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2009 J. Phys.: Condens. Matter 21 146002

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# The quantum-mechanical basis of an extended Landau–Lifshitz–Gilbert equation for a current-carrying ferromagnetic wire

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Received 25 November 2008

Published 9 March 2009

Online at [stacks.iop.org/JPhysCM/21/146002](http://stacks.iop.org/JPhysCM/21/146002)

## Abstract

An extended Landau–Lifshitz–Gilbert (LLG) equation is introduced to describe the dynamics of inhomogeneous magnetization in a current-carrying wire. The coefficients of all the terms in this equation are calculated quantum-mechanically for a simple model which includes impurity scattering. This is done by comparing the energies and lifetimes of a spin wave calculated from the LLG equation and from the explicit model. Two terms are of particular importance since they describe non-adiabatic spin-transfer torque and damping processes which do not rely on spin–orbit coupling. It is shown that these terms may have a significant influence on the velocity of a current-driven domain wall and they become dominant in the case of a narrow wall.

## 1. Introduction

The effect of passing an electric current down a ferromagnetic wire is of great current interest. If the magnetization is inhomogeneous it experiences a spin-transfer torque due to the current [1–4]. The effect is described phenomenologically by adding terms to the standard LLG equation [5, 6]. The leading term in the spin-transfer torque is an adiabatic one arising from that component of the spin polarization of the current which is in the direction of the local magnetization. However, in considering the current-induced motion of a domain wall, Li and Zhang [3, 4] found that below a very large critical current the adiabatic term only deforms the wall and does not lead to continuous motion. To achieve this effect they introduced [7] a phenomenological non-adiabatic term associated with the same spin non-conserving processes responsible for Gilbert damping. Subsequently Kohno *et al* [8] derived a torque of the Zhang–Li form quantum-mechanically using a model of spin-dependent scattering from impurities. This may arise from spin–orbit coupling on the impurities. A less explicit discussion was given by Tserkovnyak *et al* [10]. More recently Wessely *et al* [9] introduced two further non-adiabatic terms in the LLG equation in order to describe their numerical calculations of spin-transfer torques in a domain wall. These

quantum-mechanical calculations using the Keldysh formalism were made in the ballistic limit without impurities and with spin conserved. Other terms in the LLG equation, involving mixed space and time derivatives, have been considered by Sobolev *et al* [12], Tserkovnyak *et al* [10], Skadsem *et al* [11] and Thorwart and Egger [13].

The object of this paper is to give a unified treatment of all these terms in the LLG equation and to obtain explicit expressions for their coefficients by quantum-mechanical calculations for a simple one-band model with and without impurity scattering. The strategy adopted is to consider a uniformly magnetized wire and to calculate the effect of a current on the energy and lifetime of a long wavelength spin wave propagating along the wire. It is shown in section 2 that coefficients of spin-transfer torque terms in the LLG equation are directly related to  $q$  and  $q^3$  terms in the energy and inverse lifetime of a spin wave of wavevector  $q$ . The Gilbert damping parameter is the coefficient of the  $\omega$  term in the inverse lifetime, where  $\omega$  is the spin wave frequency. It corresponds to the damping of a  $q = 0$  spin wave while higher order terms  $\omega q$  and  $\omega q^2$  relate to damping of spin waves with finite wavevector  $q$ . The relation between the  $q$  term in the spin wave energy and the adiabatic spin-transfer torque has been noticed previously [2, 14]. We

find that the  $q$  term in the spin wave lifetime relates to the Zhang–Li non-adiabatic spin-transfer torque. Our result for the coefficient of the Zhang–Li term is essentially the same as that obtained by Kohno *et al* [8] and Duine *et al* [15] but our derivation appears simpler. The  $q^3$  terms in the spin wave energy and lifetime are related to the additional non-adiabatic torques we introduced into the LLG equation [9], together with an extra one arising from spin non-conserving scattering. Explicit expressions for the coefficients of these terms are obtained in section 3. In section 4 we discuss briefly the importance of the additional terms in our extended LLG equation for current-driven motion of a domain wall. Some conclusions are summarized in section 5.

## 2. The LLG equation and spin waves

We write our extended LLG equation in the dimensionless form

$$\begin{aligned} & \frac{\partial \mathbf{s}}{\partial t} + \alpha \mathbf{s} \times \frac{\partial \mathbf{s}}{\partial t} + \alpha_1 \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z \partial t} - \alpha'_1 \mathbf{s} \times \left( \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z \partial t} \right) \\ & - \alpha'_2 \mathbf{s} \times \frac{\partial^3 \mathbf{s}}{\partial z^2 \partial t} - \alpha_2 \mathbf{s} \times \left( \mathbf{s} \times \frac{\partial^3 \mathbf{s}}{\partial z^2 \partial t} \right) \\ & = \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z^2} - b_{\text{ext}} \mathbf{s} \times \mathbf{e}_z - a \frac{\partial \mathbf{s}}{\partial z} - f \mathbf{s} \times \frac{\partial \mathbf{s}}{\partial z} \\ & + a_1 \left\{ \mathbf{s} \times \left( \mathbf{s} \times \frac{\partial^3 \mathbf{s}}{\partial z^3} \right) + \left[ \mathbf{s} \cdot \frac{\partial^2 \mathbf{s}}{\partial z^2} - \frac{1}{2} \left( \frac{\partial \mathbf{s}}{\partial z} \right)^2 \right] \frac{\partial \mathbf{s}}{\partial z} \right\} \\ & - f_1 \mathbf{s} \times \left[ \mathbf{s} \times \frac{\partial}{\partial z} \left( \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z^2} \right) \right] + g_1 \mathbf{s} \times \frac{\partial^3 \mathbf{s}}{\partial z^3}. \end{aligned} \quad (1)$$

Here  $\mathbf{s}(z, t)$  is a unit vector in the direction of the local spin polarization, time  $t$  is measured in units of  $(\gamma \mu_0 m_s)^{-1}$  and the coordinate  $z$  along the wire is in units of the exchange length  $l_{\text{ex}} = (2A/\mu_0 m_s^2)^{1/2}$ . The quantities appearing here are the gyroscopic ratio  $\gamma = 2\mu_B/\hbar$ , the permeability of free space  $\mu_0$  and two properties of the ferromagnetic material, namely the saturation magnetization  $m_s$  and the exchange stiffness constant  $A$ .  $\mathbf{e}_z$  is a unit vector in the  $z$  direction along the wire. The equation expresses the rate of change of spin angular momentum as the sum of various torque terms, of which the  $\alpha_1$ ,  $\alpha'_1$ ,  $a$ ,  $f$ ,  $a_1$ ,  $f_1$  and  $g_1$  terms are proportional to the electric current flowing. The second term in the equation is the standard Gilbert term, with damping factor  $\alpha$ , while the  $\alpha'_1$  and  $\alpha'_2$  terms introduce corrections for spin fluctuations of finite wavevector. Skadsem *et al* [11] point out the existence of the  $\alpha'_2$  term but do not consider it further. It was earlier introduced by Sobolev *et al* [12] within a microscopic context based on the Heisenberg model. The  $\alpha_1$  and  $\alpha_2$  terms are found to renormalize the spin wave frequency, but for the model considered in section 3 we find that  $\alpha_1$  is identically zero. We shall argue that this result is model independent. Tserkovnyak *et al* [10] and Thorwart and Egger [13] find non-zero values of  $\alpha_1$  which differ from each other by a factor 2; they attribute this to their use of Stoner-like and  $s$ - $d$  models, respectively. Thorwart and Egger [13] also find the  $\alpha'_1$  term and they investigate the effect of  $\alpha_1$  and  $\alpha'_1$  terms on domain wall motion. Their numerical results are difficult to assess because the constant  $|\mathbf{s}| = 1$  is not maintained during the motion. In

equation (1) we have omitted terms involving the second order time derivatives, whose existence was pointed out by Thorwart and Egger [13]; one of these is discussed briefly in section 3.2.

The first term on the right-hand side of equation (1) is due to exchange stiffness and the next term arises from an external magnetic field  $B_{\text{ext}} \mathbf{e}_z$  with dimensionless coefficient  $b_{\text{ext}} = B_{\text{ext}}/\mu_0 m_s$ . The third term is the adiabatic spin-transfer torque whose coefficient  $a$  is simple and well known. In fact [3, 4]

$$a = \frac{1}{2} \frac{\hbar J P}{e \mu_0 m_s^2 l_{\text{ex}}} \quad (2)$$

where  $J$  is the charge current density and  $e$  is the electron charge (a negative quantity). The spin polarization factor  $P = (J_{\uparrow} - J_{\downarrow})/(J_{\uparrow} + J_{\downarrow})$ , where  $J_{\uparrow}, J_{\downarrow}$  are the current densities for majority and minority spin in the ferromagnet ( $J = J_{\uparrow} + J_{\downarrow}$ ). Equation (2) is valid for both ballistic and diffusive conduction. The fourth term on the right-hand side of equation (1) is the Zhang–Li torque which is often characterized [8] by a parameter  $\beta = f/a$ . The next term is the  $E_1$  term of equation (7) in [9]. It is a non-adiabatic torque which is coplanar with  $\mathbf{s}(z)$  if  $\mathbf{s}(z)$  lies everywhere in a plane. As shown in [9] it is the  $z$  derivative of a spin current, which is characteristic of a torque occurring from spin-conserving processes. In fact this term takes the form

$$a_1 \frac{\partial}{\partial z} \left[ \mathbf{s} \times \left( \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z^2} \right) - \frac{1}{2} \mathbf{s} \left( \frac{\partial \mathbf{s}}{\partial z} \right)^2 \right]. \quad (3)$$

The  $f_1$  term may be written in the form

$$-f_1 \left( \mathbf{s} \cdot \frac{\partial \mathbf{s}}{\partial z} \times \frac{\partial^2 \mathbf{s}}{\partial z^2} \right) \mathbf{s} + f_1 \frac{\partial}{\partial z} \left( \mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial z^2} \right). \quad (4)$$

If  $\mathbf{s}(z)$  lies in a plane, the case considered in [9], the first term vanishes and we recover the  $F_1$  term of equation (9) in [9]. Its derivative form indicate that it arises from spin-conserving processes so we conclude that the coefficient  $f_1$  is of that origin. This is not true of the last term in equation (1) and we associate the coefficient  $g_1$  with spin non-conserving processes. For a spin wave solution of the LLG equation, where we work only to first order in deviations from a state of uniform magnetization, the last three terms of equation (1) may be replaced by the simpler ones

$$-a_1 \frac{\partial^3 \mathbf{s}}{\partial z^3} + (f_1 + g_1) \mathbf{s} \times \frac{\partial^3 \mathbf{s}}{\partial z^3}. \quad (5)$$

Apart from additional terms, equation (1) looks slightly different from equation (7) of [9] because we use the spin polarization unit vector  $\mathbf{s}$  rather than the magnetization vector  $\mathbf{m}$  and  $\mathbf{s} = -\mathbf{m}$ . Furthermore the dimensionless coefficients will take different numerical values because we have used different dimensionless variables  $z$  and  $t$  to avoid introducing the domain wall width which was specific to [9]. The torques due to anisotropy fields were also specific to the domain wall problem and have been omitted in equation (1).

We suppose that the wire is magnetized uniformly in the  $z$  direction and consider a spin wave as a small transverse oscillation of the spin polarization about the equilibrium state

or, when a current flows, the steady state. Thus we look for a solution of equation (1) of the form

$$\mathbf{s} = (ce^{i(qz-\omega t)}, de^{i(qz-\omega t)}, -1) \quad (6)$$

where the coefficients of the  $x$  and  $y$  components satisfy  $c \ll 1$ ,  $d \ll 1$ . This represents a spin wave of wavevector  $q$  and angular frequency  $\omega$  propagating along the  $z$  axis. When (6) is substituted into equation (1) the transverse components yield, to first order in  $c$  and  $d$ , the equations

$$-i\lambda c + \mu d = 0, \quad \mu c + i\lambda d = 0 \quad (7)$$

where

$$\begin{aligned} \lambda &= \omega - aq + a_1q^3 - \alpha_2\omega q^2 + i\alpha'_1q\omega \\ \mu &= -i\alpha\omega + b_{\text{ext}} + q^2 + ifq \\ &\quad + i(f_1 + g_1)q^3 + \alpha_1\omega q - i\omega q^2\alpha'_2. \end{aligned} \quad (8)$$

On eliminating  $c$  and  $d$  from equation (7) we obtain  $\lambda^2 = \mu^2$ . To obtain a positive real part for the spin wave frequency, we take  $\lambda = \mu$ . Hence

$$\omega(1 - \alpha_1q - \alpha_2q^2) = b_{\text{ext}} + aq + q^2 - a_1q^3 + i[\omega(-\alpha - \alpha'_1q - \alpha'_2q^2) + fq + (f_1 + g_1)q^3]. \quad (9)$$

Thus the spin wave frequency is given by

$$\omega = \omega_1 - i\omega_2 \quad (10)$$

where

$$\begin{aligned} \omega_1 &\simeq (1 - \alpha_1q - \alpha_2q^2)^{-1}(b_{\text{ext}} + aq + q^2 - a_1q^3) \\ \omega_2 &\simeq (1 - \alpha_1q - \alpha_2q^2)^{-1}[\omega_1(\alpha + \alpha'_1q + \alpha'_2q^2) \\ &\quad - fq - (f_1 + g_1)q^3]. \end{aligned} \quad (11)$$

Here we have neglected terms of second order in  $\alpha$ ,  $\alpha'_1$ ,  $\alpha'_2$ ,  $f$ ,  $f_1$  and  $g_1$ , the coefficients which appear in the spin wave damping. This form for the real and imaginary parts of the spin wave frequency is convenient for comparing with the quantum-mechanical results of section 3. In this way we shall obtain explicit expressions for all the coefficients in the phenomenological LLG equation. Coefficients of odd powers of  $q$  are proportional to the current flowing whereas terms in even powers of  $q$  are present in the equilibrium state with zero current.

### 3. Spin wave energy and lifetimes in a simple model

As a simple model of an itinerant electron ferromagnet we consider the one-band Hubbard model

$$H_0 = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu_B B_{\text{ext}} \sum_i (n_{i\uparrow} - n_{i\downarrow}), \quad (12)$$

where  $c_{i\sigma}^\dagger$  creates an electron on site  $i$  with spin  $\sigma$  and  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ . We consider a simple cubic lattice and the intersite hopping described by the first term is restricted to nearest neighbours. The second term describes an on-site interaction between electrons with effective interaction parameter  $U$ ; the

last term is due to an external magnetic field. It is convenient to introduce a Bloch representation, with

$$c_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{i\sigma}^\dagger, \quad n_{\mathbf{k}\sigma} = c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (13)$$

$$\epsilon_{\mathbf{k}} = -t \sum_i e^{i\mathbf{k}\cdot\boldsymbol{\rho}_i} = -2t(\cos k_x a_0 + \cos k_y a_0 + \cos k_z a_0). \quad (14)$$

The sum in equation (13) is over all lattice sites  $\mathbf{R}_i$  whereas in equation (14)  $\boldsymbol{\rho}_i = (\pm a_0, 0, 0)$ ,  $(0, \pm a_0, 0)$ ,  $(0, 0, \pm a_0)$  are the nearest neighbour lattice sites. Then

$$H_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu_B B_{\text{ext}} \sum_{\mathbf{k}} (n_{\mathbf{k}\uparrow} - n_{\mathbf{k}\downarrow}). \quad (15)$$

To discuss scattering of spin waves by dilute impurities we assume that the effect of the scattering from different impurity sites adds incoherently; hence we may consider initially a single scattering centre at the origin. We therefore introduce at this site a perturbing potential  $u + v\mathbf{l} \cdot \boldsymbol{\sigma}$ , where  $\mathbf{l} = (\sin\theta \cos\phi, \sin\phi \sin\theta, \cos\theta)$  is a unit vector whose direction will finally be averaged over.  $u$  is the part of the impurity potential which is independent of the spin  $\boldsymbol{\sigma}$  and the spin-dependent potential  $v\mathbf{l} \cdot \boldsymbol{\sigma}$  is intended to simulate a spin-orbit  $\mathbf{L} \cdot \boldsymbol{\sigma}$  interaction on the impurity. It breaks spin rotational symmetry in the simplest possible way. Clearly spin-orbit coupling can only be treated correctly for a degenerate band such as a d-band, where on-site orbital angular momentum  $\mathbf{L}$  occurs naturally. The present model is equivalent to that used by Kohno *et al* [8] and Duine *et al* [15]. In Bloch representation the impurity potential becomes  $V = V_1 + V_2$  with

$$\begin{aligned} V_1 &= v_\uparrow \frac{1}{N} \sum_{\mathbf{k}_1\mathbf{k}_2} c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\uparrow} + v_\downarrow \frac{1}{N} \sum_{\mathbf{k}_1\mathbf{k}_2} c_{\mathbf{k}_1\downarrow}^\dagger c_{\mathbf{k}_2\downarrow} \\ V_2 &= ve^{-i\phi} \sin\theta \frac{1}{N} \sum_{\mathbf{k}_1\mathbf{k}_2} c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\downarrow} \\ &\quad + ve^{i\phi} \sin\theta \frac{1}{N} \sum_{\mathbf{k}_1\mathbf{k}_2} c_{\mathbf{k}_1\downarrow}^\dagger c_{\mathbf{k}_2\uparrow} \end{aligned} \quad (16)$$

and  $v_\uparrow = u + v \cos\theta$ ,  $v_\downarrow = u - v \cos\theta$ . To avoid confusion we note that the spin dependence of the impurity potential which occurs in the many-body Hamiltonian  $H_0 + V$  is not due to exchange, as would arise in an approximate self-consistent field treatment (e.g. Hartree-Fock) of the interaction  $U$  in a ferromagnet.

#### 3.1. Spin wave energy and wavefunction

In this section we neglect the perturbation due to impurities and determine expressions for the energy and wavefunction of a long wavelength spin wave in the presence of an electric current. The presence of impurities is recognized implicitly since the electric current is characterized by a perturbed one-electron distribution function  $f_{\mathbf{k}\sigma}$  which might be obtained by solving a Boltzmann equation with a collision term. We consider a spin wave of wavevector  $\mathbf{q}$  propagating along the  $z$  axis, which is the direction of current flow. Lengths and times used in this section and the next, except when

specified, correspond to actual physical quantities, unlike the dimensionless variables used in section 2.

We first consider the spin wave with zero electric current and treat it, within the random phase approximation (RPA), as an excitation from the Hartree–Fock (HF) ground state of the Hamiltonian (15). The HF one-electron energies are given by

$$E_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + U\langle n_{-\sigma} \rangle - \mu_B \sigma B_{\text{ext}} \quad (17)$$

where  $\sigma = 1, -1$  for  $\uparrow$  and  $\downarrow$  respectively, and  $\langle n_{-\sigma} \rangle$  is the number of  $-\sigma$  spin electrons per site. In a self-consistent ferromagnetic state at  $T = 0$ ,  $\langle n_{\sigma} \rangle = N^{-1} \sum_{\mathbf{k}} f_{\mathbf{k}\sigma}$  and  $n = \sum_{\sigma} \langle n_{\sigma} \rangle$ , where,  $f_{\mathbf{k}\sigma} = \theta(E_F - E_{\mathbf{k}\sigma})$ ,  $n$  is the number of electrons per atom, and  $E_F$  is the Fermi energy.  $N$  is the number of lattice sites and  $\theta(E)$  is the unit step function. The spin bands  $E_{\mathbf{k}\sigma}$  given by equation (17) are shifted relative to each other by an energy  $\Delta + 2\mu_B B_{\text{ext}}$  where  $\Delta = U\langle n_{\uparrow} - n_{\downarrow} \rangle$  is the exchange splitting. The ground state is given by  $|0\rangle = \prod_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} | \rangle$  where  $| \rangle$  is the vacuum state and the product extends over all states  $\mathbf{k}\sigma$  such that  $f_{\mathbf{k}\sigma} = 1$ . Within the RPA, the wavefunction for a spin wave of wavevector  $\mathbf{q}$ , excited from the HF ground state, takes the form

$$|\mathbf{q}\rangle = N_{\mathbf{q}} \sum_{\mathbf{k}} A_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow} |0\rangle \quad (18)$$

where  $N_{\mathbf{q}}$  is a normalization factor. The energy of this state may be written

$$E_{\mathbf{q}} = E_{\text{gr}} + \hbar\omega_{\mathbf{q}} = E_{\text{gr}} + 2\mu_B B_{\text{ext}} + \hbar\omega'_{\mathbf{q}} \quad (19)$$

where  $E_{\text{gr}}$  is the energy of the HF ground state and  $\hbar\omega_{\mathbf{q}}$  is the spin wave excitation energy. On substituting (18) in the Schrödinger equation  $(H_0 - E_{\mathbf{q}})|\mathbf{q}\rangle = 0$  and multiplying on the left by  $\langle 0|c_{\mathbf{k}'\uparrow}^{\dagger} c_{\mathbf{k}'-\mathbf{q}\downarrow}$ , we find

$$A_{\mathbf{k}'}(\epsilon_{\mathbf{k}'+\mathbf{q}} - \epsilon_{\mathbf{k}'} + \Delta - \hbar\omega'_{\mathbf{q}}) = \frac{U}{N} \sum_{\mathbf{k}} A_{\mathbf{k}} f_{\mathbf{k}\uparrow} (1 - f_{\mathbf{k}+\mathbf{q}\downarrow}). \quad (20)$$

Hence we may take

$$A_{\mathbf{k}} = \Delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + \Delta - \hbar\omega'_{\mathbf{q}})^{-1} \quad (21)$$

and, for small  $\mathbf{q}$ ,  $\hbar\omega'_{\mathbf{q}}$  satisfies the equation

$$1 = \frac{U}{N} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}\uparrow} - f_{\mathbf{k}+\mathbf{q}\downarrow}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + \Delta - \hbar\omega'_{\mathbf{q}}}. \quad (22)$$

This is the equation for the poles of the well-known RPA dynamical susceptibility  $\chi(\mathbf{q}, \omega)$  [16]. The spin wave pole is the one for which  $\hbar\omega'_{\mathbf{q}} \rightarrow 0$  as  $\mathbf{q} \rightarrow 0$ .

To generalize the above considerations to a current-carrying state we proceed as follows. We re-interpret the state  $|0\rangle$  such that  $\langle 0| \cdots |0\rangle$  corresponds to a suitable ensemble average with a modified one-electron distribution  $f_{\mathbf{k}\sigma}$ . When a current flows in the  $z$  direction we may consider the  $\uparrow$  and  $\downarrow$  spin Fermi surfaces as shifted by small displacements  $\delta_{\uparrow} \hat{\mathbf{k}}_z$ ,  $\delta_{\downarrow} \hat{\mathbf{k}}_z$  where  $\hat{\mathbf{k}}_z$  is a unit vector in the  $z$  direction. Thus

$$\begin{aligned} f_{\mathbf{k}\sigma} &= \theta(E_F - E_{\mathbf{k}+\delta_{\sigma} \hat{\mathbf{k}}_z, \sigma}) \\ &\simeq \theta(E_F - E_{\mathbf{k}\sigma}) - \delta_{\sigma} \delta(E_F - E_{\mathbf{k}\sigma}) \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \end{aligned} \quad (23)$$

and the charge current density carried by spin  $\sigma$  electrons is

$$\begin{aligned} J_{\sigma} &= \frac{e}{\hbar N a_0^3} \sum_{\mathbf{k}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} f_{\mathbf{k}\sigma} = -\frac{e \delta_{\sigma}}{\hbar N a_0^3} \sum_{\mathbf{k}} \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \delta(E_F - E_{\mathbf{k}\sigma}) \\ &= -\frac{e \delta_{\sigma}}{\hbar a_0^3} \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{\sigma} \rho_{\sigma}(E_F) \end{aligned} \quad (24)$$

where  $\langle (\partial \epsilon_{\mathbf{k}} / \partial k_z)^2 \rangle_{\sigma}$  is an average over the  $\sigma$  spin Fermi surface and  $\rho_{\sigma}(E_F)$  is the density of  $\sigma$  spin states per atom at the Fermi energy. We shall also encounter the following related quantities;

$$\begin{aligned} K_{\sigma} &= \frac{1}{N \Delta^2 a_0^3} \sum_{\mathbf{k}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} f_{\mathbf{k}\sigma} \\ &= \frac{\hbar J_{\sigma}}{\Delta^2 e} \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right\rangle_{\sigma} \left/ \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{\sigma} \right. \end{aligned} \quad (25)$$

$$\begin{aligned} L_{\sigma} &= \frac{1}{N \Delta^3 a_0^3} \sum_{\mathbf{k}} \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^3 f_{\mathbf{k}\sigma} \\ &= \frac{\hbar J_{\sigma}}{\Delta^3 e} \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^4 \right\rangle_{\sigma} \left/ \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{\sigma} \right. \end{aligned} \quad (26)$$

To derive equations (25) and (26),  $\delta_{\sigma}$  has been eliminated using equation (24).

To solve equation (22) for  $\hbar\omega'_{\mathbf{q}}$  we expand the right-hand side of the equation in powers of  $(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \hbar\omega'_{\mathbf{q}})/\Delta$  and make the further expansions

$$\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} = q \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} + \frac{1}{2} q^2 \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} + \frac{1}{6} q^3 \frac{\partial^3 \epsilon_{\mathbf{k}}}{\partial k_z^3} \cdots \quad (27)$$

$$\hbar\omega'_{\mathbf{q}} = Bq + Dq^2 + Eq^3 + \cdots \quad (28)$$

in powers of  $q$ . We retain all terms up to  $q^3$  except those involving  $B^2$ ; the coefficients  $B$  and  $E$  are proportional to the current and we keep only terms linear in the current. Hence we find a solution of equation (22) in the form (28) with

$$\begin{aligned} B &= \frac{1}{N_{\uparrow} - N_{\downarrow}} \sum_{\mathbf{k}} (f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow}) \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \\ &= \frac{N a_0^3}{N_{\uparrow} - N_{\downarrow}} \frac{\hbar}{e} (J_{\uparrow} - J_{\downarrow}) \end{aligned} \quad (29)$$

$$\begin{aligned} D &= \frac{1}{N_{\uparrow} - N_{\downarrow}} \left[ \frac{1}{2} \sum_{\mathbf{k}} (f_{\mathbf{k}\uparrow} + f_{\mathbf{k}\downarrow}) \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right. \\ &\quad \left. - \frac{1}{\Delta} \sum_{\mathbf{k}} (f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow}) \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right] \end{aligned} \quad (30)$$

$$\begin{aligned} E &= -\frac{a_0^2 B}{6} + \frac{B}{(N_{\uparrow} - N_{\downarrow}) \Delta} \\ &\quad \times \left[ \sum_{\mathbf{k}} (f_{\mathbf{k}\uparrow} + f_{\mathbf{k}\downarrow}) \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} - \frac{3}{\Delta} \sum_{\mathbf{k}} (f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow}) \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right] \\ &\quad - U a_0^3 \sum_{\sigma} (K_{\sigma} - \sigma L_{\sigma}). \end{aligned} \quad (31)$$

Here  $N_{\sigma}$  is the total number of  $\sigma$  spin electrons so that  $N_{\sigma} = N\langle n_{\sigma} \rangle$ .

In the absence of spin–orbit coupling the expression for  $B$  in terms of spin current is a general exact result even in the



presence of disorder, as shown in the appendix. The coefficient  $D$  is the standard RPA spin wave stiffness constant (e.g. [16]). We note that, in the limit  $\Delta \rightarrow \infty$ ,  $E$  takes the simple form  $-a_0^2 B/6$ .

On restoring the correct dimensions (as indicated after equation (1)) to the expression for  $\omega_1$  in equation (11) we may determine the coefficients  $a$  and  $a_1$  by comparing with the equation

$$\hbar\omega_{\mathbf{q}} = 2\mu_B B_{\text{ext}} + Bq + Dq^2 + Eq^3. \quad (32)$$

From the coefficient of  $q$  we have

$$a + \alpha_1 b_{\text{ext}} = B/(2\mu_B \mu_0 m_s l_{\text{ex}}). \quad (33)$$

$a$  and  $B$  are both determined directly from the spin current  $JP$  independently of a particular model (see the appendix) so that  $b_{\text{ext}}$  should not enter their relationship. We conclude quite generally that  $\alpha_1 = 0$ . In this case we find that on combining equations (33) and (29), and noting that  $m_s = -\mu_B(N_{\uparrow} - N_{\downarrow})/Na_0^3$ , equation (2) is obtained as expected. In section 3.2 we show explicitly for the present model that  $\alpha_1 = 0$ . This conflicts with the results of [10] and [13]. From the coefficients of  $q^2$  in equations (11) and (32) we find  $1 + \alpha_2 b_{\text{ext}} = D/(4\mu_B A/m_s)$ . Thus an external field slightly disturbs the standard relation  $A = Dm_s/4\mu_B$ . However in the spirit of the LLG equation we take  $A$  and  $m_s$ , which enter the units of length and time used in equation (1), to be constants of the ferromagnetic material in zero external field. The coefficients of  $q^3$  in equations (11) and (32) yield the relation (taking  $\alpha_1 = 0$ ),

$$-a_1 + \alpha_2 a = E/(2\mu_B \mu_0 m_s l_{\text{ex}}^3). \quad (34)$$

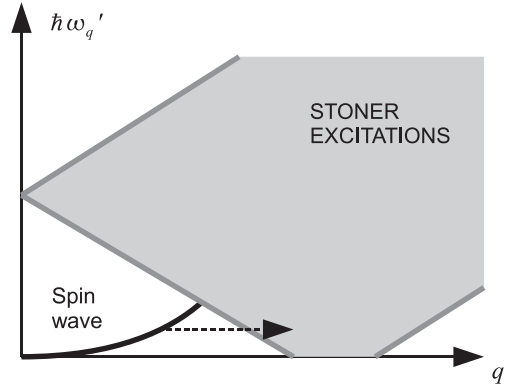
We defer calculation of  $\alpha_2$  until section 3.2 and the result is given in equation (44). Combining this with equations (34) and (31) we find

$$2\mu_B \mu_0 m_s l_{\text{ex}}^3 a_1 = \frac{a_0^2 B}{6} - \frac{2BD}{\Delta} + Ua_0^3 \sum_{\sigma} (K_{\sigma} - \sigma L_{\sigma}). \quad (35)$$

We have thus derived an explicit expression, for a simple model, for the coefficient  $a_1$  of a non-adiabatic spin torque term which appears in the LLG equation (1). We have neglected the effect of disorder due to impurities. In the absence of spin-orbit coupling the expression for the adiabatic torque coefficient  $a$ , given by equation (2), is exact even in presence of impurities. In section 3.2 we shall calculate further non-adiabatic torque terms, with coefficients  $f_1$  and  $g_1$ , as well as damping coefficients  $\alpha$ ,  $\alpha'_1$  and  $\alpha'_2$ . In the present model all these depend on impurity scattering for their existence.

### 3.2. Spin wave lifetime

The solutions of equation (22) are shown schematically in figure 1. They include the spin wave dispersion curve and the continuum of Stoner excitations  $c_{\mathbf{k}+\mathbf{q}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow} |0\rangle$  with energies  $E_{\mathbf{k}+\mathbf{q}\downarrow} - E_{\mathbf{k}\uparrow}$ . The Zeeman gap  $2\mu_B B_{\text{ext}}$  in the spin wave energy at  $\mathbf{q} = 0$  does not appear because we have plotted  $\hbar\omega'_{\mathbf{q}}$  rather



**Figure 1.** Spin-flip excitations from the ferromagnetic ground state. The dotted arrow shows the mechanism of decay of a spin wave into Stoner excitations which is enabled by the impurity potential  $V_1$ .

than  $\hbar\omega_{\mathbf{q}}$  (see equation (19)). Within the present RPA the spin wave in a pure metal has infinite lifetime outside the continuum and cannot decay into Stoner excitations owing to conservation of the momentum  $\mathbf{q}$ . However, when the perturbation  $V_1$  due to impurities is introduced (see equation (16)), crystal momentum is no longer conserved and such decay processes can occur. These are shown schematically by the dotted arrow in figure 1. If the bottom of the  $\downarrow$  spin band lies above the Fermi level there is a gap in the Stoner spectrum and for a low energy (small  $q$ ) spin wave such processes cannot occur. However the spin-flip potential  $V_2$  enables the spin wave to decay into single particle excitations  $c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}\sigma} |0\rangle$  about each Fermi surface and these do not have an energy gap.

The inverse lifetime  $\tau_{\mathbf{q}}^{-1}$  of a spin wave of wavevector  $\mathbf{q}$  is thus given simply by the ‘golden rule’ in the form

$$\tau_{\mathbf{q}}^{-1} = \frac{2\pi}{\hbar} N_{\text{imp}} (T_1 + T_2) \quad (36)$$

where  $N_{\text{imp}}$  is the number of impurity sites and

$$\begin{aligned} T_1 &= \sum_{\mathbf{k}\mathbf{p}} |\langle 0 | c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{p}\downarrow} V_1 | \mathbf{q} \rangle|^2 f_{\mathbf{k}\uparrow} (1 - f_{\mathbf{p}\downarrow}) \\ &\quad \times \delta(\hbar\omega_{\mathbf{q}} - E_{\mathbf{p}\downarrow} + E_{\mathbf{k}\uparrow}) \\ T_2 &= \sum_{\mathbf{k}\mathbf{p}\sigma} |\langle 0 | c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{p}\sigma} V_2 | \mathbf{q} \rangle|^2 f_{\mathbf{k}\sigma} (1 - f_{\mathbf{p}\sigma}) \\ &\quad \times \delta(\hbar\omega_{\mathbf{q}} - \epsilon_{\mathbf{p}} + \epsilon_{\mathbf{k}}). \end{aligned} \quad (37)$$

We first consider  $T_1$  and, using equations (16) and (18), we find

$$\begin{aligned} \langle 0 | c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{p}\downarrow} V_1 | \mathbf{q} \rangle &= \frac{N_{\mathbf{q}}}{N} f_{\mathbf{k}\uparrow} (1 - f_{\mathbf{p}\downarrow}) \\ &\quad \times [A_{\mathbf{k}} v_{\downarrow} (1 - f_{\mathbf{p}\downarrow}) - A_{\mathbf{p}-\mathbf{q}} v_{\uparrow} f_{\mathbf{p}-\mathbf{q}\uparrow}] \\ &= \frac{N_{\mathbf{q}}}{N} f_{\mathbf{k}\uparrow} (1 - f_{\mathbf{p}\downarrow}) (A_{\mathbf{k}} v_{\downarrow} - A_{\mathbf{p}-\mathbf{q}} v_{\uparrow}) \end{aligned} \quad (38)$$

for small  $q$ . The last line follows from two considerations. Firstly, because of the  $\delta$ -function in equations (37) we can consider the states  $\mathbf{k}\uparrow$  and  $\mathbf{p}\downarrow$  to be close to their respective Fermi surfaces. Secondly the  $\downarrow$  spin Fermi surface lies within

the  $\uparrow$  Fermi surface and  $q$  is small. Hence

$$T_1 = \frac{N_q^2}{N^2} \sum_{\mathbf{k}\mathbf{p}} f_{\mathbf{k}\uparrow} (1 - f_{\mathbf{p}\downarrow}) \delta(\hbar\omega_{\mathbf{q}} - E_{\mathbf{p}\downarrow} + E_{\mathbf{k}\uparrow}) \times (A_{\mathbf{k}}v_{\downarrow} - A_{\mathbf{p}-\mathbf{q}}v_{\uparrow})^2. \quad (39)$$

To evaluate this expression in the case when a current flows we use the distribution function  $f_{\mathbf{k}\sigma}$  given by equation (23). Thus, neglecting a term proportional to the square of the current, we have

$$T_1 = \frac{N_q^2}{N^2} \sum_{\mathbf{k}\mathbf{p}} \delta(\hbar\omega_{\mathbf{q}} - E_{\mathbf{p}\downarrow} + E_{\mathbf{k}\uparrow}) \times (A_{\mathbf{k}}v_{\downarrow} - A_{\mathbf{p}-\mathbf{q}}v_{\uparrow})^2 \left[ \theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow})\theta(E_{\mathbf{p}\downarrow} - E_{\mathbf{F}}) - \delta_{\uparrow}\theta(E_{\mathbf{p}\downarrow} - E_{\mathbf{F}})\delta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow}) \frac{\partial\epsilon_{\mathbf{k}}}{\partial k_z} + \delta_{\downarrow}\theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow})\delta(E_{\mathbf{F}} - E_{\mathbf{p}\downarrow}) \frac{\partial\epsilon_{\mathbf{p}}}{\partial p_z} \right]. \quad (40)$$

We wish to expand this expression, and a similar one for  $T_2$ , in powers of  $q$  to  $O(q^3)$  so that we can compare with the phenomenological expression (equations (11)) for the imaginary part of the spin wave frequency, which is given by  $\tau_q^{-1}/2$ . It is straightforward to expand the second factor in the above sum by using equations (21) and (28). We shall show that the contribution to  $T_1$  of the first term in square brackets in equation (40) leads to a contribution proportional to spin wave frequency  $\omega_{\mathbf{q}}$ . Together with a similar contribution to  $T_2$  it yields the Gilbert damping factor  $\alpha$  as well as the coefficients  $\alpha'_1, \alpha'_2$  of the terms in equations (11) which give the  $\mathbf{q}$  dependence of the damping. The remaining terms in equation (40) yield the spin-transfer torque coefficients  $f, f_1$  and  $g_1$ .

The normalization factor  $N_q^2$  which appear in equation (40) leads naturally to the factor  $(1 - \alpha_1 q - \alpha_2 q^2)^{-1}$  which appears in equations (11). From equation (18) it is given by

$$1 = \langle \mathbf{q} | \mathbf{q} \rangle = \frac{N_q^2}{N} \sum_{\mathbf{k}} (A_{\mathbf{k}}^2 f_{\mathbf{k}\uparrow} - A_{\mathbf{k}-\mathbf{q}}^2 f_{\mathbf{k}\downarrow}). \quad (41)$$

By expanding  $A_{\mathbf{k}-\mathbf{q}}^2$  in powers of  $q$ , and using equation (23), we find to  $O(q^2)$  that

$$N_q^{-2} = (N_{\uparrow} - N_{\downarrow}) \left\{ 1 + \frac{\mathbf{q}^2}{\Delta^2(N_{\uparrow} - N_{\downarrow})} \sum_{\mathbf{k}} \left( \frac{\partial\epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \times [\theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow}) - \theta(E_{\mathbf{F}} - E_{\mathbf{k}\downarrow})] \right\}. \quad (42)$$

We deduce that

$$\alpha_1 = 0 \quad (43)$$

and

$$\alpha_2 = -\frac{1}{l_{\text{ex}}^2 \Delta^2 (N_{\uparrow} - N_{\downarrow})} \sum_{\mathbf{k}} \left( \frac{\partial\epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \times [\theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow}) - \theta(E_{\mathbf{F}} - E_{\mathbf{k}\downarrow})]. \quad (44)$$

The result  $\alpha_1 = 0$ , which was predicted on general grounds in section 3.1 and in appendix 1, arises here through the

absence of a  $q$  term, proportional to current, in the spin wave normalization factor. In the derivation of equation (42) this occurs due to a cancellation involving the  $Bq$  terms in the spin energy, which appears in  $A_{\mathbf{k}}$ . Without this cancellation we would have  $\alpha_1 = 2B/l_{\text{ex}}\Delta$  which is of the form obtained by Tserkovnyak *et al* [10] and Thorwart and Egger [13].

We now return to the programme for calculating the LLG coefficients  $\alpha, \alpha'_1, \alpha'_2, f, f_1, g_1$  which was outlined after equation (40). We have seen that the  $q$  dependence of  $N_q^2$  corresponds to the prefactor in equations (11). Hence to determine the coefficients listed above we can take  $N_q^2 = N_0^2 = (N_{\uparrow} - N_{\downarrow})^{-1}$  in  $T_1$  and  $T_2$  when we expand terms in powers of  $q$  to substitute in equation (36) and compare with equations (11). We first consider the case  $q = 0$  in order to determine the Gilbert damping factor  $\alpha$ . Thus only the first term in square brackets in equation (40) contributes, since  $\partial\epsilon_{\mathbf{k}}/\partial k_z$  is an odd function  $k_z$ , and

$$T_1(\mathbf{q} = 0) = \frac{4v^2 \overline{\cos^2 \theta}}{N_{\uparrow} - N_{\downarrow}} N^{-2} \sum_{\mathbf{k}\mathbf{p}} \delta(\hbar\omega_0 - E_{\mathbf{p}\downarrow} + E_{\mathbf{k}\uparrow}) \times \theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow})\theta(E_{\mathbf{p}\downarrow} - E_{\mathbf{F}}) \quad (45)$$

where  $\overline{\cos^2 \theta}$  is an average over the angle appearing in the impurity potential  $V$  (equations (16)) and we shall assume  $\overline{\cos \theta} = 0$ . The summations in equation (45) may be replaced by energy integrals involving the density of states of per atom  $\rho_{\sigma}(\epsilon)$  of the states  $E_{\mathbf{k}\sigma}$ . Then, to order  $(\hbar\omega_0)^2$ ,

$$T_1(\mathbf{q} = 0) = \left[ \frac{4v^2 \overline{\cos^2 \theta}}{N_{\uparrow} - N_{\downarrow}} \right] \times [\hbar\omega_0 \rho_{\uparrow} \rho_{\downarrow} + \frac{1}{2} (\hbar\omega_0)^2 (\rho_{\uparrow} \rho'_{\downarrow} - \rho'_{\uparrow} \rho_{\downarrow})] \quad (46)$$

where  $\rho_{\sigma}(\epsilon)$  and its derivative  $\rho'_{\sigma}(\epsilon)$  are evaluated at  $\epsilon = E_{\mathbf{F}}$ . Similarly

$$T_2(\mathbf{q} = 0) = \left[ \frac{v^2 \overline{\sin^2 \theta}}{N_{\uparrow} - N_{\downarrow}} \right] \hbar\omega_0 (\rho_{\uparrow}^2 + \rho_{\downarrow}^2) \quad (47)$$

and no  $\omega_0^2$  terms appear. We have included the  $\omega_0^2$  term in equation (46) merely because it corresponds to a term  $\mathbf{s} \times (\mathbf{s} \times \frac{\partial^2 \mathbf{s}}{\partial t^2})$  in the LLG equation whose existence was noted by Thorwald and Egger [13]. We shall not pursue terms with second order time derivatives any further. Since the imaginary part of the spin wave frequency is given by  $\tau_q^{-1}/2$  it follows from equations (11), (36), (46) and (47) that

$$\alpha = \frac{\pi c v^2}{\langle n_{\uparrow} - n_{\downarrow} \rangle} [4 \overline{\cos^2 \theta} \rho_{\uparrow} \rho_{\downarrow} + \overline{\sin^2 \theta} (\rho_{\uparrow}^2 + \rho_{\downarrow}^2)], \quad (48)$$

where  $c = N_{\text{imp}}/N$  is the concentration of impurities, in agreement with Kohno *et al* [8] and Duine *et al* [15]. If the direction of the spin quantization axis of the impurities is distributed randomly  $\overline{\cos^2 \theta} = 1/3, \overline{\sin^2 \theta} = 2/3$  so that  $\alpha$  is proportional to  $(\rho_{\uparrow} + \rho_{\downarrow})^2$ .

To investigate the  $\mathbf{q}$  dependence of Gilbert damping, and thus evaluate  $\alpha'_1$  and  $\alpha'_2$  in equations (11), the second factor in the summation of equation (40) must be expanded in powers of  $q$ . All the terms which contribute to the sum are of separable form  $g(\mathbf{k})h(\mathbf{p})$ . The contribution to  $T_1$  of interest

here, proportional to  $\omega_{\mathbf{q}}$ , again arises from the first term in square brackets in equation (40), and similarly for  $T_2$ . The summations required in equation (40) are of the form

$$\sum_{\mathbf{k}\mathbf{p}} \delta(\hbar\omega_{\mathbf{q}} - E_{\mathbf{p}\downarrow} + E_{\mathbf{k}\uparrow})\theta(E_{\mathbf{F}} - E_{\mathbf{k}\uparrow})\theta(E_{\mathbf{p}\downarrow} - E_{\mathbf{F}})g(\mathbf{k})h(\mathbf{p})$$

$$= \langle g(\mathbf{k}) \rangle_{\uparrow} \langle h(\mathbf{k}) \rangle_{\downarrow} \rho_{\uparrow} \rho_{\downarrow} \hbar\omega_{\mathbf{q}} \quad (49)$$

where  $\langle g(\mathbf{k}) \rangle_{\sigma} = N^{-1} \sum_{\mathbf{k}} g(\mathbf{k})\delta(E_{\mathbf{F}} - E_{\mathbf{k}\sigma})$  is an average over the Fermi surface, as used previously in section 3.1. After some algebra we find

$$\alpha'_1 = 2B\alpha/\Delta l_{\text{ex}} \quad (50)$$

$$\alpha'_2 = \frac{\pi c}{\langle n_{\uparrow} - n_{\downarrow} \rangle l_{\text{ex}}^2 \Delta^2} \left\{ \rho_{\uparrow} \rho_{\downarrow} (u^2 + 5v^2 \overline{\cos^2 \theta}) \right.$$

$$\times \sum_{\sigma} \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{\sigma} - 2\rho_{\uparrow} \rho_{\downarrow} \Delta v^2 \overline{\cos^2 \theta} \sum_{\sigma} \sigma \left\langle \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right\rangle_{\sigma}$$

$$- v^2 \overline{\sin^2 \theta} \left[ \Delta \sum_{\sigma} \sigma \rho_{\sigma}^2 \left\langle \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right\rangle_{\sigma} \right.$$

$$\left. - 3 \sum_{\sigma} \rho_{\sigma}^2 \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{\sigma} \right] \left. \right\} + \frac{2D\alpha}{\Delta l_{\text{ex}}^2}. \quad (51)$$

We note that, unlike  $\alpha$  and  $\alpha'_1$ , the coefficient  $\alpha'_2$  is non-zero even when the spin-dependent part of the impurity potential,  $v$ , is zero. In this case the damping of a spin wave of frequency  $\omega$  and small wavevector  $q$  is proportional to  $\rho_{\uparrow} \rho_{\downarrow} u^2 \omega q^2$ . In zero external field  $\omega \sim q^2$  so that the damping is of order  $q^4$ . This damping due to spin-independent potential scattering by impurities was analysed in detail by Yamada and Shimizu [17]. One of the Fermi surface averages in equation (51) is easily evaluated using equations (14) and (17). Thus

$$\left\langle \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right\rangle_{\sigma} = -\frac{a_0^2}{3} \langle \epsilon_{\mathbf{k}} \rangle_{\sigma}$$

$$= -\frac{a_0^2}{3} (E_f - U \langle n_{-\sigma} \rangle + \sigma \mu_B B_{\text{ext}}). \quad (52)$$

In the spirit of the LLG equation we should take  $B_{\text{ext}} = 0$  in evaluating the coefficients  $\alpha'_2$ .

We now turn to the evaluation of the non-adiabatic spin-transfer torque coefficients  $f$ ,  $f_1$  and  $g_1$ . These arise from the second and third terms in square brackets in equation (40), and in a similar expression for  $T_2$ . The summations involved in these terms differ from those in equation (49) since one  $\theta$ -function is replaced by a  $\delta$ -function. This leads to the omission of the frequency factor  $\hbar\omega_{\mathbf{q}}$ . The Fermi surface shifts  $\delta_{\sigma}$  are eliminated in favour of currents  $J_{\sigma}$  by using equation (24).

By comparing the coefficient of  $q$  in the expansion of equation (36) with that in equation (11) we find the coefficient of the Zhang–Li torque in the form

$$f = \frac{\pi c v^2}{\mu_0 m_s^2 \Delta l_{\text{ex}}} \frac{\hbar}{e} [2 \overline{\cos^2 \theta} (\rho_{\uparrow} J_{\downarrow} - \rho_{\downarrow} J_{\uparrow})$$

$$+ \overline{\sin^2 \theta} (\rho_{\downarrow} J_{\downarrow} - \rho_{\uparrow} J_{\uparrow})]. \quad (53)$$

This is in agreement with Kohno *et al* [8] and Duine *et al* [15]. In the ‘isotropic’ impurity case, with  $\overline{\cos^2 \theta} = 1/3$ ,  $\overline{\sin^2 \theta} = 2/3$ , it follows from equations (53), (48) and (2) that

$$\beta = \frac{f}{a} = \alpha \frac{2}{U(\rho_{\uparrow} + \rho_{\downarrow})}. \quad (54)$$

In the limit of a very weak itinerant ferromagnet  $\rho_{\sigma} \rightarrow \rho$ , the paramagnetic density of states, and  $U\rho \rightarrow 1$  by the Stoner criterion. Thus in this limit  $\beta = \alpha$ . Tserkovnyak *et al* [10] reached a similar conclusion. For a parabolic band it is straightforward to show from Stoner theory that  $\beta/\alpha > 1$  and may be as large as 1.5.

As discussed in section 2 the coefficient  $f_1$  is associated with spin-conserving processes, and hence involves the spin-independent potential  $u$ . The coefficient  $g_1$  is associated with spin non-conserving processes and involves  $v$ . By comparing the coefficient of  $q^3$  in the expansion of equation (36) with that in equation (11) we deduce that

$$f_1 = \frac{\pi c}{2\mu_0 m_s^2 l_{\text{ex}}^3} u^2 (K_1 + 2L_1 + M_1) \quad (55)$$

and

$$g_1 = \frac{1}{l_{\text{ex}}^2} \left( \frac{3D}{\Delta} - \frac{a_0^2}{6} \right) f + \frac{\pi c v^2}{2\mu_0 m_s^2 l_{\text{ex}}^3}$$

$$\times [\overline{\cos^2 \theta} (5K_1 + 6L_1 - M_1) + \overline{\sin^2 \theta} (3K_2 + 4L_2)]. \quad (56)$$

Here

$$K_1 = K_{\downarrow} \rho_{\uparrow} + K_{\uparrow} \rho_{\downarrow}, \quad K_2 = K_{\downarrow} \rho_{\downarrow} + K_{\uparrow} \rho_{\uparrow}$$

$$L_1 = L_{\downarrow} \rho_{\uparrow} - L_{\uparrow} \rho_{\downarrow}, \quad L_2 = L_{\downarrow} \rho_{\downarrow} - L_{\uparrow} \rho_{\uparrow}$$

$$M_1 = \frac{\hbar}{e \Delta^3} \sum_{\sigma} \left[ 2\sigma \left\langle \left( \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_z} \right)^2 \right\rangle_{-\sigma} \right.$$

$$\left. + \Delta \left\langle \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_z^2} \right\rangle_{-\sigma} \right] J_{\sigma} \rho_{-\sigma}. \quad (57)$$

This completes the derivation of expressions for all the LLG coefficients of equation (1) within the present impurity model

#### 4. The extended LLG equation applied to current-driven domain wall motion

In a previous paper [9] we introduced the  $a_1$  and  $f_1$  terms of the extended LLG equation (cf equations (1), (3) and (4)) in order to describe numerically-calculated spin-transfer torques acting on a domain wall when it is traversed by an electric current. In that work the origin of the small  $f_1$  term for a pure ferromagnetic metal was specific to the domain wall problem; it was shown to be associated with those electronic states at the bulk Fermi surface which decay exponentially as they enter the wall. The analytic derivation of  $f_1$  in section 3 (see equation (55)) is based on impurity scattering in the bulk ferromagnet and applies generally to any slowly-varying magnetization configuration. For a ferromagnetic alloy such as permalloy both mechanisms should contribute in the domain wall situation but the impurity contribution would be expected to dominate.

To describe a domain wall we must add to the right-hand side of equation (1) anisotropy terms of the form

$$-(\mathbf{s} \cdot \mathbf{e}_y) \mathbf{s} \times \mathbf{e}_y + b^{-1} (\mathbf{s} \cdot \mathbf{e}_z) \mathbf{s} \times \mathbf{e}_z, \quad (58)$$

where  $\mathbf{e}_y$  is a unit vector perpendicular to the plane of the wire. The first term corresponds to easy plane shape anisotropy for



a wire whose width is large compared with its thickness and the second term arises from a uniaxial field  $H_u$  along the wire, so that  $b = m_s/H_u$ . The solution of equation (1), with the additional terms (58), for a stationary Néel wall in the plane of the wire, with zero external field and zero current, is

$$\mathbf{s} = (\text{sech}(z/b^{1/2}), 0, -\tanh(z/b^{1/2})). \quad (59)$$

As pointed out in [9] there is no solution of the LLG equation of the form  $\mathbf{s} = \mathbf{F}(z - v_W t)$ , corresponding to a uniformly moving domain wall, when the  $f_1$  term is included. It is likely that the wall velocity oscillates about an average value, as predicted by Tatara and Kohno [18, 19] for purely adiabatic torque above the critical current density for domain wall motion. However, we may estimate the average velocity  $v_W$  using the method of [9]. The procedure is to substitute the approximate form  $\mathbf{s} = \mathbf{F}(z - v_W t)$  in the extended LLG equation (1), with the terms (58) added, take the scalar product with  $\mathbf{F} \times \mathbf{F}'$  and integrate with respect to  $z$  over the range  $(-\infty, \infty)$ . The boundary conditions appropriate to the wall are  $\mathbf{s} \rightarrow \mp \mathbf{e}_z$  as  $z \rightarrow \pm\infty$ . Hence for  $b_{\text{ext}} = 0$  we find the dimensionless wall velocity to be

$$v_W = \frac{f \int_{-\infty}^{\infty} (\mathbf{F} \times \mathbf{F}')^2 dz + f_1 \int_{-\infty}^{\infty} (\mathbf{F} \times \mathbf{F}'')^2 dz + g_1 \int_{-\infty}^{\infty} (\mathbf{F}'')^2 dz}{\alpha \int_{-\infty}^{\infty} (\mathbf{F} \times \mathbf{F}')^2 dz + \alpha'_2 \int_{-\infty}^{\infty} (\mathbf{F}'')^2 dz}. \quad (60)$$

To estimate the integrals we take  $\mathbf{F}(z)$  to have the form of the stationary wall  $\mathbf{s}(z)$  (equation (59)) and, with the physical dimensions of velocity restored, the wall velocity is given approximately by

$$v_W = v_0 \frac{\beta}{\alpha} \frac{1 + f_1(3fb)^{-1}}{1 + \alpha'_2(\alpha b)^{-1}} \quad (61)$$

where  $v_0 = \mu_B P J / (m_s e)$ . We have neglected  $g_1$  here because, like  $f$  and  $\alpha$ , it depends on spin-orbit coupling but is a factor  $(a_0/l_{\text{ex}})^2$  smaller than  $f$  (cf equations (53) and (56)).  $f_1$  and  $\alpha'_2$  are important because they do not depend on spin-orbit coupling.

It is interesting to compare  $v_W$  with the wall velocity observed in permalloy nanowires by Hayashi *et al* [20]. We first note that  $v_0$  is the velocity which one obtains very simply from spin angular momentum conservation if the current-driven wall moves uniformly without any distortion such as tilting out of the easy plane and contraction [21]. This is never the case, even if  $f_1 = 0$ ,  $\alpha'_2 = 0$ , unless  $\beta = \alpha$ . For a permalloy nanowire, with  $\mu_0 m_s = 1 \text{ T}$ ,  $v_0 = 110 P \text{ m s}^{-1}$  for  $J = 1.5 \times 10^8 \text{ A cm}^{-2}$ . Thus, from the standard theory with  $f_1 = 0$ ,  $\alpha'_2 = 0$ ,  $v_W = 110 P \beta / \alpha \text{ m s}^{-1}$  for this current density. In fact Hayashi *et al* [20] measure a velocity of  $110 \text{ m s}^{-1}$  which implies  $\beta > \alpha$  since the spin polarization  $P$  is certainly less than 1. They suggest that  $\beta$  cannot exceed  $\alpha$  and that some additional mechanism other than spin-transfer torque is operating. However in the discussion following equation (54) we pointed out that in the model calculations it is possible to have  $\beta > \alpha$ . Even if this is not the case in permalloy we can still have  $v_W > v_0$  if the last factor in equation (61) is

greater than 1 when  $f_1$  and  $\alpha'_2$  are non-zero. We can estimate terms in this factor using the observation from [20], that  $l_W = l_{\text{ex}} b^{1/2} = 23 \text{ nm}$ , where  $l_W$  is the width of the wall. From equations (53) and (55) we find  $f_1/(fb) \sim (u/v)^2 (k_F l_W)^{-2}$ , where  $k_F$  is a Fermi wavevector. In permalloy we have Fe impurities in Ni so that in the impurity potential  $u + \mathbf{v} \cdot \boldsymbol{\sigma}$  we estimate  $u \sim 1 \text{ eV}$  and  $v \sim 0.005 \text{ eV}$ . The value for  $v$  is estimated by noting that the potential  $\mathbf{v} \cdot \boldsymbol{\sigma}$  is intended to model spin-orbit coupling of the form  $\xi \mathbf{L} \cdot \boldsymbol{\sigma}$  with  $\xi \lesssim 0.1 \text{ eV}$  and  $\langle L_z \rangle_{\text{Fe}} \sim 0.05$ ,  $L_z$  being the component of orbital angular momentum in the direction of the magnetization [22]. Hence  $u/v \sim 200$  and  $k_F l_W \sim 200$  so that  $f_1/(fb) \sim 1$ .  $\alpha'_2/(\alpha b)$  is expected to be of similar magnitude. We conclude that the  $\alpha'_2$  and  $f_1$  terms in the LLG equation (1) can be important in domain wall motion and should be included in micromagnetic simulations such as OOMMF [23]. For narrower domain walls these terms may be larger than the Gilbert damping  $\alpha$  and non-adiabatic spin-transfer torque  $f$  terms which are routinely included. Reliable estimates of their coefficients are urgently required using realistic multiband models of the ferromagnetic metal or alloy.

## 5. Conclusions

The coefficients of all the terms in an extended LLG equation for a current-carrying ferromagnetic wire have been calculated for a simple model. Two of these ( $f_1$  and  $\alpha'_2$ ) are of particular interest since they do not rely on spin-orbit coupling and may sometimes dominate the usual damping and non-adiabatic spin-transfer torque terms. One term ( $\alpha_1$ ) which has been introduced by previous authors is shown rigorously to be zero, independent of any particular model. Solutions of the extended LLG equation for domain wall motion have not yet been found but the average velocity of the wall is estimated. It is pointed out that the  $f_1$  and  $\alpha'_2$  terms are very important for narrow walls and should be included in micromagnetic simulations such as OOMMF. It is shown that there is no theoretical reason why the wall velocity should not exceed the simplest spin-transfer estimate  $v_0$ , as is found to be the case in experiments on permalloy by Hayashi *et al* [20].

## Acknowledgments

We are grateful to the EPSRC for financial support through the Spin@RT consortium and to other members of this consortium for encouragement and stimulation.

## Appendix

The simple single-band impurity model used in the main text is useful for obtaining explicit expressions for all the coefficients in the LLG equation (1). Here we wish to show that some of these results are valid for a completely general system. We suppose the ferromagnetic material is described by the many-body Hamiltonian

$$H = H_1 + H_{\text{int}} + H_{\text{ext}} \quad (\text{A.1})$$

where  $H_1$  is a one-electron Hamiltonian of the form

$$H_1 = H_k + H_{so} + V. \quad (\text{A.2})$$

Here  $H_k$  is the total electron kinetic energy,  $H_{so}$  is the spin-orbit interaction,  $V$  is a potential term,  $H_{int}$  is the coulomb interaction between electrons and  $H_{ext}$  is due to an external magnetic field  $B_{ext}$  in the  $z$  direction. Thus

$$H_{ext} = -2\mu_B S_0^z B_{ext} \quad (\text{A.3})$$

where  $S_z^0$  is the  $z$  component of total spin. Both  $H_{so}$  and  $V$  can contain disorder. Since we are interested in the energy and lifetime of a long wavelength spin wave we consider the spin wave pole, for small  $q$ , of the dynamical susceptibility.

$$\chi(\mathbf{q}, \omega) = \int dt \langle \langle S_{\mathbf{q}}^-(t), S_{-\mathbf{q}}^+ \rangle \rangle e^{-i\omega t} \quad (\text{A.4})$$

( $\omega_- = \omega - i\epsilon$ ) where  $S_{\mathbf{q}}^{\pm} = S_{\mathbf{q}}^x \pm iS_{\mathbf{q}}^y$  are Fourier components of the total transverse spin density. Here

$$\langle \langle S_{\mathbf{q}}^-(t), S_{-\mathbf{q}}^+ \rangle \rangle = \frac{i}{\hbar} \langle [S_{\mathbf{q}}^-(t), S_{-\mathbf{q}}^+] \rangle \theta(t). \quad (\text{A.5})$$

In general we shall take the average  $\langle \rangle$  in a steady state in which a charge current density  $J$  is flowing in the  $\mathbf{q}$  direction. Following the general method of Edwards and Fisher [24] we use equations of motion to find that

$$\chi(\mathbf{q}, \omega) = -\frac{2\langle S_0^z \rangle}{\hbar(\omega - b_{ext})} + \frac{1}{\hbar^2(\omega - b_{ext})^2} \times \{ \chi_c(\mathbf{q}, \omega) - \langle [C_{\mathbf{q}}^-, S_{-\mathbf{q}}^+] \rangle \} \quad (\text{A.6})$$

where  $\hbar b_{ext} = 2\mu_B B_{ext}$ ,  $C_{\mathbf{q}}^- = [S_{\mathbf{q}}^-, H_1]$  and

$$\chi_c(q, \omega) = \int dt \langle \langle C_{\mathbf{q}}^-(t), C_{-\mathbf{q}}^+ \rangle \rangle e^{-i\omega t}. \quad (\text{A.7})$$

For small  $q$  and  $\omega$ ,  $\chi$  is dominated by the spin wave pole, so that

$$\chi(q, \omega) = -\frac{2\langle S_0^z \rangle}{\hbar(\omega - b_{ext} - \omega_q)} \quad (\text{A.8})$$

where  $b_{ext} + \omega_q$  is the spin wave frequency, in general complex corresponding to a finite lifetime. Following [24] we compare (A.6) and (A.8) in the limit  $\omega_q \ll \omega - b_{ext}$  to obtain the general result

$$\omega_q = -\frac{1}{2\langle S_0^z \rangle \hbar} \left\{ \lim_{\omega \rightarrow b_{ext}} \chi_c(q, \omega) - \langle [C_{\mathbf{q}}^-, S_{-\mathbf{q}}^+] \rangle \right\}. \quad (\text{A.9})$$

Edwards and Fisher [24] were concerned with  $\text{Re } \omega_q$  whereas Kamberský [25] derived the above expression for  $\text{Im } \omega_q$  for the case  $q = 0$ , and zero current flow. His interest was Gilbert damping in ferromagnetic resonance. Essentially the same result was obtained earlier in connection with electron spin resonance, by Mori and Kawasaki [26], see also Oshikawa and Affleck [27]. Since  $S_{\mathbf{q}}^-$  commutes with the potential term  $V$ , even in the presence of disorder, we have

$$C_{\mathbf{q}}^- = [S_{\mathbf{q}}^-, H_1] = [S_{\mathbf{q}}^-, H_k] + [S_{\mathbf{q}}^-, H_{so}]. \quad (\text{A.10})$$

For simplicity we now neglect spin-orbit coupling so that

$$C_{\mathbf{q}}^- = [S_{\mathbf{q}}^-, H_k] = \hbar q J_{\mathbf{q}}^- \quad (\text{A.11})$$

where the last equation defines the spin current operator  $J_{\mathbf{q}}^-$ . For a general system, with the  $n$ th electron at position  $\mathbf{r}_n$  with spin  $\sigma_n$  and momentum  $\mathbf{p}_n$ ,

$$S_{\mathbf{q}}^- = \sum_n e^{i\mathbf{q}\cdot\mathbf{r}_n} \sigma_n^-, \quad H_k = \sum_n \mathbf{p}_n^2 / 2m. \quad (\text{A.12})$$

Hence, from equations (A.11) and (A.12),

$$\langle [C_{\mathbf{q}}^-, S_{-\mathbf{q}}^+] \rangle = N \frac{\hbar^2 q^2}{2m} + 2\hbar \sum_n \langle \sigma_n^z \mathbf{v}_n \rangle \cdot \mathbf{q} \quad (\text{A.13})$$

where  $N$  is the total number of electrons and  $\mathbf{v}_n = \mathbf{p}_n/m$  is the electron velocity, so that  $e \sum_n \langle \sigma_n^z \mathbf{v}_n \rangle$  is the total spin current. Hence from equation (A.9), we find

$$\omega_q = \frac{\hbar q^2}{2\langle S_0^z \rangle} \left[ \frac{N}{2m} - \lim_{\omega \rightarrow b_{ext}} \chi_J(0, \omega) \right] + \frac{Bq}{\hbar} \quad (\text{A.14})$$

with

$$B = \hbar \mu_B P J / e m_s. \quad (\text{A.15})$$

This expression for  $B$  has been obtained by Bazaliy *et al* [2] and Fernández-Rossier *et al* [14] for simple parabolic band,  $s$ - $d$  and Hubbard models. The derivation here is completely general for any ferromagnet, even in the presence of disorder due to impurities or defects, as long as spin-orbit coupling is neglected. Equations (2) and (A.15) are both valid for arbitrary  $b_{ext}$ , so that in equation (33) we must have  $\alpha_1 = 0$ .

*Note added in proof.* Tserkovnyak *et al* [28] have recently given a detailed discussion of the coefficient  $\alpha_2'$  in equation (1).

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