Full Micromagnetic Numerical Simulations of Thermal Fluctuations

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Thermal fluctuations for fine ferromagnetic particles are studied with the full micromagnetic analysis based on numerical integration of the spatially discretized Langevin-Landau-Lifshitz equation. These results can be used as a basis for the formulation of a standard problem to test the implementation of thermal fluctuations in numerical micromagnetic codes. To this end an example of micromagnetic analysis of thermal fluctuations in an ellipsoidal magnetic nanoparticle is presented.

Index Terms—**Micromagnetics, thermal fluctuations.**

I. Introduction

THE STUDY OF thermal fluctuations in the dynamics of nanomagnetic systems is a fundamental issue for its applications in spintronics and design of modern magnetic recording devices. In these devices, the bit-coded information is stored on a continuous magnetic thin-film medium by setting the magnetization orientation 'up' or 'down' with respect to a given direction (typically perpendicular to the plane of the medium in hard disk devices). On one hand, in order to increase the storage density, one possibility is to reduce the size of the recorded bit. On the other hand, the main problem related to the increase in the areal density is the thermal stability of the recorded bit. In fact, as the magnetic medium volume associated with the recorded bit becomes smaller and smaller, the more important the thermal agitation becomes which tends to destabilize the magnetization configuration. Of course, this process, referred to as superparamagnetic effect [1], affects the long-term stability of the information and, therefore, the reliability of magnetic recording devices [2], [3].

In order to study the influence of thermal fluctuations in magnetization dynamics, theoretical models based on micromagnetic theory have been proposed. Magnetization dynamics is described by the Landau-Lifshitz-Gilbert (LLG) equation which rules the gyromagnetic precession of magnetization vector field around the so-called micromagnetic effective field [4]. The effective field takes phenomenologically into account the interactions occurring in magnetic materials such as short-range (exchange, anisotropy) and long-range interactions (magnetostatics, Zeeman).

The most used approach, which was presented by Brown in the sixties, consists in the augmentation of the effective field by an isotropic, spatially and temporally uncorrelated Gaussian white noise random field [5]. In this context, the LLG equation becomes a stochastic differential equation (SDE) that can be studied by using two approaches: the Fokker-Planck equation and the Langevin Dynamics. The former approach gives the transient evolution of the probability density function of magnetization, whereas the latter consists in the direct numerical integration of the stochastic LLG equation in order to find the realizations of the magnetization stochastic process.

The analysis based on the Fokker-Planck equation gives synthetic and insightful information on stochastic magnetization dynamics [5], [6], but is practically limited to the case of single-domain particles since, when spatial uniformity cannot be assumed a-priori, the probability density function must be defined on a space with a very high dimensionality. For this reason, in this situation, the Langevin Dynamics approach is usually adopted [7]–[9].

In this paper, a numerical scheme for the integration of stochastic LLG equation for non uniformly magnetized bodies is presented. In addition, micromagnetic analysis of thermal fluctuations in small magnetic nanoparticles are presented and compared with the analytical results obtained by the Fokker-Planck equation approach for single-domain particles. The relevance of these results to the formulation of a meaningful standard problem to test micromagnetic numerical codes is then discussed.

II. Problem Formulation

Magnetization dynamics in a ferromagnetic body is described by the following stochastic, Langevin-type, Landau-Lifshitz-Gilbert (LLG) equation:

$$\frac{\partial \mathbf{m}}{\partial t} = -\mathbf{m} \times \left(\mathbf{h}_{\text{eff}}[\mathbf{m}] - \alpha \frac{\partial \mathbf{m}}{\partial t} \right) - \nu \mathbf{m} \times \mathbf{h}_T(t, \mathbf{r}) \quad (1)$$

where $\mathbf{m} = \mathbf{m}(\mathbf{r}, t)$ is the magnetization vector field normalized to the saturation magnetization M_{s}, time is measured in unit of $(\gamma M_{\text{s}})^{-1}$ (γ is the absolute value of the gyromagnetic ratio), α is the dimensionless damping parameter, $\mathbf{h}_T(\mathbf{r}, t)$ is the random field that describes thermal agitation, ν is a constant controlling the amplitude fluctuations, $\mathbf{h}_{\text{eff}}[\mathbf{m}(\mathbf{r}, t)]$ is the effective field operator which can be obtained by the variational derivative of the free energy functional [4]

$$\mathbf{h}_{\text{eff}}[\mathbf{m}] = -\frac{\delta g_L[\mathbf{m}]}{\delta \mathbf{m}} \quad (2)$$

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where

$$g_L[\mathbf{m}] = \frac{1}{\mathrm{V}_\Omega}\int_\Omega \left[\frac{l_{\mathrm{ex}}^2}{2}|\nabla \mathbf{m}|^2 - \frac{1}{2}\mathbf{h}_{\mathrm{m}}\cdot\mathbf{m} + \varphi(\mathbf{m}) - \mathbf{h}_{\mathrm{a}}\cdot\mathbf{m}\right]\mathrm{d}V \quad (3)$$

$\varphi(\mathbf{m})$ is the anisotropy energy density and $l_{\mathrm{ex}} = \sqrt{(2A)/\mu_0 M_{\mathrm{s}}^2}$ is the exchange length (A is the exchange constant and μ_0 the vacuum permeability), $\mathbf{h}_{\mathrm{m}}$ and $\mathbf{h}_{\mathrm{a}}$ are the demagnetizing and applied fields, respectively, and V_Ω is the body volume. In addition, the homogeneous Neumann boundary condition $\partial\mathbf{m}/\partial\mathbf{n} = 0$ is imposed at the body surface. The normalized random field $\mathbf{h}_T(\mathbf{r},t)$, introduced to describe the effects of thermal fluctuations, is assumed to be an isotropic, spatially and temporally uncorrelated, Gaussian white noise random field

$$\langle h_{Ti}(\mathbf{r},t)h_{Tj}(\mathbf{r}',t')\rangle = \delta_{ij}\delta(t-t')\delta(\mathbf{r}-\mathbf{r}') \quad (4)$$

where $\langle\cdot\rangle$ denotes ensemble average, i,j are indices labeling cartesian components.

In order to obtain a spatially discretized version of (1) we consider a partition of the region Ω in N cells Ω_k, with volume V_k and assume that the cells are small enough that the vector fields $\mathbf{m}(\mathbf{r},t)$ and $\mathbf{h}_{\mathrm{eff}}[\mathbf{m}(\mathbf{r},t)]$ can be considered spatially uniform within each cell. We denote with $\mathbf{m}_k(t)$ and $\mathbf{h}_{\mathrm{eff}\,k}$ the vectors associated with the generic k-th cell. Beside the cell vectors, we will consider also the mesh vectors $\underline{\boldsymbol{m}} = (\mathbf{m}_1,\ldots,\mathbf{m}_N)^T \in \mathbb{R}^{3N}$ containing the whole collection of cell vectors.

According to the discretization procedure outlined above, the discretized random field is the spatial average of the continuous random field over each cell

$$\nu_k h_{T,k,i}(t) = \frac{1}{V_k}\int_{\Omega_k}\nu h_{T,i}(\mathbf{r},t)\mathrm{d}V \quad (5)$$

being $h_{T,k,i}(t)$ the i-th component of a normalized white random field satisfing the condition

$$\langle h_{T,k,i}(t)h_{T,h,j}(t')\rangle = \delta_{kh}\delta_{ij}\delta(t-t'). \quad (6)$$

In order to determine ν_k, let us take into account the following identity:

$$\left\langle \int_{\Omega_k} h_{T,i}(\mathbf{r},t)\mathrm{d}V \int_{\Omega_h} h_{T,j}(\mathbf{r}',t')\mathrm{d}V' \right\rangle = V_k\delta_{kh}\delta_{ij}\delta(t-t'). \quad (7)$$

By comparing the latter equation with (5) and (6), one easily obtains that

$$\nu_k^2 = \frac{\nu^2}{V_k^2}V_k \Longrightarrow \nu_k = \frac{\nu}{\sqrt{V_k}}. \quad (8)$$

The value of the constant ν in thermodynamic equilibrium, independently from the adopted spatial discretization scheme, can be derived from the fluctuation-dissipation theorem [5], [10]

$$\nu^2 = \frac{2\alpha k_{\mathrm{B}}T}{\mu_0 M_{\mathrm{s}}^2} \Rightarrow \nu_k = \sqrt{\frac{2\alpha k_{\mathrm{B}}T}{\mu_0 M_{\mathrm{s}}^2 V_k}} \quad (9)$$

where k_{B} is the Boltzmann constant, T is the temperature, and V_k is the volume of the k-th mesh element. We now assume the following approximations:

$$\frac{1}{\mathrm{V}_k}\int_{\Omega_k}\mathbf{m}\times\mathbf{h}_{\mathrm{eff}}[\mathbf{m}]\mathrm{d}V \approx \mathbf{m}_k\times\mathbf{h}_{\mathrm{eff}_k}[\underline{\boldsymbol{m}}] \quad (10)$$

$$\frac{1}{\mathrm{V}_k}\int_{\Omega_k}\mathbf{m}\times\frac{\partial\mathbf{m}}{\partial t}\mathrm{d}V \approx \mathbf{m}_k\times\frac{d\mathbf{m}_k}{dt} \quad (11)$$

$$\frac{1}{\mathrm{V}_k}\int_{\Omega_k}\mathbf{m}\times\mathbf{h}_T(\mathbf{r},t)\mathrm{d}V \approx \frac{\nu}{\sqrt{V_k}}\mathbf{m}_k\times\mathbf{h}_{Tk}. \quad (12)$$

If the cells are small enough that $\mathbf{m}(\mathbf{r},t)$ is spatially uniform in each cell, we can reasonably assume that the magnetization amplitude is

$$|\mathbf{m}_k| = 1. \quad (13)$$

Now we can write down the discretized LLG equation in the following form that consist of a system of ordinary stochastic differential equations (SDE):

$$\frac{\mathrm{d}\mathbf{m}_k}{\mathrm{d}t} = -\mathbf{m}_k\times\mathbf{h}_{\mathrm{eff}_k}[\underline{\boldsymbol{m}}] + \alpha\mathbf{m}_k\times\frac{\mathrm{d}\mathbf{m}_k}{\mathrm{d}t} - \frac{\nu}{\sqrt{V_k}}\mathbf{m}_k\times\mathbf{h}_{Tk}(t) \quad (14)$$

where $\mathbf{m}_k$ is the average magnetization of the k-th cell. It is worth noting that the effective field in the k-th cell depends on the magnetization of the whole cell collection due to the magnetostatic interaction, namely $\mathbf{h}_{\mathrm{eff}\,k} = \mathbf{h}_{\mathrm{eff}\,k}[\underline{\boldsymbol{m}}]$.

Equation (14) can be rewritten in the standard SDE formalism [11]

$$\mathrm{d}\mathbf{m}_k = \mathbf{v}_k(\underline{\boldsymbol{m}})\mathrm{d}t - \mathbf{m}_k\times(c_\alpha\nu_k\mathrm{d}\mathbf{W}_k + \alpha'\nu_k\mathbf{m}_k\times\mathrm{d}\mathbf{W}_k) \quad (15)$$

where $c_\alpha = 1/(1+\alpha^2), \alpha' = \alpha c_\alpha$,

$$\mathbf{v}_k(\underline{\boldsymbol{m}}) = -\mathbf{m}_k\times(c_\alpha\mathbf{h}_{\mathrm{eff}\,k} + \alpha'\mathbf{m}_k\times\mathbf{h}_{\mathrm{eff}\,k}), \quad (16)$$

and

$$\mathrm{d}\mathbf{W}_k = \mathbf{h}_{Tk}\mathrm{d}t \quad (17)$$

being $\mathbf{W}_k$ the isotropic standard vector Wiener process.

Equation (15) is a SDE with multiplicative noise and, therefore, must be first complemented with the choice of the type of stochastic calculus [11]. Then, in order to numerically integrate the stochastic LLG equation, a numerical scheme consistent with the chosen calculus must be used.

We interpret (15) in the sense of Stratonovich. This choice implies that the ordinary rules of calculus apply. An important consequence is that, by multiplying both sides of (15) by $\mathbf{m}_k$, one obtains

$$d(|\mathbf{m}_k|^2) = 0. \quad (18)$$

The latter equation, along with the constraint (13), means that (15) generates in each computational cell a vector stochastic process evolving on the unit-sphere.

For the numerical solution of (15), we use the implicit midpoint rule scheme [12]. This technique is consistent with the Stratonovich interpretation of (15), namely, as the time step $\Delta t \to 0$, the numerical solution of (15) will converge to the Stratonovich solution. In addition, consistently with the property (18), the midpoint rule scheme has been shown to preserve the magnetization magnitude in each cell and also the energy balance property of the stochastic LLG dynamics [12].

The midpoint discretized version of (15) is

$$\begin{aligned}\mathbf{m}_k^{n+1} - \mathbf{m}_k^n &= -\mathbf{m}_k^{n+\frac{1}{2}} \left(c_\alpha \mathbf{h}_{\mathrm{eff}\,k}^{\,n+\frac{1}{2}} + \alpha' \mathbf{m}_k^{n+\frac{1}{2}} \times \mathbf{h}_{\mathrm{eff}\,k}^{\,n+\frac{1}{2}} \right) \Delta t \\ &\quad - \mathbf{m}_k^{n+\frac{1}{2}} \times \left(c_\alpha \nu_k \Delta \mathbf{W}_k^n + \alpha' \nu_k \mathbf{m}_k^{n+\frac{1}{2}} \times \Delta \mathbf{W}_k^n \right)\end{aligned} \tag{19}$$

where the index n refers to time instants, and the following midpoint formulas have been used [13]:

$$\mathbf{m}_k^{n+\frac{1}{2}} = \frac{\mathbf{m}_k^n + \mathbf{m}_k^{n+1}}{2}, \tag{20}$$

$$\mathbf{h}_{\mathrm{eff}\,k}^{\,n+\frac{1}{2}} = \mathbf{h}_{\mathrm{eff}\,k} \left[\frac{\underline{\boldsymbol{m}}^n + \underline{\boldsymbol{m}}^{n+1}}{2} \right]. \tag{21}$$

In addition, according to the properties of the Wiener process [11], each component of the increment

$$\Delta \mathbf{W}_k^n = \mathbf{W}_k^{n+1} - \mathbf{W}_k^n \tag{22}$$

is an independent Gaussian stochastic variable with zero-mean and variance Δt, computed for each cell and at each time step by using a pseudo-random number generator.

The solution of the time-stepping (19) requires solving a system of $3N$ nonlinear algebraic equations and provides, at each time step, the $3N$ unknowns $\mathbf{m}_k^{n+1}$ at each mesh element Ω_k. To solve this nonlinear system we use a quasi-Newton technique similar to one described in [13].

The discretized effective field in (14) is the gradient of a discretized free energy $\underline{g}_L(\underline{\boldsymbol{m}}) = \underline{g}_L(\mathbf{m}_1, \ldots, \mathbf{m}_N)$ which approximates the free energy functional $g_L[\mathbf{m}]$

$$\mathbf{h}_{\mathrm{eff}\,k} = -\frac{\partial}{\partial \mathbf{m}_k} \underline{g}_L(\mathbf{m}_1, \ldots, \mathbf{m}_N). \tag{23}$$

The effective field $\mathbf{h}_{\mathrm{eff}\,k}$ can be represented as

$$\mathbf{h}_{\mathrm{eff}\,k} = \mathbf{h}_{\mathrm{ex}k} + \mathbf{h}_{\mathrm{an}k} + \mathbf{h}_{\mathrm{m}k} + \mathbf{h}_{\mathrm{a}k} \tag{24}$$

where $\mathbf{h}_{\mathrm{ex}k}$ is the exchange field, $\mathbf{h}_{\mathrm{an}k}$ is the anisotropy field, $\mathbf{h}_{\mathrm{m}k}$ is the magnetostatic field, and $\mathbf{h}_{\mathrm{a}k}$ is the applied field. In our formulation we subdivide the magnetized domain Ω into N tetrahedral elements. The magnetostatic field contribution to the effective field is computed by means of an hybrid procedure: inside the region Ω occupied by the magnetic body, the magnetostatic problem is formulated by using the Finite Formulation scheme [14] where the magnetic vector potential is assumed as unknown. Conversely, in the exterior region extending to infinity, the magnetic scalar potential at the boundary of the magnetized domain Ω is analitically computed through an integral formulation [15]. Using this method, the resulting stiffness matrix is sparse and all coupling terms between the two formulations are on the right-end-side (RHS) [16]. Starting from a known magnetization distribution, the RHS is computed by a matrix-vector product and the resulting linear system is solved by using a direct method in which the stiffness matrix is LU factorized once and for all at the beginning of the procedure. The computational cost of the LU factorization of the stiffness matrix is $O(N^3)$ and the cost of each subsequent magnetostatic computation is $O(N)$. This scheme could also be efficiently sped-up by means of the use of Fast Multipole Method [17].

Regarding the calculation of exchange field, as vector $\mathbf{m}$ is approximated by a piecewise constant vector field (at each element Ω_k), there is not a direct way of evaluating the term $|\nabla \mathbf{m}|$ in (3). The exchange field is then computed following a procedure similar to that described by Fredkin in [18].

III. Numerical Results

In order to test the accuracy of full micromagnetic simulations, we now define a problem concerning the analysis of thermal fluctuations for a small magnetic nanoparticle. The magnetic particle has ellipsoidal shape with x, y, and z axes length equal to 3 nm, 3 nm, and 10 nm, respectively. The material parameters are: $M_{\mathrm{s}} = 8 \cdot 10^5$ A/m, negligible magneto-crystalline anisotropy, damping constant $\alpha = 0.02$. We assume temperature $\mathrm{T} = 300$ K and no external field applied.

As the dimension of the particle is comparable with the exchange length $l_{\mathrm{ex}} = 5.686$ nm, it is expected that the particle is almost uniformly magnetized. This allows one to compare the obtained numerical results with the analysis of thermal fluctuations for single-domain particles. In fact, by using the Fokker-Planck equation [5], the following equilibrium probability distribution function for the magnetization can be derived:

$$W_{\mathrm{eq}}(m_z) = \frac{1}{Z(\mu)} \exp\left(-\mu \left(N_z m_z^2 + N_y \left(1 - m_z^2 \right) \right) / 2 \right) \tag{25}$$

where

$$\mu = \frac{2\alpha}{\nu^2} = \frac{\mu_0 M_{\mathrm{s}}^2 V_\Omega}{k_{\mathrm{B}} T} \tag{26}$$

$Z(\mu)$ is the partition function which gives the correct normalization of $W_{\mathrm{eq}}(m_z), N_x = N_y = 0.4523, N_z = 0.0954$ are the demagnetizing factors and k_B is the Boltzmann constant. In our case, the values of the parameters are such that the energy barrier related to the shape anisotropy of the particle is about $\mu_0 \mathrm{M}_s^2 V_\Omega (N_y - N_z) \approx 25 k_{\mathrm{B}} T$, meaning that the role of thermal fluctuations is quite significant.

As far as micromagnetic simulations are considered, the particle has been discretized into 466 tetrahedral elements with 176 nodes. The time integration step is $\Delta t = 17.6 \cdot 10^{-3}$ (in normalized units of $(\gamma \mathrm{M_s})^{-1}$). We have performed two different set of numerical simulations. In the first set, the equilibrium distribution of the magnetization, spatially averaged over the particle's body) is computed. To this end, (15) has been integrated for a sufficiently long time (100000 in the normalized units) to have enough statistics to compute a smooth empirical probability distribution of magnetization. For symmetry arguments, we expect a symmetrical behavior of this distribution. The numerical results, reported in Fig. 1, are in good agreement with the equilibrium distribution derived from the Fokker-Planck equation approach.

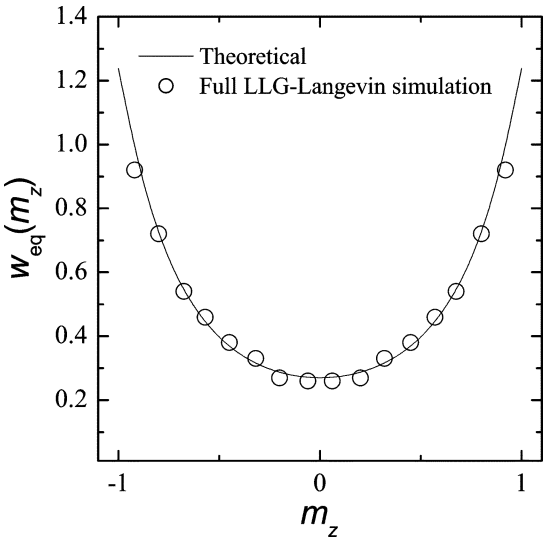

Fig. 1. Equilibrium probability distribution vs. magnetization for the chosen spheroidal particle. The values of the parameters are: $M_{\rm s} = 8 \times 10^5$ A/m, $\alpha = 0.02, V = 4.407 \times 10^{-26}$ m^3, temperature $T = 300$ K, negligible magnetocristalline anisotropy, the demagnetizing factors are $N_x = N_y = 0.4523$, and $N_z = 9.54 \times 10^{-2}$. Solid line: Equation (25). Dots: micromagnetic Langevin simulations. For the case of the single-domain particle m_z is in unit of $M_{\rm s}$. For Langevin simulations m_z is calculated by normalization to the amplitude of the spatial average of $\mathbf{M}$ which is $\sim 0.951 \cdot M_{\rm s}$.

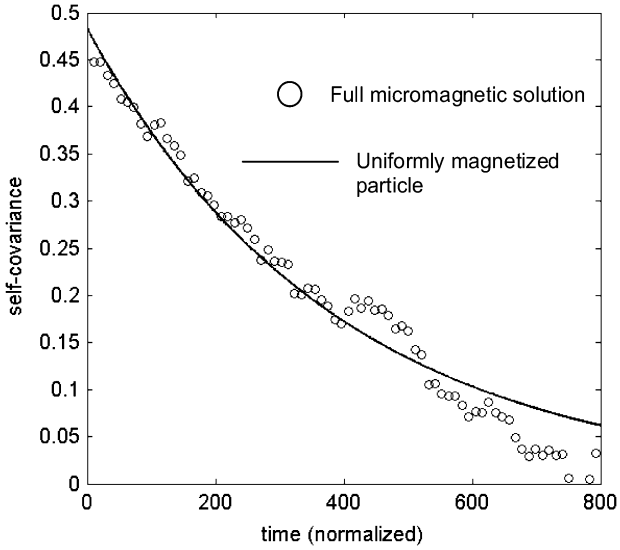

Fig. 2. Comparison between self-covariance functions for magnetization component m_z. The value of the parameters are the same as in Fig. 1. Solid line: self covariance obtained from the numerical solution of Fokker-Planck equation for the single-domain particle. Dots: computed empirical self-covariance function from full micromagnetic Langevin simulations. The number of stochastic realizations is 90. The time is expressed in units of $(\gamma \cdot M_{\rm s})^{-1} = 5.6535$ ps.

Moreover, it is found from the numerical simulations that the amplitude of the spatial average of magnetization is almost independent on time and acts as an effective saturation magnetization $\tilde{M}_{\rm s}$. We have found $\tilde{M}_{\rm s} \sim 0.951\, M_{\rm s}$. It is expected that $\tilde{M}_{\rm s} \to M_{\rm s}$ as the particle volume becomes smaller and smaller.

In the second set of numerical simulations, we have derived the empirical self-covariance function $C_{m_z}(t)$ of the spatially averaged (over the particle's body) z-component of the magnetization. To this end, we have computed $N_{\rm r}$ realizations of the stochastic LLG dynamics starting from $N_{\rm r}$ (spatially uniform) different initial conditions randomly chosen according to the equilibrium distribution (25). The time interval of each simulation has been chosen to be 5 times greater than the estimated time constant which governs the decay of $C_{m_z}(t)$. This time constant has been estimated by numerically integrating the Fokker-Planck equation and it is about 300 normalized time units. By using all this data, we have evaluated the following empirical estimate of the auto-covariance function:

$$C_{m_z}(t) = \sum_{q=1}^{N_r} \frac{\left(\overline{m_{z,q}}(0) - \langle m_z \rangle(0)\right)\left(\overline{m_{z,q}}(t) - \langle m_z \rangle(t)\right)}{N_r} \tag{27}$$

where the index $q = 1, \ldots, N_r$ denotes the q-th realization of the magnetization stochastic process and the notation $\overline{m_z}(t)$ means spatial average of m_z over the particle's body at time t. The numerical results have been compared with the results obtained by the solution of the Fokker-Planck equation for single domain particle. The comparison is shown in Fig. 2 and demonstrates a reasonably good agreement between the two results.

Finally, we would like to emphasize that the above comparison of the two independent approaches in the analysis of thermally activated dynamics of small magnetic particles can be used as a benchmark tool for testing micromagnetic codes. In fact, even if the Langevin dynamics approach is frequently used, the inclusion of thermal effects in micromagnetics using white noise is still a relatively open theoretical problem. Nevertheless, from the physical point of view, it is reasonable that the results of micromagnetic simulations coincide with the ones for single-domain particles as far as the volume is reduced.

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