Study of Spectra with Low-Quality Resonance Peaks

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***Abstract*—A Python-based software for the phenoCAVe family of resonators for plants investigations is developed to automatically extract both the center frequency and the quality factor of the main resonance peak, i.e., of the lowest transversal-magnetic mode TM_{010}, at different scan positions. Due to the specific design of the cavities, which includes large openings on the top and on the bottom of the resonators, the main peak even in the unloaded case (when no object is measured) has a sufficiently small quality factor (<350), which leads to the large influence of the higher modes on the reliability of the extracted data. Additionally, the repeated movements of the resonators and long cables usage may alter the cable influence. Moreover, continuous movements during the scans as well as a finite time of spectra sweep give a distorted peak, especially at the borders of large objects, such as plant pots, i.e., when the objects are starting to pass through a resonator. All these problems and more are taken into account in the automatic data analysis software, which allows to obtain reliable responses from noninvasive scans of the investigated plants over the whole period of their growth and further usage of these responses to calculate the important parameters for the plant growth, such as water content, dry weight, biomass, pot water content etc. Here, the whole process from the analysis of distorted spectra to the evaluation of the suitable parameters for plant growth is demonstrated. Such an analysis can be used not only for plant phenotyping platforms but also in various physical platforms supposing low-quality spectra analysis and dielectric studies of materials.**

Keywords-low-quality resonance peaks; spectra fitting.

I. INTRODUCTION

Fitting of experimental data using theoretical models is an important and well-known problem in various fields of study allowing to fulfill the understanding of investigated processes or events. There are plenty of developed tools to do so, especially when theoretical models are quite simple, such as polynomial, *Gaussian*, and *Lorentzian*, or even a convolution of the last two, often called a *Voigtian*. Such tools, for instance Origin (OriginLab Corporation, Northampton, MA, USA), Matlab-based (MathWorks, Natick, MA, USA) scripts, Python-based scripts, such as the lmfit package [1], etc., are usually used in peak fitting tasks. Nevertheless, task-specified algorithms were developed as well for the peak fitting procedure, which mainly deal with either specific data or particular cases of some processes [3]–[6].

To analyze spectra where low-quality resonance peaks are presented, a simple model of fitting these peaks cannot be used due to several reasons. First, due to the coupling of modes, they are influencing each other by changing their visible parameters on the spectrum, such as peak frequency, peak amplitude/attenuation, as well as their quality factor. Secondly, the amplitude/attenuation at each frequency can be affected by uncertainties caused by reflections in cables, noises, spurious coupling or, in case of a phenoCAVe family of resonators [2], by continuous movements of the cavities. Some of these uncertainties can be represented as baselines which are fitted together with spectra to obtain proper spectrum parameters [7][8].

Skresanov et al. [9] described a novel approach to recover coupled mode parameters from the microwave resonator amplitude-frequency response to deal with the first reason mentioned above. They used an approach from the theory of oscillation, meaning that it is always possible to select such a coordinate system, in which oscillations are independent. In this case, the total amplitude $\Gamma(f)$ of the reflected/transmitted signal can be presented as a sum of complex amplitudes of these oscillations (modes) as follows:

$$\Gamma(f) = \Gamma_S + \sum_i^n \frac{A_i \exp(j\varphi_i)}{1 + 2jQ_i\tau_i(f)}, \quad (1)$$

where Γ_S is the coefficient equal to $\Gamma(f)$ at $f \to \infty$ and is considered to be a real number, i is the ordinal number of an oscillation, n is the total number of oscillations (modes), $\tau_i(f) = (f - f_{0i}) / f_{0i}$ is the frequency tuning parameter, A_i, Q_i, f_{0i}, and φ_i are the amplitude, quality factor, resonant frequency (Center Frequency, CF [2]), and phase shift of the i-th oscillation, respectively. In the case of scattering parameters, the amplitude $\Gamma(f)$ should be considered in the logarithmic form

$$S(f) = 20\log_{10}(|\Gamma(f)| / \Gamma_0), \quad (2)$$

where $S(f)$ is the scattering parameter, e.g., S_{11}, S_{21}, etc., and Γ_0 is the amplitude of the excited signal by a signal generator.

This work presents an advanced fitting algorithm based on the approach mentioned above [9] to study low-quality resonance peaks, i.e., the peaks that have low-quality factor, disturbances, influences of other modes, etc. The developed software allows to fully-automatically analyze all the spectra

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obtained during the scans of a set of plants, which can be grown in different environmental conditions, may have different genotypes, pot sizes, soil types, etc.

In Section II, the selection of a proper approach to fit spectra obtained during the measurements by the phenoCAVe family of resonators [2] is presented, where the advantage of using (1) is clearly demonstrated (Section II.A) and compared with the simple *Lorentzian* fitting approach for the case of loaded resonators (Sections II.B and II.C). Additional problems that may appear during the fitting process caused by disturbed spectra are discussed in Section III. The spectra fitting routine and the graphical user interface of the fully-automated data analysis software based on it is shown in Section IV. The conclusions are conducted in Section V.

II. FITTING OF SPECTRA

A. Unloaded resonators

The fitting algorithm (further referred to as *complex* approach) that uses (1) to calculate parameters of up to 7 resonance modes for measured spectra is realized in so-called "Shaman" software [9]. As an example, Figure 1 shows the spectrum (black dots) which includes the resonance peaks of 5 different Transversal-Magnetic modes (TM_{010}, TM_{110}, TM_{210}, TM_{020}, and TM_{310}) as well as the fitted curve given by the software (red solid line). The obtained parameters for each mode are mentioned in TABLE 1. The matching is very close to ideal, which proves the right approach of the fitting. In many cases, especially when resonance peaks have large quality factors, the phase is not taken into account. The green dashed lines (Figure 1) are the fitted *Lorentzian* curves when each φ_i equal to zero. The difference is clearly visible, although the peaks have fairly correct positions.

B. Loaded resonators; comparison of fitting approaches

The approach when the phase is not taken into account can be realized in such a way that the data points are preselected to be as close as possible to the peak, i.e., in terms of the scattering parameter S_{21} up to 3-5 dB far from the highest point. Then, the fitting by *Lorentzian* curve is done in the following form (further referred to as *Lorentzian* approach)

$$\Gamma(f) = \frac{A}{\sqrt{1+4Q^2\tau^2(f)}}. \quad (3)$$

The last works well for the resonant oscillations, which quality factors are large enough, usually more than 10^3, to make the influence of other resonance modes negligible. Due to both the design and the large openings in the resonators used for plant investigations [2], the quality factor of the first (TM_{010}) mode even when the cavities are empty (unloaded) has far smaller values (< 350).

To demonstrate how a large error can be caused by the *Lorentzian* approach in comparison with the *complex* one, a study using both approaches was done. The analyzed spectra were obtained during the scan of a young maize plant (of about 2 g fresh weight) with its pot using resonator 1 [2]. The relative errors made by the *Lorentzian* approach are shown in Figure 2. Here, it was supposed that the *complex* approach gives the true values for the peak parameters, and the relative error was calculated using following equation

$$\text{Relative error} = \left| p_{complex} - p_{Lorentzian} \right| / \, p_{complex} \times 100\% \,, \quad (4)$$

where p denotes either peak frequency f_0 or quality factor Q. The result consists of the analysis of the 1st resonance peak only, although the fittings done by the *complex* approach included the 2nd mode too. It should be noted that the quality factor Q is the most suitable parameter in this study to demonstrate the influence of modes on each other, due to its strong dependence on the form of a resonance peak. Therefore, the relative errors were built versus Q on the plot. Decreasing of Q was stimulated by placing the resonator at different vertical positions during the scan of a maize plant with its pot [2].

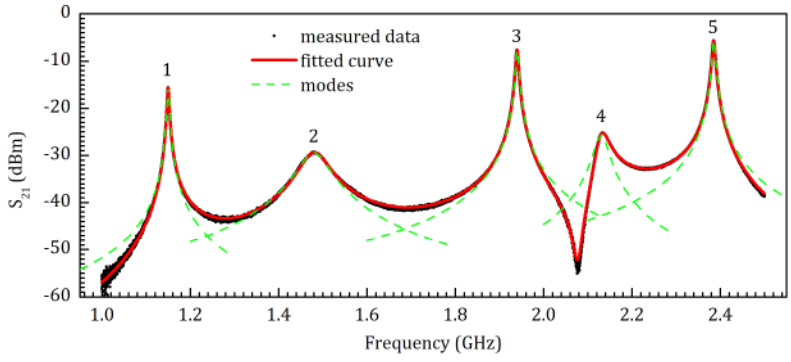

Figure 1. Transmittance spectrum with 5 resonance modes measured for unloaded resonator 1 [2] (black dots), fitting of it (red solid line), and individual resonance modes without phase shift φ_i information (green dashed line).

TABLE I. FITTED RESONANCE MODES' PARAMETERS

Modes, *i*	Parameters			
	f_{0i} (GHz)	Q_i	A_i (dBm)	φ_i
1: TM_{010}	1.14989	246.3	-15.55	0
2: TM_{110}	1.47970	23.2	-29.37	161°
3: TM_{210}	1.94015	297.4	-7.72	-5°
4: TM_{020}	2.13039	72.9	-25.60	8°
5: TM_{310}	2.38543	335.7	-5.68	-172°

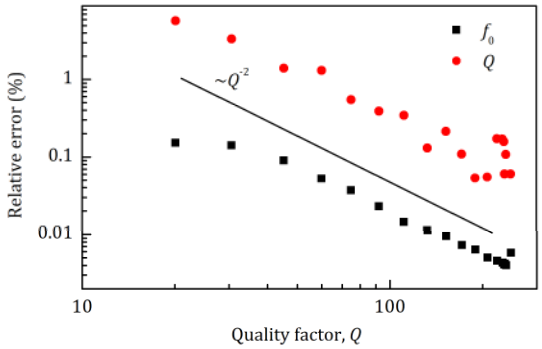

Figure 2. Relative errors of the estimated parameters, peak frequency f_0 (black squares) and quality factor Q (red circles), versus Q for the 1st resonance mode TM_{010}. The black solid line depicts the inverse square dependence on Q.

C. *The false approach leads to errors in plant water amount estimation*

It is visible that the difference between approaches may cause errors in the estimation of both f_0 and Q of up to 0.2% and 6%, respectively (see Figure 2). These errors may increase or decrease for larger or smaller measured plants, respectively. Moreover, by further estimation of the plant Water Amount (WA) [2] 0.2% by f_0 means about 2.3 MHz for the resonator 1, which in terms of the water distribution over the height of a plant gives ~1.5 µL/mm (data not published yet). This in its turn, for a young maize plant of 2 g fresh weight and about 200 mm height gives 0.3 mL of WA, or about 16% of error for the plant WA estimation (0.3[mL] / (2[g]×0.95[mL/g]) × 100% ≈ 16%)

This example demonstrates how the wrong fitting approach can affect the final measurement results. Therefore, in the phenoCAVe data analysis software, the *complex* approach instead of the simpler *Lorentzian* one was selected.

III. DISTURBED SPECTRA

A. *When a resonator is continuously moving while receiving the spectra*

Scanning of a plant by a resonator [2] involves the obtaining of a set of spectra at different positions along the height of the plant. Either a plant or a resonator can be moved against each other. The measurement setup based on the resonator 1 is supposed to shift a plant through the cavity, when the setup based on the resonator 2 displaces the cavity itself. To decrease the scanning time, these movements can be continuous at the intermediate points between the highest and the lowest positions. These lead to additional uncertainties caused by the finite sweep time of the Vector Network Analyzers (VNAs), which are used to obtain spectra, i.e., each frequency on the spectrum has its own position.

For the Screen-House setup [2], every position of the resonator is read out from the MAXON motor drive unit each 50 ms. The VNA (ZNC 3, Rohde & Schwarz GmbH, Cologne, Germany), in its case, has 87.5 µs sweep time per frequency point, i.e., one whole spectrum that consists of 801 points is measured during 70 ms. The highest speed of the resonator varies from 20 to 70 mm/s, meaning that during 70 ms the resonator can change its position by about 5 mm, which may lead to the crucial modification of the spectra, especially when the resonator is close to the plant pot. By knowing the vertical position of each point on the spectra and taking a set of spectra measured at different positions, spectra for each selected position can be recalculated using a polynomial fit of order 2. Such a polynomial fit gives a few positive effects. The first one is the automatically smoothed spectrum, and the second one is the possibility to detect outliers in combination with the Grubbs' test [10].

B. *Influence of cables and surroundings*

Both setups presented previously [2] have cables to deliver and acquire signals. The cables can be calibrated using a built-in utility of VNA and commercially available calibration kits (in our case ZV-Z132, Rohde & Schwarz GmbH, Cologne, Germany). The calibration may not properly work in some cases. For the setup based on resonator 2, even calibrated VNA showed a sinusoidal behavior on the spectrum (see Figure 3). In this case, additionally to the spectrum fitting, residuals $S_{21}^{res}(f)$ should be fitted by using a sum of sines in the following form

$$S_{21}^{res}(f) = \sum_{i}^{k} a_{i\sin} \sin(2\pi f / f_{i\sin} + \varphi_{i\sin}), \qquad (5)$$

where $a_{i\sin}$, $f_{i\sin}$, $\varphi_{i\sin}$ are the sine parameters, and k is the number of sines. The bottom plot in Figure 3 reflects this situation. Residuals may depend on the position of the resonator due to the influence of surroundings, causing the residuals fitting to be done for each spectrum. Moreover, this procedure should be circled to obtain proper parameters for the resonance peak, i.e., firstly, the spectrum (measured data)

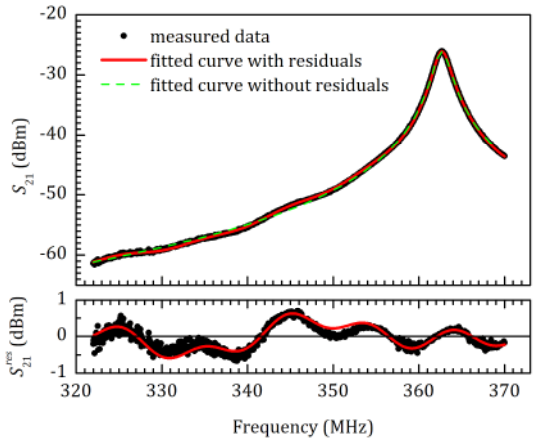

Figure 3. *Complex* fitting approach for the spectrum obtained using unloaded resonator 2 [2] (top plot) and fitting of residuals S_{21}^{res} using (4) with $k = 2$.

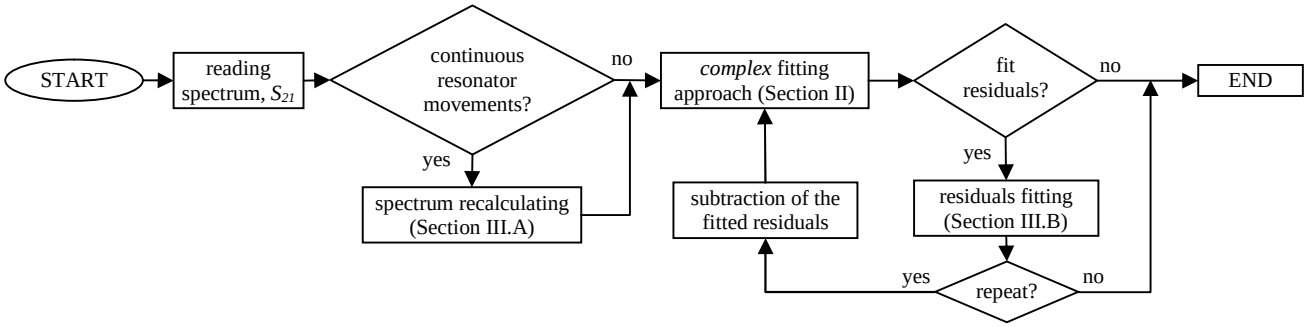

Figure 4. Suggested spectrum fitting routine.

is fitted by the *complex* approach, secondly, residuals are calculated and fitted, and finally, the obtained curve in the form (5) is subtracted from the measured data. These three steps are repeated several times to obtain a stable solution (see Figure 3).

IV. SPECTRUM FITTING ROUTINE

The suggested spectrum fitting routine is shown in Figure 4. The whole procedure starts from the reading of the spectral information (measured data) for the resonance peak at the selected position of a resonator. Then, if the resonator was continuously moving during the scan, the recalculating spectrum function is called (Section III.A). After that, the *complex* fitting approach starts (Section II), which is followed by the residuals fitting if needed (Section III.B). After subtraction of the fitted residuals, the *complex* approach can be called again, i.e., circled until obtaining a stable solution. At the end, the evaluated parameters of the resonance peak are stored for further analysis (not a part of this work). This routine is repeated for each measured spectrum at different positions of the resonator.

It should be noted that the residuals obtained at different positions are stored too for the unloaded runs of the resonator. Later, these residuals are used to simplify the fittings for the resonator runs with a measured object, e.g., a plant, a pot with soil, etc.

The fitting routine presented in Figure 4 was programmed in the fully-automatic phenoCAVe data analysis software using Python programming language. To make an interface and to deal with the mathematics behind it, a list of packages was used, such as pyqtgraph, PyQt5, scipy, numpy, lmfit, csv, itertools, fnmatch, inspect, os, bayeos, multiprocessing, sys, warnings, time, traceback, typing, copy, etc. The software tab, where spectra fitting is visible, is presented in Figure 5 with the data shown in Figure 3. The time spent to fit one spectrum from "Start" to "End" (see Figure 4) using "spectrum recalculating" and 20 iterations of "residuals fitting" was less than 5 seconds on the Intel Xeon E5-2630 v3 based computer.

Figure 5. phenoCAVe data analysis software developed using Python programming language.

V. CONCLUSIONS

The fitting approach presented in this work was mainly developed to analyze low-quality resonance peaks on measured spectra. The simple *Lorentzian* fitting approach was compared with the *complex* one, to which a preference was given. Additionally to that, issues that may arise during the measurements using partially opened resonators were shown and discussed with their possible resolution. Among them are the influences of other modes, surroundings, cables, and continuous movements of either a resonator or an investigated object. In the end, the spectrum fitting routine was suggested and the software based on it was demonstrated. The suggested *complex* fitting approach is not newly developed but the proposed fully automated fitting routine has novel ideas which can be useful for the precise analysis of spectra with low-quality resonance peaks.

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REFERENCES

[1] M. Newville et al., "LMFIT: Non-Linear Least-Squares Minimization and Curve-Fitting for Python," https://lmfit.github.io/lmfit-py/, retrieved: Apr. 2019.

[2] V. A. Sydoruk et al., "Design and Characterization of Microwave Cavity Resonators for Noninvasive Monitoring of

Plant Water Distribution," IEEE Trans. Microw. Theory Tech., vol. 64, no. 9, Sep. 2016, pp. 2894–2904, doi: 10.1109/TMTT.2016.2594218.

[3] T. Žák and Y. Jirásková, "CONFIT: Mössbauer spectra fitting program," Surf. Interface Anal., vol. 38, no. 4, Mar. 2006, pp. 710–714, doi: 10.1002/sia.2285.

[4] A. E. Hughes and B. A. Sexton, "Curve fitting XPS spectra," J. Electron Spectrosc. Relat. Phenom., vol. 46, no. 1, 1988, pp. 31–42, doi: 10.1016/0368-2048(88)80003-3.

[5] A. P. Hammersley and C. Riekel, "MFIT: Multiple spectra fitting program," Synchrotron Radiat. News, vol. 2, no. 1, Jan. 1989, pp. 24–26, doi: 10.1080/08940888908261193.

[6] A. J. Brown, "Spectral curve fitting for automatic hyperspectral data analysis," IEEE Transactions on Geoscience and Remote Sensing, vol. 44, no. 6, Jun. 2006, pp. 1601–1608, doi: 10.1109/TGRS.2006.870435.

[7] Q. Han et al., "Simultaneous spectrum fitting and baseline correction using sparse representation," The Analyst, vol. 142, no. 13, May 2017, pp. 2460–2468, doi: 10.1039/C6AN02341J.

[8] H. Hu et al., "Improved Baseline Correction Method Based on Polynomial Fitting for Raman Spectroscopy," Photonic Sensors, vol. 8, no. 4, Dec. 2018, pp. 332–340, doi: 10.1007/s13320-018-0512-y.

[9] V. N. Skresanov et al., "The novel approach to coupled mode parameters recovery from microwave resonator amplitude-frequency response," 2011 41st European Microwave Conference (EuMC 2011), IEEE Press, Oct. 2011, pp. 826–829, doi: 10.23919/EuMC.2011.6101922.

[10] "NIST/SEMATECH e-Handbook of Statistical Methods," http://www.itl.nist.gov/div898/handbook/, retrieved: Apr. 2019.

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