Multiscale phenomena which include several processes occurring simultaneously at different length scales and exchanging energy with each other, are widespread in magnetism. These phenomena often govern the magnetization reversal dynamics, and their correct modeling is important. In the present paper, we propose an approach to multiscale modeling of magnets, applying the ideas of coarse graining. We have analyzed the choice of the weighting function used in coarse graining, and propose an optimal form for this function. Simple tests provide evidence that this approach may be useful for modeling of realistic magnetic systems.

A large number of phenomena taking place in magnets include processes occurring simultaneously at different length scales. A good example is the magnetization reversal in a macroscopic piece of magnetic material possessing different kinds of defects, voids, surfaces etc. The reversal starts by a nucleation of a domain with the magnetization opposite to the initial direction. As a rule, the nucleation happens near defects, where spins can be frustrated. Here, the different length scales involved can be clearly identified. First, there is the microscopic scale with a characteristic length of the order of several interatomic distances (several tens of angstroms), which corresponds to the region of spin frustration and contains the microstructure in the vicinity of the defect. Next, there is a “micromagnetic” length scale (of order of the domain wall width, several thousands of angstroms) where the formation of the general structure of the nucleus takes place. And, finally, the truly macroscopic length scale (of order of several microns or even millimeters), where the magnons created in the course of the reversal propagate. These magnons play an important role in energy transfer and sometimes can initiate the magnetization reversal in other areas of the sample.

Processes of this type, called multiscale processes, are receiving considerable attention nowadays. Along with very interesting and rich physics, these are the very processes which govern the switching behavior of magnetic systems (coercive field, switching time, etc.), so that an adequate understanding of multiscale phenomena is of paramount importance for development and creation of new magnetic storage media. Micromagnetic simulations can provide a realistic description of the processes taking place at both micromagnetic and macroscopic length scales. On the other hand, microscopic inhomogeneities require atomistic simulations (e.g., spin dynamics modeling is an adequate tool for materials where spins are well localized at the sites of the crystalline lattice). However, for the description of real systems, all the length scales should be coupled, i.e. modeled simultaneously and seamlessly, with the possibility of energy transfer between them.

A simple scheme, where the region of micromagnetic simulations is just attached to the region of atomic spin simulations, does not give a satisfactory description of the energy transfer between the length scales. The problem is that micromagnetics does not take into account atomistic degrees of freedom; even reduction of the computational mesh in micromagnetic modeling down to atomic scale does not describe the short-wavelength excitations properly, contrary to spin dynamics simulations. The artificial sharp boundary appearing between the micromagnetic and atomistic regions leads to the unphysical scattering of magnons transferring the energy from one region to the other. To couple length scales correctly, some transition region between the micromagnetic and atomic regions is necessary, which allows for gradual exclusion of short-wavelength modes until they die out in the regions far from the defect.

Similar difficulties arise in modeling dynamics of structural defects in crystals (dislocation motion, crack propagation, etc.). The coupling of lengthscales for this class of problems has been extensively discussed in the literature. One of the most promising approaches to the solution of this problem is coarse-grained molecular dynamics (CGMD), developed in Ref. In the present paper, we apply the ideas of CGMD to magnetic materials modeling. We propose a computational scheme which employs basic concepts of nonequilibrium statistical mechanics to couple micromagnetism and the dynamic modeling of classical spins. We identify the key problems arising in the course of implementation of this scheme and their possible solutions.

To explain the idea of the method, let us consider a ferromagnet where some magnetic inhomogeneity (defect, interface, etc.) is present. We describe it as a system of classical magnetic moments $\mathbf{M}_\mu$ of fixed length $M = |\mathbf{M}_\mu|$, located at the $\mu$-th site of the crystalline lattice (greek indices enumerate the lattice sites). We assume that the system is described by the Hamilton function

$$H = \sum_\mu \mathbf{M}_\mu \cdot \mathbf{H}.$$
where $H^0$ describes the isotropic exchange interaction, while $V \ll H^0$ represents all the other, much weaker interactions present in the system, and $J_{\mu\nu}$ is the exchange integral between the sites $\mu$ and $\nu$. Let us focus on the region far from the defect, where the amplitudes of short-wavelength excitations are small (the region where their amplitudes are not small should be treated completely atomistically). Suppose, a computational grid is defined in this region, so that the magnetic state is described with required precision by defining the magnetization direction at the grid nodes: $M_j = (M_j^x, M_j^y, M_j^z)$ at the $j$-th node (below, latin indices enumerate the nodes of the mesh). These data represent the necessary number of large-scale degrees of freedom, and exact modeling of all the atomic-scale modes would be too excessive (and too expensive resourcewise). However, the atomic-scale modes can not be excluded completely, since their cumulative effect (dissipation, energy transfer, etc.) is not negligible, and should be taken into account.

This problem can be solved by invoking statistical physics, i.e. under the assumption of ergodicity the exact dynamics of short-scale modes can be replaced by their statistical distribution. For many relevant situations it has been shown that the short-scale modes relax almost immediately to the state of local quasiequilibrium determined uniquely by large-scale modes, so that knowledge of only the large-scale parameters ("gross variables") determines the dynamics of the system with necessary rigor. This description of the system, where only large-scale modes are essential (while short-scale modes are "slaved" due to the requirement of the local equilibrium), is often referred to as the coarse-grained description. The theory of local quasiequilibrium states has been developed in the 1950s-1960s, and a number of approaches exist. In the following, we will use the convenient modification of the nonequilibrium statistical operator (NSO) method. For simplicity, we do not consider the dissipation processes and quantum spin effects, but in principle they can also be included following Ref. 

It is convenient to introduce new dynamic variables $\alpha_{1,\mu}$ and $\alpha_{2,\mu}$ for the magnetic moments $M_\mu$ according to the following relations:

$$M_\mu^x = \alpha_{1,\mu} \sqrt{2M - \alpha_{1,\mu}^2 - \alpha_{2,\mu}^2}, \quad M_\mu^y = \alpha_{2,\mu} \sqrt{2M - \alpha_{1,\mu}^2 - \alpha_{2,\mu}^2}, \quad M_\mu^z = M - \alpha_{1,\mu}^2 - \alpha_{2,\mu}^2.$$  

These variables can be expressed via conventional polar $\theta_\mu$ and asimuthal $\phi_\mu$ angles as

$$\alpha_{1,\mu} = \sqrt{2M \sin (\theta_\mu/2) \cos \phi_\mu}, \quad \alpha_{2,\mu} = \sqrt{2M \sin (\theta_\mu/2) \sin \phi_\mu}.$$  

It can be checked that the variables $\alpha_{1,\mu}$ and $\alpha_{2,\mu}$ are canonically conjugated, so that Hamiltonian formalism can be used, and a computational scheme preserving the symplectic structure can be employed.

The conventional way to develop a coarse-grained description of the system is to introduce the large-scale variables $\alpha_j$ as averages of $\alpha_\mu$:

$$\alpha_{1,j} = \sum_\mu f_{\mu,j} \alpha_{1,\mu}, \quad \alpha_{2,j} = \sum_\mu f_{\mu,j} \alpha_{2,\mu},$$

where $f_{\mu,j}$ is an appropriate weighting function, satisfying the normalization condition $\sum_\mu f_{\mu,j} = 1$, and localized near the node $j$; proper choice of the weighting function $f_{\mu,j}$ will be discussed below in more detail.

Averaging is a natural way to introduce gross variables for a ferromagnet, where the local equilibrium is governed by the Hamiltonian $H^0$, so that all the magnetic moments $M_\mu$ near the node $j$ are almost parallel to $M_j$. Introduced in this way, $\alpha_{1,2,j}$ constitute collective variables of the system changing slowly with respect to quickly relaxing short-scale modes, so they can be considered as quasi-integrals of motion (for more detailed discussion see Refs. 

Following standard procedures of statistical physics, the integrals of motion are included into the distribution function via Legendre transformations, i.e. we introduce Legendre multipliers $F_j$ and $G_j$ corresponding to the node variables $\alpha_{1,j}$ and $\alpha_{2,j}$, so that the distribution function can be written as

$$\rho = Q^{-1} \exp \left( -\sum_\mu \beta_\mu H^0_\mu - \sum_j F_j \sum_\mu \beta_\mu f_{\mu,j} \alpha_{1,\mu} - \sum_j G_j \sum_\mu \beta_\mu f_{\mu,j} \alpha_{2,\mu} \right),$$

where $\beta_\mu = 1/(k_B T_\mu)$, $k_B$ is Boltzmann’s constant, $T_\mu$ is the spin temperature at the $\mu$-th site, and $Q$, as can be seen, is the normalization factor, analogous to the statistical sum of a canonical ensemble in the equilibrium case. Note that smooth variations of the temperature across the sample can be taken into account (temperature is a Legendre multiplier for the integral of energy), but to make the consideration simpler, we neglect it, assuming constant temperature, small enough to satisfy the condition $\beta J_{\mu\nu} \ll 1$.

The variables $F_j$ and $G_j$ can be considered as parameters of a local fictitious field acting on the moments $M_\mu$. Values of the parameters $F_j$ and $G_j$ should be chosen in
such a way that the resulting equilibrium values \( \alpha_{(1,2),\mu} \) averaged with the weighting function \( f_{\mu,j} \) give the required values of \( \alpha_{(1,2),j} \). It is easy to see from Eq. 6 that the values \( F^0_j, G^0_j \) producing the required values \( \alpha_{(1,2),j} \) are determined from the equations

\[
\frac{\partial F}{\partial F_j} \bigg|_{F^0_j, G^0_j} = \alpha_{1,j}, \quad \frac{\partial F}{\partial G_j} \bigg|_{F^0_j, G^0_j} = \alpha_{2,j},
\]

\[
F(F_j, G_j) = -\beta^{-1} \ln Q
\]

where \( F \) is an analog of the Gibbs’ free energy function.

Now, having all the information at hand, we can use averaging to get the equations of motion for the coarse-grained variables \( \alpha_{(1,2),j} \). The underlying dynamics of the microscopic variables \( \alpha_{(1,2),\mu} \) is Hamiltonian, i.e.

\[
\dot{\alpha}_{1,\mu} = -\frac{\partial H}{\partial \alpha_{2,\mu}}, \quad \dot{\alpha}_{2,\mu} = \frac{\partial H}{\partial \alpha_{1,\mu}},
\]

where \( H \) is the Hamilton function \( \Xi \). Using the distribution function \( \Xi \) with the values \( F^0_j \) and \( G^0_j \) determined from Eq. 6, we obtain:

\[
\dot{\alpha}_{1,j} = -\sum_{\mu} f_{\mu,j} \langle \frac{\partial V}{\partial \alpha_{2,\mu}} \rangle - \sum_{\mu} f_{\mu,j} \sum_k f_{\mu,k} G^0_k,
\]

\[
\dot{\alpha}_{2,j} = \sum_{\mu} f_{\mu,j} \langle \frac{\partial V}{\partial \alpha_{1,\mu}} \rangle + \sum_{\mu} f_{\mu,j} \sum_k f_{\mu,k} F^0_k
\]

where \( \langle \ldots \rangle \) means averaging with the distribution \( \Xi \). Note that the equations of motion are nonlocal over the node indices even if only local exchange interactions are present in the system; this important feature is totally missing in the micromagnetic description.

Direct implementation of the scheme presented above can be rather expensive computationally. To make the problem easier, we can take into account that these computations are to be performed only inside the relatively narrow “belt” of micromagnetic and atomic-scale regions (see Fig. 4), where departures of magnetization from equilibrium are already small (otherwise, Atomic-scale simulations should be used). If the \( z \)-axis of the co-ordinate frame is aligned with the equilibrium direction of magnetization the values of \( \alpha_{(1,2),\mu} \) are small, and the Hamiltonian \( H^0 \) can be expanded in terms of \( \alpha_{(1,2),\mu} \) up to second order:

\[
H^0 = \frac{1}{2} \sum_{u,v=1,2} \sum_{\mu,\nu} D_{u\mu,v\nu} \alpha_{u,\mu} \alpha_{v,\nu},
\]

where the indices \( u, v = 1, 2 \) denote the variables \( \alpha_1 \) and \( \alpha_2 \). In this case, the distribution \( \Xi \) is Gaussian, so that the integral \( Q \) and the function \( F \) in \( \Xi \) can be calculated exactly \( \Xi \). As a result, Eq. 6 determining the values of generalized torques \( F^0_j \) and \( G^0_j \) can be written as a set of linear equations:

\[
\alpha_{u,j} = \sum_{k \in \{1,2\}} T^0_{v,k} \sum_{\mu,\nu} f_{\mu,j} D_{u\mu,v\nu}^{-1} f_{v,k},
\]

where \( D_{u\mu,v\nu}^{-1} \) is the inverse of the dynamic matrix \( D_{u\mu,v\nu} \) in the linearized exchange Hamiltonian \( \Xi \), and we used the vector \( T^0_{v,k} (v = 1, 2) \) to denote both \( F^0_j \) and \( G^0_j \) as follows: \( T^0_{1,k} = F^0_k \) and \( T^0_{2,k} = G^0_k \).

Hence, the problem of dynamic coupling of length scales is reduced to two linear problems, Eqs. 6 and 7. Note that the rotation of the co-ordinate frame which brings the \( z \)-axis into coincidence with the equilibrium direction of magnetization makes the dynamic matrix independent of \( \alpha_{(1,2),j} \), so that its inverse can be calculated once and stored for further references. However, there is a subtlety in inverting \( D_{u\mu,v\nu} \); this matrix, being determined only by the isotropic exchange interactions, has a zero eigenvalue corresponding to a shift of all \( \alpha_{(1,2),\mu} \) by the same value, or, in other words, the dynamic matrix has an eigenvector \( d^0 = (1, 1, \ldots, 1) \) corresponding to the zero eigenvalue. It reflects the fact that the exchange Hamiltonian \( \Xi \) is invariant with respect to rotation of the system as a whole. Thus, when inverting numerically the dynamic matrix, a component corresponding to the zero eigenvector \( d^0 \) should be excluded.

In the present form, the essence of coarse-graining becomes especially clear. Imagine that, applying some fictitious torques \( F_j \) and \( G_j \) we brought the system into such a state that the equilibrium values of the large-scale variables \( \alpha_{(1,2),j} \) are determined. Then, the atomic magnetic moments \( \mathbf{M}_\mu \) (i.e., the microscopic variables \( \alpha_{(1,2),\mu} \)) move in such a way that, after the stage of quick relaxation is finished, their positions minimize the total energy of the system with respect to the constraints imposed by the torques \( F_j, G_j \).

The last but not least problem is an appropriate choice of the weighting function \( f_{\mu,j} \); it can be verified that an arbitrary function does not automatically give meaningful results. To study this question, let us inspect closely the basic idea of the coarse-grained description. For a general system consisting of \( N \) microscopic moments, an exact description of the system’s dynamics requires knowledge of all \( 2N \) microscopic canonical variables \( \alpha_{(1,2),\mu} \). However, we expect that under certain conditions (which are yet to be formulated), the system can be described with reasonable precision using the much smaller set of \( 2L \) gross variables \( \alpha_{(1,2),j} \). In other words, we expect that under certain approximations, we can define such a set of variables \( \alpha_{(1,2),j} \) that allows specification of all microscopic variables \( \alpha_{(1,2),\mu} \) with sufficient precision. In particular, it can be shown that, for a given weighting function \( f_{\mu,j} \), an optimal (in the least-square sense) restoration of microvariables is achieved via linear transformation

\[
\alpha_{u,\mu} = \sum_j N_{j,\mu} \alpha_{u,j},
\]
where \( N_{j,\mu} = \sum_k f_{\mu,k}(\sum_{\nu} f_{\nu,j} f_{\nu,k})^{-1} \). Thus, the problem is to find such a function \( f_{\mu,j} \) which would make the restoration (11) as accurate as possible.

In the coarse-grained region, where the linearized Hamiltonian \( \mathcal{H} \) can be used, the system’s dynamics can be represented as an independent motion of different normal modes (eigenvectors of the Hamiltonian \( \mathcal{H} \)), and the choice of the \( 2L \) gross variables becomes obvious: they should be amplitudes of the normal modes corresponding to lowest \( L \) eigenfrequencies. This choice gives an almost complete description of the system provided that the amplitudes of all the other modes, which are excluded from consideration, are much smaller. The frequencies of the excluded modes are much larger, so that their dynamics is much faster, and they can relax to local equilibrium quickly in comparison with the adiabatically slowly varying gross variables.

This choice of the gross variables is in correspondence with the dynamical approach to nonequilibrium statistical mechanics. When considering motion of the system subjected to some small rapidly varying perturbation (provided, in our case, by the fast excluded modes), the well-known basic problem is to exclude from the solution so-called secular terms, which appear due to entanglement of slow and fast motions in the system. After slow and fast modes are properly separated, the standard procedure of averaging can be performed. The use of the lowest-frequency normal modes as gross variables allows elimination of the secular terms in the coarse-grained equations of motion. An analogous procedure can be identified also in the approaches of Zwanzig [12] and Mori [13].

Thus, one possible recipe is to use the weighting function \( f_{\mu,j} = d^{ij} \), where \( d^{ij} \) is one of the lowest-frequency eigenvectors of the dynamic matrix. In real calculations it could be inconvenient to work with delocalized collective modes. It can be shown, that an equally accurate coarse-graining can be achieved with any orthonormal combination of the eigenvectors \( d^{ij} \), i.e. \( f_{\mu,j} = \sum_k C_k^j d^{\mu,k} \) is an equally good weighting function if

\[
\sum_k C_k^j C_k^{j'} = \delta_{j,j'} \quad \sum_j C_k^j C_k^{j'} = \delta_{k,k'}. \tag{12}
\]

The function \( f_{\mu,j} \) can be made well-localized using an appropriate set of \( C_k^j \).

As a specific example, we performed coarse-grained modeling of magnons in a 1-D ferromagnetic chain consisting of \( N \) classical magnetic moments with nearest-neighbor and next-nearest-neighbor exchange interactions. The corresponding Hamilton function is

\[
\mathcal{H} = \sum_{\mu} \tilde{J}_\mu^0 M_\mu (M_{\mu+1} + M_{\mu-1}) + \gamma \tilde{J}_\mu^0 M_\mu (M_{\mu+2} + M_{\mu-2}), \tag{13}
\]

and periodic boundary conditions are used. A computational mesh is imposed, consisting of \( L \) nodes, and two gross variables \( \alpha_j \) and \( \beta_j \) are attributed to each of \( L \) nodes. These two gross variables provide a coarse-grained description of a block containing \( n = N/L \) individual moments.

Several weighting functions have been used. One possible choice, giving an exact magnon spectrum, is

\[
f_{\mu,j}^{(0)} = \frac{1}{N} \sin \frac{\pi (\mu - j n)}{N} \tan \frac{\pi (\mu - j n)}{N}, \tag{14}
\]

which corresponds to an orthonormal combination of exact normal modes with coefficients \( C_k^j = (1/\sqrt{N}) \exp (-ijkn) \) where \( i = \sqrt{-1} \) (so it is a discrete analog of the Nyquist-Shannon uniform sampling). However, this function, due to its long tails, is not convenient for computations, and we tested its rescaled cutoff modification:

\[
f_{\mu,j}^{(1)} = A f_{\mu,j}^0, \quad \mu - j n \leq n, \tag{15}
\]

\[
f_{\mu,j}^{(1)} = 0, \quad \mu - j n > n,
\]

where \( A \) is the normalization factor necessary to satisfy the condition \( \sum_j f_{\mu,j} = 1 \). A second form of the weighting function

\[
f_{\mu,j}^{(2)} = 1/n, \quad \mu - j n \leq n, \tag{16}
\]

\[
f_{\mu,j}^{(2)} = 0, \quad \mu - j n > n,
\]

although very far from optimal, can be used for crude semi-qualitative computations, so we also tested its performance.

The results of our tests, the dispersion curves \( \omega(k) \) for magnons with different wave vectors \( k \), and their group velocities \( c(k) = d\omega/dk \), are calculated with different weighting functions, as shown in Fig. 2. Dispersion curves \( \omega(k) \) describe the magnon dynamics in the chain, while the group velocity curve \( c(k) \) characterizes the propagation of magnons (the latter should be tested separately since a good approximation for \( \omega(k) \) does not necessarily imply a good approximation of its derivative). For comparison, exact curves are presented, along with the results of micromagnetic calculations. The data points for \( k = 0 \) and \( k = 2\pi/n \) are not shown because the dynamic matrix formally has a singularity at these values of wave vector. For very long-wavelength magnons all types of modeling work rather well, but for shorter wave lengths the differences are large. The coarse-grained description is better than the micromagnetic even for the worst function \( f_{\mu,j}^{(2)} \). For the appropriately chosen weighting function \( f_{\mu,j}^{(1)} \), in spite of the cutoff, the difference with the exact solution is very small, even at maximal allowed wave vector values.

Summarizing, we propose an approach to modeling of multiscale processes in magnets, applying the ideas of
coarse grained molecular dynamics to magnetic modeling. The scheme proposed employs basic concepts of nonequilibrium statistical mechanics to couple length-scales. We discussed possible implementation of this approach, paying particular attention to the problem of the correct choice of the weighting function used in coarse graining. Simple tests verify our conclusions and evidence that this approach can be applicable to larger and more complicated systems.

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Fig. 1

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“Statistical coarse-graining as an approach to multiscale problems in magnetism”
Fig. 2

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"Statistical coarse-graining as an approach to multiscale problems in magnetism"