Antiferromagnetic resonance in collinear antiferromagnet: modelling f(H) dependence with easy-to-modify Octave script.

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Goals

Antiferromagnetic resonance (AFMR) is a very sensitive technique to study collective excitations of antiferromagnet. It measures resonance absorption of microwave radiation due to excitation of $q=0$ spin waves (magnons). So being limited to Brillouine zone center, AFMR spectroscopy has very high energy resolution – resolution of 1...5 GHz in the frequency domain is quite a routine, which corresponds to ~0.01 meV energy resolution, the later value is far below resolution limits of inelastic neutron scattering and other spectroscopic techniques. Thus, AFMR technique strongly compliments other spectroscopic methods.

AFMR eigenfrequencies are field dependent, the $f(H)$ dependence can be measured in multi-frequency experiment. This dependence frequently reveal zero-field gaps, which are $q=0$ magnon gaps, it usually features discontinuities of some sort at various spin-reorientation transitions, its field dependence strongly depends on mutual orientation of magnetic field and antiferromagnetic order parameter. Thus, analysis of AFMR $f(H)$ curves could provide essential information on the type of ordering, orientation of the order parameter and various phase transitions.

AFMR $f(H)$ curve could be described via semi-classical mean-field sublattices formalism [1] [2], through a cumbersome Holstein-Primakoff approach (which is described in numerous textbooks, e.g., [3]) or through a hydrodynamic approach [4]. In any case analytical expressions for a particular field orientation can be hard to handle. Hydrodynamic approach allows quite general numeric implementation of calculations, we have earlier developed such an implementation for a noncollinear antiferromagnet [5].

Here we present similar implementation for the case of collinear antiferromagnet written for Octave[1] software [6]. The Octave script can be easily modified to include arbitrary anisotropy energy, magnetic field direction and value. We hope that this script can be of use for community.

Theoretical model and its numerical implementation

We will use hydrodynamic approach of Ref.[4]. This approach is limited to the small fields (with respect to exchange fields), it can not describe spin-flip transition and similar phenomena. It

1 Script was tested in Octave 4.4.1. Script uses statistics package (used for generation of random initial guesses), it should be loaded by *pkg load statistics* command in Octave command line prompt if necessary.

describes low-energy dynamics of an antiferromagnet as oscillations of the order parameter field, which is described by Lagrangian density

$$L=\frac{\chi_\perp}{2\gamma^2}\left(\dot{\vec{l}}+\gamma[\vec{l}\times\vec{H}]\right)^2-U_A \quad ,$$

here unit vector $\vec{l}$ is an antiferromagnetic order parameter and $U_A(\vec{l})$ is the anisopy energy dependent on order parameter orientation. For the case of collinear antiferromagnet Lagrangian depends on two independent variables (e.g., polar and asimuthal angle) which yields two possible eigenfrequencies.

General procedure requires to find equilibrium position of the order parameter, which corresponds to the minimum of potential energy

$$\Pi=-\frac{\chi_\perp}{2}[\vec{l}\times\vec{H}]^2+U_A=-\frac{\chi_\perp H^2}{2}+\frac{\chi_\perp}{2}(\vec{l}\cdot\vec{H})^2+U_A$$

and then to solve set of Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{\varphi}_i}-\frac{\partial L}{\partial\varphi_i}=0 \quad ,$$

here φ_i are independent variables. We will assume $\varphi_i=0$ in equilibrium to simplify further notations.

Numerical implementation of this approach has two hidden dangers. First, due to finite accuracy of potential minimum determination, determined minimum position $\vec{l}_0$ could be slightly off-set. This could result in error in Euler-Lagrange equations. To avoid this problem we follow solution of Ref.[5] and replace "true" potential energy with its quadratic expansion

$$\Pi(\vec{l})\approx\Pi_0+\frac{1}{2}\sum_{\alpha,\beta}\left(\frac{\partial\Pi}{\partial\varphi_\alpha\partial\varphi_\beta}\right)_0\varphi_\alpha\varphi_\beta \quad ,$$

here Hessian matrix is calculated at the numerically found position $\vec{l}_0$.

Second, polar and azimuthal angle became ill defined close to Z-axis, leading to the sort of gimbal lock problem. To avoid this problem we perform a technical rotation of the polar axis to quite arbitrary position (Euler angles of this rotation are set to 0.2π , 0.1π and 0.15π , values quite unlikely to appear in any real problem).

These precautions guarantee absence of numerical problems and Euler-Lagrange equations end up in two-by-two secular equation

$$det\,M=0 \quad ,$$

where

$$M_{\alpha,\beta}=-\omega^2\frac{\chi_\perp}{\gamma^2}\left(\frac{\partial\vec{l}}{\partial\varphi_\alpha}\right)\left(\frac{\partial\vec{l}}{\partial\varphi_\beta}\right)+2i\omega\frac{\chi_\perp}{\gamma}\left(\vec{H}\left[\left(\frac{\partial\vec{l}}{\partial\varphi_\alpha}\right)\times\left(\frac{\partial\vec{l}}{\partial\varphi_\beta}\right)\right]\right)+\left(\frac{\partial^2\Pi}{\partial\varphi_\alpha\partial\varphi_\beta}\right) \quad .$$

This secular equation ends up in quadratic equation on ω^2 which is easily solvable[2]. The only problem-dependent parameters in the equations above are magnetic field vector $\vec{H}$, anisotropy energy U_A and contribution of the anisotropy energy to Hessian matrix $\frac{\partial U_A}{\partial \varphi_1 \partial \varphi_2}$.

Note also that, unless it is specially desirable to reproduce magnetization curve of the antiferromagnet, parameter $\chi_\perp$ (transverse susceptibility of the antiferromagnet) can be set to arbitrary value, e.g. to unity. Such substitution results in simple scaling of all other parameters. Since cyclic frequency enters equations as (ω/γ) one can directly calculate frequency of oscillations by choosing value of gyromagnetic ratio γ in frequency units (GHz/kOe). Finally let us note that exchange symmetry based theory [4] assumes, strictly speaking, gyromagnetic ratio to be equal to free electron value of 2.80 GHz/kOe ($\gamma_{f.e.} = 2\mu_B/h$).

User guide and test example

Algorithm is implemented in Octave (Matlab) script AFMR_collinear.m. Following description is applicable to the version 1.0 dated as February 12, 2019. Version and issue date are shown in the first line of the original script

To accommodate script to a particular problem user have to modify three code fragments:

1. To set model parameters: magnetic field direction and sweep range, anisotropy energy parameters.
2. To set the form of potential energy, which includes anisotropy energy U_A and static magnetic field contribution: $U = U_A + \frac{\chi_\perp}{2}\left(\vec{l}\,\vec{H}\right)^2$.
3. To set the form of Hessian matrix $\frac{\partial U}{\partial \varphi_1 \partial \varphi_2}$.

Details are given below.

Setting model parameters

Model parameters are set between commented separators:

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%  SETTING MODEL PARAMETERS  %%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 9-11 of original script) and

2 Note that complex part is off-diagonal and $\mathrm{Im}\,M_{12} = -\mathrm{Im}\,M_{21}$. Thus we obtain equation $A\omega^4 + B\omega^2 + C = 0$ with

$$A = \frac{\chi_\perp^2}{\gamma^4}\left(\frac{\partial \vec{l}}{\partial \varphi_1}\right)^2\left(\frac{\partial \vec{l}}{\partial \varphi_2}\right)^2 + \frac{\chi_\perp^2}{\gamma^4}\left(\left(\frac{\partial \vec{l}}{\partial \varphi_1}\right)\left(\frac{\partial \vec{l}}{\partial \varphi_2}\right)\right)^2 ,$$

$$B = -\frac{\chi_\perp}{\gamma^2}\left(\frac{\partial \vec{l}}{\partial \varphi_1}\right)^2\left(\frac{\partial^2 \Pi}{\partial \varphi_2^2}\right) - \frac{\chi_\perp}{\gamma^2}\left(\frac{\partial \vec{l}}{\partial \varphi_2}\right)^2\left(\frac{\partial^2 \Pi}{\partial \varphi_1^2}\right) -$$

$$-2\frac{\chi_\perp}{\gamma^2}\left(\left(\frac{\partial \vec{l}}{\partial \varphi_1}\right)\left(\frac{\partial \vec{l}}{\partial \varphi_2}\right)\right)\left(\frac{\partial^2 \Pi}{\partial \varphi_1 \partial \varphi_2}\right)^2 - 4\left(\frac{\chi_\perp}{\gamma}\right)^2\left(\vec{H}\left[\left(\frac{\partial \vec{l}}{\partial \varphi_\alpha}\right)\times\left(\frac{\partial \vec{l}}{\partial \varphi_\beta}\right)\right]\right)^2 , \text{ and}$$

$$C = \left(\frac{\partial^2 \Pi}{\partial \varphi_1^2}\right)\left(\frac{\partial^2 \Pi}{\partial \varphi_2^2}\right) + \left(\frac{\partial^2 \Pi}{\partial \varphi_1 \partial \varphi_2}\right)^2 .$$

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%% END OF MODEL PARAMETERS SETTINGS    %%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 42-44 of original script).

Parameters include:

- Parameters used in energy calculations. For the test example in the original script these are transverse susceptibility *chi*, gyromagnetic ratio *gamma* and anysotropy parameters *a1* and *a2*. All these parameters are combined into vector *parameters*, which will be used in call to all function calculations. All necessary parameters of particular problem should be included in this vector of parameters, which is then properly unbound in energy calculations.
- Magnetic field parameters. These are modeled field scan limits *Hstart* and *Hstop*, field increment *Hstep* and field direction given as polar and azimuthal angle in the same crystallographic frame of reference as used for anisotropy energy definition.
- Number of random minimum search attempts *Ntries*. As numerical algorithm looks for local minimum of the energy, initial approximation have to be choosen accurately. Scripts calculated energy for *Ntries* randomly distributed orientations of the order parameter and uses the one that gives minimal energy as an initial approximation.
- Filename to save modeled curves *name*.

Setting the form of potential energy

Model specific calculations are done between the commented separators

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%% U(l) CALCULATIONS START    %%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 123-125 of the original script) and

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%% U(l) CALCULATIONS END      %%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 135-137 of the original script).

Calculation of the anisotropy energy includes unbundling of the parameters vector (lines 127-130 in the test example of the original script):

```
chi=parameters(1);
gamma=parameters(2);
a1=parameters(3);
a2=parameters(4);
```

Parameters definition should be in agreement with the above section.

Then anisotropy energy is calculated. Calculations can use standard vector operations (scalar and vector product) . Predefined parameters are *vecH* for magnetic field vector, *Hx*, *Hy* and *Hz* for its projections, *l* for antiferromagnetic order parameter vector and *lx*, *ly*, *lz* for its projections. E.g. for orthorhombic anisotropy $U_A = \frac{a_1}{2} l_x^2 + \frac{a_2}{2} l_y^2$, potential energy is $U_A = \frac{a_1}{2} l_x^2 + \frac{a_2}{2} l_y^2 + \frac{\chi_\perp}{2} \left(\vec{l}\,\vec{H}\right)^2$ and calculations in the script are written as (lines 132-133 of the original script)

```
value=0.5*a1*(lx)^2+0.5*a2*(ly)^2;
value+=0.5*chi*(dot(l,vecH))^2;
```

Setting the form of Hessian matrix

Element (ij) of the Hessian matrix $\frac{\partial U}{\partial \varphi_i \partial \varphi_j}$ is calculated between the commented separators

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%% HESSIAN (ij) CALCULATIONS START   %%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 165-167 of the original script) and

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%   HESSIAN (ij) CALCULATIONS END   %%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(lines 177-179 of the original script).

Calculations are done similarly to the potential energy calculations. Besides of the predefined magnetic field and order parameters vectors *vecH* and *l*, derivatives of order parameter and their projections are predefined as well:

- *dl_i* and *dl_j* for $\frac{\partial \vec{l}}{\partial \varphi_{i,j}}$, and *dlx_i*, *dly_i*, *dlz_i*, *dlx_j*, *dly_y*, *dlz_j* for corresponding projections.
- *d2l_ij* for $\frac{\partial^2 \vec{l}}{\partial \varphi_i \partial \varphi_j}$ and *d2lx_ij*, *d2ly_ij*, *d2lz_ij* for corresponding projections.

Output and save file format

Saved file is six-columns tabulation separated file. First column is magnetic field, second and third columns are eigenfrequencies, last three columns are order parameter components. $f(H)$ curve is also plotted during the script execution.

Test example

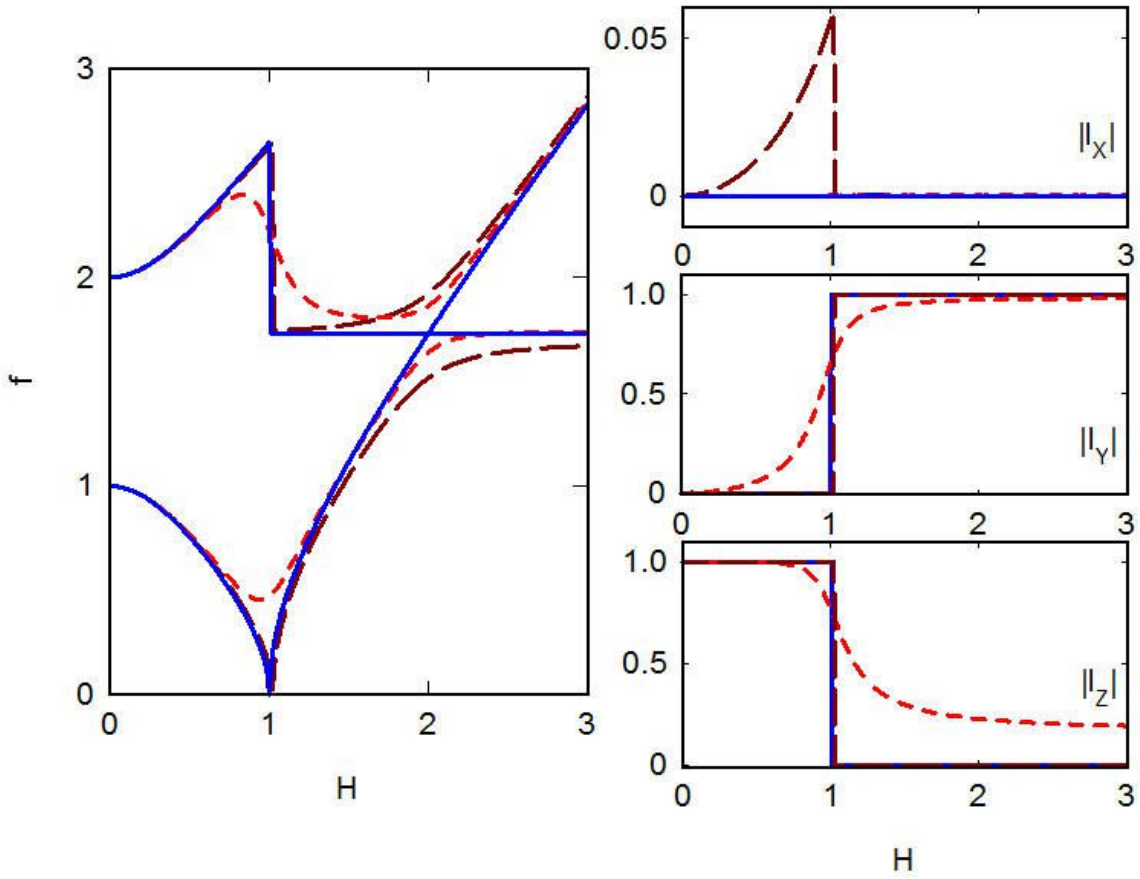

Figure 1 Results of the test modeling of AFMR $f(H)$ *dependence (left panel) and order parameter equilibrium orientation (right panels). Solid (blue) curves –* $\vec{H}\|Z$ *, short-dashed (red) curves – field inclined by* 10^0 *towards Y-axis, long-dashed (brown) curves – field inclined by* 10^0 *toward X-axis.*

Model test example included in the original script corresponds to anisotropy energy $U_A=\frac{a_1}{2}l_x^2+\frac{a_2}{2}l_y^2$ with $a_1=4$ and $a_2=1$, $\chi_\perp$ and γ were both set to unity. This anisotropy energy corresponds to bi-axial case with Z being the easy axis and X being the hard axis. Gap values are 2 and 1, for the field applied along Z axis spin-flop should be observed at $H=1$. Results of the modeling for $\vec{H}\|Z$ and for $\vec{H}$ inclined by 10^0 toward Y and X axes are shown on the Figure 1.

Literature

1: T. Nagamiya, K. Yosida and R.Kubo, Antiferromagnetism, Advances in Physics, 4,1 (1955)
2: A. G. Gurevich, G. A. Melkov, Magnetization Oscillations and Waves, CRC Press (1996)
3: M.Jascur, Quantum theory of magnetism, P.J.Safarik University, electronic textbook (2013)
4: A.F.Andreev, V.I.Marchenko, Symmetry and the macroscopic dynamics of magnetic materials, Sov. Phys. Usp., 23, 21 (1980)
5: V. Glazkov, T. Soldatov, Yu. Krasnikova, Numeric Calculation of Antiferromagnetic Resonance Frequencies for the Noncollinear Antiferromagnet, Applied Magnetic Resonance, 47, 1069 (2016)
6: Octave homepage, https://www.gnu.org/software/octave/