Extended *s-d* model for magnetization dynamics of strongly noncollinear configurations

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(Received 26 September 2008; published 26 February 2009)

In the conventional *s-d* model of magnetization dynamics, it is assumed that for an adiabatic situation the *s* magnetization is ferromagnetically aligned to the *d* magnetization. For configurations with strong noncollinearity in the *d* magnetization, this no longer holds true for all cases. In the present paper it is shown that, as a consequence of this noncollinearity between the adiabatic *s* and *d* magnetizations, there arise several additional torques in the micromagnetic equation of motion for the *d* magnetization. The equation is solved for a Néel wall driven by an external field and/or a spin-polarized current, yielding a correction term to the result of the conventional theory. By calculations with the *ab initio* density-functional electron theory, the magnitude of the correction term is estimated. It is concluded that for 3*d* metals the effects of the additional torques are very small except possibly for atomic-scale noncollinearities or for the long-term trajectories of complicated magnetization configurations.

DOI: 10.1103/PhysRevB.79.052406 PACS number(s): 75.40.Gb, 75.10.Lp, 75.40.Mg

The dynamics of noncollinear magnetization configurations driven by external magnetic fields or spin-polarized currents is often investigated by micromagnetic simulations with the Landau-Lifshitz-Gilbert (LLG) equation of motion.[1] The influence of a spin-polarized transport current thereby is treated by including two spin-torque terms (an adiabatic and a nonadiabatic spin torque) into the LLG equation. These two terms which originally have been introduced in a phenomenological manner[2] have been justified within the *s-d* model of Zhang and Li.[3] In the *s-d* model the electronic states are subdivided into "*s*" states and "*d*" states. The "*s*" states represent those electronic states (conduction electrons states) which dominate the electrical conductivity. For 3*d* (4*f*) metals these are the 4*s* and 4*p* (5*d*, 6*s*, and 6*p*) states which are strongly delocalized, i.e., itinerant. The magnetization related to these states is denoted by $\mathbf{m}(\mathbf{r},t)$. The symbol "*d*" stands for the more localized states which are the 3*d* (4*f*) states and which contribute a magnetization denoted as $\mathbf{M}_d(\mathbf{r},t)$ so that the total magnetization is given by

$$\mathbf{M}(\mathbf{r},t) = \mathbf{M}_d(\mathbf{r},t) + \mathbf{m}(\mathbf{r},t). \tag{1}$$

In the *s-d* model the dynamics of $\mathbf{M}_d(\mathbf{r},t)$ is calculated in two steps. In the first step the response of $\mathbf{m}(\mathbf{r},t)$ to a given $\mathbf{M}_d(\mathbf{r},t)$ is calculated. As soon as $\mathbf{m}(\mathbf{r},t)$ is not completely aligned to $\mathbf{M}_d(\mathbf{r},t)$, a torque density will be exerted on $\mathbf{M}_d(\mathbf{r},t)$ via the *s-d* exchange interaction,[3]

$$\mathbf{T} = \frac{1}{\tau_{\mathrm{ex}} M_d}\mathbf{m} \times \mathbf{M}_d, \tag{2}$$

with

$$\tau_{\mathrm{ex}} = \frac{\hbar}{S J_{\mathrm{ex}}}. \tag{3}$$

In Eq. (3) S is the effective spin quantum number which is related to the localized atomic moments, and J_{ex} denotes the *s-d* exchange coupling. In the second step the dynamics of $\mathbf{M}_d$ is determined from a LLG-type equation of motion,

$$\frac{\partial \mathbf{M}_d}{\partial t} = -\gamma \mathbf{M}_d \times \mathbf{H}_{\mathrm{eff},d} + \frac{1}{M_d}\mathbf{M}_d \times \alpha \frac{\partial \mathbf{M}_d}{\partial t} + \mathbf{T}, \tag{4}$$

where γ is the gyromagnetic ratio, $\mathbf{H}_{\mathrm{eff},d}$ is the effective field acting on $\mathbf{M}_d$, and α denotes the Gilbert damping constant.

In the conventional *s-d* model[3] $\mathbf{m}(\mathbf{r},t)$ is not completely aligned to $\mathbf{M}_d(\mathbf{r},t)$ because the conduction electrons experience spin-flip scattering processes [characterized by a spin-flip scattering time τ_{sf}, see Eq. (7)] and thus cannot follow $\mathbf{M}_d(\mathbf{r},t)$ instantaneously (adiabatically). To investigate this further, $\mathbf{m}$ is subdivided into two parts,

$$\mathbf{m}(\mathbf{r},t) = \mathbf{m}_0(\mathbf{r},t) + \delta\mathbf{m}(\mathbf{r},t). \tag{5}$$

Here $\mathbf{m}_0$ would be the only contribution to $\mathbf{m}$ if τ_{sf} was much smaller than the characteristic time scale τ for the dynamics of $\mathbf{M}_d$ so that $\mathbf{m}(\mathbf{r},t)$ could follow $\mathbf{M}_d(\mathbf{r},t)$ instantaneously (adiabatically). A nonadiabatic contribution $\delta\mathbf{m}(\mathbf{r},t)$ arises when the inequality $\tau_{\mathrm{sf}} \ll \tau$ is not fulfilled. In the first calculational step of the *s-d* model, $\mathbf{m}(\mathbf{r},t)$ is determined for given $\mathbf{M}_d(\mathbf{r},t)$ in a phenomenological approach from a local generalized continuity equation,[3]

$$\frac{\partial \mathbf{m}}{\partial t} = \mathbf{T}_m, \tag{6}$$

where

$$\mathbf{T}_m = -\nabla\mathbf{J} - \mathbf{T} - \frac{\delta\mathbf{m}}{\tau_{\mathrm{sf}}} \tag{7}$$

is the total torque density acting on $\mathbf{m}$. $\mathbf{J}$ is the spin-current density of the conduction electrons, and in analogy to Eq. (5) it is subdivided into an adiabatic part $\mathbf{J}_0$ and a nonadiabatic contribution $\delta\mathbf{J}$,

$$\mathbf{J}(\mathbf{r},t) = \mathbf{J}_0(\mathbf{r},t) + \delta\mathbf{J}(\mathbf{r},t), \tag{8}$$

whereby in the variant of Zhang and Li[3] the contribution of $\delta\mathbf{J}$ is finally neglected (which we will also do). The last term in Eq. (7) represents the spin relaxation due to spin-flip scattering of the conduction electrons.

In the conventional *s-d* model only the electronic states which are close to the Fermi surface and hence participate in

the transport current have been taken into account. Then $\mathbf{J}_0$ is approximated by

$$\mathbf{J}_0(\mathbf{r},t) = -\frac{\mu_B P}{e_e}\mathbf{j}_e \otimes \mathbf{e}(\mathbf{r},t), \tag{9}$$

where the symbol $\otimes$ represents the outer product, μ_B, e_e, and P denote Bohr's magneton, the elementary charge, and the norm of the spin-current polarization, $\mathbf{j}_e$ is the current density, and $\mathbf{e}(\mathbf{r},t)$ is defined via $\mathbf{m}_0(\mathbf{r},t)=m_0\mathbf{e}(\mathbf{r},t)$ with a constant prefactor m_0. Finally, an essential assumption is that

$$\frac{\mathbf{m}_0(\mathbf{r},t)}{m_0} = \frac{\mathbf{M}_d(\mathbf{r},t)}{M_d}, \tag{10}$$

i.e., that the adiabatic part of the conduction-electron magnetization is parallel to the d magnetization.

It has been outlined in Ref. 4 that in reality not only the conduction-electron states close to E_F contribute to $\mathbf{J}_0$ but all itinerant states. For situations without a transport current, the term $\nabla\cdot\mathbf{J}_0$ then describes[5–7] a torque density resulting from the dependence of the kinetic energy of the itinerant states on $\mathbf{e}(\mathbf{r},t)$. This *kinetic exchange torque density* $\mathbf{T}_{ex}$ competes with the s-d exchange torque density $\mathbf{T}$ given by Eq. (2). Whereas the latter torque density wants to align $\mathbf{m}_0(\mathbf{r},t)$ to $\mathbf{M}_d(\mathbf{r},t)$, the former torque tries to smooth out any spatial noncollinearity within $\mathbf{m}_0(\mathbf{r},t)$ induced by the noncollinearity of $\mathbf{M}_d(\mathbf{r},t)$. The result of this competition is a noncollinearity between $\mathbf{m}_0(\mathbf{r},t)$ and $\mathbf{M}_d(\mathbf{r},t)$. The objective of the present Brief Report is to include this noncollinearity into the s-d model.

To do this, we have to abandon assumption (10), i.e., the vectors $\mathbf{m}_0(\mathbf{r},t)=m_0\mathbf{e}(\mathbf{r},t)$ and $\mathbf{e}(\mathbf{r},t)$ appearing in Eqs. (5) and (9) are not parallel to $\mathbf{M}_d(\mathbf{r},t)$. Furthermore, the kinetic exchange torque density $\mathbf{T}_{ex}$ is added to the right-hand side of Eq. (7) with an ansatz which is motivated by the reasoning of Antropov[7] and which has the form of a conventional micromagnetic exchange torque for an isotropic or cubic system,

$$\mathbf{T}_{ex} = A\mathbf{m}\times\Delta\mathbf{m}, \tag{11}$$

where Δ is the Laplacian operator. In order to treat $\mathbf{T}_{ex}$ on the same footing as the s-d exchange torque density $\mathbf{T}$ of Eq. (2), we write the exchange constant in the form $A=a_0^2/(\tau_{ss}m_0)$ with the nearest-neighbor distance a_0 and with $\tau_{ss}=\hbar/(sJ_{ss})$. Here s is the effective spin quantum number which may be assigned to the atomic s-p moment defined by integrating $\mathbf{m}_0(\mathbf{r},t)$ over the atomic volume, and J_{ss} is the *kinetic exchange constant*.

Proceeding exactly in the same way as Zhang and Li,[3] we find the counterpart to their Eq. (7) (the spin-diffusion term is already omitted),

$$\begin{aligned}-\frac{1}{\tau_{ex}M_d}\delta\mathbf{m}\times\mathbf{M}_d - \frac{\delta\mathbf{m}}{\tau_{sf}} &= \frac{\partial\mathbf{m}_0}{\partial t} - \frac{\mu_B P}{e_e}(\mathbf{j}_e\cdot\nabla)\frac{\mathbf{m}_0}{m_0} + \frac{1}{\tau_{ex}M_d}\mathbf{m}_0\times\mathbf{M}_d \\ &\quad + \frac{a_0^2}{\tau_{ss}m_0}(\mathbf{m}_0\times\Delta\mathbf{m}_0).\end{aligned} \tag{12}$$

The adiabatic part $\mathbf{m}_0$ may be obtained from Eq. (12) by setting $\delta\mathbf{m}=0$, $\frac{\partial\mathbf{m}}{\partial t}=0$. If in addition the current $\mathbf{j}_e$ is small, then Eq. (12) is solved by

$$\mathbf{m}_0 = \pm\frac{m_0}{M_d}\frac{\mathbf{M}_d + r\Delta\mathbf{M}_d}{|\mathbf{e}_d + r\Delta\mathbf{e}_d|} \tag{13}$$

with $r=a_0^2(\tau_{ex}/\tau_{ss})=a_0^2(J_{ss}s/J_{ex}S)$. The $\pm$ sign holds if the coupling between $\mathbf{m}_0$ and $\mathbf{M}_d$ in the ferromagnetic ground state of $\mathbf{M}_d$ is ferromagnetic (antiferromagnetic). Finally, we find the modified torque density $\mathbf{T}$ entering equation of motion (4) for $\mathbf{M}_d$, $\mathbf{T}=\Sigma_{i=1}^{10}\mathbf{T}_i$, with

$$\mathbf{T}_1 = -\frac{1}{1+\xi^2}\frac{\partial\mathbf{m}_0}{\partial t},$$

$$\mathbf{T}_2 = \frac{1}{1+\xi^2}\frac{\xi}{M_d}\mathbf{M}_d\times\frac{\partial\mathbf{m}_0}{\partial t},$$

$$\mathbf{T}_3 = -\frac{1}{1+\xi^2}\frac{\mu_B P}{e_e m_0 M_d^2}\mathbf{M}_d\times[\mathbf{M}_d\times(\mathbf{j}_e\cdot\nabla)\mathbf{m}_0],$$

$$\mathbf{T}_4 = -\frac{1}{1+\xi^2}\frac{\mu_B P\xi}{e_e m_0 M_d}[\mathbf{M}_d\times(\mathbf{j}_e\cdot\nabla)\mathbf{m}_0],$$

$$\mathbf{T}_5 = \frac{1}{1+\xi^2}\frac{\mathbf{m}_0}{\tau_{sf}},$$

$$\mathbf{T}_6 = \frac{1}{1+\xi^2}\frac{\mathbf{M}_d}{M_d^2}\left(\mathbf{M}_d\cdot\frac{\partial\mathbf{m}_0}{\partial t}\right),$$

$$\mathbf{T}_7 = -\frac{1}{1+\xi^2}\frac{1}{\tau_{sf}M_d^2}\mathbf{M}_d(\mathbf{M}_d\cdot\mathbf{m}_0),$$

$$\mathbf{T}_8 = \frac{1}{1+\xi^2}\frac{A\xi}{M_d}\mathbf{M}_d\times(\mathbf{m}_0\times\Delta\mathbf{m}_0),$$

$$\mathbf{T}_9 = \frac{1}{1+\xi^2}\frac{A}{M_d^2}[\mathbf{M}_d\times\mathbf{m}_0(\mathbf{M}_d\cdot\Delta\mathbf{m}_0)],$$

$$\mathbf{T}_{10} = -\frac{1}{1+\xi^2}\frac{A}{M_d^2}[\mathbf{M}_d\times\Delta\mathbf{m}_0(\mathbf{M}_d\cdot\mathbf{m}_0)]. \tag{14}$$

The torque densities $\mathbf{T}_1$ and $\mathbf{T}_2$ are the counterparts to the two "temporal" torque densities of the conventional model.[3] They now depend on the temporal variation in $\mathbf{m}_0$ rather than on the temporal variation in $\mathbf{M}_d$ (as it was in the conventional model). The torque densities $\mathbf{T}_3$ and $\mathbf{T}_4$ are the counterparts to the adiabatic and nonadiabatic[3] torque densities of the conventional model, and they depend on the variation in space of $\mathbf{m}_0(\mathbf{r},t)$ rather than on the variation in $\mathbf{M}_d(\mathbf{r},t)$, as it was in the conventional model. The torque densities $\mathbf{T}_5$–$\mathbf{T}_{10}$ are completely additional: $\mathbf{T}_5$–$\mathbf{T}_7$ arise from the noncollinearity between $\mathbf{m}_0$ and $\mathbf{M}_d$ whereas $\mathbf{T}_8$–$\mathbf{T}_{10}$ are directly related to the kinetic exchange. Of course, for $\mathbf{m}_0\|\mathbf{M}_d$, as is assumed in the conventional s-d model, our $\mathbf{T}$ reduces to the

four terms given in Ref. 3. Inserting Eq. (13) into Eq. (14), it becomes obvious that for a general situation the torques $\mathbf{T}_i$ may yield contributions which are not necessarily parallel to the torques of the conventional model, i.e., the modification of $\mathbf{T}$ as compared to the conventional theory may change the results both quantitatively and qualitatively.

To give an explicit example and to explore the quantitative importance of the noncollinearity between $\mathbf{m}_0$ and $\mathbf{M}_d$, we calculated the final velocity $v(t=\infty)$ of a Néel wall with $\mathbf{M}_d=\mathbf{M}_d(x,t)$ driven by an external field $\mathbf{H}_{\text{ext}}=H_{\text{ext}}\mathbf{e}_x$ and/or by a current density $\mathbf{j}_e=j_e\mathbf{e}_x$, following the same strategy as used in Ref. 3. In order to make the problem mathematically tractable, we consider the case of small $\mathbf{H}_{\text{ext}}$ and small $\mathbf{j}_e$, and hence small $v(\infty)$ so that we can use Eq. (13) and that the out-of-plane Walker angle ϕ can be set to zero. In this situation the torque $\mathbf{T}$ of our modified theory has the same direction as the corresponding torque of the conventional theory so that the result of the conventional theory is not changed qualitatively but just quantitatively. We obtained

$$v(\infty) = \pm \frac{1}{\alpha}[\gamma H_{\text{ext}} W(\infty) - \tilde{c}_j], \tag{15}$$

where the $\pm$ signs are the same as in Eq. (13) and where $W(\infty)$ is the width of the moving domain wall. The quantity $\tilde{c}_j$ is given by

$$\tilde{c}_j = c_j\left(1 - \frac{r}{W^2(\infty)}\right), \tag{16}$$

with $c_j=Pj_e\xi/[e_eM_d(1+\xi^2)]$ and $\xi=\tau_{\text{ex}}/\tau_{\text{sf}}$ as in Ref. 3.

From Eq. (16) we see that the result of the conventional theory is corrected by a factor $(1-\frac{r}{W^2(\infty)})$, and the question arises with regards to how large this factor is in real materials. In order to answer this question, we must discuss calculations by the *ab initio* density-functional electron theory. Thereby, for systems with a ferromagnetic ground state, a static noncollinearity among the atomic moments at sites i can be generated only by applying Lagrangian fields[8] at least for some sites i. Those Lagrangian fields prescribe the orientations of the total atomic moments $\mathbf{M}_i=\mathbf{M}_{i,s}+\mathbf{M}_{i,d}$ (where "s" and "d" again stand symbolically for the contributions of the itinerant and localized states, respectively). Because $|\mathbf{M}_{i,d}| \gg |\mathbf{M}_{i,s}|$, the $\mathbf{M}_{i,d}$ then are nearly parallel to $\mathbf{M}_i$, whereas the $\mathbf{M}_{i,s}$ may be nonparallel to $\mathbf{M}_{i,d}$. In Ref. 4 Lagrangian fields were applied to all magnetic moments $\mathbf{M}_i$ in such a way that only one of these moments, $\mathbf{M}_{i=0}$, was rotated out of the perfect ferromagnetic alignment with all the other moments. It was found that for Fe and Co $\mathbf{M}_{i=0,s}$ was nearly unaffected by an arbitrary rotation of $\mathbf{M}_{i=0}$, and hence $\mathbf{M}_{i=0,d}$; moreover this could be taken as a hint that the kinetic exchange coupling among the $\mathbf{M}_{i,s}$ is much stronger than the s-d exchange coupling. However, one must take into account that, for Fe and Co (and Ni), the $\mathbf{M}_{i,s}$ are coupled antiferromagnetically to the $\mathbf{M}_{i,d}$ in the ground state. Therefore, when the Lagrangian field rotates $\mathbf{M}_{i=0,d}$ in a clockwise direction, it wants to rotate $\mathbf{M}_{i=0,s}$ in a counterclockwise direction, and this effect competes with the s-d exchange interaction which wants to rotate the two subsystems coherently. Therefore, the reluctance of $\mathbf{M}_{i=0,s}$ to follow the rotation of $\mathbf{M}_{i=0,d}$ does not necessarily mean that $(J_{ss}s)/(J_{\text{ex}}S)$ is very large.

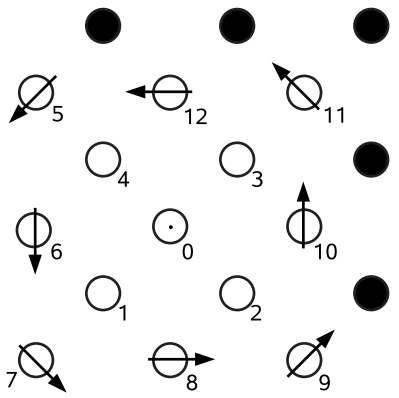

FIG. 1. Supercell used to model a minivortex in the *ab initio* calculations. The magnetic moment of atom 0 is constrained to point out of the plane, and the prescribed in-plane orientations of the magnetic moments of atoms 5–12 are given by the arrows. For atoms 1–4 no orientations are prescribed but they can develop freely. The full circles indicate vacant sites. In the *ab initio* calculation this supercell is repeated periodically in all three dimensions.

To circumvent this problem we have performed a calculation for the supercell depicted in Fig. 1 for which we considered a vortex-like magnetic configuration. We thereby applied Lagrangian fields so that the central moment $\mathbf{M}_0$ pointed out of plane whereas the moments $\mathbf{M}_5-\mathbf{M}_{12}$ showed a static in-plane circulation as shown in Fig. 1. In contrast, no Lagrangian fields were applied to the moments $\mathbf{M}_1-\mathbf{M}_4$ of the inner ring, i.e., these moments and their individual s, p, and d components could develop freely. For a ferromagnetic configuration there is an angle of 180° (antiparallel alignment) between $\mathbf{M}_{i,4s}+\mathbf{M}_{i,4p}$ and $\mathbf{M}_{i,3d}$ for Fe, Co, and Ni (Ref. 4) with $|\mathbf{M}_{i,4s}+\mathbf{M}_{i,4p}|/|\mathbf{M}_{i,3d}|=s/S=0.034$ (0.047) for Fe (Co). In contrast, for the inner ring the respective angle was 176° (169°) for Fe (Co). This shows that the magnetization $\mathbf{m}_0$ indeed is not parallel to $\mathbf{M}_d$ as a consequence of the kinetic exchange torque among the itinerant electrons. However, the misalignment is rather small, i.e., the kinetic exchange torque is smaller than the s-d exchange interaction and the parameter $(J_{ss}s)/(J_{\text{ex}}S)$ is smaller than one. Therefore, the correction factor $[1-\frac{J_{ss}s}{J_{\text{ex}}S}(\frac{a_0}{W(\infty)})^2]$ of Eq. (16) is close to one except possibly for systems such as nanowires,[9] for which the domain-wall width shrinks to atomic dimensions $[W(\infty)\approx a_0]$.

To conclude, we have investigated the influence of a noncollinearity between the d magnetization $\mathbf{M}_d$ and the adiabatic part $\mathbf{m}_0$ of the itinerant magnetization on the dissipative magnetization dynamics within the framework of the s-d model; moreover we found several additional contributions to the torque density $\mathbf{T}$ exerted on $\mathbf{M}_d$ by the itinerant magnetization $\mathbf{m}=\mathbf{m}_0+\delta\mathbf{m}$. For a 180° Néel wall, for which the additional contributions to $\mathbf{T}$ have the same orientations as the torques of the conventional s-d model (which neglects the noncollinearity between $\mathbf{m}_0$ and $\mathbf{M}_d$), the influence is extremely small for Fe and Co. It might be that for rare-earth metals the effect is larger because there the $5d$ states are the dominating itinerant states for which the magnetization is

much larger than for the 4*s* and 4*p* states of the 3*d* metals, and for which the kinetic exchange interaction among the itinerant states is also expected to be much larger. Finally, it should be noted that for more complicated magnetization configurations (e.g., vortices) those additional torques of our extended theory which have different directions than the torques of the conventional theory may have a non-negligible effect on the long-term trajectory of $\mathbf{M}_d(\mathbf{r},t)$ even though they are quantitatively very small. We thus have shown that the conventional *s*-*d* model can be used safely for 3*d* metals (as long as situations are excluded for which the dynamics for very long time scales is relevant), even if the noncollinearity between the *d* magnetization and the adiabatic conduction electron magnetization is substantial.

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