Generalised Form of the Magnetic Anisotropy Field in Micromagnetic and Atomistic Spin Models

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A general approach to the derivation of effective anisotropy fields for Landau-Lifshitz-Gilbert dynamics is presented. The approach is based on the gradient in spherical polar coordinates with the final results being expressed in Cartesian coordinates as usually applied in atomistic and micromagnetic model calculations. The approach is generally valid for all orders of anisotropies including higher order combinations of azimuthal and rotational anisotropies often found in functional magnetic materials especially permanent magnets. The anisotropies are represented in terms of spherical harmonics which have the important property of rational temperature scaling.

Index Terms—micromagnetics, atomistic, anisotropy, LLG, LLB

I. INTRODUCTION

CHARACTERISATION OF the temperature dependence of the anisotropy is extremely important for applications which involve elevated temperatures, such as permanent magnets in motor applications and heat assisted magnetic recording (HAMR) [1] where the recording medium is heated to beyond the Curie temperature to achieve writing. In some cases, specifically applications which require rotational anisotropies, the effective fields are not well known, thus limiting simulation techniques.

A feature of many applications is the use of magnetic materials with higher-order magnetic anisotropies due to their composite structure or the intrinsic properties of the material. The archetypal example is the alloy Nd₂Fe₁₄B which revolutionised the permanent magnet industry from the mid 1980s. Recently the drive for improved motors has led to the use of similar alloys in complex structures aimed at increasing the magnet energy product while reducing the rare-earth content.

Here we present a unified framework for the implementation of the full range of magnetic anisotropies, expressed in terms of spherical harmonics, in atomistic spin models that is self consistent and follows the analytically derived Callen-Callen scaling laws [2] for their separable components.

II. ANISOTROPY FIELDS

It has long been known that anisotropy can be described by spherical harmonics simplified under the constraints due to symmetries specific to the crystals in question. In order to obtain the field from the anisotropy energy, the gradient must be considered w.r.t. the spin vector \( \mathbf{S} = (S_x, S_y, S_z) \). Care must be taken when calculating derivatives of anisotropy energy w.r.t. the spin’s components, due to the assumption of partial differentiation that when differentiating w.r.t. \( S_x \), all other components are held constant. If \( S_y \) and \( S_z \) are constant, and \( S_x \) is varied, the condition that the spin is of constant length i.e., \( S_x^2 + S_y^2 + S_z^2 = \text{constant} \) is violated. In order to prevent this, the unit spin components used to represent terms in the anisotropy energy can be represented explicitly by direction cosines e.g., \( S_x \rightarrow S_x/\sqrt{S_x^2 + S_y^2 + S_z^2} \). It should be noted that atomistic and micromagnetic models use the Landau-Lifshitz-Gilbert (LLG) equation for simulations of spin dynamic processes. Due to numerical considerations computational models are generally formulated in terms of Cartesian rather than polar coordinates, however, deriving effective fields from a Cartesian representation, unless such care is taken, can lead to misleading results.

Here we give an alternative approach involving the use of a gradient function derived from the spherical-shell polar basis [3]. The results lead to a form which can be transformed to a Cartesian representation convenient for numerical simulations.

We start with the gradient in spherical polar coordinates w.r.t. \( \mathbf{m} \), equivalent to \( \partial/\partial \mathbf{m} \) which is given by

\[
\begin{align*}
\nabla &= \hat{x} \left( \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \\
&+ \hat{y} \left( \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \\
&+ \hat{z} \left( \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right)
\end{align*}
\]

where \( r = |\mathbf{S}| \), \( \theta \) is the angle of \( \mathbf{S} \) from \( \hat{z} \), and \( \phi \) the angle of \( \mathbf{S} \) from \( \hat{x} \) in accordance with the standard spherical polar system. This can be used to find \(-\nabla E_A (r, \theta, \phi)\) for evolution of systems with longitudinal as well as rotational degrees of freedom. However for the case of LLG dynamics where the spin has a constant magnitude i.e., \( |\mathbf{S}| = \mu \), and
for anisotropy expressions which have no dependence on \( r \), \( \nabla \) can be simplified to
\[
\nabla = \frac{1}{\mu} \left[ \hat{x} \left( \cos \phi \cos \theta \frac{\partial}{\partial \theta} - \sin \phi \frac{\partial}{\partial \phi} \right) + \hat{y} \left( \sin \phi \cos \theta \frac{\partial}{\partial \theta} + \cos \phi \frac{\partial}{\partial \phi} \right) - \hat{z} \sin \theta \frac{\partial}{\partial \theta} \right].
\]

III. Results

Among other anisotropies, we apply the technique to the fourth order rotational term given by
\[
E_{4,4} = -k_{4,4} \sin^4 \theta \cos 4\phi
\]
where \( k_{4,4} \) is a constant. Calculating \( -\nabla E_{4,4} \) yields the field
\[
B_{4,4} = -\frac{4k_{4,4}}{\mu} \left[ \left( S_x^4 + S_y^4 - 6S_x^2S_y^2 \right) \begin{bmatrix} S_x \\ S_y \\ S_z \end{bmatrix} + \begin{bmatrix} S_x \left( 3S_y^2 - S_x^2 \right) \\ S_y \left( 3S_x^2 - S_y^2 \right) \\ 0 \end{bmatrix} \right]
\]
where the term proportional to \( S \) gives no contribution to the torque \( \tau_{4,4} = S \times B_{4,4} \). Thus the effective field can be written as
\[
B_{4,4}^{\text{eff}} = \frac{4k_{4,4}}{\mu} \left[ \begin{bmatrix} S_x \left( S_x^2 - 3S_y^2 \right) \\ S_y \left( 3S_x^2 - S_y^2 \right) \\ 0 \end{bmatrix} \right].
\]

IV. Conclusion

We present a general technique which gives fields due to all orders of magnetocrystalline anisotropy. The results are applicable to both the LLG and LBB integration schemes when care is taken to ensure the effective field is properly employed. Results specifically for a fourth order rotational anisotropy are presented, with simulations demonstrating agreement with the Callen-Callen scaling law.

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