Supplemental Material to the article

“Equations of correlational magnetodynamics for ferromagnetic materials”

A. Lets consider calculations in finer details.

According to Gauss's theorem for smooth enough functions $g(\mathbf{m})$, $\mathbf{g}(\mathbf{m})$ $\mathbf{g}(\mathbf{m})$

$$\int\limits_{S_2} \nabla_\circ g \, d\mathbf{m} = 0, \qquad \int\limits_{S_2} \nabla_\circ \mathbf{g} \, d\mathbf{m} = 0,$$

$$\int\limits_{S_2} \mathbf{m} \nabla_\circ g \, d\mathbf{m} = -\int\limits_{S_2} \mathbf{g} \, d\mathbf{m} + \int\limits_{S_2} \mathbf{m}(\mathbf{m}\cdot\mathbf{g}) \, d\mathbf{m},$$

$$\int\limits_{S_2} \mathbf{m} \nabla_\circ \big[\mathbf{m}\times\mathbf{g}\big] \, d\mathbf{m} = -\int\limits_{S_2} \big[\mathbf{m}\times\mathbf{g}\big] \, d\mathbf{m},$$

which allows us to turn FPE into equations for $\langle\mathbf{m}\rangle$ and $\langle\eta\rangle$.

Any approximation for $f_{ij}^{(2)}$ should meet the constrains

$$\int\limits_{S_2} f_{ij}^{(2)} \, d\mathbf{m}_i = f_j, \qquad \int\limits_{S_2} f_{ij}^{(2)} \, d\mathbf{m}_j = f_i,$$

from which by taking approximation (12) into account we get

$$\frac{1}{Z^{(2)}} \int\limits_{S_2} f_j^\rho \, e^{\lambda \mathbf{m}_i \mathbf{m}_j} \, d\mathbf{m}_j \approx f_i^{1-\rho}.$$

Hence we can calculate the exchange field term (4) inside an infinitesimal volume

$$n_b J \int\limits_{S_2} \mathbf{m}_j f_{ij}^{(2)} \, d\mathbf{m}_j \approx \frac{n_b J}{Z^{(2)}} \int\limits_{S_2} \mathbf{m}_j f_i^\rho f_j^\rho e^{\lambda \mathbf{m}_i \mathbf{m}_j} \, d\mathbf{m}_j = \frac{n_b J}{Z^{(2)}} \frac{f_i^\rho}{\lambda} \nabla_{\mathbf{m}i} \int\limits_{S_2} f_j^\rho e^{\lambda \mathbf{m}_i \mathbf{m}_j} \, d\mathbf{m}_j \approx$$

$$\approx n_b J \frac{f_i^\rho}{\lambda} \nabla_{\mathbf{m}i} f_i^{1-\rho} = n_b J \frac{1-\rho}{\lambda} \nabla_{\mathbf{m}i} f_i.$$

Since this term is a part of the cross product with $\mathbf{m}_i$, then $\nabla_{\mathbf{m}i}$ may be substituted with $\nabla_{\circ i}$ without changing the result. In this notation the term clearly represents antidiffusion in the $\mathbf{m}_i$ space.

Similarly, in deriving Eq. (15)

$$\iint\limits_{S_2 S_2} (\mathbf{m}_i\cdot\mathbf{m}_j) \nabla_{\circ j} \Big[\mathbf{m}_j \times \big[\mathbf{m}_j \times \mathbf{H}^{\mathrm{L}}\big] f_{ij}^{(2)}\Big] \, d\mathbf{m}_i d\mathbf{m}_j = -\iint\limits_{S_2 S_2} \mathbf{m}_i \cdot \Big[\mathbf{m}_j \times \big[\mathbf{m}_j \times \mathbf{H}^{\mathrm{L}}\big] f_{ij}^{(2)}\Big] \, d\mathbf{m}_i d\mathbf{m}_j \approx$$

$$\approx -\Upsilon \int\limits_{S_2} \Big[\mathbf{m}_j \times \big[\mathbf{m}_j \times \mathbf{H}^{\mathrm{L}}\big]\Big] \nabla_{\mathbf{m}j} f_j \, d\mathbf{m}_j = 2\Upsilon \mathbf{H}^{\mathrm{L}} \cdot \langle\mathbf{m}\rangle_j \, .$$

Using the same considerations

$$\int\limits_{S_2} \mathbf{m}_k \frac{f_{ij}^{(2)} f_{jk}^{(2)}}{f_j} \, d\mathbf{m}_k \approx \frac{1-\rho}{\rho} \left[\frac{\nabla_{\mathbf{m}j} f_{ij}^{(2)}}{\lambda} - \mathbf{m}_i f_{ij}^{(2)} \right],$$

the coefficient $Q_\angle$ may be estimated as

$$Q_\angle = \iiint\limits_{S_2 S_2 S_2} \mathbf{m}_i \cdot \Big[\mathbf{m}_j \times \big[\mathbf{m}_j \times \mathbf{m}_k\big]\Big] \frac{f_{ij}^{(2)} f_{jk}^{(2)}}{f_j} \, d\mathbf{m}_{i,j,k} \approx$$

$$\approx \frac{1-\rho}{\rho} \left[-\frac{2}{\lambda} \langle\eta\rangle - \Big\langle \mathbf{m}_i \cdot \Big[\mathbf{m}_j \times \big[\mathbf{m}_j \times \mathbf{m}_i\big]\Big] \Big\rangle \right] = \frac{1-\rho}{\rho} \left[1 - \frac{2}{\lambda} \langle\eta\rangle - \big\langle \eta^2 \big\rangle \right].$$

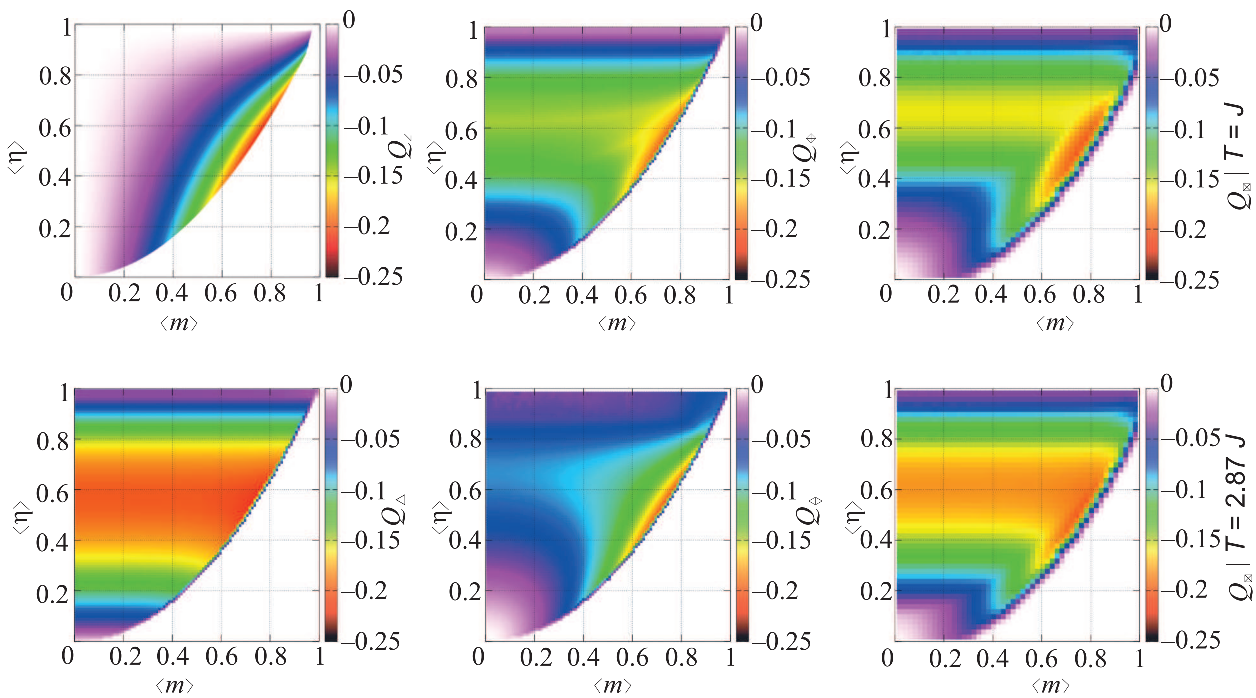

Fig. S1. The dependence of integral coefficients $Q_\angle$, $Q_\triangle$, $Q_{\oplus}$, $Q_{\diamond}$ on $(\langle m\rangle, \langle\eta\rangle)$ and dependence $Q_\boxtimes(\langle m\rangle, \langle\eta\rangle, T)$

B. Integral coefficients Q are shown on the Fig. S1. With help of the tabulated form some coefficients were fitted with analytical approximations which have accuracy $\sim 10^{-3}$:

$$\Xi_{ij} = \left\langle m_{\parallel p}^2 \right\rangle \frac{3n_{pi}n_{pj} - \delta_{ij}}{2} - \frac{\delta_{ij} + n_{pi}n_{pj}}{2}, \qquad \mathbf{n}_p = \frac{\mathbf{p}}{p},$$

where δ_{ij} is the Kronecker delta,

$$\left\langle m_{\parallel p}^2 \right\rangle \approx \frac{1}{3} + 0.4115 \cdot \langle m\rangle^2 + 0.0303 \cdot \langle m\rangle^4 + 0.3523 \cdot \langle m\rangle^6 - 0.1261 \cdot \langle m\rangle^8;$$

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

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

$$\left\langle m_{\parallel p}^3 \right\rangle \approx 0.6026 \cdot \langle m\rangle \left[1 + 0.00669 \cdot \cosh\left(5.288 \langle m\rangle\right)\right];$$

$$\Upsilon \approx \frac{1 - \langle\eta\rangle}{1 - \langle m\rangle^2} \cdot \frac{\langle m\rangle}{p} \cdot \left[1 + 0.3684 \cdot \langle\eta\rangle^2 + 0.1873 \cdot \langle\eta\rangle^3 - 0.3236 \cdot \langle\eta\rangle \langle m\rangle^2 - 0.2523 \cdot \langle\eta\rangle^2 \langle m\rangle^2\right],$$

$$\Lambda \approx \frac{1 - \langle\eta\rangle}{1 - \langle m\rangle^2} \Big[-0.6639 - 0.7617 \cdot \langle\eta\rangle + 0.2718 \cdot \langle\eta\rangle^2 - 1.367 \cdot \langle\eta\rangle^3 + 0.5078 \cdot \langle\eta\rangle^4 +$$
$$+ 0.2689 \cdot \langle\eta\rangle \langle m\rangle + 0.3472 \cdot \langle\eta\rangle \langle m\rangle^2 - 0.418 \cdot \langle\eta\rangle^2 \langle m\rangle + 1.833 \cdot \langle\eta\rangle^2 \langle m\rangle^2 \Big],$$

$$\Psi \approx \left[0.46134 \cdot \langle m\rangle^2 - 1.3836 \cdot \left(\mathbf{n}_K \cdot \langle\mathbf{m}\rangle\right)^2\right]\left(1 - \langle\eta\rangle\right)\langle m\rangle,$$

$$Q_\triangle \approx -\langle\eta\rangle \left(1 - \langle\eta\rangle\right)\left[0.69279 - 0.24455 \cdot \langle\eta\rangle + 1.1055 \cdot \langle\eta\rangle^2 - 0.53462 \cdot \langle\eta\rangle^3\right].$$

C. The generic view of the dependency $\langle m \rangle (t)$ is shown on the Fig. S2. It is hard to find the analytical approximation for such dependency, hence in all cases the relaxation time was estimated with the equation

$$\tau \approx \left(1 - \langle m \rangle_{\text{eq}}^{\text{LL}}\right) \Big/ \left.\frac{d \langle m \rangle}{dt}\right|_{t=1},$$

where $\langle m \rangle_{\text{eq}}^{\text{LL}}$ is the equilibrial magnetization value, which was calculated in the Landau–Lifshitz equations modelling.

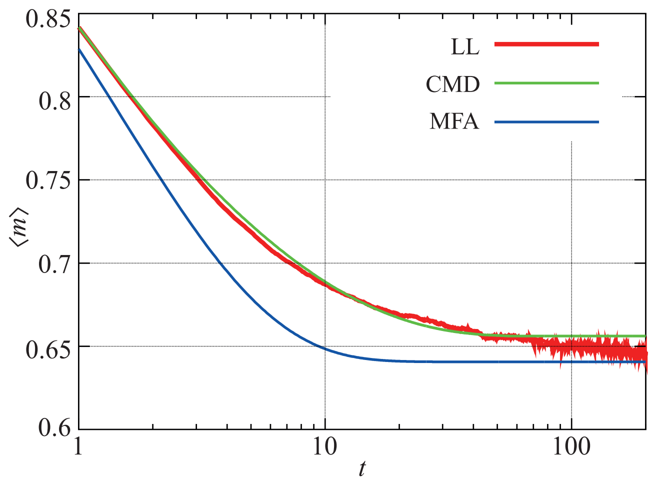

Fig. S2. Generic dependencies $\langle m \rangle (t)$ for the bcc lattice in different approaches. The system parameters are $T = 1.5J$, $H^{\text{ext}} = 0$, $K = 0$

Modelling results for systems with various lattices in the external field $H^{\text{ext}} = J$ are shown on the Fig. S3.

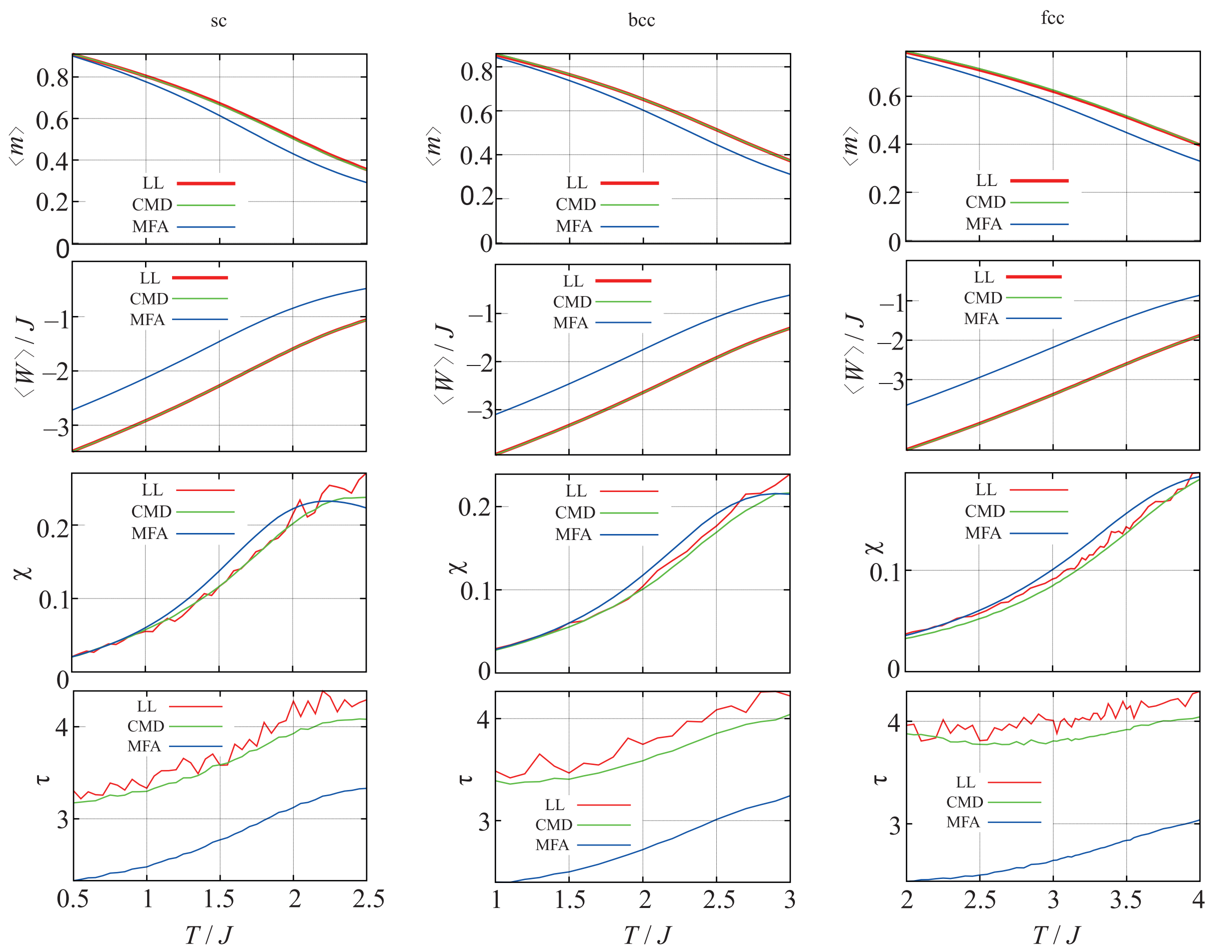

Fig. S3. The dependencies of equilibrial magnetization $\langle m \rangle$, exchange energy $\langle W \rangle$, susceptibility χ and relaxation time τ on the system temperature T, obtained in Landau–Lifshitz approach (LL), correlational magnetodynamics approximation (CMD) and mean field approximation (MFA) for systems with various lattices in the external field $H^{\text{ext}} = J$, without anisotropy $K = 0$