Magnetization reversal in a “quasi” single domain magnetic grain: a new numerical micromagnetic technique

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(February 25, 2022)

The problem of magnetization reversal in a fine single-domain grain is of great importance in magnetic recording physics. Characteristic reversal times under strong reversal magnetic field give a physical limitation to both data rates and system signal to noise ratio. Dynamic magnetization reversal depends on the system or magnetic energy relaxation mechanisms. In addition to energy absorption to the “thermal bath” of the host lattice, magnetization reversal can occur by excitation of nonlinear ‘spin-wave’ like modes. In the present paper we explore in detail the excitation of these modes in a quasi-single-domain grain. This magnetization reversal process exhibits features of several problems of nonlinear and solid state physics, such as kinetics of an orientational phase transition and energy transfer in nonlinear systems of oscillators. Therefore the problem is of interest to fundamental science.

Dynamic magnetization reversal begins when the external magnetic field reaches and exceeds the so-called ‘nucleation’ field and the original remanent state becomes unstable. Typically these dynamical processes in both single and multidomain magnetic systems are solved by integration of the Landau-Lifshitz equations with phenomenological damping. This form of magnetization dynamics describes a coherent rotation of each discretized subgrain, in which the magnetization magnitude is conserved. Such approximation is fair for small excitations, as in linear ferromagnetic resonance, or for some particular model cases when an excess of energy directly goes to the thermal bath without excitation of spin waves.

Recently we have explored magnetization reversal in quasi-single-domain grain by neglecting phenomenological damping and specifically exploring nonlinear spin-wave like magnetic excitations. By quasi-single-domain we mean grains whose dimension is on the order of the domain wall width or in some cases the exchange length. Similar analysis has also been done on reversal in thin films. In all these cases, according to Suhl’s speculation, the switching process should be rapid, governed by nonlinear spin-wave excitations. Recently spin-waves excited by large magnetization rotations have been observed experimentally.

By neglecting phenomenological damping, the total system magnetic energy is conserved. These simulations have demonstrated that the excess of Zeeman energy is transformed to the exchange, anisotropy and magneto-static energies by nonlinear spin-wave excitations. The purpose of this paper is to present a detailed study of magnetization reversal simulations focusing on magnetic interactions in a single grain.

In addition, we describe here a new numerical scheme of solving the Landau-Lifshitz equations. Typically numerical micromagnetic simulations invoke the three Cartesian coordinates of each discretization cube. At each integration time step the magnetization is modified to satisfy the condition of constant magnitude. This scheme is preferable to utilization of the natural two-parameter polar coordinate scheme because of singularities. In polar coordinates there are always two singularities at the poles. In this new scheme we utilize two coordinates per magnetization sub-cube, however here these coordinates are similar to linear combinations of the transverse magnetization components. Using a simple scheme, all singularities are avoided.

In section 2 we discuss the micromagnetic model for our quasi-single-domain grain. In section 3 we describe the implementation of our new numerical model. In sections 4, 5 results of simulations are considered in detail.
Then we discuss obtained results and draw conclusions.

II. MODEL

The magnetic energy (Hamiltonian) of the grain can be written in the form:

\[ \mathcal{H} = \int (\mathcal{U}_{\text{exch}} + \mathcal{U}_{\text{anis}} + \mathcal{U}_Z + \mathcal{U}_{\text{dmag}}) \, d\mathbf{r}. \]  

Here

\[ \mathcal{U}_{\text{exch}} = \frac{A}{M_s^2} \left[ \left( \frac{\partial \mathbf{M}}{\partial x} \right)^2 + \left( \frac{\partial \mathbf{M}}{\partial y} \right)^2 + \left( \frac{\partial \mathbf{M}}{\partial z} \right)^2 \right] \]  

is the exchange energy density,

\[ \mathcal{U}_{\text{anis}} = K_u \left[ 1 - \left( \frac{M_z}{M_s} \right)^2 \right] \]  

is the uniaxial anisotropy energy density,

\[ \mathcal{U}_Z = -\mathbf{H} \cdot \mathbf{M} \]  

is the Zeeman energy density and \( \mathcal{U}_{\text{dmag}} \) is the magnetostatic energy density.

For simplicity we shall consider a micromagnetic grain as a system of \( n = 4 \times 4 \times 4 \) (see, Fig.1) coupled cubic subgrains of the volume \( V = L^3 \), where \( L \) is the linear size of sub-cube. Each sub-cube can be characterized as a classical spin:

\[ \mathbf{S}_j = -\mathbf{M}_j V / \hbar \gamma, \]  

where \( \mathbf{M}_j \) is the vector magnetization of \( j \)-th sub-cube, \( \hbar \) is Plank’s constant and \( \gamma > 0 \) is the gyromagnetic ratio. \( |\mathbf{M}_j| = M_s \), where \( M_s \) is the saturation magnetization, and therefore, \( |\mathbf{S}_j| = S \equiv M_s V / \hbar \gamma \). Each spin is localized in the center of its sub-cube. The characterization of each sub-cube magnetization in terms of an effective spin is our choice: the problem we consider is purely classical. However the spin notation is convenient for the numerical scheme presented in Sec.3. Spin characterization also provides a bridge to quantum spin models.

The Hamiltonian Eq. (6) of the system in terms of spin notation can be written as:

\[ \mathcal{H} = \mathcal{H}_{\text{exch}} + \mathcal{H}_{\text{anis}} + \mathcal{H}_Z + \mathcal{H}_{\text{dmag}}. \]  

Here

\[ \mathcal{H}_{\text{exch}} = -\frac{J}{2} \sum_{j \neq j'} (\mathbf{S}_j \cdot \mathbf{S}_{j'} - S^2) \]  

describes the exchange interaction between the nearest neighbors, \( J = 2AL / S^2 \). Note that this form is identical to the usual micromagnetic approximation that assumes a linear variation of the magnetization between grain centers [9]. The term \(-S^2\) in Eq. (7) yields \( \mathcal{H}_{\text{exch}} = 0 \) in the case when all spins are oriented in the same direction.

\[ \mathcal{H}_{\text{anis}} = \frac{\hbar \gamma H_K S}{2} \sum_{j=1}^{N} \left[ 1 - \left( \frac{S_z}{S} \right)^2 \right] \]  

is the uniaxial anisotropy energy, where \( H_K = 2K_u / M_s \) is the anisotropy field. \( \mathcal{H}_{\text{anis}} = 0 \) corresponds to all spins parallel to the anisotropy axis.

\[ \mathcal{H}_Z = \hbar \gamma H \cdot \sum_{j=1}^{N} \mathbf{S}_j - \hbar \gamma HNS \]  

is the Zeeman energy. \( \mathcal{H}_Z = 0 \) if either \( H = 0 \) or all spins are oriented along the external magnetic field direction.

The magnetostatic interaction of the sub-cubes will be approximated by the dipole-dipole interaction energy

\[ \mathcal{H}_{\text{dmag}} = \frac{(\hbar \gamma)^2}{2} \sum_{j \neq j'} \left[ \mathbf{S}_j \cdot \mathbf{S}_{j'} - 3(\mathbf{S}_j \cdot \mathbf{r}_{jj'})(\mathbf{S}_{j'} \cdot \mathbf{r}_{jj'}) / r_{jj'}^3 \right] - \mathcal{H}_{\text{dmag}}^{(0)} \]  

where \( \mathbf{r}_{jj'} = \mathbf{r}_j - \mathbf{r}_{j'} \) and \( \mathbf{r}_j, \mathbf{r}_{j'} \) are the radius-vectors of the \( j \) and \( j' \) spins, respectively. The constant \( \mathcal{H}_{\text{dmag}}^{(0)} \) is chosen so that \( \mathcal{H}_{\text{dmag}} = 0 \) if all spins are oriented upward along the \( z \) direction.

We shall study the problem of time evolution of the normalized total magnetization

\[ \mathbf{m} = \frac{1}{NM_s} \sum_j \mathbf{M}_j = -\frac{1}{NS} \sum_j \mathbf{S}_j \]  

in the system (8) from the initial state when \( H = 0 \) and the averaged magnetization at \( t < 0 \) is oriented “upward” in the \( z \) direction. At the moment \( t = 0 \), a strong reversal magnetic field \( \mathbf{H} = (H^x, 0, H^z) \) is applied. The component \( H^z \) is negative and the transverse component \( H^x \) is taken to be relatively small (\( |H^x| \ll |H^z| \sim H_K \)). The net vector field is sufficient to give only one energy minimum corresponding to an almost “downward” orientation of the averaged magnetization. Thus the system acquires an excess of Zeeman energy which can be later transformed to nonlinear spin excitations containing magnetic anisotropy, exchange and dipole-dipole interaction energies. This transformation will cause the net magnetization magnitude \( |\mathbf{m}| \) to reduce. Mathematically the question of energy transfer is described in Appendix B.

III. NUMERICAL SCHEME

The Landau-Lifshitz equation without damping in terms of classical spin (5) can be written as
written in the form an analog of the Landau-Lifshitz equations (12) and can be
classical spin in a similar form. Schlömann [15] also presented a transformation (see Appendix). We introduce the real and dimensionless variables $q_j$ and $p_j$ (as a generalized coordinate and momentum) as follows

$$S_j^x = q_j \sqrt{(S + S_j^z)/2},$$
$$S_j^y = p_j \sqrt{(S + S_j^z)/2},$$
$$S_j^z = S - (q_j^2 + p_j^2)/2.$$  

These transformations are exact and can be considered to be a form of classical Holstein-Primakoff transformation (see Appendix). We introduce the real and dimensionless variables $q_j$ and $p_j$ (as a generalized coordinate and momentum) as follows

$$S_j^x = q_j \sqrt{(S + S_j^z)/2},$$
$$S_j^y = p_j \sqrt{(S + S_j^z)/2},$$
$$S_j^z = S - (q_j^2 + p_j^2)/2.$$  

These equations describe the evolution of coupled spin components $S_j^x$, $S_j^y$ and $S_j^z$. As time evolves, Eqs. (12), (13) give two system conservations: the net spin of each sub-grain is fixed

$$(S_j^x)^2 + (S_j^y)^2 + (S_j^z)^2 = S^2,$$  

and the total magnetic energy remains constant. Thus only two independent variables exist for each j-th site.

It is natural to write down only two differential equations for each spin in terms of spin components or other generalized variables. The most popular form of “two-variable” Landau-Lifshitz equation is known to be in spherical coordinates. However the use of spherical coordinates for an arbitrary motion of spin gives a stiff system of differential equations with singularities at the poles. Moreover, numerical calculations of trigonometric functions typically take much longer time than simple arithmetic operations. This is why the spherical coordinate approach is not usually used in micromagnetic calculations. In practice the direct method of numerical solution of the Landau-Lifshitz equation is used (see, for example, [12, 13]). Dynamic equations for all three variables are integrated with continuum numerical modification so that the Eq. (14) is maintained.

In this paper we present a new scheme for numerical solution of the Landau-Lifshitz equation (12), in which only two variables are utilized and condition (14) is automatically maintained. We introduce the real and dimensionless variables $q_j$ (as a generalized coordinate) and $p_j$ (as a generalized momentum) as follows

$$S_j^x = q_j \sqrt{(S + S_j^z)/2},$$
$$S_j^y = p_j \sqrt{(S + S_j^z)/2},$$
$$S_j^z = S - (q_j^2 + p_j^2)/2.$$  

These equations are exact and can be considered to be a form of classical Holstein-Primakoff transformation (see Appendix). Schlömann [13] also presented a classical spin in a similar form. The equations of motion for $q_j$ and $p_j$ are the exact analog of the Landau-Lifshitz equations (12) and can be written in the form

$$\frac{dq_j}{d\tau} = \frac{H_{eff,j}}{H_K} \frac{\partial S_j}{\partial p_j},$$
$$\frac{dp_j}{d\tau} = -\frac{H_{eff,j}}{H_K} \frac{\partial S_j}{\partial q_j},$$  

where a dimensionless time $\tau = \gamma H_K t$ is introduced. Corresponding spin derivatives are

$$\frac{\partial S_j^x}{\partial q_j} = \sqrt{\frac{S + S_j^z}{2}} - \frac{q_j^2}{4} \sqrt{\frac{2}{S + S_j^z}},$$
$$\frac{\partial S_j^y}{\partial p_j} = \sqrt{\frac{S + S_j^z}{2}} - \frac{p_j^2}{4} \sqrt{\frac{2}{S + S_j^z}},$$
$$\frac{\partial S_j^z}{\partial q_j} = -q_j, \quad \frac{\partial S_j^z}{\partial p_j} = -p_j.$$  

It is necessary to mention that Eqs. (16a), (16b) contain a singularity at $S + S_j^z = 0$. To avoid this singularity we shall use (16a), (16b) only in the hemisphere $|S_j| = S$ with $S_j^z > 0$. This is illustrated in Fig. 2. Following Eq. (5), negative magnetization corresponds to a positive spin and the $(p, q)$ coordinates are in the upper half hemisphere. Initially before reversal, when $M_z > 0$ it is convenient to introduce analogous variables $Q_j$ and $P_j$ (see Appendix A) for the hemisphere $|S_j| = S$ with $S_j^z < 0$:

$$S_j^x = Q_j \sqrt{(S - S_j^z)/2},$$
$$S_j^y = -P_j \sqrt{(S - S_j^z)/2},$$
$$S_j^z = -S - (Q_j^2 + P_j^2)/2.$$  

The equations of motion for $Q_j$ and $P_j$ have the form:

$$\frac{dQ_j}{d\tau} = \frac{H_{eff,j}}{H_K} \frac{\partial S_j}{\partial P_j},$$
$$\frac{dP_j}{d\tau} = -\frac{H_{eff,j}}{H_K} \frac{\partial S_j}{\partial Q_j},$$  

and spin derivatives are

$$\frac{\partial S_j^x}{\partial Q_j} = \sqrt{\frac{S - S_j^z}{2}} - \frac{Q_j^2}{4} \sqrt{\frac{2}{S - S_j^z}},$$
$$\frac{\partial S_j^y}{\partial P_j} = -\sqrt{\frac{S - S_j^z}{2}} - \frac{P_j^2}{4} \sqrt{\frac{2}{S - S_j^z}},$$
$$\frac{\partial S_j^z}{\partial Q_j} = -Q_j, \quad \frac{\partial S_j^z}{\partial P_j} = -P_j.$$  

A continuous transition from one set of variable to another one is defined by

$$q_j = Q_j \sqrt{\frac{S - S_j^z}{S + S_j^z}},$$
$$p_j = -P_j \sqrt{\frac{S - S_j^z}{S + S_j^z}}.$$  

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and

\[ Q_j = q_j \sqrt{S + S_j}, \]
\[ P_j = -p_j \sqrt{S - S_j}. \]

Thus, we begin the calculations with \( P_j(0) \) and \( Q_j(0) \). After a short integration time \( \Delta t \) we find \( P_j(\Delta t) \) and \( Q_j(\Delta t) \) and calculate corresponding \( S_j \), \( S_j^0 \) and \( S_j^1 \). If \( S_j^1 < 0 \), we continue integration of the Landau-Lifshitz equations with \( P_j \) and \( Q_j \). In the case when \( S_j^1 \geq 0 \), the \( j \)-th spin trajectory crosses the equator and enters the upper hemisphere. To avoid the singularity in the \( P_j \) and \( Q_j \) coordinates in the upper pole (see Fig.2), the new variables \( p_j \) and \( q_j \) are introduced by Eq. (21). Integration of the Landau-Lifshitz equations using \( p_j \) and \( q_j \) until the \( z \)-component of the spin changes sign \( (S_j^1 < 0) \). At that point we change back to the \( P_j \) and \( Q_j \) coordinates.

It should be noted that the Eqs. (16a), (16b), (19a) and (19b) have simple algebraic operations only and therefore numerical integration of these equations do not contain time consuming operations.

A characteristic time scale of the system is \( 1/\gamma H_K \). The role of exchange interaction is defined by the parameter \( H_e/H_K \), where \( H_e = JS/h\gamma = 2A/M_sL^2 \) is the exchange field from the nearest neighbor. One can write

\[ H_e/H_K = (n^{2/3}/16)(\delta_w/\delta_s)^2, \]

where \( \delta_w = 4(A/K_n)^{1/2} \) is the domain wall width, \( \delta_s = n^{1/3}L = 4L \) is the linear sample size. The exchange interaction energy can also be characterized by, so-called, “exchange length” \( \delta_{ex} = A^{1/2}/M_s \). Therefore one can write

\[ H_e/H_K = 2n^{2/3}(M_s/H_K)(\delta_{ex}/\delta_s)^2. \]

We shall focus on the case of relatively strong uniaxial anisotropy when \( M_s/H_K \ll 1 \) (which is valid for real magnetic recording grains). In the zeroth order of this small parameter we can neglect the dipole-dipole interaction in the system. However as it will be demonstrated in the next section that even relatively small dipole-dipole interaction, which absorbs very small amount of the Zeeman energy and reduce the magnetization.

This behavior is typical of nonlinear spin-wave processes whose amplitudes grow exponentially from an initial thermal level. The decrease in net magnetization becomes observable at virtually a critical time \( t_c \) when the magnetic moment of the (transverse) excited waves becomes comparable with the net magnetic moment. At the same time the system nonlinearities restrict the exponential growth. The oscillations in \( m_z \) that occur for \( t > t_c \) primarily correspond to the uniform rotation: the frequency increases with decreasing \( m_z \). If spin-wave excitations did not occur, oscillations in \( m_x, m_y, m_z \) would reflect uniform rotation only and at every instant sum to give constant \( |\mathbf{m}| \approx 1 \).

The equations of motion (16a), (16b), (19a), (19b) contain relative parameters only. For simulations these parameters were chosen to correspond to real magnetic recording media. For example, with \( A = 10^{-6} \text{ erg/cm} \), \( H_K = 7 \text{ kOe} \) and \( M_s = 250 \text{ Oe} \), the scaled parameters are \( \delta_w \approx 43 \text{ nm} \), \( \delta_{ex} = 40 \text{ nm} \) and \( M_s/H_K = 0.036 \).

Nonlinearities can only be excited were there are deviations in the magnetization state from perfect alignment. We include this by allowing the system to initially be in thermal equilibrium. We assign randomly a total energy deviation of \( 64\hbar^2T \). Practically we randomly deviate the magnetization of each cell within a fixed limit. This limit is adjusted to achieve the above total energy deviation. To obtain a true thermal equilibrium the Landau-Lifshitz equations are solved, given the above initialization, for a time \( \gamma H_K t_0 \approx 200 \). At this point the system is prepared for the application of the reversal field.

IV. MAGNETIZATION REVERSAL WITHOUT DIPOLE INTERACTIONS

First we shall consider the case when the dipole-dipole interactions in \( \gamma H_{ij} \) are neglected. Fig.3a,b show the time dependencies of \( m_z(t) \) and \( |\mathbf{m}(t)| \) in the case when the reverse magnetic field has a very small deviation from the anisotropy axis \( (H_e/H_z = 0.02) \). Fig.3b is simply an extension of the time axis of Fig.3a. The field magnitude is slightly less than the nucleation field for uniform rotation \( (H_{nuc} \approx -0.9H_K) \). This field corresponds (by numerical test) to the lowest reverse field required to produce nonlinear excitations. The sample dimension is 16% and 25% greater than the domain wall width and exchange length, respectively. Initially the longitudinal component of magnetization decreases monotonically from \( m_z \approx 1 \) to \( 0.7 \) and then at a ‘critical’ time \( \gamma H_K t_c \approx 70 \), oscillations of \( m_z \) occur. In contrast, the net magnitude of magnetization remains practically constant \( |\mathbf{m}| \approx 1 \) until \( t_c \) and then abruptly decreases exhibiting irregular oscillations. For times less than \( t_c \) the average magnetization simply precesses about the reverse field. For times greater \( t_c \) the excitation of nonlinear spin waves becomes pronounced. These excitations both absorb Zeeman energy and reduce the magnetization.
With increasing time the average $m_z$ continually decreases reaching, for this example an asymptotic level in the vicinity of $m_z = 0$ (at least for times less than $\gamma H_K t \approx 3000$). There is no reversal of $m_z(t)$. The average magnetization $\langle m(t) \rangle$ also decreases by about $\approx 60\%$. As time proceeds, the spin-wave oscillations exhibit increased chaotic behavior.

Fig.4 shows similar time dependences as in Fig.3 but for the case of increased angle of the reverse magnetic field from the anisotropy axis ($H_z/H = 0.10$). The field magnitude ($H_z/H = -0.70$) also corresponds to the onset of spin-wave excitation. As expected, the magnetization dynamics is much faster in this case. We can see the beginning of nonlinear spin-wave excitation at $\gamma H_K t_c \approx 30$, where the $m_z$ has reduced due to pure rotation to $\approx 0.3$. The decrease of longitudinal magnetization is more substantial, passing through zero at $\gamma H_K t_0 \approx 75$ and reaching about $\approx 55\%$ of its nominal value in the opposite direction after $\gamma H_K t \geq 1000$. Similar to the case shown in Fig.3, the average magnetization $\langle m(t) \rangle$ decreases to $\approx 60\%$. Note that the amplitudes of chaotic oscillations of $\langle m(t) \rangle$ are relatively smaller than in the case of Fig.3 (compare the long time behavior of Fig.3b and Fig.4b). Here most of the Zeeman energy is transformed into high frequency exchange-dominant spin-wave modes, which have relatively small magnetic moments.

As discussed earlier, the total magnetic energy remains constant in these dynamic processes. In Fig.5a,b we plot the evolution of the Zeeman, exchange and anisotropy energies (Fig.5b is an extended scale of Fig.5a). The reverse angle is intermediate between Fig.3 and 4. Initially, for times less than $t_c$ (in this case $\gamma H_K t_c \approx 45$), uniform rotation yields a decrease of the Zeeman energy and an increase of the anisotropy energy. At the onset of nonlinear spin-wave excitation we see, in addition, an increase of the exchange energy. The wave-like nature of these excitations can be seen in Fig.5a in the beating of the exchange and anisotropy energies. The nonlinear excitation of chaotic oscillations of the magnetization can be thought of as an “overheating of the magnetic system”. The more exchange magnetic modes that are involved in the process, the smaller the averaged magnetization $\langle m(t) \rangle$.

Fig.6a-d demonstrate the time dependences of $m_z(t)$ and $\langle m(t) \rangle$ for various magnetic fields: $-0.78 H_K$, $-0.79 H_K$, $-0.90 H_K$ and $-1.0 H_K$, respectively. As in Fig.5 the field angle is fixed at $H_z/H = 0.05$ and relative sizes are unchanged. For this angle the Stoner-Wohlfarth nucleation field is $-0.83 H_K$. In this case the onset field for nonlinear spin-wave excitation is $H_z = -0.79 H_K$. There is no reversal below this field as shown in Fig.6a. The magnetization evolution at the onset field is shown in Fig.6b (similar to Figs.3,4). Magnetization dynamics for larger fields are shown in Figs.6c,d. A notable features can be seen: the critical time for nonlinear spin-wave excitation increases with increasing field. The increase of $t_c$ allows for several cycles of uniform rotation to occur prior to the nonlinear spin-wave excitation. No reversal dynamics was observed beyond $H_z < -1.1 H_K$ (in this particular case). Essentially as the reverse field is increased beyond the spin-wave onset field, $t_c$ rapidly increases and becomes infinite. These phenomena also occur for other field angles ($H_z/H$).

As indicated in Figs.6a-d the asymptotic, long time value of $m_z$ increases with increasing applied field (i.e. less magnetization reversal occurs). In Fig.7 we explicitly plot the asymptotic values of averaged $\langle m_z(t) \rangle$ and $\langle \langle m(t) \rangle \rangle$ versus applied field. It should be noted that the excitation of nonlinear spin waves occurs only for a narrow band of applied fields.

Fig.8 shows the evolution of magnetization at various sample sizes. We see that a decrease of the sample size relative to the domain wall width leads to a suppression of magnetization reversal. This fact is also can be interpreted in terms of nonlinear spin-wave processes. By decreasing the sample size, we increase the frequencies of the non-uniform spin-wave modes and therefore restrict the number of resonance nonlinear processes that can contribute to a decay of the uniform mode. Analysis for larger sample would require finer discretization.

V. MAGNETIZATION REVERSAL WITH DIPOLE INTERACTIONS

In this section we show numerical simulations that include the dipole-dipole interactions in $\gamma H_{eff} j (13)$. The relative role of dipole-dipole interaction is small because we assume a small magnetostatic parameter $M_s/H_K \ll 1$. In this case we can not expect a noticeable absorption of the Zeeman energy solely by the dipole-dipole reservoir. Nevertheless, the dipole-dipole interaction plays an important role in the process of energy transfer: it reduces the symmetry of the system and therefore opens new channels of nonlinear spin-wave interactions.

Let us compare the results of Fig.3 obtained without dipole interaction and corresponding results in Fig.9 with the dipole interaction. The onset time $t_\nu$ of nonlinear excitation is about the same. However $m_z(t)$ decreases more rapidly, reverses and reaches an asymptotic value of $\approx -0.5$. This is in contrast to Fig.2 where the asymptotic $m_z(t)$ does not reverse. In this case the average magnetization $\langle m(t) \rangle$ decreases to $\approx 50\%$, slightly more than the $\approx 60\%$ in Fig.3. The amplitudes of chaotic oscillations of $\langle m(t) \rangle$ in this case are much smaller than occur in Fig.3. The excess Zeeman energy is transformed into exchange modes, which have smaller magnetic moments.

Plotted in Fig.10 is the magnetization dynamics for a larger field angle ($H_z/H = 0.10$). As compared with Fig.4, including magnetostatic interactions slightly increases the reversal rate. The longitudinal magnetization passes through zero at $\gamma H_K t_0 \approx 55$ and, similar to Fig.4, reaches about $\approx 55\%$ of its nominal value in the opposite direction after $\gamma H_K t \geq 500$. The average magnetization $\langle m(t) \rangle$ is decreased to $\approx 60\%$. 

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Fig. 5c,d demonstrate typical transformations of Zeeman, anisotropy and exchange energies for short (c) and long (d) time intervals for magnetization dynamics with dipole interactions. We see faster dynamics of energy transformations than shown in Fig. 5a,b. It should be noted that the energy absorbed by dipole interactions is relatively small (within $\pm 0.01$ in relative units) as expected and therefore not shown. However the magnetostatic interactions change the balance the exchange and anisotropy energies.

In Fig. 11 are shown the time dependencies $m_z(t)$ and $|n_{x}(t)|$ for various reversal fields. In agreement with Fig. 6, the reversal dynamics is suppressed with increasing the strength of reversal field but the range of reversal dynamics is much broader. We did not observe any reversal dynamics at $H_z \leq -3H_K$ in this particular case. We believe that the $4 \times 4 \times 4$ discretization is not a major limiting factor. For the case of $n = 1000$ subgrains no reversal dynamics was observed at $H_z \leq -4H_K$.

In Fig. 12 we plot the asymptotic relative change in Zeeman energy $\Delta E_Z = (1 - \langle m_z \rangle)(-H_z/H_K)$ versus the applied magnetic field for the parameters of Fig. 11 (solid dots). Even though there is less asymptotic magnetization decrease as the field is increased, the relative change in Zeeman energy does increase. After the onset of nonlinear spin-wave excitation, in this case at $H_z = -0.79H_K$, the amount of spin-wave energy that can be excited increases to a maximum value. In addition (open dots), the change in Zeeman energy is plotted corresponding to Fig. 5, for the case of no magnetostatic interaction. The same trend occurs but only over a small interval of field values.

Fig. 13 shows the evolution of magnetization at various sample sizes. As in Fig. 8, the decrease of the sample size relative to the domain wall width leads to a suppression of magnetization reversal. The minimum size for spin-wave excitation remains the same, however differences are seen in the amplitude of the chaotic excitations.

We have also examined the effect of grain size relative to the exchange length at fixed relative domain wall size ($\delta/s = 1.16$). The system evolution is more sensitive to exchange length if the dipole-dipole interaction is taken into account. The primary effect is that with a smaller relative exchange length the rate of decrease of the average magnetization is faster. As discussed above, the presence of magnetostatic interactions allows the excitation of additional spin-wave modes that were otherwise degenerate. These modes are more easily excited if the sample size is large compared to the exchange length.

### VI. DISCUSSION

Magnetization reversal occurs by reducing the Zeeman energy as the magnetization goes from an initial high energy state to one of low energy (approximately in the field direction). Typically this dynamic process is analyzed using the Landau-Lifshitz equation with an appropriate phenomenological damping term. Here we have excluded phenomenological damping and shown that substantial, rapid reversal can occur. In this case the total magnetic energy is conserved, however subject to constraints of sample size and field range, the Zeeman energy is reduced by the excitation of nonlinear spin-waves.

In the present study we have specifically focused on a cubic grain sufficiently small to be almost single domain. In this case after uniform rotation over a short time period, nonlinear spin waves are excited and the average grain magnetization decreases. For the sample sizes examined here the reduction was from positive saturation ($+M_s$) to at most, $-0.6M_s$. Due to numerical limitations we did not examine large grains and it is possible that, with sufficient discretization, almost complete reversal might occur for samples much larger than the domain wall width. In this study we considered only samples with small relative magnetostatic energy contribution. Studies have been performed on high moment low anisotropy thin films, where a large out of plane magnetization reversal torque occurs. In these cases virtually complete reversal already occurs with no phenomenological damping.

The decrease and suppression of magnetization reversal with increasing the reversal field strength initially seem unusual. In the discussion of Fig. 11 a limit is suggested as due to the saturation of the spin-wave energy. However, the problem we consider is a general system of nonlinear oscillators (nonlinear spin waves). In the oscillator problem one mode (here corresponding to coherent rotation of the magnetization) is initially strongly excited. One might expect that the system would move towards its most probable state (thermal equilibrium) by a chaotic mode mixing. With any large reverse field we would expect reversal to a new equilibrium state. However, the observed reversal decreases and suppression can be qualitatively understood as a result of nonlinear spin-wave interactions.

The processes of nonlinear spin-wave decay are defined by several factors. First, it is necessary that the frequency of the initial mode and some portion of the nonlinear spin-wave spectrum overlap. Second, we require sufficiently strong nonlinear interwave coupling. These factors determine a threshold amplitude of the decaying wave (as an effective pumping field). Third, the amplitude of initial (decaying) wave must exceed a threshold value. When the reversal field strength is increased, all these three requirements eventually are not met. As suggested in Ref. [14], increasing the reverse field shifts the spin-wave spectrum away from the uniform precession mode. Also as the reversal field is increased nonlinear coupling decreases. At a certain reversal field the threshold of nonlinear decay will exceed the amplitude of coherent magnetization rotation and the reversal process will be suppressed. Generally speaking, such a suppression of the energy transfer from the excited mode to other modes.
is a common feature of the theory of Hamiltonian systems of nonlinear oscillators (see, e.g., [17]). The most simple and popular example of nonlinear coupled oscillators is the Fermi-Pasta-Ulam chain (see, e.g., [18]).

The numerical scheme we have presented is valuable here primarily because the number of coordinates is reduced by 2/3. Thus, the computational storage requirement is correspondingly reduced. However, there is an additional advantage to this formulation. These coordinates correspond naturally to nonlinear oscillators that describe spin-wave motions. Recently, the problem of thermally agitated reversal has been analyzed in a micromagnetic grain. Using this nonlinear oscillator representation a simple exact solution has been obtained for the first passage time [19], [20], [21].

VII. CONCLUSION

Magnetization reversal in a quasi-single-domain grain can occur by nonlinear spin-wave excitation. In this process an excess of Zeeman energy is transferred to uniaxial anisotropy and exchange energies. The dipole-dipole interaction plays an important role even if small \( M_s/H_K \ll 1 \). The process of magnetization reversal in a fine grain exhibits general features of system of interacting oscillators: energy transfer by nonlinear resonance processes. This nonlinear process (diffusion) is forbidden for either a strong reversal field and/or a small grain size.

We have presented a new scheme to perform numerical integration of the Landau-Lifshitz equations. This new scheme utilizes only two variables per discretization cell, but strictly conserves the magnetization magnitude. Comparison with conventional techniques shows that both schemes require approximately the same computation time at the same level of accuracy (the new scheme takes a slightly shorter time). The main advantage of the new scheme is that it utilizes a smaller number of variables (2/3 of the total magnetization components) and therefore requires less memory.

ACKNOWLEDGMENTS

The authors are grateful to Prof. Harry Suhl for valuable comments and discussions. We also thank E. Boerner, M. E. Schabes and A. N. Slavin for interesting and helpful discussions of obtained results. This work was partly supported by matching funds from the Center for Magnetic Recording Research at the University of California - San Diego and CMRR incorporated sponsor accounts.

APPENDIX A: EQUATIONS OF MOTIONS AND CANONICAL VARIABLES

1. Classical commutations

Hamilton’s equations can be written in a general form

\[
 i\hbar \frac{d\mathcal{O}}{dt} = [\mathcal{O}, \mathcal{H}] \tag{A1}
\]

Here \( \mathcal{O} \) is a function of interest and \([\ldots, \ldots] = i\{\ldots, \ldots\}\) denotes a classical analog of commutator and \(\{\ldots, \ldots\}\) are the Poisson brackets. Plank’s constant \(\hbar\) is
used as a dimensional constant to simplify a dimensional structure of the equation and for simple correspondence with quantum mechanics.

Taking into account the Mermin’s \cite{22} formula for the Poisson brackets for a system of classical spins $S_j$, one can write:

$$[A, B] = i \sum_j S_j \cdot \frac{\partial A}{\partial S_j} \times \frac{\partial B}{\partial S_j}. \quad (A2)$$

It is simple to show that the commutation rules for the classical spins are the same as in quantum mechanics:

$$[S^j, S^k] = \pm S^k \delta_{jk}, \quad [S^j, S^k] = 2S^j \delta_{jk}. \quad (A3)$$

where $S^j = S_j^x \pm i S_j^y$ are the circular spin components.

Substituting $O = S_j$ to Eq. (A1) and taking into account that

$$[S, H] = iS \frac{\partial S}{\partial S} \times \frac{\partial H}{\partial S} = -i \frac{\partial S}{\partial S} \cdot S \times \frac{\partial H}{\partial S} = -iS \times \frac{\partial H}{\partial S},$$

one can obtain the Landau-Lifshitz equation \cite{12}.

2. Holstein-Primakoff transformations

It may be easily shown that the commutations (A3) are valid if

$$S^z = S - a^* a, \quad S^+ = a \sqrt{S + S^z}, \quad S^- = a^* \sqrt{S + S^z}. \quad (A4)$$

These relations describe the classical spin realization in terms of complex variables $a^*$ and $a$ corresponding to quantum creation and annihilation operators, respectively. The transformation (A4) in the quantum case was introduced by Holstein and Primakoff \cite{14}. Suhl \cite{23} first utilized approximate Holstein-Primakoff transformation with complex variables to describe magnetic resonance.

The classical analog of the commutator for $a^*$ and $a$ is

$$[A, B] = \frac{\partial A}{\partial a} \frac{\partial B}{\partial a^*} - \frac{\partial A}{\partial a^*} \frac{\partial B}{\partial a}. \quad (A5)$$

The Eq. (A1) with (A5) can be rewritten as

$$\frac{da}{dt} = i \frac{\partial \mathcal{H}}{\partial S} \cdot \frac{\partial S}{\partial a} - i \gamma \mathbf{H}_{\text{eff}} \cdot \frac{\partial S}{\partial a}. \quad (A6)$$

Another form of Holstein-Primakoff transformation can be written as

$$S^z = -S - b^* b, \quad S^+ = b \sqrt{S + S^z}, \quad S^- = b \sqrt{S + S^z}. \quad (A7)$$

The classical analog of commutator for $b^*$ and $b$ is

$$[A, B] = \frac{\partial A}{\partial b} \frac{\partial B}{\partial b^*} - \frac{\partial A}{\partial b^*} \frac{\partial B}{\partial b}$$

and the corresponding equation of motion has the form

$$\frac{db}{dt} = -i \frac{\partial \mathcal{H}}{\partial S} \cdot \frac{\partial S}{\partial b^*} = -i \gamma \mathbf{H}_{\text{eff}} \cdot \frac{\partial S}{\partial b^*}. \quad (A8)$$

It should be noted that Eqs. (A6) and (A8) represent other forms of the Landau-Lifshitz equation \cite{12}.

3. Real canonical variables

Let us introduce real variables $q$ and $p$ as

$$a = \frac{q + i p}{\sqrt{2}}, \quad a^* = \frac{q - i p}{\sqrt{2}}$$

Thus the Eqs. (A4) become

$$S^z = q \sqrt{(S + S^z)/2}, \quad S^y = p \sqrt{(S + S^z)/2}, \quad S^z = S - (q^2 + p^2)/2. \quad (A9)$$

These formulas are exact and can be considered as a form of classical Holstein-Primakoff transformation.

The classical commutator for $q$ and $p$ is:

$$[A, B] = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q}. \quad (A10)$$

The equations of motion for real and dimensionless $q$ and $p$ are

$$\frac{dq}{dt} = \frac{\partial \mathcal{H}}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial q} \frac{\partial S}{\partial q} \cdot \frac{\partial S}{\partial p}. \quad (A11)$$

We shall use the transformation (A3) in the case, when $S_j^z \geq 0$.

In order to exclude stiff equations, for $S_j^z < 0$ it is convenient to introduce other variables $Q$ and $P$ as follows

$$b = \frac{Q + iP}{\sqrt{2}}, \quad b^* = \frac{Q - iP}{\sqrt{2}}$$

The equations of motion for $Q$ and $P$ have the form:

$$\frac{dQ}{d\tau} = \frac{\partial \mathcal{H}}{\partial P} \frac{\partial S}{\partial Q} = \gamma \mathbf{H}_{\text{eff}} \cdot \frac{\partial S}{\partial P}, \quad \frac{dP}{d\tau} = -\frac{\partial \mathcal{H}}{\partial Q} \frac{\partial S}{\partial P} = -\gamma \mathbf{H}_{\text{eff}} \cdot \frac{\partial S}{\partial Q}. \quad (A12)$$
APPENDIX B: ENERGY TRANSFER

Mathematically the question of energy transfer between $\mathcal{H}_Z$, $\mathcal{H}_{\text{exch}}$, $\mathcal{H}_{\text{anis}}$ and $\mathcal{H}_{\text{dd}}$ is associated with the Eq. (A1) with $\mathcal{O} = \mathcal{H}_Z$:

$$i\hbar \frac{d\mathcal{H}_Z}{dt} = \left[ \mathcal{H}_Z, \mathcal{H}_Z + \mathcal{H}_{\text{exch}} + \mathcal{H}_{\text{anis}} + \mathcal{H}_{\text{dd}} \right] \quad (\text{B1})$$

It is obvious that $\left[ \mathcal{H}_Z, \mathcal{H}_Z \right] = 0$. Direct energy transfer from the Zeeman energy to the exchange energy is always forbidden, because

$$\left[ \mathcal{H}_Z, \mathcal{H}_{\text{exch}} \right] = 0. \quad (\text{B2})$$

The commutator $\left[ \mathcal{H}_Z, \mathcal{H}_{\text{anis}} \right]$ depends on the orientation of the external magnetic field. If the external magnetic field is parallel to $z$ axis ($\mathbf{H} = (0,0,H)$) then this commutator is equal to zero. However, even a slight deviation of $\mathbf{H}$ from the $z$ axis permits a possibility to transform in sequence the Zeeman energy to the anisotropy energy and the latter to the exchange energy as long as

$$\left[ \mathcal{H}_{\text{exch}}, \mathcal{H}_{\text{anis}} \right] \neq 0. \quad (\text{B3})$$

Captions

Fig.1. Model of micromagnetic grain ($4 \times 4 \times 4$ subgrains).

Fig.2. New coordinates.

Fig.3. Short (a) and long (b) time evolution of magnetization in the case of very small deviation of reversal magnetic field from the anisotropy axis.

Fig.4. Short (a) and long (b) time evolution of magnetization in the case of moderate deviation of reversal magnetic field from the anisotropy axis.

Fig.5. Transformations of Zeeman, anisotropy and exchange energies for short (a,c) and long (b,d) time intervals. The dipole interactions are neglected in (a,b) and are taken into account in (c,d). $H_z = -0.79H_K$ is the onset of reversal, $H_x/H_z = 0.05$, $\delta_w/\delta_{\text{ex}} = 1.08$.

Fig.6. Time evolution of magnetization for various reversal fields at $H_x/H_z = 0.05$, $\delta_w/\delta_{\text{ex}} = 1.08$ (dipole interactions are neglected).

Fig.7. Average asymptotic longitudinal component and absolute value of magnetization versus applied reverse field. Conditions correspond to Fig.6.

Fig.8. Time evolution of magnetization for various grain sizes $\delta_s/\delta_w$. $H_z/H_K = -0.79$, $H_x/H_z = 0.05$, $\delta_w/\delta_{\text{ex}} = 1.08$ (dipole interactions are neglected).

Fig.9. Short (a) and long (b) time evolution of magnetization in the case of very small deviation of reversal magnetic field from the anisotropy axis. The strength of reversal field corresponds to the onset of reversal (dipole interactions are taken into account).

Fig.10. Short (a) and long (b) time evolution of magnetization in the case of moderate deviation of reversal magnetic field from the anisotropy axis. The strength of reversal field corresponds to the onset of reversal (dipole interactions are taken into account).

Fig.11. Time evolution of magnetization for various reversal fields at $H_x/H_z = 0.05$, $\delta_w/\delta_{\text{ex}} = 1.08$ (dipole interactions are taken into account).

Fig.12. Relative change in Zeeman energy versus applied reversal magnetic field.

Fig.13. Time evolution of magnetization for various grain sizes $\delta_s/\delta_w$. $H_z/H_K = -0.79$, $H_x/H_z = 0.05$, $\delta_w/\delta_{\text{ex}} = 1.08$ (dipole interactions are taken into account).
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