Coarse-graining Landau–Lifshitz damping

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High speed switching in magnetic materials is usually studied with the Landau–Lifshitz (LL) equation, which describes damping through a phenomenological coefficient. The results of micromagnetic calculations based on the LL equation have been observed to depend strongly on the cell size. We take a coarse-graining or renormalization-group approach to this cell size dependence: from a simulation using cell size L, we look at the dynamics of a cell of size $2L$ and determine an effective damping coefficient that describes the larger-scale dynamics. This can be thought of as a Green–Kubo calculation of the effective damping coefficient. In principle, this makes it possible to coarse grain from the atomic scale to determine the micromagnetic damping coefficient. [DOI: 10.1063/1.1355328]

I. INTRODUCTION

Because of continuing increases in magnetic recording rates, the understanding of high-speed switching has become an important priority in micromagnetic simulation. In high-speed switching of a magnetic grain, the rapid dissipation of energy is critical, otherwise the grain will immediately switch back. However, this dissipation is not well understood or accurately modeled. Energy dissipation is normally incorporated into micromagnetic simulation through the the Landau–Lifshitz damping coefficient α, which can be measured by ferromagnetic resonance (FMR) methods. However, it has been found that the α measured in FMR experiments[1] (which involve small deviations from equilibrium) are too low to describe the damping that occurs in more violent processes such as switching. Estimates have been made of effective damping coefficients in the context of switching, by explicit simulation of energy loss during precession.[2] However, it has not been clear how to incorporate damping-coefficient variation into a micromagnetic calculation. In this article we propose a way of doing this, in which the local damping coefficient depends on the local spin temperature and on the cell size. For a simple system we actually calculate the temperature and cell size dependence of the damping coefficient, using the Green–Kubo method. The present calculation provides a partial solution to the problem of coarse-graining in magnetic systems. If we are given the parameters that describe a system on an atomic scale (in a Heisenberg type model) the methods of this article make it possible to determine the parameters (exchange and damping) that describe it on a larger (micromagnetic) scale.

The basic equation for the time evolution of the magnetization $\mathbf{M}$ of a finite element of magnetic material is the Landau–Lifshitz (LL) equation[3]

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M}\times\mathbf{H} - \frac{\alpha\gamma}{M_s}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}). \tag{1}$$

The constant γ is the gyromagnetic ratio, and α is the LL damping coefficient. In the present article, the total magnetic field $\mathbf{H}$ consists of an exchange field and a random thermal field:

$$\mathbf{H} = \sum_{\text{nbr}} J\mathbf{M}_{\text{nbr}} + \mathbf{H}_{\text{random}}, \tag{2}$$

where the sum is over the six neighbors of a cell.

The random field is taken from a Gaussian distribution centered at zero; each component has variance[4]

$$\langle H^2_{\text{random},x}\rangle = \frac{2\alpha(k_B T/V)}{\mu_0 \gamma M_s \Delta t}, \tag{3}$$

where V is the volume of a cell.

II. DAMPING-COEFFICIENT RENORMALIZATION

In atomic scale simulations one does not ordinarily use a damping term; the energy of the spin system is conserved on this scale. In macroscopic calculations (called ''micromagnetic'' calculations, confusingly in this context) one can think of the damping and random terms as an effort to include the effects of intracell degrees of freedom (''spin waves''). Intercell interactions are accounted for explicitly by the precession term of the LL equation, but fluctuations on a smaller scale can be taken into account only in a statistical sense, through damping and thermal noise. This viewpoint implies that the damping coefficient must depend on the cell size—when we simulate using larger cells, there are more intracell degrees of freedom to lose energy to, so we must use a larger damping coefficient. That is, the damping coefficient must ''renormalize'' upward when we enlarge the space scale. In this article we will adopt this ''renormalization-group'' viewpoint and show how to actually calculate the damping-coefficient renormalization, i.e., how to determine the appropriate damping coefficient for large cells from that for smaller cells.

Over long times, other sources of damping may be important, such as phonons coupled to the magnetization

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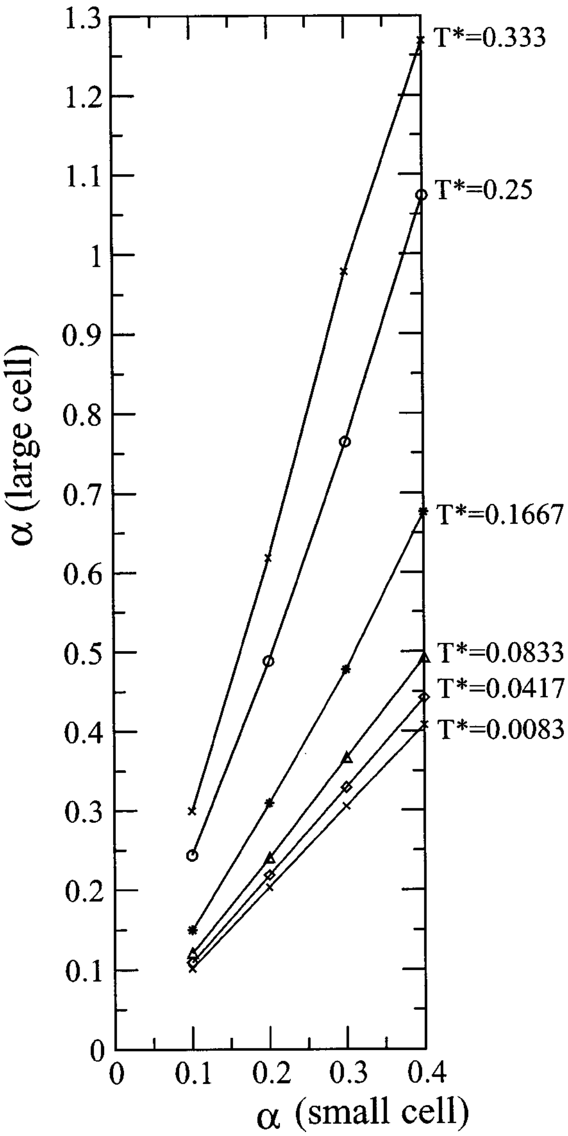

FIG. 1. Renormalized large-cell damping coefficient. We have simulated the model for six values of the dimensionless T^*, 1/120, 5/120, 1/12, 2/12, 3/12, and 4/12.

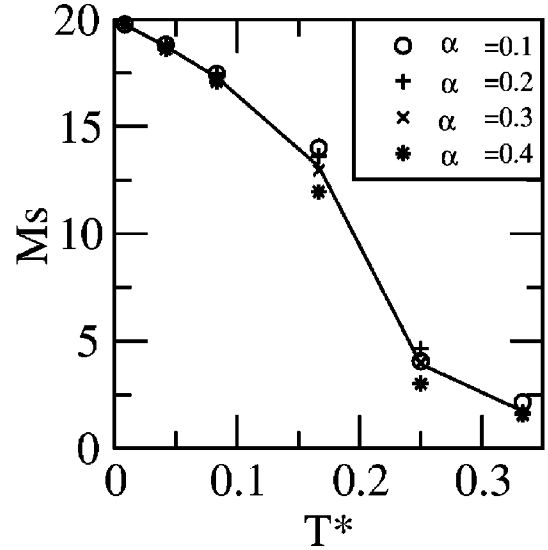

FIG. 2. Equilibrium magnetization (in kOe) of our classical Heisenberg model as a function of dimensionless temperature [Eq. (5)]. Symbols represent different values of alpha; the line is drawn through an average of these. The low temperature data are quite independent of system size, but in the critical region the magnetization is size dependent. Above the Curie temperature the magnetization vanishes in an infinite system, but has a well-defined finite value in a finite system.

through magnetostriction,[5] but it appears that over picosecond time scales in fast switching, transfer of energy into shorter wavelength spin waves is the dominant effect.

One way of viewing the present calculation is that we are assuming an equation of motion for the system with parameters appropriate for a small scale (cell size a) and calculating the parameters for a larger cell (size $2a$). Clearly this coarse-graining process can be repeated, giving the possibility of bridging all the length scales between the atomic scale of a Heisenberg model and a macroscopic (''micromagnetic'') scale by a succession of equilibrium simulations. But the method also has application to nonequilibrium processes such as switching, in which the T we use may not be a true temperature but an effective spin temperature, much higher than ambient temperature because switching has dumped a lot of Zeeman energy into the spin system. One could do a calculation in which the damping coefficient is a local variable, determined by a local average exchange energy, i.e., spin temperature.

III. GREEN–KUBO FORMULA FOR α

In this article we wish to calculate the effective damping coefficient α_L for large cells (size $2a$) from the small-cell α_S used in the simulation. In the Green–Kubo method, one calculates this in the context of an equilibrium simulation in which the magnetizations **M** are fluctuating. Note that the LL equation given above will sample an equilibrium (canonical) ensemble if we let it run for a long enough time, because of the random term. If we take the dot product of the LL equation with $\mathbf{M}\times\mathbf{M}\times\mathbf{H}$, the the precession term $(-\gamma\mathbf{M}\times\mathbf{H})$ gives zero because it is orthogonal to this. Only the damping term remains on the right hand side—if we average both sides over the equilibrium ensemble, we can solve for α:

$$\alpha=-\frac{M_s}{\gamma}\,\frac{\left\langle \dfrac{d\mathbf{M}}{dt}\cdot\mathbf{M}\times(\mathbf{M}\times\mathbf{H})\right\rangle}{\langle[\mathbf{M}\times(\mathbf{M}\times\mathbf{H})]^2\rangle}. \tag{4}$$

Both of these averages can easily be calculated in our simulation. As a consistency check, we have calculated them using the **M** and **H** of the small cells; this gives back the originally assumed value of α_S, as one would expect. If we use the large-cell **M** (the sum of eight small-cell **M**s), its rate of change $d\mathbf{M}/\mathbf{dt}$, and the large-cell **H** (the average of eight small-cell **H**s), we get a different ''renormalized'' α_L, plotted in Fig. 1.

IV. SIMULATION DETAILS

We have simulated a cubic lattice of cells with constant nearest neighbor exchange and periodic boundary conditions. We give the results here for the case of $8\times8\times8$ cells, simulated for a period of 8 ns for each value of temperature and damping coefficient. This is sufficient that the statistical errors are negligible (much less than 1%). We have chosen parameter values similar to those of iron: saturation magnetization $4\pi M_s = 20$ kOe (in SI units, $M_s = 1.59\times 10^6$ A/m), and gyromagnetic ratio $\gamma = 17.6(\mathrm{kOe\,ns})^{-1}$. We have taken the dimensionless exchange parameter $J=0.05$ [Eq. (2)]. Using the exchange constant $A = 1.3\times 10^{-11}$ J/m for iron, this implies a cell size $a = 8.2$ nm (from $a^2 = A/\mu_0 J M_s^2$).

In our simple model (no anisotropy or magnetostatic energy) there are only two energy scales: thermal and exchange. Except for trivial scaling factors, our results depend only on a ratio which we will refer to as a dimensionless spin temperature:

$$T^* = \frac{\text{thermal energy}}{\text{exchange energy}} = \frac{k_B T}{6\mu_0 J M_s^2 a^3}, \tag{5}$$

where the factor of 6 is the number of neighboring cells.

This calculation was done using a very general hierarchical object-oriented (C++) micromagnetics code, designed to be applicable to irregular or adaptive grids as well as rectangular ones. Rather than storing and updating the magnetization vector $\mathbf{M}(\mathbf{r})$ at each cell, we store a quaternion $q(\mathbf{r})$ (equivalent to a rotation matrix) which, when applied to a standard vector $(0,0,\mathbf{M}_s)$ gives $\mathbf{M}$. The algorithm for updating $q(\mathbf{r})$ to give Eq. (1) is described elsewhere;[6] for the purposes of the present article it is equivalent to a standard micromagnetics algorithm. It is basically a first order algorithm—including random forces in a higher order algorithm is much more difficult.

V. RESULTS

The main result of this article is Fig. 1, which shows the large-cell damping coefficient α_L as a function of the assumed small-cell coefficient α_S, for several values of the dimensionless spin temperature [Eq. (5)]. The curves appear to be linear within the uncertainties. Note that for the lowest temperature, the line has a slope close to 1—that is, there is almost no renormalization, consistent with the idea that it is due to intracell spin wave fluctuations. It is difficult to simulate the $\alpha_S = 0$ case because there is no thermostat, so even very small timestep errors cause the energy to drift. It may not be *a priori* obvious that the curves should go through the origin—energy can be transferred from long-wavelength to short-wavelength modes even in an energy-conserving system—but it appears that this does not happen in a system at overall equilibrium, in which the spin temperature is the same on both scales. In principle, one could use this curve to coarse grain an atomic-scale Heisenberg model description of the system up to micromagnetic scales.

In Fig. 2 we plot the equilibrium magnetization as a function of temperature. In principle, equilibrium averages like M_s are independent of α. However, we do have to avoid very small α — when the damping is small, the timestep errors can build up. In fact, in the absence of damping and random field (i.e., at zero temperature), over the periods of several nanoseconds that we have simulated, the trajectory would deviate significantly from the exact one. However, this is true of almost any stochastic simulation — stochastic simulations give correct answers anyway because these small timestep errors can be regarded as a (small) addition to the thermal noise. The results for our four different values of α are indicated by different symbols in Fig. 2; the solid line is drawn through their average. Compared to the α dependence, the Δt dependence is quite small (less than 1% at $\Delta t = 0.25$ ps) and has been removed by linear extrapolation from $\Delta t = 0.5$ ps and 0.25 ps to $\Delta t = 0$.

ACKNOWLEDGMENTS

This research was supported by the DOE under Grant No. DE-FG02-98ER45714 and by NSF MRSEC Award No. DMR-9809423.

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