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Interval Computations of Ferromagnetic Resonance Conditions in Exchange-Biased Bilayers

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The main purpose of this paper is to promote the use of interval calculus in physics. As an example we use the system consisting of two thin films, one ferromagnetic and another one antiferromagnetic, deposited one atop of the other. We successfully and accurately simulate the positions of resonance fields of such a system, as seen in ferromagnetic resonance experiment. Interval calculations have revealed the presence of 1, 2 and sometimes even 4 distinct equilibrium configurations of the system, all corresponding to the same resonance field, when the field has a component antiparallel to that of cooling field, while only 1 such position when it points in the opposite direction. In both cases only a single resonance line is observed. As an added value we show that the exchange-biased system is in the metastable state, out of true thermodynamical equilibrium.

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1. Resonance conditions

We use the model for ferromagnetic/antiferromagnetic (FM/AF) bilayers introduced by Hu et al. [1]. The relevant part (we neglect the Zeeman energy of the AF component) of the free energy per unit area of a ferro-/antiferromagnetic bilayer can be written as

$$E = \Big[2\pi \left(\boldsymbol{M}_{\mathrm{FM}} \cdot \boldsymbol{n}\right)^2 - \gamma \boldsymbol{H} \cdot \boldsymbol{M}_{\mathrm{FM}} - K^{\mathrm{in}} \left(\boldsymbol{m}_{\mathrm{F}} \cdot \boldsymbol{u}\right)^2 - K^{\mathrm{out}} \left(\boldsymbol{m}_{\mathrm{F}} \cdot \boldsymbol{n}\right)^2 \Big] t - \sigma \left(\boldsymbol{m}_{\mathrm{A}} \cdot \boldsymbol{u}\right) - J_1 \left(\boldsymbol{m}_{\mathrm{F}} \cdot \boldsymbol{m}_{\mathrm{A}}\right) + J_2 \left(\boldsymbol{m}_{\mathrm{F}} \cdot \boldsymbol{m}_{\mathrm{A}}\right)^2, \quad (1)$$

where $\boldsymbol{m}_{\mathrm{F}} = \boldsymbol{M}_{\mathrm{FM}} / \left|\boldsymbol{M}_{\mathrm{FM}}\right|$, $\boldsymbol{m}_{\mathrm{A}} = \boldsymbol{M}_{\mathrm{AF}} / \left|\boldsymbol{M}_{\mathrm{AF}}\right|$, $\boldsymbol{n} = (0,0,1)$ is the direction perpendicular to the sample plane, $\boldsymbol{u} = (1,0,0)$ is the direction of the magnetic field during cooling (an easy, in-plane direction for FM layer magnetization, $\boldsymbol{M}_{\mathrm{FM}}$), K^{in} and K^{out} are respective uniaxial anisotropy constants for FM component, σ is the domain wall energy density in the AF layer, J_1 and J_2 are the bilinear and biquadratic exchange constants at the interface, respectively. γ is the gyromagnetic ratio and t is thickness of a ferromagnetic part.

In spherical coordinates the ferromagnetic resonance (FMR) condition is

$$t^2 \left(\frac{\omega}{\gamma}\right)^2 = \frac{1}{\left|\boldsymbol{M}_{\mathrm{FM}}\right|^2 \sin^2\theta} \times \left[\frac{\partial^2 E}{\partial\theta^2}\frac{\partial^2 E}{\partial\varphi^2} - \left(\frac{\partial^2 E}{\partial\theta\partial\varphi}\right)^2\right], \quad (2)$$

where the angles θ and φ describe the orientation of magnetization of the FM layer ($\boldsymbol{M}_{\mathrm{FM}}$) at resonance and all the derivatives have to be evaluated at the equilibrium position(s) of the entire system, that is of both vectors: $\boldsymbol{M}_{\mathrm{FM}}$ and $\boldsymbol{M}_{\mathrm{AF}}$. ω is the fixed frequency of the microwave radiation, here 9.248 GHz. Our measurements were performed with external field located in the plane perpendicular to the sample plane but containing the in-plane easy axis. Other details concerning sample preparation, experiment and values of all obtained relevant parameters were already published in [2] and [3]. The nature of exchange bias effect is still poorly understood [4, 5] and the goal of our investigation was to shed some light on this phenomenon.

2. Classical simulations of the FMR spectra

To calculate the resonance field for a given orientation of an external field, one has to follow a rather tedious procedure. For each magnitude of the external field an equilibrium position(s) of the system has (have) to be found first. This step alone is a challenging task, requiring to solve a system of 4 highly non-linear equations, $\nabla E = 0$, and determining which solutions correspond to the free energy minima. Then, using Eq. (2), the resonance frequency (frequencies) is (are) determined. The field(s), at which so found resonance frequency is equal to the one used in experiment, is (are) the sought resonance field(s). It is not possible to simplify this procedure since the equilibrium position of the entire system usually differs, sometimes drastically, from the orientation of an external field and is sensitive to its magnitude; see Fig. 1. This is why the equilibrium position cannot be reliably and accurately guessed, except for rare special cases (highly symmetric ones). Needless to say that this procedure has to be repeated anew for each orientation of the external field.

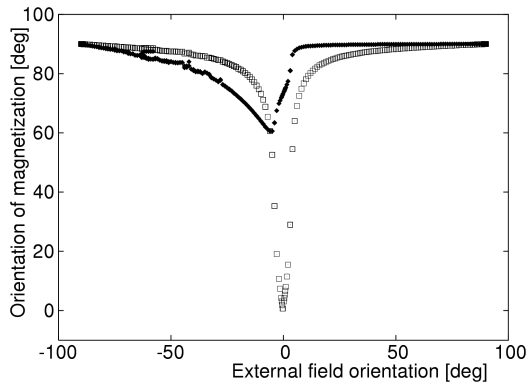

Fig. 1. The equilibrium positions at resonance for FM (squares) and AF component (diamonds) versus orientation of the external field, both given as polar angles. The field rotates in the plane perpendicular to the bilayer and containing the in-plane easy axis. Negative values mark the direction opposite to that of cooling field. The apparent "noise", in the left part of the figure, is *not* the result of numerical inaccuracies, it shows the presence of multiple equilibria, all corresponding to the same magnitude of the resonance field. Only the polar angle is shown, since azimuthal one differs no more than 1° in the whole range.

3. Interval calculus

The essence of interval calculus is to evaluate the ranges of arithmetic expressions given the ranges of their individual constituents. Interval calculations deliver the so-called guaranteed results, i.e. intervals certainly containing the true result, even when the computations are performed with finite precision (!). One should keep in mind, however, that such results are quite often too wide. The overestimation is never known precisely, but it vanishes as the width(s) of argument(s) for *continuous* functions decrease to zero. The multidimensional intervals, being the Cartesian products of ordinary intervals, are commonly called *boxes*. It has to be stressed that existing numerical algorithms only rarely can be easily converted into interval form. This is because we operate on sets rather than on ordinary numbers and some familiar computer instructions may lose their sense: think of the conditional statements like **if** $x > y$ **then** ...

Consequently, we have to get used to think in terms of boxes. More thorough introduction and some software tools can be found in [6].

4. FMR spectra simulated with interval methods

The following procedure is repeated for every particular orientation of an external field. We start with a list of 5-dimensional boxes, initially containing only one element, namely a box being the Cartesian product of the appropriate ranges for: (a) external field magnitude, $[0, \mu_0 H_{\max} = 2\ \mathrm{T}]$, (b) two angles determining the orientation of FM layer magnetization $(\theta, \varphi) = [0, \pi] \times [0, 2\pi]$, and (c) the same for AF layer. Such a box expresses our complete ignorance concerning the possible equilibrium position(s) of magnetization components at resonance(s) (full sphere for each component) as well as the magnitude of the resonance field (we set the field range to the one available in our spectrometer). The box is then subjected to the series of tests in order to determine whether or not the resonance conditions can be met somewhere in its interior. We test: whether all the components of a gradient of free energy density change sign in it, whether the free energy density is a locally convex function of its angular variables (we need to evaluate all second partial derivatives for that), and whether the range of resonance frequencies matches the one used during experiment.

Failing at least one of those tests eliminates the box immediately from further considerations (that is no further tests are attempted). The box successfully passing all the tests is bisected (halved, perpendicularly to its longest edge), the two offspring boxes are put at the end of list, and the process is repeated with the next available box. We finish when either the list is empty (no resonance found nor is possible) or contains only "small" boxes, i.e. having every edge shorter than the prescribed accuracy, which is in our case equal to 0.005 mT for magnetic field and $0.01^\circ = 1.7 \times 10^{-4}$ rad for all angles — well below experimental uncertainties. Due to the possible overestimations, the final list sometimes contains many small boxes, too many to be listed. Therefore the routine tries to "glue" them back, if they are adjacent. Effectively we finish with 1, 2 or 4 disjoint boxes in most cases. Returned are their centers and lengths of their edges, sometimes higher than intended. This way all the resonance fields are precisely determined together with the equilibrium positions of magnetization for both subsystems.

The routine is called repeatedly for subsequent orientations thus producing complete angular FMR spectrum. Processing the single orientation usually requires less than 10 s on a 1.5 GHz PC. During computations the length of list of unprocessed boxes oscillates wildly, rarely exceeding 400. For some "difficult" orientations, the computing time increases occasionally 20 times or even more and so does the instantaneous length of list.

The procedure described above, based on repeated chopping of the domain of interest into smaller parts and discarding those certainly not containing the solution(s), is typical of many interval-oriented algorithms.

5. Conclusions

We have demonstrated that the interval approach is an effective and efficient tool for precise calculation of all the resonance fields regardless of the sample orientation. This is impossible on the analytical way. Using those methods we are able to make use of all the experimental measurements, not only of those performed in specific directions, to estimate the values of important physical parameters like exchange couplings or various anisotropy constants.

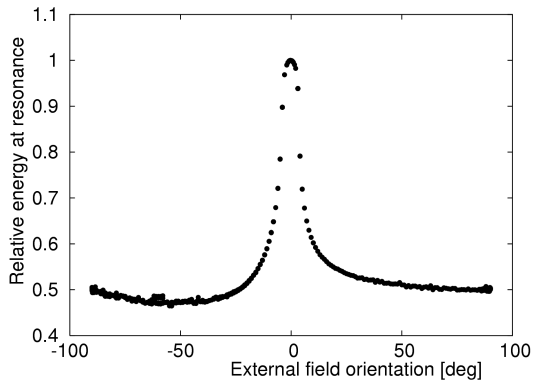

Fig. 2. The free energy of equilibrium position at resonance versus orientation of the external field. The dimensionless energy is rescaled as $(E_{\rm eq} - E_{\rm min})/(E_{\rm max} - E_{\rm min})$, where $(E_{\rm min}, E_{\rm max})$ denotes the range of free energy density for a given orientation of the resonance field.

As a side effect, our computations revealed that FMR in exchange coupled FM/AF bilayer occurs at local rather than at global free energy minimum, see Fig. 2. In the dimensionless units used there the global minimum corresponds to zero, while the resonance occurs mostly near the average height of the free energy landscape, except when the field is perpendicular to the sample plane. This indicates unambiguously that exchange-biased state is metastable, and beyond any doubt not the ground state — in full accordance with other experimental observations ("trained" hysteresis loops).

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