Length Scale Coupling for Nonlinear Dynamical Problems in Magnetism

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The dynamics of real magnets is often governed by several interacting processes taking place simultaneously at different length scales. For dynamical simulations, the relevant length scales should be coupled, and the energy transfer accurately described. We show that in this case the micromagnetic theory is not always reliable. We present a coarse-graining approach applicable to nonlinear problems, which provides a unified description of all relevant length scales, allowing a smooth, seamless coupling. The simulations performed on model systems show that the coarse-graining approach achieves nearly the precision of all-atom simulations.

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The dynamics of magnetization in real magnets is often governed by defects: impurities, vacancies, grain boundaries, etc., Because of very localized (several lattice constants) but significant changes in the magnetic interactions, the torques acting on individual atomic magnetic moments near the defect are strongly nonuniform. Atomic-scale inhomogeneities can result in large-scale (hundreds or thousands of angstroms) changes of the magnetization distribution (e.g., nucleation of a domain). At larger length scales (microns), magnons propagate into the bulk of the sample carrying away significant energy. Such multiscale phenomena are encountered in the depinning of domain walls [1–3], the influence of surfaces and interfaces on the spins in the bulk [4–6], etc., and determine basic magnetic properties such as the coercive field and the dynamics of magnetization reversal.

Accurate simulations of such phenomena might be possible if the whole system could be treated at the atomic scale [7], representing every atomic spin as a classical vector (for the phenomena discussed here, quantum spin effects can be neglected). But for a micron-size sample, the number of spins is much too large for modern supercomputers. Atomistic modeling can be used near the defects, while far from the defects one should use a micromagnetic (MM) theory [8]. Micromagnetics is a continuum approximation which treats a discrete lattice of spins as a continuous medium. It is valid for large-scale processes occurring in the bulk, but becomes inapplicable at small scales. When MM is used for numerical modeling, e.g., in the finite-element formulation [9], the continuum equations of micromagnetics are discretized again. But the size of the MM computational cell should be much larger than the lattice constant, and cannot be gradually reduced down to atomic scale, which is needed for matching atomistic simulations used near the defect. We show that neglect of this issue, and straightforward use of micromagnetics for description of small scales in dynamic multiscale problems, can give incorrect results, which differ drastically from the exact solutions obtained by all-atom simulations. Thus, MM theory *per se* cannot be used for a seamless coupling of length scales.

Here, we present an approach which treats all length scales in the same manner, enabling a seamless transition from the MM scale down to the atomistic scale. The approach is based on statistical coarse graining. A key point is the direct account of the global rotational symmetry of exchange interactions; this allows treatment of essentially nonlinear dynamical problems. The proposed approach yields reliable results which are in excellent agreement with exact atomic simulations.

The problem of length scale coupling has been discussed in the context of lattice dynamics modeling [10–12]. Analogous schemes can be constructed for *linear* magnetic problems [13], but most of the interesting problems in magnetism are essentially *nonlinear* due to the constraint $S_x^2 + S_y^2 + S_z^2 = S^2$ ($S_{x,y,z}$ are the components of the spin and S is its length; everywhere below we assume $S = 1$), and the linear scheme [11,13] gives qualitatively incorrect results. In contrast, the approach proposed here is explicitly developed for nonlinear problems.

Our approach is based on statistical coarse graining (CG), which has been used for a long time to define collective variables (''gross variables'') for description of a large number of microscopic entities. For simplicity, here we consider only the case of low temperature (much less than the other relevant energy scales), thus dealing with purely dynamical problems, where dissipation and thermal noise are negligible. We assume that the system under consideration is a ferromagnet made of identical classical spins $\mathbf{S}_\mu$ ($|\mathbf{S}_\mu| = 1$), located at the μth site of the crystalline lattice (greek indices enumerate the atomic lattice sites). The system is described by a rather general spin Hamiltonian function

$$\mathcal{H} = \mathcal{H}^0 + \mathcal{V}, \qquad \mathcal{H}^0 = \sum_{\mu,\nu} J_{\mu\nu}\mathbf{S}_\mu\mathbf{S}_\nu, \qquad (1)$$

where $\mathcal{H}^0$ describes the isotropic exchange interaction, and $J_{\mu\nu}$ is the exchange interaction between the atomic

spins at the sites μ and ν. The term $\mathcal{V} \ll \mathcal{H}^0$ represents all the other interactions (anisotropy, magnetostatics, etc.). We separate the exchange term because, at the atomic scale, the exchange interactions are much stronger than all others, even for moderately anisotropic ferromagnets such as CoPt or FePt. In the bulk, the isotropic exchange term $\mathcal{H}_0$ (in contrast with the term $\mathcal{V}$) keeps the atomic spins locally aligned, independent of their direction. Departure from alignment is noticeable only for spins separated by many lattice constants, so that the direction of many neighboring spins can be described by only a few collective variables. This is also a starting point of MM theory; both MM and CG approaches treat the small anisotropic term $\mathcal{V}$ perturbatively.

In the MM approach, the local magnetization is a gross variable, defined as a local average of individual atomic spins [8]. Similarly, in the CG method, we define the gross variables as local averages over the computational cell, with some technical differences. We use a Hamiltonian formulation of the magnetization dynamics, describing a spin by the variables $\alpha_{1\mu} = 2\sin(\theta_\mu/2)\cos\phi_\mu$ and $\alpha_{2\mu} = 2\sin(\theta_\mu/2)\sin\phi_\mu$, where θ_μ and ϕ_μ are the azimuthal and the polar angles of the spin vector, respectively. One can check that $\alpha_{1\mu}$ and $\alpha_{2\mu}$ are canonically conjugate variables, $\dot{\alpha}_{1\mu} = \partial\mathcal{H}/\partial\alpha_{2\mu}$, and $\dot{\alpha}_{2\mu} = -\partial\mathcal{H}/\partial\alpha_{1\mu}$; these are classical analogs of the Holstein-Primakoff canonical variables [14]. We assume that, for the simulations of the large-scale regions located far from defects, the finite-element method (FEM) is used. We define the local gross variables, which describe a given region of the system (at a length scale determined by the size of the computational cell), by averaging the atomic degrees of freedom: $\alpha_{1j} = \sum_\mu f_{\mu,j}\,\alpha_{1\mu}$, and $\alpha_{2j} = \sum_\mu f_{\mu,j}\,\alpha_{2\mu}$, where the index j corresponds to the FEM nodes. The weight function $f_{\mu,j}$ localized near the node j must satisfy the normalization condition $\sum_\mu f_{\mu,j} = 1$. The choice of this function was discussed in detail in Ref. [13]; we found that the piecewise-linear choice is sufficient: $f_{\mu,j} = f_0|\mu - \mu_{j-1}|/|\mu_j - \mu_{j-1}|$ for $\mu \in [\mu_{j-1}, \mu_j]$ (and symmetrically for $\mu \in [\mu_j, \mu_{j+1}]$), where μ_j is the atomic position of the jth computational node and f_0 is the normalization. This function is maximum at the jth node, decreases linearly to zero at the neighboring nodes, and is zero everywhere else.

The collective variables are similar in the CG and MM methods, but the equations of motion differ in handling the exchange interactions. The MM theory assumes that the direction of the atomic spins changes linearly between two computational nodes, and, in terms of magnetization $\mathbf{M}(\mathbf{r})$, the exchange energy density is proportional to $(\nabla\mathbf{M})^2$ for the simple cubic lattice (the result is similar for other lattices [8]). This is valid in the continuum limit (for computational cells containing a large number of atoms), but is incorrect for the cells containing only few atomic spins. The CG approach uses the framework of nonequilibrium statistical theory [15] to account for the local dynamics of the short-length scale excitations in the magnet, which MM theory treats inaccurately. Nonequilibrium statistical theory allows rigorous treatment of excitations, independently of whether they are generated dynamically (in an isolated system, as we consider here), or thermodynamically (by interactions with a heat bath) as long as they are small (so the approach is limited to temperatures much smaller than the Curie temperature). Here, we omit the finite-temperature effects for simplicity.

The main assumption of nonequilibrium statistical theory [15] is that the atomic degrees of freedom are in *local* equilibrium, i.e., the atomic spins satisfy the equilibrium Gibbs distribution, with the condition that the collective variables have their values α_{1j} and α_{2j}. The distribution function for the atomic variables is

$$\rho = Q^{-1}\exp(-\beta\mathcal{H}'), \qquad \mathcal{H}' = \mathcal{H}^0 + \sum_{\mu,j} F_j f_{\mu,j}\alpha_{1\mu} + \sum_{\mu,j} G_j f_{\mu,j}\alpha_{2\mu}, \tag{2}$$

where Q is the statistical integral. The torques F_j and G_j enforce the condition of local equilibrium, i.e., they are chosen to satisfy the conditions $\sum_\mu f_{\mu,j}\langle\alpha_{1\mu}\rangle = \partial\mathcal{F}/\partial F_j = \alpha_{1j}$, and $\sum_\mu f_{\mu,j}\langle\alpha_{2\mu}\rangle = \partial\mathcal{F}/\partial G_j = \alpha_{2j}$, where the angular brackets mean the statistical averaging with the distribution function (2), and $\mathcal{F} = (-1/\beta)\ln Q$ is the analog of the Gibbs free energy for exchange interactions. Thus, F_j and G_j are the exchange torques acting on the collective variables of the jth node; the torques originating from other (weaker) interactions in $\mathcal{V}$ will be added perturbatively to the equations of motion [15].

Because of strong exchange interactions, the atomic spins near the node j are nearly parallel to the direction defined by α_{1j} and α_{2j}, and $\mathcal{H}^0$ in Eq. (2) can be locally linearized: $\mathcal{H}^0 = (1/2)\sum_{\mu,\nu} J_{\mu\nu}(\alpha_{1\mu}\alpha_{1\nu} + \alpha_{2\mu}\alpha_{2\nu})$. Then, Q in Eq. (2) is an easily solvable Gaussian integral. But $\mathcal{H}^0$ is rotationally invariant; its value does not change if all atomic spins rotate by the same angle. The matrix $J_{\mu\nu}$ has an eigenmode describing this rotation, and the corresponding eigenvalue of J is zero (a Goldstone or zero-frequency mode). The zero-frequency mode leads to a divergence in the integral Q. Similarly "dangerous" are the slow modes which describe the spin rotations spanning large length scales: Their frequencies are small (secular terms).

These collective spin rotations are described by gross variables, and are of most interest. Their characteristic length scale, the DW width Δ, is much larger than the lattice constant a. The exchange torques affecting the gross variables are small; i.e., gross variables are much slower than the atomic-scale motions [15]. Using the modified adiabatic theory [16], we separate the slow nonlinear motion of gross variables from the fast linear motion of the atomic-scale variables. Thus, we exclude

the secular terms from Q, and also describe the nonlinear motion of the gross variables. At every node j, we define a local coordinate frame, rotated with respect to the "laboratory" frame by the angles θ_j and ϕ_j such that $\alpha_{1j} = 2\sin(\theta_j/2)\cos\phi_j$, and $\alpha_{2j} = 2\sin(\theta_j/2)\sin\phi_j$. To exclude the secular terms, we require that the local amplitude of the zero-frequency mode is zero at the jth node: $\sum_\mu f_{\mu,j}\langle\alpha_{1\mu}^{(j)}\rangle = \sum_\mu f_{\mu,j}\langle\alpha_{2\mu}^{(j)}\rangle = 0$, where $\alpha_{1\mu}^{(j)}$, $\alpha_{2\mu}^{(j)}$ are calculated in the local coordinate frame associated with the jth node. These conditions are local, since $f_{\mu,j}$ is local, and the statistical integral Q is calculated in the local coordinate frame. By averaging the canonical equations of motion for $\alpha_{1\mu}^{(j)}$, $\alpha_{2\mu}^{(j)}$, and using the definition of the gross variables ($\alpha_{pn}^{(j)} = \sum_\mu f_{\mu,n}\alpha_{p\mu}^{(j)}$, $p = 1, 2$), the equations of motion for the variables θ_j and ϕ_j can be obtained in closed form:

$$\begin{aligned}\dot\theta_j &= -\sum_\mu f_{\mu,j}\langle\partial\mathcal{V}/\partial\alpha_{2,\mu}\rangle + \sum_{kn} M_{jk}D_{kn}\alpha_{2n}^{(j)},\\ \sin\theta_j\,\dot\phi_j &= \sum_\mu f_{\mu,j}\langle\partial\mathcal{V}/\partial\alpha_{1,\mu}\rangle - \sum_{kn} M_{jk}D_{kn}\alpha_{1n}^{(j)},\end{aligned} \tag{3}$$

where $M_{jk} = \sum_\mu f_{\mu,j}f_{\mu,k}$, and $D_{jk} = D_{jk}^0 - d_jS_k/S_0 - d_kS_j/S_0 + d_0S_jS_k/S_0^2$, where $D_{jk}^0 = (\sum_{\mu\nu} f_{\mu,j}J_{\mu\nu}^{-1}f_{\nu,k})^{-1}$, S_k is the eigenvector of D_{jk}^0 corresponding to the zero eigenvalue, and $d_j = \sum_l D_{jl}^0$, $d_0 = \sum_l d_l$, $S_0 = \sum_l S_l$. To invert $J_{\mu\nu}$, which has a zero-frequency eigenmode η_μ^0, we invert the nonsingular matrix $\mathcal{K}_{\mu\nu} = J_{\mu\nu} + \epsilon\eta_\mu^0\eta_\nu^0$, and define $J_{\mu\nu}^{-1} = \mathcal{K}_{\mu\nu}^{-1} - (1/\epsilon)\eta_\mu^0\eta_\nu^0$, where ϵ is arbitrary. D_{jk}^0 is treated similarly. Because of rotational invariance of the exchange interactions, the matrix D (as well as J) does not depend on local rotations, and needs to be calculated only once, and used during all simulation time steps.

A few remarks are in order. (i) The term $\mathcal{V}$ is included perturbatively in the equations of motion (3), as is also done in MM; this is valid since $\mathcal{V} \ll \mathcal{H}^0$ (see above). These terms depend on gross variables only, and they are the same as in the MM theory (e.g., the uniaxial anisotropy term is $K\sin^2\theta_j$). (ii) The finite-temperature effects are omitted here (no heat bath), so the energy of the small-scale modes does not fluctuate. Thus, Eqs. (3) describe an isolated system (including the small-scale modes), and its energy is constant, up to small errors stemming from space-time discretization in the simulations. (iii) Above, we made no reference to the dimensionality of the system. The CG approach is applicable to 1D, 2D, or 3D systems, as long as local-equilibrium theory is valid. (iv) The nondiagonal elements of the interaction matrix D_{jk} decrease exponentially fast with the distance from the diagonal, and the product $(MD)_{jn}$ is practically banded [for the example below, $|(MD)_{jn}| < 10^{-7}$ for $|j-n| > 14$]. Since most of the computational work usually arises from the long-range magnetostatic interactions (included in $\mathcal{V}$), the increased (in comparison with MM simulations) effort in treating the exchange torques is not significant, but is essential for obtaining correct dynamics. Below, we omit the magnetostatic interactions only for simplicity; in detailed simulations they should be included.

We present one typical numeric test case out of many other simulations we have performed. We consider a 1D chain of $N = 465$ spins with ferromagnetic nearest-neighbor coupling $J = 25$, and antiferromagnetic next-nearest-neighbor coupling $J' = -\gamma J = -2.5$. 1D models can describe, e.g., thin magnetic nanowires with radius $R \ll \sqrt{J/K}$, when the nonuniformity of magnetization in the lateral dimensions is negligible. The spins possess single-ion anisotropy of easy-axis type, $K = 0.01$ (the easy-axis coincides with the z axis); the dipole-dipole interactions are neglected for simplicity. The ends of the chain are different from the bulk; this represents, e.g., a nanowire which has defects at the ends causing the parameters J, J', and K to be different from their bulk values. Thus, six spins at one end of the chain are chosen to have the following parameters: $J_{01} = 0.5J$, $J_{12} = 0.6J$, $J_{23} = 0.7J$, $J_{34} = 0.8J$, $J_{45} = J_{56} = J$, $K_0 = -0.4K$, $K_1 = -0.2K$, $K_2 = 0$, $K_3 = 0.2K$, $K_4 = 0.4K$, and $K_5 = 0.8K$. At the other end of the chain, the last six spins have the same parameters in reverse order. Initially, the chain is magnetized to saturation, so that $S_\mu^z = 1$ for all μ. At $t = 0$, the external field $H = 0.02$ is applied at the angle $\phi = -0.4\pi$ to the z axis in the y-z plane, and the spins start rotating. Since we omit dissipation and fluctuations (considering temperature $T \ll K \ll J$), the total energy of the system is conserved. Without the defects, all the spins would rotate in unison, and the magnetization dynamics would be periodic and trivial. However, in the presence of the perturbation caused by the defects, different spins rotate with slightly different rates, and the system's motion becomes chaotic. After some time, the Zeeman energy is transferred to the exchange energy, leading to a gradual decrease of the system's total magnetization [17].

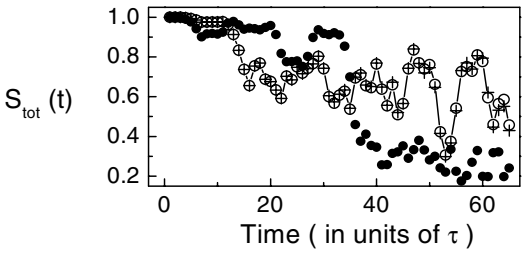

FIG. 1. Time dependence of the total magnetization $S_{\rm tot}(t)$ of the chain calculated by three methods: large white circles, atomic simulations; small black circles, MM simulations; crosses, CG scheme. Initial conditions correspond to the chain uniformly magnetized along the y axis. Since the CG results almost coincide with the atomistic ones, the crosses appear mostly in the centers of the white circles.

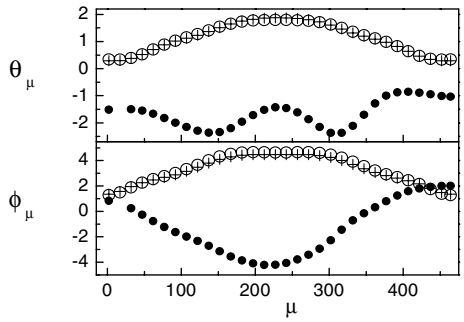

FIG. 2. The magnetization profile in the chain (the angles θ_μ and ϕ_μ) at $t = 60\tau$ calculated by three methods: large white circles, atomic simulations; small black circles, MM simulations; crosses, CG scheme. Initial conditions correspond to chain uniformly magnetized along the y axis. The values of θ_μ and ϕ_μ at the nodes of the MM grid are shown.

To compare the performance of the MM and CG schemes, we have modeled the system's dynamics by (i) atomic simulations which give the exact solution, (ii) by standard FEM micromagnetic simulations [9], with the number of spins in the cell varying from five (in the middle of the chain) to one (at the ends), and (iii) by the CG scheme described above, with the same grid as used in the MM simulations. The computational parameters have been kept the same for all schemes. The temporal dependence of the chain's total magnetization $S_{\text{tot}}(t) = \sqrt{S_x^2(t) + S_y^2(t) + S_z^2(t)}$ is shown in Fig. 1, where the time is measured in units of $\tau = 0.4\pi/|H \sin\phi| \approx 66$. The MM simulations (black circles) differ considerably from the exact atomistic solution, while the CG scheme gives results practically coinciding with the atomistic simulations. The same conclusion can be drawn from Fig. 2, where the magnetization profile in the chain is shown at $t = 60\tau$. The spin direction at every atomic site $\mathbf{S}_\mu$ is characterized by the polar θ_μ and azimuthal ϕ_μ angles.

The drastic difference between the CG and MM schemes is caused by the essential nonlinearity of magnetization dynamics. In the course of the system's motion, a considerable number of atomic-scale excitations are generated near the defects. In contrast with the MM theory, the coarse-graining approach accurately describes the collective properties of these excitations, and their effect on large-scale dynamics. We have checked different models, with different parameters J, J' (including $J' = 0$), K, and H, and different dynamical regimes (domain wall motion, linear, and nonlinear one-magnon dynamics, etc.), and found that CG scheme performs well, while the MM approach is often inadequate. Our preliminary results on 2D models also support this statement.

In summary, we have shown that the standard micromagnetic theory does not always handle correctly the dynamics of nonlinear multiscale magnetic processes. We have suggested another approach, based on statistical coarse graining, which is applicable to nonlinear problems. Numerical tests on 1D systems show that the CG scheme gives almost exact results for rather large time spans. The basic ingredient of the coarse-graining approach is the standard theory of local equilibrium, so it can be applied to a large set of 2D and 3D problems where the local-equilibrium theory is valid.

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