Python VNA-FMR Fitting Routine

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1 Initialization

1. Define folder path containing Raw S_{21} spectra vs. field
2. Define frequency window
3. Set field windowing (True/False), and set field window size (number of linewidths)
4. Create directories to save fit results
5. Import raw data
   (a) Field (H)
   (b) Re(S_{21})
   (c) Im(S_{21})
6. Define constants

$$g = 2.1 \tag{1}$$
$$\mu_B = 9.274 \times 10^{-24}\,\mathrm{J\,T^{-1}} \tag{2}$$
$$\hbar = \frac{1}{2\pi} 6.626 \times 10^{-34}\,\mathrm{J\,s} \tag{3}$$
$$\gamma = g\mu_\mathrm{B}/\hbar \tag{4}$$
$$f = \text{frequency extracted from spectrum filename, in Hz} \tag{5}$$
$$\mu_0 = 4\pi \times 10^{-7}\mathrm{H\,m^{-1}} \tag{6}$$
$$H_\mathrm{eff} = \frac{2\pi f}{\gamma\mu_0}\frac{4\pi}{10^3}\mathrm{Oe} \tag{7}$$

where the factor of $4\pi/10^3$ converts $\mathrm{A\,m^{-1}}$ to Oe, since that is the measured unit by the Hall probe in our experimental setup.

2 Data Conditioning

1. The LabVIEW code saves VNA data as the complex transmission data $\mathrm{Re}(S_{21})$ and $\mathrm{Im}(S_{21})$. Create the complex array:

$$S_{21} = \mathrm{Re}(S_{21}) + i\mathrm{Im}(S_{21}) \tag{8}$$

2. Estimate complex offset and slope in order to subtract the complex background and properly estimate the signal phase using the first and last values of the arrays:

$$\begin{aligned}
\mathrm{Re}(C_0)_{\mathrm{pre}} &= \langle \mathrm{Re}(S_{21}) \rangle & (9)\\
\mathrm{Im}(C_0)_{\mathrm{pre}} &= \langle \mathrm{Im}(S_{21}) \rangle & (10)\\
\mathrm{Re}(C_1)_{\mathrm{pre}} &= \frac{(\mathrm{Re}(S_{21})[\mathrm{end}] - \mathrm{Re}(S_{21})[0])}{(H[\mathrm{end}] - H[0])} & (11)\\
\mathrm{Im}(C_1)_{\mathrm{pre}} &= \frac{(\mathrm{Im}(S_{21})[\mathrm{end}] - \mathrm{Im}(S_{21})[0])}{(H[\mathrm{end}] - H[0])} & (12)
\end{aligned}$$

where the subscript "pre" indicates an estimated value used for the Lorentzian pre-fit of the data (Sec. 3). Correct $\mathrm{Re}(S_{21})$ and $\mathrm{Im}(S_{21})$ arrays accordingly:

$$\mathrm{Re}(S_{21})_{\mathrm{corr}} = \mathrm{Re}(S_{21}) - \left(\left[\mathrm{Re}(C_0)_{\mathrm{pre}} - \mathrm{Re}(C_1)\frac{(\max(H) + \min(H))}{2}\right] + \mathrm{Re}(C_1)_{\mathrm{pre}} * H\right) \tag{13}$$

$$\mathrm{Im}(S_{21})_{\mathrm{corr}} = \mathrm{Im}(S_{21}) - \left(\left[\mathrm{Im}(C_0)_{\mathrm{pre}} - \mathrm{Im}(C_1)\frac{(\max(H) + \min(H))}{2}\right] + \mathrm{Im}(C_1)_{\mathrm{pre}} * H\right) \tag{14}$$

3. Calculate $(S_{21})_{\mathrm{corr}}$, $|S_{21}|_{\mathrm{corr}}$, and $\arg(S_{21})_{\mathrm{corr}}$

3 Lorentzian Pre-Fit

1. Perform Lorentzian pre-fit to $|S_{21}|_{\mathrm{corr}}$ to determine initial guesses for:
   (a) amplitude, A
   (b) M_{eff}
   (c) linewidth, ΔH
   (d) phase, ϕ

using Lorentzian pre-fit equation:

$$L(H) = C_0 + C_1 H + \frac{A\Delta H^2}{(H - H_{\mathrm{res}})^2 + \Delta H^2} \tag{15}$$

where C_0 and C_1 here are real-valued and *not the same* as those used to normalize S_{21} (Eqs. 9–12 and 30). Also must generate initial guesses within the Lorentzian pre-fit function

$$\begin{aligned}
C_{0,\mathrm{Lor}} &= \frac{1}{2}\Big(|S_{21}|[\mathrm{end}] + |S_{21}|[0]\Big) && (16)\\
C_{1,\mathrm{Lor}} &= 0 && (17)\\
A_{\mathrm{Lor}} &= \max|S_{21}| - \min|S_{21}| && (18)\\
H_{\mathrm{res}} &= H[\text{index of } \max(|S_{21}|)] && (19)
\end{aligned}$$

and to generate an initial guess for the Lorentzian linewidth, ΔH:

$$\begin{aligned}
\mathrm{FHWM}_{\mathrm{min}} &= H[\text{largest index of } H \text{ where } H < H_{\mathrm{res}} \;\&\; |S_{21}| < \max|S_{21}| - \tfrac{1}{2}A_{\mathrm{Lor}}]\\
\mathrm{FHWM}_{\mathrm{max}} &= H[\text{smallest index of } H \text{ where } H > H_{\mathrm{res}} \;\&\; |S_{21}| < \max|S_{21}| - \tfrac{1}{2}A_{\mathrm{Lor}}]\\
\Delta H_{\mathrm{Lor}} &= \mathrm{FHWM}_{\mathrm{max}} - \mathrm{FHWM}_{\mathrm{min}} && (20)
\end{aligned}$$

4 Full Susceptibility Fit

1. Using results of the Lorenztian pre-fit, generate initial guesses for full complex susceptibility fit of $\mathrm{Re}(S_{21})$ and $\mathrm{Im}(S_{21})$:

$$\begin{aligned}
A_i &= 2A_{\mathrm{Lor}} && (21)\\
M_{\mathrm{eff}\,i} &= H_{\mathrm{res}} - \frac{2\pi f}{\gamma\mu_0}\left(\frac{4\pi}{10^3}\right) && (22)\\
\Delta H_i &= 2\Delta H_{\mathrm{Lor}} && (23)\\
\phi_i &= \arg(S_{21})_{\mathrm{corr}}[\text{index of } \max(|S_{21}|_{\mathrm{corr}})] && (24)\\
\mathrm{Re}(C_0)_i &= \mathrm{Re}(C_0)_{\mathrm{pre}} && (25)\\
\mathrm{Im}(C_0)_i &= \mathrm{Im}(C_0)_{\mathrm{pre}} && (26)\\
\mathrm{Re}(C_1)_i &= 0 && (27)\\
\mathrm{Im}(C_1)_i &= 0 && (28)
\end{aligned}$$

   Because $\chi_{yy} = M_{\mathrm{eff}}/\Delta H$ on resonance, re-scale A_i:

$$A_i = A_i \frac{\Delta H_i}{M_{\mathrm{eff}\,i}} \tag{29}$$

2. I force ϕ_i to lie between 0 and $+2\pi$.

3. Define upper and lower bounds for fit parameters:

Parameter	Lower Bound	Upper Bound
A	0	$+\infty$
M_{eff}	0	$+\infty$
ΔH	0	$+\infty$
ϕ	0	2π
$\text{Re}(C_0)$	$-\infty$	$+\infty$
$\text{Im}(C_0)$	$-\infty$	$+\infty$
$\text{Re}(C_1)$	$-\infty$	$+\infty$
$\text{Im}(C_1)$	$-\infty$	$+\infty$

4. Fit S_{21} data with full complex susceptibility using non-linear least squares:

$$S_{21} = C_0 + C_1 H + Ae^{i\phi}\chi_{yy} \tag{30}$$

$$\chi_{yy} = \frac{M_{\text{eff}}(H - M_{\text{eff}})}{(H - M_{\text{eff}})^2 - H_{\text{eff}}^2 + i\Delta H H_{\text{eff}}} \tag{31}$$

where C_0 and C_1 are complex offset and slope to the data, the $+i$ in the denominator is chosen for the counter-clockwise rotation convention of most VNAs, and the complex pre-factor $Ae^{+i\phi}$ is the overall signal amplitude and phase, inclusive of signal loss and phase shift due to cable length. Both $Ae^{i\phi}$ and χ_{yy} are chosen to accomodate counter-clockwise rotation.

5. Calculate H_{res} from M_{eff} fit result:

$$H_{\text{res}} = \frac{2\pi f}{\gamma\mu_0}\left(\frac{4\pi}{10^3}\right) + M_{\text{eff}} \tag{32}$$

6. Calculate insertion loss:

$$\text{IL (dB)} = 20\log_{10}\left(\sqrt{(\text{Re}(C_0) + \text{Re}(C_1)H_{\text{res}})^2 + (\text{Im}(C_0) + \text{Im}(C_1)H_{\text{res}})^2}\right) \tag{33}$$

5 Error Analysis

Define the fit function of Eq. 30 as $f(H;\mathbf{k})$ with independent variable H, and $\mathbf{k}$ is the vector of 8 fit parameters

$$\mathbf{k} = [A, M_{\text{eff}}, \Delta H, \phi, \text{Re}(C_0), \text{Im}(C_0), \text{Re}(C_1), \text{Im}(C_1)] \tag{34}$$

Python's "optimize.least_squares" routine acts to minimize an objective function of the form

$$r_i = f(H_i;\mathbf{k}) - y_i \tag{35}$$

where H_i is the array of field points at which measurements y_i are taken.

The Jacobian is defined as

$$J(\mathbf{k})_{ij} = \frac{\partial r_i(\mathbf{k})}{\partial k_j} \tag{36}$$

where $j = 1, ..., 8$ and $i = 1, ..., n$ for n field points at which measurements are acquired.

1. From the Jacobian, I calculate the Hessian as $\mathbb{H} = \mathbb{J}^T\mathbb{J}$
2. Calculate σ_r^2, the variance of the residual (a vector which is also returned by "optimize.least_squares" routine).
3. Calculate the covariance matrix: $\Sigma = \sigma_r^2(\mathbb{H}^{-1})$
4. Calculate the standard error of each of the 8 fit parameters (diagonal elements of $\sqrt{|\Sigma|}$).

6 Post-Processing

6.1 Kittel Fit

Linear fit of H_{res} vs. f (weighted by error bars of H_{res} as determined from Susceptibility Fit):

$$H_{\text{res}} = \frac{2\pi}{(g\mu_{\text{B}}/\hbar)\mu_0}\left(\frac{4\pi}{10^3}\right)f + M_{\text{eff}} \tag{37}$$

g and M_{eff} are extracted fit parameters (H_{res} and M_{eff} in [Oe]).

6.2 Linewidth Fit

Linear fit of ΔH vs. f (weighted by error bars of ΔH as determined from Susceptibility Fit):

$$\Delta H = \frac{4\pi\alpha}{\gamma\mu_0}\left(\frac{4\pi}{10^3}\right)f + \Delta H_0 \tag{38}$$

α and ΔH_0 (in [Oe]) are extracted fit parameters.

6.3 Inductance Analysis

1. The complex background is calculated as

$$\begin{aligned} Z_{\text{BG}} &= \Big[\text{Re}(C_0) + \text{Re}(C_1)H_{\text{res}}\Big] + i\Big[\text{Im}(C_0) + \text{Im}(C_1)H_{\text{res}}\Big] && (39) \\ A_{\text{BG}} &= |Z_{\text{BG}}| && (40) \\ \phi_{\text{BG}} &= \arctan\Big(\text{Im}(Z_{\text{BG}})/\text{Re}(Z_{\text{BG}})\Big) && (41) \end{aligned}$$

2. The complex signal is defined as the pre-factor of χ_{yy} in Eq. 30

$$Z = Ae^{i\phi} \tag{42}$$

where A and ϕ are fit parameters of the full susceptibility fit.

3. The complex sample inductance is calculated

$$L = \left(\frac{2Z_0}{2\pi f}\right)\frac{Z}{Z_{\mathrm{BG}}}e^{i\pi/2} \tag{43}$$

where Z/Z_{BG} is complex division, $Z_0 = 50\,\Omega$, and the additional $\pi/2$ rotation is added to convert an impedance to an inductance.

4. Linear fits to $\mathrm{Re}(L)$ vs. f and $\mathrm{Im}(L)$ vs. f are used to extract $\mathrm{Re}(L)|_{f=0}$ and $\mathrm{Im}(L)|_{f=0}$. From this, we calculate an initial guess for the anomalous phase $\phi_{\mathrm{a},i}$

$$\phi_{\mathrm{a},i} = \arctan\left(\frac{\mathrm{Im}(L)|_{f=0}}{\mathrm{Re}(L)|_{f=0}}\right) \tag{44}$$

This provides a reasonable value for the anomalous phase. However, it is best to do a simultaneous fit to $\mathrm{Re}(L)$ and $\mathrm{Im}(L)$, instead of two separate linear fits. I therefore define a 4-parameter fit, with parameters L_0, $\mathrm{Re}(\partial_f L)$, $\mathrm{Im}(\partial_f L)$, and ϕ_a. I then proceed to fit the Re and Im inductance data simultaneously with a least-squares fit where the error function is defined as:

$$\text{concatenate}\left[\frac{(f_R(L_0, \mathrm{Re}(\partial_f L), \mathrm{Im}(\partial_f L), \phi_\mathrm{a}) - \mathrm{Re}(L))}{\sigma_{\mathrm{Re}(L)}}, \right.$$
$$\left.\frac{(f_I(L_0, \mathrm{Re}(\partial_f L), \mathrm{Im}(\partial_f L), \phi_\mathrm{a}) - \mathrm{Im}(L))}{\sigma_{\mathrm{Im}(L)}}\right] \tag{45}$$

where $\sigma_{\mathrm{Re}(L)}$ and $\sigma_{\mathrm{Im}(L)}$ are the errors associated with the Re and Im parts of L, and f_R and f_I are linear equations for the Re and Im inductances:

$$f_R = [L_0 + \mathrm{Re}(\partial_f L)f]\cos(\phi_\mathrm{a}) - [\mathrm{Im}(\partial_f L)f)]\sin(\phi_\mathrm{a}) \tag{46}$$
$$f_I = [\mathrm{Im}(\partial_f L)f)]\cos(\phi_\mathrm{a}) + [L_0 + \mathrm{Re}(\partial_f L)f]\sin(\phi_\mathrm{a}) \tag{47}$$

The least squares fit minimizes the sum of the squares of the residuals between these fit functions and the data $\mathrm{Re}(L)$ and $\mathrm{Im}(L)$, and reports a final value for ϕ_a.

5. A corrected complex inductance L_{corr} is calculated as $Le^{-i\phi_\mathrm{a}}$ in order to rotate the inductance in the complex plane, to enforce that $\mathrm{Im}(L)|_{f=0} = 0$.

6. $\mathrm{Re}(L)_{\mathrm{corr}}$ and $\mathrm{Im}(L)_{\mathrm{corr}}$ are plotted vs. frequency. Each is fit to a straight line to extract:

(a) $L_0 \equiv \mathrm{Re}(L)_{\mathrm{corr}}|_{f=0}$

(b) $\partial(\mathrm{Re}(L)_{\mathrm{corr}})/\partial f$

(c) $\partial(\mathrm{Im}(L)_{\mathrm{corr}}/\partial f$

(note that $\mathrm{Im}(L)_{\mathrm{corr}}|_{f=0} = 0$, by the action of Step 5).

- Error is propagated through each of the above steps in order to provide error bars on $\mathrm{Re}(L)_{\mathrm{corr}}$ and $\mathrm{Im}(L)_{\mathrm{corr}}$.

7 Data Saving

The following results are saved:

1. Figures of the Lorentzian prefit (magnitude and phase as a function of field) are saved in \MagS21.

2. Figures of Re and Im S_{21} fits (included initial guesses (dashed lines) and final fit (solid lines)) are saved in \S21.

3. Susceptibility fit results (Freq (GHz), H_{res} (Oe), ΔH (Oe), A, ϕ (rad), $\mathrm{Re}(C_0)$, $\mathrm{Im}(C_0)$, $\mathrm{Re}(C_1)$, $\mathrm{Im}(C_1)$, insertion loss (dB), and associated errors) are saved as "Susceptibility Fit Results.csv" as tab-delimited data

4. Kittel fit figure is saved as "Kittel Fit.png"

5. Damping fit figure is saved as "Damping Fit.png"

6. Spectroscopy results (M_{eff} (Oe), g, ΔH_0 (Oe), α, and associated errors) are saved in "Spectroscopy Fit Results.csv" as tab-delimited data

7. Inductance results (Freq (GHz), $\mathrm{Re}(L)$, $\mathrm{Im}(L)$, $\mathrm{Re}(L_{\mathrm{corr}})$, $\mathrm{Im}(L_{\mathrm{corr}})$) are saved as "Inductance Results.csv" as tab-delimited data

8. Corrected inductance results (L_0 (H), dRe(L)/df (H/GHz), dIm(L)/df (H/GHz), ϕ_{a} (rad), and associated errors) are saved as "L_corr vs f Fit Results.csv" as tab-delimited data

9. Spectroscopy and inductance results from "Spectroscopy Fit Results.csv" and "L_corr vs f Fit Results.csv" are combined into a single file "All Results.csv"