$. γ is the gyromagnetic ratio. This term follows from basic quantum mechanics and is not simply phenomenological. The second term in each equation, generically labeled $\mathbf{D}$, describes the damping of the precession. Several common damping expressions are listed in Table (2.1) along with the resonance linewidth ΔH that they predict.

The Landau-Lifshitz and Gilbert equations are equivalent in the limit of small damping ($\alpha \ll 1$) and are known collectively as the Landau-Lifshitz-Gilbert (LLG) equation. α is the dimensionless Gilbert damping constant and λ is the Landau-Lifshitz damping rate. The respective damping rates can be related by $\lambda = \gamma M_s \alpha$ to first order in α . The LLG equation has become the equation of choice for describing magnetization dynamics in part because it can accurately model the results of a variety of measurements, but also due to the familiar viscous form of the damping term and the convenience of the unitless damping parameter α . For these reasons, we will use the LLG equation exclusively in the remainder of this chapter; for more details on the Bloch-Bloembergen and Callen equations see [14].

Table 2.1: Commonly used phenomenological precession damping expressions. The second column gives the damping term to be added to Eq. (2.1) to obtain the equation of motion. The third column is the resonance linewidth predicted by the damping term.

Researcher(s)	Damping Term	ΔH
Landau [15]	$-\frac{\lambda}{M_s^2} \mathbf{M} \times (\mathbf{M} \times \mathbf{H})$	$\frac{2H_0}{ \gamma M_s} \lambda$
Bloch [16, 17]	$-M_{x,y}/T_2$ and $-(M_z - M_s)/T_1$	$\frac{2}{ \gamma T_2}$
-Bloembergen		
Gilbert [18, 19]	$\frac{\alpha}{M_s} \mathbf{M} \times \dot{\mathbf{M}}$	$2H_0\alpha$
Callen [20]	$-\left(\frac{\lambda_{0k} + \lambda_{0\sigma}}{2}\right) \frac{\mathbf{H}_{\text{ext}} \times (\mathbf{M} \times \mathbf{H}_{\text{ext}})}{H_{\text{ext}}^2}$ $+ \left[\lambda_{k\sigma}(M_0 - M) + \left(\frac{MH_{\text{ext}} - \mathbf{M} \cdot \mathbf{H}_{\text{ext}}}{H_{\text{ext}}} \right) \lambda_{0\sigma} \right] \frac{\mathbf{H}_{\text{ext}}}{H_{\text{ext}}}$	$\frac{\lambda_{0k} + \lambda_{0\sigma}}{ \gamma }$

Figure (2.1) shows an example trajectory of a magnetization vector subject to LLG dynamics. In Fig. (2.2a) we plot the projection of the magnetization onto the transverse x -axis versus time to show clearly that the magnetization follows the classic "ring-down" of a damped oscillator. This damped oscillation is Fourier transformed to frequency space in Fig. (2.2b) resulting in a Lorentzian. The center of the Lorentzian is the resonant frequency of the magnetization while the Lorentzian width gives the damping rate as listed in the last column of Table (2.1).

Historically, magnetization dynamics have primarily been probed in the frequency domain by the ferromagnetic resonance technique. However, as the capabilities of ultrafast electronic circuits, pulse generators, and oscilloscopes have improved, newer time domain techniques such as pulsed inductive microwave magnetometry, magneto-optic Kerr effect, and X-ray magnetic circular dichroism have become more prevalent. In this chapter we will outline some of these measurement techniques and the information they provide.

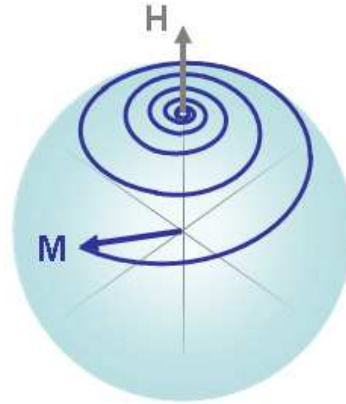


Figure 2.1: Magnetization trajectory dictated by the LLG equation. As the magnetization vector precesses about the equilibrium direction it loses energy and spirals in.

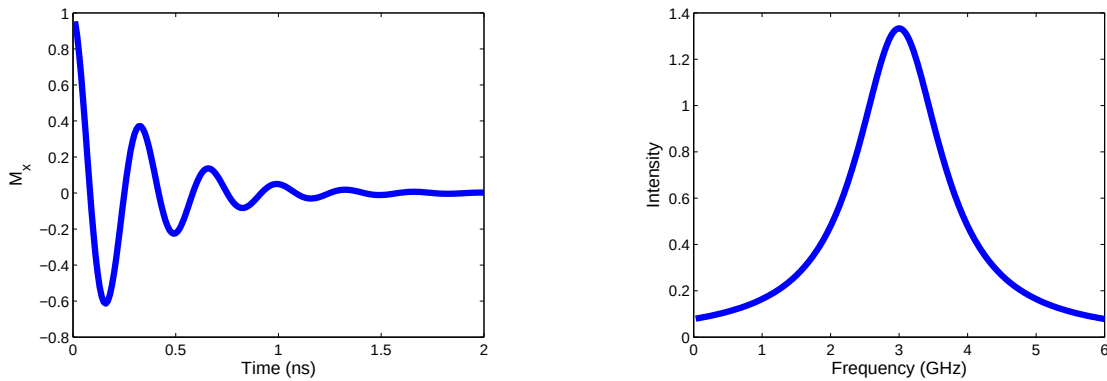


Figure 2.2: Magnetization dynamics in (a) the time domain and (b) the frequency domain. (a) shows the projection of a transverse component of the magnetization as a function of time. The transverse component undergoes a decaying oscillation. In (b) the time domain signal is Fourier transformed to the frequency domain resulting in a Lorentzian lineshape.

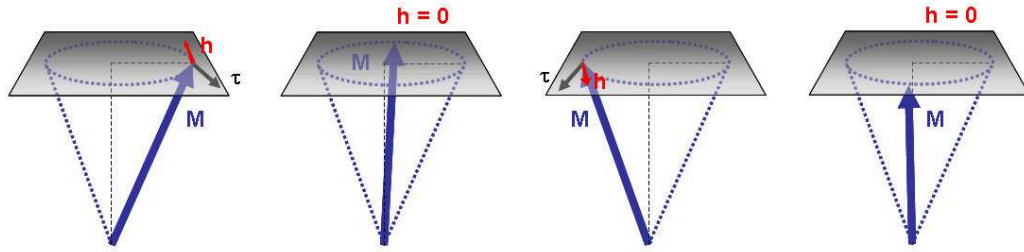


Figure 2.3: Schematic of resonance condition. Images are shown in time steps of $T/4$ where T is the precession period. When the magnetization precession frequency matches the ac field frequency the torque on the magnetization due to the ac field always pushes the magnetization out of equilibrium.

Ferromagnetic Resonance

During a typical ferromagnetic resonance (FMR) experiment, a thin film sample is mounted on top of a wave guide or inside a cavity resonator, which is centered between Helmholtz coils. The sample is subjected to both a strong dc field, which typically determines the equilibrium direction, and a weak ac field, usually between 1 and 100 GHz. The uniform precession mode of the sample has a natural frequency determined in part by the applied dc field. As the dc field strength is swept the natural frequency of the sample comes into resonance with the applied ac field. At resonance the sample absorbs significant power from the ac field (see Fig. (2.3)).

The measured quantity is the power absorbed versus dc field strength at a fixed ac frequency; this is the imaginary part of the ac susceptibility. The absorbed power versus dc field strength generally shows a Lorentzian lineshape, though it may also have a Voigt profile. The center of the Lorentzian gives the resonant frequency (energy) of the uniform mode while the linewidth serves as a measure of the damping rate (lifetime). The interpretation of the measured linewidth in terms of the damping rates as described in Table (2.1)

is significantly complicated and is the subject of the next chapter.

Pulsed Inductive Microwave Magnetometry

Pulsed inductive microwave magnetometry (PIMM) is a real-time technique for measuring magnetization dynamics. The physical apparatus for PIMM is similar to that for FMR, consisting of a thin strip-line wave guide and a perpendicular set of bias-field coil sets. The thin film sample is placed directly on top of the waveguide, at the midpoint of the coil sets. A large, short (1-10 ns) current pulse is sent down the wave guide. The intensity of the output pulse is measured at the opposite end of the wave guide. The presence of the sample will modify the pulse so that the difference between the input and output pulses will carry a signature of the magnetization dynamics.

The current pulse generates an Ampère field that is, for example, orthogonal to the dc field. This field pulse torques the magnetization, pushing it out of equilibrium and causing it to begin precessing around the equilibrium direction. Because the magnetization of the sample is precessing, the magnetic field felt by the wave guide wire is constantly changing. By Faraday's law, this changing magnetic field induces an electric field, which modulates the current pulse already flowing through the wire. This induced current either adds to or subtracts from the current pulse, depending on the phase of the precession. If the current pulse lasts 10 ns and the precession frequency of the sample is 1 GHz the magnetization will undergo about 10 oscillations during the pulse, which will appear as current oscillations in the output signal. The magnitude of the induced current depends on the deviation angle of the magnetization from the equilibrium direction. Since the precession damps out, the magnitude of the induced current decays.

The induced current is separated from the pulse current by subtracting the input current pulse from the output current pulse. The difference appears as a ring-down in the

time domain, similar to Fig. (2.2a). Fourier transforming this result, the real part of the frequency of the ring-down gives the precession frequency of the magnetization while the imaginary part gives the damping rate. Results of PIMM measurements on soft magnetic materials match the behavior expected from the LLG equation. For more details on the PIMM technique see [21].

Magneto-Optical Kerr Effect

The Kerr effect is essentially the same as the Faraday effect. In the Faraday effect, a transparent paramagnetic sample is placed in a constant uniform magnetic field. A linearly polarized beam of light propagates through the sample in the same direction as the field lines. The outgoing light is still linearly polarized, but the polarization axis is slightly rotated from that of the incoming beam.

As the light propagates through the material, the electric field component causes the electrons to oscillate linearly. However, in the presence of a strong magnetic field along the propagation direction the electrons will feel an additional component of the Lorentz force due to the magnetic field. This will drive the electrons in an elliptical orbit in a right-handed fashion about the propagation direction of the light. The linearly polarized light is equivalent to a superposition of right-circular and left-circular polarized light with a particular phase difference. The right-handed circulation of the electrons causes a small difference in the phase velocity of the right-handed and left-handed components of the light. The left-circular light lags the right-circular light in phase and the beam emerges from the material with a somewhat different phase relation as it had upon entering the material. This causes the polarization of the outgoing beam to be slightly rotated with respect to the polarization of the incoming beam.

The Kerr effect captures the same physics, but for a reflected beam. Metals reflect opti-

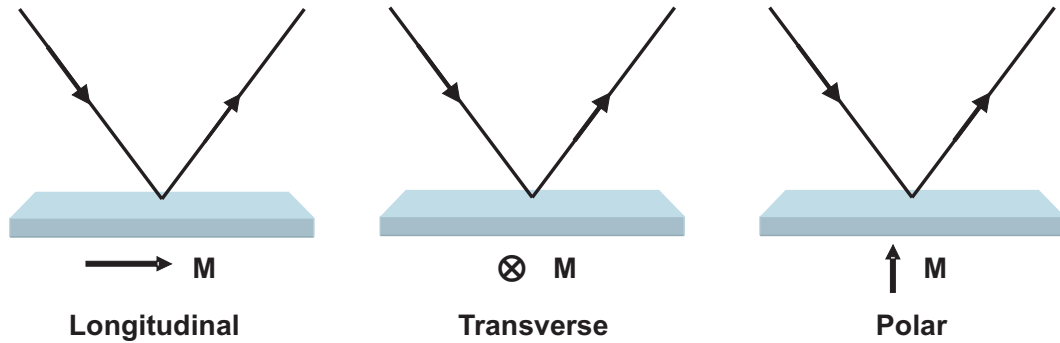


Figure 2.4: Magneto-optical Kerr effect geometries. MOKE measurements are typically made in either the longitudinal, transverse, or polar geometries. For the longitudinal case, the magnetization is in the sample plane and parallel to the plane of incidence of the light. The transverse case similarly has the magnetization in the sample plane, but perpendicular to the plane of incidence. The polar geometry has the magnetization perpendicular to the sample plane.

cal radiation, but this radiation does penetrate these materials within their skin depth. Thus, even the reflected beam travels through the material to some limited extent. For magnetized metals, this very short path length is still sufficient to cause a measurable rotation of the polarization axis of the light. The Kerr effect is usually subdivided into polar, longitudinal, and transverse geometries, shown in Fig. (2.4). In addition to the polarization axis of the outgoing beam being rotated with respect to the incoming polarization axis, the outgoing beam will generally be elliptically polarized rather than linearly polarized.

The Kerr effect is typically employed as a pump-probe technique in the time domain. The sample is subjected to a field pulse to push the magnetization out of equilibrium, beginning precession. The magnetization is then probed with a Kerr measurement after some short delay time (a few hundred fs to a few ns). By repeating the measurement with a range of delay times the dynamics can be mapped.

X-ray Magnetic Circular Dichroism

X-ray absorption spectroscopy is a synchrotron based technique for probing the electronic structure of a material. X-rays of a few hundred eV are used to promote core level electrons to the Fermi level of a material. The x-ray energy is swept and the absorption of the x-rays is measured, often by collecting electrons promoted to the vacuum level. For a given material, if the x-rays are insufficient to promote the core electrons to the Fermi level the x-rays do not get absorbed. For metals, when the x-ray energy matches the binding energy of the electrons there is a large absorption of x-rays because there are many empty states available just above the Fermi level. At higher x-ray energies the absorption drops off because there are fewer final states above the Fermi level. A further reduction of absorption occurs at higher energies due to the strong energy dependence of the light-electron matrix elements. The large spikes in the x-ray absorption only occur when the x-ray energy closely matches the binding energy of the electrons, giving this technique strong elemental specificity. X-rays of a particular energy may be absorbed strongly by one element, but not by its neighbors on the periodic table.

Since the magnitude of the absorption peak depends not only on the density of states at the Fermi level, but also on the photon absorption selection rules, this technique can be used to probe the magnetization of a material. This is accomplished by using circular polarized x-rays. For example, right circular polarized x-rays will only be absorbed by electrons that transition to a spin-up final state, and left circular x-rays will only be absorbed by electrons transitioning to a spin-down final state. Therefore, by reversing the circular polarization of light between right-handed and left-handed one can measure the ratio of the spin-up to spin-down density of states at the Fermi level, and, effectively, the magnetization [22]. This technique is known as X-ray Magnetic Circular Dichroism (XMCD).

Recent efforts have made it possible to make XMCD measurements on a sub nanosec-

ond time scale. Therefore, the trajectory of the transverse projection of the magnetization can be followed (as in Fig. (2.2a)). This has been an exciting achievement because for alloy systems, such as NiFe, the trajectories of each element may be individually mapped. It has been shown that for the case of NiFe the Ni moments precess in phase with the Fe moments [23]. It was not obvious that this would be the case because the magnetization of the ground state of NiFe is somewhat non-collinear.

CHAPTER 3

OVERVIEW OF PRECESSION DAMPING

A very important aspect of magnetization dynamics is the rate at which energy is dissipated. Magnetic damping occurs because the magnetic modes of a system (predominantly the electron spins) couple to the non-magnetic modes of the system (the electron orbits and lattice vibrations), allowing energy to be transferred back-and-forth. Since the magnetic modes are typically excited to a higher temperature than the other modes of the system, energy predominantly flows from the magnetic modes to the non-magnetic modes. As we discussed in the previous chapter, ferromagnetic resonance (FMR) probes this decay rate of the uniform precession mode.

Understanding the many coupling mechanisms and quantifying their contributions to damping has been a perennial problem for decades. It is reasonable to claim that researchers have been working on this problem at least since Landau and Lifshitz published their phenomenological equation of motion in 1935 [15]. While this chapter provides a brief overview of some of the many damping mechanisms that have been studied, this field is far too rich and expansive to do it any real justice here. For those seeking more detail on magnetism in general, I recommend the texts by Rado and Suhl [14, 24, 25] and the series edited by Bland and Heinrich [26–29]. For more specific discussions of magnetization dynamics I defer to several review papers [30–32].

In the previous chapter we investigated some of the many experimental techniques used to probe magnetization dynamics and damping. For this chapter in particular, and the remainder of this document generally, we will restrict the discussion to ferromagnetic resonance experiments. Several good general texts on this subject exist [14, 33]. One objective of a FMR experiment is to quantify the damping rate of the uniform mode of a material by

measuring the resonance linewidth. For parallel (magnetization and field in the plane of a thin film sample) and perpendicular (magnetization and field out-of-plane) configurations, the Landau-Lifshitz equation predicts that the peak-to-peak linewidth ΔH and damping rate α should be related by

$$\Delta H = \frac{2\alpha\omega_0}{\sqrt{3}|\gamma|} \quad (3.1)$$

where ω_0 is the resonant frequency, and γ is the gyromagnetic ratio. Since the experimental apparatus applies an oscillating field uniformly across the sample it overwhelmingly couples to, and excites, the uniform precession mode of the sample. Therefore, the linewidth of this resonance measures the decay rate of the uniform mode.

Contributions to the measured linewidth are logically broken down into *extrinsic* effects that are due to sample imperfections and inhomogeneities and *intrinsic* effects that originate from the interactions between the magnetic and non-magnetic modes of a system that are intrinsic to the material. Extrinsic effects are nominally avoidable and would be absent in a perfect sample, but intrinsic effects are unavoidable and operate even within a perfect sample. Extrinsic effects arise through sample inhomogeneities that can lead to a broadening of the resonance peak through various means including producing a distribution of local resonance fields across the sample, coupling the uniform mode to non-uniform mode magnons, and coupling to the phonon field. Intrinsic damping effects stem primarily from fundamental and unavoidable interactions between the magnons and the electron orbits. These interactions include generation of eddy currents and spin-orbit coupling. Additionally, damping also occurs through direct magnon-phonon scattering and a very minor intrinsic damping contribution exists through coupling of the uniform precession with the radiation field.

This work will focus solely on intrinsic damping caused by the spin-orbit interaction. However, since the measured linewidth reflects all intrinsic and extrinsic contributions it

is advisable to understand the basics of the other damping mechanisms and how to experimentally separate the intrinsic effects we are interested in from the extrinsic ones.

Extrinsic Effects

Extrinsic damping results from sample inhomogeneities. These inhomogeneities include differences in the magnetocrystalline anisotropy, variations in surface anisotropies associated with step edges, local defects, and deviations in sample thickness, magnetostriction paired with variable strains due to substrate imperfections, and other possibilities. An exact treatment of the effect of sample inhomogeneities is a very complicated problem, but it is informative to consider the limiting cases of strong inhomogeneities (when the inhomogeneous fields are large compared to the intrinsic exchange and dipole fields) and weak inhomogeneities (when the inhomogeneous field is weak compared to the exchange and dipole fields). In the strong inhomogeneity limit, different areas of the sample interact negligibly with each other and the sample appears to have a large number of local resonance fields; this is the local resonance scenario. On the other hand, when inhomogeneities are weak the magnetization of the sample maintains long range order and precesses nearly uniformly. The inhomogeneities induce mixing of the uniform mode with the non-uniform modes, causing a decoherence of the uniform mode. This limit is referred to as two-magnon scattering because the uniform mode magnon decays into non-uniform mode magnons. McMichael *et al.* have treated the local resonance limit [34], two-magnon scattering [35–37], and recently bridged these two limits with a mean field analysis [38].

Local Resonance

The limiting case to which the local resonance model applies is an ensemble of non-interacting magnetic grains that are measured simultaneously. Every grain feels the same

external field applied in the $\hat{z}$ direction. However, each grain feels a slightly different effective field due to variation in the orientations of their crystallographic axes, variations in the strength of their magnetocrystalline anisotropies, differences in defect structures and surface interactions, and other effects. Essentially, every grain feels a random contribution to its effective field, and, thus, has a unique resonance field. Therefore, even if every resonance was perfect – a delta function response with respect to the applied frequency – these local resonances would still be dispersed about some mean resonance field, producing an effective broadening of the measured resonance.

At a simple level, when the applied field is aligned with the equilibrium magnetization direction, the effect of these local resonances on the measured linewidth is given by

$$\Delta H = \Delta H_0 + \frac{2\alpha\omega_0}{\sqrt{3}|\gamma|}. \quad (3.2)$$

The linewidth is predicted to vary linearly with the resonant frequency, but also to have a non-zero intercept. The zero frequency intercept ΔH_0 has nothing to do with the damping of the uniform precession, but is a measure of the spread of the local resonance fields due to whatever inhomogeneities are present in the system. The linear increase of this linewidth with the resonant frequency would give the additional broadening due to real damping. This linear behavior of the linewidth, with non-zero intercept, is often observed [39].

Two-Magnon Scattering

The magnetic moments of a ferromagnetic system interact very strongly at short distances through the exchange interaction, which prefers parallel alignment, and at longer distances through the dipole interaction, which encourages antiparallel alignment. The competition of these two interactions leads to the formation of domains. At short distances the exchange force is stronger and spins align with their neighbors forming a ferromagnetic

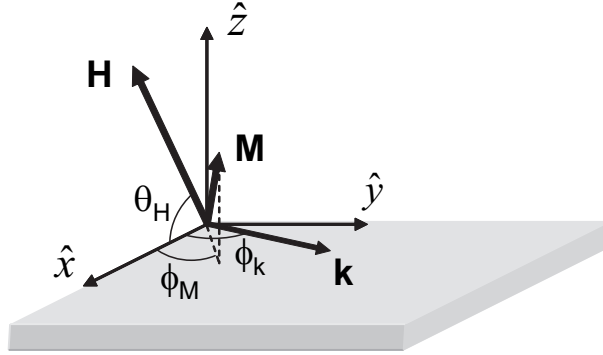


Figure 3.1: FMR sample geometry. The wavevector $\mathbf{k}$ remains in-plane, but the applied field $\mathbf{H}$ and magnetization $\mathbf{M}$ may be out-of-plane.

domain. At longer length scales the dipole interaction dominates and produces a domain wall between domains with differing magnetic orientations.

These strong interactions lead to correlations and long-range order in the system. In the present discussion we consider a single domain sample. (A sample can be forced into a single domain state by application of a strong external field.) Due to the strong interactions between spins, the magnetic excitations of the system are collective excitations of many particles rather than simple excitations of single particles. These excitations are the normal modes of the magnetic system and are known as magnons. In a perfect system the magnons can be described simply in $\mathbf{k}$ -space due to the periodicity of the crystal. The magnetic energy of the system is given as a sum over these normal modes

$$\mathcal{H}_M = \hbar\omega_0 b_0 b_0^\dagger + \hbar \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}} b_{\mathbf{q}}^\dagger. \quad (3.3)$$

Here we use $\mathbf{q}$ to designate the wavevector of the magnons. The uniform precession mode is a $\mathbf{q} = 0$ magnon and we have separated it from the summation to give it special emphasis. The magnons are created and destroyed by the $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$ operators.

Magnetic resonance experiments are typically performed on thin film samples that ap-

proximate 2-dimensional systems. The sample magnetization is uniform through the film thickness and the magnon wavevectors are restricted to lie in the sample plane. The applied field, and also the sample magnetization, may be oriented in any direction in three dimensions (see figure 3.1). The energy of the modes as a function wavevector and magnetization direction is given in [36, 40]. The magnon energy spectrum is plotted versus the magnetization direction in Fig. (3.2). The important point to note is that for a range of geometries there exist non-uniform modes that are degenerate with the uniform mode. This degeneracy is a necessary condition for scattering to occur between the uniform and non-uniform modes.

Degeneracy of modes is not sufficient to allow scattering between modes. The Hamiltonian in Eq. (3.3) does not contain any interactions, it is diagonal in $\mathbf{q}$ and, thus, does not allow scattering. This Hamiltonian is for an ideal uniform system. Real systems will have imperfections that produce inhomogeneities in the effective field. This inhomogeneous field adds off-diagonal terms to the Hamiltonian

$$\mathcal{H}_M = \hbar\omega_0 b_0 b_0^\dagger + \hbar \sum_{\mathbf{q}} \omega_{\mathbf{b}} b_{\mathbf{q}} b_{\mathbf{q}}^\dagger + \sum_{\mathbf{qp}} [M_{\mathbf{qp}} b_{\mathbf{q}}^\dagger b_{\mathbf{p}} + M_{\mathbf{qp}}^* b_{\mathbf{p}}^\dagger b_{\mathbf{q}}] , \quad (3.4)$$

which do allow scattering between the modes. The new normal modes are superpositions of the old normal modes. Fermi's golden rule gives the transition rate out of a particular mode $\mathbf{q}$ as

$$W_{\mathbf{q}} = \frac{2\pi}{\hbar} \sum_{\mathbf{p}} |M_{\mathbf{qp}}|^2 \delta(\hbar\omega_{\mathbf{q}} - \hbar\omega_{\mathbf{p}}) . \quad (3.5)$$

In particular, the line broadening due to two-magnon scattering is given by the decay rate of the uniform mode

$$\Delta\omega = \frac{2\pi}{\hbar} \sum_{\mathbf{p}} |M_{0\mathbf{p}}|^2 \delta(\hbar\omega_0 - \hbar\omega_{\mathbf{p}}) . \quad (3.6)$$

The matrix elements $|M_{0\mathbf{p}}|^2$ depend on the strength of the Fourier components of the inho-

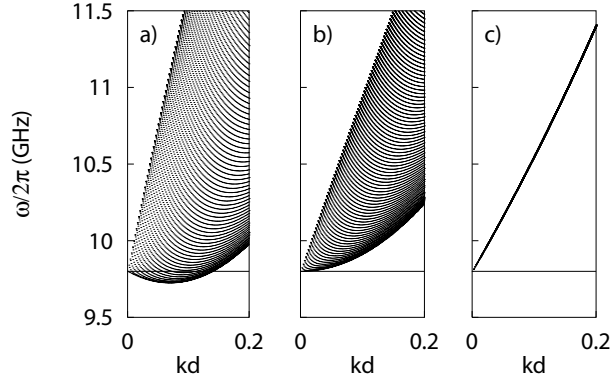


Figure 3.2: Magnon manifold versus magnetization direction. The magnon manifold was calculated for a 10 nm thick $\text{Ni}_{80}\text{Fe}_{20}$ film for the magnetization (a) in plane, (b) 45 degrees out-of-plane, and (c) perpendicular to the plane. Courtesy of R. McMichael [40].

mogeneity. The delta function enforces the requirement for degeneracy.

Two-magnon scattering is less a scattering process than a dephasing process. The uniform mode is no longer an eigenstate of the system when inhomogeneities are present. Rather, it is a superposition of new eigenmodes. These modes will dephase with each other and the uniform mode will dissolve into non-uniform modes. Therefore, the two-magnon process does not actually damp the magnetization. No energy leaves the magnetic system, energy is simply transferred from the uniform mode to non-uniform modes. However, since FMR probes only the uniform mode, this dephasing does contribute to the measured linewidth.

Figure (3.2) demonstrates that the number and wavevectors of the degenerate modes can be changed by varying the out-of-plane angle of the dc applied field. Specifically, above some critical angle there are no degenerate modes, so that measurement of the linewidth at these angles are free from two-magnon contributions. Therefore, measurement of the linewidth as a function of the out-of-plane field angle can be used to quantify the two-magnon contribution to the linewidth, and hence subtract it, even for in-plane geometries. Such measurements are shown in Fig. (3.3).

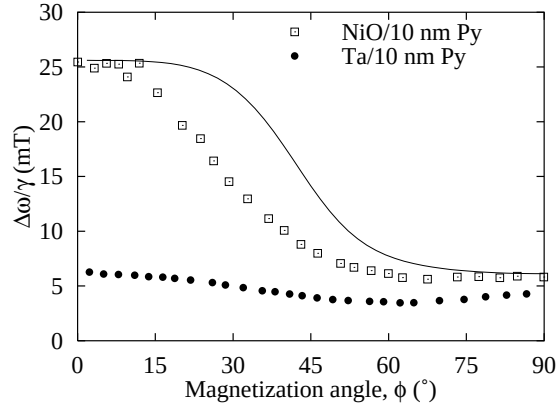


Figure 3.3: FMR linewidth versus out-of-plane magnetization angle. The resonance linewidth of a 10 nm $\text{Ni}_{80}\text{Fe}_{20}$ film on NiO (open symbols) and Ta (closed symbols) is plotted versus the out-of-plane magnetization angle. The solid curve gives the two-magnon prediction for the linewidth. As the magnetization angle increases fewer modes are degenerate with the uniform mode and the linewidth decreases. Figure courtesy of R. McMichael [40].

Phonon-Magnon Scattering

Phonons are correlated deviations of the atomic nuclei from their equilibrium positions and are present in every system. These deviations of the nuclei introduce inhomogeneities into the magnetocrystalline anisotropy field. The displacements of the nuclei alter the Coulomb energy of the electron states, enabling transitions between states. Such scattering events, which annihilate a phonon and create an electron-hole pair, must conserve angular momentum. In the absence of spin-orbit coupling, this means that the orbital moments of the initial and final electron states must be identical since the interaction does not couple to the spin. However, in systems with spin-orbit coupling, angular momentum is shared between the orbital and spin degrees of freedom. It then becomes possible that a phonon-electron scattering event can change the orbital moment of the electron, and also flip the spin of the electron.

These spin flip scattering events are a damping mechanism because they remove energy and momentum from the spins. Such scattering events occur on a time scale of approxi-

mately $\tau/(\Delta g)^2$ [41] where τ is the ordinary (non-spin flip) scattering time and Δg is the deviation of the Landé g factor from 2. For iron, cobalt, and nickel – the materials we investigate in this document – this means that the spin-flip scattering time is about 25 to 100 times longer than the ordinary scattering time. Because of this long spin-flip scattering time this damping mechanism is very weak.

Phonon-magnon scattering is an intrinsic damping mechanism because it relies on inhomogeneities produced by phonons, rather than extrinsic sample defects. However, the phonon-magnon coupling can be enhanced by extrinsic inhomogeneities. In the presence of extrinsic inhomogeneities, the uniform mode dephases into non-uniform modes, and these non-uniform modes can couple more strongly to the phonons. The coupling of the non-uniform modes is stronger because it is easier to conserve linear momentum in phonon-magnon scattering events when the magnon carries momentum (is non-uniform). However, magnon-phonon scattering is still a weak source of damping in metallic systems [42].

Intrinsic Effects

Intrinsic effects cause damping even in crystallographically perfect samples. Even in perfect crystals the magnetization is not isolated from the rest of the sample. There are unavoidable interactions between the magnetization and the other degrees of freedom and this coupling allows energy to leak from the magnetic system to the other systems. The spins couple to magnetic fields, such as those created by electron eddy currents and atomic orbits (the spin-orbit interaction). Also, the lattice is never crystallographically perfect because phonons are always present as just discussed. Lastly, as the magnetization precesses at gigahertz frequency the sample acts like an antenna and radiates energy as photons.

Eddy Currents

During a FMR measurement the magnetization, which is significant for ferromagnets, is precessing at GHz frequency. This rapidly rotating magnetic field induces a circular electric field by Faraday's law: $\nabla \times E = -\partial B/\partial t$. This circular electric field drives electrons in eddy currents. This process takes energy out of the uniform mode and puts it into the electron orbits, thus damping the magnetization. The amount of damping depends on the square of the thickness of the film: $\lambda_{\text{eddy}} \propto d^2$. Therefore, eddy current damping can be reduced by using very thin film samples. However, eddy currents become important by a thickness of just 25 nm for iron. For nickel, thicknesses of up to 100 nm have minimal damping contributions from eddy currents. Eddy current damping was investigated by Ament and Rado [43] among others.

Radiation Damping

We know from classical electrodynamics that a charge undergoing circular motion radiates energy and its orbit gradually spirals down. This concept, applied to a classical picture of the hydrogen atom, provided one of the motivations for the adoption of quantum mechanics. Similarly to this classical picture, as the magnetization of a sample precesses it acts as an antenna and radiates energy. This radiation also causes the precession to gradually spiral down [44]. While this damping effect is indeed present in all materials, its contribution to the damping rate is likely negligible.

Spin-Orbit Damping

To a first approximation the electrons in an atom have well defined orbital and spin angular momenta. ℓ , σ , ℓ_z , and σ_z are all good quantum numbers for each electron. However, this is not quite true. To understand the spin-orbit interaction we follow the approach

presented by Liboff [45]. Consider the valence electrons of an atom. They exist beyond a closed shell of electrons and feel a radial electric field $\mathbf{E}$ from the partially screened nuclear charge. Using a classical picture, as the valence electrons orbit the atom they traverse these electric field lines with velocity $\mathbf{v}$. From the rest frame of the electron the electric field appears as a magnetic field

$$\mathbf{B} = -\gamma \frac{\mathbf{v}}{c} \times \mathbf{E}. \quad (3.7)$$

$\gamma = 1/\sqrt{1 - \beta^2}$, $\beta = v/c$, and c is the speed of light. If $\beta \ll 1$ then $\gamma \approx 1$ and the electron feels a magnetic field

$$\mathbf{B} = -\frac{\mathbf{p}}{mc} \times \mathbf{E}. \quad (3.8)$$

Since the electron has magnetic moment μ there is an interaction energy $-\mu \cdot \mathbf{B}$ with the above apparent magnetic field such that

$$\mathcal{H}' = -\frac{\mu}{mc} \cdot (\mathbf{E} \times \mathbf{p}). \quad (3.9)$$

This is not quite correct. Since the electron is constantly accelerating its rest frame is non-inertial. The correction for this is the Thomas factor, 1/2. The correct interaction energy is

$$\mathcal{H}' = -\frac{\mu}{2mc} \cdot (\mathbf{E} \times \mathbf{p}). \quad (3.10)$$

For valence electrons outside a filled core it is reasonable to approximate the electric field as spherically symmetric

$$\mathbf{E} = -\frac{d\Phi}{dr} \hat{r}, \quad (3.11)$$

where Φ is the atomic electric potential. Inserting this electric field into the Hamiltonian

gives a spin-orbit energy of

$$\mathcal{H}' = \frac{1}{2mc} \left[\frac{1}{r} \frac{d\Phi}{dr} \right] (\mathbf{r} \times \mathbf{p}) \cdot \boldsymbol{\mu}. \quad (3.12)$$

The cross product $\mathbf{r} \times \mathbf{p}$ is the angular momentum $\mathbf{L}$ and the magnetic moment is $\boldsymbol{\mu} = (e/mc)\mathbf{S}$. Therefore, the spin-orbit interaction is

$$\hat{\mathcal{H}}_{so} = \frac{e}{2m^2c^2} \left[\frac{1}{r} \frac{d\Phi}{dr} \right] \hat{\mathbf{L}} \cdot \hat{\mathbf{S}} = \xi(r) \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}. \quad (3.13)$$

This result holds also for solids, though in metals the orbital moment is largely quenched as the valance electrons occupy Bloch states.

One important consequence of the spin-orbit interaction is that ℓ_z and σ_z are no longer good quantum numbers. Rather, $j_z = \ell_z + \sigma_z$ is the good azimuthal quantum number. Therefore, the spin and orbital moments can trade momentum back-and-forth as the magnetization precesses. j precesses with constant j_z , but ℓ and σ are misaligned and exert a torque on each other that causes them both to precess about j such that their z components are not constants of the motion (see Fig. (3.4)). Since the spin carries a larger magnetic moment than the orbit, μ_z is not a constant of the motion.

During a FMR measurement, the spins will be in an excited state, but the orbits will be essentially in the ground state. Therefore, as j precesses energy is pumped from the spin degrees of freedom into the orbital degrees of freedom. This process is frequently interrupted by electron-lattice scattering events. These scattering events alter the orbital moment, removing energy from the electron and leaving the orbit in a lower energy configuration. The spin moment is not affected. This process is illustrated in Fig. (3.4). Damping through the spin-orbit interaction is a two step process: the orbital moments are pumped into a high energy configuration by the spins, and then this energy is scattered to the lattice.

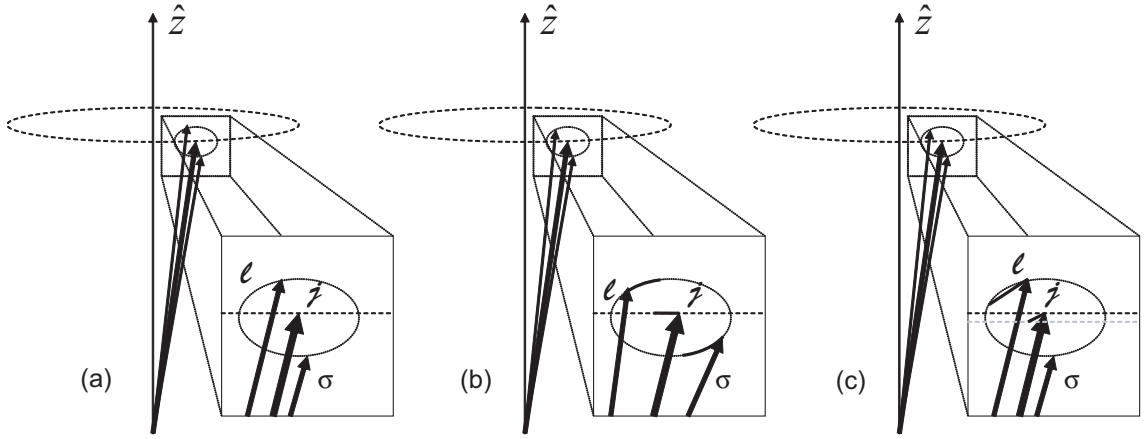


Figure 3.4: Schematic of spin-orbit damping. Main figure depicts the precession cone. Insets for (a) and (b) show that as j precesses ℓ and σ precess about j . Heavy black curves indicate the trajectories of the vectors. Electron-lattice scattering, occurring between (b) and (c), does not affect the spin direction σ , but removes energy from the orbits, aligning ℓ , and hence j , more closely to the equilibrium direction $\hat{z}$. The process then repeats until equilibrium is reached and the magnetization is pointed along $\hat{z}$.

Prospectus

While investigations into intrinsic damping in metallic ferromagnets have focused on the spin-orbit interaction for some time [46–53], much work still remained to be done on this topic at the outset of this project. The remainder of this thesis recites the contributions we have made. One theory of precession damping by Kamberský [49] seemed particularly promising as it qualitatively matched temperature dependent FMR results. However, up until this point it had not been possible to quantitatively evaluate the expression he put forth 4.1 due to the significant computational requirements. The theory seemed to be largely forgotten over the years, but we resolved to understand and evaluate it. Chapter 4 presents the results of our numerical evaluation of Kamberský’s torque-correlation expression 4.1 for iron, cobalt, and nickel. However, the results give the damping rate as a function of the electron-lattice scattering rate. Since measurements report the damping rate as a function of temperature, and the electron-lattice scattering rate is generally not known as a func-

tion of temperature, comparison between the calculations and measurements is restricted. Therefore, we also calculate the resistivity as a function of the scattering rate. The damping rate is then plotted versus resistivity for better comparison to experimental results. Chapter 5 discusses our physical understanding of the damping process, addressing the questions of how the damping rate depends on different material parameters and how experimentalists might adjust the damping rates of materials.

The final two chapters are intended as appendices and contain the theoretical and numerical details that represent the bulk of the work behind the results in Chapters 4 and 5. Kamberský's derivation of the expression for the damping rate quoted in [49] is rather complicated to follow and tedious to reproduce, but does not exist in full in that paper or elsewhere in the literature. Therefore, we include a full derivation of the damping expression in Chapter 6 for any that may continue this work. This appendix also contains a derivation of the resistivity. The final chapter is a numerical appendix that provides details on the density functional theory methods used to evaluate the damping rate and resistivity.

CHAPTER 4

RESULTS

Precession damping in metallic ferromagnets results predominantly from a combined effort of spin-orbit coupling and electron-lattice scattering [49, 54]. The role of lattice scattering was studied in early experimental work through the temperature dependence of damping rates [55, 56]. Measurement of damping rates versus temperature revealed two primary contributions to damping, an expected part that increased with temperature, and an unexpected part that decreased with temperature. In cobalt these two opposing contributions combine to produce a minimum damping rate near 100 K, for nickel the increasing term is weaker leading to a temperature independent damping rate above 300 K, while for iron the damping rate becomes independent of temperature below room temperature. Heinrich *et al.* later noted that the temperature dependence of the increasing and decreasing contributions matched that of the resistivity and conductivity, respectively [57, 58], and so dubbed the two contributions conductivity-like for the decreasing piece and resistivity-like for the increasing part.

Among the many theories on intrinsic precession damping [44, 46–49, 51, 53, 59–61], Kamberský’s torque-correlation model [49] is unique in qualitatively matching this non-monotonic temperature dependence. Kamberský’s theory describes precession damping as due to two processes: the decay of magnons into electron-hole pairs and the scattering of the electrons and holes with the lattice. The spin-orbit torque annihilates a uniform mode magnon and excites an electron, generating an electron-hole pair. The electron-hole pair is then collapsed through lattice scattering. The electron and hole are dressed through lattice interactions and are best thought of as a single quasiparticle with indeterminate energy and a lifetime given by the electron-lattice scattering time. The dressed electron and hole can

occupy the same band, which we call an *intraband* transition, or two different bands, an *interband* transition.

The derivation of the damping rate due to the spin-orbit interaction is complicated and we put it off to an appendix in Chapter 6. The result obtained for the damping rate of small amplitude uniform precession is

$$\lambda = \pi \hbar \frac{\gamma^2}{\mu_0} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} |\Gamma_{mn}^-(\mathbf{k})|^2 \int d\epsilon_1 A_{nk}(\epsilon_1) A_{mk}(\epsilon_1) \eta(\epsilon_1). \quad (4.1)$$

The gyromagnetic ratio is $\gamma = g\mu_0\mu_B/\hbar$, g is the Landé g factor, μ_0 is the permeability of space, n and m are band indices, and $\mathbf{k}$ is the electron wavevector. The matrix elements $|\Gamma_{mn}^-(\mathbf{k})|^2$ describe the torque between the spin and orbital moments that arises as the spins precess. Terms with $n = m$ ($n \neq m$) give the intraband (interband) contribution. $\eta(\epsilon)$ is the derivative of the Fermi function $-df/d\epsilon$, which is a positive distribution peaked about the Fermi level that restricts scattering events to the neighborhood of the Fermi surface. The electron spectral functions $A_{nk}(\epsilon)$ are Lorentzians in energy space centered at band energies with widths determined by the electron scattering rate. They phenomenologically account for electron-lattice scattering.

Expression (4.1) for the damping rate is appropriate for low power FMR measurements conducted at frequencies ranging between a few GHz and tens of GHz at temperatures from a few Kelvin to several hundred Kelvin. In the derivation of Eq. (4.1) we assume that the electronic system can be described by a thermodynamic equilibrium distribution among states found using a ground state density. At higher temperatures the actual electronic configuration could differ significantly from the ground state density, altering the effective band structure.

This expression does not capture the decay of non-uniform modes, for which the electron-hole pair would carry the momentum of the magnon. Therefore, this expression is likely

not suited to describe large amplitude dynamics or damping when there is a significant population of non-uniform modes. The damping expression could be modified to include damping of non-uniform modes by relaxing the constraint that the initial and final states in the torque matrix elements have the same wavevector. Modes with wavevector $\mathbf{q}$ would be damped by torque matrix elements between electron states with wavevectors $\mathbf{k}$ and $\mathbf{k} + \mathbf{q}$.

In this chapter we present the results of our calculations of the damping rates of iron, cobalt, and nickel according to Eq. (4.1). These calculations give the damping rate as a function of the electron-lattice scattering rate. Heinrich *et al.* [57, 58] have shown experimentally that at all but the lowest temperatures, the intraband and interband damping rates are proportional to the electrical conductivity and resistivity, respectively. This evidence supports the assumption that the important scattering rate in the damping calculation is the same as the resistivity scattering rate. Therefore, we also calculate the electrical resistivity as a function of the same scattering rate, and plot the damping rate versus the resistivity. A comparison to experimental results is made.

The Damping Rate

Figure 4.1 shows the results of our calculations for the damping constants of Fe, Co, and Ni as a function of electron scattering rate. The curves are separated into their intraband and interband contributions to clearly demonstrate that these two terms represent different processes. Measured curves have analogously been separated into conductivity- and resistivity-like pieces. The intraband contributions are given by the downward sloping lines. These terms are proportional to the scattering time, hence inversely proportional to the scattering rate, and dominate for low scattering rates (low temperatures). The interband terms are initially proportional to the scattering rate (for low scattering rates), but gradually saturate as the scattering rate is increased, particularly for Ni. This contribution domi-

nates for large scattering rates (high temperatures). The calculated intraband terms give the conductivity-like contribution to the measured data while the interband terms match the resistivity-like portion.

The dependence of the intraband and interband terms on the scattering rates enters through the integration over the spectral functions. The spectral functions are Lorentzians in energy space. For very long scattering times the energies of the electron states are well defined and the spectral functions are nearly delta functions. As the state lifetimes decrease the spectral functions broaden. The height of the spectral functions is proportional to the scattering time while the width is inversely proportional to the scattering time. The η function in the energy integral in Eq. (4.1) is essentially a delta function at the Fermi energy. Therefore, the value of the integral is determined by the overlap of the spectral functions at the Fermi level. For the intraband terms, the two spectral functions are the same and the integral is proportional to the peak height of the spectral function. For the interband terms, the integral depends on both the width of the spectral functions and the distance between the central energies. The overlap of the spectral functions initially increases as the scattering rate increases, but then decreases with significant broadening since the spectral intensity at the Fermi level goes to zero. These trends are described pictorially in Fig. (4.2).

Damping curves are measured as a function of temperature, but our calculations are made as a function of electron scattering rate. Since the relation between scattering rate and temperature is not known sufficiently well, it is not possible to directly compare these curves in their entirety. However, since the intraband and interband contributions have opposite scattering rate dependencies, the damping curve of each material exhibits a minimum at some scattering rate. What we can meaningfully do is compare these calculated minima to the smallest values measured as a function of temperature. This is done in Table 4.1.

As we discuss in Chapter 6, during the derivation of the damping rate we make the

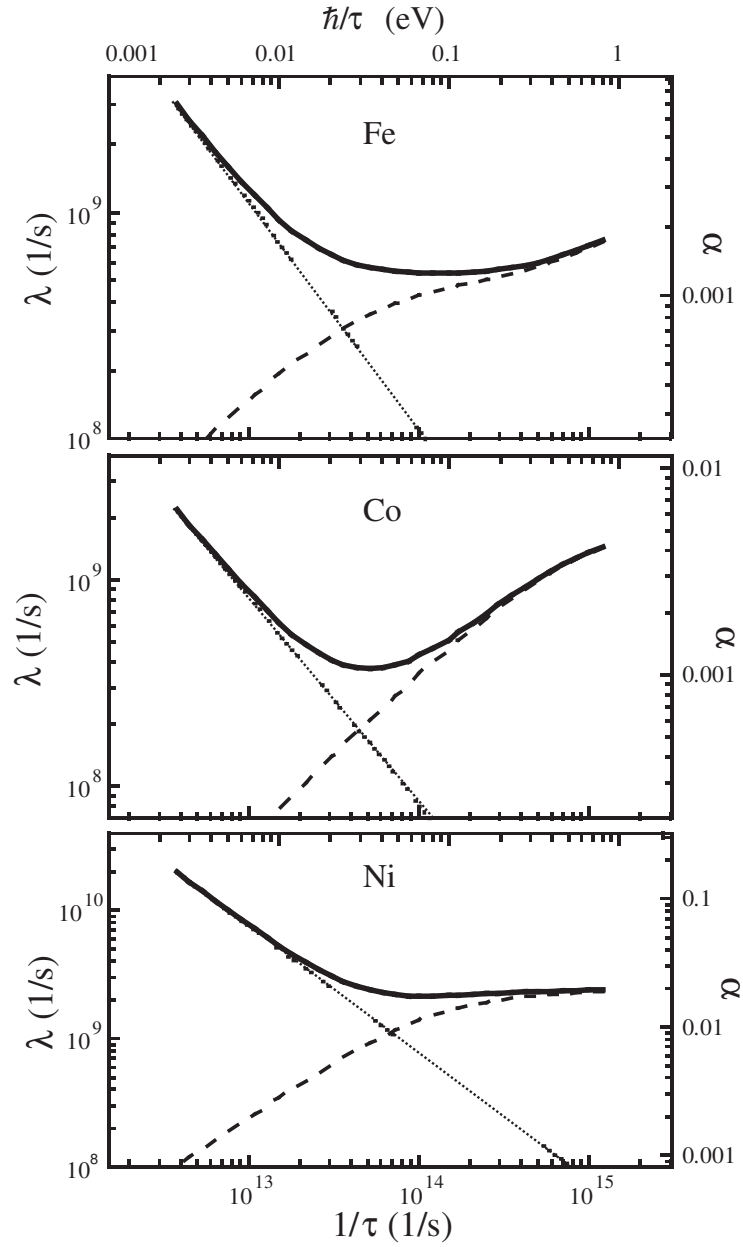


Figure 4.1: Calculated Landau-Lifshitz damping constant for Fe, Co, and Ni. Thick solid curves give the total damping parameter while dotted lines give the intraband and dashed curves the interband contributions. Values for λ are given in SI units. The right axis is the equivalent Gilbert damping parameter and the top axis is the full-width-half-maximum of the electron spectral functions.

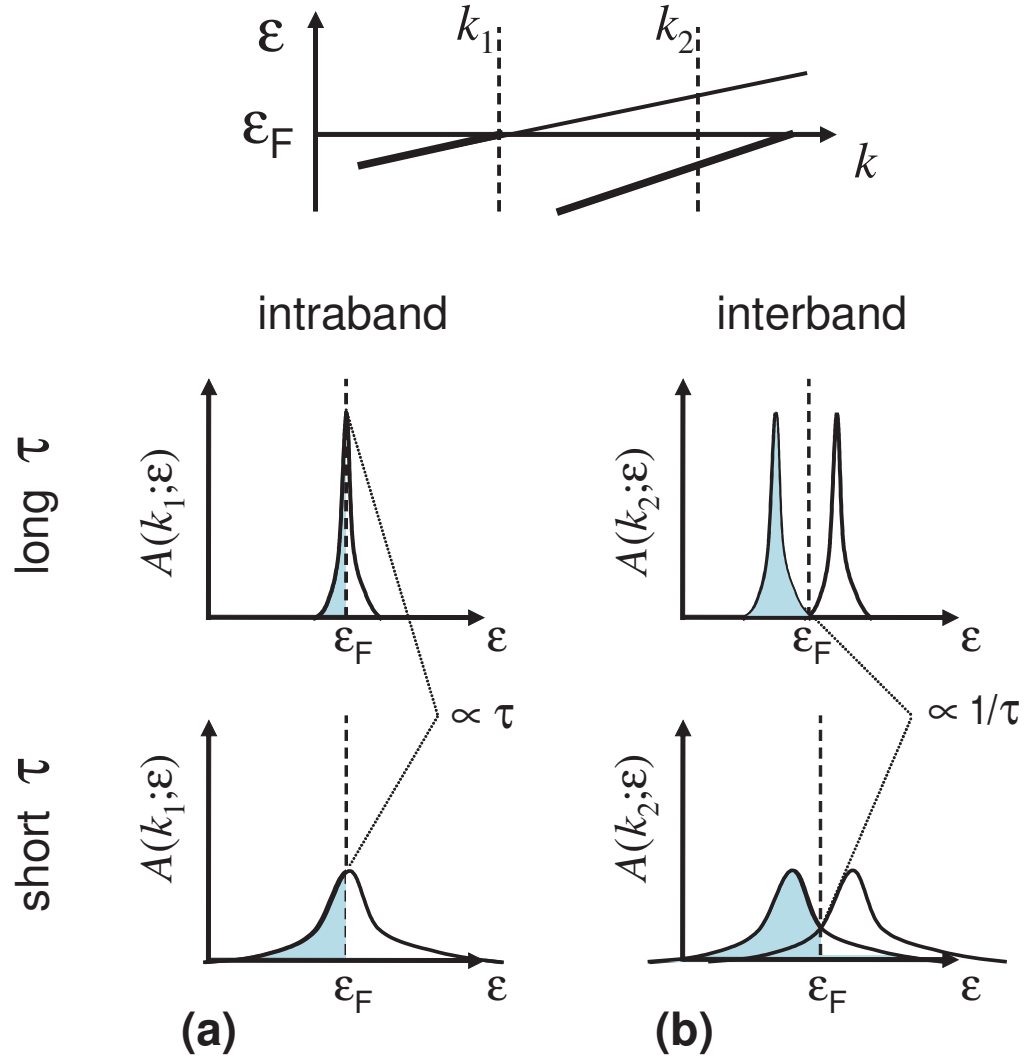


Figure 4.2: Schematic diagram of the scattering time dependence of the intraband and interband spectral overlap integral. Top diagram is a close-up of a portion of a band structure showing two bands. Heavy lines below the Fermi level indicate filled states while lighter lines above the Fermi level indicate empty states. The four images below represent slices through the band structure in energy space at fixed wavevector. The top two diagrams are for a long scattering time and the bottom two are for a short scattering time. The images on the left (a) are for wavevector k_1 and indicate an intraband transition, images on the right (b) are for wavevector k_2 and show an interband transition. Shaded regions below the Fermi level indicate filled states. The strength of the intraband transitions is shown to be proportional to τ while the interband transitions increase with $1/\tau$.

Table 4.1: Calculated and measured damping parameters. Values for λ are reported in 10^9 s^{-1} while those for α are dimensionless. The values indicate minima of the calculated or measured curves. Published numbers from [55] have been multiplied by 4π to convert from the cgs unit system to SI.

	α_{calc}	λ_{calc}	λ_{meas}	$\lambda_{\text{calc}}/\lambda_{\text{meas}}$
bcc Fe $\langle 001 \rangle$	0.0013	0.54	0.88	0.61
bcc Fe $\langle 111 \rangle$	0.0013	0.54	—	—
hcp Co $\langle 0001 \rangle$	0.0011	0.37	0.9	0.41
fcc Ni $\langle 111 \rangle$	0.017	2.1	2.9	0.72
fcc Ni $\langle 001 \rangle$	0.018	2.2	—	—

approximation that the magnetic moment of each electron is due solely to its spin; we neglect the orbital contribution to the magnetization. This approximation is reasonable because the orbital moments are largely quenched in metals. To maintain consistency with this approximation, we should set the Landé g factor in Eq. (4.1) equal to 2. Using this value for g we find the agreement between the calculated and measured minimal values is about 70 % for Ni, 60 % for Fe, and 40 % for Co. Since the expression for λ contains a factor of g^2 , if we were to use the measured g values the agreement would improve to 86 % for Ni, 67 % for Fe, and 48 % for Co. This is the first time that calculated damping rates of the correct order of magnitude for these metals have been quantitatively compared to measurements. For the reasons we now discuss, obtaining results within a factor of two of the measured values for all three systems is a significant accomplishment.

The comparison between the calculated and measured minima is most reliable in the case of nickel. The first reason for this is that the nickel data express both the conductivity-like and resistivity-like contributions, and, hence, the data contains the damping minimum, unlike the case with iron. The second reason is that the uncertainty in interpreting the measured linewidths is much less for nickel than for cobalt. Therefore, of the three materials, only nickel has a clean set of data that contains the damping minimum. Not surprisingly

then, the agreement between the calculated and measured minima is best for nickel. The agreement for iron and cobalt is also good, within a factor of two of the experimental values, but not as strong as the nickel match. The comparison for iron is complicated by the fact that the iron data shows only a resistivity-like (interband) contribution. We suspect that this is because the scattering rate in iron is higher than the other metals, forbidding measurement from probing the region in which the conductivity-like (intraband) term dominates. Therefore, the iron data do not reach the damping minimum. Also, factoring the temperature dependence of the damping constant out of the temperature dependence of the linewidth is more difficult for iron than for nickel, so there is more uncertainty in these measurements. The uncertainty in the cobalt measurement is quite large as separating the temperature dependence of the damping constant from other temperature dependent quantities is very challenging for this system. Consequently, the uncertainties in these measurements are very substantial. Therefore, a factor of two difference between our calculation and the measurement should not be viewed as a significant discrepancy.

It is important also to note that we do not expect complete agreement. We have calculated only the first-order contribution to damping of the uniform mode due to the spin-orbit interaction. Further, we have made several approximations to make the calculation more tractable. We neglected the orbital magnetic moment. The orbital moment is partially parallel to the spin moment and partially perpendicular to the spin moment. The error associated with neglecting the parallel component should be close to a factor of $(g/2)^2$, as we estimated in a previous paragraph. The cost of neglecting the perpendicular component is not clear. As we discuss in Chapter 6, this component contributes both a spin-orbit and an orbit-spin correlation function to the moment-moment correlation function that we treat. We also assume that the electron-hole pairs are created with low enough density that the pairs do not interact with each other. Again, it is not clear how reasonable this assumption is. At higher temperatures, the presence of thermally generated electron-hole pairs may

make pair-pair interactions significant. Additionally, there are damping mechanisms other than the spin-orbit interaction simultaneously at work. As we discussed in the previous chapter, damping also occurs through direct magnon-phonon scattering, though this is estimated to be a very small effect [42]. Lastly, we have set the scattering rates of all states equal, though surely there will be some variation. We will relax this constraint later in this chapter and find an improved agreement between the calculations and the measurements.

On the numerical side, the wavefunctions used were found through the mean field approach of the local spin density approximation (LSDA). The exchange interaction depends on non-local spin correlations. The LSDA neglects the non-local nature of the exchange interaction and approximates it using only a local spin density. This shortcoming appears not to be critical for the transition metals that we study.

In Chapter 7 we will discuss the numerical methods used to evaluate Eq. (4.1) in detail. However, we make a few brief comments on this matter here. The evaluation of Eq. (4.1) required the single particle eigenstates and energies of each metal. These were found using the linear augmented plane wave method in the LSDA. The calculations are converged to within a standard deviation of 3 %, which required including 7 bands for iron, 15 for cobalt, and 6 for nickel. The necessary k -point sampling was $(160)^3$ k -points for Fe, $(140)^3$ for Ni, and $(100)^2$ k -points in the basal plane by 57 along the c -axis for Co.

The Resistivity

We calculated the damping rate as a function of the electron-lattice scattering rate, but the damping rate has been measured as a function of temperature. Since the scattering rate is not known very well as a function of temperature we could only compare the minimal values of the calculated damping curves to the minima of the measured curves. To get around this problem we calculated the electrical resistivity of each metal as a function of

the scattering rate. Therefore, it is now possible to plot the damping rate as a function of the resistivity. Since analogous plots can be constructed from experimental data these new curves allow comparison of the damping rates for any temperature.

The derivation of the electrical conductivity is presented in Chapter 6 with the result that

$$\sigma = \pi \frac{e^2}{\hbar} \sum_n \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \left(\frac{\partial \epsilon_{nk}}{\partial k_z} \right)^2 \int d\epsilon_1 \eta(\epsilon_1) A_{n,k}^2(\epsilon_1). \quad (4.2)$$

Since the conductivity contains only intraband terms it is proportional to the scattering time. Therefore, the resistivity $\rho = 1/\sigma$ is proportional to the scattering rate. A simple way to present the results of our calculations of the resistivities of the three metals we investigated is as the single number ρ/γ where $\gamma = 1/\tau$ is the scattering rate. These values are listed in Table 4.2. The resistivities per scattering rate for the three metals are very similar and just above $1 \times 10^{-21} \Omega \cdot m \cdot s$. For a clean sample with a scattering rate of $10^{14} s^{-1}$ this gives a resistivity on the order of $10^{-7} \Omega \cdot m$, which is reasonable.

Table 4.2: Sample resistivity. Resistivity per scattering rate for Fe, Co, and Ni in units of $10^{-21} \Omega \cdot m \cdot s$.

	Fe	Co	Ni
ρ/γ	1.30	1.24	1.18

With these results we can parameterize out the poorly known scattering rate in the presentation of the damping rates. Figure (4.3) presents the damping rates versus the directly measurable resistivity instead of versus the indirectly inferred scattering rate, as we had previously presented our calculations in Fig. (4.1). This presentation allows the entire damping curves to be compared to experimental results, whereas previously we were only able to compare the minima of the curves. These curves place the damping minimum of each metal near a sample resistivity of $10^{-7} \Omega \cdot m$. Unfortunately, we do not yet have exper-

imental results for the damping rate versus the resistivity, so at this time we are unable to make a full comparison of our calculations. Based on these curves and previous damping measurements made versus temperature [55, 56], we expect the cleanest samples to have a resistivity range of roughly 10^{-8} to $10^{-6} \Omega \cdot m$ for nickel and cobalt, and for that range to be increased about half an order of magnitude for iron, which appear to be reasonable numbers.

The fundamental assumption that we make in deriving Eq. (4.2) for the conductivity is that the resistivity is dominated by electron-lattice interactions and that electron-electron interactions play a minimal role. Such a simplistic approach appears to be validated by the success of the Boltzmann equation approach to transport. The Kubo formula approach that we employ is a more formal treatment of the physics used in the Boltzmann equation. Therefore, our result should hold for the same conditions of the resistivity being dominated by scattering from dilute impurities and phonons.

The Scattering Time

The results may not be as straight-forward as suggested in Fig. (4.3). Thus far we have been assuming that the lifetimes of all electronic states are the same. This is surely not the case. There will be some range over which the lifetimes of the many states are spread. Determining the lifetime of each state separately would involve a very arduous investigation of electron-phonon scattering, and would also require knowledge of the impurities. This is not a task that we will undertake. Instead, we relax the assumption of a universal scattering time in a more feasible way. We allow the lifetimes of states with opposite spin to differ. (We have in mind that the spin-up and spin-down lifetimes may be inversely proportional to the spin-up and spin-down densities of states at the Fermi level.) We define two lifetimes $\tau_{\uparrow}$ and $\tau_{\downarrow}$ for the up-spin and down-spin states. However, since we include the spin-orbit

interaction in solving for the wavefunctions, the eigenstates of the Hamiltonian are not pure spin states. We use this to our advantage and assign a separate lifetime to each state based on how much the state is spin-up versus how much it is spin-down. Specifically, for a state ψ_{nk} the relaxation time becomes

$$\tau_{nk} = \alpha_{nk}\tau_{\uparrow} + \beta_{nk}\tau_{\downarrow}. \quad (4.3)$$

The coefficients α_{nk} and β_{nk} are the up and down components of the spin vector for the state ψ_{nk} .

We now investigate what effect varying the ratio $r = \tau_{\downarrow}/\tau_{\uparrow}$ has on the damping rate and the resistivity. Figures (4.4-4.6) show the damping rates for the three metals for several values of r while Fig. (4.7) similarly presents the resistivity. In Fig. (4.8) we combine these new sets of results for the damping and resistivity to plot the damping rate versus the resistivity for several lifetime ratios. Unfortunately, we do not presently have experimental data for the damping rate versus sample resistivity for any of these metals. Therefore, we cannot yet check the accuracy of our results. Hopefully, this data will be available for such a comparison in the future.

One objective of calculating the resistivity was to eliminate the one free parameter in the damping calculation: the scattering rate. The plots in Fig. (4.3) show this result. We then modified our calculation to allow for the fact that different states may have different scattering rates. This modification put a free parameter – the spin-down to spin-up lifetime ratio r – back into the results. Therefore, the damping curves of Fig. (4.3) became the family of curves presented in Fig. (4.8). While the true spin-dependent lifetime ratio r may be probed experimentally, we are not aware of such measurements on the systems we are considering. Therefore, we do not know which member of each of the sets of curves in Fig. (4.8) we expect to match the experimental result. Further, the ratio r may vary

with temperature. However, it seems reasonable that the spin-down to spin-up lifetime ratio r follows the ratio of the spin-up to spin-down density of states at the Fermi level r_F . (The scattering rate of states of a given spin should be proportional to the number of states available to scatter into. Therefore, the state lifetime for a given spin should be inversely proportional to the density of states for that spin direction at the Fermi level. Based on this argument, we then estimate a lifetime ratio $r = r_F$ of 3.6 for Fe, 0.25 for Co, and 0.12 for Ni.)

An interesting observation can be made from inspecting the sets of curves in Fig. (4.8). In a previous section we compared the minimal calculated damping rates to the minimal measured damping rates (see Table 4.1). Figure (4.8) shows that the minimal calculated damping rates depend on the ratio r . In Table (4.3) we reconsider the comparison of the minimal damping rates by setting $r = 4$ for iron, $r = 1/4$ for cobalt, and $r = 1/8$ for nickel (to closely match the spin-polarized densities of states ratios). We find that the comparison improves in each case, rising from 71% to 95% for nickel, 61% to 70% for iron, and 41% to 47% for cobalt.

Table 4.3: Minimal damping rates. Measured (λ_{meas}) and calculated minimal damping rates. λ_1 is the minimal damping rate using a spin-down to spin-up lifetime ratio of $r = 1$. λ_F is the minimal damping rate when the ratio r is set to the spin-up to spin-down density of states ratio at the Fermi level r_F . The agreement with the measured minima is improved when r is set to r_F . Damping rates are reported in 10^9 s^{-1} in SI units. $g = 2$ was used.

	λ_1	λ_F	λ_{meas}
Fe $\langle 100 \rangle$	0.54	0.62	0.88
Co $\langle 0001 \rangle$	0.37	0.42	0.9
Ni $\langle 111 \rangle$	2.14	2.76	2.9

Summary

In this chapter we calculated the damping rates of iron, cobalt, and nickel. The first set of results presented the damping rates versus the electron-lattice scattering rate. The minima of these calculations were compared to the minimal measured damping rates of these metals. The calculations agreed with the experimental results at a level of 70 % for nickel, 60 % for iron, and 40 % for cobalt, using $g = 2$. If instead, the measured g values were used, the agreement improved to 86 % for Ni, 67 % for Fe, and 48 % for Co. To eliminate the scattering time from the presentation of the results the resistivity was calculated. Once experimental results of the damping rate versus the resistivity become available it will be possible to compare the full measured and calculated damping curves.

We further refined the calculation of the damping rate (and resistivity) by introducing a new parameter – the ratio of the spin-down to spin-up lifetimes. This ratio can be determined experimentally and we predict that it should correlate strongly with the ratio of the spin-up to spin-down density of states at the Fermi level. When we choose the damping versus resistivity curves for which the lifetime ratio is close to the density of states ratio we find an enhanced agreement of the calculated minimal damping rates with the measured minimal damping rates. The agreement improves from 71% to 95% for nickel, 61% to 70% for iron, and from 41% to 47% for cobalt.

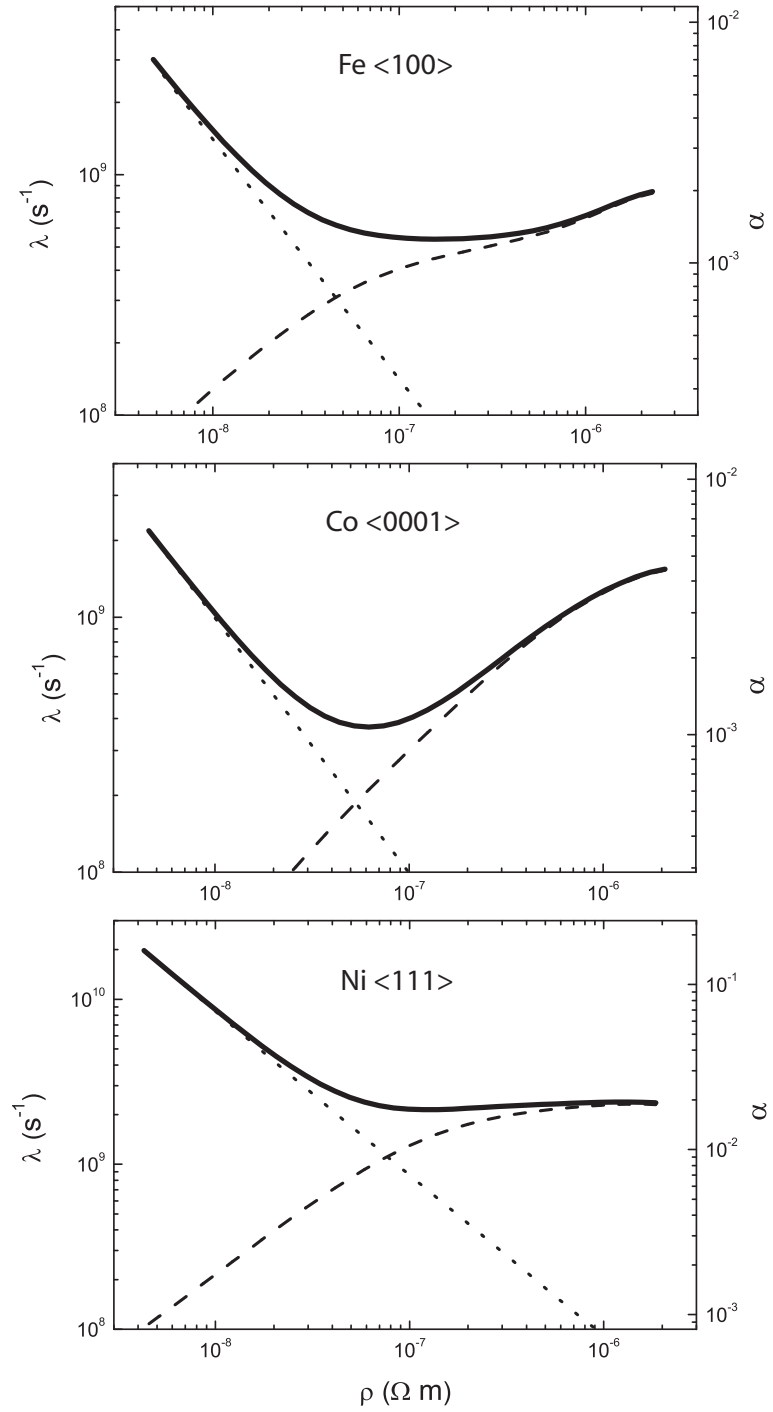


Figure 4.3: Damping rate versus resistivity. The solid curves give the damping rates for iron (top), cobalt (middle), and nickel (bottom), versus sample resistivity. Dotted lines are the intraband contribution and dashed curves give the interband rates.

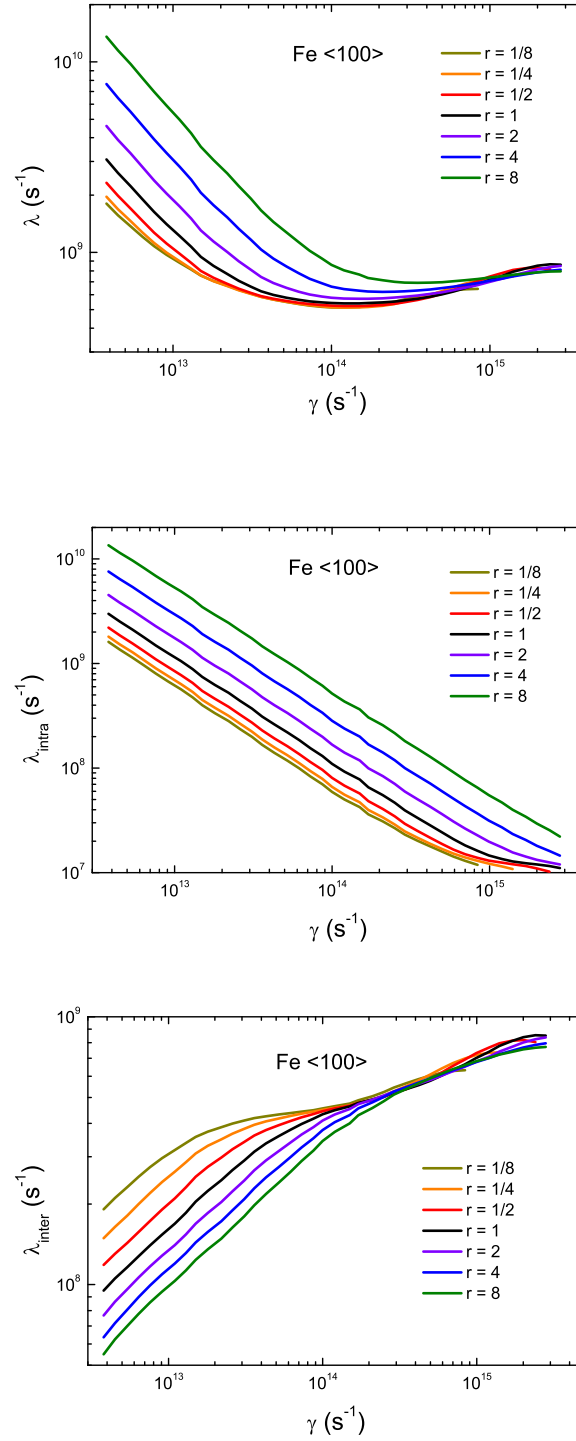


Figure 4.4: Iron damping rate versus scattering rate. Top row total damping rate, middle row intraband contribution, bottom row interband contribution. Different curves represent different values of the lifetimes for spin-up versus spin-down states.

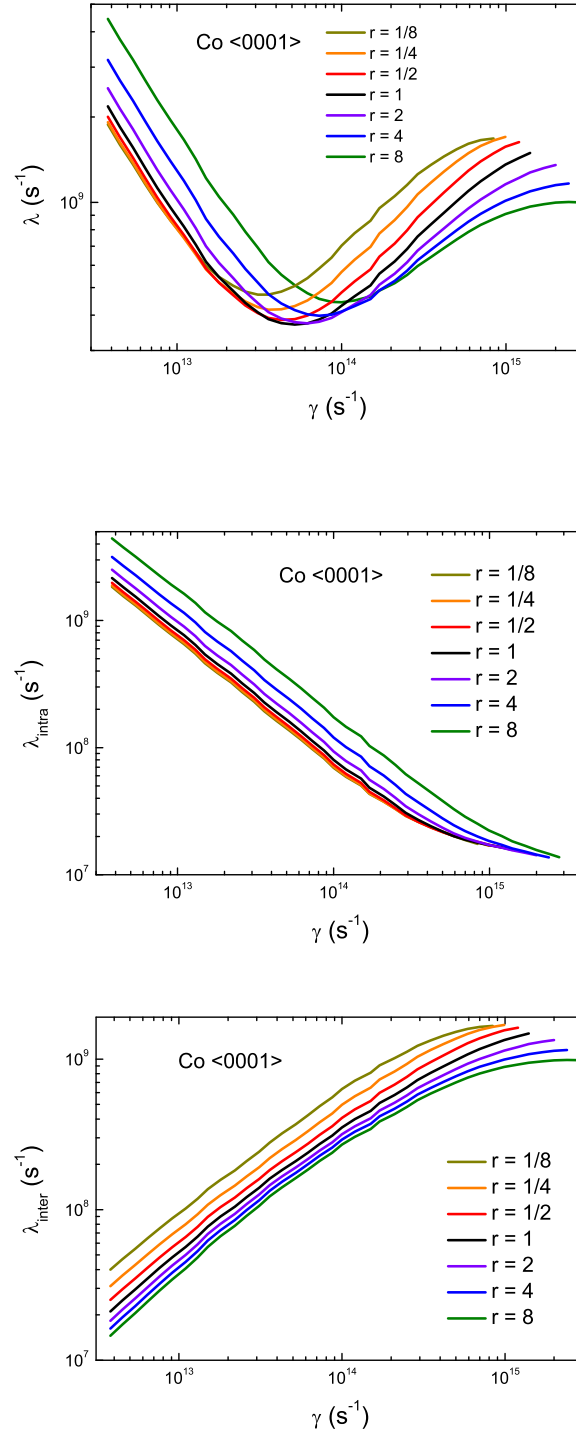


Figure 4.5: Cobalt damping rate versus scattering rate. Top row total damping rate, middle row intraband contribution, bottom row interband contribution. Different curves represent different values of the lifetimes for spin-up versus spin-down states.

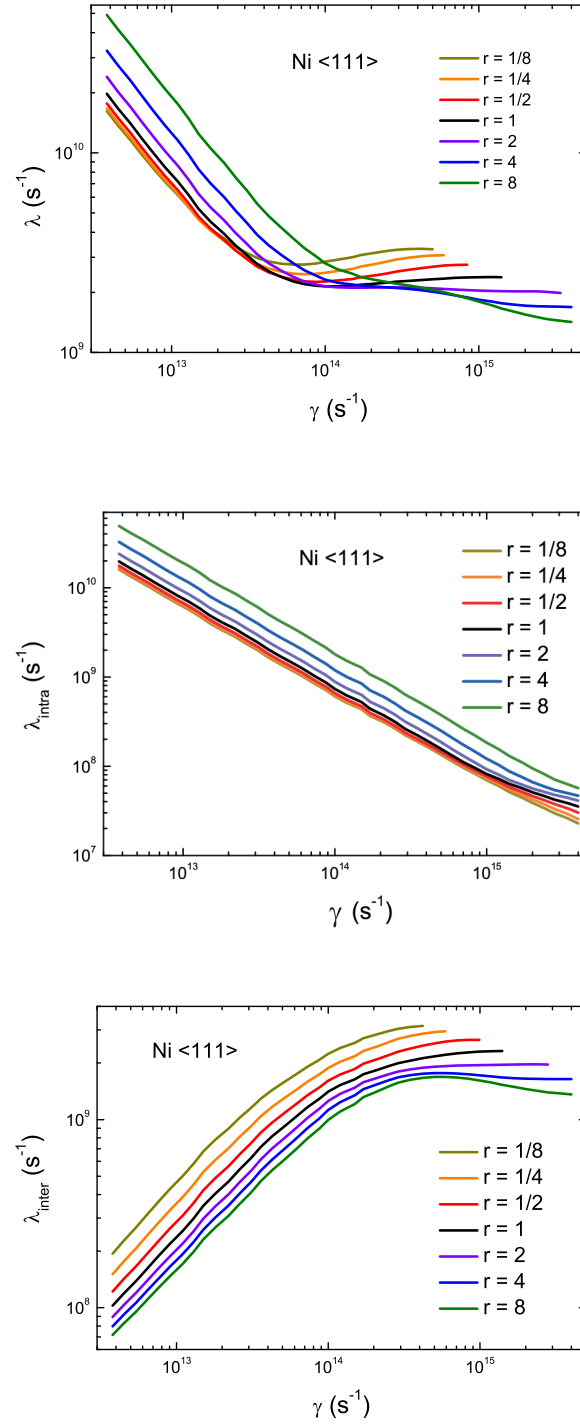


Figure 4.6: Nickel damping rate versus scattering rate. Top row total damping rate, middle row intraband contribution, bottom row interband contribution. Different curves represent different values of the lifetimes for spin-up versus spin-down states.

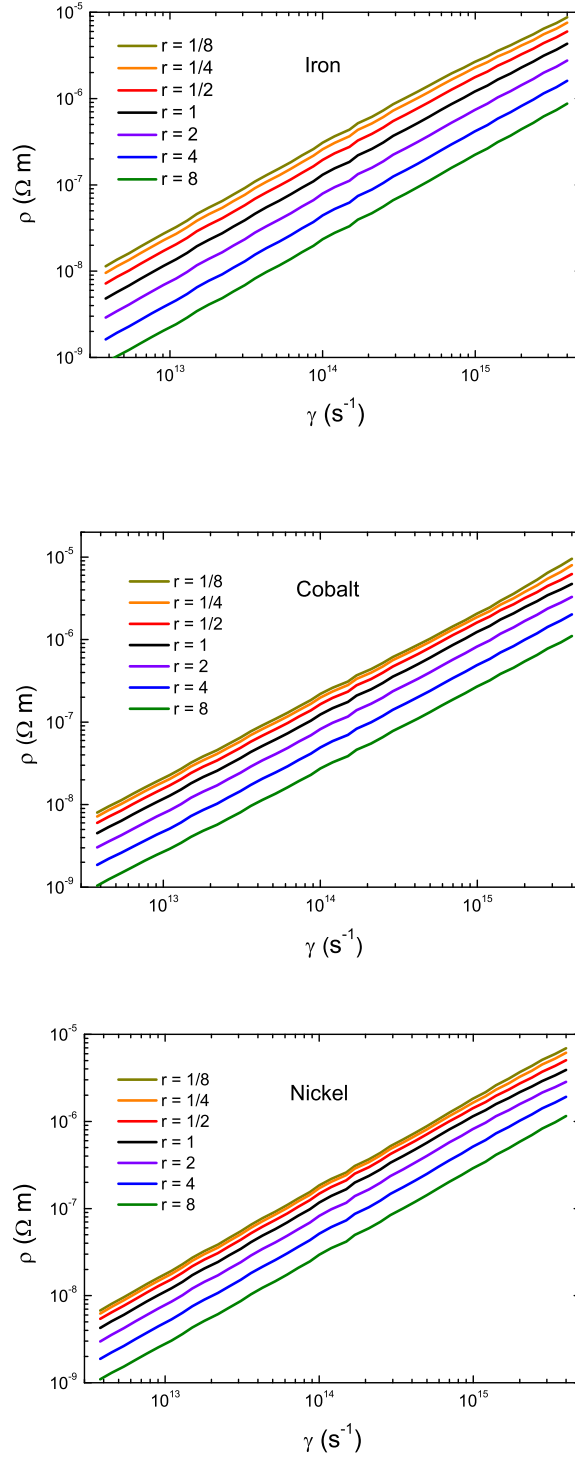


Figure 4.7: Resistivity versus scattering rate. Top iron, middle cobalt, bottom nickel. Different curves represent different values of the lifetimes for spin-up versus spin-down states.

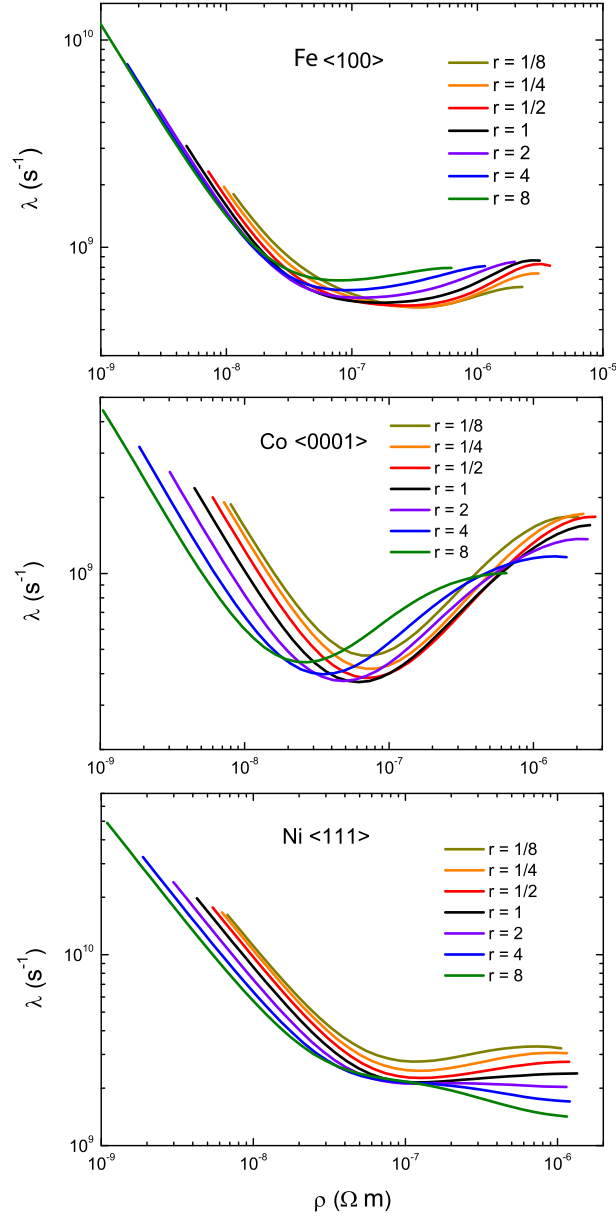


Figure 4.8: Damping rate versus resistivity. The damping rate is plotted versus sample resistivity for a set of ratios of the spin-down to spin-up lifetimes. Based on the ratio of the spin-up to spin-down densities of states at the Fermi level, the expected lifetime ratios are approximately 4 for Fe, 1/4 for Co, and 1/8 for Ni. Curves for which $r = 1$ are identical to those presented in Fig. (4.3).

CHAPTER 5

PHYSICAL UNDERSTANDING

We have shown that the expression for the damping rate Eq. (4.1) produces accurate results for iron, cobalt, and nickel. However, the formal derivation of this expression, which we put off until the next chapter, fails to illuminate the physical processes involved or give insight into how one might alter the damping rate through sample manipulation. In order to provide a more tangible explanation of precession damping we rederive Eq. (4.1) using an informal effective field approach in this chapter.

The magnetization dynamics are governed by an effective field, which is defined as the variation of the electronic energy with respect to the magnetization direction $\mu_0 \mathbf{H}^{\text{eff}} = -\partial E / \partial \mathbf{M}$. The magnitude of the magnetization M is considered constant within the Landau-Lifshitz formulation, only the direction $\hat{M}$ of the magnetization changes. The total electronic energy of the system can be approximated by $E = \sum_{nk} \rho_{nk} \epsilon_{nk}$, which is a summation over the single electron energies ϵ_{nk} weighted by the state occupancies ρ_{nk} .

The effective field will include both reversible and irreversible terms. The reversible part of the effective field originates from holding the state occupancies ρ_{nk} at their equilibrium values. The effective field resulting from this procedure is equivalent to the magnetocrystalline anisotropy [62]. The irreversible contribution to the effective field comes from allowing the state occupancies to deviate from their equilibrium populations in response to the perturbation of the applied oscillating field. This irreversible part of the effective field produces the damping in Eq. (4.1).

As the magnetization precesses the energies of the states change through variations in the spin-orbit contribution and transitions between states occur. These two effects, the changing energies of the states and the transitions between states, produce a contribution

to the effective field

$$\mathbf{H}^{\text{eff}} = -\frac{1}{\mu_0 M} \sum_{nk} \left[\rho_{nk} \frac{\partial \epsilon_{nk}}{\partial \hat{M}} + \frac{\partial \rho_{nk}}{\partial \hat{M}} \epsilon_{nk} \right]. \quad (5.1)$$

The first term in the brackets describes the variation in the spin-orbit energies of the states as the magnetization direction changes. This effect, which has been discussed and evaluated before [47, 51, 52], is generally referred to as the breathing Fermi surface model. The spin-orbit torque does not cause transitions between states in this picture, but does cause the Fermi surface to swell and contract as the magnetization precesses. We will show that this portion of the effective field gives the intraband terms of Eq. (4.1). The second term in the brackets has previously been neglected in effective field treatments, but accounts for changes in the system energy due to transitions between states. This term does not change the energies of the states, but does create electron-hole pairs by exciting electrons from lower bands to higher bands. This process can be pictured as a bubbling of individual electrons on the Fermi surface. We will demonstrate that this portion of the effective field gives the interband terms of Eq. (4.1).

Intraband Terms

In the absence of spin-orbit coupling and any external fields the energies of the single particle states would be independent of the spin direction. However, the spin-orbit interaction breaks this degeneracy. As the magnetization precesses the spin-orbit energy of each state fluctuates periodically. At any particular time, some occupied states originally just below the Fermi level get pushed above the Fermi level and simultaneously some unoccupied state originally above the Fermi level may be pushed below it. This process takes the system, which was originally in the ground state, and pushes it out of equilibrium into an excited state creating electron-hole pairs in the absence of any scattering events. Scattering,

which occurs with a rate given by the inverse of the relaxation time τ , brings the system to a new equilibrium. The relaxation time approximation determines how far from equilibrium the system can get.

$$\rho_{nk} = f_{nk} - \tau \frac{df_{nk}}{dt}. \quad (5.2)$$

The occupancy ρ_{nk} of each state ψ_{nk} deviates from its equilibrium value f_{nk} by an amount proportional to the scattering time. How quickly the system damps depends on the magnitude of this deviation.

The rate of change of the equilibrium distribution df_{nk}/dt depends on how much the distribution changes as the energy of the state changes $df_{nk}/d\epsilon_{nk}$, how much the state energy changes as the precession angle changes $d\epsilon_{nk}/d\hat{M}$, and how quickly the spin direction is precessing $d\hat{M}/dt$. These can be combined with a chain rule

$$\frac{df_{nk}}{dt} = \frac{df_{nk}}{d\epsilon_{nk}} \frac{d\epsilon_{nk}}{d\hat{M}} \frac{d\hat{M}}{dt}. \quad (5.3)$$

Combining this result with the relaxation time approximation Eq. (5.2) and substituting these state occupancies into the first term of the effective field in Eq. (5.1) gives

$$\mathbf{H}_{\text{bfs}}^{\text{eff}} = \mathbf{H}_{\text{bfs}}^{\text{ani}} + \mathbf{H}_{\text{bfs}}^{\text{damp}}, \quad (5.4)$$

$$\mathbf{H}_{\text{bfs}}^{\text{ani}} = -\frac{1}{\mu_0 M} \sum_{nk} f_{nk} \frac{\partial \epsilon_{nk}}{\partial \hat{M}}, \quad (5.5)$$

$$\mathbf{H}_{\text{bfs}}^{\text{damp}} = -\frac{1}{\mu_0 M} \sum_{nk} \tau \left(-\frac{df_{nk}}{d\epsilon_{nk}} \right) \left(\frac{d\epsilon_{nk}}{d\hat{M}} \right)^2 \frac{d\hat{M}}{dt}. \quad (5.6)$$

$\mathbf{H}_{\text{bfs}}^{\text{ani}}$ is a contribution to the magnetocrystalline anisotropy field and $\mathbf{H}_{\text{bfs}}^{\text{damp}}$ is the damping field from the breathing Fermi surface model. When we compare this damping field to the

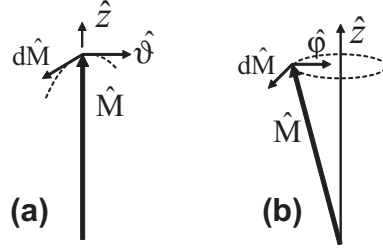


Figure 5.1: Schematic description of precession geometry. Within the breathing Fermi surface model (a) the damping rate is calculated as the magnetization passes through a specific point in a given direction. The torque correlation model (b) gives the damping rate for precessing about a given direction. The dashed curves indicate the precession trajectory.

damping field postulated by the Landau-Lifshitz-Gilbert equation

$$\mathbf{H}_{\text{LLG}}^{\text{damp}} = -\frac{\lambda}{\gamma^2 M} \frac{d\hat{M}}{dt} \quad (5.7)$$

we find that the damping rate is

$$\lambda_{\text{bfs}} = \tau \frac{\gamma^2}{\mu_0} \sum_{nk} \eta(\epsilon_{nk}) \left(\frac{\partial \epsilon_{nk}}{\partial \hat{M}} \right)^2. \quad (5.8)$$

As in Eq. (4.1), $\eta(\epsilon)$ is the negative derivative of the Fermi function and is a positive distribution peaked about the Fermi energy.

As described in Fig. (5.1a), the result of the breathing Fermi surface model Eq. (5.8) describes the damping rate of a material as the magnetization rotates through a particular point $\hat{z}$ about a given axis $\hat{\vartheta}$. When $\hat{M}$ is instantaneously aligned with $\hat{z}$ the direction of the change in the magnetization $d\hat{M}$ will be perpendicular to $\hat{z}$, in the $\hat{x}$ - $\hat{y}$ plane. On the other hand, the torque correlation model Eq. (4.1) gives the damping rate when the magnetization is undergoing small angle precession about the $\hat{z}$ direction (see Fig.(5.1b)). When $\hat{z}$ is a high symmetry direction the change in the magnetization will stay in the $\hat{x}$ - $\hat{y}$ plane. In each scenario – rotating $\hat{M}$ through $\hat{z}$ in the breathing Fermi surface model and rotating $\hat{M}$ about

$\hat{z}$ in the torque correlation model – $d\hat{M}$ is confined to the $\hat{x}$ - $\hat{y}$ plane. Therefore, rotating through $\hat{z}$ and rotating about $\hat{z}$ are equivalent in the small angle limit when $\hat{z}$ is a high symmetry direction. With this observation we now show that the intraband contributions of the torque correlation model are equivalent to the breathing Fermi surface result under these conditions.

The only energy that changes as the magnetization rotates is the spin-orbit energy $\mathcal{H}_{\text{so}}$. As the spin of the state $|nk\rangle$ rotates about the $\hat{\vartheta}$ direction by angle ϑ its spin-orbit energy is given by

$$\epsilon(\vartheta) = \langle nk | e^{i\sigma \cdot \vec{\vartheta}} \mathcal{H}_{\text{so}} e^{-i\sigma \cdot \vec{\vartheta}} | nk \rangle \quad (5.9)$$

where $\vec{\vartheta} = \vartheta \hat{\vartheta}$. Taking the derivative of this energy with respect to ϑ in the limit that ϑ goes to zero shows that the energy derivatives are

$$\frac{\partial \epsilon}{\partial \vartheta} = i \langle nk | [\sigma \cdot \hat{\vartheta}, \mathcal{H}_{\text{so}}] | nk \rangle. \quad (5.10)$$

Figure (5.1) shows that the derivative $\partial \epsilon / \partial \vartheta$ is identical to $\partial \epsilon / \partial \hat{M}$ and that when $\hat{M} = \hat{z}$ the rotation direction $\hat{\vartheta}$ lies in the $x - y$ plane. The two components of the transverse torque operator Γ^x and Γ^y can be obtained (up to factors of i) by setting $\hat{\vartheta}$ equal to $\hat{x}$ or $\hat{y}$, respectively. From this observation we find

$$|\langle nk | \Gamma^- | nk \rangle|^2 = \left(\frac{\partial \epsilon}{\partial x} \right)^2 + \left(\frac{\partial \epsilon}{\partial y} \right)^2. \quad (5.11)$$

When the magnetization direction $\hat{z}$ is pointed along a high symmetry direction the transverse directions $\hat{x}$ and $\hat{y}$ are equivalent and $|\Gamma^-|^2 = 2(\partial \epsilon / \partial \hat{M})^2$.

Substituting the torque matrix elements for the energy derivatives in Eq.(5.8) gives a

damping rate of

$$\lambda_{\text{bfs}} = \frac{\tau\gamma^2}{2\mu_0} \sum_{nk} |\Gamma_n^-(k)|^2 \eta(\epsilon_{nk}). \quad (5.12)$$

For the intraband terms in Eq. (4.1) the integration over the spectral functions reduces to $2\tau\eta(\epsilon_{nk})/\pi\hbar$ so we find

$$\lambda_{\text{bfs}} = \pi \frac{\mu_0\mu_B^2 g^2}{\hbar} \sum_n \int \frac{d^3k}{(2\pi)^3} |\Gamma_n^-(k)|^2 \int d\epsilon_1 A_{nk}^2(\epsilon_1) \eta(\epsilon_1), \quad (5.13)$$

which matches the intraband terms of Eq. (4.1).

Calculation of the damping rate from Eq. (5.8) requires evaluation of the microscopic anisotropies for a given spin orientation and has been conducted by other researchers [51, 52]. Since the damping is linear in the scattering time it is typical to report results from Eq. (5.8) as the ratio λ/τ . The intraband term in our calculation Eq. (5.13) also results in a damping rate that is proportional to the electron lifetime. Table 5.1 compares the ratio λ/τ found from the breathing Fermi surface model Eq. (5.8) to that obtained from the intraband contributions Eq. (5.13) of the torque correlation model. The agreement is quite remarkable given the very different approaches of the two calculations and numerically verifies our analytical demonstration that these approaches are equivalent. The agreement is also reassuring because the scattering events in the torque-correlation model can be difficult to understand, but we have now shown that the intraband scattering events describe the same physics as the more understandable breathing Fermi surface picture.

The intraband terms describe scattering from one state to itself by the torque operator, which lowers the angular momentum of the state. The matrix elements of this operator acting between some state and itself can be appreciably non-zero because the spin-orbit interaction mixes small amounts of the opposite spin direction into each state. Since the initial and final states are the same, the operation is naturally spin conserving. The matrix

Table 5.1: Comparison of the breathing Fermi surface to the intraband terms of the torque correlation model. The damping rates due to the intraband contribution from Eq. (4.1) are compared to previous results from the breathing Fermi surface model [52]. Values for λ/τ are given in 10^{22} s^{-2} . Published numbers from [52] have been multiplied by 4π to convert from the cgs unit system to SI.

	$(\lambda/\tau)_{\text{intra}}$	$(\lambda/\tau)_{\text{bfs}}$
bcc Fe $\langle 001 \rangle$	1.01	0.968
bcc Fe $\langle 111 \rangle$	1.35	1.29
hcp Co $\langle 0001 \rangle$	0.786	0.704
fcc Ni $\langle 111 \rangle$	6.67	6.66
fcc Ni $\langle 001 \rangle$	8.61	8.42

elements do not describe a real transition, but rather provide a measure of the energy of the electron-hole pairs that are generated as the spin direction changes. The electron-hole pairs are subsequently annihilated by a real electron-lattice scattering event.

Interband Terms

The set of states ψ_{nk} that we use are eigenstates only when the magnetization is pointed along the $\hat{z}$ direction. As the magnetization rotates away from $\hat{z}$ the spin-orbit energy of the states change and this acts as a perturbation. Therefore, when the magnetization precesses about $\hat{z}$ the states that are occupied are not eigenstates and transitions occur between them. Since the spin-orbit energy is small the transition rate may be found from first order perturbation theory. The perturbation is

$$V(t) = e^{i\sigma \cdot \varphi(t)} \mathcal{H}_{so} e^{-i\sigma \cdot \varphi(t)} - \mathcal{H}_{so}(0) \approx i[\sigma \cdot \varphi(t), \mathcal{H}_{so}]. \quad (5.14)$$

This approximation results from linearizing the exponents, which is appropriate in the small angle limit. The time dependence of the rotation axis is $\hat{\varphi}(t) = \cos \omega t \hat{x} + \sin \omega t \hat{y}$, up to

a phase factor. This perturbation causes band transitions between the states ψ_{nk} and ψ_{mk} . The initial and final states have the same wavevector because these transitions are caused by the uniform precession, which has a wavevector of zero. The transition rate between states due to this perturbation is

$$W_{mn}(k) = \frac{2\pi}{\hbar} |\Gamma_{mn}^-(k)|^2 \delta(\epsilon_{mk} - \epsilon_{nk} - \hbar\omega). \quad (5.15)$$

The variations of the occupancies of the states with respect to the magnetization direction are given by the master equation

$$\frac{\partial \rho_{nk}}{\partial t} = \sum_{m \neq n} W_{mn}(k) [\rho_{mk} - \rho_{nk}]. \quad (5.16)$$

The second term in the effective field Eq. (5.1) contains the factor $\partial \rho_{nk} / \partial \hat{M}$ which is $(\partial \rho_{nk} / \partial t) / (\partial \hat{\varphi} / \partial t)^2 \cdot (\partial \hat{M} / \partial t)$ where $\partial \hat{\varphi} / \partial t = \omega$. Inserting these expressions into the second term in the effective field and rearranging the sums gives

$$\mathbf{H}^{\text{eff}} = -\frac{1}{2\mu_0 M} \sum_{nk} \sum_{m \neq n} \frac{W_{mn}(k)}{\omega^2} [\rho_{nk} - \rho_{mk}] [\epsilon_{mk} - \epsilon_{nk}] \frac{d\hat{M}}{dt}. \quad (5.17)$$

Comparing this result to the effective field predicted by the Landau-Lifshitz-Gilbert equation (5.7) we find a damping rate of

$$\lambda = \frac{\gamma^2}{2\mu_0} \sum_{nk} \sum_{m \neq n} W_{mn}(k) \frac{[\rho_{nk} - \rho_{mk}]}{\omega} \frac{[\epsilon_{mk} - \epsilon_{nk}]}{\omega}. \quad (5.18)$$

The finite lifetime of the states is introduced with the spectral functions

$$\lambda = \frac{\hbar^2 \gamma^2}{2\mu_0} \sum_{nk} \sum_{m \neq n} \int d\epsilon_1 A_{nk}(\epsilon_1) \int d\epsilon_2 A_{mk}(\epsilon_2) W_{mn}(k) \frac{[f(\epsilon_1) - f(\epsilon_2)]}{\hbar\omega} \frac{[\epsilon_2 - \epsilon_1]}{\hbar\omega}. \quad (5.19)$$

Inserting the transition rate Eq. (5.15), integrating over ϵ_2 , and taking the limit that ω goes to zero leaves

$$\lambda = \pi \frac{\mu_0 \mu_B^2 g^2}{\hbar} \sum_n \sum_{m \neq n} \int \frac{d^3 k}{(2\pi)^3} |\Gamma_{mn}^-(k)|^2 \int d\epsilon_1 A_{nk}(\epsilon_1) A_{mk}(\epsilon_1) \eta(\epsilon_1), \quad (5.20)$$

which are the interband terms of Eq. (4.1).

In this derivation of the bubbling Fermi surface contribution to the damping we have ignored an additional, reversible term that contributes to the magnetocrystalline anisotropy. This contribution arises from changes in the equilibrium state occupancies as the magnetization direction changes. This contribution to the magnetocrystalline anisotropy is localized to the Fermi surface while the contribution discussed in the intraband section is spread over all of the occupied levels.

Modifying the Damping Rate

In Chapter 4 we demonstrated that the torque correlation model Eq. (4.1) accurately predicts the precession damping rates of the transition metals iron, cobalt, and nickel. So far in the present chapter we have shown that this expression for the damping rate can be described simply within an effective field picture. We now investigate the degree to which the damping rate may be modified by adjusting certain material parameters. Inspection of Eq. (4.1) reveals that the damping rate depends on the convolution of two factors: the torque matrix elements and the integral over the spectral functions. We separate the quantitative analysis of the damping rates into their dependencies on these two factors, beginning with the spectral weight.

Spectral Overlap

For the intraband terms, the integral over the spectral functions is essentially proportional to the density of states at the Fermi level. Therefore, it appears reasonable to suspect that the intraband contribution to the damping rate of a given material should be roughly proportional to the density of states of that material at the Fermi level. To test this claim numerically, we artificially varied the Fermi level of the metals within the d-bands and calculated the intraband damping rate as a function of the Fermi level. The results of these calculations are superimposed on the calculated densities of states of the materials in Fig. 5.2. The correlation between the damping rates and the densities of states, while not exact, is certainly strong, indicating that increasing the density of states of a system at the Fermi level will generally increase the intraband contribution to damping.

The dependence of the interband terms on the spectral overlap is more complicated than that of the intraband terms. The spectral overlap depends on the energy differences $\epsilon_m - \epsilon_n$, which can vary significantly between bands and over k-points. When the scattering rate $\hbar/\tau$ is much less than these energy gaps the interband terms are proportional to the scattering rate. However, this proportionality only holds at low scattering rates when the interband contribution is much less than the intraband contribution. The proportionality breaks down at higher scattering rates when $\hbar/\tau$ becomes comparable to the band gaps. After this point the damping rate gradually plateaus with respect to the scattering rate. Despite the inability to analytically predict the dependence of the interband damping rate on the density of states it was possible to conduct the test numerically. Figure 5.3 presents the interband damping rate for a high scattering rate as the Fermi level was artificially varied through the d-bands. Superposing the squared density of states upon these results shows a very strong correlation. It is not clear why the interband damping rate should be proportional to the density of states squared, however, this trend is observed in each metal.

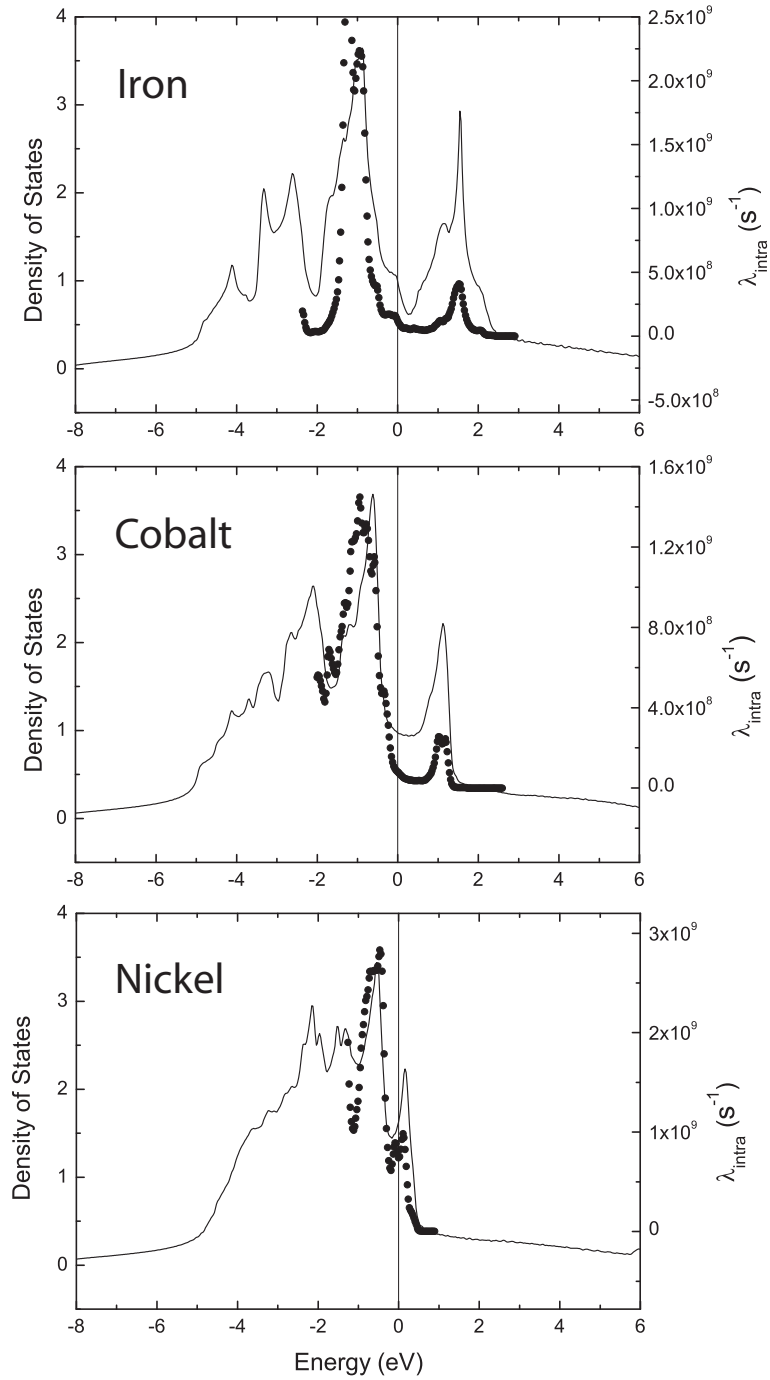


Figure 5.2: Intraband damping rate versus Fermi level superimposed upon density of states. A strong correlation between the intraband damping rate versus Fermi level (●) and the density of states (solid curves) is observed. Vertical black lines indicates true Fermi energy calculated by density functional theory.

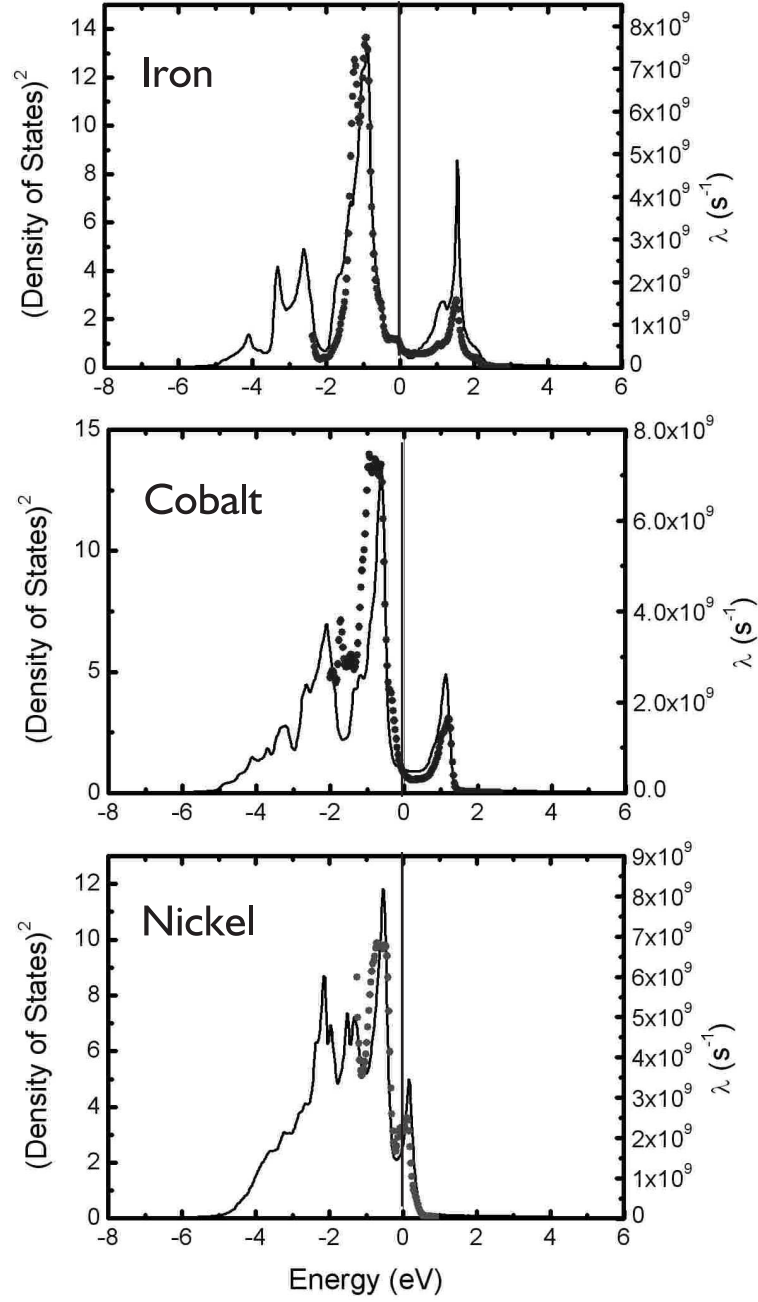


Figure 5.3: Interband damping rate versus Fermi level superimposed upon squared density of states. A strong correlation between the interband damping rate versus Fermi level (●) and the density of states squared (solid curves) is observed. Vertical black lines indicates true Fermi energy calculated by density functional theory.

Torque Matrix Elements

The damping rate also depends on the square of the torque matrix elements. A goal of doping is often to modify the effective spin-orbit coupling of a sample. While doping does more than this, such as introducing strong local scattering centers, it is nevertheless useful to estimate the dependence of the matrix elements on the spin-orbit parameter ξ . We begin with pure spin states ψ_n^0 and treat the spin-orbit interaction $V = \xi V'$ as a perturbation. The states can be expanded in powers of ξ as

$$\psi_n = \psi_n^0 + \xi \psi_n^1 + \xi^2 \psi_n^2 + \dots \quad (5.21)$$

The superscripts refer to the unperturbed wavefunction (0) and the additions (i) due to the perturbation to the i th order while the subscript n is the band index, which includes the spin direction, up or down. Since the torque operator also contains a factor of the spin-orbit parameter the matrix elements have terms in every order of ξ beginning with the first order. Therefore, the squared matrix elements have contributions of order ξ^2 and higher.

To determine the importance of these terms we artificially tune the spin-orbit interaction from zero to full strength, calculating the damping rate over this range. We then fit the intraband and interband damping rates separately to polynomials. In each material, this fitting showed that for the intraband terms the ξ dependence of the damping rate was primarily third order, with smaller contributions from the second and fourth order terms. Restricting the fit to only the third order term produced a very reasonable result, shown in Fig. (5.4). For the interband terms, polynomial fitting was dominated by the second order term, with all other powers contributing only negligibly. The second order fit is shown in Fig. (5.4).

To understand the difference in the ξ dependence of the intraband and interband contri-

butions it is useful to define the torque operator

$$\Gamma^- = \xi(\ell^- \sigma^z - \ell^z \sigma^-). \quad (5.22)$$

The torque operator lowers the angular momentum of the state it acts on. This can be accomplished either by lowering the spin momentum $\ell^z \sigma^-$, a spin flip, or lowering the orbital momentum $\ell^- \sigma^z$, an orbital excitation. Therefore, both the intraband and interband contributions each have two sub-mechanism: spin flips and orbital excitations.

The second order terms for the intraband case are $\xi^2 |\langle \psi_n^0 | (\ell^z \sigma^- - \ell^- \sigma^z) | \psi_n^0 \rangle|^2$. Since the unperturbed states ψ_n^0 are pure spin states the spin flip part $\ell^z \sigma^-$ of the torque returns zero. Therefore, only the orbital excitations exist to lowest order in ξ , reducing the strength of the second order term in the intraband case. However, the interband terms contain matrix elements between several states, some with the same spin direction, but others with opposite spin direction. Therefore, both spin flips and orbital excitations contribute in second order to the interband contribution.

Conclusions

This chapter and the previous one have presented the results of this project, but have avoided much of the technical discussion to make the content accessible to a general solid state audience. The remaining two chapters contain the analytical and numerical details behind these results. These details are included because they represent the significant portion of the work behind this project, but are not intended for a general audience. The final two chapters can be treated as appendices intended for those who wish to extend this work. Therefore, at this point we give a summary of our work and an outlook toward future projects.

We began this project by identifying a precession damping mechanism [49] that, based

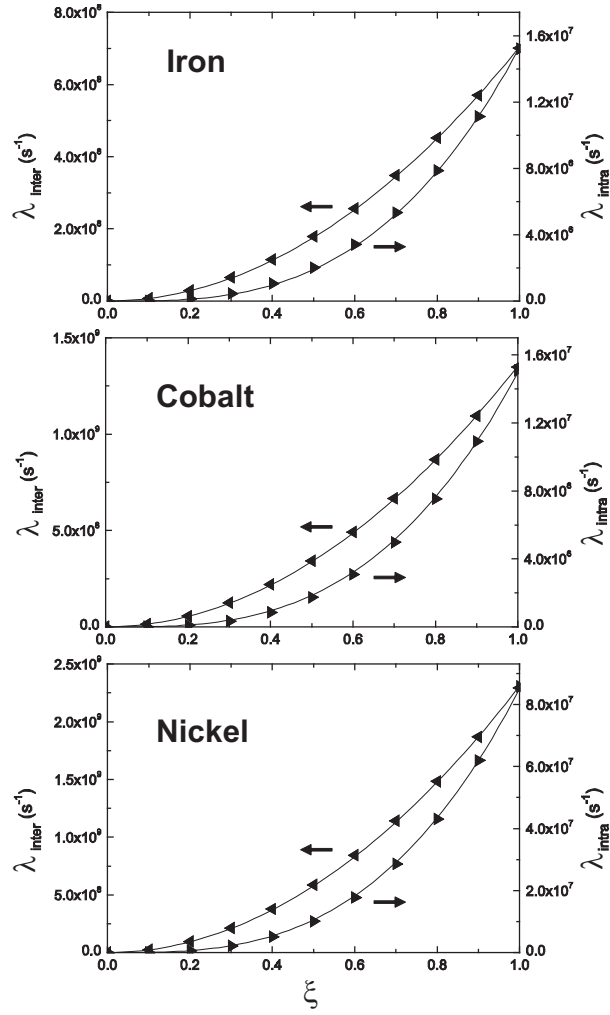


Figure 5.4: ξ dependence of intraband and interband damping rates. Damping rates were calculated for a range of spin-orbit interaction strengths between off ($\xi = 0$) and full strength ($\xi = 1$). ξ^2 fits were made to the interband damping rates (left axes and $\blacktriangleleft$ symbols) and ξ^3 fits to the intraband rates (right axes and $\blacktriangleright$ symbols).

on qualitative arguments, appeared a promising candidate for quantitatively matching experimental damping rates. We evaluated this expression numerically using density functional theory techniques within the linear augmented plane wave and local spin density framework. We developed and evaluated an expression for the resistivity in a similar fashion. The damping rates that we calculated matched the measured damping rates to within 95 % for nickel, 70 % for iron, and 47 % for cobalt.

To gain a better physical understanding of the damping process we extended the previous effective field formulation. The previously existing effective field treatment of damping, called the breathing Fermi surface model, provided a simple and understandable explanation of precession damping in metallic ferromagnets. However, since it only produced the intraband contribution to damping and not the interband terms, it is only applicable to very pure systems at low temperatures. Our objective was to extend this effective field model to reproduce the torque correlation model, which accurately predicts damping rates of systems with imperfections from low temperatures to above room temperature. We discovered that the breathing Fermi surface model accounts for only one of the two terms in the effective field. By constructing an effective field with the previously studied breathing Fermi surface contribution and also the new bubbling effect we have shown that this simpler picture may be mapped onto the torque correlation model such that the breathing terms match the intraband contribution and the bubbling terms match the interband contribution.

Since there is considerable interest in understanding how to manipulate the damping rates of materials, we investigated the dependence of the intraband and interband damping rates on both the spectral overlap integral and the torque matrix elements. For the intraband terms, the spectral overlap is proportional to the density of states and we found a strong correlation between the intraband damping rate and the density of states of the material. The interband case is significantly complicated by the range of band gaps present in materials. No simple relation was found between the strength or scattering rate dependence of the

interband terms and common material parameters. The importance of the torque matrix elements to the damping rates was characterized through their dependence on the spin-orbit parameter. The intraband damping rates were found to vary as the spin-orbit parameter cubed while the interband damping rates went as the spin-orbit parameter squared. This difference was explained by noting that the torque operator changes the angular momentum of states either through spin flips, or by changing the orbital angular momentum. Spin-flip excitations do not occur to second order in ξ for the intraband terms, but do contribute at second order for the interband terms.

It is desirable to understand the relative differences in damping rates among various materials, such as why the damping rate for nickel is higher than that for cobalt and iron. We have shown that the relative damping rates of these materials depend in part on the differences of their densities of states and spin-orbit coupling strengths. However, they also depend in an intricate way on the energy gap spectra of each metal. For the interband terms the dependence on the gap spectrum enters through the spectral overlap integral. For the intraband terms the energy gaps appear in the denominators of the matrix elements. Therefore, states with very small splittings can dominate the k-space convolution. The abundance of such states in nickel appears to contribute to the larger damping rate in this material [63].

Doping is a common technique for modifying damping rates. Doping has a number of consequences on a sample and these effects vary with the method of doping. Dopants can increase the electron-lattice scattering rate, introduce magnetic inhomogeneities that act as local scattering centers, alter the density of states, and change the effective spin-orbit parameter. We have investigated the consequences of modifying the densities of states and spin-orbit parameter on the damping rate, and demonstrated the scattering rate dependence of the damping rate, however, it is not clear what new damping mechanisms arise when rare-earth elements are added to a transition metal host.

There are a few obvious projects to investigate next. These include small angle precession damping in transition metal alloys, large amplitude damping in single element metals, and ultrafast demagnetization. The spin-orbit torque damping mechanism that we have investigated appears suitable for describing damping in crystalline and magnetically collinear alloys such as CoFe in various stoichiometries. Extending the spin-orbit torque picture to non-collinear systems, such as NiFe, would require including a new exchange-exchange torque [53]. This does not appear overly burdensome. It is not clear, however, what other processes take place in amorphous materials.

Large amplitude dynamics would prove a challenging, but interesting endeavor. The Kubo formula used here would have to be extended to include non-linear terms. One should also abandon the constraint that the magnitude of the magnetization is constant during the dynamics. Further, non-uniform modes would likely play a significant role in large amplitude dynamics. Describing large amplitude dynamics would be complicated, but of significant interests as many commercial and industrial applications of magnetization dynamics involve the complete reversal of the magnetization direction of a material. A particularly interesting result would be a clear characterization of under what conditions the LLG equation breaks down and how the resulting dynamics should be described.

Lastly, ultrafast magnetization dynamics and demagnetization have recently become the center of intense experimental investigation. Such processes are used in the heat assisted magnetic reversal technique discussed in the first chapter. Light, sometimes circularly polarized, is used to excite the electrons of a material on a time scale of a few hundred femtoseconds. This often results in the decrease of the magnetization of the material and a softening of the magnetocrystalline anisotropy. Similar techniques are used to change FeRh from the antiferromagnetic phase to the ferromagnetic phase on similar time scales. Understanding these processes on a quantum mechanical level would be a serious undertaking requiring careful treatment of excited non-equilibrium electronic configurations.

CHAPTER 6

THEORETICAL DETAILS

The Damping Rate

In this section we derive Eq. (4.1) for the precession damping rate. The damping rate is found experimentally by studying the response of the magnetization to an applied field, which is the susceptibility. We begin by assuming that the Landau-Lifshitz-Gilbert equation accurately describes the dynamics of the magnetization, and constructing the phenomenological susceptibility that the LLG equation predicts. We then express the damping rate in terms of the imaginary part of the susceptibility. The next step is to derive the susceptibility from a Kubo formula for the magnetization. Taking the imaginary part of this susceptibility then gives the damping rate according to the relation determined from the LLG equation.

LLG Susceptibility

The magnetization dynamics of ferromagnets are well described by the Landau-Lifshitz equation

$$\dot{\mathbf{M}} = -|\gamma| \mathbf{M} \times \mathbf{H} - \frac{\lambda}{M_s^2} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}) . \quad (6.1)$$

In the limit of small amplitude oscillations of the magnetization vector this equation can be linearized to derive an expression for the susceptibility and the damping constant λ . During small amplitude dynamics, the magnetization will point essentially in the equilibrium z-direction and have a small oscillating transverse response

$$\mathbf{M} = (m_x, m_y, M_s) . \quad (6.2)$$

By small amplitude dynamics we mean that $m_{x,y} \ll M_s$. During a FMR measurement, a strong dc field is applied in the z-direction with a small transverse oscillating component in the x-y direction. Including an isotropic demagnetizing field the total applied field is

$$\mathbf{H} = (h_x - Nm_x, h_y - Nm_y, H_0 - NM_s). \quad (6.3)$$

We now write down the linear expansion for each of the three terms in 6.1. The derivative of the magnetization is

$$\dot{\mathbf{M}} = -i\omega \begin{bmatrix} m_x \\ m_y \end{bmatrix}. \quad (6.4)$$

To first order in the transverse components of the magnetization, the cross product in the precession term is

$$\begin{aligned} \mathbf{M} \times \mathbf{H} &= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ m_x & m_y & M_s \\ (h_x - Nm_x) & (h_y - Nm_y) & (H_0 - NM_s) \end{vmatrix} \\ &= [m_y H_0 - h_y M_s] \hat{x} + [h_x M_s - m_x H_0] \hat{y}. \end{aligned} \quad (6.5)$$

The demagnetizing field N cancels to first order in $m_{x,y}$ because the magnetization essentially remains in the equilibrium direction. The damping term is

$$\begin{aligned} \mathbf{M} \times \mathbf{M} \times \mathbf{H} &= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ m_x & m_y & M_s \\ (m_y H_0 - h_y M_s) & (h_x M_s - m_x H_0) & 0 \end{vmatrix} \\ &= [m_x M_s H_0 - h_x M_s^2] \hat{x} + [m_y M_s H_0 - h_y M_s^2] \hat{y}. \end{aligned} \quad (6.6)$$

Substituting these linear approximations into the equation of motion (6.1) gives

$$-i\omega \begin{bmatrix} m_x \\ m_y \end{bmatrix} = -|\gamma| \begin{bmatrix} m_y H_0 - h_y M_s \\ h_x M_s - m_x H_0 \end{bmatrix} - \frac{\lambda}{M_s^2} \begin{bmatrix} m_x M_s H_0 - h_x M_s^2 \\ m_y M_s H_0 - h_y M_s^2 \end{bmatrix}. \quad (6.7)$$

Collecting the $m_{x,y}$ terms on the left and the $h_{x,y}$ terms on the right gives

$$\begin{bmatrix} -i\omega + \lambda H_0/M_s & |\gamma|H_0 \\ -|\gamma|H_0 & -i\omega + \lambda H_0/M_s \end{bmatrix} \begin{bmatrix} m_x \\ m_y \end{bmatrix} = \begin{bmatrix} \lambda & |\gamma|M_s \\ -|\gamma|M_s & \lambda \end{bmatrix} \begin{bmatrix} h_x \\ h_y \end{bmatrix}. \quad (6.8)$$

We introduce two frequencies $\omega_0 = |\gamma|H_0$ and $\omega_M = |\gamma|M_s$ to simplify the above result to

$$\begin{bmatrix} -i\omega + \lambda\omega_0/\omega_M & \omega_0 \\ -\omega_0 & -i\omega + \lambda\omega_0/\omega_M \end{bmatrix} \begin{bmatrix} m_x \\ m_y \end{bmatrix} = \begin{bmatrix} \lambda & \omega_M \\ -\omega_M & \lambda \end{bmatrix} \begin{bmatrix} h_x \\ h_y \end{bmatrix} \quad (6.9)$$

and finally

$$\begin{bmatrix} m_x \\ m_y \end{bmatrix} = \begin{bmatrix} -i\omega + \lambda\omega_0/\omega_M & \omega_0 \\ -\omega_0 & -i\omega + \lambda\omega_0/\omega_M \end{bmatrix}^{-1} \begin{bmatrix} \lambda & \omega_M \\ -\omega_M & \lambda \end{bmatrix} \begin{bmatrix} h_x \\ h_y \end{bmatrix}. \quad (6.10)$$

ω_0 is the precession frequency. We could also add an anisotropy field to Eq. (6.3). If we were to align the easy axis with the z-direction then the precession frequency would become $\omega_p = \omega_0 + \omega_a$ where $\omega_a = |\gamma|H_a$ and H_a is the anisotropy field.

The linear response of a magnetic material to an applied field is $\mathbf{m} = \chi \mathbf{h}$ where χ is the magnetic susceptibility. To get the susceptibility, we assume weak damping $\lambda/\omega_M = \alpha \ll$

1, and carry the matrix multiplication in the above expression to first order in λ/ω_M .

$$\begin{aligned}\chi(\omega) &= \frac{1}{\omega_0^2 + (\lambda\omega_0/\omega_M - i\omega)^2} \begin{bmatrix} (1 + \lambda^2/\omega_M^2)\omega_0\omega_M - i\omega\lambda & -i\omega\omega_M \\ i\omega\omega_M & (1 + \lambda^2/\omega_M^2)\omega_0\omega_M - i\omega\lambda \end{bmatrix} \\ &\approx \frac{-\omega_M}{\omega_0^2 - \omega^2 - 2i\omega\lambda\omega_0/\omega_M} \begin{bmatrix} -\omega_0 + i\omega\lambda/\omega_M & i\omega \\ -i\omega & -\omega_0 + i\omega\lambda/\omega_M \end{bmatrix}. \quad (6.11)\end{aligned}$$

Experiments typically probe the transverse susceptibility, which is the diagonal term.

$$\begin{aligned}\chi^\perp(\omega) &= \frac{\omega_0\omega_M - i\omega\lambda}{\omega_0^2 - \omega^2 - 2i\omega\lambda\omega_0/\omega_M} \\ &= \frac{[\omega_0\omega_M - i\omega\lambda] \cdot [(\omega_0^2 - \omega^2) + 2i\omega\lambda\omega_0/\omega_M]}{(\omega_0^2 - \omega^2)^2 + (2\omega\lambda\omega_0/\omega_M)^2} \\ &= \frac{\omega_0\omega_M(\omega_0^2 - \omega^2) + 2\omega^2\lambda^2\omega_0/\omega_M - i\omega\lambda(\omega_0^2 - \omega^2) + 2i\omega\lambda\omega_0^2}{(\omega_0^2 - \omega^2)^2 + (2\omega\lambda\omega_0/\omega_M)^2}. \quad (6.12)\end{aligned}$$

Our objective is to relate the damping rate λ to the susceptibility. There are many ways to relate the two quantities, but the simplest result comes from taking the imaginary part of the above expression in the limit of the frequency going to zero.

$$\begin{aligned}\text{Im } \chi^\perp(\omega) &= \frac{\omega\lambda\omega_0^2 + \omega^3\lambda}{(\omega_0^2 - \omega^2)^2 + (2\omega\lambda\omega_0/\omega_M)^2} \\ \lim_{\omega \rightarrow 0} \text{Im } \chi^\perp(\omega)/\omega &= \frac{\lambda}{\omega_0^2} \\ \lambda &= \omega_0^2 \lim_{\omega \rightarrow 0} \text{Im } \chi^\perp(\omega)/\omega. \quad (6.13)\end{aligned}$$

Taking the limit that $\omega \rightarrow 0$ does not imply that ω is small compared to the other frequencies. In fact, during the FMR experiment the frequency ω gets tuned to the precession frequency ω_0 , and can be larger than the frequency ω_M . We could have taken the limit that $\omega \rightarrow \omega_0$, but the result would be less useful. The above is a simple and mathematically true result that we will make use of. In the following we will derive an expression for

the susceptibility. The imaginary part of this expression will give the damping rate. We will end this chapter by presenting the results of our calculations of the damping rates and comparing these results to the experimental values.

Kubo Formula

A distinguishing feature of ferromagnetic materials is a strong non-zero equilibrium magnetization $\langle \mathbf{m} \rangle_0$. Ferromagnetic materials are useful in part because this magnetization may be pushed out of equilibrium with an external field. The magnetization $\mathbf{m}$ of a solid is given by its equilibrium magnetization plus a contribution that depends on how susceptible the material is to being perturbed by an external field.

$$\langle \mathbf{m}(\mathbf{r}, t) \rangle = \langle \mathbf{m}(\mathbf{r}, t) \rangle_0 + \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \chi(\mathbf{r}, \mathbf{r}'; t, t') \cdot \mathbf{h}(\mathbf{r}', t'). \quad (6.14)$$

The magnetization at coordinates $(\mathbf{r}, t)$ depends on the applied field $\mathbf{h}$ at all earlier coordinates $(\mathbf{r}', t')$. To find the susceptibility we will derive an expression for the magnetization, which will be proportional to the driving field $\mathbf{h}$. The proportionality will be the susceptibility.

Our system has some Hamiltonian $\mathcal{H}$ to which we add a perturbation $\mathcal{V} = -\mathbf{m} \cdot \mathbf{h}$ by applying the oscillating external field $\mathbf{h}$. The Hamiltonian $\mathcal{H}$ has some set of N-particle eigenstates $|\Psi\rangle$. At any time t' we can define a time independent Schrödinger equation for $\mathcal{H}' = \mathcal{H} + \mathcal{V}$ as $\mathcal{H}'(t') |\Psi'_i(t')\rangle = E_i(t') |\Psi'_i(t')\rangle$. The subscript i orders the eigenvalues E_i . We can define a complete set of time dependent N-particle states for $\mathcal{H}'$ as the states $|\Psi'_i\rangle$ that track the eigenstates of the time independent Schrödinger equation for all t' . The magnetization may be written symbolically as

$$\langle \mathbf{m}(\mathbf{r}, t) \rangle = \left\langle \left\langle \hat{\Psi}'(t) | \hat{\mathbf{m}}(\mathbf{r}, t) | \hat{\Psi}'(t) \right\rangle \right\rangle. \quad (6.15)$$

The outer set of angled brackets indicate a thermodynamic average over the set of states. The hats over the wavefunctions and the operator indicate that these are given in the interaction representation. This expression for the magnetization is not particularly useful because we do not know what the states $|\Psi'\rangle$ are. Our first task is to replace the perturbed states $|\Psi'\rangle$ with the unperturbed states $|\Psi\rangle$.

The time dependence of the wavefunctions can be expressed using the time evolution operator

$$\langle \mathbf{m}(\mathbf{r}, t) \rangle = \left\langle \left\langle \hat{\Psi}'(-\infty) \left| U^\dagger(t, -\infty) \hat{\mathbf{m}}(\mathbf{r}, t) U(t, -\infty) \right| \hat{\Psi}'(-\infty) \right\rangle \right\rangle. \quad (6.16)$$

By writing $t = -\infty$ we really mean a time before the perturbation $\mathcal{V}$ has been turned on. Since $\mathcal{V}$ is zero at $t = -\infty$, the states $\Psi'_i(t)$, which solve the time independent Schrödinger equation of $\mathcal{H}'$ for all t , must match the N-particle eigenstates Ψ_i of the unperturbed Hamiltonian. Therefore, $\left| \hat{\Psi}'(-\infty) \right\rangle = \left| \hat{\Psi}(0) \right\rangle$, up to some phase factor.

At $t = 0$ the Heisenberg, Schrödinger, and interaction pictures are all the same so $\left| \hat{\Psi}(0) \right\rangle = |\Psi(0)\rangle$ and we can drop the hats over the states. Since the time argument of the states will remain 0 for the rest of this section we will further simplify the notation to $|\Psi(0)\rangle = |\Psi\rangle$.

The time evolution operator contains the perturbation in an exponential

$$U(t, -\infty) = \text{T exp} \left[-\frac{i}{\hbar} \int_{-\infty}^t dt' \hat{\mathcal{V}}(t') \right]. \quad (6.17)$$

T is the time ordering operator and the above expression is really a shorthand notation for an infinite series in powers of the perturbation. The Kubo formula approximation is to

truncate this series after the linear term; hence, this gives the linear response.

$$U(t, -\infty) \approx 1 - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \hat{\mathcal{V}}(\mathbf{r}', t'). \quad (6.18)$$

And similarly for the Hermitian conjugate

$$U^\dagger(t, -\infty) \approx 1 + \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \hat{\mathcal{V}}(\mathbf{r}', t'). \quad (6.19)$$

This gives a manageable expression for the magnetization:

$$\begin{aligned} \langle \mathbf{m}(\mathbf{r}, t) \rangle &\approx \langle \langle \Psi | \left(1 + \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \hat{\mathcal{V}}(\mathbf{r}', t') \right) \hat{\mathbf{m}}(\mathbf{r}, t) \\ &\quad \cdot \left(1 - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \hat{\mathcal{V}}(\mathbf{r}', t') \right) | \Psi \rangle \rangle \\ &\approx \langle \langle \Psi | [\hat{\mathbf{m}}(\mathbf{r}, t) \\ &\quad - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' [\hat{\mathbf{m}}(\mathbf{r}, t) \hat{\mathcal{V}}(\mathbf{r}', t') - \hat{\mathcal{V}}(\mathbf{r}', t') \hat{\mathbf{m}}(\mathbf{r}, t)]] | \Psi \rangle \rangle \\ &= \langle \mathbf{m}(\mathbf{r}, t) \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \langle \langle \Psi | [\hat{\mathbf{m}}(\mathbf{r}, t), \hat{\mathcal{V}}(\mathbf{r}', t')] | \Psi \rangle \rangle \end{aligned} \quad (6.20)$$

When we compare this result to our original expression (6.14) we find

$$\begin{aligned} &-\frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \langle \langle \Psi | [\hat{\mathbf{m}}(\mathbf{r}, t), \hat{\mathcal{V}}(\mathbf{r}', t')] | \Psi \rangle \rangle \\ &= \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d^3 r' \tilde{\chi}(\mathbf{r} - \mathbf{r}'; t - t') \cdot \mathbf{h}(\mathbf{r}', t'). \end{aligned} \quad (6.21)$$

The susceptibility is a tensor, and component-wise we find

$$\chi_{ij}(\mathbf{r}, \mathbf{r}'; t, t') \cdot h_j(\mathbf{r}', t') = -\frac{i}{\hbar} \Theta(t - t') \langle \langle \Psi | [\hat{m}_i(\mathbf{r}, t), \hat{\mathcal{V}}_j(\mathbf{r}', t')] | \Psi \rangle \rangle \quad (6.22)$$

where $\Theta(t - t')$ is the Heaviside step function. Substituting in the perturbation, which

as we noted before is $\mathcal{V}_j(\mathbf{r}', t') = -m_j(\mathbf{r}', t') h_j(\mathbf{r}', t')$, leaves the Kubo formula for the susceptibility

$$\chi_{ij}(\mathbf{r}, \mathbf{r}'; t, t') = \frac{i}{\hbar} \Theta(t - t') \langle \langle \Psi | [\hat{m}_i(\mathbf{r}, t), \hat{m}_j(\mathbf{r}', t')] | \Psi \rangle \rangle. \quad (6.23)$$

This accomplishes the first step of writing the susceptibility in terms on the unperturbed N-particle eigenstates.

The magnetization has both spin and orbital components. For transition metal systems the orbital moments are largely quenched and the magnetization is dominated by the spin moment. We can simplify our problem by approximating the magnetization operator as $\mathbf{m}(\mathbf{r}, t) = g\mu_B\sigma(\mathbf{r}, t)$. The Landé g factor quantitatively accounts for the orbital contribution to the magnetization that is parallel to the spin direction and σ is the spin operator. This simplification gives

$$\tilde{\chi}_{ij}(\mathbf{r}, \mathbf{r}'; t, t') = -g^2\mu_B^2 \mathcal{S}_{ij}(\mathbf{r}, \mathbf{r}'; t, t') \quad (6.24)$$

$$\mathcal{S}_{ij}(\mathbf{r}, \mathbf{r}'; t, t') = -\frac{i}{\hbar} \Theta(t - t') \langle \langle \Psi | [\hat{\sigma}_i(\mathbf{r}, t), \hat{\sigma}_j(\mathbf{r}', t')] | \Psi \rangle \rangle. \quad (6.25)$$

Since FMR measurements excite uniform precession we are interested primarily in the decay of the uniform mode, which has wavevector $\mathbf{q} = 0$. Therefore, it is useful to transform the spin response function from position-time space to wavevector-frequency space. The spin response at fixed wavelength is

$$\begin{aligned} \mathcal{S}_{ij}(\mathbf{q}; t, t') &= -\frac{i}{\hbar} \Theta(t - t') \int_{-\infty}^{\infty} d\mathbf{r} \int_{-\infty}^{\infty} d\mathbf{r}' e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \langle \langle \Psi | [\sigma_i(\mathbf{r}, t), \sigma_j(\mathbf{r}', t')] | \Psi \rangle \rangle \\ &= -\frac{i}{\hbar} \Theta(t - t') \left\langle \left\langle \Psi \left| \left[\int_{-\infty}^{\infty} d\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \sigma_i(\mathbf{r}, t), \int_{-\infty}^{\infty} d\mathbf{r}' e^{-i\mathbf{q} \cdot \mathbf{r}'} \sigma_j(\mathbf{r}', t') \right] \right| \Psi \right\rangle \right\rangle \\ &= -\frac{i}{\hbar} \Theta(t - t') \langle \langle \Psi | [\sigma_i(-\mathbf{q}, t), \sigma_j(\mathbf{q}, t')] | \Psi \rangle \rangle. \end{aligned} \quad (6.26)$$

Because our system remains in a steady state near equilibrium during the experiment the spin response function depends only on the time difference $\tau = t - t'$. The time-frequency transform then gives

$$\begin{aligned}\mathcal{S}_{ij}(\mathbf{q}; \omega) &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} d(t - t') e^{-i\omega(t-t')} \Theta(t - t') \langle \langle \Psi | [\sigma_i(-\mathbf{q}, t), \sigma_j(\mathbf{q}, t')] | \Psi \rangle \rangle \\ &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} \Theta(\tau) \langle \langle \Psi | [\sigma_i(-\mathbf{q}, \tau), \sigma_j(\mathbf{q}, 0)] | \Psi \rangle \rangle.\end{aligned}\quad (6.27)$$

Finally, we note that $\sigma(-\mathbf{q}, \tau) = \sigma^\dagger(\mathbf{q}, \tau)$. The expression for the susceptibility that we must now evaluate is

$$\mathcal{S}_{ij}(\mathbf{q}; \omega) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} \Theta(\tau) \left\langle \left\langle \Psi \left| [\sigma_i^\dagger(\mathbf{q}, \tau), \sigma_j(\mathbf{q}, 0)] \right| \Psi \right\rangle \right\rangle, \quad (6.28)$$

$$\chi_{ij}(\mathbf{q}; \omega) = -g^2 \mu_B^2 \mathcal{S}_{ij}(\mathbf{q}; \omega). \quad (6.29)$$

Torque Correlation Function

Equation 6.29 is the expression that we would like to evaluate, however we are not able to do so directly because the states $|\Psi\rangle$ are N-particle states, but our calculations return only single particle states $|\psi\rangle$ obtained within the independent particle approximation. These single particle states lack some of the correlations that exist in the N-particle states. For instance, the exchange field is held in the z-direction and does not track the magnetization precession. As the spins precess, this exchange field, which should track the spin direction, remains static. The spin response function will contain the unphysical very large real-valued frequency Δ corresponding to precession about this artificial exchange field. To work around this problem we begin by defining the independent particle transverse spin

response function

$$\mathcal{S}_0^\perp(\mathbf{q}; \omega) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle \langle \psi | [\sigma^-(\mathbf{q}, \tau), \sigma^+(\mathbf{q}, 0)] | \psi \rangle \rangle \quad (6.30)$$

and put the correlations back in with the appropriate self energy in a Dyson equation

$$\chi^\perp(\mathbf{q}; \omega) = -\hbar\omega_M \frac{\mathcal{S}_0^\perp(\mathbf{q}; \omega)}{1 + \Sigma_0^\perp(\mathbf{q}; \omega) \mathcal{S}^\perp(\mathbf{q}; \omega)}. \quad (6.31)$$

The frequency ω_M is $\mu_0\mu_B^2g^2/\hbar$ and the self energy $\Sigma^\perp(\mathbf{q}; \omega)$ is defined to make the equality true. Finding the self energy for the independent particle susceptibility is difficult. We will settle for a mean field approximation and set $\Sigma^\perp = \hbar\Delta/P$ where $P = -2\langle\sigma^z\rangle$ is the spin polarization and Δ is the exchange frequency. This approximation for the self energy shifts the resonant frequency of the single electron spins back down by the exchange field, removing the spurious high frequency precession, but does not contribute to the damping because it is real valued. As a reminder, the damping rate is found from the transverse susceptibility according to $\lambda = \omega_0^2 \lim_{\omega \rightarrow 0} \text{Im}[\chi^\perp(\omega)/\omega]$.

Evaluation of the independent particle spin response function is complicated for numerical reasons. The high frequency precession due to the static exchange field will swamp the much smaller imaginary damping frequency we are after. The solution to this situation is to separate the spin motion into the very fast precession about the exchange field and the damping torque caused by the spin-orbit interaction. When we take the imaginary part of the susceptibility the real valued exchange precession will be dropped and we will be left with the spin-orbit torque that we are after.

We begin by defining a general response function in both the time and frequency do-

mains

$$G(A(\tau), B(0)) = -i\Theta(\tau)\langle[A(\tau), B(0)]\rangle, \quad (6.32)$$

$$G(A, B; \omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(A(\tau), B(0)). \quad (6.33)$$

These expressions are true for any set of operators A and B . Specifically, the transverse spin response function is

$$G(\sigma^-(\tau), \sigma^+) = -i\Theta(\tau)\langle[\sigma^-(\tau), \sigma^+]\rangle, \quad (6.34)$$

$$G(\sigma^-, \sigma^+; \omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\sigma^-(\tau), \sigma^+). \quad (6.35)$$

To separate out the spin-orbit contribution to the spin response function we use the equation of motion technique. This begins with taking the derivative of the integrand of Eq. (6.35).

$$\begin{aligned} \frac{d}{d\tau} \{e^{i\omega\tau} G(\sigma^-(\tau), \sigma^+)\} &= i\omega e^{i\omega\tau} G(\sigma^-(\tau), \sigma^+) - ie^{i\omega\tau} \delta(\tau) \langle[\sigma^-(\tau), \sigma^+]\rangle \\ &\quad - ie^{i\omega\tau} \Theta(\tau) \langle[\sigma^-(\tau), \mathcal{H}]/i\hbar, \sigma^+\rangle. \end{aligned} \quad (6.36)$$

Since we wish to implicate the spin-orbit interaction in damping we separate the Hamiltonian into a spin polarized term $\mathcal{H}_{\text{sp}}$ and the spin-orbit interaction $\mathcal{H}_{\text{so}}$ in the last commutator. The spin polarized Hamiltonian does not cause any damping, but does induce precession at frequency Ω , which is the sum of the frequency ω_0 due to the applied field plus anisotropy field, and the frequency Δ originating from the fictitious exchange field. Thus, $[\sigma^-, \mathcal{H}_{\text{sp}}] = \hbar\Omega\sigma^-$. The commutator of the spin operator with the spin-orbit Hamiltonian is defined as the spin-orbit torque $\Gamma^- = [\sigma^-, \mathcal{H}_{\text{so}}]$. Therefore, the last commutator

in Eq. (6.36) contains two terms

$$\langle [[\sigma^-(\tau), \mathcal{H}]/i\hbar, \sigma^+] \rangle = -i\Omega \langle [\sigma^-(\tau), \sigma^+] \rangle - i \langle [\Gamma^-(\tau), \sigma^+] \rangle / \hbar. \quad (6.37)$$

Now we integrate Eq. (6.36)

$$\begin{aligned} \int_{-\infty}^{\infty} d\tau \frac{d}{d\tau} \{ e^{i\omega\tau} e^{-\delta\tau} G(\sigma^-(\tau), \sigma^+) \} &= e^{i\omega\tau} e^{-\delta\tau} G(\sigma^-(\tau), \sigma^+) \Big|_{-\infty}^{\infty} = 0 - 0 = 0. \\ i\omega \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\sigma^-(\tau), \sigma^+) &= i\omega G(\sigma^-, \sigma^+; \omega). \\ -i \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \delta(\tau) \langle [\sigma^-(\tau), \sigma^+] \rangle &= -i \langle [\sigma^-, \sigma^+] \rangle = -iP. \\ -i\Omega \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\sigma^-(\tau), \sigma^+) &= -i\Omega G(\sigma^-, \sigma^+; \omega). \\ -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) &= -i/\hbar G(\Gamma^-, \sigma^+; \omega). \end{aligned}$$

In the first term the extra factor $e^{-\delta\tau}$ has been added to make the integral converge. This captures the fact that eventually the oscillating field will be turned off. This factor is, of course, present in each term.

Combining these results according to Eq. (6.36) we find that we can write the spin response function in terms of a new response function

$$\begin{aligned} 0 &= i\omega G(\sigma^-, \sigma^+; \omega) - iP - i\Omega G(\sigma^-, \sigma^+; \omega) - i/\hbar G(\Gamma^-, \sigma^+; \omega) \\ (\omega - \Omega)G(\sigma^-, \sigma^+; \omega) &= P + G(\Gamma^-, \sigma^+; \omega)/\hbar. \end{aligned} \quad (6.38)$$

We now apply the same process to this new response function

$$\begin{aligned} \frac{d}{d\tau} \{ e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) \} &= i\omega e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) - ie^{i\omega\tau} \delta(\tau) \langle [\Gamma^-(\tau), \sigma^+] \rangle \\ &\quad - ie^{i\omega\tau} \Theta(\tau) \langle [\Gamma^-, [\sigma^+(-\tau), \mathcal{H}]/i\hbar] \rangle \end{aligned} \quad (6.39)$$

The last line above needs some justification, which is

$$\begin{aligned}
\frac{d}{d\tau} \langle |[\Gamma^-(\tau), \sigma^+] | \rangle &= \frac{d}{d\tau} \langle | \{ e^{i\mathcal{H}\tau/\hbar} \Gamma^- e^{-i\mathcal{H}\tau/\hbar} \sigma^+ - \sigma^+ e^{i\mathcal{H}\tau/\hbar} \Gamma^- e^{-i\mathcal{H}\tau/\hbar} \} | \rangle \\
&= \langle | \left\{ \frac{i}{\hbar} e^{i\mathcal{H}\tau/\hbar} \mathcal{H} \Gamma^- e^{-i\mathcal{H}\tau/\hbar} \sigma^+ - \frac{i}{\hbar} e^{i\mathcal{H}\tau/\hbar} \Gamma^- \mathcal{H} e^{-i\mathcal{H}\tau/\hbar} \sigma^+ \right. \\
&\quad \left. - \frac{i}{\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \mathcal{H} \Gamma^- e^{-i\mathcal{H}\tau/\hbar} + \frac{i}{\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \Gamma^- \mathcal{H} e^{-i\mathcal{H}\tau/\hbar} \right\} | \rangle \\
&= \frac{i}{\hbar} \langle | \{ \Gamma^- e^{-i\mathcal{H}\tau/\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \mathcal{H} - \Gamma^- \mathcal{H} e^{-i\mathcal{H}\tau/\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \\
&\quad - e^{-i\mathcal{H}\tau/\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \mathcal{H} \Gamma^- + \mathcal{H} e^{-i\mathcal{H}\tau/\hbar} \sigma^+ e^{i\mathcal{H}\tau/\hbar} \Gamma^- \} | \rangle \\
&= \frac{i}{\hbar} \langle | (\Gamma^- [\sigma^+(-\tau), \mathcal{H}] - [\sigma^+(-\tau), \mathcal{H}] \Gamma^-) | \rangle \\
&= \frac{i}{\hbar} \langle | [\Gamma^-, [\sigma^+(-\tau), \mathcal{H}]] | \rangle . \tag{6.40}
\end{aligned}$$

Within the expectation value the operators may be cycled without changing the result.

Considering the last commutator in Eq. (6.39), we again separate $\mathcal{H}$ into $\mathcal{H}_{\text{sp}}$ and $\mathcal{H}_{\text{so}}$. The two resulting commutators for the spin operator are $[\sigma^+, \mathcal{H}_{\text{sp}}] = -\hbar\Omega\sigma^+$ and $[\sigma^+, \mathcal{H}_{\text{so}}] = -\Gamma^+$. These give the result that

$$\langle [\Gamma^-, [\sigma^+(-\tau), \mathcal{H}]] / i\hbar \rangle = -i\Omega \langle [\Gamma^-(\tau), \sigma^+] \rangle - i \langle [\Gamma^-(\tau), \Gamma^+] \rangle / \hbar . \tag{6.41}$$

The integral of Eq. (6.39) is

$$\begin{aligned}
\int_{-\infty}^{\infty} d\tau \frac{d}{d\tau} \{ e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) \} &= e^{i\omega\tau} e^{-\delta\tau} G(\Gamma^-(\tau), \sigma^+) \Big|_{-\infty}^{\infty} = 0 - 0 = 0 \\
i\omega \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) &= i\omega G(\Gamma^-, \sigma^+; \omega) \\
-i \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \delta(\tau) \langle [\Gamma^-(\tau), \sigma^+] \rangle &= -i \langle [\Gamma^-, \sigma^+] \rangle = -iQ \\
-i\Omega \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\Gamma^-(\tau), \sigma^+) &= -i\Omega G(\Gamma^-, \sigma^+; \omega) \\
-i \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\Gamma^-(\tau), \Gamma^+) &= -iG(\Gamma^-, \Gamma^+; \omega) / \hbar
\end{aligned}$$

With these results we can write the new response function in terms of the torque response function

$$\begin{aligned} 0 &= i\omega G(\Gamma^-, \sigma^+; \omega) - iQ - i\Omega G(\Gamma^-, \sigma^+; \omega) - i/\hbar G(\Gamma^-, \Gamma^+; \omega) \\ (\omega - \Omega)G(\Gamma^-, \sigma^+; \omega) &= Q + G(\Gamma^-, \Gamma^+; \omega)/\hbar. \end{aligned} \quad (6.42)$$

The commutator $Q = \langle [\Gamma^-, \sigma^+] \rangle = 0$. With the results Eq. (6.38) and Eq. (6.42) we can write the spin correlation function in terms of the torque correlation function

$$\begin{aligned} \hbar^2(\omega - \Omega)^2 G(\sigma^-, \sigma^+; \omega) &= \hbar(\omega - \Omega)P + \hbar(\omega - \Omega)G(\Gamma^-, \sigma^+; \omega) \\ &= \hbar(\omega - \Omega)P + G(\Gamma^-, \Gamma^+; \omega) \\ G(\sigma^-, \sigma^+; \omega) &= \frac{P}{\hbar(\omega - \Omega)} + \frac{G(\Gamma^-, \Gamma^+; \omega)}{\hbar^2(\omega - \Omega)^2} \\ \mathcal{S}(\omega) &= \frac{P}{\hbar(\omega - \Omega)} + \frac{\mathcal{F}(\omega)}{\hbar^2(\omega - \Omega)^2} \end{aligned} \quad (6.43)$$

In the last line we have defined the torque correlation function as $\mathcal{F}(\omega) = G(\Gamma^-, \Gamma^+; \omega)$.

Having converted the spin response function to a torque response function we can now return to the susceptibility, Eq. (6.29). With the result of Eq. (6.43) the susceptibility becomes

$$\begin{aligned} \chi_{\perp}(\omega) &= -\hbar\omega_M \frac{\frac{P}{\hbar(\omega - \Omega)} + \frac{\mathcal{F}(\omega)}{\hbar^2(\omega - \Omega)^2}}{1 + \hbar\Delta/P \left\{ \frac{P}{\hbar(\omega - \Omega)} + \frac{\mathcal{F}(\omega)}{\hbar^2(\omega - \Omega)^2} \right\}} \\ &= -\hbar\omega_M \frac{\hbar(\omega - \Omega)P + \mathcal{F}(\omega)}{\hbar^2(\omega - \Omega)^2 + \hbar^2(\omega - \Omega)\Delta + \hbar\Delta/P \mathcal{F}(\omega)}. \end{aligned} \quad (6.44)$$

We now take the imaginary part of this expression

$$\text{Im } \chi_{\perp}(\omega) = \frac{-\hbar\omega_M \text{Im } \mathcal{F}(\omega)}{\hbar^2(\omega - \Omega + \Delta)^2 + 2\hbar\Delta/P \frac{(\omega - \Omega + \Delta)}{(\omega - \Omega)} \text{Re } \mathcal{F}(\omega) + \Delta^2/P^2 \frac{|\mathcal{F}(\omega)|^2}{(\omega - \Omega)^2}}. \quad (6.45)$$

Next we divide this expression by ω and take the limit that $\omega \rightarrow 0$. Since the spin-orbit torque vanishes as the spin motion ceases, the torque response function goes to zero in the limit that the frequency goes to zero. Therefore, we have

$$\lim_{\omega \rightarrow 0} \text{Im } \chi_{\perp}(\omega)/\omega = -\hbar\omega_M \frac{\lim_{\omega \rightarrow 0} \text{Im } \mathcal{F}(\omega)/\omega}{\hbar^2(\Delta - \Omega)^2}. \quad (6.46)$$

In the denominator $\Omega - \Delta = \omega_0$ so the damping rate is

$$\lambda = \omega_0^2 \lim_{\omega \rightarrow 0} \chi^{\perp}(\omega)/\omega = -\omega_M \lim_{\omega \rightarrow 0} \text{Im } \mathcal{F}(\omega)/\hbar\omega. \quad (6.47)$$

Evaluation of the Correlation Function

The torque correlation function is

$$\mathcal{F}(\omega) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \Theta(\tau) \langle \langle \psi | [\Gamma^-(\tau), \Gamma^+(0)] | \psi \rangle \rangle. \quad (6.48)$$

The outer angled brackets indicate a summation over the single particle states weighted by the Fermi-Dirac distribution

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \int_0^{\infty} d\tau e^{i\omega\tau} \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} f(\epsilon_{nk}) \\ & \times \{ \langle \psi_{nk} | \Gamma^-(\mathbf{q}, \tau) \Gamma^+(\mathbf{q}, 0) | \psi_{nk} \rangle - \langle \psi_{nk} | \Gamma^+(\mathbf{q}, 0) \Gamma^-(\mathbf{q}, \tau) | \psi_{nk} \rangle \} \end{aligned} \quad (6.49)$$

We insert another set of states

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \int_0^{\infty} d\tau e^{i\omega\tau} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} f(\epsilon_{nk}) \\ & \times \{ \langle \psi_{nk} | \Gamma^-(\mathbf{q}, \tau) | \psi_{mk'} \rangle \langle \psi_{mk'} | \Gamma^+(\mathbf{q}, 0) | \psi_{nk} \rangle \\ & - \langle \psi_{nk} | \Gamma^+(\mathbf{q}, 0) | \psi_{mk'} \rangle \langle \psi_{mk'} | \Gamma^-(\mathbf{q}, \tau) | \psi_{nk} \rangle \} \end{aligned} \quad (6.50)$$

and switch the indices in the second term

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \int_0^\infty d\tau e^{i\omega\tau} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} [f(\epsilon_{nk}) - f(\epsilon_{mk'})] \\ & \times \langle \psi_{nk} | e^{i\mathcal{H}\tau/\hbar} \Gamma^-(\mathbf{q}) e^{-i\mathcal{H}\tau/\hbar} | \psi_{mk'} \rangle \langle \psi_{mk'} | \Gamma^+(\mathbf{q}) | \psi_{nk} \rangle . \end{aligned} \quad (6.51)$$

We now act with the Hamiltonian operators

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \int_0^\infty d\tau e^{i\omega\tau} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} [f(\epsilon_{nk}) - f(\epsilon_{mk'})] \\ & \times |\langle \psi_{nk} | \Gamma^-(\mathbf{q}) | \psi_{mk'} \rangle|^2 e^{i\tilde{\omega}_{nk}\tau} e^{-i\tilde{\omega}_{mk'}\tau} . \end{aligned} \quad (6.52)$$

We can condense this a little with the shorthand notation

$$|\langle \psi_{nk} | \Gamma^-(\mathbf{q}) | \psi_{mk'} \rangle|^2 = |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 . \quad (6.53)$$

The torque correlation function is then

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} [f(\epsilon_{nk}) - f(\epsilon_{mk'})] \\ & \times |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_0^\infty d\tau e^{i\omega\tau} e^{i(\tilde{\omega}_{nk} - \tilde{\omega}_{mk'})\tau} . \end{aligned} \quad (6.54)$$

The states ψ_{nk} are single particle eigenstates for the perfect crystal systems at zero temperature. To incorporate the reality that measured samples are neither perfect crystals nor are they at zero temperature, we push the ideal eigenenergies $\hbar\omega_{nk}$ off the real axis making them complex valued. The imaginary part of the energies constitute decay terms that reflect the fact that scattering occurs between different states (true eigenstates would have infinite lifetimes and not undergo any scattering). We write the imaginary frequencies as $\tilde{\omega} = \omega + i\gamma/\hbar$ where γ is the scattering rate.

Before doing the τ integral we make a variable transformation for the two state energies, changing their complex values $\tilde{\omega}$ to real frequencies ω' via

$$e^{i\tilde{\omega}\tau} = \int_{-\infty}^{\infty} d\hbar\omega' \delta(\hbar\omega' - \hbar\tilde{\omega}) e^{i\omega'\tau}. \quad (6.55)$$

The principle part of the above integral gives a Lorentzian weighting function for the single particle propagator

$$\text{P} \int_{-\infty}^{\infty} d\hbar\omega' \delta(\hbar\omega' - \hbar\tilde{\omega}) e^{i\omega'\tau} = \int_{-\infty}^{\infty} d\hbar\omega' A_{\omega'}(\hbar\tilde{\omega}) e^{i\omega'\tau} \quad (6.56)$$

where the Lorentzian spectral function $A_{\omega'}(\hbar\tilde{\omega})$ is

$$A_{\omega'}(\hbar\tilde{\omega}) = \frac{1}{\pi} \frac{\gamma}{\hbar^2(\omega' - \omega)^2 + \gamma^2}. \quad (6.57)$$

With these substitutions the torque correlation function becomes

$$\begin{aligned} \mathcal{F}(\mathbf{q}; \omega) = & -\frac{i}{\hbar} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_0^{\infty} d\tau \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \\ & \times [f(\epsilon_1) - f(\epsilon_2)] A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) e^{i(\hbar\omega + \epsilon_1 - \epsilon_2)\tau/\hbar} e^{-\delta\tau/\hbar}. \end{aligned} \quad (6.58)$$

As discussed earlier, the decaying exponential term has been added to the driving frequency

ω so that the integral will converge. At this point we do the time integration to get

$$\begin{aligned}
\mathcal{F}(\mathbf{q}; \omega) &= -\frac{i}{\hbar} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \\
&\quad \times [f(\epsilon_1) - f(\epsilon_2)] A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) \frac{-\hbar}{i(\hbar\omega + \epsilon_1 - \epsilon_2) - \delta} \\
&= \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \\
&\quad \times [f(\epsilon_1) - f(\epsilon_2)] A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) \frac{1}{(\hbar\omega + \epsilon_1 - \epsilon_2) + i\delta}. \quad (6.59)
\end{aligned}$$

Recalling Eq. (6.47), that the damping rate depends on the imaginary part of the torque correlation function, we now take the imaginary part of the above expression. The only imaginary part is the infinitesimal energy in the denominator. When we take the imaginary part this will leave a delta function on the energy difference of the scattering products.

$$\begin{aligned}
\text{Im } \mathcal{F}(\mathbf{q}; \omega) &= \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \\
&\quad \times [f(\epsilon_1) - f(\epsilon_2)] A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) [-\pi\delta(\hbar\omega + \epsilon_1 - \epsilon_2)] \\
&= -\pi \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_{-\infty}^{\infty} d\epsilon_1 \\
&\quad \times [f(\epsilon_1) - f(\epsilon_1 + \hbar\omega)] A_{nk}(\epsilon_1) A_{mk'}(\epsilon_1 + \hbar\omega). \quad (6.60)
\end{aligned}$$

Again, in accordance with our expression for the damping rate Eq. (6.47), we now divide by ω and take the limit of $\omega \rightarrow 0$. The important contribution is

$$\lim_{\omega \rightarrow 0} \frac{f(\epsilon_1) - f(\epsilon_1 + \hbar\omega)}{\hbar\omega} = -\frac{\partial f}{\partial \epsilon_1} = \eta(\epsilon_1). \quad (6.61)$$

The η function is essentially a positive delta function at the Fermi energy. We are left with

$$\lambda = \pi \frac{\mu_0 \mu_B^2 g^2}{\hbar} \sum_{nm} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k}, \mathbf{q})|^2 \int_{-\infty}^{\infty} d\epsilon_1 \eta(\epsilon_1) A_{nk}(\epsilon_1) A_{mk'}(\epsilon_1). \quad (6.62)$$

Both terms with $m = n$ and with $m \neq n$ exist in this result. Since n and m are band indices the terms for which $m = n$ are referred to as the intraband terms and those with $m \neq n$ are called interband terms. When a magnon decays an electron-hole pair is created; these labels indicate whether the electron-hole pair exists within a single band (intraband) or is spread over two bands (interband).

Review of Approximations

In deriving the damping rate we have made several approximations that should be kept in mind. We have restricted our study to simplest case of the decay of small amplitude uniform oscillations in single element bulk materials. These conditions simplified the expression for the susceptibility obtained from the LLG equation. Terms beyond first order in the transverse magnetization were dropped, which also removed any effects of the demagnetizing field. A further simplification was made when we assumed that the damping rate was small compared to the precession frequency ($\lambda \ll |\gamma| M_s$). This last assumption is easily met for the materials we studied; $\alpha_{Ni} \approx 10^{-2}$ and $\alpha_{Fe,Co} \approx 10^{-3}$. Even for materials such as permalloy $\alpha \approx 0.02$, which is still small compared to 1.

We have assumed that the perturbed N-particles states may be expressed in terms of the unperturbed N-particle states by $|\Psi'(-\infty)\rangle = |\Psi(0)\rangle$. The assumption here is that the ground states of the perturbed system may be obtained by adiabatically adjusting the unperturbed ground states. It is not clear that this condition would be satisfied in pulsed measurements. Next, we truncated the infinite series expansion for the time evolution operator after the first order to obtain the Kubo formula. This approximation is appropriate in

the limit that the the rf field is much smaller than the other fields, such as the applied dc field and the internal fields. This will be a safe approximation for typical FMR measurements, but would not be satisfied when the applied field is sufficient to switch the magnetization. We have further assumed that the frequency ω of the applied field (about 10^{10} s^{-1}) is very small compared to the electron-lattice scattering rate (roughly 10^{14} s^{-1}). This assumption holds for rf measurements even when samples are very pure and cold (perhaps a scattering rate of only 10^{13} s^{-1}). The additional assumption was made that $\hbar\omega \ll k_B T$, but this condition could be violated when both the frequency is high $\omega \approx 100 \text{ GHz}$ and the temperature is low $T \leq 10 \text{ K}$.

We have assumed that the magnetization is due entirely to the electron spins, neglecting the orbital component of the magnetization. This approximation occurs when we replace the commutator $[m^-(\tau), m^+(0)]$ with the commutator $g^2 \mu_B^2 [\sigma^-(\tau), \sigma^+]$. The commutator is really $\mu_B^2 [(\ell^- + 2\sigma^-)(\tau), (\ell^+ + 2\sigma^+)(0)]$, but since the orbital momentum is nearly quenched in metallic systems it is typically safe to approximate $\ell + 2\sigma \approx g\sigma$ with g close to 2. This neglects the component of the orbital momentum that is transverse to the spin momentum. A more thorough derivation of the damping rate would include the $[\ell^-(\tau), \sigma^+]$ and $[\sigma^-(\tau), \ell^+]$ terms.

In transforming the spin response function from the space-time domain to the wavevector-frequency domain we make two assumptions. First, that the sample is globally uniform so that the spin response function depends only on the distance between the two spins and not on their absolute positions. This assumption would not be appropriate in lower dimensional systems when surfaces and edges break translational symmetry. Second, we assume that the difference in environments seen by the spins at times t and t' is independent of the absolute time t . This assumption is appropriate for steady-state situations, such as occur during FMR. For pulsed techniques such as PIMM and MOKE one would have to assess how small $t - t'$ is compared to the time scales of the experiment.

The Resistivity

In the previous section we developed the torque-correlation model that describes the precession damping that results from the spin-orbit interaction. We expressed the damping rate as a function of the electron-lattice scattering rate. Unfortunately, the scattering rate is difficult to pin down experimentally, so it acts nearly as a free parameter. On the other hand, measurements of the damping rate have been made as a function of temperature. While the scattering rate is a function of temperature, the scattering rate of a given sample at a given temperature is typically not known very well. Therefore, it is not possible to simply overlay the calculated damping curves upon the measured curves to look for agreement. The most we can do is compare the minimal damping rates of the calculated and measured curves. This comparison produced satisfying agreement as seen in section 4.1. To present our calculations such that they may be compared in full to measured data we calculated the resistivity in section 4.2. In the following we derive the expression for the resistivity.

The Kubo Formula

The conductivity σ is defined as the tensor that converts electric field $\mathbf{E}$ to current density $\mathbf{j}$

$$j_{\mu}(\mathbf{r}, t) = \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \sum_{\nu} \sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') E_{\nu}(\mathbf{r}', t'). \quad (6.63)$$

The derivation of the conductivity will largely parallel that of the susceptibility, except that in this case we will be spared any acrobatics associated with conversions between

correlation functions. The current density is

$$\begin{aligned}
\langle j_\mu(\mathbf{r}, t) \rangle &= \left\langle \left\langle \hat{\Psi}'(t) \left| \hat{j}_\mu(\mathbf{r}, t) \right| \hat{\Psi}'(t) \right\rangle \right\rangle \\
&= \left\langle \left\langle \hat{\Psi}'(-\infty) \left| U^\dagger(t, -\infty) \hat{j}_\mu(\mathbf{r}, t) U(t, -\infty) \right| \hat{\Psi}'(-\infty) \right\rangle \right\rangle \\
&= \left\langle \left\langle \hat{\Psi}(0) \left| U^\dagger(t, -\infty) \hat{j}_\mu(\mathbf{r}, t) U(t, -\infty) \right| \hat{\Psi}(0) \right\rangle \right\rangle . \tag{6.64}
\end{aligned}$$

Again we have converted between the complete set of states $|\Psi'\rangle$ for the Hamiltonian that includes the perturbation $\mathcal{V}$ and the eigenstates $|\Psi\rangle$ of the Hamiltonian in the absence of the external electric field. As before, we assume that $|\Psi'(-\infty)\rangle = |\Psi(0)\rangle$ and write $|\Psi(0)\rangle = |\Psi\rangle$. To first order the time evolution operator is

$$U(t, -\infty) \approx 1 - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \hat{\mathcal{V}}(\mathbf{r}', t'). \tag{6.65}$$

The current density may also be expressed as a commutator in a Kubo formula

$$\begin{aligned}
\langle j_\mu(\mathbf{r}, t) \rangle &= \left\langle \left\langle \hat{\Psi} \left| \left(1 + \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \hat{\mathcal{V}}(\mathbf{r}', t') \right) \hat{j}_\mu(\mathbf{r}, t) \right. \right. \\
&\quad \left. \left(1 - \frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \hat{\mathcal{V}}(\mathbf{r}', t') \right) \hat{\Psi} \right\rangle \right\rangle \\
&\approx -\frac{i}{\hbar} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \left\langle \left\langle \Psi \left| [\hat{j}_\mu(\mathbf{r}, t), \hat{\mathcal{V}}(\mathbf{r}', t')] \right| \Psi \right\rangle \right\rangle . \tag{6.66}
\end{aligned}$$

The equilibrium current $\langle \Psi | j_\mu | \Psi \rangle$ is of course zero in the absence of any field. The perturbation is

$$\hat{\mathcal{V}}(\mathbf{r}', t') = -\frac{1}{c} \hat{\mathbf{j}}(\mathbf{r}', t') \cdot \hat{\mathbf{A}}(\mathbf{r}', t') = \frac{i}{\omega} \hat{\mathbf{j}}(\mathbf{r}', t') \cdot \hat{\mathbf{E}}(\mathbf{r}', t') \tag{6.67}$$

so that the current density

$$\langle j_\mu(\mathbf{r}, t) \rangle = -\frac{i}{\hbar} \frac{i}{\omega} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \sum_\nu \left\langle \left\langle \Psi \left| [\hat{j}_\mu(\mathbf{r}, t), \hat{j}_\nu(\mathbf{r}', t') \hat{E}_\nu(\mathbf{r}', t')] \right| \Psi \right\rangle \right\rangle \tag{6.68}$$

can now be expressed in terms of the current correlation function

$$\langle j_\mu(\mathbf{r}, t) \rangle = \frac{i}{\hbar\omega} \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\mathbf{r}' \sum_{\nu} \zeta_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') E_\nu(\mathbf{r}', t') \quad (6.69)$$

which is

$$\zeta_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') = -\frac{i}{\hbar} \Theta(t - t') \left\langle \left\langle \Psi \left| [\hat{j}_\mu(\mathbf{r}, t), \hat{j}_\nu(\mathbf{r}', t')] \right| \Psi \right\rangle \right\rangle. \quad (6.70)$$

Comparing the two expressions for the current density Eq. (6.63) and Eq. (6.69) we find

$$\begin{aligned} \int_{-\infty}^t dt' \int_{-\infty}^{\infty} d\mathbf{r}' \sum_{\nu} \sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') E_\nu(\mathbf{r}', t') \\ = \frac{i}{\omega} \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\mathbf{r}' \sum_{\nu} \zeta_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') E_\nu(\mathbf{r}', t') \end{aligned} \quad (6.71)$$

and that the conductivity is

$$\sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t') = \frac{i}{\omega} \zeta_{\mu\nu}(\mathbf{r}, \mathbf{r}'; t, t'). \quad (6.72)$$

It is again useful to transform from position-time space to wavevector-frequency space. The response at fixed wavelength is found from Fourier transforming over the position variables

$$\begin{aligned} \zeta_{\mu\nu}(\mathbf{q}; t, t') &= -\frac{i}{\hbar} \Theta(t - t') \int_{-\infty}^{\infty} d\mathbf{r} \int_{-\infty}^{\infty} d\mathbf{r}' e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \left\langle \left\langle \Psi \left| [\hat{j}_\mu(\mathbf{r}, t), \hat{j}_\nu(\mathbf{r}', t')] \right| \Psi \right\rangle \right\rangle \\ &= -\frac{i}{\hbar} \Theta(t - t') \left\langle \left\langle \Psi \left| \left[\int_{-\infty}^{\infty} d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} \hat{j}_\mu(\mathbf{r}, t), \int_{-\infty}^{\infty} d\mathbf{r}' e^{i\mathbf{q} \cdot \mathbf{r}'} \hat{j}_\nu(\mathbf{r}', t') \right] \right| \Psi \right\rangle \right\rangle \\ &= -\frac{i}{\hbar} \Theta(t - t') \left\langle \left\langle \Psi \left| [\hat{j}_\mu(-\mathbf{q}, t), \hat{j}_\nu(\mathbf{q}, t')] \right| \Psi \right\rangle \right\rangle. \end{aligned} \quad (6.73)$$

The time-frequency transform also proceeds as in the case of the susceptibility.

$$\begin{aligned}
\zeta_{\mu\nu}(\mathbf{q}; \omega) &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} d(t-t') e^{-i\omega(t-t')} \Theta(t-t') \left\langle \left\langle \Psi \left| [\hat{j}_{\mu}(-\mathbf{q}, t), \hat{j}_{\nu}(\mathbf{q}, t')] \right| \Psi \right\rangle \right\rangle \\
&= -\frac{i}{\hbar} \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} \Theta(\tau) \left\langle \left\langle \Psi \left| [\hat{j}_{\mu}(-\mathbf{q}, \tau), \hat{j}_{\nu}(\mathbf{q}, 0)] \right| \Psi \right\rangle \right\rangle \\
&= -\frac{i}{\hbar} \int_0^{\infty} d\tau e^{-i\omega\tau} \left\langle \left\langle \Psi \left| [\hat{j}_{\mu}^{\dagger}(\mathbf{q}, \tau), \hat{j}_{\nu}(\mathbf{q}, 0)] \right| \Psi \right\rangle \right\rangle . \tag{6.74}
\end{aligned}$$

For the case of the susceptibility, switching from the N-particle states $|\Psi\rangle$ to the single particle states $|\psi\rangle$ was complicated because the spins of a ferromagnet constitute a highly correlated system. Therefore, it was necessary to build in a self energy for these interactions when we shifted to the single particle states. If we assume that the dominant source of resistive scattering is electron-lattice than electron-electron then the electron correlations are not as significant a problem for the case of the current. In this case it will be a reasonable approximation to just replace the N-particle states with the single particle states. We can then evaluate the current correlation function just as we evaluated the torque correlation function in the previous chapter. We first expand the commutator

$$\begin{aligned}
\zeta_{\mu\nu}(\mathbf{q}, \omega) &= -\frac{i}{\hbar} \int_0^{\infty} d\tau e^{-i\omega\tau} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} f(\epsilon_{n,k}) \\
&\quad \times \left\{ \left\langle \psi_{nk} \left| \hat{j}_{\mu}^{\dagger}(\mathbf{q}, \tau) \right| \psi_{mk'} \right\rangle \left\langle \psi_{mk'} \left| \hat{j}_{\nu}(\mathbf{q}, 0) \right| \psi_{nk} \right\rangle \right. \\
&\quad \left. - \left\langle \psi_{nk} \left| \hat{j}_{\nu}(\mathbf{q}, 0) \right| \psi_{mk'} \right\rangle \left\langle \psi_{mk'} \left| \hat{j}_{\mu}^{\dagger}(\mathbf{q}, \tau) \right| \psi_{nk} \right\rangle \right\} . \tag{6.75}
\end{aligned}$$

Then switch the band indices in the second term

$$\begin{aligned}
\zeta_{\mu\nu}(\mathbf{q}, \omega) &= -\frac{i}{\hbar} \int_0^{\infty} d\tau e^{-i\omega\tau} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} [f(\epsilon_{n,k}) - f(\epsilon_{m,k'})] \\
&\quad \times \left\langle \psi_{nk} \left| e^{iH\tau/\hbar} \hat{j}_{\mu}^{\dagger}(\mathbf{q}) e^{-iH\tau/\hbar} \right| \psi_{mk'} \right\rangle \left\langle \psi_{mk'} \left| \hat{j}_{\nu}(\mathbf{q}) \right| \psi_{nk} \right\rangle \tag{6.76}
\end{aligned}$$

and act on the states with the exponential operators

$$\begin{aligned} \zeta_{\mu\nu}(\mathbf{q}, \omega) = & -\frac{i}{\hbar} \int_0^\infty d\tau e^{-i\omega\tau} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \\ & \times \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) [f(\epsilon_{n,k}) - f(\epsilon_{m,k'})] e^{i\tilde{\omega}_{nk}\tau} e^{-i\tilde{\omega}_{mk'}\tau}. \end{aligned} \quad (6.77)$$

We have introduced the shorthand $\mathcal{J}_{nm}^\mu(k, k') = \langle \psi_{nk} | j_\mu | \psi_{mk'} \rangle$ for the matrix elements.

The single particle energies are complex, but may be expressed as an integration over a real valued energy weighted by spectral functions.

$$\begin{aligned} \zeta_{\mu\nu}(\mathbf{q}, \omega) = & -\frac{i}{\hbar} \int_0^\infty d\tau e^{-i\omega\tau} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) \int d\epsilon_1 \int d\epsilon_2 \\ & \times A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) [f(\epsilon_1) - f(\epsilon_2)] e^{i\epsilon_1\tau/\hbar} e^{-i\epsilon_2\tau/\hbar}. \end{aligned} \quad (6.78)$$

The τ integration is performed by adding an infinitesimal decaying piece δ to the frequency ω giving

$$\begin{aligned} \zeta_{\mu\nu}(\mathbf{q}, \omega) = & -\frac{i}{\hbar} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) \int d\epsilon_1 \int d\epsilon_2 \\ & \times A_{nk}(\epsilon_1) A_{mk'}(\epsilon_2) [f(\epsilon_1) - f(\epsilon_2)] \frac{-1}{i(\hbar\omega + \epsilon_1 - \epsilon_2) - \delta}. \end{aligned} \quad (6.79)$$

Measurement probes the real part of the conductivity, which from Eq. (6.72) is $-\text{Im } \zeta / \omega$.

Taking the imaginary part of the current correlation function introduces a delta function

$$\begin{aligned} \text{Re} [\sigma(\omega)] = & \frac{\hbar\pi}{\hbar\omega} \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) \int d\epsilon_1 \int d\epsilon_2 \\ & \times A_{n,k}(\epsilon_1) A_{m,k'}(\epsilon_2) [f(\epsilon_1) - f(\epsilon_2)] \delta(\hbar\omega + \epsilon_1 - \epsilon_2) \end{aligned} \quad (6.80)$$

which may be integrated over to leave

$$\begin{aligned} \text{Re}[\sigma(\omega)] &= \hbar\pi \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) \\ &\times \int d\epsilon_1 A_{n,k}(\epsilon_1) A_{m,k'}(\epsilon_1 + \hbar\omega) \frac{[f(\epsilon_1) - f(\epsilon_1 + \hbar\omega)]}{\hbar\omega}. \end{aligned} \quad (6.81)$$

For the dc conductivity we take the limit that ω goes to zero

$$\begin{aligned} \lim_{\omega \rightarrow 0} \text{Re}[\sigma(\omega)] &= \hbar\pi \sum_{nm} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \mathcal{J}_{nm}^{\mu\dagger}(k, k') \mathcal{J}_{mn}^\nu(k', k) \\ &\times \int d\epsilon_1 A_{n,k}(\epsilon_1) A_{m,k'}(\epsilon_1) \eta(\epsilon_1). \end{aligned} \quad (6.82)$$

The function η is the derivative of the Fermi distribution as before. In the limit that $q = 0$ the wavevectors k and k' must be equal and the matrix elements become

$$|\mathcal{J}_{nm}^{\mu\nu}(k, k')|^2 = \left(\frac{e}{\hbar}\right)^2 \left(\frac{\partial \epsilon_{mk'}}{\partial k_\mu}\right) \left(\frac{\partial \epsilon_{nk}}{\partial k_\nu}\right) \delta_{mn} \delta_{kk'}. \quad (6.83)$$

The delta function on the band indices is present because the dc field will not induce transitions between bands. This simplifies the result by eliminating the interband terms.

$$\lim_{\omega \rightarrow 0} \text{Re}[\sigma(\omega)] = \hbar\pi \left(\frac{e}{\hbar}\right)^2 \sum_n \int \frac{d^3k}{(2\pi)^3} \left(\frac{\partial \epsilon_{nk}}{\partial k_\mu}\right) \left(\frac{\partial \epsilon_{nk}}{\partial k_\nu}\right) \int d\epsilon_1 A_{n,k}^2(\epsilon_1) \eta(\epsilon_1). \quad (6.84)$$

For the cubic systems Fe and Ni the conductivity is diagonal in the basis aligned with the cubic axes. Further, the conductivity is symmetric with respect to x , y , and z . Therefore, it is sufficient to calculate $\lim_{\omega \rightarrow 0} \text{Re}[\sigma(\omega)]_{zz}$

$$\lim_{\omega \rightarrow 0} \text{Re}[\sigma(\omega)]_{zz} = \hbar\pi \left(\frac{e}{\hbar}\right)^2 \sum_n \int \frac{d^3k}{(2\pi)^3} \left(\frac{\partial \epsilon_{nk}}{\partial k_z}\right)^2 \int d\epsilon_1 \eta(\epsilon_1) A_{n,k}^2(\epsilon_1). \quad (6.85)$$

Calculating the zz -component of the conductivity is also sufficient for cobalt since our goal is just to parameterize out the scattering rate. The resistivity is $\rho = 1/\text{Re}[\sigma]$.

Review of Approximations

The primary assumption that we made while deriving the above expression for the resistivity is that electron-electron scattering is not significant. The Kubo formula approach we have taken uses the same physical concepts as the Boltzmann equation. Therefore, we expect our result to be appropriate under the same set of conditions for which the Boltzmann equation gives reasonable answers. Since the Boltzmann equation generally yields reasonable results for metals, the above expression should be satisfactory.

As with the susceptibility, the typical Kubo formula assumptions were made. We have assumed that the perturbed N -particles states may be expressed in terms of the unperturbed N -particle states by $|\Psi'(-\infty)\rangle = |\Psi(0)\rangle$. This assumes that the states of the perturbed system may be obtained by adiabatically adjusting the unperturbed states. Next, we truncated the infinite series expansion for the time evolution operator after the first order to obtain the Kubo formula. This approximation is appropriate in the limit that the Coulomb energy of the electrons with the applied field is small compared to the other energy terms in the system, such as the electron-electron and electron-nuclei terms. If the applied field becomes large, higher order terms may need to be included. One could test experimentally whether the induced current is linear in the applied field. We have further assumed that the applied field is dc, rather than ac. That is, the frequency ω of the applied field is very small, $\hbar\omega$ is a negligible energy and does not cause transitions between states.

We have taken a semi-classical approach to treating the applied electric field. Instead of calculating matrix elements for the current operators we instead calculate energy derivatives, the effective velocities of the electrons. This simplification is likely appropriate in

the dc limit, but would not be sufficient to treat ac fields.

A constant assumption throughout this document is that the samples we investigate are fully uniform in three dimensions. This assumption may become inappropriate for small device structures such as those used in magnetic recording media. We have also assumed that the electronic population of the systems remain near equilibrium. It is not clear that this approximation holds during complete magnetic reversals.

CHAPTER 7

NUMERICAL DETAILS

In this thesis I have presented the results of calculations of the precession damping rate and the electrical resistivity of iron, cobalt, and nickel. This appendix will discuss the linear augmented planewave (LAPW) implementation of the density functional theory (DFT) technique used to find the electronic structure of the three metals. We will also discuss a few computational routines added to evaluate the velocity and torque matrix elements, as well as perform the numerical integration over the spectral functions. Lastly, we will show the tests made to insure proper convergence of the calculations.

Numerical Methods

The two expressions that we evaluated in this work are

$$\lambda = \pi \frac{\mu_0 \mu_B^2 g^2}{\hbar} \sum_{nm} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} |\Gamma_{nm}^-(\mathbf{k})|^2 \int d\epsilon \eta(\epsilon) A_{nk}(\epsilon) A_{mk}(\epsilon), \quad (7.1)$$

$$\sigma = \pi \frac{e^2}{\hbar} \sum_n \int \frac{d^3 \mathbf{k}}{(2\pi)^3} |v_{nk}|^2 \int d\epsilon \eta(\epsilon) A_{nk}(\epsilon) A_{nk}(\epsilon). \quad (7.2)$$

Before evaluating these expressions it is necessary to first find the converged ground state electronic density for each metal. This task was accomplished prior to the start of this project [62]. Finding the ground state electronic density is the realm of density functional theory. DFT can be implemented in several ways; for transition metals the linear augmented planewave method works very well. The code that we use to obtain the ground state density was written by Don Hamann [64] and Mark Stiles [62], and uses the local density approximation (LDA). They have demonstrated that the code produces accurate results of the electronic structure for transition metals.

To evaluate the expressions (7.1 and 7.2) I modified the code of Hamann and Stiles. The program reads in a properly converged ground state density, from which it constructs the single electron wavefunctions, and obtains the eigenenergies and Fermi level. Either the electron velocities – for the resistivity – or the torque matrix elements – for the damping rate – are then evaluated. Finally, the energy integration over the spectral functions is performed. We will first very briefly and generally outline the LAPW/DFT code of Hamann and Stiles. Next, we will discuss the routines I wrote to evaluate the resistivity and damping rate. We will end by presenting some convergence tests for the numerical integrations.

The Existing Code

Density functional theory is based on the theorem of Hohenberg and Kohn [65] that states that the total energy of an interacting electron system subject to some potential is given exactly as a functional of the ground state electron density. This means that the energy does not depend on the details of the single electron wavefunctions, but only on the total electronic density. The important points are first that the electronic density that minimizes the total energy is the true ground state density of the system, and second that other ground state properties of the system can be found from this density. The whole trick, of course, is to find the correct ground state density.

For a given electronic density ρ , the energy of the system is

$$E[\rho] = T_e[\rho] + E_{ei}[\rho] + E_{ii}[\rho] + E_{ee}[\rho] . \quad (7.3)$$

$T_e[\rho]$ is the single particle kinetic energy, $E_{ei}[\rho]$ is the electron-ion Coulomb interaction, $E_{ii}[\rho]$ is the ion-ion Coulomb interaction, and $E_{ee}[\rho]$ contains all the electron many-body interactions. $E_{ee}[\rho]$ is the challenging energy term. It is typical to approximate the electron-electron interactions with the Hartree and exchange-correlation terms. Many codes, such as

the one we use, employ the local density approximation, which makes the approximation that the non-local exchange-correlation interaction should depend only on the local density. This approximation may be extended by including the gradient of the density within the generalized gradient approximation (GGA). However, the LDA often does well enough and the GGA sometimes even makes the results worse. Within the LDA, the electron-electron interactions are

$$E_H[\rho] = \frac{e^2}{2} \int d\mathbf{r} d\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (7.4)$$

$$E_{xc}[\rho] = \int d\mathbf{r} \rho(\mathbf{r}) \epsilon_{xc}(\rho(\mathbf{r})). \quad (7.5)$$

Due to the approximations made for the electron-electron energy terms, DFT codes do not find the true ground state density, but they typically come close enough to accurately calculate physical properties of interest.

Obtaining the ground state density is accomplished through the iterative process layed out by Kohn and Sham [66] and outlined in Fig.(7). An initial guess is made for the electronic density. This density is used to construct the potentials

$$V_H(\mathbf{r}) = e^2 \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (7.6)$$

$$V_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}. \quad (7.7)$$

A set of single particle wavefunctions is then obtained by solving the Kohn-Sham equations

$$\{T + V_{ei}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})\} \varphi_j(\mathbf{r}) = \epsilon_k \varphi_j(\mathbf{r}). \quad (7.8)$$

Once the single particle wavefunctions and eigenenergies are found a new density is con-

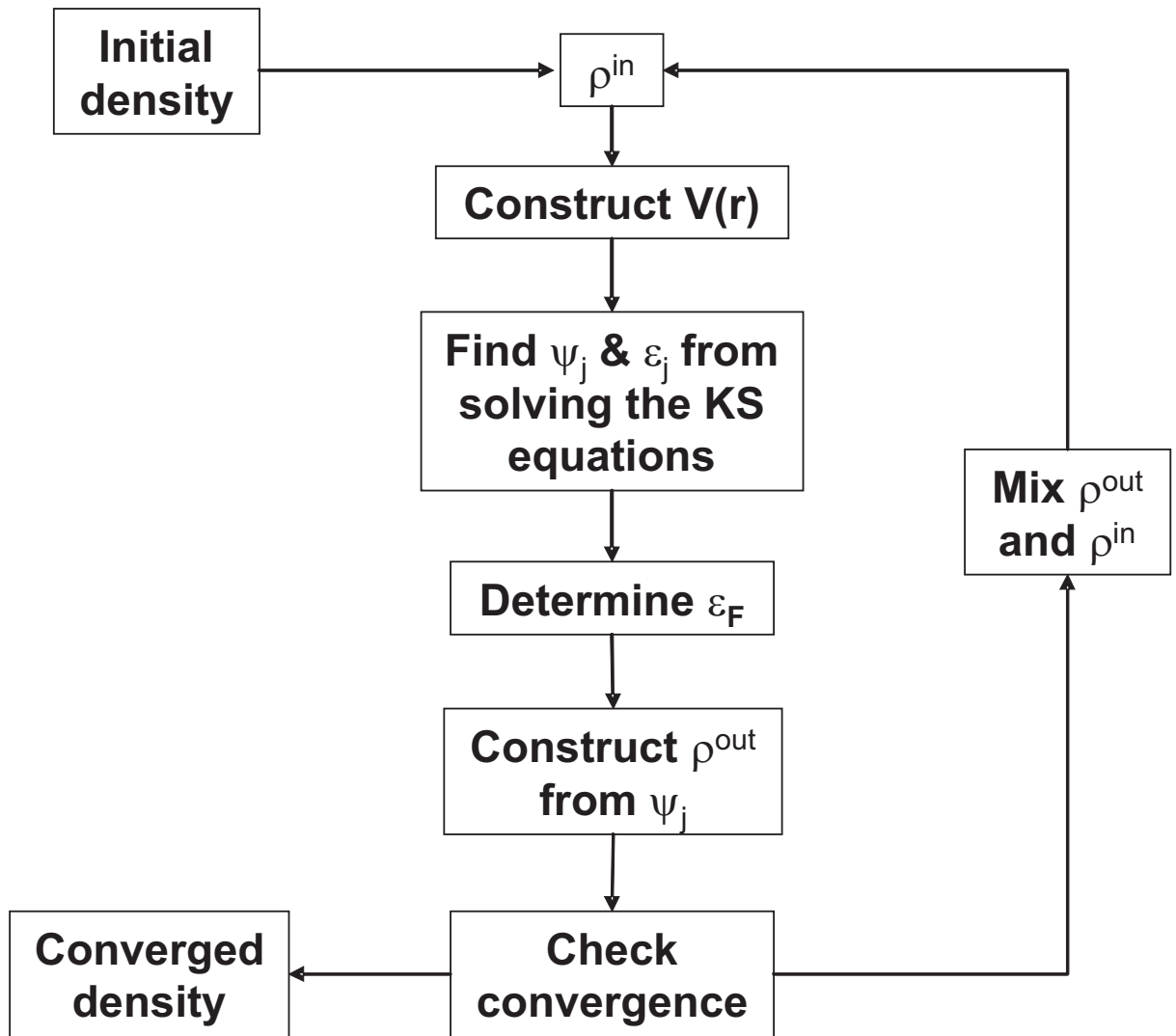


Figure 7.1: Density functional theory self consistency loop.

structed by summing the single particle densities of all the occupied states

$$\rho'(\mathbf{r}) = \sum_j \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}). \quad (7.9)$$

Only states with energies below the Fermi level are counted in the summation. If this new density differs significantly from the starting density then part of the new density is mixed with the old density and the process is reiterated until the density converges.

Within each self-consistency iteration of a DFT code the potentials in the Kohn-Sham equations must be constructed from the starting density, the Kohn-Sham equations must be solved, the Fermi level found, and the new density built from the occupied orbitals. Different DFT techniques, for example pseudopotential versus LAPW, use different basis sets and muffin tin potentials for the Kohn-Sham equations. The LAPW method divides space within the crystal into two regions: non-overlapping spheres centered on the nuclei (the muffin tins) and the interstitial region between these spheres. The interstitial region I uses a plane wave basis while the muffin tin spheres S use spherical harmonics

$$\psi_{\mathbf{k}}(\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} D_{\mathbf{G}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} & \mathbf{r} \in I \\ \sum_{lm} [A_{lm} u_l(\mathbf{r}) + B_{lm} \dot{u}_l(\mathbf{r})] Y_{lm}(\mathbf{r}) & \mathbf{r} \in S \end{cases} \quad (7.10)$$

Ω is the unit cell volume and $\mathbf{G}$ form a set of reciprocal lattice vectors. u_l solve the radial equations

$$\left\{ -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r) - E_l \right\} r u_l = 0 \quad (7.11)$$

and $\dot{u}_l$ is the energy derivative of u_l . A_{lm} and B_{lm} and $D_{\mathbf{G}}$ are expansion coefficients.

The augmented plane waves consist of the interstitial plane waves augmented by the

spherical harmonics inside the spheres, and the Kohn-Sham orbitals are linear combinations of these augmented plane waves

$$\varphi_j(\mathbf{r}) = \sum_k c_{jk} \psi_k(\mathbf{r}). \quad (7.12)$$

With this substitution the Kohn-Sham equation may be rewritten as

$$(\mathcal{H} - \epsilon_j \mathcal{S}) \mathbf{c}_j = 0. \quad (7.13)$$

$\mathcal{H}$ is the Hamiltonian on the left hand side of the Kohn-Sham equation (7.8), $\mathcal{S}$ is the overlap integral for the augmented plane waves, and $\mathbf{c}_j$ is the vector of coefficients c_{jk} . The Hartree and exchange-correlation potentials are constructed from the starting potential in terms of the augmented plane wave basis and the above secular equation is solved for the eigenenergies ϵ_j and eigenvectors $\mathbf{c}_j$.

For considerably more detail about the DFT and LAPW methods see [67] or [68]. More specifics about the code used in this work may be found in [64] and [62].

Evaluation of the Velocities

The code used in the present work reads in a density that has been converged to the ground state by the procedure outlined above. This density is then used to construct the single electron wavefunctions, and find the energies of the states and the Fermi level. The spin-orbit interaction is included in constructing the wavefunctions. The states are labeled by the interstitial wavevector $\mathbf{k}$. We define the velocity of each state as $(1/\hbar) \partial \epsilon_{nk} / \partial k_z$. The velocity is not necessarily isotropic. However, for our purpose, which is to relate the electron-lattice scattering time to a measurable resistivity, choosing one particular current direction is sufficient.

To evaluate the velocity of an electron state the energy of a particular $\mathbf{k}$ state was found, a very small addition δk was made to k_z , the energy was recalculated, and $\delta\epsilon/\delta k$ was computed. A test was made to ensure that the velocity $\delta\epsilon/\hbar\delta k$ was insensitive to small changes in the magnitude of δk for the particular δk that we used.

Construction of the Torque Matrix

The torque matrix elements are required to evaluate the damping rate. The torque operator is defined as $\Gamma^- = [\sigma^-, \mathcal{H}_{so}]$. The evaluation of the spin-orbit Hamiltonian $\mathcal{H}_{so}$ is described in [62], but we will briefly discuss it here. We use an independent electron approximation for the spin-orbit Hamiltonian writing $\mathcal{H}_{so} = \sum_i \xi_i \ell_i \cdot s_i$, where the spin orbit parameter is taken as

$$\xi_i = \frac{1}{2m^2c^2} \frac{1}{r_i} \frac{dV}{dr_i}, \quad (7.14)$$

$$\frac{dV}{dr_i} = -\frac{e^2}{4\pi\epsilon_0} \sum_j \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|^3}. \quad (7.15)$$

With $\ell = \mathbf{r} \times \mathbf{p}$ the spin-orbit interaction becomes

$$\mathcal{H}_{so} = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{2m^2c^2} \sum_{ij} \frac{(\mathbf{r}_i - \mathbf{r}_j) \times \mathbf{p}_i}{|\mathbf{r}_i - \mathbf{r}_j|^3} \cdot \frac{2\sigma_i}{\hbar}. \quad (7.16)$$

To write this as a functional of the density we introduce the number, momentum, and spin

densities

$$n(\mathbf{r}) = \sum_{i\mu} f_i \psi_{i\mu}^*(\mathbf{r}) \psi_{i\mu}(\mathbf{r}) , \quad (7.17)$$

$$\mathbf{p}(\mathbf{r}) = -\frac{i}{m} \sum_{i\mu} f_i \psi_{i\mu}^*(\mathbf{r}) \nabla \psi_{i\mu}(\mathbf{r}) , \quad (7.18)$$

$$\sigma(\mathbf{r}) = \sum_{i\mu\mu'} f_i \psi_{i\mu}^*(\mathbf{r}) \hat{\sigma} \psi_{i\mu'}(\mathbf{r}) . \quad (7.19)$$

In the above μ and μ' are spin indices. With these definitions the spin-orbit energy is

$$\mathcal{H}_{so} = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{m^2 c^2 \hbar} \int d\mathbf{r} \int d\mathbf{r}' n(\mathbf{r}') \frac{(\mathbf{r} - \mathbf{r}') \times \mathbf{p}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|^3} \cdot \sigma(\mathbf{r}) . \quad (7.20)$$

The charge and spin densities are largely spherically symmetric within the muffin tins. If we approximate them as spherically symmetric the inverse square potential becomes

$$\frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = \frac{1}{r^2} \Theta(r_i - r_j) \hat{\mathbf{r}} . \quad (7.21)$$

This gives us

$$\mathcal{H}_{so} = \frac{\alpha^2 \mathcal{E}_H a_0^3}{4} \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 \int d\Omega \int d\Omega' \frac{n(r')}{r^2} \Theta(r - r') (\mathbf{L}(r) \cdot \sigma(r)) . \quad (7.22)$$

where $\alpha = e^2/4\pi\epsilon_0$, $\mathcal{E}_H = 4\pi\epsilon_0 \hbar^2/mc^2$, and $a_0 = mc^4/(4\pi\epsilon_0 \hbar)^2$. We calculate the matrix elements of $\mathcal{H}_{so}$ by contracting it against the muffin tin wavefunctions $\psi_i(\mathbf{r}) = \varphi_i(r) Y_{l_i m_i}(\Omega)$.

$$\langle \mathcal{H}_{so} \rangle_{ji} = \frac{\alpha^2 \mathcal{E}_H a_0^3}{4} \int_0^\infty dr \varphi_j^*(r) \varphi_i(r) \int_0^r dr' r'^2 n(r') \int d\Omega Y_{l_j m_j}^*(\Omega) \mathbf{L} Y_{l_i m_i}(\Omega) \cdot \sigma_{\mu_j \mu_i} . \quad (7.23)$$

σ is the Pauli spin vector and here we have put it into an up/down basis with respect to the

direction of the exchange field. This direction is defined by the unit vector $\hat{\mathbf{s}}$ and with two additional orthonormal vectors we can write

$$\begin{aligned}
 \hat{\sigma} &= \sigma^z \hat{\mathbf{s}} + \sigma^x \hat{\mathbf{u}} + \sigma^y \hat{\mathbf{v}} \\
 &= \sigma^z \hat{\mathbf{s}} + \frac{1}{2} \sigma^- (\hat{\mathbf{u}} + i \hat{\mathbf{v}}) + \frac{1}{2} \sigma^+ (\hat{\mathbf{u}} - i \hat{\mathbf{v}}) \\
 &= \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \hat{\mathbf{s}} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} (\hat{\mathbf{u}} + i \hat{\mathbf{v}}) + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} (\hat{\mathbf{u}} - i \hat{\mathbf{v}}) \right]. \quad (7.24)
 \end{aligned}$$

Since the torque operator is $\Gamma^- = [\sigma^-, \mathcal{H}_{so}]$ we now need to commute σ^- with Eq. (7.23). Because σ^- commutes with the orbital angular momentum operator we only need the commutator with the spin vector,

$$\begin{aligned}
 [\sigma^-, \hat{\sigma}] &= [\sigma^-, \sigma^z] \hat{\mathbf{s}} + [\sigma^-, \sigma^-/2] (\hat{\mathbf{u}} + i \hat{\mathbf{v}}) + [\sigma^-, \sigma^+/2] (\hat{\mathbf{u}} - i \hat{\mathbf{v}}) \\
 &= \sigma^- \hat{\mathbf{s}} + 0 (\hat{\mathbf{u}} + i \hat{\mathbf{v}}) - \sigma^z (\hat{\mathbf{u}} - i \hat{\mathbf{v}}) \\
 &= \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} \hat{\mathbf{s}} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (\hat{\mathbf{u}} - i \hat{\mathbf{v}}) \\
 &= \begin{pmatrix} -\hat{\mathbf{u}} + i \hat{\mathbf{v}} & 0 \\ 2\hat{\mathbf{s}} & \hat{\mathbf{u}} - i \hat{\mathbf{v}} \end{pmatrix}. \quad (7.25)
 \end{aligned}$$

Given that the exchange field is directed in the (θ, ϕ) direction with respect to some z-direction, defined, for example, by the crystal lattice, the unit vectors used above are

$$\hat{\mathbf{s}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \quad (7.26)$$

$$\hat{\mathbf{u}} = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta) \quad (7.27)$$

$$\hat{\mathbf{v}} = (-\sin \phi, \cos \phi, 0). \quad (7.28)$$

The commutator finally is

$$[\sigma^-, \hat{\sigma}] = \begin{pmatrix} (-\cos \theta \cos \phi - i \sin \phi, -\cos \theta \sin \phi + i \cos \phi, \sin \theta) \\ (2 \sin \theta \cos \phi, 2 \sin \theta \sin \phi, 2 \cos \theta) \\ 0 \\ (\cos \theta \cos \phi + i \sin \phi, \cos \theta \sin \phi - i \cos \phi, -\sin \theta) \end{pmatrix} \quad (7.29)$$

Making the torque operator

$$\begin{aligned} \langle \hat{\Gamma}^- \rangle_{ij} &= \frac{\alpha^2 E_h a_0^3}{4} \int_0^\infty dr \varphi_i(r) \varphi_j(r) \frac{1}{r} \left[-4\pi \int_0^r dr' r'^2 n(r') \right] \\ &\times \left[\int d\Omega Y_{l_i m_i}^*(\Omega) \mathbf{L} Y_{l_j m_j}(\Omega) \cdot [\sigma^-, \hat{\sigma}]_{\mu_i \mu_j} \right]. \end{aligned} \quad (7.30)$$

The Energy Integral

Both the expression for the damping rate (7.1) and the conductivity (7.2) contain an integration over the electron spectral functions

$$\int d\epsilon \eta(\epsilon) A_{nk}(\epsilon) A_{mk}(\epsilon), \quad (7.31)$$

though for the conductivity only intraband scattering ($m = n$) occurs. The spectral functions are Lorentzians,

$$A_{nk}(\epsilon) = \frac{1}{\pi} \frac{\hbar/2\tau_{nk}}{(\epsilon - \epsilon_{nk})^2 + (\hbar/2\tau_{nk})^2}, \quad (7.32)$$

centered at the band energies ϵ_{nk} with widths determined by the scattering time τ_{nk} . The spectral functions are weighted by $\eta(\epsilon) = -\partial f / \partial \epsilon$ the negative derivative of the Fermi function, which is a positive distribution peaked about the Fermi level. The integrand

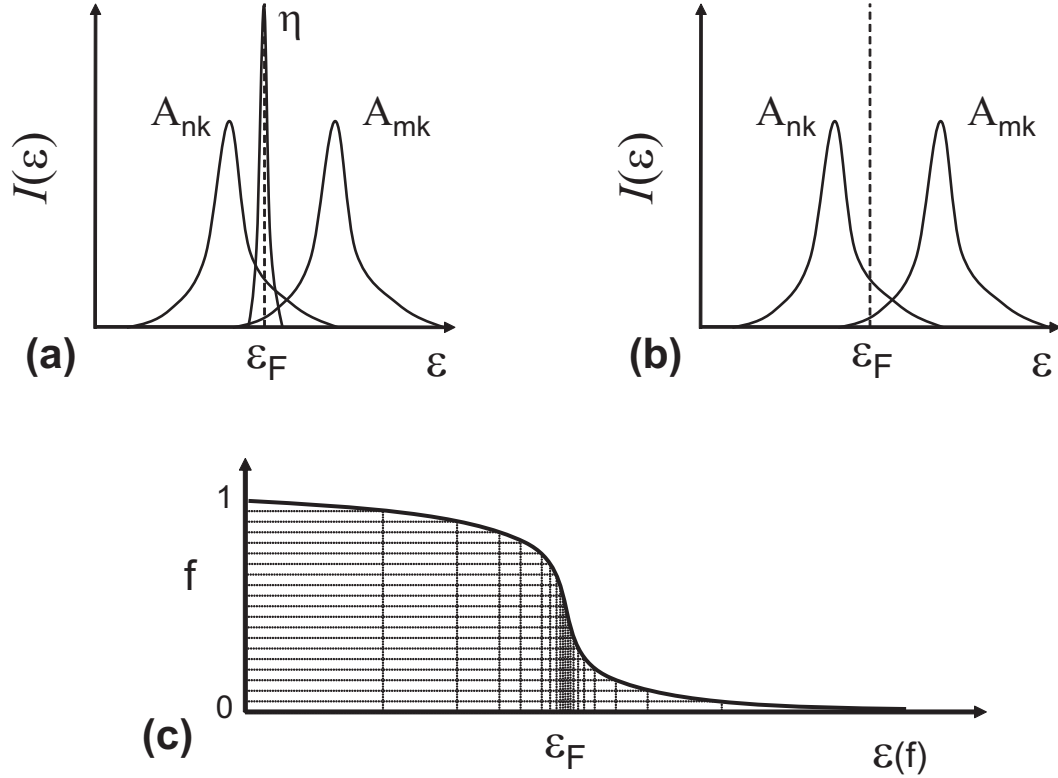


Figure 7.2: Technique for evaluating the energy integration. The functions of the energy integrand are shown in (a). The broadening $\hbar/2\tau$ of the spectral functions A is typically significantly larger than the broadening $k_B T$ of the η function. Figure (b) shows the integrand after changing the integration variable from ϵ to f . The solid curve in (c) is the Fermi function. This figure demonstrates the conversion of unbiased f point sampling to biased ϵ sampling to make the integration over the functions in (b) equivalent to the unbiased integration over the functions in (a).

consists of three peaked functions, which we sketch in Fig. (7a).

To evaluate 7.31 we first change variables from ϵ to f

$$\int_{-\infty}^{\infty} d\epsilon \eta(\epsilon) A_n(\epsilon) A_m(\epsilon) = \int_{-\infty}^{\infty} d\epsilon \left(-\frac{df}{d\epsilon} \right) A_n(\epsilon) A_m(\epsilon) \rightarrow - \int_1^0 df A_n(\epsilon(f)) A_m(\epsilon(f)). \quad (7.33)$$

The integrand now only consists of the two spectral functions, the η function has been removed, as shown in Fig. (7b). However, the integral is no longer performed directly over

energy space, but over the distribution function f . The η function now indirectly weights the spectral functions by biasing the energy sampling $\epsilon(f)$ to values near the Fermi level. Uniform sampling of values of the distribution function f equates to weighted sampling of the energy, as demonstrated in Fig. (7c). Specifically, we find $\epsilon(f)$ from the Fermi function:

$$f(\epsilon) = \frac{1}{1 + e^{\beta(\epsilon - \epsilon_F)}} \quad (7.34)$$

$$\epsilon(f) = \epsilon_F + \frac{1}{\beta} \ln(1/f - 1). \quad (7.35)$$

Note that the Fermi-Dirac function f is unitless and takes on values between 0 and 1. β is $1/k_B T$. The integration over energy can be written as a summation over the Fermi distribution using the midpoint method

$$\int_{-\infty}^{\infty} d\epsilon \eta(\epsilon) A_n(\epsilon) A_m(\epsilon) \rightarrow \frac{1}{N} \sum_{f=\delta/2}^{1-\delta/2} A_n(\epsilon(f)) A_m(\epsilon(f)). \quad (7.36)$$

The spectral functions are evaluated at the N points $f_i = (n_i + 1/2)\delta$ between 0 and 1 where $n_i \in \{0, N-1\}$. $\delta = 1/N$ is the distance between these evenly spaced points.

Convergence Tests

The calculations that we have performed in this work take as input a previously converged density. Therefore, the painstaking work of ensuring that the density is properly converged with respect to the many numerical parameters in a DFT program had already been done. However, to calculate the damping rate and conductivity we needed to expand these converged densities into wavefunctions and evaluate the k -space and energy integrals described above. The results of these steps depended on several factors such as the number

of k points sampled, the number of bands included, the number of steps used in the energy integration, and the artificial temperature used to broaden the Fermi function. In what follows we present tests for convergence of the damping rate and resistivity with respect to these parameters.

Damping

The convergence tests for the damping rate with respect to the number of bands, the energy integration mesh, and the number of k -points are presented in Figs. (7.3-7.5). For iron, the damping rate is largely independent of the number of bands included in the calculation beyond 7 bands, while the results for cobalt required the inclusion of 15 bands (twice as many because the hcp structure has a two atom basis), and nickel was well converged after 6 bands. For iron and nickel, the result of the damping calculation exhibits a roughly damped oscillatory behavior with respect to the number of k points sampled. Satisfactory convergence required $(160)^3$ k points for iron, and $(140)^3$ points for nickel. As seen in Fig. (7.5), the situation is a little different for cobalt. The result of the calculation alternates between a converged number and an incorrect larger value. The incorrect larger value slowly converges, with respect to the number of k points, to the correct result. Since the damping rate evaluated with a relatively small number of k points, $(100)^2$ in the basal plane and 57 along the c -axis, is very close to the apparent converged value, this sampling was used.

The energy integral was converted to a summation over values of the Fermi distribution as discussed above. The summation sampled N energy points. Figure (7.4) shows the convergence of the damping rate with respect to the number of energy points sampled in this summation. For each metal 100 points were sufficient to obtain good convergence of the energy integration.

The energy integration also depended on the the broadening of the Fermi distribution. The Fermi distribution was broadened by including an artificial temperature. Figure (7.6) shows results of the damping calculations for several temperatures between 50 K and 800 K. The results are largely independent of this temperature. The results depend little on this temperature because even for a temperature of 1000 K the broadening of the Fermi distribution is still much less than the broadening of the spectral functions.

Resistivity

Figures (7.7-7.9) show the results of the convergence tests for the resistivity. The convergence criteria for the k space integration for the resistivity are similar to those found for the damping rate. Convergence requires the use of 6 bands for iron, 12 for cobalt, and 6 for nickel. Convergence with respect to the number of bands occurs with slightly fewer bands in this case, as compared to the damping rate, because the resistivity expression does not include interband transitions. The k point convergence for the resistivity requires a somewhat larger number of k points than found for the damping rate. $(180)^3$ k points were used for iron, $(160)^2$ by 91 k points were used for cobalt, and $(160)^3$ were used for nickel. For the energy integration, the results were again well converged for 100 summation steps. As seen in Fig. (7.10) The resistivity is very insensitive to the artificial temperature used to broaden the Fermi function.

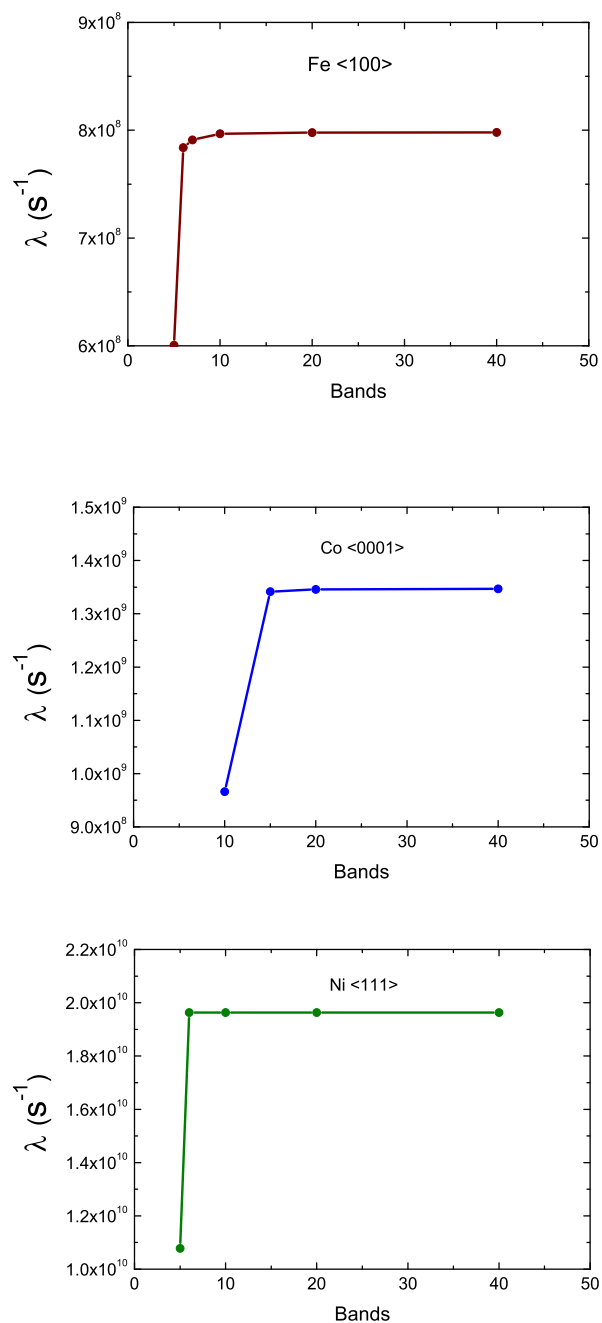


Figure 7.3: Convergence of the damping rate with respect to number of bands. The plots show convergence with respect to the number of bands for iron (top), cobalt (middle), and nickel (bottom).

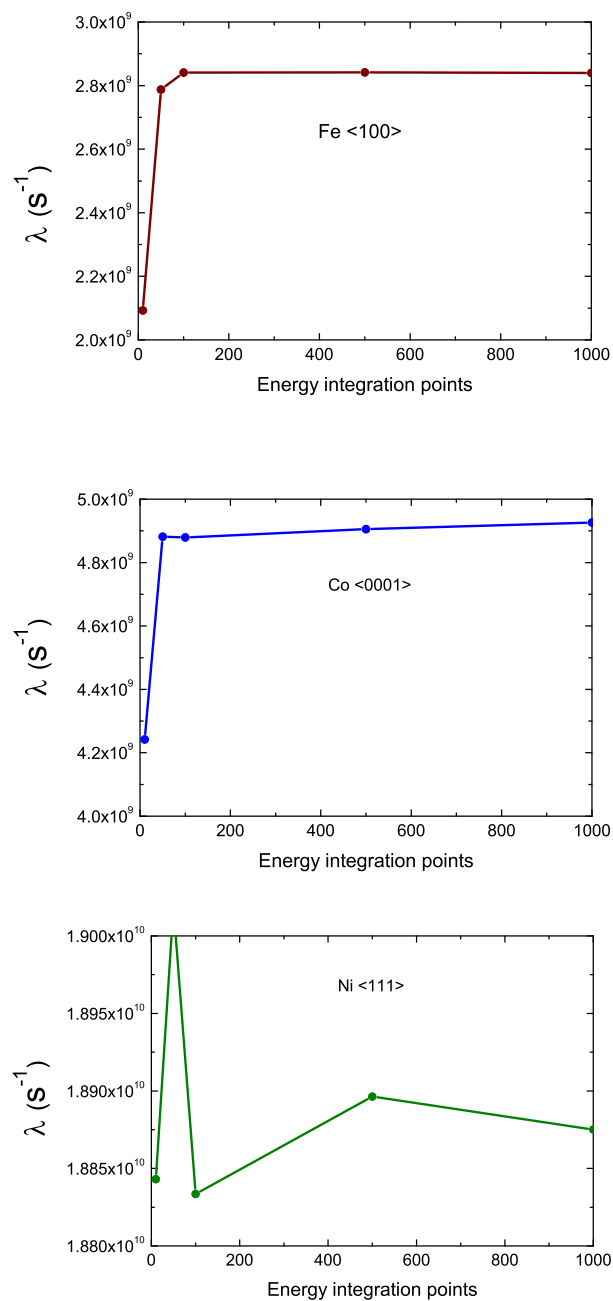


Figure 7.4: Convergence of the damping rate with respect to number of energy integration steps. The plots show convergence with respect to the number of energy integration steps for iron (top), cobalt (middle), and nickel (bottom).

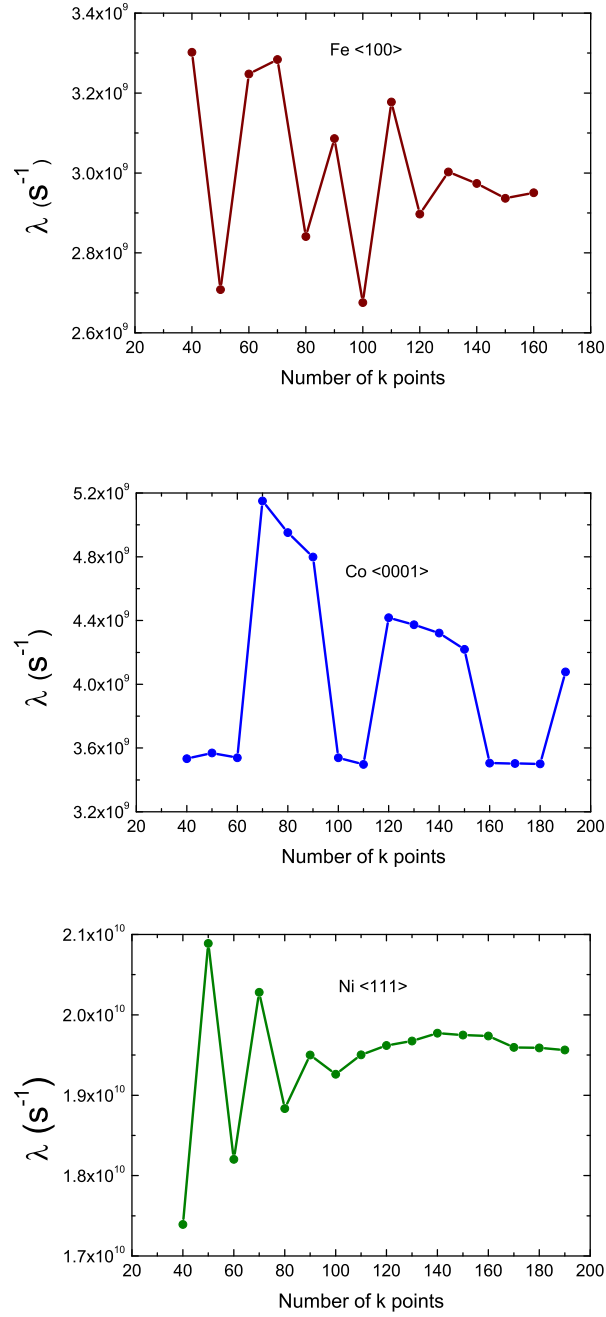


Figure 7.5: Convergence of the damping rate with respect to k point sampling. The plots show convergence with respect to the number of k points used in the integration for iron (top), cobalt (middle), and nickel (bottom).

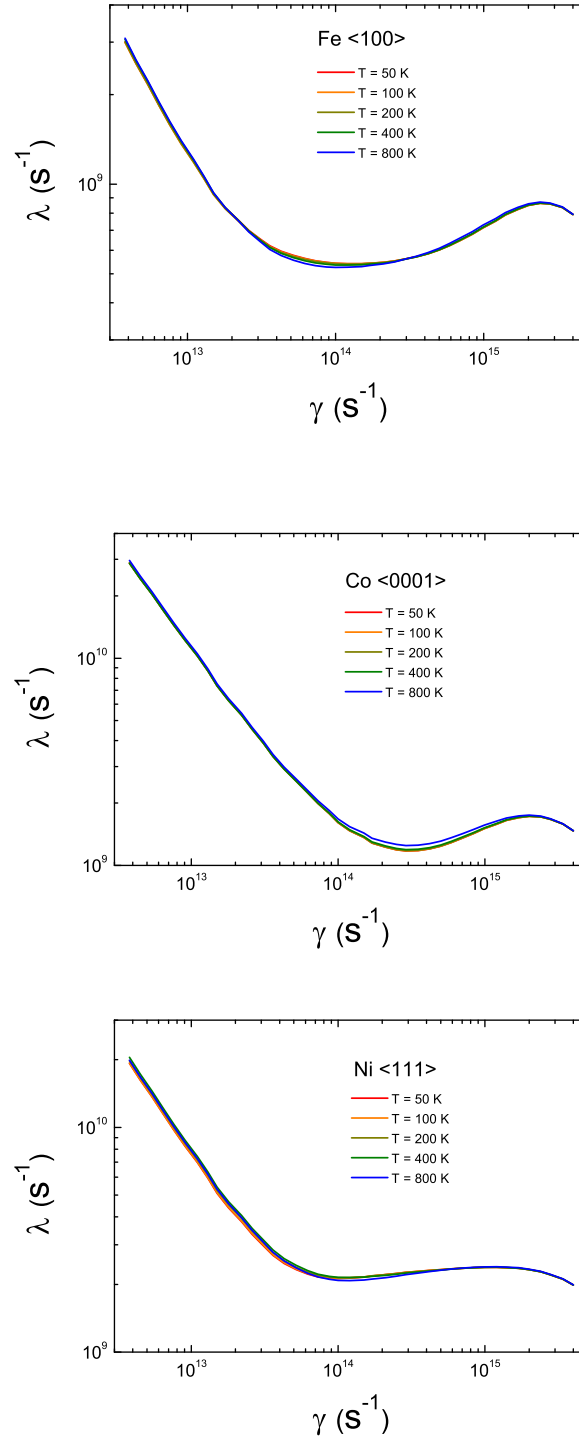


Figure 7.6: Damping rate dependence on Fermi function broadening. Damping rates calculated for several artificial temperatures. This temperature is used to broaden the Fermi function in the energy integral.

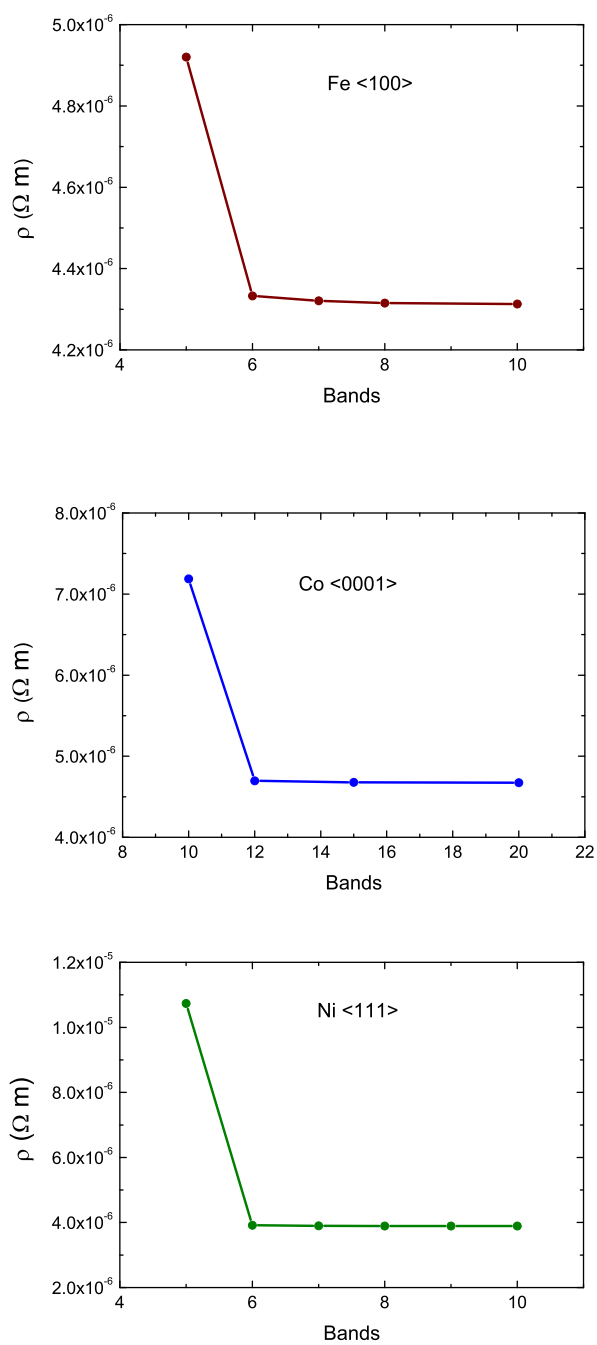


Figure 7.7: Convergence with respect to the number of bands for the resistivity. The plots show the convergence of the resistivity with respect to the number of bands for iron (top), cobalt (middle), and nickel (bottom).

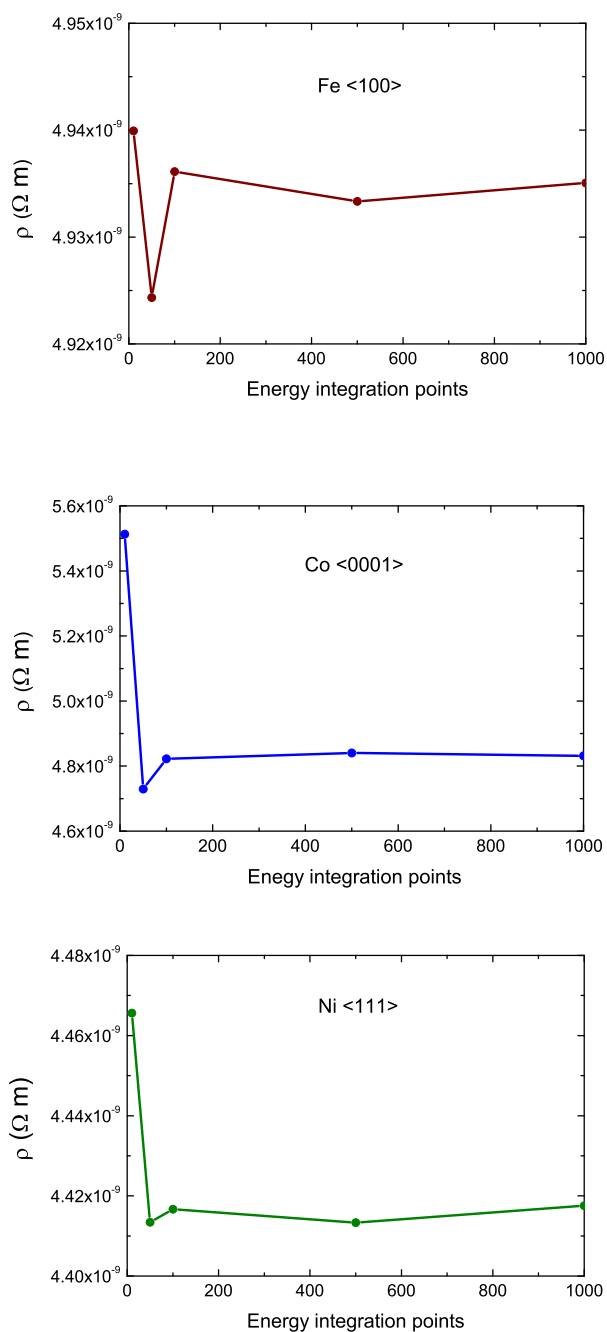


Figure 7.8: Convergence with respect to the number of energy integration steps for the resistivity. The plots show the convergence of the resistivity with respect to the number of energy integration steps for iron (top), cobalt (middle), and nickel (bottom).

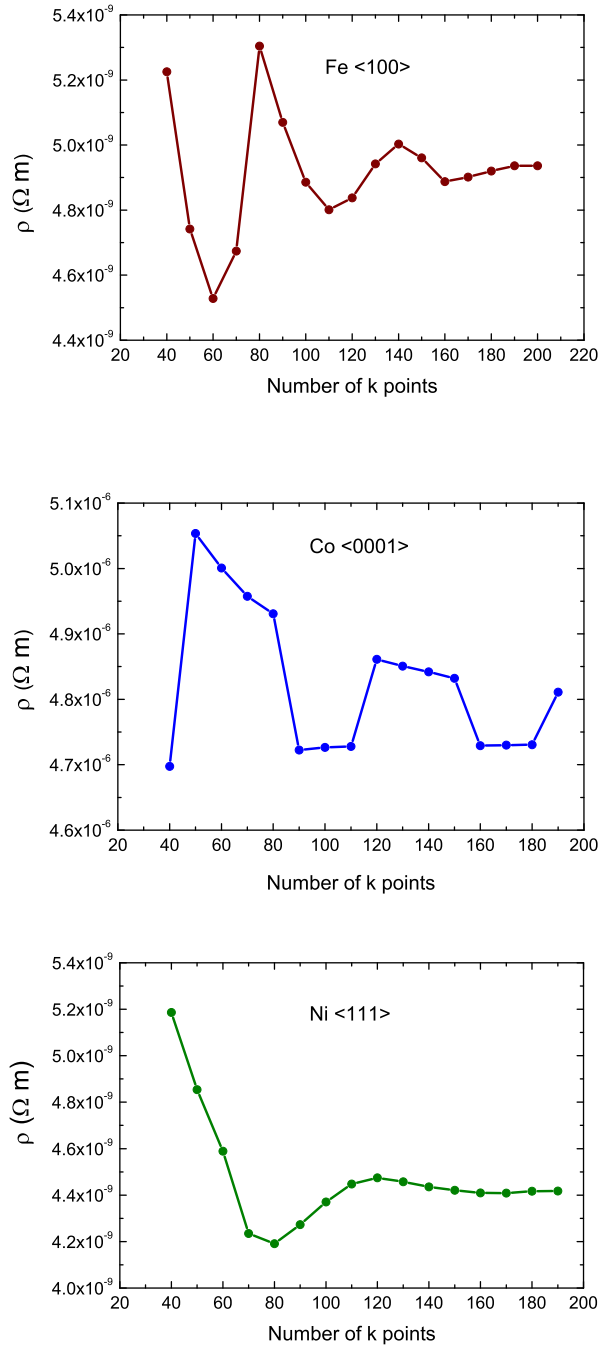


Figure 7.9: Convergence with respect to the number of k points for the resistivity. The plots show the convergence of the resistivity with respect to the number of k points used in the integration for iron (top), cobalt (middle), and nickel (bottom).

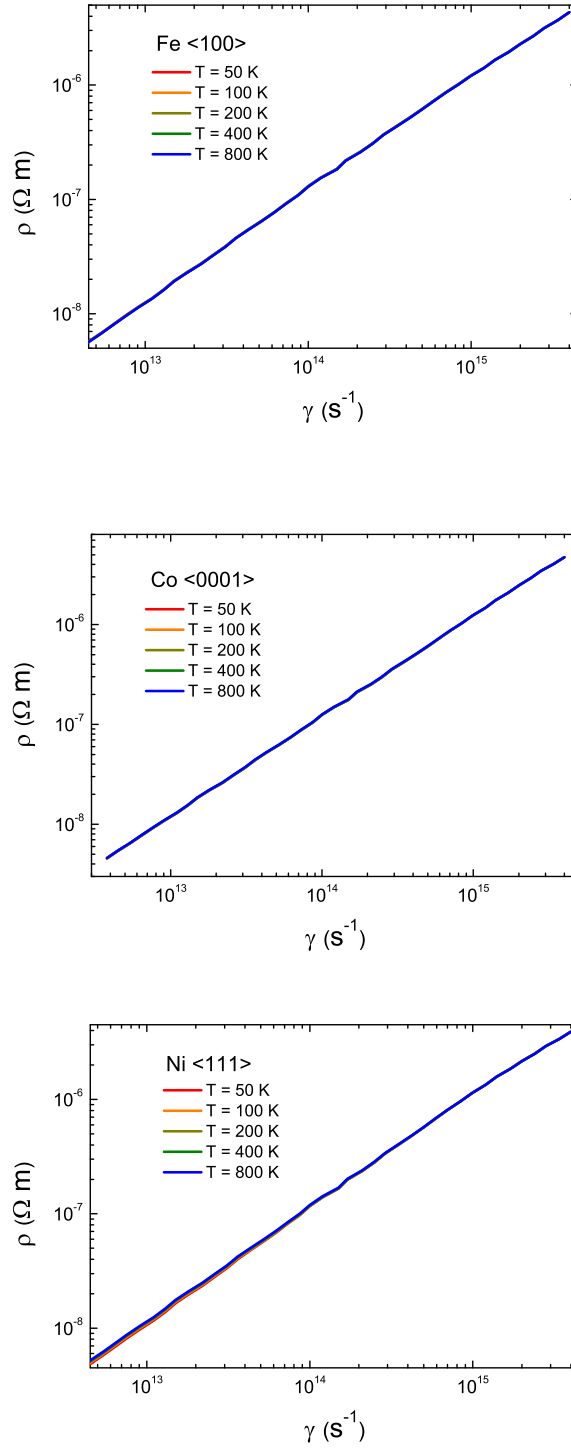


Figure 7.10: Resistivity dependence on Fermi function broadening. Damping rates calculated for several artificial temperatures. This temperature is used to broaden the Fermi function in the energy integral.

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