

BROWNIAN DYNAMICS APPROACH TO INTERACTING MAGNETIC MOMENTS

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The question of how to introduce thermal fluctuations in the equation of motion of a magnetic system is addressed. Using the approach of the fluctuation-dissipation theorem we calculate the properties of the noise for both, the fluctuating field and fluctuating torque (force) representation. In contrast to earlier calculations we consider the general case of a system of interacting magnetic moments without the assumption of axial symmetry. We show that the interactions do not result in any correlations of thermal fluctuations in the field representation and that the same widely used formula can be used in the most general case. We further prove that close to the equilibrium where the fluctuation-dissipation theorem is valid, both, field and torque (force) representations coincide, being different far away from it. We also show that the uncorrelated character of the noise is due to the form of the Landau-Lifshitz (or Gilbert) damping and under different damping formalisms, the normal mode analysis is proper.

INTRODUCTION

The problem of how to correctly introduce temperature induced fluctuations into the equation of motion of a magnetic system has gained in importance as a result of the technological requirements of magnetic recording industry [1–3]. This is associated with the need to perform calculations of magnetization dynamics at finite temperatures. Open problems include fast magnetization switching, thermal stability and magnetic viscosity, among others. The correct solution of the problem is still far from being understood. The main difference between the magnetic problem and the standard molecular dynamics approach is that the magnetic moment dynamics is governed by the Landau-Lifshitz equation which includes the precession of a magnetic moment around the local field direction. It comprises coupled first-order equations for the magnetization components, and the requirement of conservation of the magnetization amplitude. As a consequence, no analogue of mass and kinetic energy exist in the system, thus making it impossible to introduce the temperature through this mechanism.

Consequently, the temperature is introduced through small deviations from the equilibrium configuration. Therefore, strictly speaking, this approach is only valid when these deviations are small and it cannot be used for fast magnetization switching.

Let us briefly summarize the original approach from W. Brown [4, 5]. The underlying equation of motion is the

Landau-Lifshitz-Gilbert equation which can be written in the form

$$\frac{d\vec{M}_i}{d\tau} = -\vec{M}_i \times \vec{H}_i - \alpha \vec{M}_i \times (\vec{M}_i \times \vec{H}_i), \quad (1)$$

where

$$\tau = \frac{\gamma_0}{(1 + \alpha^2)} t, \quad \vec{H}_i = -\frac{1}{M_s V_i} \frac{\delta E}{\delta \vec{M}_i} \quad (2)$$

γ_0 is the gyromagnetic ratio α is the damping constant i is the particle site and V_i is the particle volume. The magnetic moment \vec{M} is normalized to the saturation value M_s . The energy E contains all the necessary energy contributions: anisotropy, exchange, magnetostatic and Zeeman.

W. Brown proposed the inclusion of thermal fluctuations via a random field, added to the internal field, Eq. 2. For the calculation of the properties of the random field he outlined two methods: (i) based on the fluctuation-dissipation theorem (see also [6]) and (ii) by imposing the condition that the equilibrium solution of the corresponding Fokker-Planck equation is the Boltzmann distribution (see also [7]). As a result of these the thermal field statistical properties are given by

$$\langle \xi_\alpha \rangle = 0, \quad \langle \xi_\alpha(0) \xi_\beta(\tau) \rangle = \frac{2\alpha k_B T}{M_s V_i (1 + \alpha^2)} \delta_{\alpha\beta} \delta(\tau), \quad (3)$$

where α, β denote Cartesian components x, y, z . Different approaches based, for example, on the Landau-

Lifshitz rather than on the Landau-Lifshitz-Gilbert equation were also introduced [7, 8].

However, the properties of the thermal noise, Eqs. 3, were derived only for one isolated particle. Moreover, Brown considered in his paper [4] only the simplest axially symmetric case. Nevertheless, in the past the formulas above provided the basis for practically every numerical method [2, 9–11] for the computation of magnetization dynamics taking into account thermal fluctuations.

But the investigated magnetic systems usually comprise interacting particles [12–17] due to magnetostatic and/or exchange couplings. For that case the thermal field may be expected to be influenced by correlations between different particles [10]. In fact, in interacting liquids and gases, the requirement of thermal equilibrium often imposes the correlation conditions on the thermal term [18]. This has led many authors to introduce thermal fluctuations via the normal modes for strongly interacting systems [6, 19–21]. Hence, it is necessary to generalize Brown's result to the case of interacting magnetic moments. To the best of our knowledge, this has never been done before.

BROWNIAN DYNAMICS

In what follows we start with the Brownian dynamics approach (see [22]) which was originally applied to magnetic systems by A. Lyberatos et al. [6, 10]. However, we consider the general case of an interacting system with a non-axially-symmetric potential around a general stationary equilibrium $\{\bar{M}_0^i\}$ which is not necessary a saturation. All our calculations are going to be valid indistinguishably for interacting magnetic particles or for discretization units of a continuous magnetic material (micromagnetics). Following the standard approach, we introduce the temperature into the motion of the magnetic moments as a result of the application of the fluctuation-dissipation theorem (via its formulation in the kinetic coefficient theory). Consequently, this approach is only valid when small deviations from equilibrium are considered.

We first consider torque fluctuations. In next section we consider the situation when thermal fluctuations are introduced via the local field.

Additive noise and torque fluctuations

The general Langevin equation of motion is written in the form

$$\frac{dx_i}{dt} = -\sum_j \gamma_{ij} X_j + f_i, \quad X_j = -\frac{\partial S}{\partial x_j}, \quad (4)$$

where the γ_{ij} are the so-called kinetic coefficients, X_j are variables which are thermodynamically conjugate to x_j ,

and S is the entropy of the magnetic system. For a closed system in an external medium,

$$X_j = \frac{1}{k_B T} \frac{\partial E}{\partial x_j}. \quad (5)$$

In Eq. 4, f_i is a random force representing thermal fluctuations in the system having the properties

$$\langle f_i(t) \rangle = 0 \quad \text{and} \quad \langle f_i(0) f_j(t) \rangle = \mu_{ij} \delta(t) \quad (6)$$

where

$$\mu_{ij} = \gamma_{ij} + \gamma_{ji}. \quad (7)$$

A linear equation of motion of the form

$$\frac{dx_i}{dt} = \sum_j L_{ij} x_j, \quad (8)$$

with the associated energy

$$E = E_0 + \frac{1}{2} \sum_{i,j} A_{ij} x_i x_j, \quad (9)$$

can be rewritten as

$$\frac{dx_i}{dt} = -\sum_j L_{ij} x_j = -\sum_j \gamma_{ij} \frac{1}{k_B T} \sum_k A_{kj} x_k, \quad (10)$$

so that the matrix L_{ik} is related to the kinetic coefficients γ_{ik} in the following way [6]:

$$L_{ik} = -\frac{1}{k_B T} \sum_j \gamma_{ij} A_{kj} \quad (11)$$

In micromagnetics the motion of a magnetic moment \mathbf{M} is governed by the deterministic LLG equation (Eq. 1). For the equilibrium state of the system Brown's condition

$$\vec{M}_i^0 \times \vec{H}_i^0 = 0 \quad (12)$$

must be satisfied, implying that here \vec{H}_i^0 and \vec{M}_i^0 are parallel. Close to equilibrium, the LLG equation can be linearized using small deviations

$$\vec{m}_i = \vec{M}_i - \vec{M}_i^0, \quad \vec{h}_i = (\vec{H}_i - \vec{H}_i^0)/M_s \quad (13)$$

from their equilibrium values, yielding

$$\frac{dm_i}{d\tau} = \sum_{j=1}^{3N} L_{ij} m_j. \quad (14)$$

Here, the indices i, j count the particles sites $1, \dots, N$ as well as their x, y, z coordinates. The internal fields h_j play the role of the variables which are thermodynamically conjugate to m_j ,

$$X_j = \frac{1}{k_B T} \frac{\partial E}{\partial m_j} = -\frac{M_s^2 V_i}{k_B T} h_j. \quad (15)$$

Thus, the LLG equation should be rewritten in the form

$$\frac{dm_i}{d\tau} = \frac{M_s^2 V_i}{k_B T} \sum_{j=1}^{3N} \gamma_{ij} h_j \quad (16)$$

which is an easier way to calculate the kinetic coefficients than the use of Eq. 11. The representation of the LLG equation in the form of Eq. 4 means that in what follows the thermal fluctuations are introduced as a fluctuating torque (a generalized force rather than a field). Later we will show that in the linear approximation this is equivalent to the standard fluctuating field representation. Alternatively, Eq. 16 could be viewed as a polar representation of the magnetization vector $m_i^1 = \theta_i, m_i^2 = \varphi_i$, in this case the conjugate variables are the polar projections of the internal fields (h_θ, h_φ) and the fluctuations f_i will stand for the random field polar components. This latter approach was used originally by W. Brown [4].

We continue by writing the energy of the system in the form

$$E = \sum_i^N \left(-\vec{M}_i \cdot \vec{H}_i + \frac{\lambda}{2} M_s \vec{M}_i^2 \right) V_i M_s. \quad (17)$$

where λ is the Lagrange multiplier. In the zero order approximation one obtains

$$M_s \vec{M}_i^0 = \frac{1}{\lambda} \vec{H}_i^0 \quad (18)$$

which corresponds to Brown's condition, Eq. 12. The linear approximation leads to the equilibrium condition

$$-\vec{M}_i^0 \cdot \vec{h}_i - \vec{H}_i^0 \cdot \vec{m}_i + \lambda \vec{M}_i^0 \cdot \vec{m}_i = 0, \quad (19)$$

which leaves us only the quadratic form for the energy expression near the equilibrium,

$$E^* = E/(V_i M_s^2) = E_0 - \sum_i^N \left(\vec{m}_i \cdot \vec{h}_i(\{\vec{m}_i\}) - \frac{\lambda}{2} \vec{m}_i^2 \right), \quad (20)$$

where $\vec{h}_i(\{\vec{m}_i\})$ is the deviation of the internal field acting on the particle at site i from its equilibrium value.

Most of the magnetic energy expressions are quadratic in the magnetization components (apart from the Zeeman term which is included in the equilibrium field \vec{H}_i^0 and condition 19). In micromagnetic methods [23–25] the expressions for discretized magnetic interaction matrix are available explicitly. Some other terms, as for example the cubic anisotropy, are not quadratic. In this case the Taylor expansion around the equilibrium should be made. These expressions should be used in Eq. 11 to find the kinetic coefficients. However, the remarkable form of the Landau-Lifshitz-Gilbert equation make the kinetic coefficients independent of the concrete system

under consideration. The only supposition we are making so far is that the energy has the most general form of the quadratic expression:

$$h_i^\alpha = \sum_{j,\beta} B_{ij}^{\alpha\beta} m_j^\beta = -\frac{\partial E^*}{\partial m_i^\alpha} + \lambda m_i^\alpha \quad (21)$$

where λm_i^α is the field due to the kinematic interaction expressing the ferromagnetic constraints and λ is a Lagrange multiplier. Also from now on it is convenient to separate the indices corresponding to different particle sites (Latin) and to different magnetization and field components (Greek). The value of the Lagrange multiplier is normally found from the equilibrium condition 19. However, its actual value is not necessary for these calculations due to the fact that the LLG equation conserves the magnetization length.

The expressions for the kinetic coefficients are normally obtained by using directly the expressions 11 and the explicit form of the expression 21. In this approach it seems that the final result could also include correlations between different particles [10]. But in the particular case of the Landau-Lifshitz-Gilbert damping the direct calculations show that this is not true. Moreover, the kinetic coefficients can easily be obtained by representing the linearized LLG equation in the form of Eq. 16 yielding

$$\gamma_{ij}^{xx} = \frac{\alpha k_B T}{M_s V_i} \left[(M_i^{0,y})^2 + (M_i^{0,z})^2 \right] \delta_{ij} \quad (22)$$

$$\gamma_{ij}^{xy} = \frac{k_B T}{M_s V_i} \left[-M_i^{0,z} + \alpha M_i^{0,x} M_i^{0,y} \right] \delta_{ij} \quad (23)$$

$$\gamma_{ij}^{yx} = \frac{k_B T}{M_s V_i} \left[M_i^{0,z} + \alpha M_i^{0,x} M_i^{0,y} \right] \delta_{ij} \quad (24)$$

$$\gamma_{ij}^{yy} = \frac{\alpha k_B T}{M_s V_i} \left[(M_i^{0,x})^2 + (M_i^{0,z})^2 \right] \delta_{ij}. \quad (25)$$

The other coefficients can be obtained by symmetry. Note, that there are no correlations between different particles. Also, the kinetic coefficients have obviously reversible parts (coming from rotation) and irreversible parts (from damping). The reversible antisymmetric parts do not contribute to the thermal fluctuations after adding the kinetic coefficients to calculate the matrix μ from Eq. 7, yielding

$$\mu_{ij}^{xx} = \frac{2\alpha k_B T}{M_s V_i} \left[(M_i^{0,y})^2 + (M_i^{0,z})^2 \right] \delta_{ij} \quad (26)$$

$$\mu_{ij}^{xy} = \frac{2\alpha k_B T}{M_s V_i} M_i^{0,x} M_i^{0,y} \delta_{ij}. \quad (27)$$

Once again, the others can be obtained by symmetry. Note that in a general system of coordinates there are correlations between different magnetization components but no correlations between different particles. However, if we choose a local coordinate system such that the z axis coincides with the equilibrium magnetization direction, $M_i^{0,x} = 0, M_i^{0,y} = 0, M_i^{0,z} = 1$, for each magnetic

moment, these correlations disappear and we have the same thermal fluctuations in x and y directions but no fluctuations in z direction,

$$\mu_{ij}^{xx} = \mu_{ij}^{yy} = \frac{2\alpha k_B T}{M_s V_i} \delta_{ij} \quad \text{and} \quad \mu_{ij}^{zz} = 0. \quad (28)$$

Thus, the torque fluctuations produce effectively correlations and different values of thermal fluctuations in all other systems of coordinates different from the special local system, where one of the axes is parallel to the equilibrium magnetization direction and where the equation of motion for this component disappears. We stress that the expansion is made around any stationary equilibrium solution, like, for example, a stationary domain wall. Use of the special local coordinate system renders the μ matrix free of inter-particle correlations according to Eqs. 26–27.

Field fluctuations

It is customary to introduce thermal fluctuations in the field components (see [9] and originally W. F. Brown [4]) instead of the torque fluctuations as derived above. This has its origin in the representation of the LLG equation in a spherical system of coordinates in form of Eq. 4. However, in both of these papers above only the axially symmetric case without interactions was considered. The big difference between these two approaches is the *multiplicative* character of the field noise versus the *additive* noise of the torque. This turns out to be important for larger magnetization deviations. But first we will show that in the local coordinate system both approaches, torque and field, give the same result, as long as the magnetization deviations from the equilibrium are small.

Let us use a decomposition of the field components according to $H_i^\mu \rightarrow H_i^\mu + \xi_i^\mu$, where ξ_i^μ are the components of the thermal fluctuation part of the field and H_i^μ are the components of the internal field at the i -th particle. When this is done we obtain the following expansion of the equations of motion,

$$\begin{aligned} \frac{dM_i^\eta}{d\tau} &= -\varepsilon^{\eta\zeta\nu} M_i^\zeta H_i^\nu - \alpha H_i^\zeta \left[M_i^\zeta M_i^\eta - \delta^{\zeta\eta} \right] \\ &\quad - \varepsilon^{\eta\zeta\nu} M_i^\zeta \xi_i^\nu - \alpha \xi_i^\zeta \left[M_i^\zeta M_i^\eta - \delta^{\zeta\eta} \right] \\ &= A_i^\eta(M_i^\mu, H_i^\nu) + B_i^{\eta\zeta}(M_i^\mu) \xi_i^\zeta. \end{aligned} \quad (29)$$

where A_i^η stands for the deterministic part of the equation and $B_i^{\eta\zeta}$ stands for the thermal part. Furthermore, in the special local system of coordinates we linearize the magnetization by the decomposition $M^\eta \rightarrow M_0^\eta + m^\eta$, where m^η are small fluctuations around the equilibrium values M_0^η , and apply the constraint condition, $|\vec{M}| = 1$. For simplicity below we drop in the formulas the particle index i .

The components in the specified coordinate system are then

$$\frac{dm^x}{d\tau} = A^x(\{\vec{m}\}) - (m^y + \alpha m^x) \xi^z + f^x, \quad (30)$$

$$\frac{dm^y}{d\tau} = A^y(\{\vec{m}\}) + (m^x - \alpha m^y) \xi^z + f^y, \quad (31)$$

$$\frac{dm^z}{d\tau} = (m^x + m^y) (\xi^x - \alpha \xi^y), \quad (32)$$

where $\vec{A}(\{\vec{m}\})$ stands for the linearized deterministic part of the LLG equation and

$$f^x = \xi^y + \alpha \xi^x, \quad f^y = -\xi^y + \alpha \xi^x. \quad (33)$$

The constraint condition implies that in a first order approximation it is $m^z(\tau) = 0, \forall \tau$. This is compatible with Eq. 32 only if the field fluctuations ξ^i can be considered to be small quantities, in which case products of the ξ^i with the m^i can be ignored in Eqs. 30 and 31. These equations suggest that the field fluctuations contribute *additively*. From Eqs. 33 one can also obtain Brown's formulas for the field fluctuations (Eq. 3).

It is important to note that the equation $m^z(\tau) = 0, \forall \tau$ is satisfied for any fluctuation field value due to the character of the LLG damping term. Thus the f^z value (or ξ^z) is in this case undefined. This is different from what happens with the torque fluctuations where the z component should be set to zero explicitly following Eq. 28. In any case the component ξ^z is not efficient since it acts parallel to the magnetization direction. The assumption made in the paper of A. Lyberatos and R. Chantrell [9] is that the field components are isotropic and that

$$\langle (\xi^x)^2 \rangle = \langle (\xi^y)^2 \rangle = \langle (\xi^z)^2 \rangle. \quad (34)$$

This assumption in the local coordinate system (where the fluctuation-dissipation theorem is applied) leads to the remarkable symmetry (Eq. 34) of the field components in all the systems of coordinates and to the absence of correlations. This can be checked by making change to an arbitrary system or coordinates. Furthermore, it is assumed that this property is valid through the magnetization reversal.

For the torque fluctuations the reasonable hypothesis to mimic the field ones would be the assumption that there are never torque (force) fluctuations along the magnetization direction. In this case the correlations between different noise components would appear in all other systems of coordinates different from the local one. While equivalent near the equilibrium, these two approaches will be different far from it. At this point, we would like to restate the fact that the whole theory is valid for small fluctuations around the equilibrium where both approaches coincide.

We should note here that the remarkable property of the non-correlated noise is due to the form of the Landau-Lifshitz-Gilbert equation in which each term is linearly

proportional to the effective field. The linearized form of the Gilbert equation is the same (apart from the additional multiplier $(1 + \alpha^2)$) and all the results presented here are valid for this equation as well. Even if the damping in this case is introduced in form of the torque (as in the case of Ref. [8]) effectively, it falls into the class of the field damping of the present paper, since due to its functional dependence, the component parallel to the magnetization direction could be chosen arbitrarily.

Thermal fluctuations under a different damping mechanism

We should recall that the Landau-Lifshitz-Gilbert damping is just a phenomenological model. Alternatively, many other phenomenological damping mechanisms, as the famous Bloch damping, were proposed [26–28]. In each case the application of the fluctuation-dissipation theorem should be checked separately. Consider, for example a phenomenological damping term

$$G = -\Gamma \vec{M} \times (\vec{M} \times \vec{M}^0) \quad (35)$$

which was derived by D. Garanin [26] from the Fokker-Planck equation for a classical ferromagnet for small temperatures. In this case, the damping term is not proportional to the internal field, and the general formula (Eq. 11) must be used. As an example, let us consider a chain of uniform magnetic particles with uniaxial anisotropy and exchange coupling. The energy of the chain is written as:

$$E = V \sum_i \left(-\frac{K^*}{2} (M_i^z)^2 - J^* M_s^2 (\vec{M}_{i+1} - \vec{M}_i)^2 \right) \quad (36)$$

where J^* is the effective exchange constant and K^* the effective uniaxial anisotropy constant. Direct linearization of the equation of motion around the equilibrium $(0, 0, 1)$ gives the following equations:

$$\frac{dm_i^x}{d\tau} = M_s (-h_i^y + \Gamma m_i^x), \quad (37)$$

$$\frac{dm_i^y}{d\tau} = M_s (h_i^x - \Gamma m_i^y). \quad (38)$$

The internal fields can be expressed through magnetization as

$$h_i^\alpha = J^* m_{i-1}^\alpha - 2(K^* + J^*) m_i^\alpha + J^* m_{i+1}^\alpha \quad (39)$$

for $\alpha = x, y$ and

$$h_i^z = 0. \quad (40)$$

Consequently,

$$\mathbf{m}^x = \tilde{B}^{-1} \mathbf{h}^x, \quad \mathbf{m}^y = \tilde{B}^{-1} \mathbf{h}^y, \quad \mathbf{m}^z = 0 \quad (41)$$

where \tilde{B} is a band matrix with $B_{ii} = -2(K^* + J^*)$ and $B_{i,i+1} = B_{i,i-1} = J^*$. Using the notation β_{ij} for the elements of the inverse of the matrix \tilde{B} , we obtain:

$$\gamma_{ij}^{xx} = -\gamma_{ij}^{yy} = \frac{2\Gamma k_B T}{VM_s} \beta_{ij}, \quad (42)$$

$$\gamma_{ij}^{xy} = -\gamma_{ij}^{yx} = \frac{2\Gamma k_B T}{VM_s} \delta_{ij}, \quad (43)$$

$$\gamma_{ij}^{\alpha z} = \gamma_{ij}^{z\alpha} = 0, \quad \alpha = x, y, z \quad (44)$$

Therefore, in this case the noise components should contain correlations between different particles. Of course, a transformation to normal modes which will make the matrix \tilde{B} diagonal and the corresponding noise components non-correlated, may be performed. Note also that according to Eq. 11, the mean squared deviation of the thermal field for each individual normal mode in the system of coordinates of normal modes is going to be inversely proportional to its eigenvalue. The Safonov damping [27] as well as the Baryakhtar one [28] will also result into correlated fluctuations in all systems of coordinates different from the normal modes ones.

CONCLUSIONS

In conclusion, the application of the Brownian dynamics approach to the motion of a magnetic particle system shows that interactions do not introduce correlations into thermal fluctuations introduced as both, either a fluctuating torque or a fluctuating field when a standard damping of the Landau-Lifshitz-Gilbert or the Gilbert form is considered. Correlations may appear between different magnetization components as a result of the conservation of the value of the magnetic moment. The reasonable hypothesis that all the fluctuating field components are equivalent leads to Brown's well-known formulas for the fluctuating fields values without correlations. Our results show that the uncorrelated fluctuations are completely in agreement with the fluctuation-dissipation theorem. The introduction of temperature into normal modes should lead to the same equilibrium properties. This validates all previously done micromagnetic calculations where this kind of assumption was made. However, different damping mechanisms may lead to the appearance of correlations

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