INTERVAL METHODS FOR FMR SPECTRA SIMULATION

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Part of author’s statutory activity in:
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Marek W. Gutowski, Mądralin, August 29th – September 1st, 2002
What is interval calculus?

A branch of (numerical) mathematics, which makes possible to evaluate ranges (bounds) of algebraic expressions over finite domains, not just for specific values of their parameters.

The results obtained on different computers may differ, i.e. the bounds are usually overestimated, but always include the true result.

Examples:

\[ ([ -2, 3 ])^2 = [ 0, 9 ] \]

\[ [-2, 3] + [0, 1] = [-2, 4] \]

but, surprisingly

\[ [0, 1] - [0, 1] = [-1, +1] \]
What is FMR?

**Ferromagnetic resonance** is the resonance absorption of electromagnetic radiation by magnetic bodies placed in an external magnetic field.

The magnetization vector of the ferromagnetic body, which is located in an external magnetic field, is freely precessing around the field vector with some frequency. The precession is damped and spontaneously decays. The relation between the field strength and the precessing frequency is simple:

$$\omega = \gamma H_{eff}$$

where $H_{eff}$ is an **effective field** acting on the body, and $\gamma$ is a constant known as **gyromagnetic ratio**.

$H_{eff}$ includes: **external** magnetic field, **demagnetizing** field, due to the sample’s geometry (shape), and **anisotropy** field.
Two types of measurements

There are two possible kinds of experiments:

1. with fixed external magnetic field and variable frequency, and

2. with fixed (microwave) frequency and variable external field

We will talk about the spectra obtained with the second method. Here the resonance absorption is observed only for some magnitudes of an external field, called resonance fields. Due to the presence of various internal fields, the observed resonance fields will be generally different for different orientations of the sample in the external field.
The resonance condition

The resonance condition is usually written in the form of the well known relation:

\[
\left( \frac{\omega}{\gamma} \right)^2 = \frac{1}{(M \sin \theta)^2} \left[ \frac{\partial^2 E}{\partial \theta^2} \cdot \frac{\partial^2 E}{\partial \varphi^2} - \left( \frac{\partial^2 E}{\partial \theta \partial \varphi} \right)^2 \right] \tag{1}
\]

where the second derivatives of the free energy \( E(H_{ext}, M, \ldots) \) are taken at equilibrium position of the magnetization vector \( M \), and \((\theta, \varphi)\) describe the orientation of this vector in the polar reference frame.

In order to find the equilibrium position of \( M \), one needs first to solve the system of equations

\[
\begin{align*}
\frac{\partial E}{\partial \theta} &= 0 \\
\frac{\partial E}{\partial \varphi} &= 0
\end{align*}
\]

and making sure that its solution(s) are indeed at the minimum of the free energy, i.e. that the r.h.s. of (1) is strictly positive.
Outline of classical calculation method

1. fix the orientation and magnitude of the external field

2. find numerically the equilibrium position of magnetization vector \(\mathbf{M}\) and verify that it is stable

3. calculate the resonance frequency \(\omega\)

4. if \(\omega\) coincides with the frequency used in experiment then we have found the resonance field, otherwise the calculations should be repeated for other value of \(H_{ext}\) (with the same orientation).

The equilibrium position of \(\mathbf{M}\) may be hard to find (and thus inexact), since even in amorphous, i.e. non-crystalline, samples, usually \(\mathbf{M}\) and \(H_{ext}\) are NOT parallel.
Interval method

The list of 3D boxes $\Delta \varphi \times \Delta \theta \times \Delta H_{ext}$ is systematically reviewed, starting from the single initial box

\[ [0, 2\pi] \times [0, \pi] \times [0, H_{max}] \]

For each box in succession the series of tests are applied, leading either to elimination of the box from the list or to its splitting into two (smaller) offspring boxes. Failing any of the tests below (answer: NO) eliminates the box from list

- does the interval $\partial E/\partial \varphi$ contains zero?
- does the interval $\partial E/\partial \theta$ contains zero?
- does the interval describing r.h.s of relation (1) contains positive numbers?
- does the interval $\omega$, computed from relation (1) contains the experimental frequency $\omega_{exp}$?
Interval method — some details

Boxes not failing applied tests remain on the list. The largest of them is then selected and divided into two parts, each of which are tried again. We continue this procedure until the list is empty or contains only small boxes, i.e. in our case $\Delta \varphi = \Delta \theta \leq 2 \cdot 10^{-6}$ rad $\approx 10^{-4}$ degree, $\Delta H = 0.005$ Oe. The maximum length of list is usually close to 200, but occasionally, for some ”difficult” orientations, it exceeds 2000. On exit, the small neighboring boxes are 'glued' together, if necessary. In rare cases, for some directions of $\mathbf{H}$, this procedure leads to higher inaccuracy in determining $H_{res}$.

For amorphous wire, depending on orientation of $\mathbf{H}_{ext}$, zero, one, two or even more boxes (resonance fields) are returned, see figures.

Typical running time, for $\theta_{ext} = 0^\circ, 2^\circ, 4^\circ, \ldots 180^\circ$ is around 12 min. on a 100 MHz PC.
Advantages of interval method

- no resonance field is ever missed

- complete elimination of numerical inaccuracies

- the equilibrium positions are calculated exactly, without any simplifications, even when the anisotropies are quite complicated

- reliable replacement for other methods

- the method may be easily extended to reliably reconstruct the values of unknown anisotropy constants and other material parameters, together with their uncertainties, from experimental data, thus replacing the usual trial-and-error procedures. In this case no classical counterpart — other than guessing — exists.
Disadvantages of interval method

• negligible or non-existent knowledge of interval methods among the practitioners in the field and, generally, among physicists at large\(^1\)

• increased requirements for the raw computing power (moderate)

\(^1\)To find more on interval methods click on the URL:
http://www.cs.utep.edu/interval-comp/
List of figures

All figures simulated with: $\omega_{exp} = 2\pi \times 9.243$ GHz, 
g = 2.00 and $4\pi M_s = 6400$ Gs. Anisotropy constants 
$K_u$ and $K_4$ are given in $10^5 \times \text{erg/cm}^3$, angles ($x$-axis) 
in degrees, and resonance fields ($y$-axis) – in Gs.

1. No anisotropy at all, $K_u = K_4 = 0$
2. $K_u = -1.11$, $K_4 = 0$
3. $K_u = +0.20$, $K_4 = -K_u$
4. $K_u = +2.00$, $K_4 = +4.41$
5. $K_u = +1.59$, $K_4 = +2.85$
6. $K_u = +1.19$, $K_4 = -2.38$
7. $K_u = -0.19$, $K_4 = +2.90$
8. $K_u = -1.19$, $K_4 = +7.16$
9. $K_u = -1.39$, $K_4 = +3.18$
10. $K_u = -5.96$, $K_4 = -1.19$
11. $K_u = -7.16$, $K_4 = +4.77$
12. $K_u = -1.39$, $K_4 = +2.38$
Figure 1: No anisotropy at all, $\kappa = \kappa = 0$. 

$\kappa = 0$
Figure 2: \( K_u = -1.11 \times 10^5 \), \( K_4 = 0 \)
Figure 3: $K_u = +0.20 \times 10^5$, $K_4 = -K_u$. 
Figure 4: $K_u = +2.00 \times 10^5$, $K_4 = +4.41 \times 10^5$. 

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Figure 5: $K_u = +1.59 \times 10^5$, $K_4 = +2.85 \times 10^5$.
Figure 6: $K_u = +1.19 \times 10^5$, $K_4 = -2.38 \times 10^5$. 

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Figure 7: $K_u = -0.19 \times 10^5$, $K_4 = +2.90 \times 10^5$
Figure 8: $K_\theta = -1.19 \times 10^5 + 7.16 \times 10^5 K_4 = \frac{n}{\pi}$.
Figure 9: $K_u = -1.39 \times 10^5$, $K_4 = +3.18 \times 10^5$,
Figure 10: $K_u = -5.96 \times 10^5$, $K_4 = -1.19 \times 10^5$
Figure 11: \( K_u = -7.16 \times 10^5, \ K_4 = +4.77 \times 10^5 \)
Figure 12: $K_u = -1.39 \times 10^5$, $K_4 = +2.38 \times 10^5$