Resonance parameter estimation from spectral data: Cramér–Rao lower bound and stable algorithms with application to liquid sensors

T Voglhuber-Brunnmaier¹,², A O Niedermayer², R Beigelbeck¹,³ and B Jakoby²

¹ Center for Integrated Sensor Systems, Danube University Krems, Viktor Kaplan Str. 2, 2700 Wiener Neustadt, Austria
² Institute for Microelectronics and Microsensors, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria
³ Institute of Sensor and Actuator Systems, Vienna University of Technology, Gusshausstrasse 27-29, A-1040 Vienna, Austria

E-mail: thomas.voglhuber@donau-uni.ac.at

Received 4 April 2014, revised 17 July 2014
Accepted for publication 22 July 2014
Published 15 September 2014

Abstract
A recently introduced method for robust determination of the parameters of strongly damped resonances is evaluated in terms of achievable accuracy. The method extracts and analyzes the locus of the resonant subsystem of noisy recorded complex spectra, such that the interfering influences of many environmental factors are eliminated. Estimator performance is compared to the absolute lower limit determining the Cramér–Rao lower bound (CRLB) for the variance of the estimated parameters. A generic model that is suitable for representation of a large class of sensors is used and analyzed. It is shown that the proposed robust method converges to the CRLB for low measurement noise.

Keywords: resonant sensor, fluid sensing, estimation theory, minimum variance, quartz, QCM

(Some figures may appear in colour only in the online journal)

1. Introduction

The resonance frequency and the quality factor ($Q$ factor) of resonant sensors are the most important intermediate parameters in the determination of desired physical quantities. For example, quartz crystal resonators (QCRs) can be used as microbalances (QCMs) to measure mass deposits on the resonator surface [1]. The increased resonator mass results in a reduced resonance frequency. More generally, dissipative overlayers can also be detected with such a sensor [2, 3]. If the surface of the QCM is in contact with a viscous liquid, the mass drag causes a frequency shift and the viscosity of the fluid reduces the initially high quality factor of the resonator. Examples of resonant sensors are limited to liquid sensors in this work, although the illustrations are just as valid for a variety of other resonant sensors like pressure sensors, force sensors, accelerometers and mass flow sensors [4, p 225]. We consider applications where the resonance can be strongly attenuated and thus determination of the resonance parameters is critical. Since viscosity may vary within a large dynamic range, it is important that the parameter estimation algorithms perform reliable for a wide range of $Q$ factors and resonance frequency shifts, as well. Further important aspects and an overview of the current state of the art with respect to fluid sensors can be found in [5, 6].

Unfortunately, there is no strict consensus in the literature about how resonance frequency shifts and $Q$ factors are to be
measured best. In cases where only the amplitude response is known, the −3 dB method is commonly used. For example, the resonance frequency \( f_j \) and the resonator bandwidth \( B \) are estimated at the maximum amplitude and by the frequency range between the points at which the signal has decreased by a factor of \( 1 / \sqrt[4]{2} \) on both sides of the maximum. The \( Q \) factor is calculated from \( \hat{Q} = \frac{f_j}{\hat{B}} \), where estimated parameters are marked with a hat symbol. Particularly in the presence of larger spurious components and low \( Q \) factors, the −3 dB criterion is not meaningful, as the maximum amplitude point and the resonance point differ. Furthermore, drifts of the spurious effects are difficult to separate from changes in the quantity to be measured. Although alternative approaches like Lorentzian curve fit [7] and resonance curve area [8] are more sophisticated, they also do not perform well under these conditions.

When complex spectra are available, the additional phase information should be considered in the signal processing. The approaches used in this work follow [9] and are based on various modified methods summarized in the review paper of Petersen and Anlage [7]. We assume that complex spectra, e.g. from quadrature-demodulated signals are available. The locus plot in the vicinity of an undisturbed resonance closely resembles a circle, which can be modeled by a linear second-order lumped element system, such as an RLC in series or in parallel connection. In agreement with common literature [10–12] on quartz crystal resonators, this part is termed a motional arm. The signal of the motional arm is extracted from the measurement data and the resonance parameters are determined. Therefore, the results do not depend on spurious phase shifts and signal components.

In general, estimation of the resonance parameters from complex spectra by direct optimization methods, such as the non-linear least squares method (nLSQ), shows poor performance. This is mainly caused by ill-conditioned equation systems. The stability of the estimation method can be greatly improved if the geometric properties of resonance curves in the complex plane are considered as proposed in [9]. This, and modified approaches, have been successfully applied to resonances of QCMs [13], Lorentz force actuated double diaphragm sensors [14], pressure wave viscometers [15], cantilevers and U-shaped wire sensors [16] and vibrating platelets [17].

The paper is structured as follows: Starting with acquisition of noisy steady state oscillations, the noise on the spectrum in terms of variances, covariances and the covariance matrix is determined in section 2. In section 3, reasonable signal models for linear second-order resonances are shown. The Cramér–Rao lower bound for this function and present noise is derived in section 4. The realizable and stable estimator as proposed in [9] is outlined and the probabilistic properties of the estimator are derived in section 5.

2. Acquisition of complex spectra

In this section, the transfer of measurement noise to the frequency spectra is described. The spectra are calculated by a Fourier transform of noisy sampled time signals. The basic finding is that the real and imaginary parts of the spectra are approximately Gaussian, linearly independent and of equal variance.

The resonance parameters are determined from complex spectra obtained with an impedance analyzer (e.g. Agilent 4294A) or the YAPIA circuit [18]. Both systems generate harmonic oscillations at discrete and known frequencies \( f_j \) and analyze the oscillation after sufficient settling time. The commercial impedance analyzer uses analogous demodulation, whereas the YAPIA design samples the electrical current signal at the instants \( t_i \) and calculates the admittance \( \frac{y_m}{y_A} \) with

\[
y_m[f_j; t_i] = A_j \cos (2\pi f_j t_i + \phi_j) + \delta[f_j; t_i] \tag{1}
\]

with \( i \in 0...L - 1, j \in 0...M - 1 \).

The signal \( y_m[f_j; t_i] \) is inevitably affected by noise \( \delta[f_j; t_i] \). In order to determine the spectral properties \( A_j \) and \( \phi_j \) from \( y_m[f_j; t_i] \), the Goertzel algorithm [19, p 633] is applied to each discrete time signal vector \( y_m[t_0, ..., t_L-1; f_j] \), yielding the admittance spectrum \( \sum_m f_j \).

\[
\sum_m f_j = \mathbf{Y} \mathbf{f}_j + \xi \mathbf{f}_j. \tag{2a}
\]

The spectrum transform can be represented by

\[
\mathbf{Y} \mathbf{f}_j = \sum_{i=0}^{L-1} \mathbf{E} [t_i; f_j] \ y[t_i; f_j] \tag{2b}
\]

\[
\xi \mathbf{f}_j = \sum_{i=0}^{L-1} \mathbf{E} [t_i; f_j] \ \delta[t_i; f_j]. \tag{2c}
\]

\[
\mathbf{E} [t_i; f_j] = \frac{1}{L} e^{-2i \pi f_j t_i} \text{ with } i = \sqrt{-1}. \tag{2d}
\]

A scaling factor of \( 1/L \) is used in (2d) to obtain spectral amplitudes independent of the sample number \( L \). The readout electronics records the oscillations of different frequencies \( f_j \) with integer periods, such that inner products

\[
\sum_{i=0}^{L-1} \mathbf{E} [t_i; f_j] \mathbf{E} [t_i; f_k] \ \forall j \neq k, \tag{2e}
\]

vanish and consequently the amplitude and phase in (1) are related to \( \mathbf{Y} \) by

\[
A_j = 2|\mathbf{Y} \mathbf{f}_j | \ \text{and} \ \phi_j = \text{arg} (\mathbf{Y} \mathbf{f}_j). \tag{3}
\]

Additive noise on the data yields additive complex noise on the spectrum, which is not correlated with the parameters (see (2a)–(2d)). The variances and the covariance are

\[
\text{var} \{ \xi \} = \sigma^2 = \frac{\sigma^2_f}{L}, \tag{4a}
\]

\[
\text{var} \{ \text{Re}\{\xi\} \} = \text{var} \{ \text{Im}\{\xi\} \} = \frac{\sigma^2_f}{2}, \tag{4b}
\]

\[
\text{cov} \{ \text{Re}\{\xi\}, \text{Im}\{\xi\} \} = 0. \tag{4c}
\]

4. Sampled data are indicated by square brackets.

5. The Goertzel algorithm is a computationally efficient implementation of the discrete Fourier transform of a single spectral line.

6. The underlines denote complex valued quantities.
For a large number of sampling points, the restrictions on
the measurement noise $\delta$ can be relaxed to independent, iden-
tically distributed random variables with finite variance, as a
result of the central limit theorem [20, p 44]. The definition
of variance and covariance can be given in terms of expected
values $E\{x\}$ (i.e. $E\{x\}$ is an average of $x$) by
\[
\text{var}\{x\} = E\{x^2\} - (E\{x\})^2, \quad (5a)
\]
\[
\text{cov}\{x, y\} = E\{x y^*\} - E\{x\} E\{y^*\}. \quad (5b)
\]
A unified representation of variances and covariances for a
vector of complex random variables $\mathbf{x}$ is given by the covari-
ance matrix $\mathbf{C}(\mathbf{x})$
\[
\mathbf{C}(\mathbf{x}) = E\{\mathbf{x} \mathbf{x}^H\} - E\{\mathbf{x}\} E\{\mathbf{x}^H\},
\]
where the superscript $H$ indicates Hermitian transposition. On
the main diagonal of $\mathbf{C}$ are the variances (real valued) and
on the off-diagonal elements are the covariances in complex
conjugate pairs.

### 3. Sensor models of fluid sensors

Statements about the principal achievable accuracies of esti-
mation algorithms are based on a specific signal model. The
models used are reduced representations of the actual systems
(partial differential equations in general) and in the form of
electrical lumped element circuits. Although, the fundamental
sensor typically exhibits many different vibrational modes,
these equivalent circuits are valid representations. For each
mode, the potential and kinetic energy can be calculated, from
which in turn equivalent mass-spring-damper systems for a
generalized coordinate can be deduced (see e.g. [21, p 22]).
Equivalent electrical circuits consisting of passive elements
\footnote{The superscript asterisks denote complex conjugates.}
can be determined for every system, such that the proposed
lumped element circuits are well founded.

The frequency response of, e.g. a liquid loaded QCM or a
piezoelectric tuning fork sensor can be modeled by the lumped
element Butterworth–Van Dyke equivalent circuit [22, 23],
as shown in figure 1 (left). The parameters $f_0$ and $Q$ denote
the undamped resonance frequency and the quality factor of
the motional arm $(L_m, C_m, R_m)$, respectively. Changes of the
mass-density and viscosity of the liquid under test change
these parameters. The shunt capacitance $C_0 = \varepsilon A/h$ is basically
determined by the electrode area $A$, permittivity $\varepsilon$ and reso-
nator thickness $h$. This parameter can vary strongly if there
are changes of the electrical parameters (permittivity and con-
ductivity) of the liquid under test as shown e.g. in [24]. On
the right side of figure 1, an equivalent circuit, valid for many
Lorentz force actuated and inductively read out sensors (e.g.
[16, 25–27]), is shown. In many setups, the inductive cross-
talk between excitation and readout path is significant and is
modeled by the inductor $L_0$. The ideal transformer couples
the electrical and mechanical systems. The coupling strength
is represented by the transformer ratio $n$ and depends on the
external magnetic field required for excitation and readout.

Due to wiring, sensor interface and calibration errors a phase shift and additional spurious elements
may be present for both setups.

\[
\mathcal{Y}(f) = \mathcal{Y}(f)/\mathcal{Y}(f)
\]
\[
\mathcal{Y}(f) = \left( \frac{Y_0 + i 2\pi f C_0}{1 + i Q \left( \frac{f}{f_0} - \frac{f}{Q} \right)} \right) \mathcal{Y}_f + \mathcal{Y}_k + \mathcal{Y}_l(f), \quad (7a)
\]

Figure 1. Left: the Butterworth–Van Dyke model for QCM consists of a motional arm $(R_m, C_m, L_m)$ and a shunt capacitance $(C_0)$. Right: equivalent circuit for Lorentz force actuated sensors. Due to wiring and calibration errors a phase shift and additional spurious elements may be present for both setups.
where the spurious components are modeled by a complex offset $Y_k = k_R + ik_i$, a complex linear frequency part $Y_f = f_R + if_i$ and a phase shift $\phi$.

One fact that will be exploited is that the locus plot of the motional arm alone resembles a circle with diameter $\frac{1}{2}Y$ centered at $\frac{1}{2}Y$. The additional part $Y_I$ causes a significant distortion of the circular shape at $Q$ factors lower than approximately 1000. In fluid sensing especially, the $Q$ factors are much lower and the impact of the shunt capacitance, as shown in figure 2, or the inductive crosstalk is relevant.

Figure 2. Locus plots of the quartz admittance (—) versus the motional arm (– –) admittance for $Q = \{1000, 500, 200, 100\}$. Deviations are significant at low $Q$, but can largely be eliminated by adequate preprocessing.

4. Cramér–Rao lower bound

In this section, the limits of the achievable accuracies of the estimated resonance parameters for the model from the previous section are shown. It is demonstrated that the spurious elements lead to larger errors compared to the spurious-free case, and that the choice of the frequency sampling points of the spectrum also has a certain influence.

Since resonant sensors may be represented by different models, and the parameters of each model react differently to measurement noise, the case is considered where the sensor can be described by a series RLC arm with additional phase shift (e.g. caused by wiring or calibration errors) and broadband spurious elements, which may be due to the sensor as for the QCR and owing to signal conditioning (e.g. signal
transformers [28]). The Cramér–Rao lower bound (CRLB) defines a lower bound for the variance of the estimated parameters [29, p 27]. This limit can always be found for the considered class of sensors, even though the existence of an estimator achieving this bound is not assured. For the signal model in (7a), additive Gaussian noise \( \xi \) [f, j] and multiple real parameters \( \theta = [f, Q, \bar{Y}, \phi, k_0, k_1, k_2, h_1]^T \), the CRLB \( (C_\theta) \) can be specified by (see [29, p 525])

\[
C_\theta = I(\theta)^{-1}
\]  

(8a)

with

\[
I_i(\theta) = 2\text{Re} \left\{ \left[ \frac{\partial Y(\theta)}{\partial \theta} \right]^\dagger \left[ \frac{\partial Y(\theta)}{\partial \theta} \right] \right\} + \text{trace} \left\{ C_\bar{Y}^{-1}(\theta) \frac{\partial C_\bar{Y}(\theta)}{\partial \theta_k} C_\bar{Y}^{-1}(\theta) \frac{\partial C_\bar{Y}(\theta)}{\partial \theta_l} \right\},
\]

(8b)

\[
Y(\theta) = \left[ Y[0; \theta], \ldots, Y[M-1; \theta] \right]^T,
\]

(8c)

where \( I(\theta) \) represents the so-called Fisher information and \( C_\bar{Y} \) the covariance matrix of the spectral data. This form can only be used for independent and equal variances of the real and imaginary parts of \( \xi \), which was verified in section 2. Equation (8b) can be simplified in the present case where the covariance matrix of the data is a diagonal matrix with identical entries independent of the parameters \( (C_\bar{Y} = \sigma^2 E, \text{with identity matrix } E) \). The vector and matrix multiplications in (8b) are replaced by summation, yielding

\[
I_i(\theta) = \frac{2}{\sigma^2} \text{Re} \left\{ \sum_{j=0}^{M-1} \frac{Y[j; \theta]^* Y[j; \theta]}{\partial \theta_k} \right\}.
\]

(9)

The achievable variance depends on the distribution of the samples around the locus plot. The lowest variances are obtained for frequency distributions with uniform arc lengths in (10a) and shown in figure 3.

\[
f_j = \frac{f}{2Q} \left( (4Q^2 + \text{cot}^2(\alpha_j/2))^{1/2} - \text{cot} (\alpha_j/2) \right),
\]

(10a)

\[
\alpha_j = \frac{1 + 2j}{M}.
\]

(10b)

In [9], an equidistant frequency distribution centered around the resonance \( f_i \) is proposed. Using this frequency vector does not yield closed form expressions for the CRLB and generally larger values. The differences between equidistant arc lengths and equidistant frequency distributions are examined in appendix A. It can be argued that for this frequency vector the resonance parameters \( Q \) and \( f_i \) must be known \textit{a priori}. In order to obtain usable measurement results, it is evident that the resonance frequency and the \( Q \) factor must be coarsely known. The results in appendix A show no drastic changes for deviations from the sample frequencies in (10a).

The entries of the Fisher information are determined by (9) and are given by

\[
I_{11} = \frac{M\bar{Y}^2}{\sigma^2} + \frac{12Q^2}{4f_i^2}, \quad I_{14} = \frac{M\bar{Y}^2}{\sigma^2} + \frac{24Q^2}{16f_iQ},
\]

\[
I_{15} = -\frac{M\bar{Y}}{\sigma^2} \frac{8Q^2 - \sin \phi}{8f_iQ}, \quad I_{16} = \frac{M\bar{Y}}{\sigma^2} \frac{8Q^2 - \cos \phi}{8f_iQ},
\]

\[
I_{17} = \frac{M\bar{Y}}{\sigma^2} \frac{8Q^2 + 3}{16Q^2} \sin \phi + \frac{4Q^2 - 1}{4Q} \cos \phi,
\]

\[
I_{18} = -\frac{M\bar{Y}}{\sigma^2} \frac{8Q^2 + 3}{16Q^2} \sin \phi - \frac{4Q^2 - 1}{4Q} \cos \phi,
\]

\[
I_{22} = \frac{M\bar{Y}^2}{\sigma^2} 2Q, \quad I_{23} = -\frac{M\bar{Y}}{\sigma^2} 2Q, \quad I_{25} = -\frac{M\bar{Y}}{\sigma^2} \frac{\cos \phi}{2Q}, \quad I_{26} = -\frac{M\bar{Y}}{\sigma^2} \frac{\sin \phi}{2Q},
\]

\[
I_{37} = -\frac{M\bar{Y}}{\sigma^2} \frac{\cos \phi}{4Q^2} \sin \phi - \frac{4Q^2 + 1}{4Q} \cos \phi,
\]

\[
I_{38} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q - \sin \phi}{4Q}, \quad I_{44} = \frac{M\bar{Y}^2}{\sigma^2} \frac{\cos \phi}{4Q}, \quad I_{45} = -\frac{M\bar{Y}}{\sigma^2} \frac{\sin \phi}{2Q}, \quad I_{46} = \frac{M\bar{Y}}{\sigma^2} \frac{\cos \phi}{2Q},
\]

\[
I_{47} = -\frac{M\bar{Y}}{\sigma^2} \frac{2Q + 1}{4Q} \sin \phi - \frac{4Q^2 - 1}{4Q} \cos \phi,
\]

\[
I_{48} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q - \sin \phi}{4Q}, \quad I_{55} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q - \cos \phi}{4Q}, \quad I_{56} = \frac{M\bar{Y}^2}{\sigma^2} \frac{\cos \phi}{4Q},
\]

\[
I_{57} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q + 1}{4Q} \cos \phi + \frac{4Q^2 - 1}{4Q} \sin \phi,
\]

\[
I_{58} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q - \cos \phi}{4Q}, \quad I_{59} = \frac{M\bar{Y}^2}{\sigma^2} \frac{2Q - \sin \phi}{4Q}, \quad I_{60} = \frac{M\bar{Y}^2}{\sigma^2} \frac{\sin \phi}{4Q},
\]

The matrix is symmetric (i.e. \( I_j = I_{jj} \)) and only the non-zero values of the upper triangular part are shown. The thick printed expressions are approximated with relative errors below 2% at \( Q = 2 \) and below 0.02% at \( Q = 10 \). To the best of our knowledge, no suitable approximation for \( I_{37} \) and \( I_{58} \) is known.

The Fisher-information matrix in (11) can also be used to determine the CRLB for various reduced models. If some parameters of \( \theta = [f_i, Q, \bar{Y}, \phi, k_0, k_1, k_2, h_1]^T \) are known \textit{a priori}, the corresponding columns and rows can be eliminated from \( I(\theta) \).
If there are dependencies between parameters (i.e., correlation between the columns of $\mathbf{H}$), then the variances on the remaining estimated parameters are decreased. In the following, the CRLB for a single RLC series arm, (i.e. free from spurious elements) is derived and compared to the full signal model in (7a).

### 4.1. CRLB for spurious-free second-order resonance

In this case, only the upper left $3 \times 3$ submatrix of $\mathbf{I}(\theta)$ is relevant

$$\mathbf{I}(\theta) = \frac{M}{\sigma^2} \begin{bmatrix} \frac{\bar{Y}^2 + 12Q^2}{4Q} & 0 & 0 \\ 0 & \frac{\bar{Y}^2}{4Q} - \frac{\bar{Y}}{4Q} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (12)$$

The expressions in (12) are exact, but only valid for the given frequency distribution in (10a). The inverse of $\mathbf{I}(\theta)$ yields the covariance matrix for this problem with the single variances

$$\text{var}\{\hat{f}_c\} = \frac{4\bar{Y}^2}{M(1 + 12Q^2)} \approx \frac{\bar{Y}^2}{3M^2Q}, \quad \text{var}\{\hat{\theta}\} = \frac{128f_c^2Q^2}{M(64Q^2 - 16Q^2 - 5)}, \quad \text{var}\{\hat{\theta}\} \approx 6\bar{Y}^2, \quad \text{var}\{\hat{\phi}\} \approx \frac{128f_c^2Q^2}{M(64Q^2 - 16Q^2 - 5)}, \quad \text{var}\{\hat{\phi}\} \approx 6\bar{Y}^2/\sqrt{2}, \quad \text{var}\{\hat{k}_l\} \approx \frac{3\sigma_0^2}{2M}.$$

The variance on the frequency estimate is approximately six times higher and the variance on the $Q$ factor is twice as large as in the spurious-free case. The estimation of the offset introduces also covariances with all parameters, which are not further discussed because the main interest is in the resonance frequency and quality factor, as they are in close relationship with the relevant fluid parameters. Although the spurious components are of minor interest for sensing applications, they have to be taken into account when present and unknown as they increase the variances of the relevant parameters.

Adding lines/rows 7 and 8 of the matrix influences all parameters and the expressions become very bulky. However, the resulting variances of the resonance parameters, as shown in figure 4, are close to the previous results in (15a)–(15e), such that these expressions provide good approximations.

The CRLB for the parameter estimation problem in (7a) is determined. The calculation of the CRLB in this manner is continued in Appendix B for various submodels and additional spurious components. In the next section, the variances of the stable estimation algorithm are calculated and compared with the lower bound.

### 5. Performance of the stable estimator

In this section, a stable estimation procedure, as outlined in [9], is analyzed. It will be shown that the variances of this estimator converge to the CRLB for small noise amplitudes. The robust method is based on the investigation of the locus plots of the complex spectra. In a first step, additive, linearly frequency dependent components are removed using so-called off-resonance measurements (ORMs) [9]. The ORMs are acquired at both sides and at a significant distance from the resonance and are used for linear
regression. The accuracy of the regression depends on the separation and the number of ORMs. (The effect of higher-order background functions are discussed in appendix C in more detail.) Subsequently, the center of the resonance circle is estimated using the hyperaccurate circle fit [30, 31], which is free from essential bias. We used the implementation of the algorithm in MATLAB available from the web page of Nikolai Chernov.9 The phase of the residual function of the algorithm in MATLAB available from the web page of Nikolai Chernov.

The circle center is estimated using the hyperaccurate circle fit [30, 31], which is free from essential bias. We used the implementation of the algorithm in MATLAB available from the web page of Nikolai Chernov.9 The phase of the residual function of the algorithm in MATLAB available from the web page of Nikolai Chernov.

The model function in (7a) is rearranged such that the function in brackets is centered at 0 + 0i

$$Y_m(f) = \left( \frac{\tilde{Y}}{1 + iQ} \right)^2 - \tilde{Y} \right) e^{i\phi} + Y_C + e(f),$$

(16a)

$$Y_C = Y_k + \frac{\tilde{Y}}{2} e^{i\phi}.$$  

(16b)

The circle center $Y_C = k_R + i k_I$ is estimated from

$$Y_mC[Y] = \frac{\tilde{Y}}{2} \cos(\alpha_j - \phi) + k_R$$

$$+ \left( \frac{\tilde{Y}}{2} \sin(\alpha_j - \phi) + k_I \right) + e[Y].$$

(17)

For angles equally distributed (see (10a)) around the circle center, the minimum variances of estimating the circle center and the diameter are

$$\mathrm{var} \{k_R \} = \mathrm{var} \{k_I \} = \frac{\sigma^2}{2M},$$

(18a)

$$\mathrm{var} \{\tilde{Y}\} = \frac{2M}{\sigma^2},$$

(18b)

9 http://people.cas.uab.edu/~mosya/cl/MATLABcircle.html

**Figure 4.** Deviations of the variances of $\hat{k}$ and $\hat{\tilde{Y}}$ with estimation of the parameters $k_R$ and $k_I$ relative to the results in (15a)–(15b).

The phase of the residual function has a smooth profile and the resonance parameters are derived using a nLSQ method. For convergence, a reasonable initial guess of the parameters is still mandatory, but their range is increased such that simple heuristic methods are sufficient.

The phase angle $\phi_m$ of the admittance in (19) and the phase of the noise and bias-free model function are given by

$$\phi_m = \arg(Y_mC[Y]).$$

(20a)

$$\phi_{\psi} = \phi - 2 \arctan \left( Q \left( \frac{f_j - f_j}{f_i - f_i} \right) \right).$$

(20b)

Equation (20a) is a smooth function and can be inverted numerically using Newton’s method [32, p 146] to obtain the parameters $\hat{\theta} = [\hat{f}, \hat{Q}, \hat{\phi}]^T$. Starting with an initial guess $\hat{\theta}_0$, the iteration in (21a) is repeated until the updates fall below the numerical noise floor. The estimation problem is real valued and given by

$$\hat{\theta}_{n+1} = \hat{\theta}_n + H_{\psi}(\hat{\theta}_n) \left( \phi_m - \phi(\hat{\theta}_n) \right)$$

(21a)

with the pseudo-inverse denoted by the superscript $\dagger$.

$$\phi_m = [\phi_{m,0} \ldots \phi_{m,M-1}]^T, \quad \phi(\hat{\theta}_n) = [\phi(\hat{f}), \ldots \phi(\hat{f})]^T$$

(21b)

$$H_{\psi}(\hat{\theta}_n) = \left( H_{\psi}(\hat{\theta}_n) \right)^T H_{\psi}(\hat{\theta}_n) + S_{\psi}(\hat{\theta}_n)^{-1} H_{\psi}(\hat{\theta}_n)^T$$

(21c)

$$H_{\psi}(\hat{\theta}_n) = \frac{\delta \phi(\hat{\theta}_n)}{\delta \theta}, \quad i = 0 \ldots M - 1, \quad \hat{\theta}_n = [\hat{f}_n, \hat{Q}_n, \hat{\phi}_n]^T,$$

(21d)
φ

Figure 5. Left: standard deviation of the resonance parameters relative to the CRLB. Right: parameter estimation bias relative to the optimum standard deviation.

\[ S_{\varphi,i},(\hat{\varphi}_m) = \sum_{i=0}^{M-1} \left( \varphi_m[i] - \varphi[i, \hat{\varphi}_m] \right) \frac{\partial \varphi[i]}{\partial \varphi[i]}, \quad k, l \in 0 \ldots 2, \quad (21e) \]

\[ H_{\varphi}(\hat{\varphi}_m) = \begin{bmatrix}
\frac{1}{\mu_\varphi} & \frac{1}{\mu_\varphi} & \ldots & \frac{1}{\mu_\varphi} \\
\frac{1}{\mu_\varphi} & \frac{1}{\mu_\varphi} & \ldots & \frac{1}{\mu_\varphi} \\
\frac{1}{\mu_\varphi} & \frac{1}{\mu_\varphi} & \ldots & \frac{1}{\mu_\varphi} \\
\frac{1}{\mu_\varphi} & \frac{1}{\mu_\varphi} & \ldots & \frac{1}{\mu_\varphi} \\
\end{bmatrix} \frac{\partial \varphi}{\partial \varphi} \quad (21f) \]

The observation matrix \( H_{\varphi} \) contains first derivatives and \( S_{\varphi} \) second derivatives. It is observed that \( S_{\varphi} \) can be neglected for the present case, which results in the Gauss–Newton method. Furthermore, the convergence behavior of the iteration is not enhanced notably by \( S_{\varphi} \). For a poor initial guess, it is appropriate to replace \( S_{\varphi} \) by a scaled identity matrix \( \mu E \) where the scalar value \( \mu \) is reduced towards zero during the iteration. By choosing a suitable positive \( \mu \), the search direction of the iteration is continuously directed to a local minimum of the residual (i.e. \( \varphi_m - \varphi[i, \hat{\varphi}_m] \)), resulting in a stable iteration. This approach is also known as the Levenberg–Marquardt modification [32, p 145]. For small second derivatives, the essential bias can be assumed small compared to the parameter noise, and the estimation yields values close to the correct parameter. Therefore, the deviation from the correct parameter can be estimated for small errors (\( \Delta \varphi \ll \varphi \)) by

\[ \Delta \varphi = H_{\varphi}^T \Delta \varphi. \quad (22a) \]

Phase deviations are caused by errors of the center estimation and by the measurement noise

\[ \Delta \varphi = \Delta \varphi_\text{bias} + \Delta \varphi_\text{bias}. \quad (22b) \]

The bias and phase distortion function resemble scaled and phase shifted sinusoidal functions for \( \Delta \varphi \ll \varphi \)

\[ \Delta \varphi_{\text{bias},j} \approx -\frac{2}{\varphi} \left( b_{\text{bias}} \cos(\phi - \alpha) + b_{\text{bias}} \sin(\phi - \alpha) \right), \quad (22c) \]

\[ \Delta \varphi_{\text{bias}} \approx - \frac{2}{\varphi} \left( \varepsilon \cos(\phi - \alpha) + \varepsilon \sin(\phi - \alpha) \right), \quad (22d) \]

Consequently, the covariance matrix for \( E[\Delta \varphi] \approx 0 \) reduces to

\[ C_\varphi = E[\Delta \varphi \Delta \varphi^T] = E[\Delta \varphi]E[\Delta \varphi^T], \quad (23a) \]

\[ C_\varphi = \left( H_{\varphi}^T H_{\varphi} \right)^{-1} H_{\varphi}^T E[\Delta \varphi \Delta \varphi^T] H_{\varphi} \left( H_{\varphi}^T H_{\varphi} \right)^{-1}, \quad (23b) \]

\[ C_\varphi \approx \frac{\sigma^2}{\varphi M^2} \begin{bmatrix}
\frac{16Q^2}{8Q^2 - 4Q + 5} & 0 & -\frac{20Q^2}{5Q^2 - 1} \\
0 & 8Q^2 & 0 \\
-\frac{20Q^2}{5Q^2 - 1} & 0 & \frac{8Q^2}{5Q^2 - 1} \\
\end{bmatrix}. \quad (23c) \]

The result for \( f \) in (23c) seems to fall below the CRLB in (15a) for \( Q < 1.8 \). At such low \( Q \), the approximations used for the derivation of the CRLB are inaccurate. By using accurate numerical calculations, the CRLB is shown to be always lower for any constellation. The interesting variances are approximately

\[ \text{var}(\hat{f}) \approx \frac{2\varepsilon^2}{\varphi M^2}, \quad (24a) \]

\[ \text{var}(\hat{\varphi}) \approx \frac{8Q^2}{\varphi M} \sigma^2, \quad (24b) \]

and thus close to the CRLB in (15a) and (15b). Although this holds only for small noise amplitudes, the convergence to the CRLB is remarkable, because this implies that the method uses the information provided by the data efficiently. The critical operation, which could reduce the information content of the data, is the calculation of the phase angle of (19) yielding (20a). In general, also the magnitude spectrum must be considered to prevent loss of information. However, in the present case, the circle center was subtracted such that the magnitude spectrum is constant and contains no information but noise. All of the information is therefore passed to the phase and it is possible to achieve an optimum result with the benefit of a largely
increased numerical stability compared to direct numerical approaches. Figure 5 (left) shows the standard deviation of the parameters relative to the optimum standard deviation. The empirical standard deviations are calculated based on 100,000 simulated measurements with $M = 100$ frequency points per locus plot. Furthermore, locus plots at different noise levels are shown. The right graph shows the bias relative to the standard deviation. Although the results show a slight bias at higher noise levels, this bias is practically irrelevant as long as it is much smaller than the standard deviation of the parameters.

6. Conclusions

We demonstrated that the approach for circle estimation in the locus plot and subsequent data processing is not only numerically stable but also an efficient approach to determine the resonance parameters of the motional arm of resonators. The method was successfully applied to piezoelectric transducers and Lorentz force actuated and inductively read out sensors in [14, 16, 17]. The approach in [9] uses more advanced model functions with arbitrary and polynomial frequency dependencies. The same approach, as shown in this paper, can be used to assess the performance of these methods. When the discussed method is employed for fluid sensing, an interesting coincidence is observed in that the real and imaginary parts of the acoustic impedance of the fluid layer can be estimated with equal accuracy.

Acknowledgments

This work was supported by the Austrian COMET program (Austrian Center of Competence in Mechatronics, ACCM) and by the Austrian Science Fund (FWF, research grant L657-N16). The CISS gratefully acknowledges partial financial support from the European Regional Development Fund and the province of Lower Austria.

Appendix A. The effect of non-uniform frequency distributions

A frequency distribution resulting in a uniformly sampled locus plot was chosen in favor of closed form expressions of the variances. In [13], a frequency distribution with constant frequency increment was proposed and an extensive numerical analysis was performed to determine the optimum frequency span, which was found to be around three times the resonator bandwidth ($3B = 3f_r/Q$). This result is reproduced by using the sampling frequencies in (A.1) ranging from $f_r - bB/2$ to $f_r + bB/2$ and calculating the variances numerically for various $b$ using (9)

$$f_j = f_r \left(1 + b \left(\frac{j}{M} - \frac{1}{2}\right)\right), \quad j \in 0, ..., M - 1. \quad (A.1)$$

Figure A1 shows the variances of $f_r$, $Q$ and $\tilde{Y}$ relative to the CRLB for equal distribution on the locus plot. It can be observed that the curves for $Q$ and $f_r$ are indistinguishable. Furthermore, there is no $b$ such that the linear frequency vector yields better results, but a minimum ($\approx 1.13$) around $b \approx 2.9$ exists. At $b = 2.33$ the variance of the $\tilde{Y}$ estimate approaches $\sigma^2_Y$ up to a relative deviation of $8 \times 10^{-7}$.

The proposed frequency distribution in (10a) is a reasonable choice but similarly good performance can be obtained by using a linear frequency vector with a span around three times the resonator bandwidth. To generate the frequency vectors, such as in (10a) and (A.1), the resonance frequency and $Q$ factor must be known a priori. However, this is not a significant limitation when sensor excitation and signal processing can be performed in an iterative loop.

Appendix B. Cramér–Rao lower bound for various models

The variances for the case where some parameters are assumed known are shown below to illustrate the sensitivity of the results to certain model assumptions. The values in
Appendix C. Background components of higher order

The Fisher-information matrix can also be extended to encompass higher-order background functions such as \( f_n \) or arbitrary functions. Because the explicit calculation of the variances in the same fashion as shown before is difficult for higher-order terms, simulation results for background spectra comprising first- to

| Parameters | \( \text{var} \left\{ \hat{\theta} \right\} / \sigma_{\hat{\theta}}^2 \) | \( \text{var} \left\{ \hat{\theta} \right\} / \sigma_{\hat{\theta}}^2 \) |
|------------|----------------|----------------|
| \( f, Q, \bar{Y} \) | 1 | 1 |
| \( f, Q, \bar{Y}, \phi \) | 4 | 1 |
| \( f, Q, \bar{Y}, k_R, k_l \) | \( \frac{6}{5} \) | \( \frac{3}{2} \) |
| \( f, Q, \bar{Y}, k_R, l_l \) | \( \frac{6}{5} \) | \( \frac{3}{2} \) |
| \( f, Q, \bar{Y}, \phi, k_R, k_l \) | 6 | \( \frac{3}{2} \) |
| \( f, Q, \bar{Y}, \phi, k_R, k_l \) | 6 | \( \frac{3}{2} \) |
| \( f, Q, \bar{Y}, k_R \) | \( 4 \cdot \frac{2 - \cos 2\phi}{7 - 3 \cos 2\phi} \) | \( 2 \cdot \frac{4 - \cos 2\phi}{7 - 3 \cos 2\phi} \) |
| \( f, Q, \bar{Y}, l_l \) | \( 4 \cdot \frac{2 - \cos 2\phi}{7 - 3 \cos 2\phi} \) | \( 2 \cdot \frac{4 - \cos 2\phi}{7 - 3 \cos 2\phi} \) |
| \( f, Q, \bar{Y}, k_l \) | \( 4 \cdot \frac{2 + \cos 2\phi}{7 - 3 \cos 2\phi} \) | \( 2 \cdot \frac{4 + \cos 2\phi}{7 + 3 \cos 2\phi} \) |
| \( f, Q, \bar{Y}, l_l \) | \( 4 \cdot \frac{2 + \cos 2\phi}{7 - 3 \cos 2\phi} \) | \( 2 \cdot \frac{4 + \cos 2\phi}{7 + 3 \cos 2\phi} \) |
| \( f, Q, \bar{Y}, \phi, k_R \) | \( 5 - \cos 2\phi \) | \( \frac{1}{4} \) |
| \( f, Q, \bar{Y}, \phi, k_l \) | \( 5 + \cos 2\phi \) | \( \frac{1}{4} \) |

Figure C1. The variances of \( f \) and \( Q \) estimates are normalized to the case where \( \{ f, Q, \bar{Y}, \phi, k_R, k_l \} \) (marked as \( \{ f \} \), black) are estimated. Adding a higher-order frequency-dependent function results in increased variances. Estimation of \( \{ f, Q, \bar{Y}, \phi, k_R \times f^n, k_l \times f^n \} \) yields reduced variances at large sample counts \( M \). The curves are shown for \( Q = 100 \). Small deviations result only at \( Q < 10 \).

Table B1 are relative to the achievable variances when only this quantity is estimated. Increasing the number of estimated parameters increases the variances of non-orthogonal parameters.

\[
\sigma_{\hat{\theta}}^2 \approx \frac{f^2}{3YQ^3M} \sigma^2, \quad \sigma_{\hat{\theta}}^2 \approx \frac{16Q^2}{3Y^2M} \sigma^2 \quad (B.1)
\]
third-order terms are shown in figure C1. Stepwise increasing the order from offset only \((f^1)\) to \((f^2), (f^3), (f^4), (f^5)\) and \((f^6), (f^7), (f^8), (f^9)\) shows increased variances for small \(M\). An interesting effect is observed when the offset \((f^0)\) is assumed known and single higher-order contributions \((f^1), (f^2)\) and \((f^3)\) are added. The variances approach the half values of \(\sigma_f^2\) and \(\sigma_q^2\) for large \(M\).

References

[1] Sauerbrey G 1959 Verwendung von Schwingquarzen Zur Wägung dünner Schichten und zur Mikrowägung Z. Phys. 155 206–22
[2] Ferrari V, Marioli D and Taroni A 2001 Improving the accuracy and operating range of quartz microbalance sensors by a purposely designed oscillator circuit IEEE Trans. Instrum. Meas. 50 1119–22
[3] Lucklum R, Behling C and Hauptmann P 1999 Role of mass accumulation and viscoelastic film properties for the response of acoustic-wave-based chemical sensors Anal. Chem. 71 2488–96
[4] Elwenspoek M and Wiegerink R 2001 Mechanical Microsensors (Berlin: Springer)
[5] Jakoby B, Beigelbeck R, Keplinger F, Lucklum F, Niedermayer A, Reichel E K, Riesch C, Voglhuber-Brunnmaier T and Weiss B 2010 Miniaturized sensors for the viscosity and density of liquids: performance and issues IEEE Trans. Ultrason. Ferroelectr. Freq. Control 57 111–20
[6] Dufour I et al 2012 The microcantilever: a versatile tool for measuring the rheological properties of complex fluids J. Sensors 2012 719898
[7] Petersan P J and Anlage S M 1998 Measurement of resonant frequency and quality factor of microwave resonators: comparison of methods J. Appl. Phys. 84 3392–402
[8] Miura T, Takahashi T and Kobayashi M 1994 Accurate Q-factor evaluation by resonance curve area method and its application to the cavity perturbation IEEE Trans. Electron. 77 900–7
[9] Niedermayer A O, Voglhuber-Brunnmaier T, Sell J and Jakoby B 2012 Methods for the robust measurement of the resonant frequency and quality factor of significantly damped resonating devices Meas. Sci. Technol. 23 085107
[10] Armia Vives A 2008 Piezoelectric Transducers and Applications (New York: Springer)
[11] Parzen B and Ballato A 1983 Design of Crystal and Other Harmonic Oscillators (New York: Wiley)
[12] Rosenbaum J F 1988 Bulk Acoustic Wave Theory and Devices (Boston: Artech House)
[13] Niedermayer A O 2013 Measurement system design for resonant sensors: excitation, acquisition and signal processing PhD Thesis Johannes Kepler University, Austria
[14] Voglhuber-Brunnmaier T, Heinisch M, Reichel E K, Weiss B and Jakoby B 2013 Derivation of reduced order models from complex flow fields determined by semi-numerical spectral domain models Sensors Actuators A 202 44–51
[15] Beigelbeck R, Antlinger H, Cerimovic S, Clara S, Keplinger F and Jakoby B 2013 Resonant pressure wave setup for simultaneous sensing of longitudinal viscosity and sound velocity of liquids Meas. Sci. Technol. 24 125101
[16] Heinisch M, Reichel E K and Jakoby B 2013 U-Shaped wire based resonators for viscosity and mass density sensing Proc. SENSOR 2013 (Linz: Johannes Kepler University) pp 52–7
[17] Abdallah A, Lucklum F, Heinisch M, Niedermayer A O and Jakoby B 2012 Viscosity measurement cell utilizing electrodynamic-acoustic resonator sensors: issues and improvements IEEE Int. Instrumentation and Measurement Technology Conf. (I2MTC) (Graz, Austria, 13–16 May 2012) pp 2458–63
[18] Niedermayer A O, Reichel E K and Jakoby B 2009 Yet another precision impedance analyzer (YAPIA): readout electronics for resonating sensors Sensors Actuators A 156 245–50
[19] Oppenheim A V and Schafer R W 1999 Discrete-Time Signal Processing 2nd edn (Englewood Cliffs, NJ: Prentice Hall)
[20] Gardner W A 1990 Introduction to Random Processes: with Applications to Signals and Systems vol 31 (New York: McGraw-Hill)
[21] Bendat J S and Piersol A G 1980 Engineering Applications of Correlation and Spectral Analysis vol 1 (New York: Wiley)
[22] Butterworth S 1914 On electrically-maintained vibrations Proc. Phys. Soc. Lond. 27 410
[23] Van Dyke K S 1928 The piezo-electric resonator and its equivalent network Proc. Inst. Radio Eng. 16 742–64
[24] Niedermayer A O, Voglhuber-Brunnmaier T, Sell J K and Jakoby B 2012 Evaluating the robustness of an algorithm determining key parameters of resonant sensors Procedia Eng. 47 330–3
[25] Reichel E, Jakoby B and Riesch C 2007 A novel combined rheometer and density meter suitable for integration in microfluidic systems IEEE Sensors (Atlanta, GA, 28–31 October 2007) pp 908–11
[26] Etchart I, Chen H, Dryden P, Junji I, Harrison C, Hsu K, Marty F and Mercier B 2008 Mems sensors for density–viscosity sensing in a low-flow microfluidic environment Sensors Actuators A 141 266–75
[27] Rust P and Dual J 2011 Novel method for gated inductive readout for highly sensitive and low cost viscosity and density sensors 16th Int. Solid-State Sensors, Actuators and Microsystems Conf. (TRANSDUCERS) (Beijing, China, 5–9 Jun 2011) IEEE pp 1088–91
[28] Niedermayer A O, Voglhuber-Brunnmaier T and Jakoby B 2010 Smart analog compensation of spurious signals for a fully differential interface for resonating sensors IEEE Sensors (Waikoloa, HI, USA, 1–4 November 2010) pp 1445–58
[29] Kay S M 1993 Fundamentals of Statistical Signal Processing Volume I: Estimation Theory (Englewood Cliffs, NJ: Prentice Hall)
[30] Rangarajan P and Kanatani K 2009 Improved algebraic methods for circle fitting Electron. J. Stat. 3 1075–82
[31] Chernov N 2010 Circular and Linear Regression: Fitting Circles and Lines by Least Squares (Boca Raton, FL: Taylor and Francis)
[32] Chong E K P and Zak S H 2001 An Introduction to Optimization 2nd edn, vol 76 (New York: Wiley)