Implementation of the mean field quantum LLB for the python package *udkm1dsim*

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I will try to document the progress on the implementation of magnetization dynamics in the above mentioned python package in this document. Both the code and this small documentation are very incomplete and I will update them ongoingly.

THE MEAN FIELD QUANTUM LLB

The Landau-Lifshitz-Bloch (LLB) equations are a set of micromagnetic formulas to describe the dynamics of the spin system in a magnetic compound. The equations are equipped to describe a set of macrospins, which in turn are a collection of atomistic spins. Analytical formulations of dynamical parameters in the LLB can describe the behaviour of these macrospins by statistically avering the behaviour of atomistic spins. While this description is lacking in precision in comparison to atomistic LLG methods, it is computationally cheaper and able to describe and predict a wide range of magnetic dynamical properties. Here, I will focus on the **mean field quantum LLB**, meaning the temperature dependence of parameters such as exchange coupling, susceptibility, anisotropy etc. is based on the temperature dependence of the mean field equilibrium magnetization. The quantum LLB is an extension of the classical LLB for systems with assumed effective spin $S < \infty$, which affects the formulation of the damping parameters.

DEFINITION OF COMMONLY USED TERMS

Importantly, as stated above, the LLB is not an atomistic model. Thus magnetic properties are not assigned to single atomistic spins but rather to **grains** within the one dimensional sample structure of about 5 nm of depth. These grains behave unifomrly internally, thus one needs to assign **material** parameters on this dimension. Temperature dependence of parameters for certain alloys as for instance FeGd have already been investigated, many complex constructions of unit cells however lack treatment in literature. To investigate magnetization dynamics for complex systems without undergoing a tedious and rather phenomenological fitting process should be simulated using atomistic simulations.

General LLB equations

The code I write shall produce the iterative solution of the following differential equation for the reduced magnetization $\mathbf{n}(T) = \mathbf{m}/m_e(T)$ at temperature T and (equilibrium) magnetization $m_{(eq)}$:

$$\dot{\mathbf{n}} = \gamma[\mathbf{n} \times \mathbf{H}_{\text{eff}}] - \frac{\gamma\alpha_\perp}{n^2}[\mathbf{n} \times [\mathbf{n} \times \mathbf{H}_{\text{eff}}]] + \frac{\gamma\alpha_\parallel}{n^2}[\mathbf{n} \cdot \mathbf{H}_{\text{eff}}]\mathbf{n} \tag{1}$$

$$\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{int}} + \frac{m_e(T)}{2\chi_\parallel}(1 - n^2)\mathbf{n} \tag{2}$$

A graphic sketch of the three terms in Eq. (1) is shown in figure 1. The first term describes precession of the magnetization vector around the effectivemagnetic field $\mathbf{H}_{\text{eff}}$ with the Lamor frequency, where γ is the gyromagnetic ratio. $\mathbf{H}_{\text{eff}}$ contains the internal fields $\mathbf{H}_{\text{int}}$ (Zeeman, Heisenberg, Anisotropy, magnetic dipole) and a thermal field (second term). The second term in Eq. (1) describes transverse damping of the magnetization vector with damping parameter $\alpha_\perp$ and thus a **correlated precession** of atomistic spins within the grain on which the macrospin is defined. The third term describes longitudinal damping of the magnetization with damping parameter $\alpha_\parallel$ and thus uncorrelated precession of atomistic spins that lead to an increase or decrease of the magnetization amplitude.

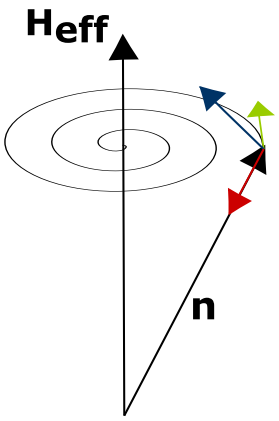

FIG. 1: Sketch of the direction of terms of the LLB.The colored arrows show the direction of the terms in Eq. (1). The spiral sketches the trajectory of the reduced magnetization.

In the presence of a strong thermal field, as in the case of ultrafast laser heating, the longitudinal damping dominates the magnetization dynamics on short timescales ($\approx$ ps).

PREPARATION OF TEMPERATURE DEPENDENT PARAMETERS

To model the LLB equation, it is very useful to define the temperature dependence of all parameters and interactions before starting the dynamical simulation. Therefore, a temperature map of the mean field magnetization for all materials in the sample is constructed first. This is the evaluation of the self consistent equation

$$m(T) = B_S(m,T) \tag{3}$$

$$B_S(m,T) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}\frac{Jm}{k_BT}\right) - \frac{1}{2S}\coth\left(\frac{1}{2S}\frac{Jm}{k_BT}\right), \tag{4}$$

where S is the **effective spin** of the material, $J = 3S/(S+1)k_BT_C$ is the exchange coupling constant, T_C the Curie temperature.

Thus, in the material class, the function **material.create_mean_mag_map(self)** is called. This function constructs a grid of temperatures in $[0, T_C]$ and solves Eq. (3) using *scipy.optimize.fsolve* on this temperature grid. The resulting array is then interpolated with *scipy.interpolate.interp1d*, which is the output of the function. By calling this function in **__init__(self, *params)** the map is computed only once, saved as **material.mean_mag_map** and can be called by **material.get_mean_mag(self, T)** to evaluate the function for an array of temperatures. The same procedure is done for the derivative $\frac{dm_{\rm eq}}{dT}$. (Plotting functions are inlcuded as dummies to visualize the above functions of the materials with random parameters I have defined.) [ALL THE TEMERTAURE DEPENDENT PARAMETERS WILL BE LISTED AND EXPLAINED HERE]

CONNECTION TO STRUCTURE CLASS

Of course, the macrospins are interacting with each other, which is usually restricted to nearest neighbours (NNs). When a sample consists of several materials which are stack onto each other, it is useful to predefine the needed interactions of the grains. The function **get_exch_coup_sam(materials, sample)** creates a $(N \times 2)$ dimensional array for the sample containing N grains and each grain being coupled to its 2 NN. This structure is created once

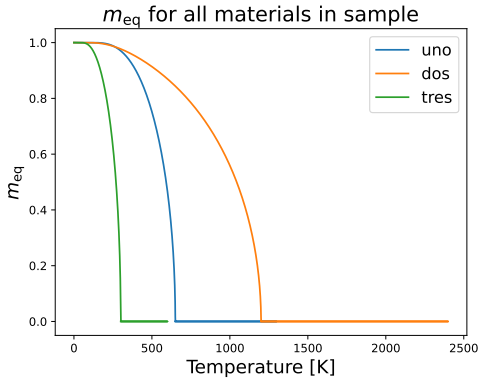

FIG. 2: Mean field magnetization for three test samples with different effective spins and T_C plotted for $T \in [0, 2material.Tc]$

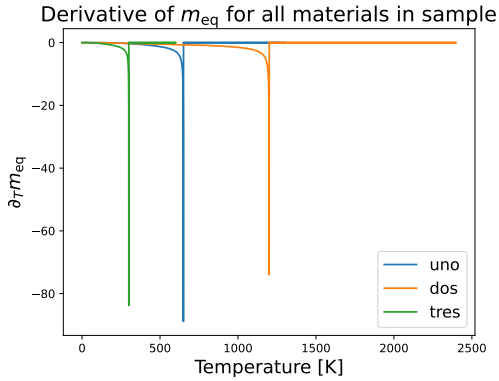

FIG. 3: Derivative of the mean field equilibrium magnetization for the same materials

and can then at each site be read out to get the corresponding exchange coupling between the nieghbouring grains. For the case that identical materials neighbour each other, it gives the mean field exchange coupling constant, else it gives coupling constants that need to be defined manually.