Micromagnetic Modeling with Account for the Correlations Between Closest Neighbors

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Introduction | Main equations | Theory | Correlations | Results | Conclusion

In the development of spintronic devices, a large amount of numerical computations is essential [1]. For a correct description of device operation, temperature fluctuations must be taken into consideration, since they play a major role in the device behavior. Some devices require a model that is correct for a wide range of temperatures, including the vicinity of the phase transition. The atomistic approach is the most adequate for the task, but its computational complexity is unacceptably high for engineering problems.

In terms of the balance between computational complexity and model adequacy, micromagnetic approach is optimal. The influence of the temperature fluctuations is described with the LLBE (Landau–Lifshitz–Bloch equation [2]). In the LLBE derivation, the mean field approximation (MFA) was used for the closure of the BBGKY hierarchy. With such approximation, correlations between magnetic moments of the closest atoms are neglected. Such neglect leads to various artifacts in modeling results, the most noticeable of which is that the relaxation time might become less by an order of magnitude.

References

[1] A. Knizhnik, I. Goryachev, G. Demin, K. Zvezdin, E. Zipunova, A. Ivanov, I. Iskandarova, V. Levchenko, A. Popkov, S. Solov’ev, and B. Potapkin, “A software package for computer-aided design of spintronic nanodevices,” Nanotechnologies in Russia 12, 208–217 (2017).

[2] D. A. Garanin, “Fokker-Planck and Landau-Lifshitz-Bloch equations for classical ferromagnets,” Phys. Rev. B 55, 3050 (1997).

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Main equations

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

$$\mathbf{H}_i^{\text{eff}} = -\nabla_{\mathbf{m}_i} W = \mathbf{H}_i^{\text{exch}} + \mathbf{H}_i^{\text{anis}} + \mathbf{H}_i^{\text{dip}} + \mathbf{H}^{\text{ext}},$$

$$\mathbf{H}_i^{\text{exch}} = \sum_j J_{ij}\mathbf{m}_j, \qquad \mathbf{H}_i^{\text{anis}} = 2K\sum_i \mathbf{n}_K(\mathbf{n}_K \cdot \mathbf{m}_i), \qquad \mathbf{H}_i^{\text{dip}} = \sum_j \frac{3(\mathbf{m}_j \cdot \mathbf{r}_{ij})\mathbf{r}_{ij} - \mathbf{m}_j r_{ij}^2}{r_{ij}^5}, \qquad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j,$$

where γ is the gyromagnetic ratio, α is the damping parameter, W is full energy, T is temperature measured in energy units,
ξ(m,t) is three-dimensional white noise, which doesn't change the absolute value of the magnetic moment and provides unit directional dispersion [3],
∇m_i is the operator ∇ for magnetic moment m_i, H_{exch} is the exchange magnetic field,
J_{ij} is the exchange integral (it is equal to zero almost everywhere except for the closest neighbors),
H_{anis} is the anisotropy magnetic field, K is the anisotropy coefficient, n_K is the orientation of the anisotropy axis,
H_{dip} is the dipole interaction (magnetostatic) field, H_{ext} is the external magnetic field. Hereafter we work in the specific unit system.
The Fokker-Planck (Brown) equation for one-particle distribution function f(m, r) for magnetization:

$$\frac{\partial f(\mathbf{m},\mathbf{r},t)}{\partial t} + \gamma\nabla_\circ[\mathbf{m} \times \mathbf{H}^{\text{eff}}]f = \alpha\gamma\nabla_\circ[\mathbf{m} \times [\mathbf{m} \times (\mathbf{H}^{\text{eff}} - T\nabla_\circ)f]], \quad \mathbf{H}_i^{\text{exch}} = \frac{1}{f(\mathbf{r}_i, \mathbf{m}_i)}\sum_j J_{ij}\int_{\text{sph}} \mathbf{m}_j f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j)\,d\mathbf{m}_j, \qquad \langle W \rangle = \ldots - \frac{1}{2}J_{ij}\iint_{\text{sph}} \mathbf{m}_i \cdot \mathbf{m}_j f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j)\,d\mathbf{m}_i\,d\mathbf{m}_j.$$

References

[3] A. V. Ivanov, "Kinetic modeling of magnetic's dynamic," Matem. Mod. 19, 89–104 (2007).

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Landau-Lifshitz-Bloch equation

The mean field approximation:

$$f_{ij}^{(2)} \approx f_i \cdot f_j \qquad \mathbf{H}_{\mathrm{MFA}}^{\mathrm{exch}} = a^2 J \Delta_{\mathbf{r}} \langle \mathbf{m} \rangle + n_b J \langle \mathbf{m} \rangle,$$

where a is the distance between the closest neighbors,
J is integral of exchange between the closest neighbors,
n_b is the number of the closest neighbors.
Equation for mean magnetization evolution $\langle m \rangle (r)$:

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

$$\mathbf{H}^{\mathrm{L}} = \mathbf{H}^{\mathrm{ext}} + a^2 J \Delta_{\mathbf{r}} \langle \mathbf{m} \rangle + \mathbf{H}^{\mathrm{demag}}, \quad \mathbf{\Phi} = \langle \mathbf{m} \times \mathbf{n}_K (\mathbf{m} \cdot \mathbf{n}_K) \rangle, \quad \mathbf{\Theta} = \langle \mathbf{m} \times [\mathbf{m} \times \mathbf{n}_K] (\mathbf{m} \cdot \mathbf{n}_K) \rangle,$$

where H_L depends on $\langle m \rangle$ linearly, $\varepsilon_G < 1$ is the Garanin coefficient. One needs ε_G to obtain the right critical temperature [4].

References

[4] D. A. Garanin, "Self-consistent Gaussian approximation for classical spin systems: Thermodynamics," Phys. Rev. B 53, 11593 (1996).

Correlation magneto-dynamics equation

Let's approximate two-particle function as in [5]:

$$f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j, t) \approx \frac{1}{Z^{(2)}} \left[f_i(\mathbf{m}_i, t) f_j(\mathbf{m}_j, t) \right]^{\rho} e^{\lambda \mathbf{m}_i \cdot \mathbf{m}_j},$$

$$Z^{(2)} = \iint_{\mathrm{sph}} \left[f_i(\mathbf{m}_i, t) f_j(\mathbf{m}_j, t) \right]^{\rho} e^{\lambda \mathbf{m}_i \cdot \mathbf{m}_j} \, d\mathbf{m}_i \, d\mathbf{m}_j,$$

$$\rho = \arg\min \int_{\mathrm{sph}} \left[f_i(\mathbf{m}_i, t) - \int_{\mathrm{sph}} f_{ij}^{(2)}(\mathbf{m}_i, \mathbf{m}_j, t) \, d\mathbf{m}_j \right]^2 d\mathbf{m}_i,$$

Exchange field may be computed as:

$$\mathbf{H}_{\mathrm{CMD}}^{\mathrm{exch}} = a^2 J \Delta_{\mathbf{r}} \langle \mathbf{m} \rangle + n_b J \Upsilon \frac{\nabla_{\mathbf{m}} f}{f}, \qquad \Upsilon = \frac{1-\rho}{\lambda}.$$

Multiplying Fokker-Planck equation by m and integrating over dm we obtain

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

References

[5] A. V. Ivanov, "Calculation of the statistical sum and approximation of multiparticle distribution functions for magnetics in the heisenberg model," Keldysh Institute preprints 104, 12 (2019).

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Correlation magneto-dynamics equation

One more equation for couple correlations (exchange energy per link) is needed to calculate: $\langle\eta\rangle = \iint\limits_{\text{sph}} \mathbf{m}_i\cdot\mathbf{m}_j\, d\mathbf{m}_i\, d\mathbf{m}_j.$

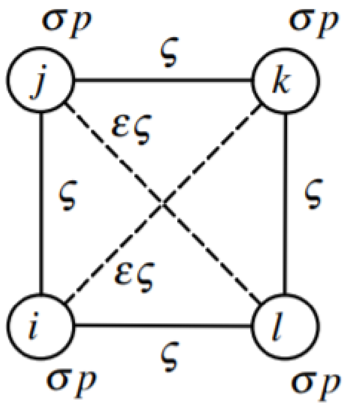
The second link in BBGKY hierarchy describes the evolution of $f_{ij}^{(2)}$. Thus, multiplying it by $(m_i \cdot m_j)$ and integrating over $dm_i\; dm_j$ for BCC lattice we obtain:

$$-\frac{\langle\dot{\eta}\rangle}{2\alpha\gamma} = -2\mathbf{H}^{\mathrm{L}}\cdot\langle\mathbf{m}\rangle\Upsilon + 2K\Psi + J\left[\Lambda + 6Q\right] + 2T\langle\eta\rangle,$$

$$\Psi = \left\langle \mathbf{m}_i\cdot\left[\mathbf{m}_j\times\left[\mathbf{m}_j\times\mathbf{n}_K\right]\right]\left(\mathbf{m}_j\cdot\mathbf{n}_K\right)\right\rangle,\quad Q = \left\langle \mathbf{m}_i\cdot\left[\mathbf{m}_j\times\left[\mathbf{m}_j\times\mathbf{m}_k\right]\right]\right\rangle,\quad \Lambda = \frac{1-2\rho}{\rho}\left(1-\langle\eta^2\rangle\right) - 2\frac{1-\rho}{\rho\lambda}\langle\eta\rangle.$$

To calculate Q the three-particle distribution function $f_{ijk}^{(3)}$ is required. The following steps depend on the structure of crystal lattice. For BCC lattice we consider symmetrical four-particle distribution function $f_{ijkl}^{(4)}$. Diagonal links ες in such function are defined only by indirect correlations.

$$f_{ijkl}^{(4)} = \frac{1}{Z^{(4)}}\exp\Big[\varsigma\left(\mathbf{m}_i\cdot\mathbf{m}_j + \mathbf{m}_j\cdot\mathbf{m}_k + \mathbf{m}_k\cdot\mathbf{m}_l + \mathbf{m}_l\cdot\mathbf{m}_i\right) + \varepsilon\varsigma\left(\mathbf{m}_i\cdot\mathbf{m}_k + \mathbf{m}_j\cdot\mathbf{m}_l\right) + \sigma\mathbf{p}\cdot\left(\mathbf{m}_i + \mathbf{m}_k + \mathbf{m}_j + \mathbf{m}_l\right)\Big]$$



Consequently, $Q(\langle m\rangle, \langle\eta\rangle, T)$ is computed numerically and is defined as a tabulated function.
The expressions for $\Upsilon(\langle m\rangle, \langle\eta\rangle)$, $\Psi(\langle m\rangle, \langle\eta\rangle)$, $\Lambda(\langle m\rangle, \langle\eta\rangle)$ can be approximated analytically [6].

$$f_{ijk}^{(3)} = \int\limits_{\text{sph}} f_{ijkl}^{(4)}\, d\mathbf{m}_l,\qquad \varsigma - \varepsilon\varsigma \approx \frac{J}{T} \;\rightarrow\; \varepsilon \approx \frac{1}{\varsigma}\left[\varsigma - \frac{J}{T}\right],\quad 0\le\varepsilon\le 1.$$

References

[6] A. V. Ivanov, “The account for correlations between nearest neighbors in micromagnetic modeling,” Keldysh Institute preprints 118, 30 (2019).

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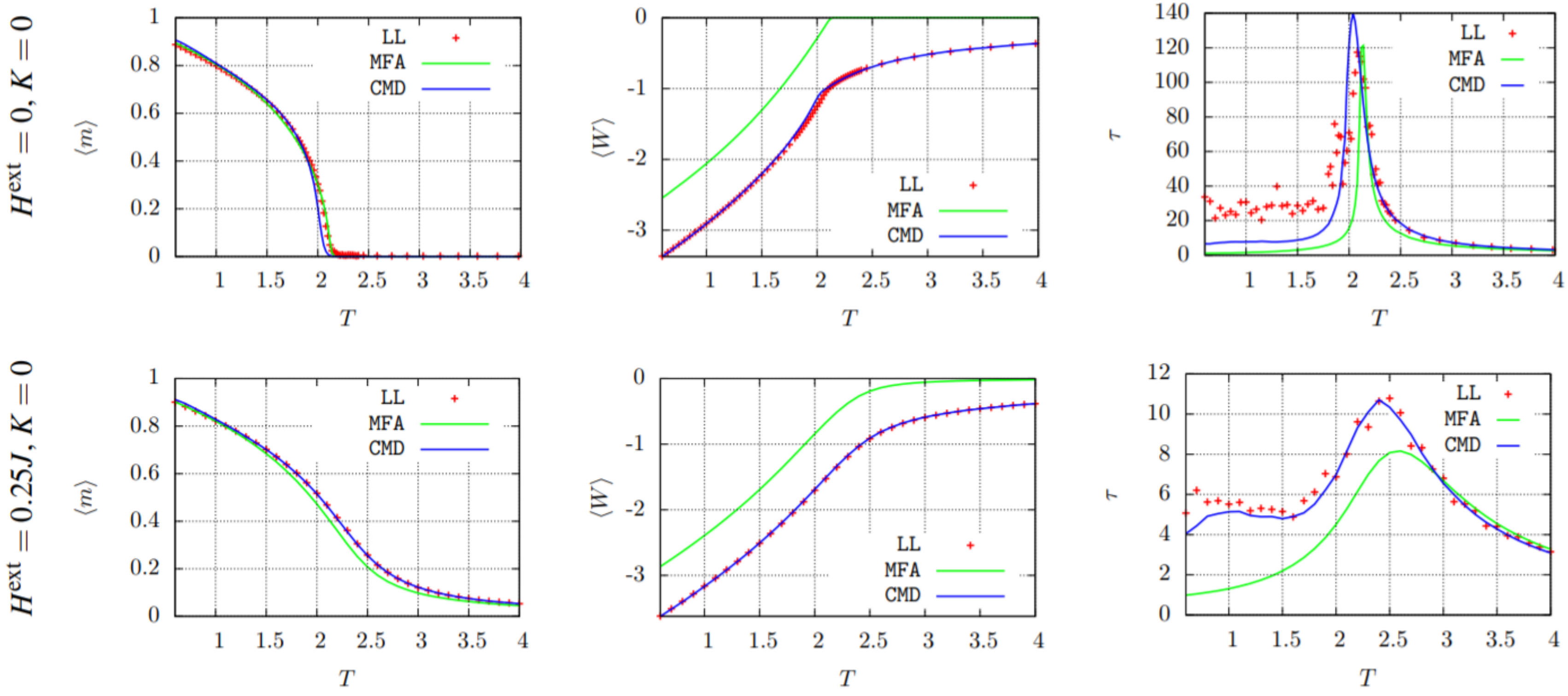
Modeling results



Results of modeling with atomistic (LL), LLBE (MFA) and CMD approaches for differents H ext and K: dependence of the mean magnetisation hmi, mean full energy $\langle W \rangle$ and relaxation time τ on the temperature T.

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In this work, the micromagnetic equation of the LLBE type is obtained with the use of the two-particle distribution function which takes into account correlations between nearest neighbors. Furthermore, the equation for pair correlations (exchange energy) is derived. Thus, a system of CMD equations is derived. This was made for a BCC lattice, wich has two sublattices. An analogous system of equations can be obtained for multi-sublattice cases. The equation for pair interactions would include different coefficients. Unlike the traditional Landau–Lifshitz–Bloch equation, which is obtained in mean field approximation, the CMD equations describe the energy and relaxation process in magnetic materials correctly. It allows achieving better accuracy in the modeling of spintronic devices and magnetic nanoelectronics.

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