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Approximating Landau–Lifshitz–Bloch Coefficients in Micromagnetic Simulation

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Approximating Landau–Lifshitz–Bloch Coefficients in Micromagnetic Simulation

At this time, the Landau–Lifshitz–Bloch equation is the principal tool used to describe the evolution of magnetization and to account for temperature fluctuations when creating spintronics and magnetism-based microelectronics. These equation coefficients depend on average magnetization at a given point in space, and are calculated as the higher moments of a model distribution function.

For the coefficients to be computed, a transcendental equation must first be solved to determine the parameters of the distribution function. In addition, a rather crude approximation is used as a rule that does not account for the significant differences in the structure of the anisotropy field versus that of the other fields.

This paper presents an analytic approximation of the Landau–Lifshitz–Bloch coefficients assuring an accuracy up to the third significant digit and helping increase the adequacy of micromagnetic simulation and computation speed.

Keywords: Landau–Lifshitz–Bloch equation, micromagnetic simulation

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Аппроксимация коэффициентов уравнения Ландау–Лифшица–Блоха при микромагнитном моделировании

Уравнение Ландау–Лифшица–Блоха в настоящий момент является основным инструментом для описания эволюции намагниченности с учетом температурных флуктуаций при создании устройств спинтроники и магнитной микроэлектроники. Коэффициенты уравнения зависят от средней намагниченности в данной точке пространства и вычисляются как старшие моменты модельной функции распределения.

Вычисление коэффициентов требует предварительно решения трансцендентного уравнения для определения параметров функции распределения, кроме того, как правило используется достаточно грубая аппроксимация, не учитывающая существенного отличия в структуре поля анизотропии и остальных полей.

В данной работе представлена аналитическая аппроксимация коэффициентов уравнения Ландау–Лифшица–Блоха, обеспечивающая точность до третьего знака, позволяющая повысить адекватность микромагнитного моделирования и увеличить темп вычислений.

Ключевые слова: уравнение Ландау–Лифшица–Блоха, микромагнитное моделирование

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Translated by Michael Y. Tovbin

Table of Contents

1. Introduction

Creating spintronics and microelectronic devices using magnetic effects requires extensive numerical simulation [1–3]. At the same time, the best sufficiency versus computational complexity is offered by the Landau–Lifshitz–Bloch Equation [4] that describes the evolution of a continuous distribution of average magnetization in space. Initially, the coefficients of this equation are written as some higher moments of a model distribution function, and although they can be expressed in terms of analytic functions, they are too ungainly in the general case. The situation is further complicated by the fact that for these coefficients to be calculated based on an average magnetization vector, a transcendental equation must first be solved every time. Overall, the computational complexity of this approach for the purposes of numerical simulation is unacceptably high; therefore, a fairly crude analytic approximation is utilized to compute these coefficients, which has a detrimental effect on the sufficiency of the outcome.

In particular, the primary disadvantage of the conventional approximation of the Landau–Lifshitz–Bloch coefficients is the uniform treatment of the external field, the exchange field, the dipolar coupling field, and the anisotropy field [5,6]. The anisotropy field, however, unlike the other fields, is dependent on the higher moments of the model distribution function which results in totally different effective dependencies on average magnetization.

This paper builds an approximation for the Laundau–Lifshitz–Bloch coefficients in the form of analytic functions of the average magnetization component vector. The resulting approximation assures an accuracy to the third significant digit and may be used for fast micromagnetic computations for a broad spectrum of tasks [7].

2. Landau–Lifshitz–Bloch Equation

A magnetic substance is best modeled using a system of Landau–Lifshitz equations describing the evolution of N magnetic moments $\mathbf{m}_i(t)$, $|\mathbf{m}_i(t)| = 1$ located at the nodes of a crystalline lattice with coordinates $\mathbf{r}_i$:

$$\begin{aligned}
\frac{d\mathbf{m}_i}{dt} &= -\gamma\big[\mathbf{m}_i \times \mathbf{H}_i^{\text{eff}}\big] - \alpha\gamma\big[\mathbf{m}_i \times \big[\mathbf{m}_i \times \mathbf{H}_i^{\text{eff}}\big]\big] + 2\sqrt{\alpha\gamma T}\boldsymbol{\xi}(\mathbf{m}_i, t); \qquad (1)\\
\mathbf{H}_i^{\text{eff}} &= -\nabla_{\mathbf{m}_i} W = \mathbf{H}_i^{\text{exch}} + \mathbf{H}_i^{\text{anis}} + \mathbf{H}_i^{\text{dip}} + \mathbf{H}^{\text{ext}};\\
W^{\text{exch}} &= -\frac{1}{2}\sum_{i,j} J_{ij}\big(\mathbf{m}_i \cdot \mathbf{m}_j\big), \qquad \mathbf{H}_i^{\text{exch}} = \sum_j J_{ij}\mathbf{m}_j;\\
W^{\text{anis}} &= -K\sum_i \big(\mathbf{n}_K \cdot \mathbf{m}_i\big)^2, \qquad \mathbf{H}_i^{\text{anis}} = 2K\sum_i \mathbf{n}_K\big(\mathbf{n}_K \cdot \mathbf{m}_i\big);\\
\mathbf{H}_i^{\text{dip}} &= \sum_j \frac{3\big(\mathbf{m}_j \cdot \mathbf{r}_{ij}\big)\mathbf{r}_{ij} - \mathbf{m}_j r_{ij}^2}{r_{ij}^5}, \qquad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j;\\
W^{\text{ext}} &= -\sum_i \mathbf{m}_i \cdot \mathbf{H}^{\text{ext}};
\end{aligned}$$

where γ stands for the gyromagnetic ratio; α is the attenuation parameter; $\mathbf{H}^{\text{eff}}$ is the effective magnetic field; W stands for the total energy of the system; T represents the system temperature in terms of energy units; $\boldsymbol{\xi}(\mathbf{m}, t)$ represents a random source that maintains the magnitude of the magnetic moment and assures unit dispersion in all directions [8]; $\nabla_{\mathbf{m}i}$ is the ∇ operator for magnetic moment $\mathbf{m}_i$; W^{exch} and $\mathbf{H}^{\text{exch}}$ represent the exchange interaction energy and field; J_{ij} is the exchange integral (normally, non-zero only for the nearest neighbors); W^{anis} and $\mathbf{H}^{\text{anis}}$ are the anisotropy energy and field; K is the anisotropy parameter; $\mathbf{n}_K$ represents the anisotropy axis direction, $|\mathbf{n}_K| = 1$; $\mathbf{H}^{\text{dip}}$ is the dipolar coupling (magnetostatic) interaction field [9]; W^{ext} is uniform external field interaction energy. Both here and below, we will be using a dimensionless system of units.

The starting point for deriving the Landau–Lifshitz–Bloch equation is the Fokker–Planck equation [10] which describes the evolution of a distribution function $f(\mathbf{m}, \mathbf{r}, t)$ that is continuous in configuration space $\mathbf{r}$ and describes the distribution of magnetic moments $\mathbf{m}$, $|\mathbf{m}| = 1$ by direction which can be obtained using the Bogolyubov hierarchy in a mean-field approximation [8, 11]:

$$\begin{aligned}
\frac{\partial f(\mathbf{m}, \mathbf{r}, t)}{\partial t} - \gamma\nabla_\circ\big[\mathbf{m} \times \mathbf{H}^{\text{eff}}\big] f &= \gamma\alpha\nabla_\circ\Big[\mathbf{m} \times \big[\mathbf{m} \times \big(\mathbf{H}^{\text{eff}} - T\nabla_\circ\big) f\big]\Big], \qquad (2)\\
\mathbf{H}^{\text{eff}} &= \mathbf{H}^{\text{exch}} + \mathbf{H}^{\text{dip}} + 2K\mathbf{n}_K\big(\mathbf{n}_K \cdot \mathbf{m}\big) + \mathbf{H}^{\text{ext}},\\
\mathbf{H}^{\text{exch}} &= J\Big[a^2\Delta_{\mathbf{r}}\langle\mathbf{m}\rangle + \varepsilon_G n_b\langle\mathbf{m}\rangle\Big],
\end{aligned}$$

where a represents the distance between atoms in a crystalline lattice; $\Delta_{\mathbf{r}}\langle\mathbf{m}\rangle$ is the

Laplace operator for space with respect to average magnetization $\langle \mathbf{m} \rangle$ (by components of $\langle \mathbf{m} \rangle$); ε_G is the Garanin factor to account for mean-field fluctuations [12] (for a body-centered crystalline lattice $\varepsilon_G \approx 0.795$); n_b is the number of an atom's nearest neighbors; $\nabla_\circ$ is the spherical magnetization gradient:

$$\nabla_\circ = \nabla_{\mathbf{m}} - \frac{\mathbf{m}\left(\mathbf{m} \cdot \nabla_{\mathbf{m}}\right)}{\mathbf{m}^2}.$$

Taking advantage of Gauss' Law, multiplying both sides of (2) by $\mathbf{m}$ and integrating over a sphere, we obtain

$$\begin{aligned} -\frac{1}{\gamma}\frac{\partial \langle \mathbf{m} \rangle}{\partial t} = \langle \mathbf{m} \rangle \times \left(\mathbf{H}^{\text{ext}} + \mathbf{H}^{\text{exch}} + \mathbf{H}^{\text{dip}}\right) + 2K \left\langle \mathbf{m} \times \mathbf{n}_K \left(\mathbf{m} \cdot \mathbf{n}_K\right) \right\rangle + \\ + \alpha \left\langle \mathbf{m} \otimes \mathbf{m} - \widehat{I} \right\rangle \left(\mathbf{H}^{\text{ext}} + \mathbf{H}^{\text{exch}} + \mathbf{H}^{\text{dip}}\right) + \\ + 2\alpha K \left\langle \mathbf{m} \times \left[\mathbf{m} \times \mathbf{n}_K\right] \left(\mathbf{m} \cdot \mathbf{n}_K\right) \right\rangle + 2\alpha T \langle \mathbf{m} \rangle , \end{aligned} \quad (3)$$

where $\widehat{I}$ is the unit matrix (angle brackets represent averaging)

$$\langle A \rangle \equiv \int\limits_{\text{sph}} A f(\mathbf{m}, \mathbf{r}, t)\, d\mathbf{m},$$

$\int_{\text{sph}} \ldots d\mathbf{m}$ represents integration over a unit sphere.

To obtain the closed form of the resulting equation (compute the relationship between the higher moments of the distribution function based on $\langle \mathbf{m} \rangle$), the form of the distribution function must be specified which is analogous to introducing an equation of state when deriving fluid dynamics equations from the Bolzmann equation. The following is a good approximation

$$f(\mathbf{m}, \mathbf{r}, t) = \frac{e^{\mathbf{p}(\mathbf{r},t)\cdot\mathbf{m}}}{Z}, \quad Z = \int\limits_{\text{sph}} e^{\mathbf{p}\cdot\mathbf{m}}\, d\mathbf{m} = 2\pi \int\limits_0^\pi e^{p\cos\theta}\, \sin\theta\, d\theta = \frac{4\pi}{p}\,\text{sh}\, p, \quad (4)$$

$$\langle \mathbf{m} \rangle = \frac{1}{Z}\int\limits_{\text{sph}} \mathbf{m}\, e^{\mathbf{p}\cdot\mathbf{m}}\, d\mathbf{m} = \mathbf{n}_p L(p), \qquad L(p) = \text{cth}\, p - \frac{1}{p}, \qquad \mathbf{n}_p = \frac{\mathbf{p}}{p},$$

where $\mathbf{p}$ is a vector that serves as a parameter in model distribution function $\mathbf{p} \parallel \langle \mathbf{m} \rangle$, L is the Langevin function. Multiple comparisons against the results of ''atom–to–atom'' direct numerical simulations [13, 14] demonstrate that the error of this approximation of a one-particle distribution function at the current parameter values is on the order of the second significant digit, which is a fairly satisfactory result.

Customarily, following a number of manipulations and additional assumptions, the Landau–Lifshitz–Bloch equation is written as follows [4, 5]:

$$\begin{aligned}
\frac{1}{\gamma}\frac{\partial \langle \mathbf{m} \rangle}{\partial t} =& - \left[\langle \mathbf{m} \rangle \times \mathbf{H}^{\text{LLB}} \right] + \alpha_{\parallel} \left(\langle \mathbf{m} \rangle \cdot \mathbf{H}^{\text{LLB}} \right) \cdot \langle \mathbf{m} \rangle - \\
& - \alpha_{\perp} \left[\langle \mathbf{m} \rangle \times \left[\langle \mathbf{m} \rangle \times \mathbf{H}^{\text{LLB}} \right] \right], \qquad (5) \\
\alpha_{\parallel} = \frac{2\alpha T}{3T_c}, \qquad & \alpha_{\perp} = \begin{cases} \alpha \left[1 - T/3T_c \right], & \text{при} \quad T \le T_c, \\ \alpha_{\parallel}, & \text{при} \quad T > T_c, \end{cases} \\
\mathbf{H}^{\text{LLB}} =& \mathbf{H}^{\text{dip}} + 2K\mathbf{n}_K \left(\mathbf{n}_K \cdot \langle \mathbf{m} \rangle \right) + \mathbf{H}^{\text{ext}} + Ja^2 \Delta_{\mathbf{r}} \langle \mathbf{m} \rangle + \\
& + \begin{cases} \dfrac{1}{2\chi} \left(1 - \dfrac{\langle m \rangle^2}{\langle m \rangle_{\text{eq}}^2} \right) \langle \mathbf{m} \rangle, & \text{при} \quad T \le T_c, \\ -\dfrac{1}{\chi} \left(1 + \dfrac{3}{5} \dfrac{T_c \langle m \rangle^2}{T - T_c} \right) \langle \mathbf{m} \rangle, & \text{при} \quad T > T_c, \end{cases}
\end{aligned}$$

where T_c is the Curie temperature; $\langle m \rangle_{\text{eq}} = \langle m \rangle_{\text{eq}}(T)$ is the equilibrium magnetization; $\chi = \chi(T)$ stands for longitudinal susceptibility

$$\chi = \frac{L'}{T - \varepsilon_G n_b J L'}, \qquad L' = \frac{dL}{dp}\left(\frac{\varepsilon_G n_b J \langle m \rangle_{\text{eq}}}{T} \right), \qquad \langle m \rangle_{\text{eq}} = L\left(\frac{\varepsilon_G n_b J \langle m \rangle_{\text{eq}}}{T} \right).$$

Here and elsewhere below, we use the notation

$$\langle m \rangle \equiv |\langle \mathbf{m} \rangle|.$$

The Landau–Lifshitz–Bloch equation as shown in (5) does not have serious computational advantages with respect to the original form (3), because it requires that the vector $\mathbf{p}(\langle \mathbf{m} \rangle) = L^{-1}(|\langle \mathbf{m} \rangle|) \langle \mathbf{m} \rangle / |\langle \mathbf{m} \rangle|$ be computed at every point based on a solution of a transcendental equation. At the same time, (5) makes the transition as follows

$$\begin{aligned}
\left\langle \mathbf{m} \times \mathbf{n}_K (\mathbf{m} \cdot \mathbf{n}_K) \right\rangle &\sim \left[\langle \mathbf{m} \rangle \times \mathbf{n}_K \right] \left(\langle \mathbf{m} \rangle \cdot \mathbf{n}_K \right), \\
\left\langle \mathbf{m} \times \left[\mathbf{m} \times \mathbf{n}_K \right] (\mathbf{m} \cdot \mathbf{n}_K) \right\rangle &\sim \left[\langle \mathbf{m} \rangle \times \left[\langle \mathbf{m} \rangle \times \mathbf{n}_K \right] \right] \left(\langle \mathbf{m} \rangle \cdot \mathbf{n}_K \right),
\end{aligned}$$

which might result in an incorrect relationship between the anisotropy field and the other fields and impact the sufficiency of the numerical simulation results.

Tensor $\left\langle \mathbf{m} \otimes \mathbf{m} - \widehat{I} \right\rangle$ included in (3) depends only on average magnetization $\langle \mathbf{m} \rangle$ whereas higher moments $\left\langle \mathbf{m} \times \mathbf{n}_K (\mathbf{m} \cdot \mathbf{n}_K) \right\rangle$ and $\left\langle \mathbf{m} \times \left[\mathbf{m} \times \mathbf{n}_K \right] (\mathbf{m} \cdot \mathbf{n}_K) \right\rangle$ depend on the average magnitude of magnetization $\langle m \rangle$ and the relative orientation of magnetization and anisotropy axis direction $\mathbf{n}_K$. Thus, computations require that

an analytic approximation of these quantities be constructed based on $\langle \mathbf{m} \rangle$ with the accuracy of the approximation possibly being limited because a random source in a special form is added to the Landau–Lifshitz–Bloch equation to account for temperature fluctuations.

It should be noted that the original Fokker–Planck equation (2) obtained through a mean-field approximation has a marked disadvantage: the mean-field approximation cannot easily be applied to ferromagnets because it does not account for correlations between the nearest neighbors. At the same time, strong exchange interactions in magnets are of a local nature and result in there being strong correlations between the nearest neighbors even in the paramagnetic phase [11, 15]. Therefore, the mean-field approximation produces an incorrect critical temperature T_c (which can be compensated for by factor ε_G [12]), exchange energy, and relaxation times with the difference in the relaxation times for some conditions possibly as much as an order of magnitude. Discussing and accounting for these effects is outside the scope of this paper, in which we will focus on constructing an approximation for the coefficients of the original Landau–Lifshitz–Bloch equation in (3).

3. Coefficients Associated with External and Linear Fields

For the purposes of this paper, linear fields will be defined as $\mathbf{H}^{\text{exch}}$ and $\mathbf{H}^{\text{dip}}$ and will be linearly dependent on average magnetization. $\langle \mathbf{m} \rangle$.

As a starting point, let us consider the higher moments of function $f(\langle \mathbf{m} \rangle)$. These can be obtained by computing the relevant integrals in spherical coordinates

$$\left\langle m_{\parallel p}^2 \right\rangle = 1 - \frac{2\langle m \rangle}{p}, \qquad \lim_{\langle m \rangle \to 0} \left\langle m_{\parallel p}^2 \right\rangle = \frac{1}{3}, \qquad \langle m_{\perp p}^2 \rangle = \frac{1 - \left\langle m_{\parallel p}^2 \right\rangle}{2},$$

$$\left\langle m_{\parallel p}^3 \right\rangle = \left[1 + \frac{6}{p^2}\right] \langle m \rangle - \frac{2}{p}, \quad \left\langle m_{\parallel p}^3 \right\rangle \approx \frac{3}{5} \langle m \rangle \text{ при } \langle m \rangle \ll 1, \quad \langle m_{\perp p}^3 \rangle = 0,$$

with $\left\langle m_{\parallel p}^{2,3} \right\rangle$ representing the components of the higher moments parallel to vector $\mathbf{p}$, and $\left\langle m_{\perp p}^{2,3} \right\rangle$ components normal to vector $\mathbf{p}$.

Given that $\mathbf{n}_p$ is the principal axis of symmetric tensor $\langle \mathbf{m} \otimes \mathbf{m} \rangle$, the components of tensor $\left\langle \mathbf{m} \otimes \mathbf{m} - \widehat{I} \right\rangle$ can be expressed as

$$\langle m_i m_j \rangle - \delta_{ij} = \left\langle m_{\parallel p}^2 \right\rangle \frac{3 n_{pi} n_{pj} - \delta_{ij}}{2} - \frac{\delta_{ij} + n_{pi} n_{pj}}{2}, \qquad \lim_{\langle m \rangle \to 0} \langle m_i m_j \rangle - \delta_{ij} = -\frac{2}{3} \delta_{ij},$$

where δ_{ij} is the Kronecker delta.

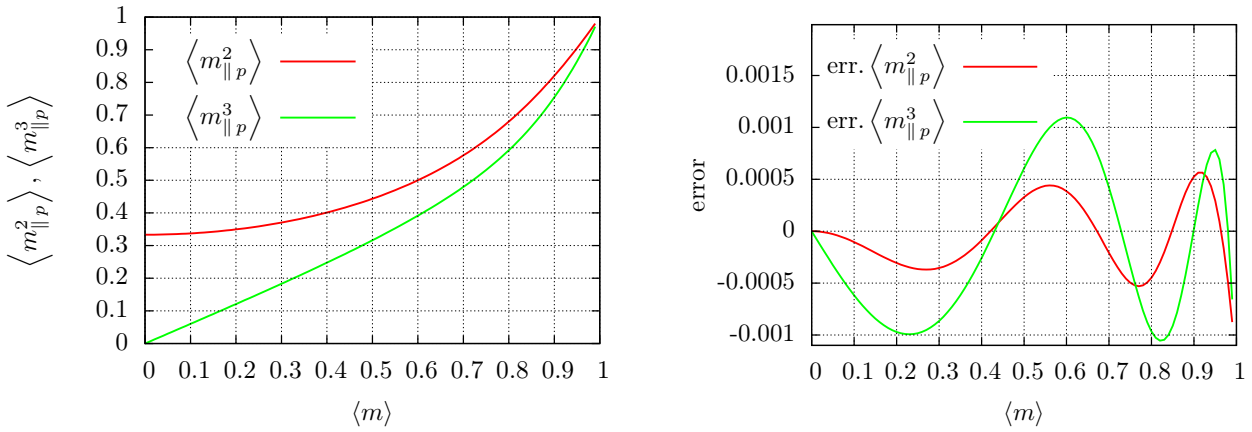


Fig. 1. Form of functions $\left\langle m^{2,3}_{\|p}\right\rangle$ ($\langle m\rangle$) and their approximation errors

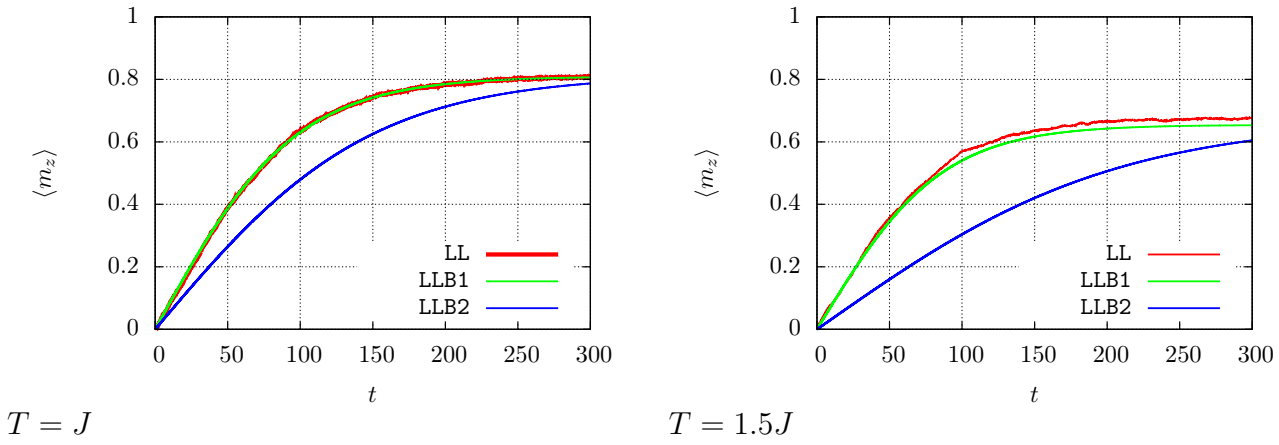
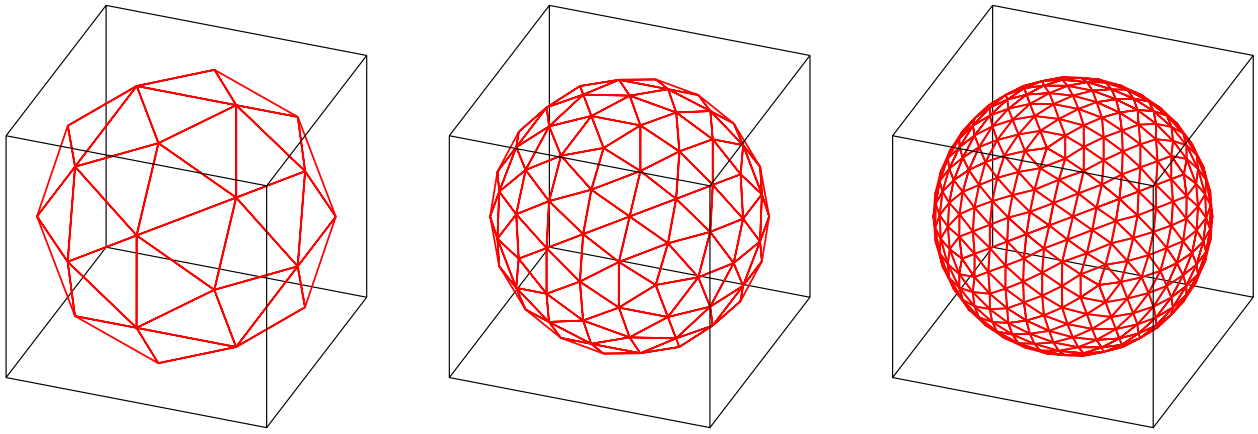


Fig. 2. Evolution of component $\langle m_z\rangle$ for original ‘‘atom-to-atom’’ simulation (LL) of Landau–Lifshitz–Bloch equation with constructed approximation of tensor $\left\langle \mathbf{m}\otimes\mathbf{m}-\widehat{I}\right\rangle$ (LLB1) and conventional approximation (LLB2)

The relations $\left\langle m^{2,3}_{\|p}\right\rangle$ ($\langle m\rangle$) can be approximated on the interval $\langle m\rangle \in [0, 0.98]$ with an absolute error not exceeding 10^{-3} (Fig. 1) as

$$\left\langle m^2_{\|p}\right\rangle \approx \frac{1}{3} + 0.4115\cdot\langle m\rangle^2 + 0.0303\cdot\langle m\rangle^4 + 0.3523\cdot\langle m\rangle^6 - 0.1261\cdot\langle m\rangle^8,$$
$$\left\langle m^3_{\|p}\right\rangle \approx 0.6026\cdot\langle m\rangle\left[1 + 0.00669\cdot \mathrm{ch}\left(5.288\,\langle m\rangle\right)\right].$$

The constructed approximation of tensor $\left\langle \mathbf{m}\otimes\mathbf{m}-\widehat{I}\right\rangle$ turns out to be much more compact than the conventional one in (5) and fully matches the original equation in (3). Let us compare the results obtained through the constructed approximation with those of the conventional approximation as well as those of the ‘‘atom-to-atom’’ direct simulation of a magnet with a body-centered crystalline lattice given an initial magnetization $\langle\mathbf{m}\rangle_0 = (\langle m\rangle_{\text{eq}},0,0)$, an external field $\mathbf{H}^{\text{ext}} = (0,0,0.1)$



a *b* *c*

Fig. 3. Spherical grid constructed by recursively dividing a pentakis dodecahedron: no division (*a*), single division (*b*), double division (*c*)

for temperatures $T = J$ и $T = 1.5J$. If exchange integral $J = 1$, then Curie temperature $T_c = 2.12J$, the dipolar coupling and anisotropy are null, and we will assume magnetization spatial distribution to be uniform. Figure 2 shows that for these conditions, the constructed approximation of tensor $\left\langle \mathbf{m} \otimes \mathbf{m} - \widehat{I} \right\rangle$ turns out to be much closer to the original ‘‘atom-to-atom’’ simulation than the conventional approximation.]

4. Coefficients Associated with Anisotropy

When computing the anisotropy term, the integration over a sphere was performed using a grid constructed by recursively dividing a pentakis dodecahedron (Fig. 3) and implemented with the `aiwlib` [16] library. Unlike conventional spherical coordinates, this grid is isotropic, made up of almost regular spherical triangles, and instead of having two strong singularities at the poles, it has twelve weak singularities corresponding to the centers of the faces of the original pentakis dodecahedron. In addition, at a specified resolution (cell size), this grid required half (and when using a dual hexagonal grid, a quarter of) the nodes of a conventional uniform spherical coordinate grid.

Let us introduce parameter $\beta = \mathbf{n}_p \cdot \mathbf{n}_K = \langle \mathbf{m} \rangle \cdot \mathbf{n}_K / \langle m \rangle$. For reasons of symmetry, it follows that

$$\left\langle \mathbf{m} \times \mathbf{n}_K \big(\mathbf{m} \cdot \mathbf{n}_K \big) \right\rangle \parallel \big[\langle \mathbf{m} \rangle \times \mathbf{n}_K \big] \quad \rightarrow \quad \left\langle \mathbf{m} \times \mathbf{n}_K \big(\mathbf{m} \cdot \mathbf{n}_K \big) \right\rangle = \big[\langle \mathbf{m} \rangle \times \mathbf{n}_K \big] \Phi(p, \beta),$$

and based on a review of the results of numerical integration for different $\langle m \rangle$, β,

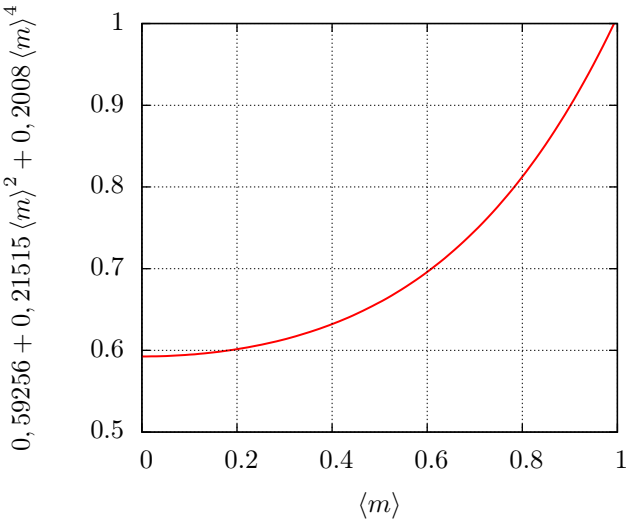


Fig. 4. Coefficient for term $\Big[\,\langle\mathbf{m}\rangle \times \mathbf{n}_K\big(\,\langle\mathbf{m}\rangle \cdot \mathbf{n}_K\big)\Big]$

an approximation can be constructed with an absolute error smaller than $2 \cdot 10^{-3}$ (Fig. 4, 5):

$$\big\langle \mathbf{m} \times \mathbf{n}_K\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big\rangle \approx \Big(0.59256{+}0.21515{\cdot}\langle m\rangle^2{+}0.2008{\cdot}\langle m\rangle^4\Big)\big(\,\langle\mathbf{m}\rangle{\cdot}\mathbf{n}_K\big)\big[\,\langle\mathbf{m}\rangle{\times}\mathbf{n}_K\big].$$

It is easy to see that conventional approximation

$$\big\langle \mathbf{m} \times \mathbf{n}_K\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big\rangle \approx \Big[\,\langle\mathbf{m}\rangle \times \mathbf{n}_K\big(\,\langle\mathbf{m}\rangle \cdot \mathbf{n}_K\big)\Big]$$

differs in coefficient $\Big(0.59256 + 0.21515 \cdot \langle m\rangle^2 + 0.2008 \cdot \langle m\rangle^4\Big)$, which could result in an error of up to 40% at small $\langle m\rangle$.

From the approximation standpoint, the term $\big\langle \mathbf{m} \times \big[\mathbf{m} \times \mathbf{n}_K\big]\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big\rangle$ is the most troublesome. For symmetry considerations

$$\big\langle \mathbf{m} \times \big[\mathbf{m} \times \mathbf{n}_K\big]\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big\rangle = \langle\mathbf{m}\rangle\,\Psi_{\parallel}(\langle\mathbf{m}\rangle) + \Big[\,\langle\mathbf{m}\rangle \times \big[\,\langle\mathbf{m}\rangle \times \mathbf{n}_K\big]\Big]\Psi_{\perp}(\langle\mathbf{m}\rangle),$$

and based on a review of the results of numerical integration for different $\langle\mathbf{m}\rangle$, $\mathbf{n}_K$ (Fig. 6, 7), an approximation can be constructed with an absolute error that is $2 \cdot 10^{-3}$:

$$\big\langle \mathbf{m} \times \big[\mathbf{m} \times \mathbf{n}_K\big]\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big\rangle \approx \langle\mathbf{m}\rangle \left[\frac{\big\langle m_{\parallel p}^3\big\rangle}{\langle m\rangle} - 1\right]\frac{3\beta^2 - 1}{2} + \\ + \Big[\,\langle\mathbf{m}\rangle \times \big[\,\langle\mathbf{m}\rangle \times \mathbf{n}_K\big]\Big]\frac{\big\langle m_{\parallel p}^3\big\rangle}{\langle m\rangle^2}\beta.$$

It is obvious from Figure 8 that the difference between the conventional approximation and the one constructed in this paper could be as high as 50%.

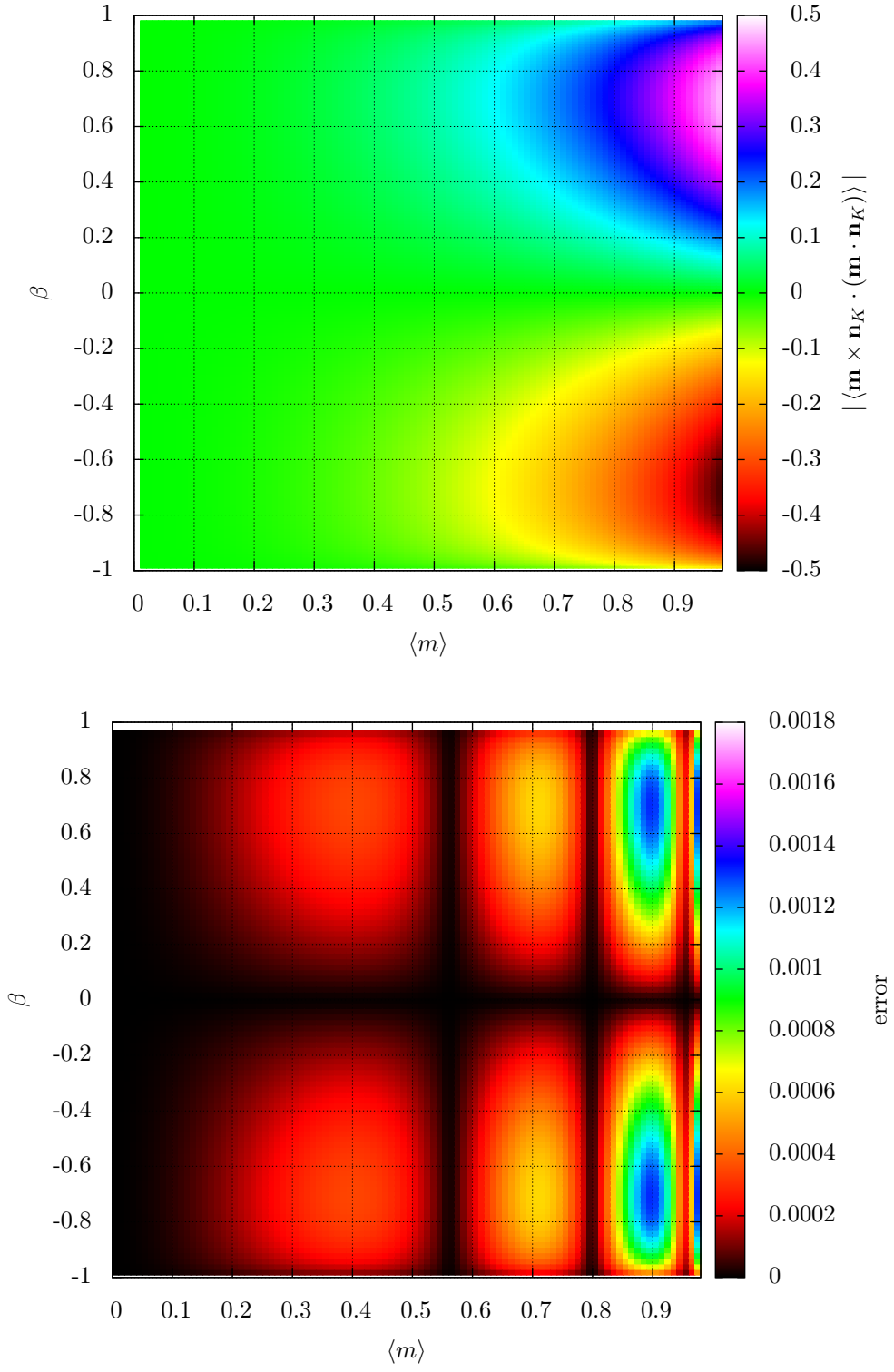


Fig. 5. Magnitude of vector $\langle \mathbf{m} \times \mathbf{n}_K(\mathbf{m} \cdot \mathbf{n}_K) \rangle$ as a function of parameters $\langle m \rangle$, β, and its approximation error

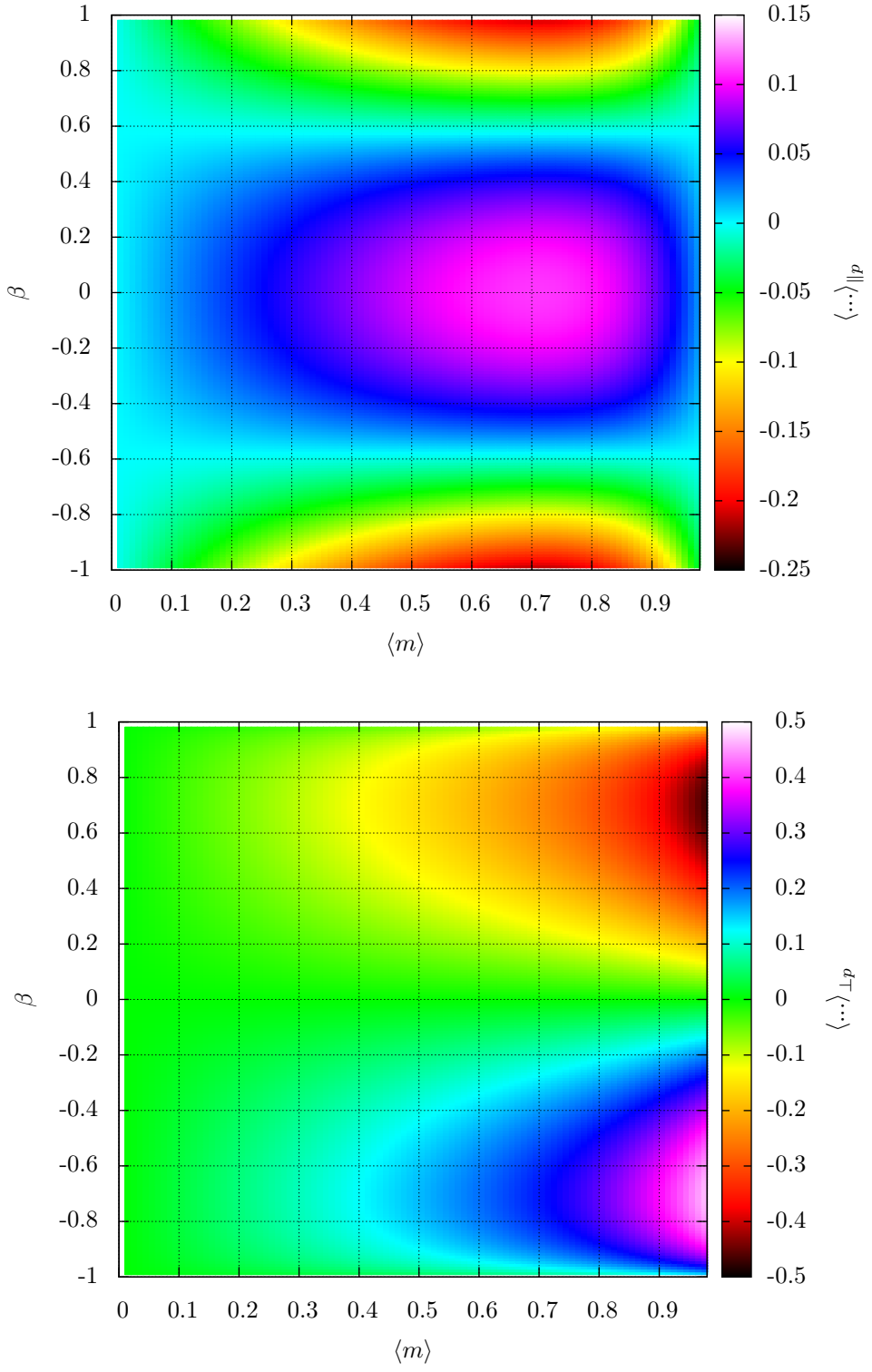


Fig. 6. Components of vector $\left\langle \mathbf{m} \times \left[\mathbf{m} \times \mathbf{n}_K \right] \left(\mathbf{m} \cdot \mathbf{n}_K \right) \right\rangle$ as a function of parameters $\langle m \rangle$, β

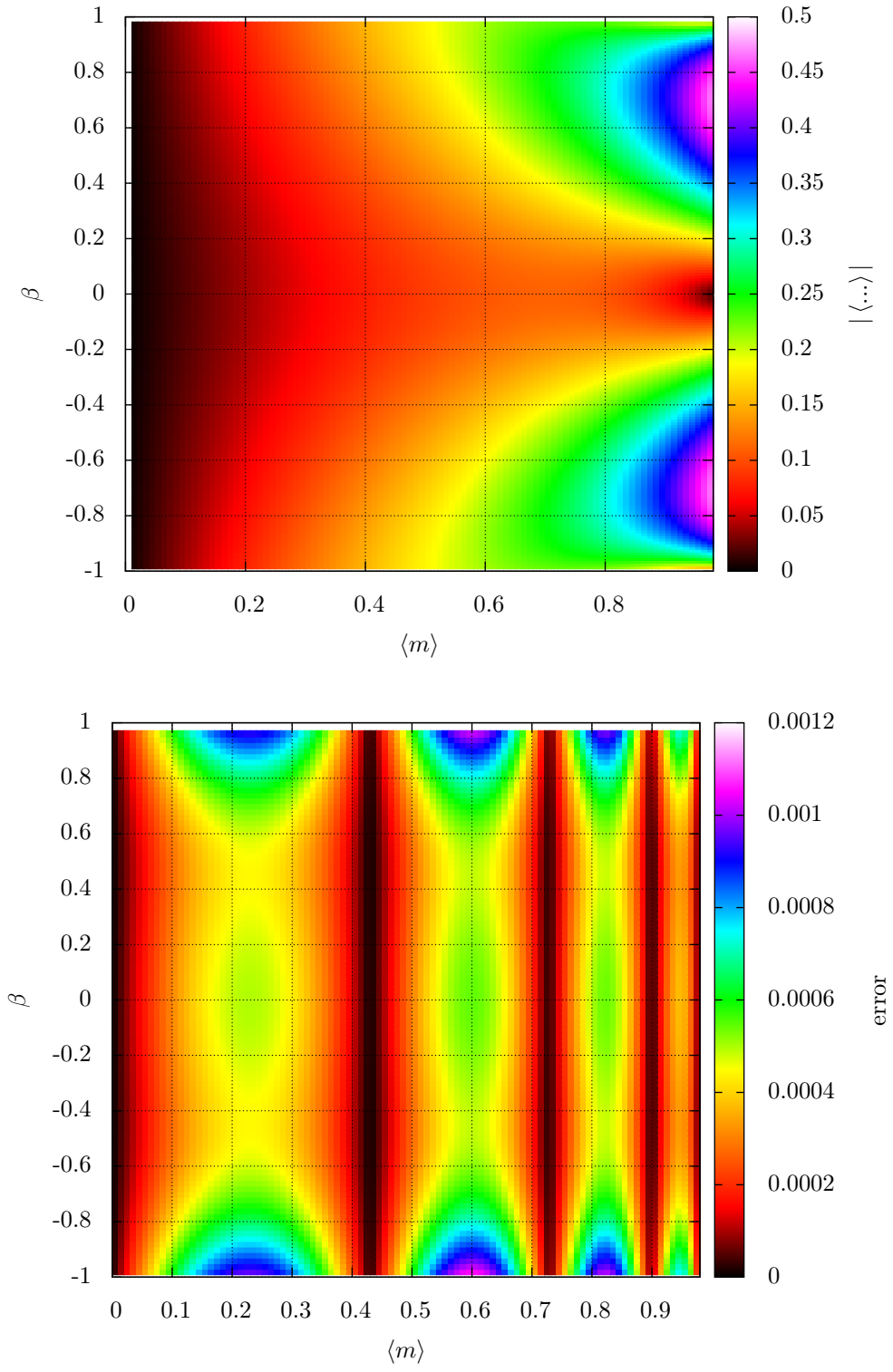


Fig. 7. Magnitude of vector $\left\langle \mathbf{m} \times \left[\mathbf{m} \times \mathbf{n}_K \right] \left(\mathbf{m} \cdot \mathbf{n}_K \right) \right\rangle$ as a function of parameters $\langle m \rangle$, β and its approximation error

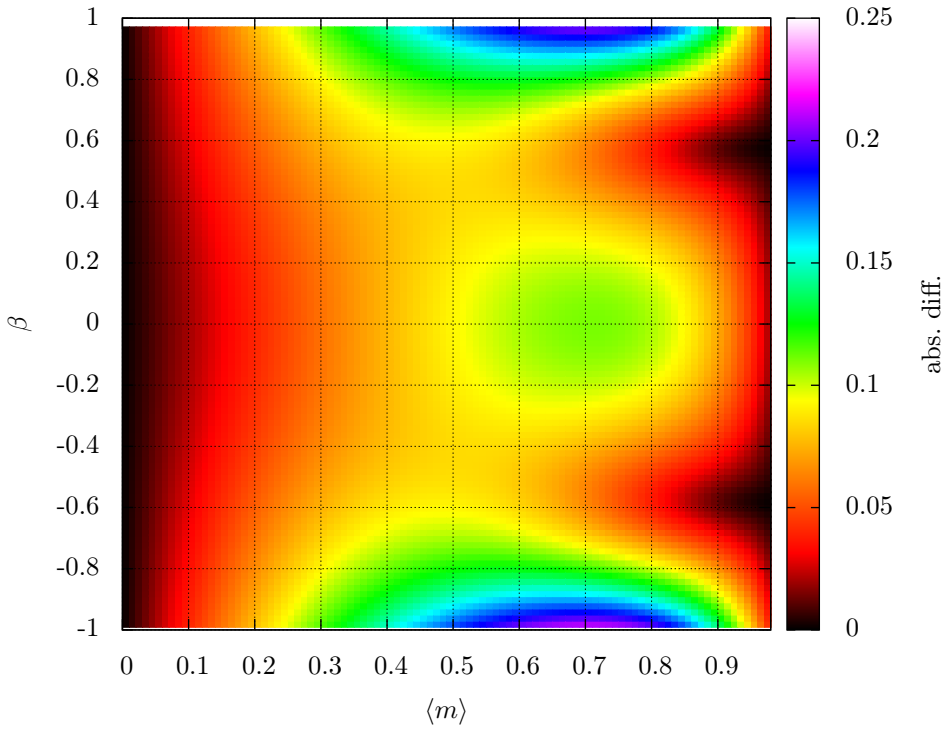


Fig. 8. Magnitude of difference between $\Big[\langle\mathbf{m}\rangle \times \big[\langle\mathbf{m}\rangle \times \mathbf{n}_K\big(\langle\mathbf{m}\rangle \cdot \mathbf{n}_K\big)\big]\Big]$ and $\big\langle\mathbf{m} \times \big[\mathbf{m} \times \mathbf{n}_K\big(\mathbf{m} \cdot \mathbf{n}_K\big)\big]\big\rangle$ as a function of parameters $\langle m\rangle$ and β

5. Conclusion

The approximations constructed for the Landau–Lifshitz–Bloch coefficients are implemented in the `llbe` C++ header file and the `aiwlib` [16] library containing functions to compute coefficients using single-precision floating-point arithmetic. This turns out to be sufficient given the temperature fluctuations and the limited precision of the constructed approximation to the third significant digit.

As compared to the conventional solution, the constructed approximations account for the structural differences between the external and the linear fields and the anisotropy field, which could be especially important when simulating the switching of magnetoresistive memory cells.

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