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Significance of nutation in magnetization dynamics of nanostructures

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The dynamics of magnetic moments in nanostructures is closely linked to that of gyroscopes. The Landau-Lifshitz-Gilbert equation describes precession and relaxation but does not include nutation. Both precession and relaxation have been observed in experiments, in contrast to nutation. The extension of the atomistic Landau-Lifshitz-Gilbert equation by a nutation term allows us to study the significance of nutation in magnetization dynamics of nanostructures: for a single magnetic moment, a chain of Fe atoms, and Co islands on Cu(111). We find that nutation is significant at low-coordination sites and on the time scale of about 100 fs; its observation challenges strongly today's experimental techniques.

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Investigations of the magnetization dynamics in nanoscale systems have become very important in the recent past. Hot topics comprise, for example, current-induced domain-wall motion[1] and demagnetization effects upon femtosecond laser pulses.[2,3] On time scales from microseconds down to femtoseconds, the dynamics of magnetic systems is well characterized by the Landau-Lifshitz-Gilbert (LLG) equation

$$\frac{\partial \boldsymbol{M}}{\partial t} = \boldsymbol{M} \times \left(-\gamma \boldsymbol{B}^{\text{eff}} + \frac{\alpha}{M_{\text{s}}} \frac{\partial \boldsymbol{M}}{\partial t} \right) \tag{1}$$

for the average magnetic moment $\boldsymbol{M}$ (Ref. 4). It describes the precession of $\boldsymbol{M}$ around and its relaxation towards the effective field $\boldsymbol{B}^{\text{eff}}$ (Ref. 5).

Precession is well known from the classical mechanics of a gyroscope. If an external force tilts the rotation axis of the gyroscope off the direction of the gravity field, then the gyroscope starts to precess around the gravitational field with a tilt angle ψ (Fig. 1, large circle). Because of the inertia, the rotation axis shifts to larger angles than ψ. Thus, the rotation axis does not coincide with the angular-momentum direction, which results in an additional precession of the gyroscope around the angular-momentum axis (Fig. 1, small circle), called nutation. The trajectory is a cycloid with the tilt angle $\phi(t) = \bar{\phi}[1 - \cos(\omega_{\text{n}} t)]$ and the azimuthal angle $\theta(t) = \bar{\phi}[\omega_{\text{n}} t - \sin(\omega_{\text{n}} t)]$. In most cases, nutation is small compared to precession ($\bar{\phi} < \psi$).

Given the similarity of gyroscope dynamics and magnetization dynamics, Döring introduced the concepts of mass and inertia in macrospin systems,[6] especially for domain walls. De Leeuw and Robertson proved the existence of a domain-wall mass experimentally.[7] Spin nutation was first predicted in Josephson junctions.[8–12] It was shown that in a magnetic tunnel junction, a local spin inserted into the junction can be electrically controlled, using short bias voltage pulses. Ciornei *et al.*[13,14] studied the role of inertia in damped dynamics using a macrospin approach, thereby neglecting the magnetic exchange interaction within the sample, and concluded that nutation will have a lifetime of picoseconds.

Up to now, nutation has not been observed in magnetization dynamics, possibly because the effect is too small and appears on the time scale of the magnetic exchange interaction. However, with respect to the recent enormous progress in ultrafast spectroscopies (e. g., Ref. 15), experimental techniques will access the femtosecond time scale soon. This raises the question under what circumstances nutation can be observed in magnetic nanostructures.

In this paper, we give an answer to the above question for selected nanostructures by means of the atomistic Landau-Lifshitz-Gilbert equation. The spin Hamiltonian comprises the exchange interactions, the magnetocrystalline anisotropy, as well as an external magnetic field. The Heisenberg exchange and the anisotropy constants are calculated from first principles. Starting from an almost collinear magnetic state, an external magnetic field $\boldsymbol{B}$ is switched on abruptly, resulting in nutation of the local magnetic moments. We consider model systems such as a single moment (atom), Fe chains of various lengths, and Co islands on Cu(111).

The magnetization dynamics is described by an atomistic Landau-Lifshitz-Gilbert equation[16,17]

$$\frac{\partial \boldsymbol{m}_i}{\partial t} = \boldsymbol{m}_i \times \left(-\gamma \boldsymbol{B}_i^{\text{eff}} + \frac{\alpha}{m_i} \frac{\partial \boldsymbol{m}_i}{\partial t} + \frac{\gamma \iota}{m_i} \frac{\partial^2 \boldsymbol{m}_i}{\partial t^2} \right), \tag{2}$$

which is extended by a nutation term. $\boldsymbol{m}_i$ is the local atomic moment ($|\boldsymbol{m}_i| = m_i$) at site i. γ and $\alpha \ll 1$ are the gyromagnetic ratio and the Gilbert damping, respectively. The magnetic moment of inertia ι is expressed as $\iota = \frac{\alpha\tau}{\gamma}$ (taken from Ref. 13), with the relaxation time τ that enlarges or reduces the period of the nutation cycloid. The nutation part (usually not considered in magnetization dynamics) is treated as in Refs. 13 and 18, following Döring's concept of magnetic-moment mass.[6] Temperature effects are neglected.

The first term in Eq. (2) accounts for the precession of $\boldsymbol{m}_i$ around the local effective field $\boldsymbol{B}_i^{\text{eff}}$, whereas the second term describes the relaxation of $\boldsymbol{m}_i$ toward $\boldsymbol{B}_i^{\text{eff}}$ due to inelastic processes. The third term models the nutation due to a change in $\boldsymbol{B}_i^{\text{eff}}$. The local effective field $\boldsymbol{B}_i^{\text{eff}} = -\partial \hat{H} / \partial \boldsymbol{m}_i$ is obtained from the Hamiltonian

$$\hat{H} = \hat{H}_{\text{ex}} + \hat{H}_{\text{mca}} + \hat{H}_{\text{dd}} + \hat{H}_{\text{ext}}. \tag{3}$$

$\hat{H}_{\text{ex}}$ is the Heisenberg exchange interaction

$$\hat{H}_{\text{ex}} = -\sum_{ij} J_{ij} \boldsymbol{m}_i \cdot \boldsymbol{m}_j, \tag{4}$$

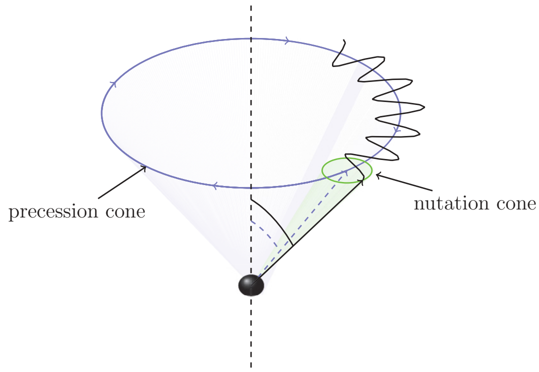

FIG. 1. (Color online) Precession and nutation of a gyroscope or a magnetization vector. The large circle sketches the precession cone around the effective magnetic field (marked as blue (dark gray) line). The inertia leads to the nutation, i. e., an additional precession [green (gray) small circle]. The trajectory is thus a cycloid (black wavy line).

where J_{ij} are the Heisenberg exchange constants. The magnetocrystalline anisotropy

$$\hat{H}_{\text{mca}} = \sum_i K_i (\boldsymbol{m}_i \cdot \boldsymbol{e}_{\text{mca}})^2 \tag{5}$$

is assumed uniaxial, with "easy axis" $\boldsymbol{e}_{\text{mca}}$ and anisotropy constants K_i. The demagnetization field yields the shape anisotropy

$$\hat{H}_{\text{dd}} = -\frac{1}{2}\frac{\mu_0}{4\pi}\sum_{ij}\frac{3(\boldsymbol{m}_i \cdot \boldsymbol{r}_{ij})(\boldsymbol{m}_j \cdot \boldsymbol{r}_{ij}) - (\boldsymbol{m}_i \cdot \boldsymbol{m}_j)\boldsymbol{r}_{ij}^2}{\boldsymbol{r}_{ij}^5}. \tag{6}$$

$\boldsymbol{r}_{ij} \equiv \boldsymbol{r}_i - \boldsymbol{r}_j$ is the distance between sites i and j (μ_0 vacuum permeability). Eventually, the Zeeman term

$$\hat{H}_{\text{ext}} = -\mu_{\text{B}}\boldsymbol{B} \cdot \sum_i \boldsymbol{m}_i \tag{7}$$

accounts for an external field $\boldsymbol{B}$.

Prior to the magnetization-dynamics calculations, we computed the electronic and magnetic structures of bulk Fe and a 2-monolayer-thick Co film on Cu(111) from first principles, using a multiple-scattering approach.[19] Our relativistic Korringa-Kohn-Rostoker method[20] relies on the local spin-density approximation to density-functional theory, with Perdew-Wang exchange-correlation potential.[21] Based on the *ab initio* calculations, both the exchange constants J_{ij} and the anisotropy constants K_i were computed from the magnetic-force theorem (e. g., Ref. 22).

The nutation term in the LLG equation (2) can be interpreted as follows: The Heisenberg model describes the transfer of angular momentum $\boldsymbol{L}$ between two atomic moments, where the total angular momentum is conserved within the entire system. This results in precession because $\frac{\partial \boldsymbol{L}}{\partial t} = \boldsymbol{M}$. An external field $\boldsymbol{B}$ can also transfer angular momentum and tilts the moment off the angular-momentum axis, analogous to the classical gyroscope. However, the moments respond inert and start to nutate on a femtosecond time scale because they are coupled by the Heisenberg exchange interaction. The cycloid period of the nutation is affected by the relaxation time τ. An increased Gilbert damping leads on one hand to a decrease of the nutation effect and on the other hand increases the inertia. Nutation becomes important if the time scale of the change of $\boldsymbol{B}$ is smaller than the angular-momentum relaxation time. The latter can be estimated from the Heisenberg exchange parameters ($J \approx 12$ meV for nearest neighbors in bulk Fe) and the relaxation time to be in the order of tens of femtoseconds.

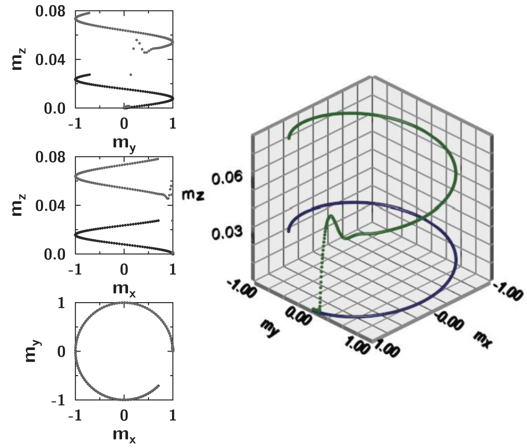

FIG. 2. (Color online) Nutation of a single magnetic moment. The external magnetic field $\boldsymbol{B}$ along z is abruptly increased from 1 to 51 T. Blue (green) line: trajectory without (with) the nutation term in the LLG equation (2). The panels on the left-hand side show the vector components [dark gray (gray): without (with) nutation term]; note the different scales of the Cartesian axes. Relaxation time $\tau = 1$ ps, Gilbert damping $\alpha = 0.005$, total duration 600 fs.

Application 1: Single magnetic moment. It suggests itself that a single moment should have the strongest nutation.[13] If an external magnetic field $\boldsymbol{B}$ is applied, e. g., in z direction, the magnetic moment precesses around the external field with the Larmor frequency $\omega = \gamma B$. An abrupt increase of $\boldsymbol{B}$ changes the angular velocity of the precession: Without the nutation term in Eq. (2), the precession becomes only faster (blue line in Fig. 2). However, with the nutation term in Eq. (2), nutation shows up as a cycloid with a small lifetime (green line): the abrupt increase of the z component of the magnetic moment is due to the huge external magnetic field which is, admittedly unphysically, suddenly increased.

Despite the unphysical parameters (given in Fig. 2), the nutation amplitude is very weak. We attribute this finding to a change of the *strength* of $\boldsymbol{B}$, rather than a change of its *direction* (cf. Ref. 13 in which a pronounced nutation is found for the latter case).

Our finding supports that nutation is hard to observe in a macrospin system under realistic physical conditions. It suggests that nutation is more significant when changing the external-field direction or by taking into account the effective field coming from nearby magnetic moments [Eq. (4); the single magnetic moment of this model system is apparently not affected by other magnetic moments]. This supposition is proved in the next examples.

Application 2: Chain of Fe atoms. The role of angular-momentum transfer due to Heisenberg exchange is investigated by means of Fe chains of finite lengths. The exchange constants J_{ij} are deliberately taken from bulk Fe ($J = 12.6$ meV for nearest neighbors and $J = 11.3$ meV for next-nearest neighbors); since the exchange parameters depend on the dimensionality ($\approx \frac{1}{r^{\mathrm{dim}}}$), this is an approximation, the anisotropies K_i are set to zero. The system is initially prepared in a slightly noncollinear state to which the external field is applied after 1 ps; because of the typical relaxation time of about 5 ps, this intermediate state is still not perfectly collinear. As in the first example, we apply a sudden increase of the external field.

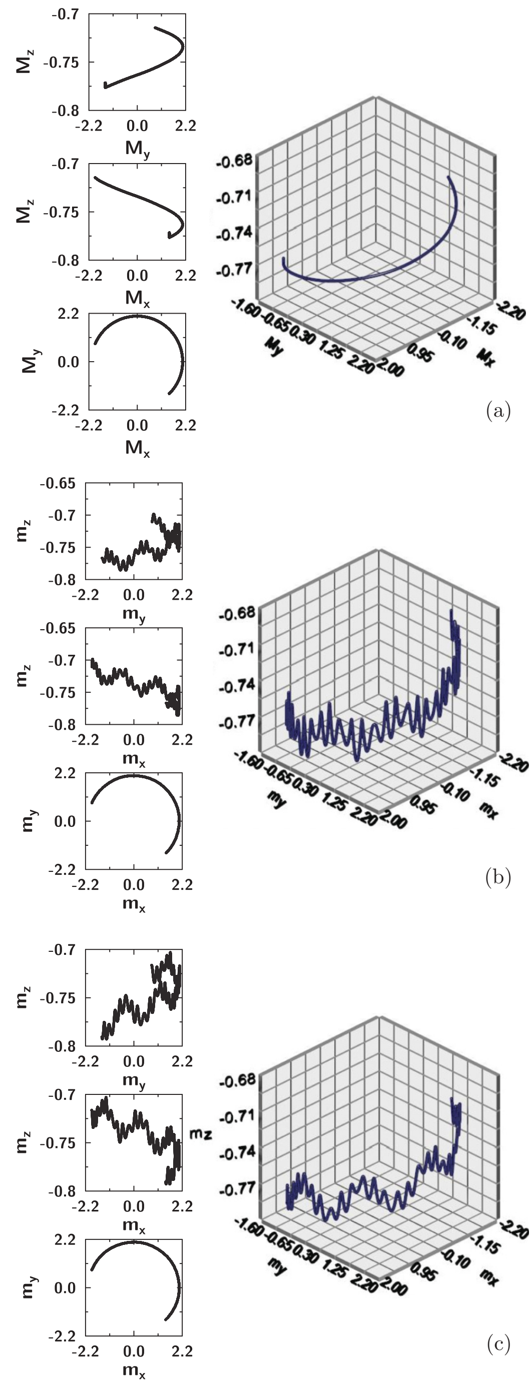

FIG. 3. (Color online) Nutation in an Fe chain with five atoms. A magnetic field of 10 T in the z direction is applied abruptly to the collinear ground state. (a)–(c) Trajectories of the average magnetization (a), the central moment (b), and an edge moment (c). The panels on the left-hand side show the vector components; note the different scales of the Cartesian axes. Relaxation time $\tau = 1$ fs, Gilbert damping $\alpha = 0.004$, atomic distance 2.863 Å, total duration 2 ps.

We exemplify our findings for a chain of five atoms. The nutation is small compared to the precession: the typical amplitude is about $0.2\,\mu_{\mathrm{B}}$–$0.4\,\mu_{\mathrm{B}}$ for a single moment. The average magnetization $\boldsymbol{M}$ shows no considerable effect [Fig. 3(a)], similar to the single magnetic moment in the first application. In the present case, however, the reason is a phase shift between single magnetic moments due to the noncollinear initial state, the magnetic coupling, and the inertia that leads to cancellation [Figs. 3(b) and 3(c)].

The amplitude of the nutation depends also on the number of interacting neighbors in the ensemble: smaller for the central moment [Fig. 3(b)], larger for an edge moment [Fig. 3(c)]. The correlation between the magnetic moments increases with the coordination number, which results on one hand in a larger effective field and on the other hand in a reduced nutation lifetime and amplitude.

With increasing damping α, both magnitude and lifetime of the nutation decrease. A high damping speeds up the relaxation towards the collinear configuration. Depending on the ratio of exchange field and magnetic field, different forms of cycloids occur (not shown here): an elongated or an abbreviated cycloid.

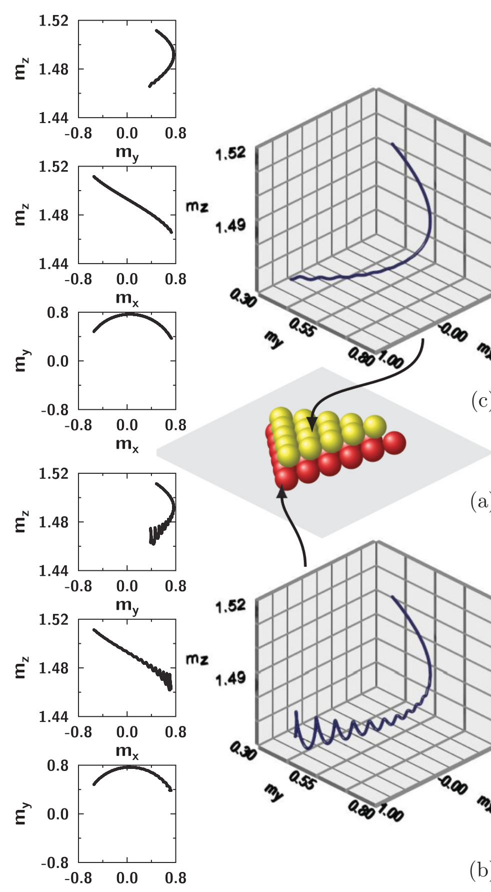

FIG. 4. (Color online) Nutation in 2-monolayer-thick Co island on Cu(111) with 36 atoms. (a) Schematic illustration of the triangular-shaped Co island. The Cu substrate is not shown. (b) and (c) Trajectory of a corner atom (b) and a center atom (c), respectively. The panels on the left-hand side show the vector components; note the different scales of the Cartesian axes. $\tau = 1$ fs, $\alpha = 0.02$, total duration 2 ps.

Especially, the first form is due to collective excitations (e. g., from excitations of magnons perpendicular to the magnetic field).

Application 3: Co nanoislands on Cu(111). As seen before, the nutation strength of a local moment depends on the coordination number of the respective atom. This effect becomes even stronger in a nanoisland as compared to a chain. To support this observation further, we address a 2-monolayer-thick Co island on Cu(111) with 36 atoms in total. Here, the effective field incorporates the magnetocrystalline anisotropy, calculated from *ab initio* (for details see Ref. 23). The chosen Gilbert damping α of 0.02 is typical for nanostructures (Refs. 16 and 23). The abrupt magnetic-field increase of 5 T perpendicular to the island results in a stronger nutation at a corner atom [Fig. 4(b)] as compared to that for a center atom [Fig. 4(c)]. For even larger islands (not shown here), the nutation at a center atom can vanish completely, but that at a corner atom remains. Because of the angular-momentum conservation, the average magnetic moment exhibits no nutation (not shown here).

We estimate the range of nutation lifetimes to about 100 fs up to 500 fs (a lifetime of a few ps was found in Ref. 13). This rather short time scale corroborates why nutation has not been measured so far. The dependence on the coordination number suggests that nutation is negligible in bulk materials. An increase of the relaxation time τ enlarges the cycloid period because the system reacts more inert; increasing the damping constant reduces the cycloid amplitude and the nutation decays much faster.

Temperature effects are usually incorporated in the LLG equation by a white-noise ansatz, i. e., $\boldsymbol{B}_i^{\text{eff}}$ is replaced by $\boldsymbol{B}_i^{\text{eff}} + \boldsymbol{b}_i(t)$ where $\boldsymbol{b}_i(t)$ is an uncorrelated random field.[16] However, this approach does not hold in the presence of the nutation term: the process is no longer a Markov process due to the second derivative in the LLG equation. The occurring temporal correlations can be included by a color-noise approach.[24] Using nevertheless white noise, the random fields result in a broadening of the trajectories because both the nutation as well as the precession axes are varied randomly. Hence, the nutation effects reported are significantly reduced (not shown here).

Concluding remarks. Nutation is significant on the femtosecond time scale since a typical damping constant of $0.01 \ldots 0.1$ reduces the nutation lifetime to about 100 fs. It shows up preferably in low-dimensional systems, e. g., at edges and corners but with a small amplitude with respect to the precession. These findings lead to the conclusion that the observation of nutation effects is a strong challenge for experimental investigations.

Since the inertia of moment and the dissipation depend on the environments of the local magnetic moments, one could improve the theory by replacing the damping constant and the moment-of-inertia constant by respective tensors, both of which could be computed from first principles.[18,25,26] Further, there is, to our knowledge, no theoretical foundation for a Langevin dynamics including nutation at finite temperatures.

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