Approximation of Multiparticle Distribution Function in Micromagnetic Modeling

Anton Ivanov, Sergey Khilkov and Zipunova Elizaveta
Keldysh Institute of Applied Mathematics, Miusskaya sq., 4, Moscow, 125047, Russia
E-mail: aiv.racs@gmail.com

Abstract. We propose the new system of equations for magnetodynamics. It is based on BBGKY hierarchy and uses a new approximations of mult-particles distribution functions, which takes nearest-neighbour correlations into account. Thus we call the new system of equations correlational magnetodynamics system (CMD). It consists of well known Landau–Lifshitz–Bloch (LLB) equation complemented with an equation for two-particles correlations. Compared to traditional LLB equation, numerical simulations with CMD produces results that are closer to atomistic simulations.

1. Introduction
In systems with the strong coupling the derivation of continuous medium equations from atomistic ones is a great challenge. In that respect magnetic system appeared to be simpler than fluid one due to different shape of the phase space. The aforementioned transition requires approximation of two- and three-particles distribution functions as a functional on one-particle distribution. Usually these approximation are based on strong assumptions with vague physical evidences at best.

The simplest form of a multi-particles distribution approximation is the multiplication of one-particle distribution functions. It corresponds to the mean field approximation. It leads to LLB equation [1] for magnetics, which describes the evolution of the magnetisation \( \langle m \rangle \) distribution in space \( r \) and time \( t \). The main drawbacks of the LLB equation approach are the vanishing of the exchange energy in the paramagnetic phase and the underestimated system relaxation time. The later is quite important for engineering applications. The flaws are caused by the fact that mean field approximation lose the information about nearest neighbours correlations which is important in case of a strong exchange interaction.

Taking the nearest neighbours correlations into account in the multi-particles distribution approximation allows us to write the correction term for LLB equation complemented with equation for two-particles correlation (exchange energy) \( \langle \eta \rangle = \langle m_i \cdot m_j \rangle \). Here \( m_i \) and \( m_j \) are magnetic moments of the adjacent atoms. This equation resembles the energy conservation equation in the fluid dynamics. All coefficients in the CMD system are expressed as a functions of \( \langle m \rangle \) and \( \langle \eta \rangle \). Those functions could either be evaluated numerically or approximated with the analytical functions.
2. The derivation of the LLB equation

Let's consider the magnetic system of $N$ particles with magnetic moments $\mathbf{m}_i(t)$ nailed to lattice points $\mathbf{r}_i$. Landau–Lifshitz equations govern the motion of the system

\[
\frac{d\mathbf{m}_i}{dt} = -\gamma [\mathbf{m}_i \times \mathbf{H}^{\text{eff}}] - \alpha [\mathbf{m}_i \times [\mathbf{m}_i \times \mathbf{H}^{\text{eff}}]] + \sqrt{2\alpha \gamma T} [\mathbf{m}_i \times \xi_i(t)],
\]

where

\[
\mathbf{H}^{\text{eff}} = -\nabla_{\mathbf{m}_i} W = \mathbf{H}^{\text{exch}} + \mathbf{H}^{\text{anis}} + \mathbf{H}^{\text{dip}} + \mathbf{H}^{\text{ext}}, \quad \mathbf{H}^{\text{exch}} = \sum_{j} J_{ij} \mathbf{m}_j,
\]

\[
\mathbf{H}^{\text{anis}} = 2K \mathbf{n}_K (\mathbf{n}_K \cdot \mathbf{m}_i), \quad \mathbf{H}^{\text{dip}} = \sum_{j} \frac{3 (\mathbf{m}_j \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij} - \mathbf{m}_j \mathbf{r}_{ij}^3}{r_{ij}^5}, \quad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j.
\]

Here $\gamma$ is the electron gyromagnetic ratio and $\alpha$ is the damping parameter. The full energy and the temperature of the system are labeled $W$ and $T$ correspondingly. The $\delta$-correlated three-dimensional white noise $\xi_i(t)$ has zero mean value and dispersion equals to the identity matrix. $\nabla_{\mathbf{m}_i}$ is the differential operator in $\mathbf{m}_i$ space. The effective field $\mathbf{H}^{\text{eff}}$ is the combination of exchange field $\mathbf{H}^{\text{exch}}$, the linear anisotropy field $\mathbf{H}^{\text{anis}}$, $\mathbf{H}^{\text{dip}}$ which denotes the field caused by dipole-dipole (magnetostatic) interaction and the external field $\mathbf{H}^{\text{ext}}$. The exchange integral $J_{ij}$ is usually nonzero only for adjacent particles. From now on we will assume that the value of exchange integral for adjacent particles is constant thus we can omit indices. Finally uniaxial linear anisotropy is described in terms of anisotropy parameter $K$ and easy axis $\mathbf{n}_K$ ($|\mathbf{n}_K| = 1$). For brevity we are using dimensionless units.

The equations of motion (1) are describing the stochastic process. Suppose $f^{(N)}(\mathbf{m}_1, ..., \mathbf{m}_N, t)$ is the $N$-particles distribution function for the process, then

\[
f_i(\mathbf{m}_i, t) = \int \cdots \int f^{(N)} d\mathbf{m}_{i-1,i+1,...}, \quad f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j, t) = \int \cdots \int f^{(N)} d\mathbf{m}_{i-1,i+1...j-1,j+1...}.
\]

We use notation $\int_{S_2^N} d\mathbf{m}$ to describe the integral over a unit sphere.

With help of BBGKY hierarchy one can relatively derive from the equations (1) the Fokker–Plank equation for continuous medium (for the scale much greater than lattice constant). This equation describes the evolution of one-particle distribution function $f(\mathbf{m}, \mathbf{r}, t)$

\[
\frac{\partial f(\mathbf{m}, \mathbf{r}, t)}{\partial t} + \gamma \nabla_{\mathbf{m}} [\mathbf{m} \times \mathbf{H}^{\text{eff}}] f = \alpha \nabla_{\mathbf{m}} [\mathbf{m} \times (\mathbf{H}^{\text{eff}} - T \nabla_{\mathbf{m}}) f],
\]

where

\[
\mathbf{H}^{\text{eff}} = \mathbf{H}^{\text{exch}} + \mathbf{H}^{\text{dip}} + 2K \mathbf{n}_K (\mathbf{n}_K \cdot \mathbf{m}) + \mathbf{H}^{\text{ext}}.
\]

Here $\nabla_{\mathbf{m}} = \nabla_{\mathbf{m}_i} - \mathbf{m}_i (\nabla_{\mathbf{m}_i} \mathbf{m}_i) / m_i^2$, stands for the gradient in the space tangent to sphere.

Similar equation for superparamagnetics (without the exchange interaction) was derived by Brown [2]. In general case the main issue in equation (2) arises from exchange field approximation

\[
\mathbf{H}^{\text{exch}} = a^2 J \Delta_r <\mathbf{m}(\mathbf{r})> + \frac{1}{f(\mathbf{r}_i, \mathbf{m}_i)} \sum_{j} J_{ij} \int_{S_2} \mathbf{m}_j f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j) d\mathbf{m}_j,
\]

where $a$ is the length of the link between atoms and $n_b$ is the number of adjacent atoms.

Conventional way to obtain the closed system of equations is to use mean field approach, i.e. assume that $f_{ij}^{(2)} \approx f_i \cdot f_j$. That leads to the following form of exchange field term

\[
\mathbf{H}^{\text{exch}}_{\text{MFA}}(\mathbf{r}) = a^2 J \Delta_r <\mathbf{m}(\mathbf{r})> + n_b J <\mathbf{m}(\mathbf{r})>.
\]
Multiplication of the equation (2) by \( \mathbf{m} \) and than integrating it over \( d\mathbf{m} \) we obtain the continuous medium equations for magnetisation \( \langle \mathbf{m} \rangle(\mathbf{r}) \)

\[
\dot{\langle \mathbf{m} \rangle} = -\gamma \left[ (\mathbf{m}) \times \mathbf{H}^L \right] - 2\gamma K \left[ \Phi + \alpha \Theta \right] - \alpha \gamma \langle \mathbf{m} \otimes \mathbf{m} - \mathbf{I} \rangle \cdot \left( \mathbf{H}^L + n_b \varepsilon_G J(\mathbf{m}) \right) - 2\alpha \gamma T(\mathbf{m}),
\]

where \( \otimes \) means the tensor product and \( \varepsilon_G < 1 \) is the factor introduced by Garanin to take the mean field fluctuations into account [3]. This factor also helps to get correct critical temperature. Integral coefficients \( \Phi, \Theta, \langle \mathbf{m} \otimes \mathbf{m} \rangle \) depend on high-order moments of single-particle distribution function. Thus we have to approximate it in order to calculate the coefficients

\[
f(\mathbf{m}, \mathbf{r}, t) \approx e^{\mathbf{p} \cdot \mathbf{m}} / \mathcal{L}(p), \quad \mathcal{L}(p) = \int_{S^2} e^{\mathbf{p} \cdot \mathbf{m}} d\mathbf{m} = 4\pi \sin \frac{p}{p}, \tag{5}
\]

Here \( \mathbf{p} = \mathbf{p}(\mathbf{r}, t) \) is the approximation parameter, \( \mathbf{p} \parallel \mathbf{m} \), \( |\langle \mathbf{m} \rangle| = \coth p - 1/p \equiv \mathcal{L}(p) \), where \( \mathcal{L}(p) \) is the Langevin function. Coefficients \( \Phi, \Theta, \langle \mathbf{m} \otimes \mathbf{m} \rangle \) may be calculated numerically as well as approximated analytically [4].

The mean field approximation does a good job describing long distance collective interactions like the demagnetisation field. In transition to continuous medium model the mean field approximation produces the term \( a^2 J \Delta_r(\mathbf{m}) \) adequately corresponding to exchange interaction between infinitesimal volumes. However the term \( n_b J(\mathbf{m}) \) is off the mark due to correlations between adjacent atoms distributions that was neglected. Thus we have to introduce \( \varepsilon_G \) factor to obtain correct temperature of phase transition.

3. Accounting for nearest neighbours correlations

To take the nearest neighbours correlations into consideration we use another approximation of the two-particles distribution function

\[
f^{(2)}_{ij}(\mathbf{m}_i, \mathbf{m}_j, t) \approx \frac{1}{Z} \left[ f_i(\mathbf{m}_i, t) f_j(\mathbf{m}_j, t) \right]^\rho e^{\lambda m_i \cdot m_j}, \tag{6}
\]

\[
Z_{ij}^{(2)} = \int_{S^2} \left[ f_i(\mathbf{m}_i, t) f_j(\mathbf{m}_j, t) \right]^\rho e^{\lambda m_i \cdot m_j} d\mathbf{m}_i d\mathbf{m}_j,
\]

\[
\rho = \arg \min_{\frac{1}{2} \leq \rho \leq 1} \int_{S^2} \left[ f_i(\mathbf{m}_i, t) - \int_{S^2} f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j, t) d\mathbf{m}_j \right]^2 d\mathbf{m}_i. \tag{7}
\]

Where \( \lambda \geq 0 \) is the parameter describing correlations (indirect included) between adjacent magnetic moments \( \mathbf{m}_i \) and \( \mathbf{m}_j \). The exponent \( \frac{1}{2} \leq \rho \leq 1 \) is introduced to meet the constraint \( f_i = \int_{S^2} f_{ij}^{(2)} d\mathbf{m}_j \). The approximation could be applied for any two-particle function but we concern about only adjacent ones. Farther reasons for such approximation form are presented in [5].

For \( \lambda \ll 1 \) the approximation (6) converges to mean field approach while \( \rho \to 1 \). Another corner case \( \lambda \gg 1 \) implies that exponential function in the approximation (6) shrinks to Dirac delta \( \delta(\mathbf{m}_i \cdot \mathbf{m}_j) \) and \( \rho \to \frac{1}{2} \). Regardless of power \( \rho \) the dimension of the approximation stays correct due to the factor \( 1/Z^{(2)} \).
With the approximation (6) field (3) becomes
\[ H_{\text{CMD}}^{\text{exch}} = a^2 J \Delta_r \langle m \rangle + n_b J \Upsilon \frac{\nabla m f}{f}, \quad \Upsilon = \frac{1 - \rho}{\lambda}. \quad (8) \]

The exchange field inside infinitesimal volume results in antidiffusion (proportional to \( n_b J \Upsilon \)) in the magnetic moment directions space. Meanwhile the temperature fluctuations produce the diffusion term (proportional to \( T \)). The balance between these terms defines the equilibrium magnetisation value \( \langle m \rangle \). It is also responsible for the phase transition.

Despite the fact that coefficient \( \Upsilon \) directly depends on \( \lambda \) and \( \rho = \rho(\langle |m| \rangle, \lambda) \) it is convenient to describe it as a function \( \Upsilon(\langle |m| \rangle, \langle \eta \rangle) \) depending on magnetisation \( \langle m \rangle \) and the level of two-particles correlation \( \langle \eta \rangle \).

Again the multiplication of the equation (2) by \( m \) integration by \( dm \) leads to LLB-like equation
\[ \dot{\langle m \rangle} = -\gamma \left[ \langle m \rangle \times H^L \right] - 2\gamma K \left( \Phi + \alpha \Theta \right) - \alpha \gamma \langle m \otimes m - I \rangle \cdot H^L - 2\alpha \gamma (T - n_b JT) \langle m \rangle, \quad (9) \]
where \( \Phi \) and \( \Theta \) are the integral contribution of anisotropy same as for LLB (4).

In order to calculate \( \Upsilon \) we introduce another equation for two-particles correlations \( \langle \eta \rangle = \langle m_i \cdot m_j \rangle \). We integrate the second equation (for two-particles distribution \( f(t)^{(2)} \)) of BBGKY hierarchy with the factor \( m_i \cdot m_j \) to get
\[ \frac{\langle \eta \rangle}{2\alpha \gamma} = -2H^L \cdot \langle m \rangle \Upsilon + 2K \Psi + J \Omega + 2T \langle \eta \rangle, \quad \Omega = \langle \eta^2 \rangle - 1 + \sum_{k \in nb, j, k \neq i} Q_k, \quad (10) \]
\[ \Psi = \langle m_i \cdot [m_j \times [m_j \times n_K]] (m_j \cdot n_K) \rangle, \quad Q_k = \langle m_i \cdot [m_j \times [m_j \times m_k]] \rangle. \]

Here the summation is performed over all atoms \( k \) adjacent to the atom \( i \). The coefficient \( Q_k \) depends on three-particles distribution functions \( f^{(3)}_{ijk} \).

The three-particles distribution function depends on relative positions of atoms \( i, j \) and \( k \) which in turn relies on the type of the crystal lattice. In this paper we study only cubic and body-centered cubic (BCC) lattices. The similar formulations for face-centered lattice introduce some complications.

For far enough atoms \( i \) and \( k \) we can neglect correlations (fig. 1, a). Then
\[ f^{A}_{ijk} \approx f^{(2)}_{ij} \cdot f^{(2)}_{jk} / f_j, \quad (11) \]
Figure 2. Integral coefficients Υ(⟨m⟩, ⟨η⟩) and Λ(⟨m⟩, ⟨η⟩) calculated numerically

that corresponds to mean field approach generalised fir multi-particles functions. In both cubic and BCC lattices for a pair of adjacent atoms i and j there is only one such three-particles function. For all other cases we introduce the symmetric four-particles function for cubic and BCC lattices correspondingly (fig. 1, b, c).

\[ f_{ijkl}^B = \frac{1}{Z^{(4)B}} \exp \left[ \varsigma (m_i \cdot m_j + m_j \cdot m_k + m_k \cdot m_l + m_l \cdot m_i) + \varepsilon \varsigma (m_i \cdot m_k + m_j \cdot m_l) + \sigma p \cdot (m_i + m_k + m_j + m_l) \right], \] (12)

To farther simplify calculations we assume that the indirect part of correlations are the same for directly connected atoms and for diagonal positioning without direct link. Hence we assume that the only difference between those two positioning variants is the presence of the exchange interaction

\[ \varsigma - \varepsilon \varsigma \approx \frac{J}{T} \rightarrow \varepsilon \approx \frac{1}{\varsigma} \left[ \varsigma - \frac{J}{T} \right], \quad 0 \leq \varepsilon \leq 1, \quad f_{ijkl}^B = \int_{S_2} f_{ijkl}^B \, dm_l. \] (13)

For a given pair of adjacent atoms i and j in cubic lattice there are exactly four free-particles functions of that kind (fig. 1, b). The BCC lattice on the other hand has six functions for every pair. The obtained equations (9), (10) become the system of the correlational magnetodynamics equations (CMD).

Functions Υ, Ψ and Λ depend on ⟨m⟩ and ⟨η⟩, while \( Q^B \) also depends on temperature, \( Q^B = Q^B(⟨m⟩, ⟨η⟩, T) \). In this work we use the numerically calculated tables for them. However they also have analytical approximations [6], which are developed as a part of aiwlib library [7].

4. Simulation results

In this section we are comparing the results of direct atomistic calculations based on equations (1) with CMD and LLB modeling results for different parameters \( T, H^\text{ext} \) and \( K \).

We used uniform magnetisation \( m_i|_{t=0} = m_{\text{start}} \forall i \), as the initial conditions for atomistic simulation. The solution \( ⟨m⟩(t) \) could be estimated as \( ⟨m⟩(t) \approx ⟨m⟩_{eq} + C e^{-t/\tau} \), where \( ⟨m⟩_{eq} \) is the equilibrium magnetisation and \( C \) is some constant. Relaxation time \( \tau \) may be evaluated for a given \( ⟨m⟩(t) \) with aid of least squares method (as a best fit).

Atomistic model had BCC lattice with 64^3 atoms and periodic boundary conditions. The equations (1) were solved by Runge–Kutta fourth order method [8]. For LLB and CMD we considered the space-uniform case.
For all models the equilibrium magnetisation values are the same. Exchange energy value and total relaxation time in CMD approach turns out to be closer to atomistic results than LLB results (fig. 3).

5. Conclusions
A semi-phenomenological approximations for the two- and three-particle distribution functions in a magnetic device are developed. They take correlations between neighboring atoms and the lattice structure into account. With the use of the obtained approximation, the new system of equations of correlation magnetodynamics (CMD) is derived on the base of the BBGKY hierarchy. It consists of a modified Landau-Livshitz-Bloch equation and an equation for two-particle correlations (exchange energy). In contrast with the conventional Landau-Livshitz-Bloch equation, which is obtained in the mean-field approximation, the new CMD system of equations describes the energy and relaxation process correctly. That improves the quality of simulations for spintronic and magnetic nanoelectronic devices.

References
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