Damping of spin dynamics in nanostructures: An *ab initio* study

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Based on the Fermi surface breathing model of Kamberský, a phenomenological extension of the *ab initio* density-functional electron theory is used to derive an equation of motion for the spin dynamics in magnets. It is shown that even in the simple case of a homogeneous magnetization $\mathbf{M}$ the damping term $(1/M)\mathbf{M} \times [\alpha d\mathbf{M}/dt]$ of the commonly used Gilbert equation with the damping scalar α has to be replaced by a term of the form $(1/M)\mathbf{M} \times [\underline{\alpha}(\mathbf{M}) \cdot d\mathbf{M}/dt]$ with a damping matrix $\underline{\alpha}$ which depends on the orientation of $\mathbf{M}$. Explicit calculations are performed for bulk, monolayers, and monatomic wires of Fe, Co, and Ni. The variation of $\underline{\alpha}$ with an orientation of $\mathbf{M}$ is quite substantial already for the bulk materials (up to a factor of 4 in hcp Co) but most dramatic in the monolayers and monatomic wires in which for some orientations the damping is even zero. This represents an additional option for optimizing the magnetization reversal process in a magnetic nanostructure. It is shown that there is no simple relation between damping and magnetic anisotropy energy.

I. INTRODUCTION

In the past few years there has been extensive research activity to achieve a basic understanding of ultrafast magnetization processes in magnetically ordered materials. From the viewpoint of fundamental research this issue is very interesting and demanding because it requires a combination of methods of electron theory with methods of irreversible thermodynamics. From the viewpoint of magnet technology a strong impetus came from the promising possible applications of magnetization dynamics in micro- and nanosized magnets for advanced information storage and data processing devices.[1,2] In these applications it is essential to have a reliable control of the temporal magnetization reversal under the action of an external field $\mathbf{B}_{\text{ext}}(t)$. For example, for a given $\mathbf{B}_{\text{ext}}(t)$, such a reversal process depends[3] on the shape of the sample and on the intrinsic material parameters of the magnet, including those characterizing the damping of the spin dynamics. This damping is often described by a single scalar damping parameter α entering the Gilbert equation[4] for the magnetization $\mathbf{M}(\mathbf{r}, t)$,

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M} \times \mathbf{H}_{\text{eff}} + \frac{1}{M} \mathbf{M} \times \alpha \frac{d\mathbf{M}}{dt}. \quad (1)$$

Here γ is the gyromagnetic ratio, and $\mathbf{H}_{\text{eff}}$ is the effective field composed of the external field as well as the exchange, anisotropy, and dipolar fields. One of the objectives of micromagnetic simulations based on Eq. (1) so far has been to optimize the magnetization reversal with respect to the damping scalar α.

In the present paper we discuss the damping of the ultrafast spin dynamics in the adiabatic regime on the basis of a semiempirical extension of the *ab initio* density-functional electron theory introduced by Kamberský.[5] In its most general form the theory includes all effects on the adiabatic spin dynamics apart from contributions arising from transport spin and orbital currents (i. e., currents which cannot be written as the curl of a corresponding magnetization). Nevertheless, it is not the objective of the theory to identify the de-

tailed microscopic mechanisms of the energy transfer from the spin system to other degrees of freedom which are the origin for spin damping; these mechanisms appear via phenomenological relaxation times. The scope is to investigate for given relaxation times the influence of the specific electronic structure of a given material on the damping, with special emphasis on the modifications which appear when going to systems with reduced dimensionality. We will show that in the framework of this theory an equation of motion similar to Eq. (1) can be obtained only if the magnetization is homogeneous, and even in this situation the damping term of Eq. (1) with the damping scalar α has to be replaced by a term of the form $(1/M)\mathbf{M} \times (\underline{\alpha} \cdot d\mathbf{M}/dt)$ with a damping matrix $\underline{\alpha}(\mathbf{M})$, which depends on the orientation of the magnetization. This damping matrix has been calculated by Kuneš and Kamberský[6] for special orientations of $\mathbf{M}$ in bulk Fe, Co, and Ni, and in the present paper we extend the calculations to more general orientations. It will be shown that even for these bulk materials the damping shows a considerable variation for different orientations of the magnetization in the crystal. This anisotropy of the damping becomes very large when going to magnets with reduced dimensions like monolayers or atomic wires which will become increasingly important for future technological applications due to the dramatic improvement concerning the controlled fabrication of the nanomagnets. It will be shown that in the monolayers and monatomic wires there are orientations for which no damping appears at all. This yields a further option to optimize a magnetization reversal process by choosing a magnetization trajectory which is most appropriate from the viewpoint of damping.

The paper is organized as follows. In Secs. II and III we describe and comment on the theory of Kamberský which is the basis for our calculations, and in Sec. IV it is discussed how the various quantities entering this theory are determined within an *ab initio* band-structure calculation. Numerical results and group theoretical investigations for bulk systems, atomic monolayers, and atomic wires are given in Sec. V, and conclusions as well as an outlook are given in Sec. VI.

II. BASIC THEORY

In order to derive an equation of motion (EOM) for the ultrafast magnetization dynamics we adopt various assumptions and approximations. In the first step we confine ourselves to spin dynamics in the adiabatic regime which encompasses processes on the timescale typically between nanoseconds and several picoseconds. (The spin dynamics on the femtosecond timescale which has received growing interest in the past few years[7] will not be discussed.) In the adiabatic approximation it is assumed[8–10] that for the situation under consideration the fast spin degrees of freedom arising from single-electron spin fluctuations can be integrated out and that only the dynamics of the atomic spin moments $\mathbf{M}_{\mathrm{s,R}}$ at atoms $\mathbf{R}$ on a timescale defined by the inverse frequencies of typical long-wavelength magnons is relevant. The magnetic spin moment $\mathbf{M}_{\mathrm{s,R}}$ thereby is defined in the common way as an integral of the magnetic spin density $\mathbf{m}(\mathbf{r})$ over a suitably defined atomic volume $\Omega_{\mathbf{R}}$,

$$\mathbf{M}_{\mathrm{s,R}} = M_{\mathrm{s,R}}\mathbf{e}_{\mathrm{s,R}} = \int_{\Omega_{\mathbf{R}}} \mathbf{m}(\mathbf{r})d^3r. \tag{2}$$

In particular, in systems with reduced dimensionality there is in addition to the magnetic spin moment $\mathbf{M}_{\mathrm{s,R}}$ also a magnetic orbital moment $\mathbf{M}_{\mathrm{l,R}}$, and the total magnetic moment is given by $\mathbf{M}_{\mathbf{R}}=\mathbf{M}_{\mathrm{s,R}}+\mathbf{M}_{\mathrm{l,R}}$. In the present chapter we neglect the contribution $\mathbf{M}_{\mathrm{l,R}}$, and we consider only systems for which the magnitudes $|\mathbf{M}_{\mathrm{s,R}}|$ do not depend on the orientations of the spin moments $\mathbf{M}_{\mathrm{s,R}}$. For simplicity, we suppress the label s. A generalization to the case of large orbital contributions and variable moment magnitudes will be given in Sec. III.

In the theory of Kamberský[5] an EOM is derived for the $\mathbf{M}_{\mathbf{R}}$ within the framework of a one-electron theory neglecting the contribution $\mathbf{M}_{\mathrm{l,R}}$. Thereby a semiempirical extension is required to incorporate the effects of spin damping which arise because energy flows from the system of magnetic moments to nonmagnetic degrees of freedom, e.g., vibrational degrees of freedom of the lattice. Because we want to arrive at an EOM exclusively for the magnetic moments, we must assume that we can integrate out these other degrees of freedom and that we can represent their effects on the timescale of the adiabatic approximation by quantities which depend only on the magnetic moments $\mathbf{M}_{\mathbf{R}}(t)$. In general, such a procedure introduces[11] terms in the EOM for the $\mathbf{M}_{\mathbf{R}}$ that depend on the entire history of the $\mathbf{M}_{\mathbf{R}}$, and we have to figure out under what circumstances a Gilbert-like EOM is found where the terms depend only on the current state $\mathbf{M}_{\mathbf{R}}(t)$. We just want to mention two examples where a nonlocal time dependence of the magnetization is taken into account, at least in principle. The first one is the phenomenological treatment of magnetization damping via magnetoelastic coupling to the lattice,[11] and the second one is the time-dependent density-functional theory for the damping of the magnetization on a long timescale via electronic spin-spin interactions on short time scales.[12]

In the second step we assume that the effect of damping may be included into a dissipative free-energy functional $F_{\mathrm{diss}}[\mathbf{M}_{\mathbf{R}}]$. It is well known that various nonequilibrium processes may be described by a dissipative free-energy functional, but it is, of course, not guaranteed that this procedure encompasses all types of dissipation, especially when we drive the system far out of the thermodynamic equilibrium. In the context of magnetization dynamics a phenomenological dissipation free-energy functional has been written down, e.g., by Brown[13] by including in the free energy a Rayleigh dissipation function. If an appropriate functional exists, the EOM is derived from

$$\frac{d\mathbf{e}_{\mathbf{R}}}{dt} = -\gamma(\mathbf{e}_{\mathbf{R}} \times \tilde{\mathbf{H}}_{\mathrm{eff,R}}), \tag{3}$$

with the effective field

$$\tilde{\mathbf{H}}_{\mathrm{eff,R}} = -\frac{1}{M_{\mathbf{R}}}\frac{\delta F_{\mathrm{diss}}}{\delta \mathbf{e}_{\mathbf{R}}}, \tag{4}$$

which encompasses the contributions from damping.

In the third step we have to make contact with the electronic level. We do this within the framework of the *ab initio* density-functional electron theory. If we consider zero temperature for the moment, the free energy is given by the total energy.

For the following it will be important to incorporate the effect of spin-orbit coupling on the total energy which is a relativistic effect of order $1/c^2$. We may also include the dipolar interaction energy which is of the same order, as well as the Zeeman interaction energy with an external field. In the present paper these two terms are not taken into account when calculating the damping. When considering situations with directions $\mathbf{e}_{\mathbf{R}}$ which do not correspond to the ground-state directions, we have to fix these directions by an appropriate measure, e.g., by a Lagrangian constraining field.[14,15] In the present paper we will instead use an approximate constraining scheme[16] by prescribing within the framework of an atomic-sphere approximation for the orientations $\mathbf{e}_{\mathbf{R}}^{\mathrm{SQA}}$ of the spin quantization axes (SQA) for the atomic sites $\mathbf{R}$ (see Sec. IV), and we will confine ourselves to situations where the moment directions $\mathbf{e}_{\mathbf{R}}$ which result from the density-functional calculations are very close to the respective $\mathbf{e}_{\mathbf{R}}^{\mathrm{SQA}}$. The total energy then is given by the conventional total energy expression of the density-functional theory,

$$E[n,\{\mathbf{e}_{\mathbf{R}}(t)\}] = \sum_{j\mathbf{k}} n_{j\mathbf{k}}\varepsilon_{j\mathbf{k}} + E_{\mathrm{dc}}[n]. \tag{5}$$

In Eq. (5) j and $\mathbf{k}$ denote the band index and the wave vector for the single-particle states (we consider periodic systems) derived from the effective single-particle equations. In a system with collinear magnetic moments and zero spin-orbit coupling, the single-particle states can be classified in addition by the spin quantum number m_{s}. For nonzero spin-orbit coupling and/or for noncollinear situations this is no longer possible. The quantities $n_{j\mathbf{k}}$ and $\varepsilon_{j\mathbf{k}}$ are the occupation numbers and the eigenvalues for these states.

The first term in Eq. (5) is the band-structure term and the second term is the double-counting term. The band-structure term depends on the orientations $\{\mathbf{e}_{\mathbf{R}}(t)\}$ both explicitly via the prescription of the spin quantization axes and implicitly

via $n = [\rho(\mathbf{r}, \{\mathbf{e}_\mathbf{R}(t)\}); m(\mathbf{r}, \{\mathbf{e}_\mathbf{R}(t)\})]$ where $\rho(\mathbf{r})$ is the charge density. In contrast, E_{dc} depends on the $\{\mathbf{e}_\mathbf{R}(t)\}$ only implicitly via n.

To determine the effective field $\widetilde{\mathbf{H}}_{\text{eff},\mathbf{R}}$ according to Eq. (4), we must calculate in the third step the variation of E due to an infinitesimal change $\delta\mathbf{e}_\mathbf{R}$ of $\mathbf{e}_\mathbf{R}$,

$$\delta E = E[n(\mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}] - E[n(\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R}]$$
$$= E[n(\mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}] - E[n(\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}]$$
$$+ E[n(\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}] - E[n(\mathbf{e}_\mathbf{R}), \mathbf{e}_\mathbf{R}]. \quad (6)$$

In Eq. (6) the difference between the first two terms vanishes because the total energy is stationary with respect to a small variation $\delta n = n(\mathbf{e}_\mathbf{R} + \delta\mathbf{e}_\mathbf{R}) - n(\mathbf{e}_\mathbf{R})$. The difference between terms three and four in Eq. (6) is determined exclusively by the band-structure contribution to E because E_{dc} does not depend explicitly on $\mathbf{e}_\mathbf{R}$, yielding

$$\delta E = \sum_{j\mathbf{k}} \delta n_{j\mathbf{k}} \varepsilon_{j\mathbf{k}} + \sum_{j\mathbf{k}} n_{j\mathbf{k}} \delta \varepsilon_{j\mathbf{k}}. \quad (7)$$

For the following we assume that changes of the occupation numbers $n_{j\mathbf{k}}$ due to a change of the orientations $\{\mathbf{e}_\mathbf{R}\}$ occur nearly exclusively for states close to the Fermi energy ε_F. (This is certainly a good approximation when we consider only the change in orientation for a collinear spin system, because then the energies $\varepsilon_{j\mathbf{k}}$ are modified only by the generally weak spin-orbit interaction. The assumption is much more critical for processes in noncollinear spin systems which modify the relative orientations of the magnetic moments on an atomic scale.) Based on this assumption one obtains[17]

$$\sum_{j\mathbf{k}} \delta n_{j\mathbf{k}} \varepsilon_{j\mathbf{k}} \approx \varepsilon_F \sum_{j\mathbf{k}} \delta n_{j\mathbf{k}} = 0. \quad (8)$$

In Eq. (8) the fact is used that the total number of states is conserved. From Eqs. (7) and (8) we then find

$$\widetilde{\mathbf{H}}_{\text{eff},\mathbf{R}} = -\frac{1}{M_\mathbf{R}} \frac{\partial E}{\partial \mathbf{e}_\mathbf{R}} = -\frac{1}{M_\mathbf{R}} \sum_{j\mathbf{k}} n_{j\mathbf{k}}[\{\mathbf{e}_{\mathbf{R}'}(t)\}] \frac{\partial \varepsilon_{j\mathbf{k}}[\{\mathbf{e}_{\mathbf{R}'}(t)\}]}{\partial \mathbf{e}_\mathbf{R}}. \quad (9)$$

In the fourth step we want to introduce the semiempirical extension[5] of the density-functional theory in order to incorporate dissipative processes. For a static situation the occupation numbers $n_{j\mathbf{k}}$ are identical to the Fermi-Dirac occupation numbers, which depend on the $\mathbf{e}_\mathbf{R}$ because the $\varepsilon_{j\mathbf{k}}$ depend on them. When changing the $\mathbf{e}_\mathbf{R}$, the $\varepsilon_{j\mathbf{k}}$ also change and the Fermi surface is modified ("breathing Fermi surface"). This requires a redistribution of the occupation numbers $n_{j\mathbf{k}}$ provided by scattering processes between various electronic states $j\mathbf{k}$ around the Fermi surface. For quasistatic changes the characteristic time scale $\tau_\mathbf{e}$ for the changes of the moment directions is much longer than the characteristic time scale τ_s for these scattering processes, $\tau_\mathbf{e} \gg \tau_s$, and then $n_{j\mathbf{k}}[\{\mathbf{e}_\mathbf{R}(t)\}] \equiv n_{j\mathbf{k}}(t)$ is given by the Fermi-Dirac distribution $f(\varepsilon_{j\mathbf{k}}[\{\mathbf{e}_\mathbf{R}(t)\}]) \equiv f_{j\mathbf{k}}(t)$ at any instant. In the general case, however, $n_{j\mathbf{k}}$ never catches up with $f_{j\mathbf{k}}$, and the deviation between $n_{j\mathbf{k}}$ and the fictitious equilibrium distribution $f_{j\mathbf{k}}$

generates the dynamical evolution of $n_{j\mathbf{k}}$. In Kamberský's theory[5] this process is described by a relaxation ansatz

$$\frac{dn_{j\mathbf{k}}(t)}{dt} = -\frac{1}{\tau_{j\mathbf{k}}}[n_{j\mathbf{k}}(t) - f_{j\mathbf{k}}(t)] \quad (10)$$

with the relaxation times $\tau_{j\mathbf{k}}$, which in general will depend on the electronic states $j\mathbf{k}$.

Before proceeding, we want to make some comments on Eq. (10). First, the whole information about the scattering processes is included in the relaxation times $\tau_{j\mathbf{k}}$. No statement is made on the physical origin of the scattering process; different processes just will result in different relaxation times $\tau_{j\mathbf{k}}$. Second, only scattering among states close to the Fermi surface are involved, in contrast to the spin dynamics investigated in typical experiments on the femtosecond timescale.[7] Therefore, there is little hope that we can directly learn much about the relaxation times that are relevant for the adiabatic regime from the experiments for the femtosecond timescale. It is more promising to gain appropriate information on the $\tau_{j\mathbf{k}}$ from measurements of spin-dependent electronic transport which involves also only processes close to the Fermi surface. Finally, a relaxation time ansatz, in general, is used only for intraband scattering processes but not for interband scattering processes.

In the fifth step we introduce an approximation for the exact solution of Eq. (10),

$$n_{j\mathbf{k}}(t) = \int_{t_0}^{t} \frac{1}{\tau_{j\mathbf{k}}} f_{j\mathbf{k}}(t') e^{-(t-t')/\tau_{j\mathbf{k}}} dt' + n_{j\mathbf{k}}(t_0) e^{-(t-t_0)/\tau_{j\mathbf{k}}}. \quad (11)$$

Obviously the momentary $n_{j\mathbf{k}}$ depends on the orientation $\mathbf{e}_\mathbf{R}(t')$ for all former times, introducing a time-memory term into the EOM for the $\mathbf{e}_\mathbf{R}$ as discussed above. Neglecting the second term in Eq. (11) for $t_0 \to -\infty$ and evaluating $f_{j\mathbf{k}}(t')$ around $t' = t$ into a Taylor series, we find a power series in $\tau_{j\mathbf{k}}$,

$$n_{j\mathbf{k}}(t) = f_{j\mathbf{k}}(t) - \tau_{j\mathbf{k}} \frac{df_{j\mathbf{k}}}{dt} + \cdots, \quad (12)$$

which converges for $\tau_{j\mathbf{k}} \ll \tau_\mathbf{e}$.

In the sixth step we confine ourselves to a homogeneous situation where $\mathbf{M}_\mathbf{R} = \mathbf{M} = M\mathbf{e}$ for all sites $\mathbf{R}$. This assumption, of course, limits the direct applicability of our theory to homogeneous situations, for instance, to a ferromagnetic resonance of the $\mathbf{q} = 0$ mode or to homogeneous magnetization reversal processes (often magnetization reversal processes will involve spatially inhomogeneous magnetization configurations). We will see in Sec. V that even in this simple case the EOM is in general more complicated than the Gilbert equation which is used very often for inhomogeneous situations. (Note also the remark at the end of Sec. VI.) Inserting Eq. (12) into Eq. (9) then yields

$$\widetilde{\mathbf{H}}_{\text{eff},\mathbf{R}} = \widetilde{\mathbf{H}}_{\text{eff}} = \mathbf{H}_{\text{aniso}} + \mathbf{H}_{\text{damp}}. \quad (13)$$

The higher-order terms in Eq. (12) would generate further damping terms which are not considered in the present calculation. In Eq. (13) the first term is the anisotropy field,

$$\mathbf{H}_{\text{aniso}} = -\frac{1}{M}\sum_{j\mathbf{k}} f_{j\mathbf{k}} \frac{\partial \varepsilon_{j\mathbf{k}}(\mathbf{e})}{\partial \mathbf{e}}, \tag{14}$$

whereas $\mathbf{H}_{\text{damp}}$ is the damping term described by

$$\mathbf{H}_{\text{damp}} = -\frac{1}{\gamma M}\underline{\underline{\alpha}} \cdot \frac{d\mathbf{M}}{dt} \tag{15}$$

with the damping matrix

$$\alpha_{lm} = -\frac{\gamma}{M}\sum_{j\mathbf{k}} \tau_{j\mathbf{k}} \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \left.\frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_l}\right|_{\mathbf{M}} \left.\frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_m}\right|_{\mathbf{M}}. \tag{16}$$

We note the similarity of Eq. (16) with the Drude equation for the conductivity tensor $\underline{\underline{\sigma}}$ in semiclassical approximation,

$$\sigma_{lm} = -e_0^2\sum_{j\mathbf{k}} \tau_{j\mathbf{k}} \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial k_l} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial k_m}, \tag{17}$$

where e_0 denotes the elementary charge.

In the seventh step we assume that the relaxation time $\tau_{j\mathbf{k}}$ for processes appearing at the Fermi surface are independent of the state $(j\mathbf{k})$, i.e., $\tau_{j\mathbf{k}} \equiv \tau$, yielding

$$\frac{\alpha_{lm}}{\tau} = -\frac{\gamma}{M}\sum_{j\mathbf{k}} \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \left.\frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_l}\right|_{\mathbf{M}} \left.\frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_m}\right|_{\mathbf{M}}. \tag{18}$$

Equation (18) enables us to relate the ratios α_{lm}/τ directly to the electronic properties of the considered material via the derivatives $\partial \varepsilon_{j\mathbf{k}}/\partial e_i|_{\mathbf{M}}$, and we can figure out how this ratio changes when going to systems with various dimensionalities. Assuming that the main temperature dependence of both $\underline{\underline{\alpha}}$ and $\underline{\underline{\sigma}}$ is given by the temperature dependence of τ, we can conclude that with the approximations discussed so far the damping has a similar temperature dependence as the conductivity. Experimentally, it has been shown[18] that the temperature dependence of the damping scalar α as obtained by ferromagnetic resonance experiments has two contributions, one proportional to the conductivity and the other one proportional to the resistivity. Within the framework of our approximations we obviously cannot get the second contribution. Possible reasons might be the use of the relaxation time ansatz, which may not be appropriate for describing interband relaxations and/or the failure of our assumption $\tau_{j\mathbf{k}} \ll \tau_{\mathbf{e}}$.

It should be noted that numerical values for α in bulk materials of the order of magnitude of the experimental values are found if inserting typical relaxation times τ as obtained from conductivity measurements.[6]

Introducing Eqs. (13)–(15) into Eq. (3) yields the EOM for the direction $\mathbf{e}$ of the homogeneous magnetization. Because for homogeneous magnetization the modulus M of $\mathbf{M}$ depends only very slightly on $\mathbf{e}$ we finally obtain the Gilbert-like EOM for homogeneous magnetization,

$$\frac{d\mathbf{M}}{dt} = -\gamma\mathbf{M} \times \mathbf{H}_{\text{aniso}} + \frac{1}{M}\mathbf{M} \times \left(\underline{\underline{\alpha}} \cdot \frac{d\mathbf{M}}{dt}\right), \tag{19}$$

which looks very similar to the original Gilbert equation, Eq. (1), with the only difference that the damping scalar α of the Gilbert equation is replaced by a matrix $\underline{\underline{\alpha}}$. Therefore, in general, $\mathbf{H}_{\text{damp}}$ is not parallel to $d\mathbf{M}/dt$. A Gilbert equation is

obtained only for the special case that $d\mathbf{M}/dt$ corresponds to an eigenvector of $\underline{\underline{\alpha}}(\mathbf{M})$, and then the damping scalar is given by the corresponding eigenvalue of $\underline{\underline{\alpha}}$.

Multiplying Eq. (19) with $\mathbf{M}$ yields $\mathbf{M}\cdot d\mathbf{M}/dt=0$, i.e., the change of $\mathbf{M}$ is perpendicular to $\mathbf{M}$. When we choose $\mathbf{M} = M\mathbf{e}_z$ we thus obtain $d\mathbf{M}/dt = (dM_x/dt, dM_y/dt, 0)$, and if $\underline{\underline{\alpha}}$ attains the form

$$\underline{\underline{\alpha}} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{20}$$

then the damping term of Eq. (19) reduces to the Gilbert damping term $(1/M)\mathbf{M} \times \alpha(d\mathbf{M}/dt)$ with a damping scalar α. It can be shown that Eq. (16) yields the form of $\underline{\underline{\alpha}}$ given by Eq. (20) if the magnetization is aligned parallel to a three-fold or fourfold symmetry axis of the system.

A matrix form of magnetization damping has been introduced ad hoc also by Safonov,[19] however, not in a Gilbert-type equation but in a Landau-Lifshitz type equation,

$$\frac{d\mathbf{M}}{dt} = -\gamma^{\text{LL}}\mathbf{M} \times \mathbf{H}_{\text{eff}} - \gamma^{\text{LL}}\frac{\mathbf{M}}{M} \times [\underline{\underline{\alpha}}^{\text{LL}} \cdot (\mathbf{M} \times \mathbf{H}_{\text{eff}})]. \tag{21}$$

Whereas for the case of a damping scalar the Gilbert equation and the Landau-Lifshitz equation can be transformed into each other, yielding relations between (γ, α) and $(\gamma^{\text{LL}}, \alpha^{\text{LL}})$, this is no longer possible for a matrix form of the damping, and therefore $\underline{\underline{\alpha}}^{\text{LL}}$ cannot be related to $\underline{\underline{\alpha}}$ from Eq. (15) in a simple way (see Sec. V). This becomes also obvious from the fact that Safonov derives $\underline{\underline{\alpha}}^{\text{LL}}$ from $\delta^2 E[\mathbf{M}]/\delta\mathbf{M}^2$ which in our approach would relate $\underline{\underline{\alpha}}^{\text{LL}}$ to the second derivatives of $\varepsilon_{j\mathbf{k}}$ with respect to $\mathbf{M}$ whereas our $\underline{\underline{\alpha}}$ is related to products of the first derivatives of $\varepsilon_{j\mathbf{k}}$. It should be noted that a matrix form of the magnetization damping was obtained also in the time-dependent density-functional theory of Capelle and Gyorffy.[12] In this theory a special mechanism of damping via short-time spin-spin interactions is discussed, i.e., the angular momentum of the whole electronic system is conserved. In contrast, the breathing Fermi surface model encompasses in principle all processes, including spin-lattice relaxation, which leads to a redistribution of the single electronic states.

III. GENERALIZATION TO SYSTEMS WITH ORBITAL MOMENTS AND WITH VARIABLE MAGNETIC MOMENT MAGNITUDES

In the preceding sections we have considered systems for which the orbital moments can be neglected, and for such systems we have determined the damping matrix $\underline{\underline{\alpha}}$, Eqs. (10)–(18). We now want to give arguments for the conjecture that this damping matrix is of central importance also for systems for which the orbital moments cannot be neglected. To do this, we derive an EOM for the total magnetic moment $\mathbf{M_R} = |\mathbf{M_R}|\mathbf{e_R} = \mathbf{M_{s,R}} + \mathbf{M_{l,R}}$ with the spin moment $\mathbf{M_{s,R}} = |\mathbf{M_{s,R}}|\mathbf{e_{s,R}}$ and the orbital moment $\mathbf{M_{l,R}} = |\mathbf{M_{l,R}}|\mathbf{e_{l,R}}$. The derivation of this EOM is based on assumptions [see Eqs.

(28)–(30) and the corresponding text], the validity of which we cannot prove in full generality. We have checked by our *ab initio* calculations that they are fulfilled for the situations considered in the paper, i.e., monolayers and monatomic wires. It may be that there are situations for which these assumptions are not fulfilled, then the EOM derived in this section is not applicable. Motivated by the results of this section, we nevertheless think that the matrix $\underline{\alpha}$ calculated from Eqs. (16)–(18) should play a central role for the damping of the total magnetization even in these situations.

In general $\mathbf{e}_{s,\mathbf{R}}$ is not parallel to $\mathbf{e}_{l,\mathbf{R}}$, and the magnitudes $|\mathbf{M}_\mathbf{R}|$, $|\mathbf{M}_{s,\mathbf{R}}|$ and $|\mathbf{M}_{l,\mathbf{R}}|$ are not constant but depend on the magnetic configuration of the system.[10,20,21] We confine ourselves to homogeneous situations for which we can omit the site label $\mathbf{R}$. The considerations of this section will show that the damping matrix enters the EOM for the magnetic moment also in this generalized situation.

Again we adopt an adiabatic approximation by assuming that the basic adiabatic variable is the direction $\mathbf{e}_s$ of the spin moment, and that all the other quantities are "slaved" by $\mathbf{e}_s$, i.e., are univalued functions of $\mathbf{e}_s$, for instance,

$$\mathbf{M}_s = \mathbf{M}_s(\mathbf{e}_s), \tag{22}$$

$$\mathbf{M}_l = \mathbf{M}_l(\mathbf{e}_s), \tag{23}$$

$$\mathbf{M} = \mathbf{M}(\mathbf{e}_s), \tag{24}$$

$$\mathbf{J} = \mathbf{J}(\mathbf{e}_s). \tag{25}$$

Here $\mathbf{J}$ is the expectation value $\langle \hat{\mathbf{J}} \rangle$ of the total angular momentum,[22]

$$\langle \hat{\mathbf{J}} \rangle = \langle \hat{\mathbf{L}} \rangle + \langle \hat{\mathbf{S}} \rangle, \tag{26}$$

with the operators $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$ of the orbital moment and the spin moment, and where e_0, m, and c denote the elementary charge, the electron mass, and the speed of light, respectively. The total magnetic moment is given by

$$\mathbf{M} = -\frac{e_0}{2mc}(\langle \hat{\mathbf{L}} \rangle + 2\langle \hat{\mathbf{S}} \rangle). \tag{27}$$

The justification, for instance, of Eq. (22) is that the spin length M_s would be an independent dynamical variable only if we took into account the longitudinal fluctuations of the spin variable arising from the fast single-electron spin fluctuations which, however, are neglected in our adiabatic approximation. The justification of Eqs. (23)–(25) is that, in general, the spin-orbit interaction, which is responsible for the formation of the orbital moments $\mathbf{M}_l$, is much smaller than the exchange interactions which are responsible for the spin moments $\mathbf{M}_s$.

The adiabatic approximation means that we can determine the dynamics of all the quantities $\mathbf{M}_s, \mathbf{M}_l, \mathbf{M}, \mathbf{J}$, etc. from the dynamics of $\mathbf{e}_s$ by using Eqs. (22)–(25). In the following we will make use of Eqs. (24) and (25). We thereby assume that the inverse relations,

$$\mathbf{e}_s = \mathbf{e}_s(\mathbf{M}), \tag{28}$$

$$\mathbf{e}_s = \mathbf{e}_s(\mathbf{J}), \tag{29}$$

also represent univalued functions. Combining Eqs. (24) and (29) we get

$$\mathbf{M} = \mathbf{M}(\mathbf{J}). \tag{30}$$

We then can determine the dynamics of $\mathbf{M}$ from the dynamics of $\mathbf{J}$ by making use of Eq. (30). To get the explicit relations (22)–(30) for a system under consideration we can, e.g., perform static calculations for $\mathbf{M}_s = -(e_0/mc)\langle \hat{\mathbf{S}} \rangle$, $\mathbf{M}_l = -(e_0/2mc)\langle \hat{\mathbf{L}} \rangle$, $\mathbf{J}$ according to Eq. (26) and $\mathbf{M}$ according to Eq. (27) within the framework of the *ab initio* density-functional theory for prescribed directions $\mathbf{e}_s$.

To obtain the dynamics of $\mathbf{J}$ we write down the classical equation of motion for the angular momentum which holds via Ehrenfest's theorem also for the expectation value of a quantum mechanical operator,

$$\frac{d\mathbf{J}}{dt} = \mathbf{M} \times \tilde{\mathbf{H}}_{\mathrm{eff}}. \tag{31}$$

Equation (31) is the equation which tells that a change of an angular momentum is obtained by exerting a torque. In the present situation the torque on the magnetic moment $\mathbf{M}$ is given by $\mathbf{M} \times \mathbf{H}_{\mathrm{eff}}$ with the effective field $\tilde{\mathbf{H}}_{\mathrm{eff}}$, the components $\tilde{H}_{\mathrm{eff},i}$ of which are again obtained from

$$\tilde{H}_{\mathrm{eff},i} = -\frac{\partial F_{\mathrm{diss}}}{\partial M_i} = -\frac{\partial F_{\mathrm{diss}}}{\partial e_{s,j}}\frac{\partial e_{s,j}}{\partial M_i}, \tag{32}$$

where we made use of Eq. (28).

It should be noted that in a general quantum mechanical description there are additional contributions to the torque arising from transport spin and orbital currents. In line with the usual assumption of the *ab initio* spin dynamics simulations[9,15,20] we do not take them into account explicitly. The appearance of such additional contributions would allow that the spin length M_s changes, and this is taken into account implicitly by Eqs. (22) and (23).

For the calculation of $\partial F_{\mathrm{diss}}/\partial e_{s,j}$ we use the formalism described in the preceding section, as well as Eq. (29), which yields $de_{s,k}/dt=(\partial e_{s,k}/\partial J_m)(dJ_m/dt)$. We then obtain

$$\tilde{H}_{\mathrm{eff},i} = \tilde{H}_{\mathrm{aniso},i} + \tilde{H}_{\mathrm{damp},i} \tag{33}$$

with

$$\tilde{H}_{\mathrm{aniso},i} = MH_{\mathrm{aniso},j}\frac{\partial e_{s,j}}{\partial M_i} \tag{34}$$

and

$$\tilde{H}_{\mathrm{damp},i} = \alpha_{ln}\eta_{im}^{nl}\frac{dJ_m}{dt}. \tag{35}$$

Here H_{aniso} and α_{ln} are the anisotropy field and the damping matrix calculated in the preceding section, and η_{im}^{nl} is given by

$$\eta_{im}^{nl} = \frac{M}{\gamma}\frac{\partial e_{s,n}}{\partial M_i}\frac{\partial e_{s,l}}{\partial J_m}. \tag{36}$$

For a system without orbital contributions and with fixed moment length we have $\eta_{im}^{nl} = \delta_{ni}\delta_{lm}$, $\partial e_{s,j}/\partial M_i = (1/M)\delta_{ij}$, and $\mathbf{M} = \gamma\mathbf{J}$ and the theory reduces to the one of the preceding section.

Altogether before starting to solve the EOM (31) for $\mathbf{J}$, we have to provide as input information $\mathbf{e}_s(\mathbf{M})$, $\mathbf{e}_s(\mathbf{J})$, $\mathbf{M}(\mathbf{e}_s)$, $\mathbf{J}(\mathbf{e}_s)$, and $\mathbf{J}(\mathbf{M})$ from static *ab initio* calculations. The EOM then is solved numerically. In each time step we thereby calculate $\mathbf{e}_s(t)$ from $\mathbf{J}(t)$ via Eq. (29) and then the quantities $\mathbf{M}$, $\partial e_{s,j}/\partial M_i$, $\alpha_{ln}(\mathbf{e}_s)$, and $\eta_{im}^{nl}(\mathbf{e}_s)$ which enables us to calculate the momentary value of the right-hand side of Eq. (31).

IV. DETAILED CALCULATIONAL PROCEDURE

In this section we describe the calculation of the damping matrix given by Eq. (16) by an *ab initio* band-structure approach. We hereby consider a system with spin-orbit coupling, and we confine ourselves to homogeneous magnetization configurations.

Our calculations are based on the local-spin-density approximation[23] (LSDA) for the exchange-correlation functional $E_{xc}[\rho(\mathbf{r}), \mathbf{m}(\mathbf{r})]$ of the density-functional theory

$$E_{xc}^{ASA} = \sum_{\mathbf{R}} \int_{\Omega_{\mathbf{R}}} \rho(\mathbf{r})\varepsilon_{xc}(\rho(\mathbf{r}), |\mathbf{m}(\mathbf{r})|)d^3r, \qquad (37)$$

where ε_{xc} is the LSDA exchange-correlation energy per electron and where $|\mathbf{m}(\mathbf{r})|$ is the modulus of the magnetization density. In the following, we replace E_{xc} by the corresponding expression in atomic-sphere approximation (ASA) for the spin direction.[16] To do this, we prescribe for the atomic sphere at each site $\mathbf{R}$ a spin quantization axis (SQA) with direction $\mathbf{e}_{\mathbf{R}}^{SQA}$ with respect to which the Pauli spin matrices in that sphere are defined. Then E_{xc} is approximated by

$$E_{xc}^{ASA} = \sum_{\mathbf{R}} \int_{\Omega_{\mathbf{R}}} \rho(\mathbf{r})\varepsilon_{xc}(\rho(\mathbf{r}), \mathbf{e}_{\mathbf{R}}^{SQA}\cdot\mathbf{m}(\mathbf{r}))d^3r. \qquad (38)$$

The introduction of the spin ASA breaks the rotational invariance of the original LSDA exchange-correlation functional (37), because now the exchange-correlation field $\mathbf{B}_{xc}^{ASA} = -\delta E_{xc}^{ASA}/\delta\mathbf{m}(\mathbf{r})$ is parallel to $\mathbf{e}_{\mathbf{R}}^{SQA}$ in each atomic sphere, i.e., due to this approximation the physics depends on the choice of the SQA whereas in the original LSDA it does not. For noncollinear spin systems we can choose different orientations of the SQA for different sites; for a homogeneous magnetization we take $\mathbf{e}_{\mathbf{R}}^{SQA} = \mathbf{e}^{SQA}$ for all $\mathbf{R}$. In the ground state the magnetization is parallel to the easy axis of the crystal, and we choose $\mathbf{e}^{SQA}$ parallel to this direction. When changing $\mathbf{e}^{SQA}$ then the spin magnetization $\mathbf{M} = M\mathbf{e}$ as obtained from the calculation will stay almost parallel to the spin quantization axis for the case normally present that the on-site exchange interactions (represented by $\mathbf{B}_{xc}^{ASA}$) are much stronger than the spin-orbit interactions, and we then can adopt the approximation $\mathbf{e} = \mathbf{e}^{SQA}$. For more details of this well-known procedure to approximately prescribe the magnetization direction, see Ref. 16. The effective Hamiltonian $\hat{H}$ for the single-electron states $\psi_{j\mathbf{k}}$ of the density-functional theory for the crystal then depends explicitly on $\mathbf{e}$, on the one hand via $\mathbf{B}_{xc}^{ASA}$ and on the other hand via the spin-orbit coupling term

$$\hat{H}_{SO} = \sum_{\mathbf{R}} \xi_{\mathbf{R}}(r)\hat{\mathbf{l}}_{\mathbf{R}}\cdot\hat{\mathbf{s}}_{\mathbf{R}}(\mathbf{e}), \qquad (39)$$

where $\xi_{\mathbf{R}}(r)$ is the spin-orbit coupling coefficient and $\hat{\mathbf{l}}_{\mathbf{R}}$ is the angular momentum operator. The spin operator $\hat{\mathbf{s}}_{\mathbf{R}}(\mathbf{e})$ thereby depends explicitly on $\mathbf{e}$ via the definition of the spin quantization axis.

Because the direction of the spin quantization axis plays the role of an external parameter, we can use the theorem of Hellmann and Feynman[24] to calculate the derivatives occurring in Eq. (16), i.e.,

$$\frac{\partial\varepsilon_{j\mathbf{k}}}{\partial\mathbf{e}} = \langle\psi_{j\mathbf{k}}|\frac{\delta\hat{H}}{\delta\mathbf{e}}|\psi_{j\mathbf{k}}\rangle. \qquad (40)$$

The right-hand side of Eq. (40) may be calculated by use of the transverse torque operator[6,17] $\hat{\mathbf{T}}$,

$$\langle\psi_{j\mathbf{k}}|\frac{\delta\hat{H}}{\delta\mathbf{e}}|\psi_{j\mathbf{k}}\rangle = \langle\psi_{j\mathbf{k}}|\hat{\mathbf{T}}|\psi_{j\mathbf{k}}\rangle = \mathbf{T}_{j\mathbf{k}}, \qquad (41)$$

with

$$\hat{\mathbf{T}} = \mathbf{e}\times\sum_{\mathbf{R}}\xi_{\mathbf{R}}(r)\hat{\mathbf{l}}_{\mathbf{R}}\times\hat{\mathbf{s}}_{\mathbf{R}}(\mathbf{e}). \qquad (42)$$

Introducing the matrix T with

$$\mathsf{T}_{lm} = \sum_{j\mathbf{k}} -\frac{\partial f_{j\mathbf{k}}}{\partial\varepsilon_{j\mathbf{k}}}\mathbf{T}_{j\mathbf{k},l}\mathbf{T}_{j\mathbf{k},m} \qquad (43)$$

we can finally write the damping matrix, Eq. (16), as

$$\frac{\alpha_{lm}}{\tau} = \frac{\gamma}{M}\mathsf{T}_{lm}. \qquad (44)$$

The summation $\Sigma_{\mathbf{k}}$ over the Brillouin zone in Eq. (43) is performed by a summation over $\mathbf{k}$ vectors of the irreducible part of the Brillouin zone and a subsequent symmetrization with respect to the star of each $\mathbf{k}$ vector. If the combined rotation $\hat{R}$ by an angle φ in real space and spin space is a symmetry operation of the system, then the spinor $\Psi_{j\hat{R}\mathbf{k}}$ is obtained from $\Psi_{j\mathbf{k}}$ via

$$\Psi_{j\hat{R}\mathbf{k}} = \exp\left[-\frac{i}{\hbar}\varphi(\hat{\mathbf{l}}+\hat{\mathbf{s}})\right]\Psi_{j\mathbf{k}}, \qquad (45)$$

and therefore the quantity $\mathbf{T}_{j\mathbf{k}}$ transforms under $\hat{R}$ like a pseudovector. It then can be shown that as a consequence the matrices T and $\underline{\underline{\alpha}}$ attain the form of Eq. (20) if the magnetization is oriented parallel to a threefold or fourfold symmetry axis of the system, so that the damping term in the EOM reduces to a Gilbert-like damping term with a damping scalar α (Sec. II).

In the present paper the matrix T is calculated by the *ab initio* density-functional electron theory in LSDA both without and with the orbital polarization term.[25] This term takes into account at least in part the orbital correlation effects, which become very important in systems with reduced

dimensionality.[26] We use the tight-binding linear-muffin-tin-orbital (LMTO) method in the atomic-sphere approximation[27] in which we have implemented the spin-orbit coupling.[28]

For the monatomic layer and for the monatomic wire the calculations are performed by the supercell formalism, i.e., large supercells containing the layer or the wire and in addition empty atomic spheres, i.e., spheres without a nucleus, are repeated periodically. The supercell for the monolayer calculation is given by an A^*BCABC close-packed stacking of hexagonal layers in the z direction (the y axis was oriented parallel to a densely packed atom row in the hexagonal plane), where layer A^* consists of the respective transition metal atom and layers A, B, and C are composed of atomic spheres without nuclear potential. We use the same nearest-neighbor distance for the atoms in the bulk, monatomic layer and monatomic wire. The supercell for the wire calculation is given by an A^*BAB close-packed stacking of hexagonal layers in the z direction, where layer A^* contains the wire running in the y direction and in addition three parallel wires composed of empty spheres, whereas layers A and B are entirely composed of empty spheres. For the layers (wires) the dispersion of the bands in the z (x and z) direction was negligibly small, and therefore we used $N_{k_z}=1$ ($N_{k_x}=N_{k_z}=1$ or 2) for the sampling of the Brillouin zone in Eq. (43) and converged with respect to $N_{k_x}=N_{k_y}$ (N_{k_y}). A Gaussian smearing method[29] was applied, fixing either the smearing parameter σ or the product σN_{k_y}.

V. RESULTS

In this section we present our results for the damping matrix $\underline{\alpha}$ in the bulk and in free-standing monatomic layers and monatomic wires of Fe, Co, and Ni. Special attention will be given to the question how $\underline{\alpha}$ changes when going to systems with more and more reduced dimensionality. Thereby we want to investigate whether the change in $\underline{\alpha}$ is closely related to the change in magnetic anisotropy which, in general, increases strongly when decreasing the dimensionality of the system.[30] (Examples for calculations dealing with the strong dependence on the dimensionality of other magnetic properties of transition metals are in Refs. 26 and 31.) For the discussion of ultrafast spin dynamics it is often assumed that the damping is the larger, the larger the magnetic anisotropy is. From the inspection of our Eqs. (14) and (16), it becomes clear that this is not at all trivial. The anisotropy field $\mathbf{H}_{aniso}$ contains the derivatives $\partial \varepsilon_{j\mathbf{k}}/\partial \mathbf{e}$ linearly. These derivatives may exhibit positive and negative values which may compensate to a large extent when performing the summation in Eq. (14), and this is the reason why the calculation of the magnetic anisotropy energy often is a very delicate numerical problem. In contrast, the derivatives enter quadratically when calculating α_{ll} from Eq. (16) (and therefore there is a hope that the calculation of α_{ll} is less demanding), and hence, in general, there will be no simple relation between magnetic anisotropy and damping.

The case of monatomic wires deserves a little more discussion. As it becomes obvious from the discussion of Sec. II, the breathing Fermi surface model is tightly related to the notion of a Fermi liquid behavior of the system whereas in a one-dimensional system there is a Luttinger liquid behavior. However, in reality monatomic wires of magnetic atoms are grown on substrates.[30] Our basic assumption is that the coupling to the substrate is large enough to transform a Luttinger liquid behavior to a Fermi liquid behavior, but it is on the other hand nevertheless so small that the energy dispersion relations which we calculate for the freestanding monatomic wire are very similar to those of the corresponding wire grown on the substrate. Having accepted the Fermi liquid behavior, it is easy to see that the system exhibits a breathing Fermi surface when changing the direction of the magnetization: When introducing spin-orbit coupling to the system, the dispersion relations will differ from those which we get when neglecting spin-orbit coupling, e.g., their curvature will be modified. This will change the energy-resolved density of states and the Fermi energy, and there will be a dependence of the single-particle energies at the Fermi level on the direction of the magnetization, i. e., all the preconditions for the application of Eqs. (14) and (16) are fulfilled.

In the following we present our results for the eigenvalues $\tilde{\alpha}_p$ of the damping matrix as a function of the direction of the magnetic spin moment. Choosing for the moment without loss of generality $\mathbf{e}=\mathbf{e}_z$, we obtain the general form

$$\mathbf{T}_{j\mathbf{k}} = \begin{pmatrix} a_{j\mathbf{k}} \\ b_{j\mathbf{k}} \\ 0 \end{pmatrix} \tag{46}$$

and hence

$$\underline{\alpha} = \begin{pmatrix} a^2 & ab & 0 \\ ab & b^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{47}$$

This shows that there are at most two different eigenvalues $\tilde{\alpha}_p$, $p=1,2$ of $\underline{\alpha}$, and that the two eigenvectors $\mathbf{e}_1$ and $\mathbf{e}_2$ which are orthogonal to $\mathbf{e}$ are in addition orthogonal to each other (due to the symmetry of $\underline{\alpha}$).

For a mode $d\mathbf{M}/dt$ which corresponds to the pth eigenvector the damping term $\mathbf{M} \times (\underline{\alpha} \cdot d\mathbf{M}/dt)$ reduces to $\tilde{\alpha}_p \mathbf{M} \times d\mathbf{M}/dt$. For a general $\dot{\mathbf{M}}=d\mathbf{M}/dt$ we can subdivide $\underline{\alpha} \cdot \dot{\mathbf{M}}$ into a component parallel to $\dot{\mathbf{M}}$ and another one perpendicular to $\dot{\mathbf{M}}$, and then the EOM (19) may be rewritten as

$$\frac{d\mathbf{M}}{dt} = -\tilde{\gamma}(\dot{\mathbf{M}},\mathbf{M})\mathbf{M} \times \mathbf{H}_{eff} + \tilde{\alpha}(\dot{\mathbf{M}},\mathbf{M})\frac{1}{M}\mathbf{M} \times \dot{\mathbf{M}}. \tag{48}$$

The "momentary" gyromagnetic ratio

$$\tilde{\gamma}(\dot{\mathbf{M}},\mathbf{M}) = \frac{\gamma}{1 - \tilde{\alpha}^{\perp}(\dot{\mathbf{M}},\mathbf{M})} \tag{49}$$

and the "momentary" damping parameter

TABLE I. Values of $\gamma M \tilde{\alpha} / \tau$ (in 10^{20} sec^{-2}) with the Landé factor taken as $g=2$ for special orientations of the magnetization in bulk Fe, Co, and Ni, as obtained in LSDA and LSDA plus orbital polarization. The numbers are given in the same units as in Ref. 6 where the values in parentheses are taken from. These were obtained by the same general procedure as in the present paper but from LSDA full-potential-linearized-augmented-plane-wave band-structure calculations.

	LSDA	FLAPW	LSDA+OP
bcc Fe $\langle 001 \rangle$	7.2	(7)	7.7
bcc Fe $\langle 111 \rangle$	10.0		10.3
hcp Co $\langle 0001 \rangle$	4.1	(4)	5.6
fcc Ni $\langle 001 \rangle$	57	(60)	67
fcc Ni $\langle 111 \rangle$	46	(50)	53

$$\tilde{\alpha}(\dot{\mathbf{M}}, \mathbf{M}) = \frac{1}{\dot{\mathbf{M}}^2} [\tilde{\alpha}_1(\mathbf{M}) [\dot{\mathbf{M}} \cdot \mathbf{e}_1(\mathbf{M})]^2$$

$$+ \tilde{\alpha}_2(\mathbf{M}) [\dot{\mathbf{M}} \cdot \mathbf{e}_2(\mathbf{M})]^2] / [1 - \tilde{\alpha}^\perp(\dot{\mathbf{M}}, \mathbf{M})] \tag{50}$$

with

$$|\tilde{\alpha}^\perp(\dot{\mathbf{M}}, \mathbf{M})| = \left| \left\langle \left(\underline{\underline{\alpha}}(\mathbf{M}) - \frac{\dot{\mathbf{M}}}{\dot{M}} \underline{\underline{\alpha}}(\mathbf{M}) \frac{\dot{\mathbf{M}}}{\dot{M}} \right) \frac{\dot{\mathbf{M}}}{\dot{M}} \right\rangle \right| \tag{51}$$

thereby all depend on the momentary values of $\mathbf{M}$ and $\dot{\mathbf{M}}$. Thus, the EOM (19) with the damping matrix $\underline{\underline{\alpha}}(\mathbf{M})$ may be rewritten for each instant into the momentary Gilbert equation (48) with a momentary damping scalar $\tilde{\alpha}$ which, however, depends on $\mathbf{M}$ and $\dot{\mathbf{M}}$. [This also makes it possible to transform the momentary Gilbert equation at any instant to a corresponding momentary Landau-Lifshitz equation, see Eq. (21).]

All the results presented in Sec. V B (apart from Table I) are obtained exclusively from calculations including the orbital polarization term. Whereas for the monatomic layer and the monatomic wire this inclusion is indispensable[26] its influence is smaller for bulk materials (see Table I).

A. Results from group theory

In the present section it will be shown that for special orientations $\mathbf{e}$ of the spin magnetization (which we simply call magnetization in the following) in a monatomic layer or in a monatomic wire there is no damping at all. According to Eq. (16) this is the case if the eigenvalues do not change when changing $\mathbf{e}$, i.e., $\partial \varepsilon_{j\mathbf{k}} / \partial \mathbf{e} = \mathbf{T}_{j\mathbf{k}} = 0$. Then such a change of the magnetization direction does not require any scattering processes at the Fermi surface and no damping appears. In several situations it is intuitively clear that the eigenvalues do not change when changing the magnetization direction. For instance, for an arbitrary orientation of the magnetization in a wire the eigenvalues will not change when rotating the magnetization around the wire axis. In other situations we require help from group theory to show that for special ori-

entations of the magnetization the $\mathbf{T}_{j\mathbf{k}}$ and hence the damping are zero for any change $d\mathbf{M}/dt$. We will show this for a monatomic layer with magnetization parallel to a perpendicular twofold symmetry axis, and for a monatomic wire with perpendicular magnetization or magnetization in chain direction. In all these cases the twofold rotation around the magnetization direction is a symmetry operation of the system.

As a starting point of our considerations we have shown that for the above-mentioned cases all the irreducible corepresentations of the magnetic double group are one dimensional at each $\mathbf{k}$ point. Then we have for each unitary element $\hat{U}$ of the magnetic double group the relation

$$\hat{U} \psi_{j\mathbf{k}} = \chi_{j\mathbf{k}} \psi_{j\mathbf{k}}, \tag{52}$$

with $|\chi_{j\mathbf{k}}|^2 = 1$, i.e.,

$$\langle \hat{U} \psi_{j\mathbf{k}} | \hat{T}_l | \hat{U} \psi_{j\mathbf{k}} \rangle = \langle \psi_{j\mathbf{k}} | \hat{T}_l | \psi_{j\mathbf{k}} \rangle. \tag{53}$$

On the other hand we have

$$\langle \hat{U} \psi_{j\mathbf{k}} | \hat{T}_l | \hat{U} \psi_{j\mathbf{k}} \rangle = \langle \psi_{j\mathbf{k}} | \hat{U}^\dagger \hat{T}_l \hat{U} | \psi_{j\mathbf{k}} \rangle = \langle \psi_{j\mathbf{k}} | \hat{U}^{-1} \hat{T}_l \hat{U} | \psi_{j\mathbf{k}} \rangle. \tag{54}$$

We choose $\mathbf{e} = (0, 0, 1)$ for the direction of the magnetization. Then $\hat{T}_z = 0$, and we must consider $\hat{T}_{x,y} = \xi(r)(\hat{l}_{x,y} \hat{s}_z - \hat{l}_z \hat{s}_{x,y})$. Under the action of a twofold rotation around the z axis we get $\hat{U}^{-1} \hat{l}_z \hat{U} = \hat{l}_z$ and $\hat{U}^{-1} \hat{l}_{x,y} \hat{U} = -\hat{l}_{x,y}$ and analogous relations for $\hat{s}$. From a comparison of Eq. (53) with Eq. (54) we therefore obtain $\langle \psi_{j\mathbf{k}} | \hat{T}_{x,y} | \psi_{j\mathbf{k}} \rangle = -\langle \psi_{j\mathbf{k}} | \hat{T}_{x,y} | \psi_{j\mathbf{k}} \rangle$ and hence $\langle \psi_{j\mathbf{k}} | \hat{T}_{x,y} | \psi_{j\mathbf{k}} \rangle = 0$ and according to Eqs. (43) and (44), $\underline{\underline{\alpha}} = 0$.

B. Numerical results

When discussing our numerical data we cannot consider the matrix $\underline{\underline{\alpha}}$ itself but just $\underline{\underline{\alpha}} M / \gamma \tau$ [see Eq. (18)]. Instead of this quantity which has the dimension of an energy we will discuss the matrix $(\mu_B / \hbar)^2 \underline{\underline{\alpha}} M / \gamma \tau$ which has the dimension sec^{-2}. For the sake of simplicity we will denote this quantity in the following nevertheless as damping matrix $\underline{\underline{\alpha}}$.

1. Bulk materials

In the present section we report on the results for bcc Fe, fcc Ni, and hexagonal Co at experimental lattice constants. Figure 1 shows the convergence tests with respect to the number of $\mathbf{k}$ points. To obtain reliable results for $\underline{\underline{\alpha}}$ we have to use much more $\mathbf{k}$ points than for the spin or the orbital moment.

Figure 2 shows the results for the eigenvalues of $\underline{\underline{\alpha}}(\mathbf{M})$ for different orientations of $\mathbf{M}$ in bulk Fe, Co, and Ni. It becomes obvious that the eigenvalues $\tilde{\alpha}_p(\mathbf{M})$ depend rather sensitively on the orientation of $\mathbf{M}$ in the crystal. This holds especially for the case of Co for which the eigenvalues for different orientations differ by factors of up to 4. Altogether, it becomes obvious that the Gilbert Eq. (1) with a damping scalar α which does not depend on the orientation of the magnetization may be violated rather strongly even in the case of bulk materials.
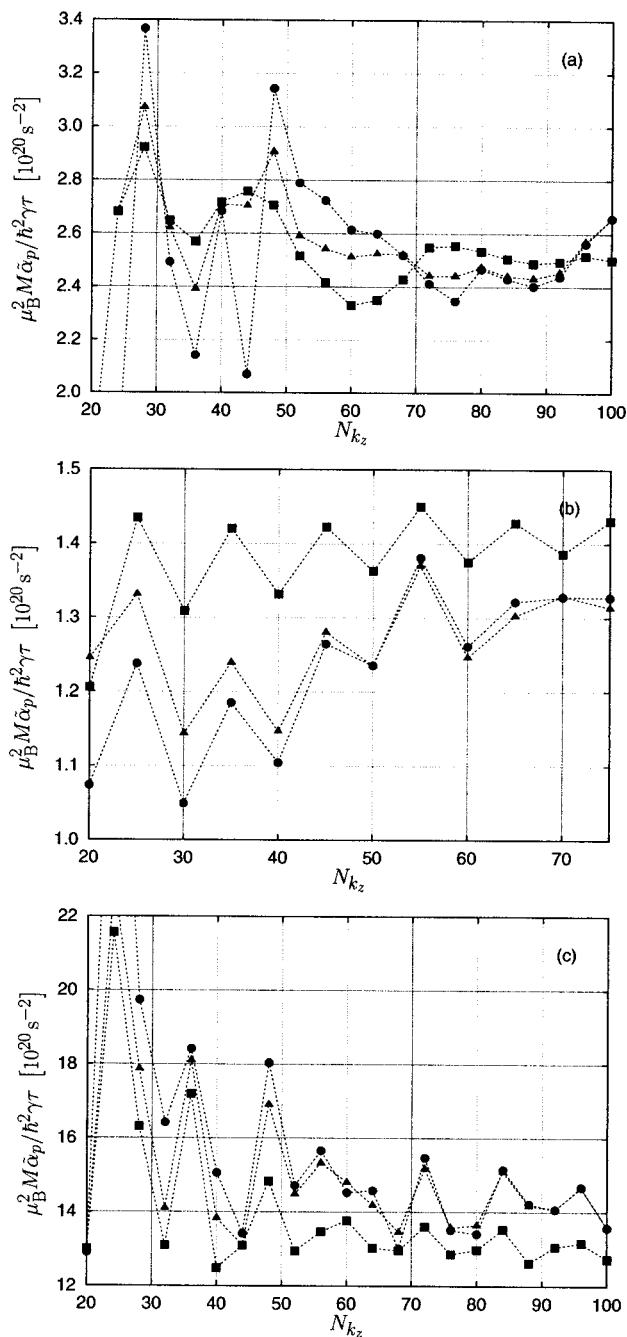
FIG. 1. Convergence tests for the eigenvalue of $\underline{\alpha}$ in bcc Fe (a), hcp Co (b), and fcc Ni (c), with $N_{k_x}=N_{k_y}=N_{k_z}$ for Fe and Ni and $N_{k_x}=N_{k_y}=\frac{8}{5}N_{k_z}$ for Co. For Fe and Ni the magnetization is along the $\langle 111 \rangle$ axis, for Co along the hexagonal axis. All calculations are performed in LSDA including the orbital polarization term. The different curves are $\sigma=5$ mRy ($\blacksquare$), $\sigma=1$ mRy ($\bullet$), and $N_{k_x}\sigma=0.1$ Ry ($\blacktriangle$) for Fe and Ni, respectively, $N_{k_x}\sigma=0.05$ Ry ($\blacktriangle$) for Co.

2. Hexagonal monatomic layers

Figure 3 shows the convergence tests with respect to the number of **k** points. It is startling that the results depend rather sensitively on the question whether we fix σ or σN_{k_y}. The results for Co converge better than those for Ni. Figure 4 shows the results for the two eigenvalues of $\underline{\alpha}(\mathbf{M})$ for
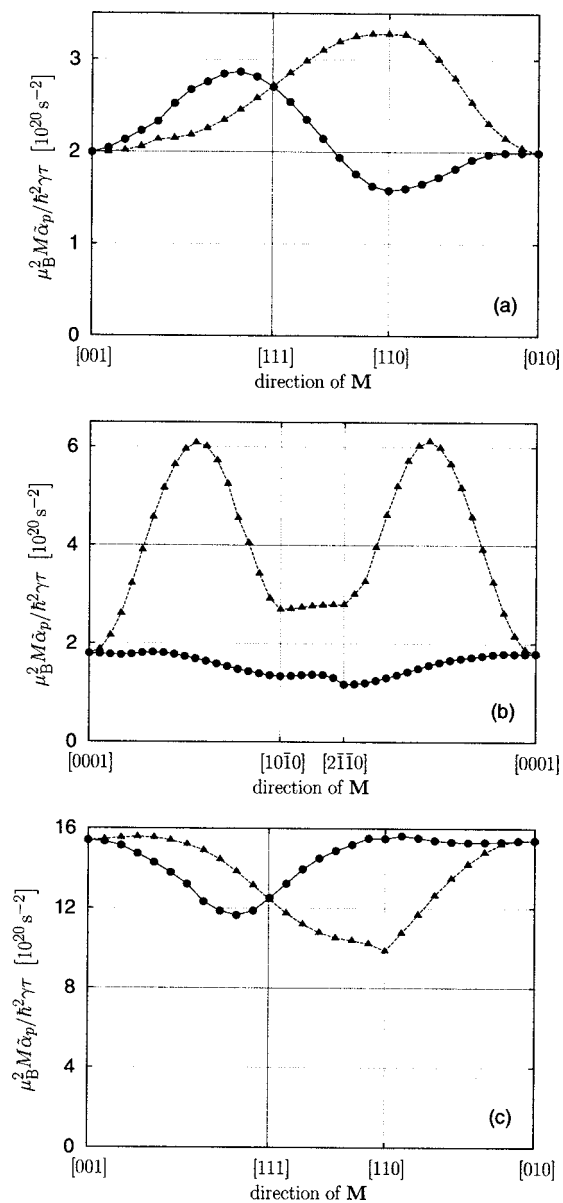
FIG. 2. The two eigenvalues of $\underline{\alpha}$ for different orientations of **M** in bcc Fe (a), hcp Co (b), and fcc Ni (c). The full (symbol $\bullet$) and dashed (symbol $\blacktriangle$) lines give the two eigenvalues $\tilde{\alpha}_p$. The calculations were performed for $N_{k_z}=40$ (Fe, Ni) and $N_{k_z}=15$ (Co), with $\sigma=5$ mRy.

different orientations of **M** in the monolayers of Co and Ni.

As discussed in Sec. V A, the eigenvalues are zero if the magnetization is perpendicular to the layer, i.e., there is no damping at all for this case. Very interesting is the case of in-plane magnetization: The eigenvalue corresponding to the out-of-plane eigenvector perpendicular to **M** is almost zero so that for each in-plane orientation an out-of-plane change $d\mathbf{M}/dt$ perpendicular to **M** is nearly undamped. For an orientation of **M** along the x or y direction this eigenvalue is exactly zero, and this can be shown by arguments from group theory on the line discussed in Sec. V A. In contrast, the eigenvalues corresponding to the in-plane eigenvector are large.
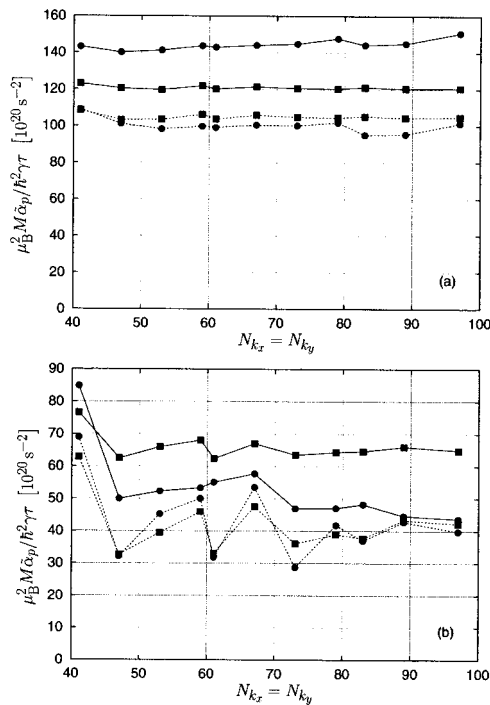
FIG. 3. Convergence tests for the two eigenvalues $\tilde{\alpha}_p$ of $\underline{\underline{\alpha}}$ (corresponding to the full or dashed lines) for hexagonal monatomic layers of Co (a) and Ni (b). The magnetization is declined from the z axis towards the x axis by an angle of 40° (Co) and 35° (Ni). The symbols (● and ■) are for $\sigma N_{k_y}=0.1$ Ry ($\sigma=5$ mRy).
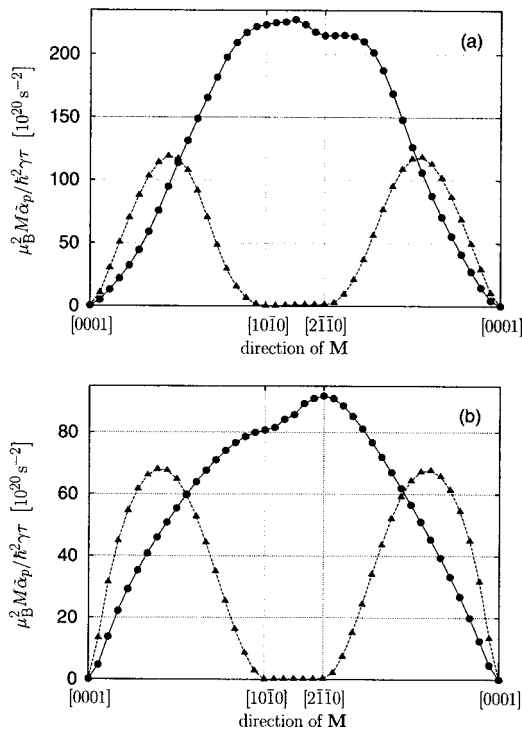

FIG. 5. The magnetic anisotropy energy for hexagonal monolayers of Co (a) and Ni (b). For Co (Ni) the calculations were performed for $N_{k_x}=N_{k_y}=21$ (59) and $\sigma=5$ mRy.


FIG. 4. The two eigenvalues of $\underline{\underline{\alpha}}$ (corresponding to the full or dashed lines) for different orientations of **M** in hexagonal monolayers of Co (a) and Ni (b). The full (symbol ●) and dashed (symbol ▲) lines give the two eigenvalues $\tilde{\alpha}_p$. The calculations for Co (Ni) were performed with $N_{k_x}=N_{k_y}=21$ (59) with $\sigma=5$ mRy.
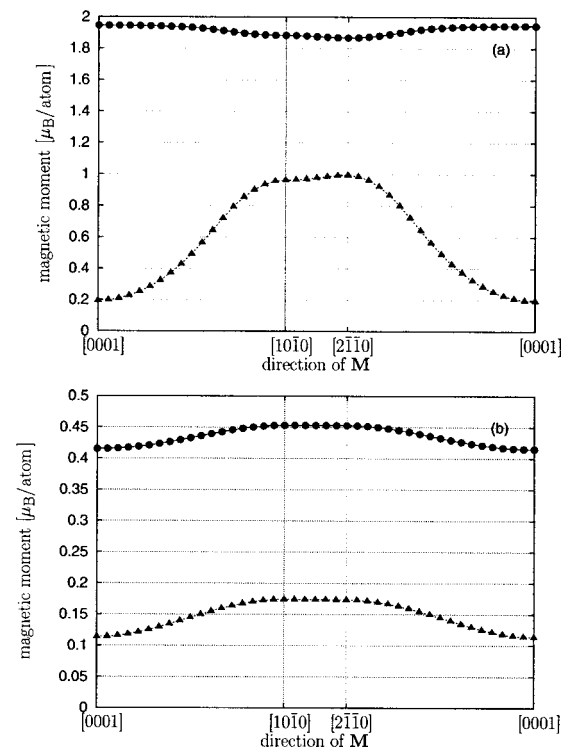
FIG. 6. The spin (●) and orbital (▲) moments for the hexagonal monolayers of Co (a) and Ni (b). For Co (Ni) the calculations were performed for $N_{k_x}=N_{k_y}=21$ (59) and $\sigma=5$ mRy.
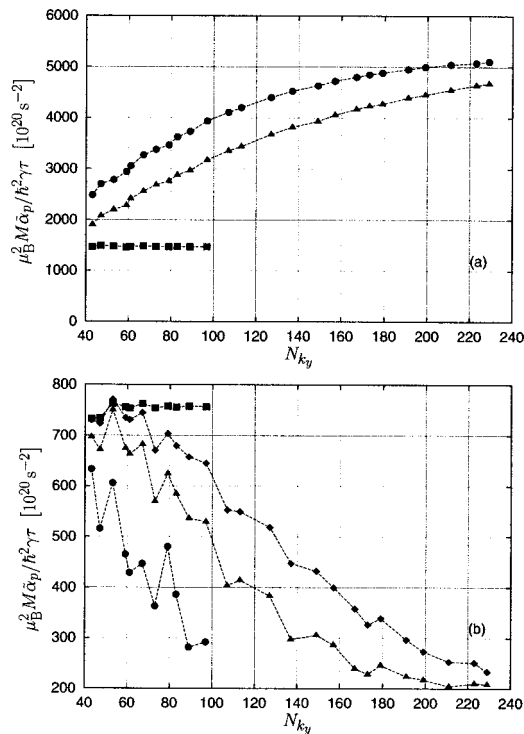
FIG. 7. Convergence tests for the finite eigenvalue $\tilde{\alpha}_p$ of $\underline{\underline{\alpha}}$ for monatomic wires of Co (a) and Ni (b). The magnetization is declined from the z axis towards the wire (y axis) by an angle of 20° (Co) and 40° (Ni). The symbols are for $\sigma=5$ mRy ($\blacksquare$), σN_{k_y} =0.1 Ry ($\bullet$), σN_{k_y}=0.15 Ry ($\blacktriangle$) and σN_{k_y}=0.2 Ry ($\blacklozenge$), only for Ni. The calculations are for $N_{k_x}=N_{k_z}=1$.
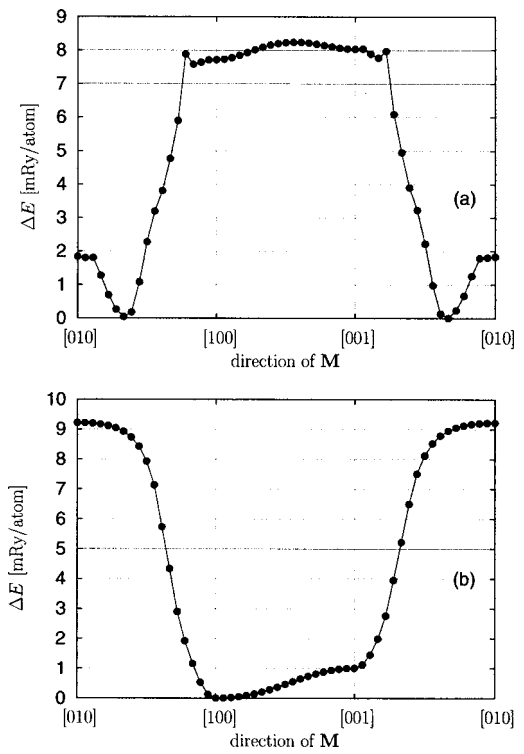

FIG. 9. The magnetic anisotropy energy for monatomic wires of Co (a) and Ni (b). For Co (Ni) the calculations were performed for $N_{k_y}=199$ and $\sigma=0.5$ mRy ($\sigma=0.75$ mRy). The wire is along [010].

FIG. 8. The two eigenvalues $\tilde{\alpha}_p$ of $\underline{\underline{\alpha}}$ (symbols $\bullet$ and $\blacktriangle$) for different orientations of **M** in a monatomic wire of Co (a) and Ni (b). For Co (Ni) the calculations were performed for $N_{k_y}=199$ and $\sigma=0.5$ mRy ($\sigma=0.75$ mRy). The wire is along [010].
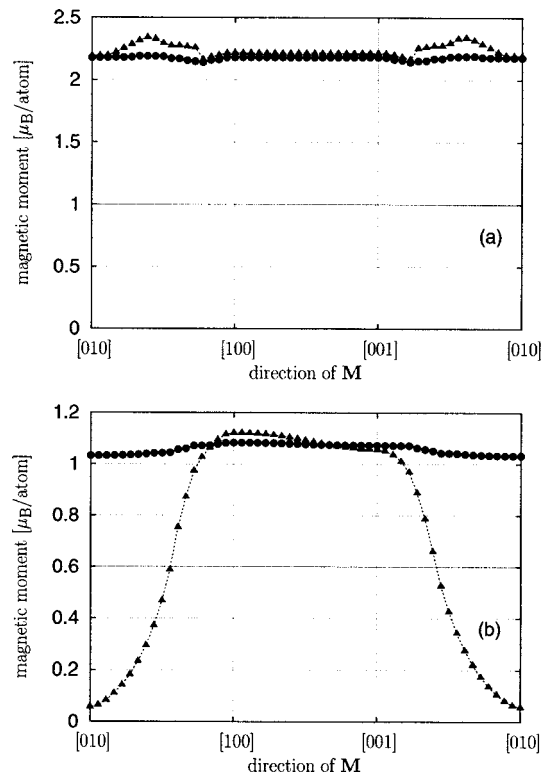

FIG. 10. The spin ($\bullet$) and orbital ($\blacktriangle$) moments for the monatomic wires of Co (a) and Ni (b). For Co (Ni) the calculations were performed for $N_{k_y}=199$ and $\sigma=0.5$ mRy ($\sigma=0.75$ mRy). The wire is along [010].
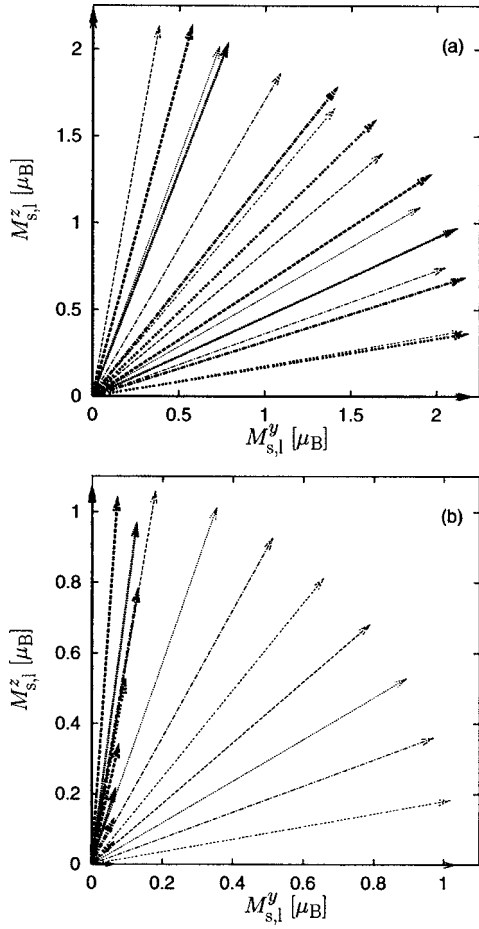
FIG. 11. z and y components of the atomic spin moment $\mathbf{M}_s$ (thin lines) and the atomic orbital moments $\mathbf{M}_l$ (thick lines) of a monatomic wire of Co (a) and Ni (b) for a rotation of the magnetization from the z direction around the x axis versus the wire direction. Arrows with the same structure (full, dashed, dotted, etc.) belong together.

Figure 5 shows the magnetic anisotropy energy. Both for the Co and Ni monolayer the easy axis is in the monolayer.

Figure 6 shows the variation of the magnitudes of the spin and orbital moment with variation of the magnetization direction. Whereas the spin moment is rather stable, the orbital moment varies strongly and attains a rather large value of about $1\mu_B$ ($0.15\mu_B$) for the in-plane orientation in Co (Ni).

3. Monatomic wires

Figure 7 shows the convergence tests with respect to the number of **k** points.

Figure 8 shows the results for the two eigenvalues of $\underset{=}{\alpha}(\mathbf{M})$ for different orientations of **M** in monatomic wires of Co and Ni. As discussed in Sec. V A, the eigenvalues are zero for an orientation perpendicular to the wire or in wire direction. In addition, for an arbitrary orientation the eigenvalue corresponding to a rotation of the magnetization around the wire axis is also zero, whereas the second eigenvalue is large.

Figure 9 shows the magnetic anisotropy energy. For the Co wire the easy axis is perpendicular to the z axis and

TABLE II. The maximum eigenvalues $\mu_B^2 M \widetilde{\alpha}_p / \hbar^2 \gamma \tau$ (in 10^{20} s^{-2}) and the maximum anisotropy energies ΔE_{magn} (in mRy/atom) for Co and Ni bulk, monolayer, and wire. The magnetic anisotropy of Co and Ni bulk has not been calculated in the present paper. The experimental room temperature anisotropy constants for bulk Fe, Co, and Ni are $K_1 = 4.6 \times 10^5, 4.1 \times 10^6, -5 \times 10^4$ and $K_2 = 1.5 \times 10^5, 1 \times 10^6, -3 \times 10^4$.

	Bulk	Monolayer	Wire
Co			
$\mu_B^2 M \widetilde{\alpha}_p / \hbar^2 \gamma \tau$	6	230	6500
ΔE_{magn}/atom		6	8
Ni			
$\mu_B^2 M \widetilde{\alpha}_p / \hbar^2 \gamma \tau$	15.5	95	250
ΔE_{magn}/atom		0.1	9

inclined to the wire by 30°. For the Ni wire the easy axis is perpendicular to the wire. Note that the slight variations of the energy for a rotation of the two magnetization directions perpendicular to the wire result from the fact that in the LMTO-ASA method the vacuum is structured by the ABAB stacking of the empty spheres.

Figure 10 shows the variation of the spin and orbital moment with variation of the magnetization direction. As in the case of a monolayer, the spin moment is rather stable whereas the orbital moment shows a substantial variation, especially for the Ni wire. For Co the orbital moment is even larger than the spin moment.

From Fig. 11 it becomes obvious that for the monatomic wires there may be a very strong deviation from collinearity between orbital and spin moment. Please note that for the case of Co (Ni) the orbital moment is closer to the wire axis (z axis) than the spin moment (strong deviations appear also for the monolayers). As outlined in Sec. III the damping matrix $\underset{=}{\alpha}$ nevertheless has a well-defined meaning in the context of the generalized EOM [see Eqs. (31)–(35)].

VI. DISCUSSION AND CONCLUSIONS

The most important result of the present paper is that the Gilbert EOM for the magnetization dynamics with a damping term of the form $(1/M)\mathbf{M} \times \alpha(d\mathbf{M}/dt)$ and a damping scalar α which does not depend on the orientation of **M** is strictly valid only for a few special situations. Even for the case of a homogeneous magnetization the damping term has to be replaced by a more general term of the form $(1/M)\mathbf{M} \times (\underset{=}{\alpha}(\mathbf{M}) \cdot d\mathbf{M}/dt)$ with a damping matrix $\underset{=}{\alpha}(\mathbf{M})$ which depends on the orientation of the magnetization. The orientation dependence of $\underset{=}{\alpha}$ is already substantial in bulk materials (e.g., variations of up to a factor of 4 in hexagonal Co), and it is very strong for systems with reduced dimensionality like monatomic layers or monatomic wires. In these systems there are orientations for which the damping is identically zero and other orientations for which the damping is very large. Altogether, the dependence of the damping on the orientation of **M** represents an additional option to optimize

a magnetization reversal process in a nanostructured system by choosing a magnetization trajectory which is most appropriate from the viewpoint of damping.

We hope that our results will initiate further experimental study of the dependence of the damping on $\mathbf{M}$ and $d\mathbf{M}/dt$. For thick (bulklike) layers of Co, e.g., this could be done by ferromagnetic resonance experiments, for monolayers or monatomic wires the technique of x-ray magnetic circular dichroism imaging is probably useful. For instance, an anisotropy of the ferromagnetic resonance linewidth has been reported in Ni.[18]

Another important result is that there is no simple relation between damping and magnetic anisotropy. For bulk Fe, Co, and Ni, the values α/τ given in Table I differ only by a factor of at most about 16. In contrast, the magnetic anisotropy of Co is about a factor of 10 larger than the anisotropy of Fe, which in turn is about one order of magnitude larger than the one of Ni. Table II shows the maximum eigenvalues and the maximum anisotropy energy for bulk, monolayers, and monatomic wires of Co and Ni. For the monolayer the maximum eigenvalue is a factor of about 2.4 larger in Co than in Ni whereas the maximum anisotropy energy is a factor of 60 larger in Co. Finally, for the monatomic wire the damping is a factor of 26 larger in Co but the anisotropy energy is very similar.

We have already started to generalize the theory to the case of noncollinear magnetization configurations. For strong noncollinearities on an atomic scale like in the center of a vortex[2] or in narrow domain walls in nanowires[32] the electronic eigenvalues $\varepsilon_{j\mathbf{k}}$ change strongly when changing the magnetic configuration and this should result in a very strong damping.

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