Investigation of an Extended Magnetization Vector Constraint

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In continuum micromagnetics, the classical "fixed" length constraint for a magnetization vector $\mathbf{M}$ is well known, while at the same time, some experimental conditions suggest the condition clearly breaks down, e.g., finite temperature. Assuming a fixed length for an elementary moment and using the definition of a magnetization vector as its volume average, along with existing continuum exchange theory, it can be shown that this constraint does not explicitly follow, but rather an extended form of it which includes exchange. Using this extended constraint, consequent equilibrium (and dynamic) continuum micromagnetics formulations are numerically solved to examine differences in current and this "extended" formulation. The classical problem of the transition of nanoparticles from flower to vortex states is considered for illustration. The use of the extended constraint suggests greater potential for nonuniformity at smaller particle sizes. Considering dynamics, it is also observed that new contributions from exchange are present in the direction of "damping," which have the effect of speeding up magnetization "motion," thus minimally damped systems may still demonstrate fast reversal, contrary to current intuition based on the LLG.

***Index Terms*—Micromagnetics, magnetization constraint, Landau–Lifshitz–Gilbert (LLG), extended LLG (eLLG).**

I. INTRODUCTION

THE Landau–Lifshitz–Gilbert (LLG) equation (or variants of it) is probably the most widely used micromagnetics formulation for describing the spatiotemporal evolution of a continuous magnetization vector $\mathbf{M}$ [1]–[3], where $\mathbf{M}$ is defined as the dipole moment (or elementary moment) per unit volume. For the LLG, it is well known that it conserves the length of $\mathbf{M}$, maintaining the equilibrium constraint given by

$$|\mathbf{M}|^2 = M_{\mathrm{s}}^2. \tag{1}$$

There is an intuition already that this condition relates to the behavior of exchange. This is because it assumes that interatomic exchange forces are much stronger than energies that may effectively reduce exchange, e.g., thermal energy and possibly even sample size [4], [5]. Another relevant point to consider, for example, is the known behavior of paramagnetic materials that spontaneously form $\mathbf{M}$ upon the application of an external field. As temperature increases, ferromagnetic materials transition to paramagnetic, and therefore, it is quite possible that the length of $\mathbf{M}$ is not conserved, even below the Curie temperature. Some currently investigated potential technologies like heat-assisted magnetic recording are good examples that motivate these kinds of concerns. This departure from the constraint in (1) is therefore of importance in describing $\mathbf{M}$ in finite temperature, at minimum.

Recently, an analysis using the definition of $\mathbf{M}$, the (dipole) elementary moment per unit volume, along with continuum exchange theory, has been carried out to explicitly obtain a relationship between $\mathbf{M}$ and its saturation magnetization M_{s} [6]. This constraint has the form of an extension to (1). Consequently, if used, it leads to extended forms of the equations of motion. In this paper, using these extended equations, computations solving the LLG and this extended LLG (eLLG) are discussed computing equilibrium states for cubic nanoparticles evolving from flower to vortex states. Rather striking implications from the eLLG on dynamics are also observed and highlighted.

A summary of the extended constraint is given in Section II. Section III presents the extended equations of motion. In Section IV, numerical computations investigating solutions from both the eLLG and LLG are discussed.

II. EXTENDED MAGNETIZATION CONSTRAINT

The critical results from continuum exchange theory used here include the following: 1) the number N of elementary moments $\mathbf{m}$ in a unit volume are sufficiently large; and 2) the expansions of the direction cosines of these elementary moments are all truncated above third-order terms, where $|\mathbf{m}| = M_{\mathrm{s}}$, however it is *not* assumed that $|\mathbf{M}| = M_{\mathrm{s}}$.

Let us begin with a unit volume, where the magnetization $\mathbf{M}$ may be defined in terms of the elementary moment $\mathbf{m}$ as

$$\mathbf{M} = \frac{1}{N}\sum_{j=1}^{N}\mathbf{m}_j. \tag{2}$$

A constraint between $\mathbf{M}$ and M_{s} may be obtained directly by dotting $\mathbf{M}$ with itself and using known results from continuum exchange theory [7]. Dotting $\mathbf{M}$ with itself and introducing direction cosines and M_{s}, one can obtain the following constraint for $\mathbf{M}$ [6]:

$$|\mathbf{M}|^2 = M_s^2 + \kappa\ell_x^2\mathbf{M}\cdot\nabla^2\mathbf{M}. \tag{3}$$

ℓ_x is a material parameter, e.g., exchange length, which is on the order of the variation of $\mathbf{m}$, i.e., $\ell_x \sim \min(\sqrt{A_X/K}, \sqrt{2A_X/\mu_0 M_{\mathrm{s}}^2})$ (in SI units). A_X is the exchange stiffness corresponding to interatomic exchange energy, and K is the anisotropy constant. The parameter κ is introduced here as a convenient scaling parameter and is on the order of unity [6]. By inspection, the fixed length constraint is seen to be a lower-order approximation of (3).

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Digital Object Identifier 10.1109/TMAG.2011.2145366

III. Extended Equations of Motion

The equilibrium equations of motion follow from the Lagrangian of the system [8], which, taking the extended constraint into consideration, leads to an extended equilibrium condition given by

$$\mathbf{H}_{\mathrm{T}} \propto \mathbf{M}^{*} \equiv \mathbf{M} - \kappa \ell_x^2 \nabla^2 \mathbf{M}. \tag{4}$$

$\mathbf{H}_{\mathrm{T}}$ is the total effective magnetic field that includes external fields, effective anisotropy, exchange fields, etc. From (4), a consistent extended 'precession" term is then given by

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M}^{*} \times \mathbf{H}_{\mathrm{T}}. \tag{5}$$

In obtaining the dissipative part of the equation, it is noted that there are infinitely many choices for the damping terms. Here, the introduction of a phenomenological damping term follows the form proposed by Gilbert [3] as it includes effects on both precessional and rotational motion [9] leading to

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \left(\mathbf{M} - \kappa \ell_x^2 \nabla^2 \mathbf{M}\right) \times \left(\mathbf{H}_{\mathrm{T}} - \eta \frac{\partial \mathbf{M}}{\partial t}\right). \tag{6}$$

IV. Results and Discussion

Considering this extended constraint and equations of motion, the classical problem of the equilibrium states of nanosized cubes are recomputed for different particle sizes along with switching in an external field. These calculations, solving the LLG, were done previously by Schabes and Bertram [10] and others [11]. From the resulting magnetization distributions after reducing an external field to zero, the remanence is computed and compared between the fixed length (LLG) and extended formulation (eLLG). Fig. 1 shows the results from simulations for cubic particles using parameters similar to those in [10] and [11].

The extended formulation predicts potentially smaller critical particle sizes, where the transition occurs, compared to the fixed-length LLG formulation ($\kappa = 0$). Thus, the extended formulation suggests a Stoner–Wohlfarth behavior may deteriorate faster than normally predicted using a fixed-length formulation, depending on the material. This behavior is due to the fact that both curling and vector length contraction (or magnetization vector shortening) is allowed, thus leading to smaller observed remanance values.

Another implication, and perhaps more surprising, concerns the dynamics of the eLLG. Relative to the LLG, a new torque term is present involving exchange, given by

$$\mathbf{T}_{\mathrm{new}} = \gamma \kappa \ell_x^2 \nabla^2 \mathbf{M} \times \left[\mathbf{H}_{\mathrm{T}} - \eta \frac{\partial \mathbf{M}}{\partial t}\right]. \tag{7}$$

This additional torque term gives rise to an effective enhancement or increase in damping, in the problem considered, and this effect is illustrated in the bottom figure showing faster switching times with increasing κ parameter value for a fixed Gilbert damping constant ($\alpha = 0.1$) and external field of 10^6 A/m ($\sim$1.25 T) to promote 180° switching.

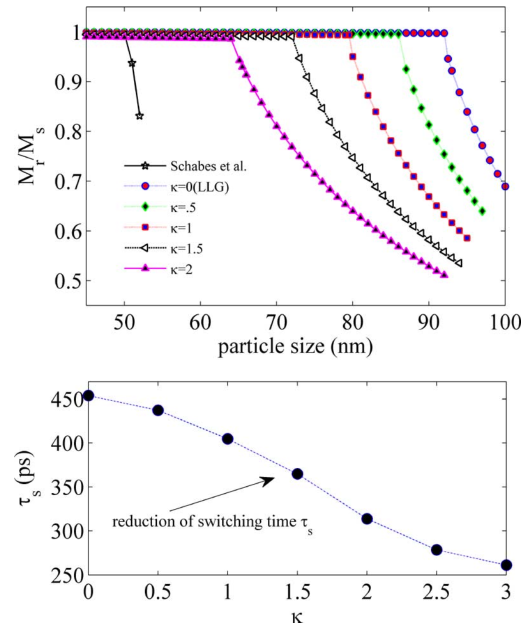

Fig. 1. *(top)* Computed remanance versus particle size using LLG and eLLG. Equilibrium states computed in zero applied field. Note: A factor of 1/2 is used here with the demagnetization field in $\mathbf{H}_{\mathrm{T}}$ in the dynamic equations. It is not used in [10], [11], etc., and if omitted, exact results from [10] are obtained ($\sim$52 nm critical particle size for LLG). *(bottom)* Switching times of 90-nm cubic particle varying κ in extended constraint.

V. Conclusion

We have discussed results from investigating an extended continuum micromagnetics formulation derived from using an extended form of the constraint on a magnetization vector. Equilibrium states were computed for the transition of cubic nanoparicles from flower to vortex states, showing effects of the additonal terms due to the extended constraint. It was shown that great nonuniformity or curling is possible in some materials at smaller particle sizes. Additionally, the damping has been shown to be enhanced giving rise to faster switching, independent of the damping parameter.

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