Fitting Code Explanation

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1 Introduction

This document explains the theory behind, and the operation of the python file, fitS21.py, which were are using to fit the transmission of our resonators. The code is designed to extract the relevant data from the .csv files which are saved by the vector network analyzer (VNA) in the lab, fit this data to the resonators transmission equation (derived below), and from this fit, extract the resonators resonant frequency, f_r, total quality factor, Q, and its intrinsic and coupling quality factors, Q_i and Q_c.

2 Derivation of Equations

Figure 1 shows the model of a parallel LC resonant circuit, coupled to two transmission lines of impedance, Z_0 (3). This can be simplified to a shunt admittance Y, coupled to two transmission lines with admittances, Y_1 and Y_2, as in Figure 2. RF circuit theory describes the S-paramaters for such a circuit (see (1)).

$$\begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \frac{1}{D_S} \begin{bmatrix} Y_1 - Y_2 - Y & \sqrt{2Y_1Y_2} \\ \sqrt{2Y_1Y_2} & Y_1 - Y_2 - Y \end{bmatrix}$$

Here, $D_S = Y + Y_1 + Y_2$.
Thus, this gives:

$$S_{21} = \frac{2\sqrt{Y_1Y_2}}{Y + Y_1 + Y_2} \tag{1}$$

From 1, the admittance of the transmission lines are given by:

$$Y_1 = Y_2 = \frac{1}{Z_0} = Y_0 \tag{2}$$

Moreover, with the admittance of an inductor given by $Y_L = \frac{1}{j\omega L}$, and the admittance of a capacitor as $Y_C = j\omega C$, this gives:

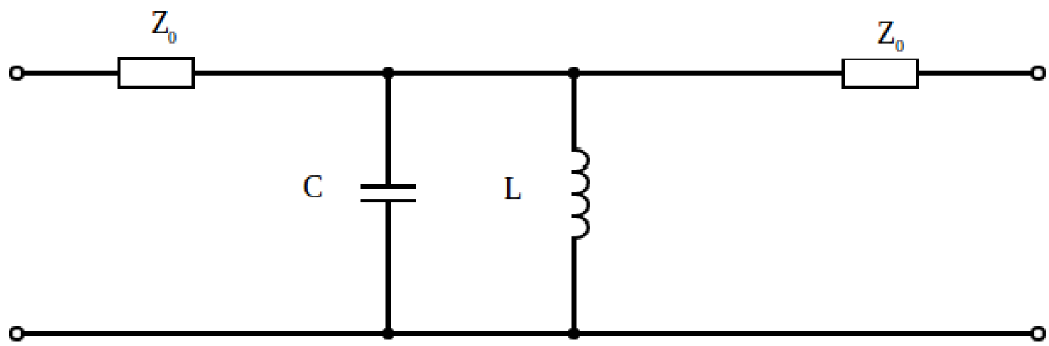

Figure 1: LC Resonator Circuit

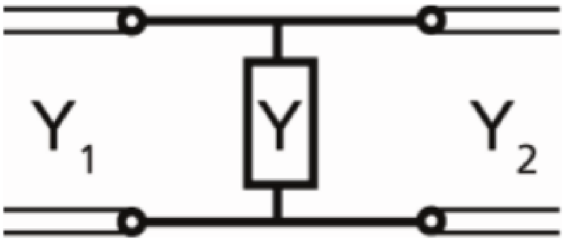

Figure 2: Shunt Admittance Circuit

$$Y = \frac{1}{j\omega L} + j\omega C \tag{3}$$

Thus, S_{21} can be written as:

$$S_{21} = \frac{2\sqrt{Y_0 Y_0}}{Y + Y_0 + Y_0} \tag{4}$$

$$\implies S_{21} = \frac{2Y_0}{Y + 2Y_0} \tag{5}$$

$$\implies S_{21} = \frac{2}{2 + \frac{Y}{Y_0}} \tag{6}$$

$$\implies S_{21} = \frac{2}{2 + YZ_0} \tag{7}$$

Substituting in the equation for Y gives:

$$\implies S_{21} = \frac{2}{2 + Z_0(\frac{1}{j\omega L} + j\omega C)} \tag{8}$$

$$\implies S_{21} = \frac{2}{2 + Z_0(j\omega C - \frac{j}{\omega L})} \tag{9}$$

$$\implies S_{21} = \frac{2}{2 + j(Z_0\omega C - \frac{Z_0}{\omega L})} \tag{10}$$

$$\implies S_{21} = \frac{2}{2 + 2j(\frac{Z_0\omega C}{2} - \frac{Z_0}{2\omega L})} \tag{11}$$

$$\implies S_{21} = \frac{1}{1 + j(\frac{Z_0\omega C}{2} - \frac{Z_0}{2\omega L})} \tag{12}$$

$$\implies S_{21} = \frac{1}{1 + j(\frac{Z_0\omega C}{2} - \frac{Z_0\omega C}{2}\frac{1}{\omega L}\frac{1}{\omega C})} \tag{13}$$

$$\implies S_{21} = \frac{1}{1 + j\frac{Z_0\omega C}{2}(1 - \frac{1}{\omega^2 LC})} \tag{14}$$

It can be easily shown that for an LC resonator circuit the resonant frequency of the circuit is $\omega_0 = \frac{1}{\sqrt{LC}}$, and its quality factor is $Q = \frac{\omega_0 Z_0 C}{2}$.

Thus, S_{21} can be further simplified to:

$$S_{21} = \frac{1}{1 + jQ(1 - \frac{\omega_0{}^2}{\omega^2})} \tag{15}$$

For the sake of simplicity, this is then rewritten in terms of x, where $\delta x = \frac{\omega - \omega_0}{\omega_0}$.
For small perturbations from the resonant frequency $\delta x = \frac{\delta\omega}{\omega_0} \ll 1$ and $\omega = \omega_0 + \delta\omega$.
This allows the equation for S_{21} to be rewritten as:

$$S_{21} = \frac{1}{1 + jQ(1 - \frac{{\omega_0}^2}{(\omega_0+\delta\omega)^2})} \tag{16}$$

$$\implies S_{21} = \frac{1}{1 + jQ(1 - (\frac{\omega_0}{\omega_0+\omega_0\delta x})^2)} \tag{17}$$

$$\implies S_{21} = \frac{1}{1 + jQ(1 - (\frac{1}{1+\delta x})^2)} \tag{18}$$

$$\implies S_{21} = \frac{1}{1 + jQ(\frac{(1+\delta x)^2-1}{(1+\delta x)^2})} \tag{19}$$

$$\implies S_{21} = \frac{1}{1 + jQ(\frac{1+2\delta x+(\delta x)^2-1}{1+2\delta x+(\delta x)^2})} \tag{20}$$

Since, $\delta x \ll 1$, $(\delta x)^2 \approx 0$.

$$\implies S_{21} = \frac{1}{1 + jQ(\frac{2\delta x}{1+2\delta x})} \tag{21}$$

And, since $\delta x \ll 1$

$$S_{21} = \frac{1}{1 + jQ(2\delta x)} \tag{22}$$

$$\implies S_{21} = \frac{1}{1 + 2jQ\delta x} \tag{23}$$

Note fitting to a complex equation with Python is extremely susceptible to the initial guess. Thus, it is found that it is better to instead fit to $|S_{21}|^2$, where:

$$|S_{21}| = \frac{1}{\sqrt{1 + 4Q^2\delta x^2}} \tag{24}$$

$$\implies |S_{21}|^2 = \frac{1}{1 + 4Q^2\delta x^2} \tag{25}$$

Substituting in $\delta x = \frac{\omega-\omega_0}{\omega_0}$ gives,

$$\implies |S_{21}|^2 = \frac{1}{1 + 4Q^2(\frac{\omega-\omega_0}{\omega_0})^2} \tag{26}$$

This is then used to fit the data to a skewed Lorentzian model, with constant background A_1, background slope A_2, maximum A_3 and skew A_4 (2) (4):

$$|S_{21}(\omega)|^2 = A_1 + A_2(\omega - \omega_0) + \frac{A_3 + A_4(\omega - \omega_0)}{1 + 4Q^2(\frac{\omega-\omega_0}{\omega_0})^2} \tag{27}$$

Note that while here $|S_{21}|^2$ is being used, the phase of S_{21}, θ can also be used.

Fitting the VNA data to the above, gives us values for the resonant frequency of the resonator ω_0, and its total quality factor Q. These are then used to calculate the intrinsic quality factor Q_i, and coupling quality factor Q_c, using (5) (2):

$$Q_i = \frac{Q}{min(|S_{21}|)} \tag{28}$$

And,

$$Q_c = \frac{Q}{1 - min(|S_{21}|)} \tag{29}$$

References

[1] F. Caspers. Rf engineering basic concepts: S-parameters, 2012.

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