Closed-Form Relations for Resonance Detection Error Using Statistical Analysis of Amplitude Noise

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Abstract—The optimization of resonance-tracking sensors relies critically on proper estimation of resonance detection error. We study this error in two common resonance detection algorithms: the absolute minimum method and the linear regression method. Closed-form relations for the error originating from additive noise are presented. The formulation accommodates the majority of line-shapes of practical interest and a wide variety of noise statistics. Lorentzian and Fano line shapes are studied here with further detail for their practical importance. It is discussed that while the performance of the absolute minimum method depends on the tail of the noise probability distribution function, for the linear regression method the total noise power is the determining characteristic of the noise. This fact is explained for the specific case of quantization noise. The results of this study enable a quantitative comparison of the performance of resonance-based sensors, which is a center piece in the optimization of their limit of detection.

Index Terms—Limit of detection, noise, resonance detection.

I. INTRODUCTION

RESONANCE-based sensors are capable of detecting minute amounts of material, even down to individual molecules [1]–[3]. To achieve its full potentials, the sensor has to be adequately optimized. This optimization has two facets: highest sensitivity and least vulnerability to system noises. The evaluation of the effect of noise on resonance detection requires efficient numerical and analytical tools to determine how each type of noise affects the accuracy of the resonance detection.

The random error in resonance detection results from various system noises. This error can be quantified in terms of the standard deviation of the detected resonance. We refer to this standard deviation as the error (in resonance detection) throughout this paper. The error caused by amplitude noise is not linearly dependent on noise level in general. Electronic, shot, or thermal noise in the system are examples of amplitude noise in resonance spectrum measurements. The aggregate effect of these noises can be represented by an effective random noise on the measured samples [4], [5]. Basically, the components of the aggregate noise fall into two general components of light intensity-dependent and light intensity-independent noises [6]. For small noise levels, the noise level can be assumed almost constant around the resonance, although its dependence on the intensity should be considered in the calculations. The relations for estimating the error from amplitude noise are especially important as they help estimate the power consumption of the sensor. That is because the higher the amplitude noise, the higher the required signal power to achieve a target level of error. The target level of error is determined by the limit of detection (LOD) or the false-positive rate that we desire the sensor to achieve [7]. Hence, the relation between noise and the error is useful to calculate the power consumption of the sensor.

A widely used method for resonance detection is to scan the spectrum point by point, and then to retrieve the resonance by spectral data analysis. The spectral measurement approach is especially of interest for spectrally multiplexed sensors (consisting of multiple resonators) in which tracking resonators one by one is costly and complicated. To analyze the measured spectral data, a variety of processing algorithms have been proposed including parametric fits [8], polynomial fits [9], [10], parametric regression [11], centroid method [12], [13], and optimal linear data analysis [14], [15]. The resulting error in each of these algorithms has a idiosyncratic behavior specific to that algorithm. Having a closed-form formula for this unique behavior obviates the need for extensive Monte Carlo simulations. Monte Carlo method is an effective tool to estimate the error originating from system noises [16]. However, a blind Monte Carlo simulation in a multi-dimensional optimization space is time-consuming, and it does not provide the designer with an insight on system trends. Curve fitting to Monte Carlo simulation data has been used to propose ad hoc formula for the error when the resonance of a Lorentzian lineshape is detected subject to a white Gaussian noise [17]. Such a formula for the error not only depends on the lineshape and noise statistics, but also on the specifics of the measurement technique and the resonance detection algorithm. Analytical relations have also been proposed for the estimation of the error on a case-by-case basis. For example Nenninger et al. [18] studied the noise in surface-plasmon-resonance sensors and provided an analytical framework, which can be used along with computer simulations to estimate the effect of noise. Homola [19] proposed a closed-form relation for the error in the centroid data processing method. However, similar relations are lacking in the literature for other commonly used processing methods.
In this article, we derive closed-form relations for the error in the two most commonly used resonance detection methods: (1) **absolute minimum** method, which denotes the resonance as the wavelength of the readout sample with minimum (or maximum) detector recording [17], (2) **linear regression** method, which finds the resonance using a quadratic fit to the data. The majority of the lineshapes of practical interest are quadratic around their resonance, and thus a quadratic fit is usually adequate [20].

A mentionable characteristic of these two methods is their relatively low computational load. We use a simple additive model for noise, which is sufficiently comprehensive for the majority of practical cases [6], [21].

Our analysis clarifies the effect of sampling resolution on the error in the above mentioned methods. The ensuing formulas accommodate a large class of noise statistics and resonance lineshapes. Empirical data on the statistics of the aggregate amplitude noise in a conventional laser-scanning setup is presented in Section II. In Section III, a theoretical framework based on extreme value theory is developed to propose a parametric formula for the error in the absolute minimum method. In Section IV, a closed-form relation is derived for the error when the resonance is detected by the linear regression method. For both methods, the proposed formulas are compared against Monte Carlo simulations. Next, we discuss the fundamental difference between the trends of the absolute minimum method and the linear regression method in Section V. The implications of these trends in the presence of quantization noise are also elaborated. Final conclusions are made in Section VI.

II. EXPERIMENTAL NOISE MEASUREMENT

Laser-scanning setups are common configurations to scan the spectrum of photonic resonators and detect their resonances. Fig. 1(a) shows the scanning electron micrograph (SEM) of a microring resonator coupled to a waveguide in a silicon nitride on oxide material platform. Fig. 1(b) shows the transmitted power of the structure shown in Fig. 1(a) as a function of wavelength \( \lambda \) measured using a laser-scanning setup. (The details of fabrication and characterization are explained in Reference [7], and they are not repeated here for brevity.) Fig. 1(c) shows an enlarged view of the recorded spectrum samples along with a Lorentzian fit and a quadratic fit obtained by the linear regression method. Within this wavelength window, these methods result in closely similar fits. Fig. 1(d) shows the detected resonance according to the absolute minimum method and the linear regression method. The difference between the two methods is visible.

We use the laser-scanning setup mentioned above to measure the amplitude noise statistics. The light from a tunable laser (Newport TLB 6305, 652–660 nm, operated at a constant current of 43.5 mA) is passed through a polarizer and then detected by a photodetector (without passing through the integrated device). The photodetector gain is 40 dB, and its analog output is connected to a data acquisition device (National Instrument USB-6211) that samples the data and sends the digital readout to a computer. The setup is controlled by LabView software to synchronously scan the laser wavelength and record the photodetector readout. Laser scan rate is 6 nm/s; and the spectrum sampling resolution is 250 fm. The setup is run at its normal measurement condition (i.e., scanning from 652 to 660 nm) for a fixed polarizer angle. Since the laser output is partially polarized, the polarizer is meant to act as a simple attenuator.

Noise analysis is carried out on the data in the 654–659 nm window to exclude the power oscillations occasionally observed at the beginning or at the end of the scan window. Since laser output power slowly varies over the scan window, the baseline of the readout is calculated by applying a 100-point moving average filter to the data. The difference between the raw readout and its baseline is regarded as the amplitude noise. This noise excludes lower frequency components such as optical Fabry–Perot oscillations (from the optical components such as the glass/air interfaces of the polarizer) and the harmonics of the power grid frequency. Since the behavior and characteristics of such noises are known, they can be removed from transmission measurements using parametric fitting or filtering. Although the recorded samples correspond to different wavelengths of the laser, we assume the amplitude noise not to depend strongly on the wavelength. Fig. 2(a) and (b) show the noise, extracted as explained above, and its probability distribution function (p.d.f.) in this scan, average light intensity on the detector is 68 mV.

Next, we repeated this experiment with the laser light physically blocked. The photodetector readout is shown in Fig. 2(c), which demonstrates the quantized values of the readout. The quantization leads to a multi-peak p.d.f, shown in Fig. 2(d).
Since the same setup is also used for the spectral measurements of photonic resonators, Fig. 2(d) essentially represents the amplitude noise of the setup on a near-zero resonance dip. The measurements presented here will inform our discussion in Section VI.

III. ABSOLUTE MINIMUM METHOD

In the absolute minimum method, the resonance wavelength ($\lambda_{res}$) is defined as $\lambda_{res} = \lambda_i$, where $i = \text{argmin} \{D_i\}$, and $D_i$ is $i$-th detector readout. The wavelength of the $i$-th data point is $\lambda_i = i \delta$, where $\delta$ is the sampling resolution in the wavelength domain. Based on the Monte Carlo simulations for a Lorentzian resonance lineshape with unity height (amplitude extinction) and subject to a white Gaussian noise, White and Fan [17] have proposed the following relation for the estimation of the error when absolute minimum method is used:

$$\sigma_\lambda \approx \frac{1}{4.5} \Lambda \sqrt{\sigma_n},$$

(1)

where $\sigma_\lambda$ is the standard deviation of resonance wavelength detection, $\Lambda$ is the full width at half maximum (FWHM) of the Lorentzian lineshape, and $\sigma_n$ is the standard deviation of the white Gaussian noise. Using extreme value theory in Appendix A, we have shown that the $\Lambda \sqrt{\sigma_n}$ trend in Eq. (1) is in fact the dominant term of the Taylor series expansion of the error ($\sigma_\lambda$). It is worth mentioning that our argument in Appendix A holds for a general quadratic lineshape (i.e., non-zero second order coefficient in its Taylor expansion around the resonance wavelength). Thus, the $\Lambda \sqrt{\sigma_n}$ trend can be generalized to other quadratic lineshapes such as Fano. However, the scaling factor depends on the noise p.d.f and the sampling resolution. Following Eq. (A.13), we let this scaling factor to be a function of $\delta/\Lambda$ and denote it by $\alpha_1$ to represent the error as:

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) = \Lambda \sqrt{\sigma_n} \alpha_1 \left(\frac{\delta}{\Lambda}\right).$$

(2)

The analysis in Appendix A provides us the parametric model given in Eq. (A.19), which is based on the asymptotic trend of $\alpha_1$. To verify that model, we use Monte Carlo simulations to calculate $\alpha_1(\delta/\Lambda)$ for three separate cases with Gaussian, uniform, and Laplacian noises. Noise standard deviation is assumed $\sigma_n = 0.01$ in all the cases, and the lineshape is Lorentzian as defined in Eq. (A.5) with $\Lambda = 1$. After adding the random noise to the lineshape, the resonance is detected by the absolute minimum method, and this test is repeated $10^4$ times. The standard deviation of the resulting resonances is $\sigma_\lambda$ from which we can calculate $\alpha_1 = \sigma_\lambda/\sigma_n$. Finally, the parametric model of Eq. (A.19) is fitted to the numerical data for $\alpha_1(\delta/\Lambda)$ to estimate optimal parameters. The results are shown in Table I.

Even though suggested parametric relations are derived from the asymptotic behavior of $\alpha_1(\delta/\Lambda)$, the parametrization allows for the extension of these relations to non-asymptotic regimes of $\delta/\Lambda$. As demonstrated in Fig. 3, the parametric models fit very well to the numerical data over a large range of sampling resolutions. The data point that corresponds to the estimate provided by Eq. (1), i.e. Gaussian noise and $\alpha_1 = 1/4.5$, is marked by an arrow on this figure. Fig. 3 clearly shows that for a fixed Lorentzian linewidth ($\Lambda$) and noise standard deviation ($\sigma_n$), the error ($\sigma_\lambda$) changes considerably depending on the noise p.d.f and the sampling resolution ($\delta$).

Next, we undertake the extension of this result to other lineshapes. First, note that in Appendix A we replaced the real resonance lineshape with a quadratic approximation early on in the argument. Hence, the $\sigma_n \sim \Lambda$ behavior is expected to be true for any general lineshape with a quadratic form around its resonance. But to extend the results beyond a Lorentzian lineshape, we need a general definition for the linewidth. According to Appendix A, if the functional variation of the resonance lineshape with wavelength ($\lambda$) is given by $R(\lambda)$, the parameter $\Lambda$
is in fact related to the second order derivative of $R(\lambda)$ at the resonance wavelength as:

$$\frac{\partial^2 R}{\partial \lambda^2}|_{\lambda_{res}} = \frac{8}{\Lambda^2}. \quad (3)$$

Thus, $\Lambda$ can be defined more rigorously as:

$$\Lambda = \sqrt{\frac{8}{|\partial^2 R/\partial \lambda^2|(\lambda_{res})}}. \quad (4)$$

In order to show the versatility of the definition in Eq. (4), we discuss it for a Fano lineshape. Following reference [22], we define Fano lineshape as:

$$R(\lambda) = R_0 \left(\frac{F\gamma + \lambda}{\lambda^2 + \gamma^2}\right)^3, \quad (5)$$

where $F$ is the so-called Fano parameter, and $\gamma$ is the width in wavelength domain. Fano lineshape is quadratic around both extrema and their respective second order derivatives are

$$\lambda_{min} = -\gamma F, \quad \frac{\partial^2 R}{\partial \lambda^2}|_{\lambda_{min}} = 2R_0 \frac{1}{\gamma^2 (1 + F^2)}; \quad (6a)$$

$$\lambda_{max} = \gamma F, \quad \frac{\partial^2 R}{\partial \lambda^2}|_{\lambda_{max}} = -2R_0 \frac{F^4}{\gamma^2 (1 + F^2)}. \quad (6b)$$

Hence, by plugging Eqs. (6) in (4) and (2), the resonance detection error at the maximum and minimum points of a Fano lineshape are given by

$$\sigma_{\lambda}^{(min)} = 2\gamma \sqrt{1 + F^2} \sqrt{\frac{\sigma_n}{R_0}} \alpha_1; \quad (7a)$$

$$\sigma_{\lambda}^{(max)} = 2\gamma \sqrt{1 + F^2} \frac{\sigma_n}{F^2} \sqrt{\frac{\sigma_n}{R_0}} \alpha_1. \quad (7b)$$

The factor $\alpha_1$ in these equations is the same as that presented in Fig. 3. We will use this relation in our discussion in Section V.

Fig. 3. The scaling factor $\alpha_1$ in Eq. (2) for various amplitude noise p.d.f.s (Gaussian: circles, uniform: squares, Laplacian: diamonds). The standard deviation of the error ($\sigma_1$) is calculated for each noise p.d.f, the corresponding parametric model presented in Table I is fitted to the numerical results to find optimal $A$ and $B$ coefficients.

Fig. 4. The Monte Carlo simulations (circles) and theoretical estimates (dashed lines) of the resonance detection error ($\sigma_1$) for linear regression method. The theoretical estimate is obtained from Eq. (9). The Monte Carlo simulations are performed for $\Lambda = 1$, uniform noise p.d.f, $N$ being the closest integer to $\Lambda/10^{6}$, and $10^3$ iterations. The number next to each curve is the SNR defined as $20 \log \sigma_n$. The Lorentzian amplitude is unity, as in Eq. (A.5).

IV. LINEAR REGRESSION METHOD

Another conventional method of resonance detection is fitting a parametric function to the lineshape around the resonance wavelength [20], [23]. Specifically, linear regression can be used to fit a quadratic function to the data with a relatively small computational load. The fitting function, $f(\lambda)$, is

$$f(\lambda) = p_1 \lambda^2 + p_2 \lambda + p_3, \quad (8)$$

from which, the resonance wavelength is estimated as $\lambda_{res} = -p_2/2p_1$. Using the matrix representation of linear regression [20], we have calculated the error approximately as

$$\sigma_{\lambda}(A, \sigma_n, \delta) = \sqrt{\frac{3}{N^3}} \Lambda^2 \sigma_n \frac{4\delta}{\alpha_1}. \quad (9)$$

The window length (i.e., the number of samples used for the linear regression) is denoted by $N$. We have made three assumptions in deriving Eq. (9): 1) $N$ is large ($\gg 1$), so that only the dominant terms in $N$ are kept in the calculations. 2) The fitting window of $N$ samples is symmetrically positioned around the actual resonance wavelength. A fairly accurate positioning for this window can be achieved either by running a few iterations of the linear regression method, or by the absolute minimum method provided that its error is relatively small. 3) The resonance linewidth, i.e., $\Lambda$ in Eq. (A.5), is known. So, we let $p_1 = 4/\Lambda^2$. This is a reasonable assumption as in most practical cases the resonance shift does not alter the linewidth considerably.

Fig. 4 compares the results of the Monte Carlo simulations ($\Lambda = 1$, uniform noise p.d.f, $N$ being the closest integer to $\Lambda/10^6$ and $10^3$ iterations) and those estimated by Eq. (9). In these simulations, we assume an estimation window symmetrically positioned around the actual resonance wavelength, and calculate the resonance wavelength using $\lambda_{res} = -p_2 \Lambda^2/8$ (assuming a known $\Lambda$). The good agreement between the two sets of results is evident from Fig. 4.
Since our definition of lineshape is similar to that in Appendix A, the result of Eq. (9) can be extended to any lineshape with quadratic behavior around the extremum point. Hence, the $\Lambda$ calculated from the Eqs. (4) and (6) can be plugged in Eq. (9), to give the $\sigma_n$ error when linear regression is used on a Fano resonance:

$$
\sigma_{\lambda}^{(\text{min})} = \sqrt{\frac{3}{N^3 R_0} \frac{\gamma^2 (1 + F^2)}{\delta}}, \quad (10a)
$$

$$
\sigma_{\lambda}^{(\text{max})} = \sqrt{\frac{3}{N^3 R_0} \frac{\gamma^2 (1 + F^2)}{\delta F^4}}. \quad (10b)
$$

Finally, it is worth discussing the implications of Eqs. (2) and (9) for the optimization of LOD in resonance-based sensors. A conventional definition for LOD is $3\sigma_\gamma/S$, with $S$ being the sensitivity of the resonance [7]. Subject to a fixed $\delta/\Lambda$, $\tau$ (detector integration time per sample, affecting $\sigma_n$), and $(N\delta)/\Lambda$; we have $\text{LOD} \sim 3\sigma_\gamma \sim 1/Q \left( Q = \lambda_{\text{res}}/\Lambda \right)$. This result is observed both for the absolute minimum method in Eqs. (2) and for the linear regression method in Eq. (9). Whereas, if we use the linear regression method with fixed $\delta$, $\tau$, and $(N\delta)/\Lambda$; Eq. (9) results in $\text{LOD} \sim 3\sigma_\gamma \sim 1/\sqrt{Q}$ (as opposed to $\sim 1/Q$). This example shows the importance of resonance detection method in determining what figure of merit should be used. Similar to our argument above, for any arbitrary case with its specific restrictions, Eqs. (2) and (9) provide proper analytical tools to optimize LOD based on the specifics of the sensor system.

V. DISCUSSION: STATISTICS TAIL VERSUS AVERAGE NOISE POWER

Although our estimates of $\sigma_{\lambda}$ for both methods depend on noise standard deviation ($\sigma_n$), the interpretation of $\sigma_n$ is fundamentally different in these two cases. In the absolute minimum method, the resonance is determined by the sample that has the smallest (i.e., largest negative) noise. Thus, the tail section of the noise p.d.f (i.e., the section corresponding to extreme values) most critically affects the resonance detection. That is to say, if we keep the negative tail of the noise p.d.f intact and replace the rest of the p.d.f arbitrarily, we do not expect the absolute minimum method to produce much different $\sigma_{\lambda}$. In marked contrast to this rationale, the linear regression method leads to a linear relationship between the noise standard deviation ($\sigma_n$) and the error ($\sigma_{\lambda}$), no matter what the noise p.d.f is. Thus, $\sigma_n$ is directly related to and represented by the noise power in the linear regression method.

To better discern the $\sigma_n$ interpretations, we carried out a numerical experiment on a Fano resonance subject to a two-level quantization noise. Quantization noise is especially important for near-zero measurements. One such example is a resonance dip (see Fig. 2(d)). We let the noise p.d.f, $p_n(n)$, be comprised of two similar Gaussian peaks with different centers $\mu_1$ and $\mu_2$:

$$
p_n(n) = \frac{1}{2 \sigma_0 \sqrt{2\pi}} \exp\left(-\frac{(x - \mu_1)^2}{2\sigma_0^2}\right) + \frac{1}{2 \sigma_0 \sqrt{2\pi}} \exp\left(-\frac{(x - \mu_2)^2}{2\sigma_0^2}\right). \quad (11)
$$

By changing the spacing between the quantization levels ($|\mu_1 - \mu_2|$), the standard deviation of the noise changes while the overall tail stays almost the same. In this situation, for the tail-dependent absolute minimum method, we do not expect $\sigma_n$ to change with the spacing between the quantization levels. Whereas, for the linear regression method, $\sigma_n$ is expected to change almost linearly with the spacing between the quantization levels.

For this numerical experiment, we use a Fano lineshape as defined by Eq. (5) with $F = 1$, $R_0 = 1$, and $\gamma = 1$, and we focus on the detection of the Fano dip at $\lambda = -1$. The sampling resolution is $\delta = 0.01$, and the standard deviation of each individual Gaussian peak in Eq. (11) is $\sigma_0 = 0.01$. Linear regression is applied in a window of $N = 30$ samples around the Fano resonance peak. The results presented in Fig. 5 confirm the hypothesis that the performance of the absolute minimum method depends on the tail of the noise p.d.f, while in the linear regression method the noise standard deviation is the determining factor.

It should be noted that the invariability of the error ($\sigma_{\lambda}$) with the noise standard deviation ($\sigma_n$) for the absolute minimum method in this experiment does not contradict the $\sigma_n \sim \sqrt{\gamma}$ trend implied by Eq. (2). The $\sqrt{\gamma}$ trend there was derived for a self-similar noise p.d.f subject to merely a linear scaling. However, the standard deviation of noise in the numerical experiment of Fig. 5 changes by a shift in the individual peaks, and not a linear scaling. Thus, the $\alpha_1$ factor also changes when $|\mu_1 - \mu_2|$ varies. The combined variation of $\sigma_n$ and $\alpha_1$ results in the nearly invariant behavior of $\sigma_{\lambda}$ in Fig. 5. This numerical experiment also demonstrates considerable variations of $\alpha_1$ for noise p.d.f.s other than the Gaussian distribution. This fact entails caution and due diligence in using the $\Lambda \sqrt{\sigma_n}$ trend for absolute minimum method in general.

Fig. 5. The error in the absolute minimum method (circles) and the linear regression method (squares), in the presence of a bi-level quantization noise. The resonance is a Fano dip with $F = 1$, $R_0 = 1$, and $\gamma = 1$, as shown in inset (a). The standard deviation of the noise ($\sigma_n$) is changed by increasing the spacing between the two Gaussian peaks in the noise p.d.f, shown in the inset (b). Each of the two quantized levels is represented by a Gaussian with $\sigma_0 = 0.01$. Dashed lines demonstrate the theoretical formula for: the absolute minimum method, with $\alpha_1 = 0.25$ and $\sigma_n = \sigma_0$ in Eq. (7b); and the linear regression method, with $\sigma_n$ in Eq. (10b) being the total standard deviation of the noise (which is the same parameter shown on the horizontal axis in this figure).
According to Eqs. (2) and (9), the performance of the linear regression method degrades faster than that of the absolute minimum method when the SNR is decreased, or the sampling becomes sparser. Beyond a certain threshold, the latter outperforms the former. Fig. 5 represents as an example in which the absolute minimum method outperforms the linear regression method (for \( \sigma_n > 0.04 \)).

The formulas derived in Eqs. (2) and (9) for the resonance detection error allow for the systematic optimization of resonance-based sensors in a large set of applications. Compared to previous results (e.g., Eq. (1)), our closed-form formulas are not limited to specific cases such as Gaussian noise or Lorentzian lineshape.

**VI. CONCLUSIONS**

We presented closed-form formulas for the estimation of the error in resonance detection. The focus of the article is on two algorithms with low computational load: absolute minimum method, and linear regression method. The proposed formulas accommodate a wide class of noise statistics and resonance lineshapes. Noise measurements in a conventional laser-scanning setup revealed a dominant quantization noise for near-zero signals. The two above mentioned methods are juxtaposed in the specific case of quantization noise, to discuss that while in the former the error depends on the tail behavior of the noise p.d.f, in the latter the total power of noise is the important noise characteristic. The presented formulas remarkably simplify the optimization process of resonance-tracking sensors.

**APPENDIX A**

**ANALYSIS OF ABSOLUTE MINIMUM METHOD**

In this appendix, the error resulting from amplitude noise is calculated for absolute minimum method. We start from the exact form of p.d.f for the error of resonance detection; derive proper scaling rules under self-similarity assumption of noise p.d.f, and employ these rules in a parameter-reduction process; and simplify the problem by discussing different terms of the Taylor expansion of the error. Finally, the asymptotic behavior of the error is calculated using extreme value theory [24], and a parametric relation for the error is presented.

The amplitude of the \( i \)-th measured sample, \( D_i \), is

\[
D_i = R_i + n_i, \quad (A.1)
\]

where the resonance function \( R_i \) is the ideal resonance function (power transmission of the device) for the wavelength at which the \( i \)-th sample is measured, i.e. \( R(\lambda_i) \). \( n_i \) is the amplitude noise of this measurement. The probability of the \( i \)-th sample to be the absolute minimum is:

\[
p(i) = \int_{n_i = -\infty}^{+\infty} \prod_{j \neq i} P(R_i + n_i < R_j + n_j)p_n(n_i)dn_i
\]

\[
= \int_{n_i} \prod_{j \neq i} P(n_j > R_i - R_j + n_i)p_n(n_i)dn_i
\]

where the function \( P(\cdot) \) denotes the probability that the condition inside the parentheses is true. \( Q(\cdot) \) is defined as:

\[
Q(x) = \int_{x = -\infty}^{+\infty} p_n(n)dn,
\]

\[
= \sum_{i} (i\delta)^2 \int_{n_i} \prod_{j \neq i} Q(R_i - R_j + n_i)p_n(n_i)dn_i. \quad (A.4)
\]

For small-noise cases, where \( \sigma_n \) is much smaller than resonance linewidth, the resonance can be approximated by its leading Taylor expansion term. For a Lorentzian resonance with a normalized amplitude we have

\[
R(\lambda) = 1 - \frac{1}{1 + (2\lambda/\Lambda)^2} \quad (A.5a)
\]

\[
\approx \frac{4}{\Lambda^2} \lambda^2, \quad (A.5b)
\]

where \( \Lambda \) denotes the FWHM linewidth. Sampling this function with a resolution (i.e., the wavelength difference between adjacent samples) of \( \delta \) results in \( R_i \approx (2i\delta/\Lambda)^2 \). The rest of our analysis here is based on the assumption that the resonance function can be approximated by a quadratic function around its resonance, which is for instance the case for Lorentzian and Fano resonances (Although Fano resonance is asymmetric, for small intervals around its extremum points it can be considered a symmetric quadratic function). Thus,

\[
\sigma_n^2 = \sum_{i} (i\delta)^2 \int_{n_i} \prod_{j \neq i} Q\left(\left(\frac{2\delta}{\Lambda}\right)^2 (i^2 - j^2) + n\right)p_n(n)dn.
\]

\[
(A.6)
\]

We assume that the noise samples are independent and identically distributed (iid), and replace \( n_i \) with \( n \) from this point. The three parameters of our interest here are \( \Lambda, \sigma_n \) (noise standard deviation), and \( \delta \). It can be seen from Eq. (A.6) that for any arbitrary \( \alpha > 0 \),

\[
\sigma_1(\Lambda, \sigma_n, \alpha \delta) = \alpha \sigma_n \frac{\sigma_2(\Lambda/\alpha, \sigma_n, \delta)}{\Lambda}, \quad (A.7)
\]

\[
\sigma_2(\Lambda, \alpha \sigma_n, \delta) = \sigma_2(\sqrt{\alpha \Lambda}, \sigma_n, \delta). \quad (A.8)
\]

In the above equations, the noise p.d.f is assumed to be self-similar for various values of standard deviation, so that when we scale the standard deviation by \( \alpha \) we have \( p_n(n) = p_n(n/\alpha)/\alpha \). The scaling rules allow us to reduce the three initial parameters to one parameter by defining the function \( \sigma \) as

\[
\sigma_2(\Lambda, \sigma_n, \delta) = \delta \sigma_2 \left( \frac{\Lambda}{\delta} \sqrt{\sigma_n} \right). \quad (A.9)
\]
Using the Taylor expansion of $\bar{\sigma}_2(\lambda \sqrt{\sigma_n}/\delta)$, i.e.:

$$\bar{\sigma}_2\left(\frac{\lambda}{\delta} \sqrt{\sigma_n}\right) \approx \alpha_0 + \alpha_1 \frac{\lambda}{\delta} \sqrt{\sigma_n} + \alpha_2\left(\frac{\lambda}{\delta} \sqrt{\sigma_n}\right)^2 + \ldots,$$  \hspace{1cm} (A.10)

we get

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) \approx \delta \alpha_0 + \Lambda \sqrt{\sigma_n} \alpha_1 + \frac{1}{\delta}(\Lambda \sqrt{\sigma_n})^2 \alpha_2 + \ldots$$ \hspace{1cm} (A.11)

In order for $\sigma_\lambda(\Lambda, \sigma_n, \delta)$ to be non-singular at $\delta \to 0$, we should have $\alpha_i = 0$ for $i > 1$. Therefore, the dominant term in Eq. (A.11) at the limit of $\delta \to 0$, is the second term:

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) \approx \Lambda \sqrt{\sigma_n} \alpha_1.$$  \hspace{1cm} (A.12)

Note that the $\sigma_\lambda \sim \Lambda \sqrt{\sigma_n}$ trend is not limited to a Gaussian noise, although the parameter $\alpha_1$ does depend on the specifics of the noise distribution. Following a similar line of discussion, it can be shown that if the first non-zero term is the fourth order term we would have $\sigma_\lambda \sim \Lambda \sqrt{\sigma_n}$.

According to the above analysis, the behavior of $\sigma_\lambda$ is mainly dominated by $\Lambda$ and $\sigma_n$. In the next step, in order to include the smaller effect of $\delta$ as well, we let $\alpha_1$ be a function of $\delta$ (normalized to the linewidth $\Lambda$) so that:

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) \approx \Lambda \sqrt{\sigma_n} \alpha_1 \left(\frac{\delta}{\Lambda}\right).$$  \hspace{1cm} (A.13)

Finding a general relation for $\alpha_1$ is involved. However, the asymptotic behavior of $\alpha_1(\delta/\Lambda)$ at $\delta/\Lambda \to 0$ provides helpful insight. Although in practice we may design the system at non-asymptotic regimes of sampling resolution, the study of this regime reveals the principle trends in $\sigma_\lambda$, based on which some parametric models can be proposed to cover both asymptotic and non-asymptotic regimes accurately. The importance of these parametric models is discussed in Section III.

Let us assume that the resonance function is densely sampled so that $\delta \ll \Lambda, \sigma_\lambda$. Now consider the case of doubling the sampling density. We can assume that each single sample will be replaced by a bundle of two adjacent samples, $\delta/2$ apart in their wavelengths. Within each bundle represented by $\{D_i, D_{i+1}\}$, we can discard the larger sample, because that sample will not be the absolute minimum of the whole data set. Since $\delta \ll \Lambda$, we have $R_i \approx R_{i+1}$. So, the same argument for $D$ can be extended to the noise because $D_i = R_i + n_i$. That is to say, within each bundle, the sample with larger noise ($n_i$ or $n_{i+1}$) will be discarded; and we only keep the sample with smaller noise as the dominant sample of the bundle. The dominant noise of this bundle will then be a random variable defined as $n_{m_{\text{min}}(2)} = \min\{n_i, n_{i+1}\}$. As a result, doubling the sampling resolution (as far as $\sigma_\lambda$ is concerned) is equivalent to replacing the distribution function of $n$ with that of $n_{m_{\text{min}}(2)}$ (without doubling the sampling resolution). Similar argument can be made for the case of an $m$-fold increase in the sampling resolution: changing the sampling resolution from $\delta$ to $\delta/m$ is equivalent to replacing $p_n(n)$ with $p_{\lambda m}(n)$, where $p_{\lambda m}(n)$ is the p.d.f of the random variable $N$ defined as the minimum of $m$ i.i.d. random variables with a p.d.f of $p_n(n)$.

According to extreme value theory, for any well-behaved [25] p.d.f $p_n(n)$, there exists scaling factors $a_m > 0$ and $b_m$ such that:

$$\lim_{m \to \infty} Q_N(a_m^{-1} n + b_m) = Q_n^\prime(a_m^{-1} n + b_m) \to G(n) \equiv e^{-e^{-n}},$$  \hspace{1cm} (A.14)

where $Q_n$ and $Q_N$ are defined according to Eq. (A.3) for the noise ($n$), and for the minimum of a bundle of $m$ noise samples ($N$). In general, $G(n)$ is the cumulative distribution function of one of three well known extreme distributions: Gumbel, Frechet, and Weibull. However, for the majority of noise statistics of practical interest, $G(n)$ is the Gumbel distribution as defined in Eq. (A.14). Thus,

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) = \sigma_{G, \lambda}(\Lambda, \frac{1}{a_m} \sigma_n, m\delta).$$  \hspace{1cm} (A.15)

Note that the $\sigma_\lambda$ on the left corresponds to any arbitrary distribution function within Gumbel domain of attraction [24], while the $\sigma_{G, \lambda}$ on the right corresponds to that for a Gumbel distribution. Using Eqs. (A.7) and (A.8) we have

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) = \frac{1}{\sqrt{a_m}} \sigma_{G, \lambda}(\Lambda, \sigma_n, m\delta).$$  \hspace{1cm} (A.16)

To simplify the relations, we define:

$$k \equiv m\sqrt{a_m} \approx A_1 m^{1+\epsilon},$$  \hspace{1cm} (A.17)

with which Eq. (A.16) turns to

$$\sigma_\lambda(\Lambda, \sigma_n, \delta) = \frac{1}{\sqrt{a_m}} \sigma_{G, \lambda}(\Lambda, \sigma_n, k\delta).$$  \hspace{1cm} (A.18)

This relation is important as it expresses the scaling behavior of $\sigma_\lambda$ with $\delta$. Changing the sampling resolution from $\delta$ to $\delta/k$ scales $\sigma_\lambda$ with $1/\sqrt{a_m}$, where $m \approx A_2 k^{1+\epsilon} \approx A(\Lambda/\delta)^{1+\epsilon}$. This approximation leads to

$$\alpha_1(\frac{\delta}{\Lambda}) = \frac{A}{\sqrt{a_m}}; \text{ where } m = B \left(\frac{\Lambda}{\delta}\right)^{1+\epsilon}.\hspace{1cm} (A.19)$$

$A$, $B$, and $\epsilon$ parameters depend on the noise statistics. We will use this parametric model in Section III to propose accurate estimates for $\alpha_1(\frac{\delta}{\Lambda})$.

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