UWA Research Summary

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Abstract

To utilize specific resonant mode (Whispering Gallery Mode) of crystal resonators to characterize its property, an efficient and robust peak finding algorithm is needed for distinguishing and locating resonant peaks in transmission spectrum. Traditional peak finding functions, for example, *peak_find* function in python, mainly focus on detecting Lorentzian curve in transmission amplitude vs. frequency image. There is an intrinsic drawback of this method: it only makes use of amplitude data, while both amplitude and phase data are measured in experiment. In this research, an algorithm was developed which distinguishes resonant modes with both amplitude and phase data (2.1), based on the fact that complex transmission coefficients of a resonant mode form a circle on complex plane (1.2). Then this algorithm was used to search for resonant modes in a KTO resonator's spectrum. The results show that this algorithm is more robust in atypical situations and more precise when two peaks are extremely close to each other (2.2). Finally, I packed this algorithm in a Python GUI for further using by others and in that, some interactive functions are implemented for convenience and simplicity.

CONTENT

1. Basic Theory

1.1. Resonance[1]

A typical resonator circuit is showed in Figure 1. the input impedance of it is

$$Z_{LCR} = \left(\frac{1}{i\omega L_n} + i\omega C + \frac{1}{R}\right) \approx \frac{R}{1 + 2iRC(\omega - \omega_n)}$$

and internal quality factor

$$Q_{int} = \omega_n RC = \frac{n\pi}{2\alpha l}$$

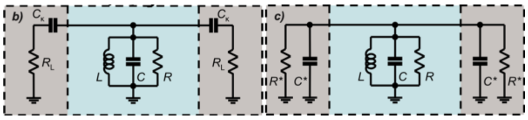

Figure 1. Lumped element representation of resonator circuit. The second picture shows how coupling capacitors are taken into consideration.

where L_n represents the inductance of nth mode and α is the attenuation coefficient. Taking coupling capacitor C_κ into consideration, we get

$$\frac{1}{Q_L} = \frac{1}{Q_{int}} + \frac{1}{Q_{ext}}$$

where $Q_{ext} = \frac{\omega_n R^* C}{2}$.

The ABCD matrix of this system is

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & Z_{in} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix}_{LCR} \begin{pmatrix} 1 & Z_{out} \\ 0 & 1 \end{pmatrix}.$$

$Z_{in/out}$ describes the coupling port of this system and t_{ij} represents the matrix of LCR circuit, which is

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}_{LCR} = \begin{pmatrix} 1 & 0 \\ 1/Z_{LCR} & 1 \end{pmatrix}$$

According to Reference[2], scattering matrix element S_{21} is

$$S_{21}(f) = \frac{2}{A + \frac{B}{Z_0} + CZ_0 + D} \propto \frac{Q_{int}}{1 + 2Q_{int} i \left(\frac{f}{f_r} - 1\right)}$$

So, by measuring circuits transmission response S_{21} under different frequency we can determine the property of this resonator. If we plot S_{21} values of different frequencies onto complex plane, they form a circle as shown in Figure 2. This is the theory basis of following resonant peaks detection method.

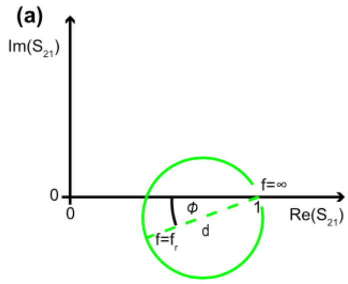

Figure 2. S_{21} circle on complex plane[3]

In our experiment, the physical resonator is a metal cavity with dielectric materials (cylinder sapphire) filled in. Electromagnetic field in this cavity will oscillate in Whisper Gallery Modes (WHG modes). Space is separated into three parts to describe these modes

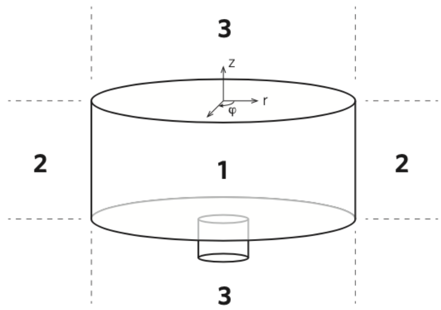

Figure 3. Cylindrical coordinate of EMF in a sapphire resonator[4]

$$E_{z1} = A_1 J_m(k_E r)\cos(\beta z)\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

$$E_{z2} = A_2 K_m(k_{out} r)\cos(\beta z)\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

$$E_{z3} = A_3 J_m(k_E r)\mathrm{e}^{-\alpha z}\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

$$H_{z1} = B_1 J_m(k_H r)\cos(\beta z)\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

$$H_{z2} = B_2 K_m(k_{out} r)\cos(\beta z)\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

$$H_{z3} = B_3 J_m(k_E r)\mathrm{e}^{-\alpha z}\begin{cases}\cos(m\varphi)\\ \sin(m\varphi)\end{cases}$$

where k_E, k_H and k_{out} are the dielectric propagation constants for E-modes, H-modes, and free space in that order, α and β are axial decay constant outside the dielectric and longitudinal propagation constant.

The degeneracy ($\sim MHz$) caused by $\cos(m\varphi)$ and

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1 *Journal of Applied Physics* 104, 113904 (2008)
2 Microwave Engineer, David M. Pozar, 3rd version
3 *Review of Scientific Instruments* 86, 024706 (2015); doi: 10.1063/1.4907935
4 Effects of Electron Spin Resonance in a Cryogenic Sapphire Whispering Gallery Mode Maser, Daniel L. Creedon.

$sin(m\varphi)$ can be detected in following chapters.

1.2. Circle Detection Using Hough Algorithm

As shown in last part, resonant peaks will appear as a circle in transmission data on complex plane. Traditional peak finding methods mainly focus on looking for peaks in transmission amplitude, $|S_{21}|$, because $|S_{21}|$ spectrum has a typical Lorentzian shape which is well investigated and easy to fit. Most professional calculation software has internal function for fitting Lorentzian curve. So, in most cases this is the best and most efficient way to find resonant peaks.

But there is an intrinsic drawback of this method: it only exploits amplitude information from the experiment and most measuring devices (like Vector Network Analyzer) gives both amplitude and phase of transmission coefficient. Under some special circumstances shown in following parts, where noise or imperfection factors dominate, we need to exploit as much information as we can to extract useful parameters and guarantee precision. This is why we choose S_{21} circle detecting as substitution of Lorentzian fitting.

This method aims to detect arcs (or a complete circle) in transmission data using Hough transformation. Because complex transmission coefficients contain all information from experiment, this method exploits both amplitude and phase information of the resonator, which helps to increase detection sensitivity and fitting precision. Following is an introduction of Hough Transformation:

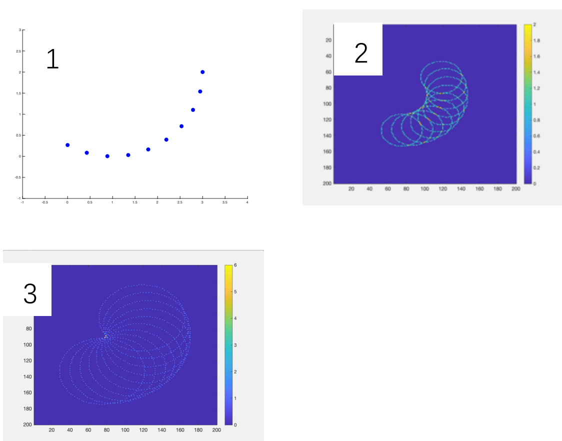
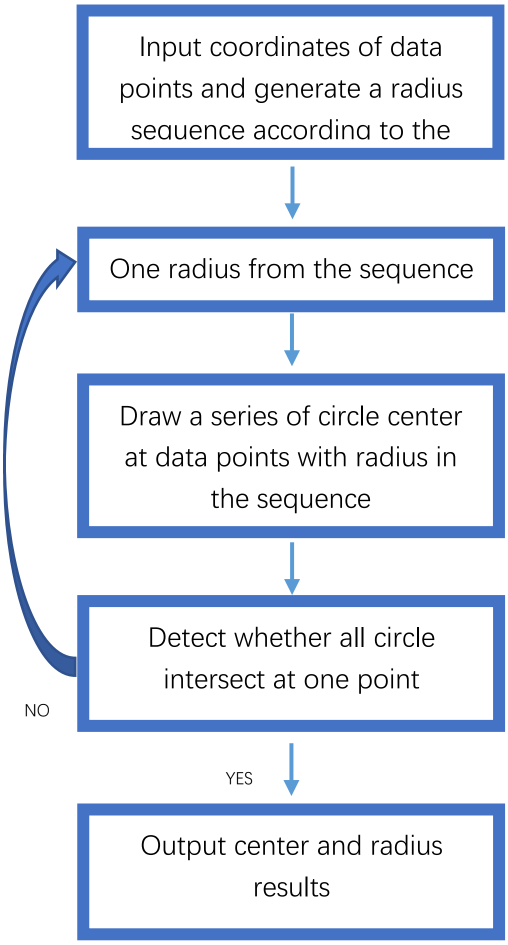


Figure 3. Hough Transformation process (double click the second picture to view the video). 1. The first picture shows the data points on an unknown circle and 2. the second picture shows how Hough Transformation find the intersection points among iterations of radius. 3. The third picture shows the result found.

When a circle is described by

$$x = a + r \cdot \cos\varphi$$
$$y = b + r \cdot sin\varphi$$

and we have coordinates of many sample points (x, y), we can draw a circle with every point with the point as center and a specific radius r. If r equals the radius of the circle which all data points belong to, all circles we draw intersect at one point (where is the center of data formed circle). So, the algorithm runs as:



This process is shown in Figure 3. and a video is used to manifest how it tests different radius and find the wanted circle according to intersection between drawn circles. Result of this example is shown in Figure 3.

1.3. Cable Delay

According to reference[5], cable delay may distort the S_{21} circle to highly spiral shape and it must be eliminated before use Hough detection. Cable delay can be described by

$$S_{21}^{delay}(f) = e^{-2\pi i f\tau} S_{21}(f)$$

[5] Review of Scientific Instruments 86, 024706 (2015); doi: 10.1063/1.4907935

where τ is the result of it. With cable delay, phases of S_{21}^{dalay} have a uniform non-zero gradient along f axis. This can be shown by experiment result:

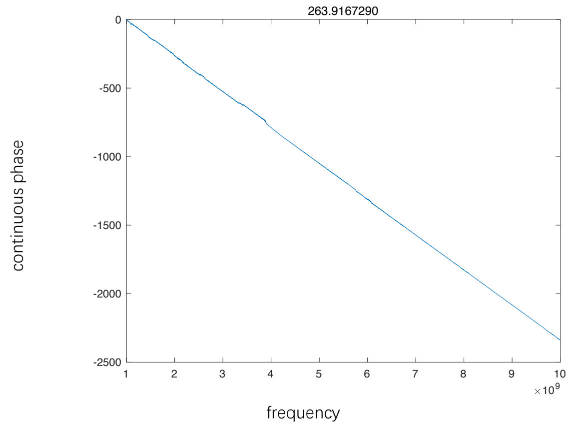


Figure 4. Continuous phase (not limited between $-\pi$ and π) of transmission coefficients. A uniform gradient over whole frequency band is shown.

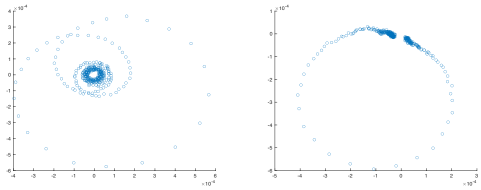


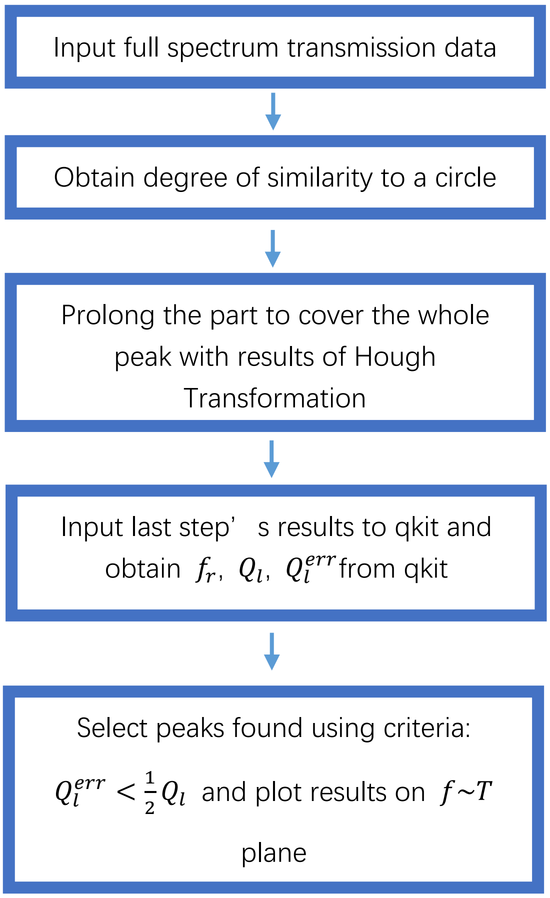
Figure 5. S_{21} of one resonant peak on complex plane before and after revision.

It is easy to revise cable delay: Using linear fitting model we obtain the gradient of the continuous phase data, $k = -\tau$, then multiply this term, $e^{-2\pi i k f}$, with experiment data and the cable delay is revised. The results are shown in Figure 5, which is good enough for Hough Algorithm to detect circle in data.

2. Algorithm Realization

2.1. Procedure of Peak Detecting

As mentioned in 1.2, the problem of recognizing resonant peaks is transformed to detecting circles in complex transmission coefficient data.



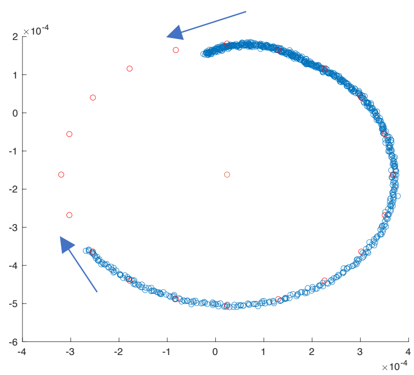


Figure 6. Prolong the found sequence. Blue points are selected raw data and red points denote the theoretical circle which blue points belong to. More data points will be selected if they fall in a certain range near the circle.

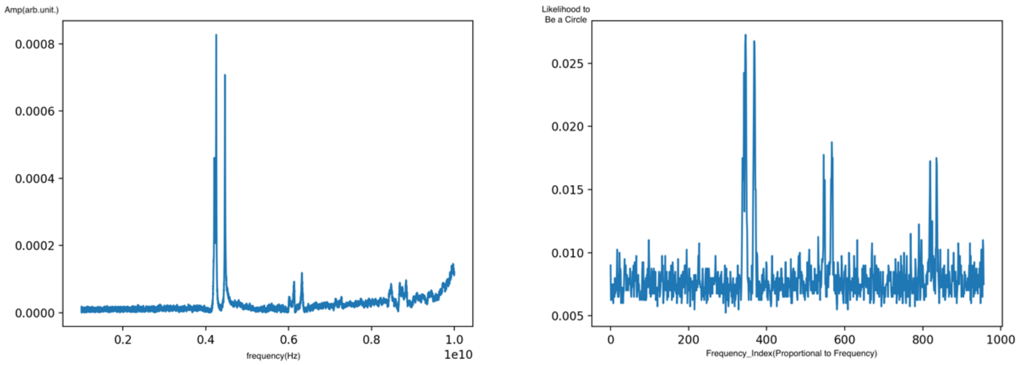


Figure 7. (Left) Transmission spectrum of KTO resonator under 285K. (Right) Degree of similarity to a circle of transmission spectrum calculated by Hough algorithm.

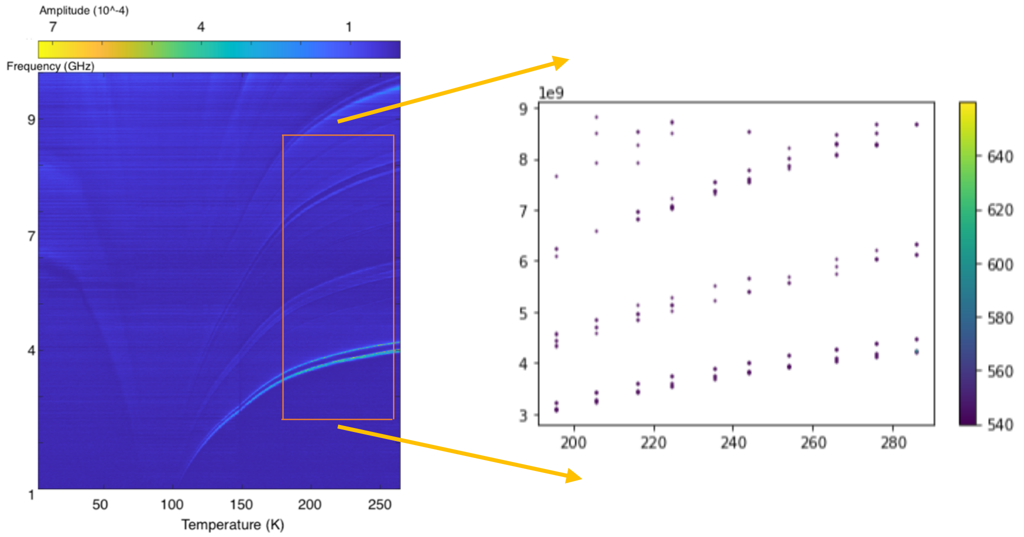


Figure 8. Transmission spectrum under different temperature. The color map shows resonant peaks by light color and the region in red rectangular was used to search for peaks. Searching results are plotted in right with each point represents a resonant peak and its color represents its quality factor. The error of fitting quality factor is used to filter out bad results. Plot all found peaks on Frequency ~ Temperature plane, a temperature dependence of resonance frequency is clearly showed.

Raw data from experiment contains transmission coefficients of a resonator under different frequencies and temperatures (See Figure 8). For example, transmission data under 285K is shown in Figure 7 Left. Full spectrum data is divided into small pieces and the algorithm will calculate the similarity between the shape that data in each piece forms and a circle. High similarity implies that there is probably a resonant peak in that region. Once the similarity surpasses a certain threshold, this piece of data is selected. All selected pieces are prolonged and this process is shown in Figure 6: since the length of data pieces is determined empirically, actual resonant peaks may contain a wider frequency span that the preset piece length. So, once a sequence of data is selected, Hough algorithm will also give out the circle it belongs to. On each edge of this sequence, the algorithm tests adjacent point out of this piece to see whether it falls near enough to the circle. If true, this point is added to the selected sequence to consist a complete resonant peak.

2.2. The Reason Why Use Hough Algorithm.

2.2.1. Resonant Valley

According to analysis above, a resonance peaks appears as a peak in transmission spectrum which is the basic principle of most traditional algorithm. But sometimes environment factors distort the shape of peaks so seriously that to a valley. This phenomenon is showed as following. Under this situation, peak-finding methods won' t even have a chance to detect it because of its valley-like shape. In Figure 9, although the transmission coefficient amplitudes look like random noise and the amplitude is just the opposite of peak-a valley, the fitting results shows the complex amplitudes was on a circle.

Furthermore, the amplitude and phase of fitting results agreed well with experiment data, which confirms that this is indeed a resonant peak. Unfortunately, this is not a rare phenomenon in spectrum data. The reason why some resonant modes appear as a valley is that cross talk between resonator and unknown element results in

$$S_{21}^{shift} = S_{21} + S_c$$

$$= \frac{Q_{int}}{1 + 2Q_{int} i \left(\frac{f}{f_r} - 1\right)} + S_{cr} + iS_{cx}.$$

Thus, the circle represents complex transmission coefficients is shifted on the complex plane. Once the circle is shifted towards origin, a resonant valley appears.

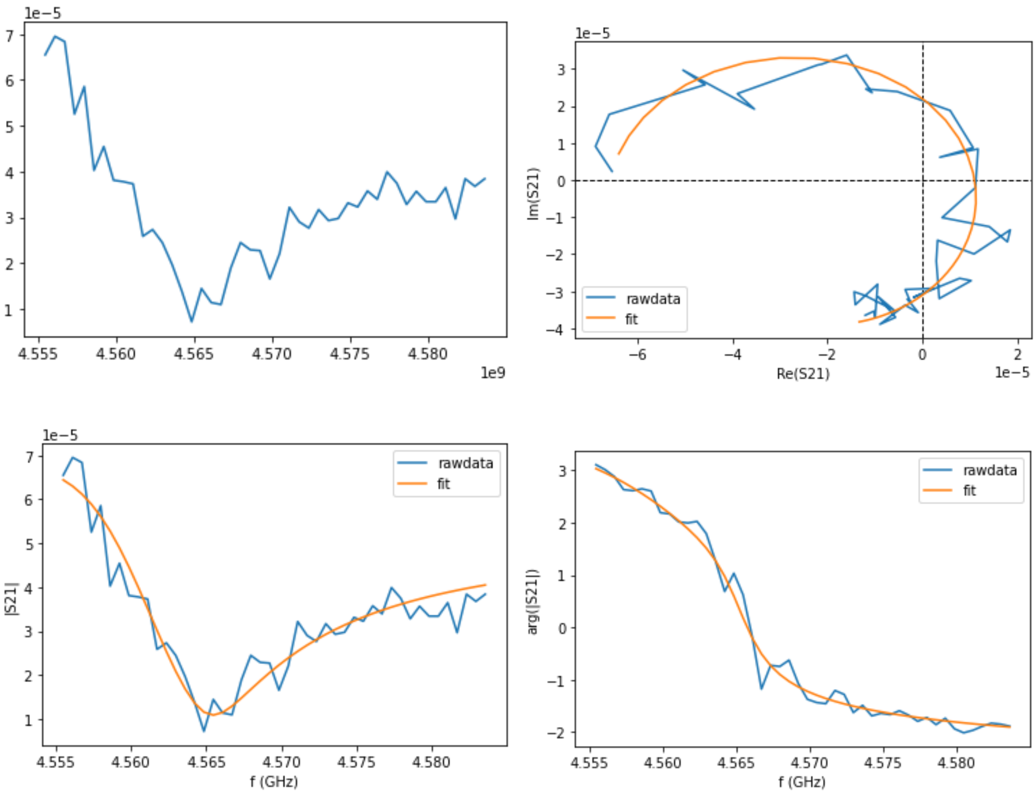


Figure 9. Detection of a resonant valley

2.2.2. Distinguish overlapped peaks caused by frequency degeneracy

In Dr. Daniel Creedon' s PhD thesis, an argument is made that in Whisper Gallery modes, the difference between $sin\varphi$ and $cos\varphi$, for example

$$E_{z1} = A_1 J_m(k_E r)\cos(\beta z)\begin{cases}\cos(m\varphi) \\ \sin(m\varphi)\end{cases}'$$

can lead to difference in resonant frequency due to imperfections in the sapphire. But the difference is very small. In his thesis, the difference between two modes is approximately $10^5 Hz$, with a resonant frequency several $GHz(10^9 Hz)$. So, the two overlapped peaks are a little bit (0.01%) away from each other.

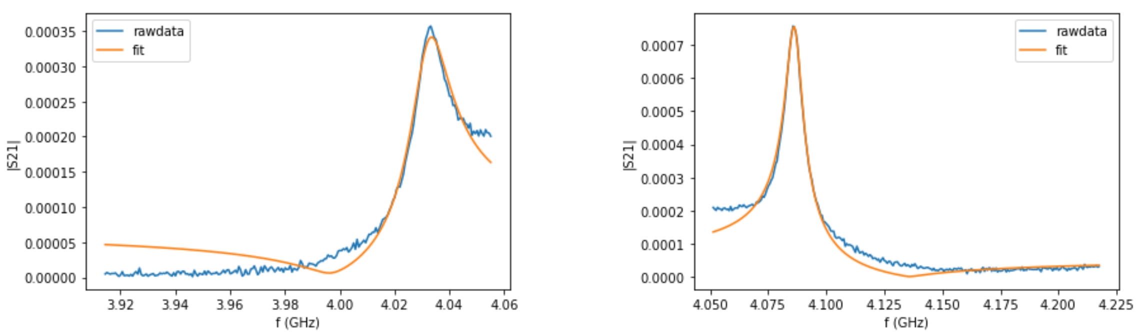


Figure 10. Two overlapped peaks detected by Hough Algorithm.

The fitted resonant frequencies of modes shown in Figure 10 are:

f_{left}: $4032064923.5181355\ Hz$; f_{right}: $4086349009.0768647\ Hz$

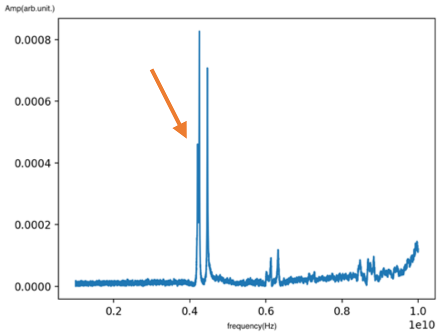


Figure 11. The part of spectrum showed in Figure 10.

2.2.3. Comparison with python *find_peaks* Function

Python' s internal function *find_peaks* can also detect peaks at fast speed at cost of ignoring some useful information. The same spectrum showed in Figure 6. is processed by *find_peaks*. Results are shown in Figure 12. Prominence is a fitting parameter need to be set manually and according to the explanation in its documents, its function is similar to threshold: it requires the peak to be prominent enough to be regarded as effective. Apparently, when prominence is low, many noisy signals are considered as effective peaks and when prominence is high, the function missed useful information in the spectrum.

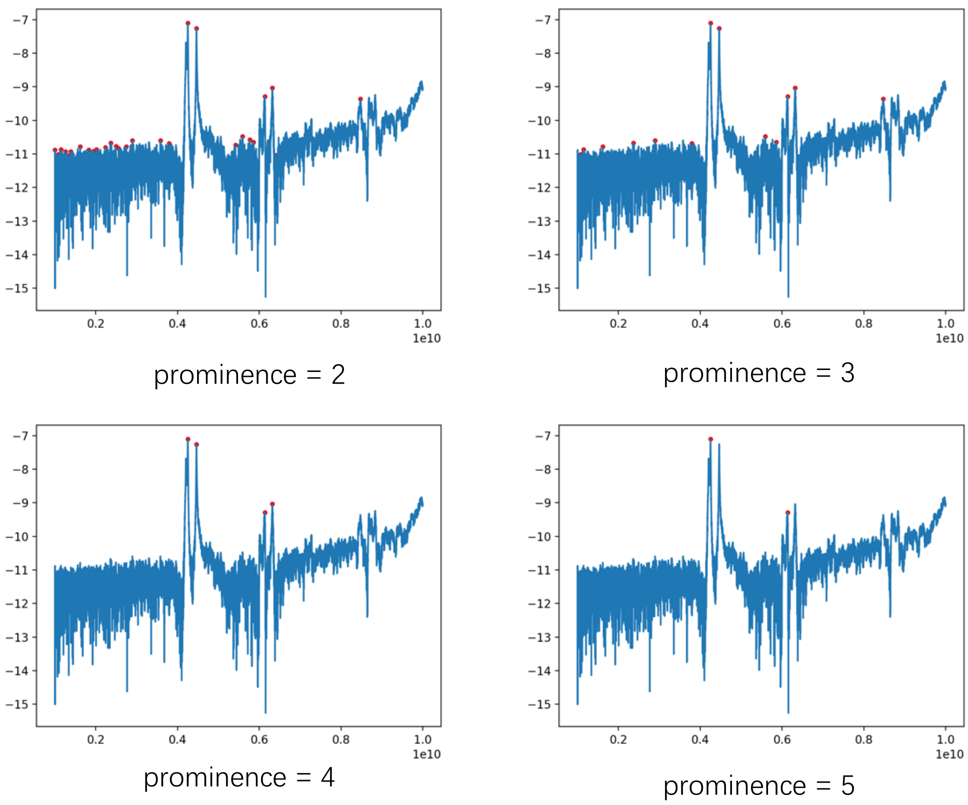


Figure 12. find_peaks result under different standard. Amplitudes are plotted in logarithm form. find_peaks either finds too much peaks under small prominence threshold or too less under big prominence. Especially, it never detects the degeneracy phenomenon around $4\mathrm{GHz}$*, which is shown in details in Figure 13.*

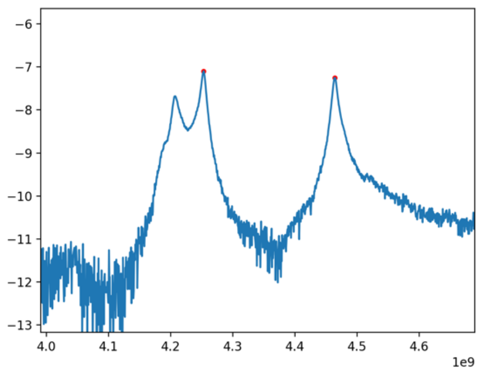


Figure 13. Overlapped peaks due to frequency degeneracy. The same part of spectrum is shown in Figure 10., where the overlapped peaks are detected and fitted successfully.

2.3. Python GUI and Interactive Processing

For conveniently using this algorithm without the need to understand all the principle above, I package all the program as a python GUI and all a user need to do is:

1) Choose the file folder where you load data.
2) Fitting parameters setting, only the estimated width of resonant peaks and a threshold between 0 and 1 is required.
3) If several modes are detected and a frequency ~ temperature dependent relation of a specific mode is wanted, just click on points belong to the target

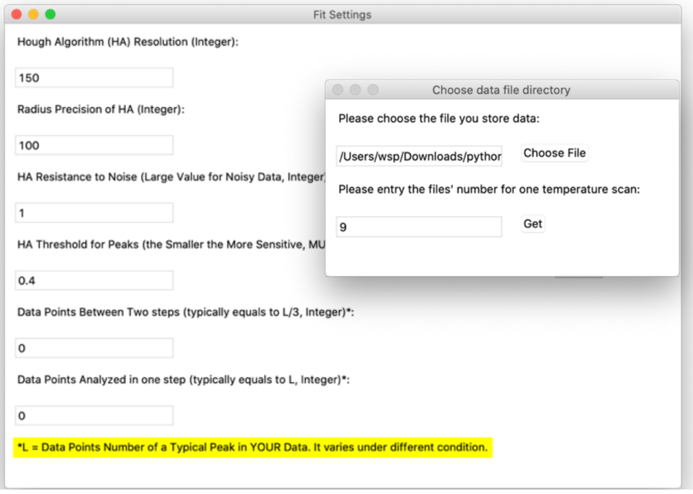


Figure 14. GUI windows for data readout and parameter setting.

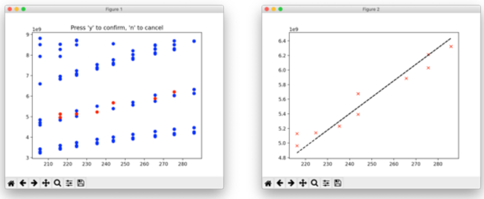


Figure 15. Interactive Mode: Select data points by mouse click (red points are clicked). Clicked points are used to fit a frequency ~ temperature dependent relation.

Now I have already uploaded this project on GitHub (https://github.com/Einspiao/Hough-Algorithm). The Qkit package by *Qkitgroup* on GitHub is also included. There is also a readme text for detailed description.