Effect of multiplicative noise on least-squares parameter estimation with applications to the atomic force microscope

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Measurement of the power spectral density of (stochastic) Brownian fluctuations of micro- and nano-devices is used frequently to gain insight into their mechanistic properties. Noise is always present in these measurements and can directly influence any parameter estimation obtained through a least-squares analysis. Importantly, measurements of the spectral density of stationary random signals, such as Brownian motion, inherently contain multiplicative noise. In this article, we theoretically analyze the impact of multiplicative noise on fit parameters extracted using a least-squares analysis. A general analysis is presented that is valid for any fit function with any number of fit parameters. This yields closed-form expressions for the expected value and variance in the fit parameters and provides a rigorous theoretical framework for *a priori* determination of the effect of measurement uncertainty. The theory is demonstrated and validated through Monte Carlo simulation of synthetic data and by comparison to power spectral density measurements of the Brownian fluctuations of an atomic force microscope cantilever – analytical formulas for the uncertainty in the fitted resonant frequency and quality factor are presented. The results of this study demonstrate that precise measurements of fit parameters in the presence of noise are inherently problematic – individual measurements of the power spectral density are capable of yielding fit parameters that are many standard deviations away from the mean, with finite probability. This is of direct relevance to a host of applications in measurement science, including those connected with the atomic force microscope. *© 2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4709496]

I. INTRODUCTION

Least-squares analysis is used widely to extract quantitative information from experimental data.[1–9] This is achieved by formulating a residual function that is based on the mean-squared difference between the measured data and a fit function (model).[10,11] This residual function is then minimized with respect to the fit parameters of the chosen model. Knowledge of the functional form of the experimental data ensures selection of an appropriate fit function, and hence meaningful interpretation of the extracted fit parameters.

Estimation of the spectral properties of stationary random processes is required frequently in physical measurements – for example, the Brownian motion of micro- and nano-devices. This can provide fundamental insight into the underlying thermodynamic and mechanical processes within these devices, and is employed extensively in their characterization.[3,4,7,12–18] Such studies often make use of least-squares analysis to interpret the measured power spectral density (PSD). The power spectral density is commonly estimated from the Fourier transform of finite time series of the stochastic (Brownian) motion of the device.[4,13–17,19] This inherently introduces noise into the estimate, which is proportional to the PSD, i.e., the noise is multiplicative – its variance is proportional to the square of the PSD.[19] While this sampling noise can be reduced by averaging multiple independent measurements, it is always present and must be considered in any interpretation of experimental data.

Uncertainty in the fit parameters obtained from a least-squares analysis, due to the presence of noise, can be estimated through use of simplified formulas derived under the assumption of linear regression and additive noise,[20] and/or Monte Carlo simulation which implicitly ignores the functional form of the experimental data or fit function;[21] the latter approach is computationally expensive. However, these approaches do not allow for rigorous analysis of measurement uncertainty and/or design of experimental protocols to minimize the effect of noise. For example, the resonant frequency and quality factor of atomic force microscope (AFM) cantilevers are commonly deduced by fitting a Lorentzian to the measured thermal noise spectrum of the device using a least-squares analysis. Yet no rigorous theory currently exists for determining the uncertainty in these measured (fit) parameters.[18] Standard least-squares analyses are commonly used in applications involving the atomic force microscope. While an alternate approach based on a weighted least-squares analysis is also possible,[22,23] we do not consider weighted least-squares here.

In this article, we address this issue and investigate the effect of multiplicative noise on fit parameters determined through a least-squares analysis of data derived from a stochastic process – a general fit function with an arbitrary number of parameters is considered. The fit function and the data are also considered arbitrary in this general formulation, which is then applied to the special case where the noiseless

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data and fit function have identical functional forms. Analytical formulas are derived for both the expected value and standard deviation of the fit parameters, due to the presence of multiplicative noise. This allows for *a priori* analysis of the fit procedure, its optimization, and evaluation of the standard deviation of all fit parameters resulting from a least-squares analysis.

The validity of this theoretical framework is explored using Monte Carlo simulation of synthetic data and experimental measurements of the PSD of stochastic fluctuations of an AFM cantilever. An overriding practical question is how does noise in the PSD affect the precision and distribution of fit parameters resulting from a least-squares analysis of these signals? Despite the well-defined properties of these mechanical systems, the extracted fit parameters are observed to follow Gaussian distributions. Thus, there exists a finite probability of obtaining fit parameters from a single measurement that are many standard deviations away from the true value (or mean). This is true even in the case where the noise is uniformly distributed and of finite amplitude, as in the presented synthetic data.

The theoretical origin of this property and its implication to 'single-shot measurements' on seemingly well-defined systems in the presence of noise are discussed. It has clear implications to both quantitative and qualitative interpretation of data obtained from a least-squares fit. By 'single-shot measurement' we mean, for example, fit parameters extracted from a single estimate of the PSD – as opposed to using multiple estimates of the PSD and averaging the resulting fit parameters. Note that any estimate of the PSD inherently contains multiplicative noise due to finite sampling.[19] Thus, multiple estimates of the PSD from independent time series measurements will each be different, and yield fit parameters that differ. This study highlights the importance of performing statistically significant measurements on multiple realizations of the PSD and the inherent uncertainty in all physical measurements.

We commence by presenting a general theoretical framework for calculating fit parameter uncertainty in the presence of multiplicative noise. No restriction is placed on the data to be fitted nor the fit function. This theory is then applied to the case where the fit function and noiseless data are identical in form, and explicit results are derived for the expected value and variance in fit parameter uncertainty. The practical case of a Lorentzian distribution is considered and a comparison to simulations of synthetic data is presented. The theory is then applied to analysis of the PSD of a stationary random signal, and compared to measurements of an atomic force microscope cantilever. Explicit formulas for the uncertainty in the fitted resonant frequency and quality factor are derived, which are found to be in excellent agreement with experimental measurements. We conclude with a discussion of the implications of this study to practical measurements.

Previous work on dynamic atomic force microscopy also yielded an explicit formula for the uncertainty in the measured resonant frequency.[24] However, in those applications the cantilever is actively excited at or near its resonant frequency, with finite oscillation amplitude. Brownian fluctuations of the cantilever superimpose on this excited sinusoidal motion, which limits the precision with which the oscillation frequency can be determined. Increasing the oscillation amplitude thus reduces the relative effect of Brownian motion, which improves measurement sensitivity. This previously examined problem differs fundamentally from the present study. Here, we explore the effect of sampling noise in the PSD of Brownian fluctuations on resulting fits to a specified function – the cantilever is not actively excited. Thus, all formulas in this article are independent of any oscillation amplitude, in contrast to previous studies.[24–27] This feature will be examined in Sec. III.

II. GENERAL THEORY

The general problem entails fitting a specified fit function to data that contains multiplicative noise. The (idealized) noiseless data, $G(x)$, depends on a single variable x that is evaluated at discrete values $x = x_k$; this is the frequency variable in a PSD. The fit function, $F(x, \boldsymbol{\alpha})$, contains a vector $\boldsymbol{\alpha}$ with an arbitrary but specified number (N) of adjustable fit parameters. The (true) noisy data contains multiplicative noise. The goal of the least-squares analysis is to determine the fit parameter vector, $\boldsymbol{\alpha}$, such that the residual,

$$\Delta \equiv \sum_k [F(x_k, \boldsymbol{\alpha}) - (1 + \epsilon z_k) G(x_k)]^2, \tag{1}$$

is minimized, where ϵ is the noise amplitude, which is assumed to be small ($0 < \epsilon \ll 1$) and $\{z_k\}$ is a set of independent $O(1)$ random variables. Thus, the fit parameter vector $\boldsymbol{\alpha}$ satisfies the equation,

$$\sum_k [F(x_k, \boldsymbol{\alpha}) - (1 + \epsilon z_k) G(x_k)] \nabla F(x_k, \boldsymbol{\alpha}) = \mathbf{0}, \tag{2}$$

where ∇ is the gradient with respect to $\boldsymbol{\alpha}$, and $\nabla F(x_k, \boldsymbol{\tau})$ denotes ∇F evaluated at $x = x_k$ and $\boldsymbol{\alpha} = \boldsymbol{\tau}$.

To proceed, the solution for $\boldsymbol{\alpha}$ is expanded in the small parameter ϵ,

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}_0 + \epsilon \boldsymbol{\alpha}_1 + o(\epsilon), \tag{3}$$

where $\boldsymbol{\alpha}_0$ is the solution in the absence of noise, i.e., when $\epsilon = 0$, and $\epsilon \boldsymbol{\alpha}_1$ is the leading-order deviation that results from the presence of noise. The fit function, $F(x, \boldsymbol{\alpha})$, then becomes

$$F(x, \boldsymbol{\alpha}) = F(x, \boldsymbol{\alpha}_0) + \epsilon \boldsymbol{\alpha}_1 \cdot \nabla F(x, \boldsymbol{\alpha}_0) + o(\epsilon). \tag{4}$$

Substituting Eqs. (3) and (4) into Eq. (2) gives the required solution for the deviation in the fit parameters due to multiplicative noise in the data,

$$\boldsymbol{\alpha}_1 = \sum_k z_k G(x_k) \, \mathbf{A}^{-1} \cdot \nabla F(x_k, \boldsymbol{\alpha}_0), \tag{5}$$

where the symmetric second-order tensor $\mathbf{A}$ is

$$\mathbf{A} = \sum_k [\nabla F(x_k, \boldsymbol{\alpha}_0) \nabla F(x_k, \boldsymbol{\alpha}_0) + (F(x_k, \boldsymbol{\alpha}_0) - G(x_k)) \nabla\nabla F(x_k, \boldsymbol{\alpha}_0)]. \tag{6}$$

A. Identical data and fit function

We consider the special case where $F(x_k, \boldsymbol{\alpha}_0) = G(x)$, i.e., the noiseless data and fit function that minimizes the resulting residual, Δ, have identical forms. This case is often encountered in practice.[4,8,13,15–18,28,29] The interval on which the analysis is performed is $x_k \in [x_{\min}, x_{\max}]$ and we take $x_k = x_{\min} + k\delta x$, where δx is the spacing between fitting points in Eq. (1). Assuming the spacing to be sufficiently fine that the sums can be replaced by integrals, and averaging over the noise variables $\{z_k\}$, yields the required results for the expected value and variance of the m-th component, $\alpha_{1|m}$, of $\boldsymbol{\alpha}_1$,

$$E[\alpha_{1|m}] = E[z_1]\int_{x_{\min}}^{x_{\max}} F(x,\boldsymbol{\alpha}_0) \times [\mathbf{B}^{-1}\cdot\nabla F(x,\boldsymbol{\alpha}_0)]_m\,dx,$$
$$\mathrm{Var}[\alpha_{1|m}] = \mathrm{Var}[z_1]\delta x\int_{x_{\min}}^{x_{\max}} (F(x,\boldsymbol{\alpha}_0) \times [\mathbf{B}^{-1}\cdot\nabla F(x,\boldsymbol{\alpha}_0)]_m)^2 dx, \tag{7}$$

where in the integrands, $[\mathbf{v}]_m$ denotes the m-th component of the vector $\mathbf{v}$, and

$$\mathbf{B} = \int_{x_{\min}}^{x_{\max}} \nabla F(x,\boldsymbol{\alpha}_0)\nabla F(x,\boldsymbol{\alpha}_0)\,dx. \tag{8}$$

This theoretical framework can also be used to evaluate the uncertainty in a function, $H(\boldsymbol{\alpha})$, that depends on the extracted fit parameters. Applying the above theory to the relative difference in H due to the presence of noise, i.e., $\gamma \equiv H(\boldsymbol{\alpha})/H(\boldsymbol{\alpha}_0) - 1$, yields the leading-order results,

$$E[\gamma] = \frac{\epsilon E[z_1]}{H(\boldsymbol{\alpha}_0)}\int_{x_{\min}}^{x_{\max}} F(x,\boldsymbol{\alpha}_0) \times [\mathbf{B}^{-1}\cdot\nabla F(x,\boldsymbol{\alpha}_0)]\cdot\nabla H(\boldsymbol{\alpha}_0)\,dx,$$
$$\mathrm{Var}[\gamma] = \frac{\epsilon^2 \mathrm{Var}[z_1]}{H^2(\boldsymbol{\alpha}_0)}\delta x\int_{x_{\min}}^{x_{\max}} \{F(x,\boldsymbol{\alpha}_0) \times [\mathbf{B}^{-1}\cdot\nabla F(x,\boldsymbol{\alpha}_0)]\cdot\nabla H(\boldsymbol{\alpha}_0)\}^2 dx. \tag{9}$$

III. RESULTS AND DISCUSSION

We now explore application of the above formulas to some cases of practical interest. One common application involves fitting a Lorentzian function,

$$F(x, A, f_R, Q) = \frac{A}{4Q^2\left(\dfrac{x}{f_R} - 1\right)^2 + 1}, \tag{10}$$

to noisy experimental data, e.g., estimates for the PSD of optical and mechanical resonators.[3,4,7,13,15,28–31] Equation (10) contains three adjustable fit parameters: the resonant frequency, f_R, quality factor, Q, and the amplitude at resonance, A. The frequency variable is x.

We assume that the fit function and the noiseless data are both Lorentzian; the noiseless data has the values $f_R = f_0$ and $Q = Q_0$, as per the above notation. The residual and related formulas in Eqs. (7)–(9) are evaluated over the finite interval $x_{\min} \le x \le x_{\max}$, with $x_{\min} = f_0(1 - \beta/Q_0)$ and $x_{\max} = f_0(1 + \beta/Q_0)$, where β is a constant.

Results for the expected value and variance of deviations in the fit parameters that result from multiplicative noise in the data are calculated in the asymptotic limit of large Q and β. The area under Eq. (10) over the interval $x_{\min} \le x \le x_{\max}$, denoted Π, is also calculated and the effect of deviations in the fit parameters on Π is determined using Eq. (9). Equations (7) and (9) give the required results for the expected values of the deviations,

$$\frac{E[A_1]}{A_0} = \frac{E[\Pi_1]}{\Pi_0} = E[z_1], \qquad \frac{E[f_1]}{f_0} = \frac{E[Q_1]}{Q_0} = 0, \tag{11}$$

and for the standard deviations,

$$\frac{\mathrm{SD}[A_1]}{A_0} = \mathrm{SD}[z_1]\sqrt{\frac{13Q_0\delta x}{2\pi f_0}\left(1 + \frac{6}{13\pi\beta^3} + O\left(\frac{1}{\beta^5}\right)\right)},$$
$$\frac{\mathrm{SD}[f_1]}{f_0} = \frac{\mathrm{SD}[z_1]}{Q_0}\sqrt{\frac{7Q_0\delta x}{8\pi f_0}\left(1 + \frac{2}{5\pi\beta^5} + O\left(\frac{1}{\beta^7}\right)\right)},$$
$$\frac{\mathrm{SD}[Q_1]}{Q_0} = \mathrm{SD}[z_1]\sqrt{\frac{6Q_0\delta x}{\pi f_0}\left(1 + \frac{13}{6\pi\beta^3} + O\left(\frac{1}{\beta^5}\right)\right)},$$
$$\frac{\mathrm{SD}[\Pi_1]}{\Pi_0} = \mathrm{SD}[z_1]\sqrt{\frac{3Q_0\delta x}{2\pi f_0}\left(1 + \frac{16}{9\pi\beta^3} + O\left(\frac{1}{\beta^5}\right)\right)}, \tag{12}$$

where the subscripts 0 and 1 are as defined in Eq. (3).

The standard deviations of all parameters increase as the fit range is reduced, i.e., β decreases. It is therefore desirable to use the largest fitting range in practical applications. The resonant frequency, f_R, is most insensitive to the fit range, which is not unexpected since this parameter defines the peak position. The standard deviation of the fitted resonant frequency decreases with increasing quality factor, since a higher quality factor yields a sharper peak. Even so, the effect of fit window is small, because the leading-order correction is $O(\beta^{-5})$ for the resonant frequency and $O(\beta^{-3})$ for all other parameters; see Eq. (12).

The parameter $Q_0\delta x/f_0$ appears in all formulas for the standard deviation. This parameter is inversely proportional to the number of sample points in the immediate vicinity of the peak.[32] Increasing its value leads to greater averaging of the data noise and reduces uncertainty in fits, as reflected in Eq. (12).

A. Comparison to synthetic noisy data

We now compare the predictions of Eq. (12) to synthetic noisy data. This was generated by taking a reference Lorentzian function (with specified f_0, Q_0, and A_0), discretizing the function in x, multiplying each discrete value by a uniformly distributed random variable, ϵz_k, where $z_k \in [-1, 1]$ and ϵ is a specified small constant, and adding the result to the reference Lorentzian. A total of 100 000 individual realizations of such noisy data were generated in this manner. Each realization was then fitted to a second Lorentzian function (with adjustable fit parameters f_R, Q, and A) using a least-squares analysis that incorporated a method of steepest decent. All simulations were performed in Mathematica.

Representative data for the fitted parameters of the 100 000 noisy Lorentzians are given in Fig. 1. It is

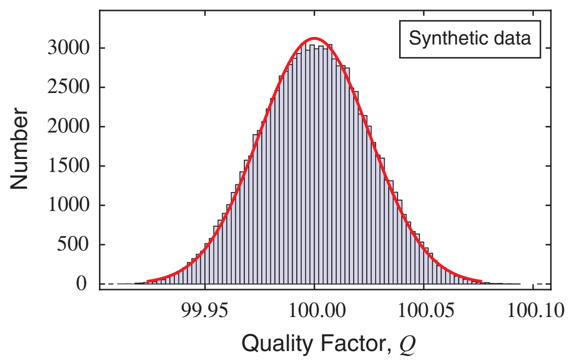

FIG. 1. Histogram of the quality factor, Q, obtained from fits to synthetic data of a noisy Lorentzian; $\epsilon = 0.001$, $A_0 = 1$, $f_0 = 1$, $Q_0 = 100 \gg 1$, and $\beta = 5$. Similar results are obtained for all other fit parameters, and for a narrower fit range of $\beta = 2$ (not shown). Fit to Gaussian distribution (solid line).

striking that histograms for all fit parameters precisely follow Gaussian distributions, despite the noise being uniformly distributed. This is in accord with the central limit theorem of probability theory, which stipulates this property regardless of the original noise distribution.[33] This has important implications to interpretation of the resulting fit parameters, allowing for fit values many standard deviations away from the mean, e.g., the larger values in the histogram in Fig. 1 lie at ∼4.3 standard deviations from the true value. Since the histogram is normally distributed, the probability of attaining a measurement at least M standard deviations above the mean is

$$\Pr[X - \mu \geq M\sigma] = \frac{1}{2}\mathrm{erfc}\left(\frac{M}{\sqrt{2}}\right), \tag{13}$$

where X is the fit parameter and μ and σ are its mean and standard deviation, respectively. Equation (13) thus yields a probability of ∼1/120 000 of attaining a value that lies at least 4.3 standard deviations from the mean, which is consistent with the large number of samples in Fig. 1. The implications of this finding will be explored further below.

Table I provides a comparison of standard deviations in the fit parameters, as obtained from Eq. (12) and the simulation data (Fig. 1). Agreement between the presented theory and simulations is excellent. Since the random variable z_k, used to generate the synthetic data has zero mean, the expected values in Eq. (11) are zero.

B. Power spectral density of stationary random signal

Next, we apply the theory to analysis of the PSD of a stationary random signal, for which we derive explicit analytical formulas. This PSD, $P(x)$, is often estimated by computing the discrete Fourier transform (DFT) of finite time series of the signal, yielding the so-called periodogram.[19] A consistent estimate of $P(x)$ is obtained by averaging N_{ave} individual periodograms, giving $S(x)$ with a variance,[19]

$$\mathrm{Var}[S(x)] \approx \frac{1}{N_{\mathrm{ave}}} P^2(x). \tag{14}$$

Comparing Eqs. (1) and (14) establishes that multiplicative noise in $S(x)$ is characterized by

$$\epsilon\, \mathrm{SD}[z_1] = \frac{1}{\sqrt{N_{\mathrm{ave}}}}. \tag{15}$$

Frequency division in the DFT is given by the reciprocal of the time series duration, T. If a single time series is subdivided into N_{ave} segments, and the DFT of each subdivision computed, the frequency division of the resulting averaged periodogram is $\delta x = N_{\mathrm{ave}}/T$. As such, the multiplicative noise term in Eq. (12) is completely determined and given by

$$\epsilon\, \mathrm{SD}[z_1]\sqrt{\delta x} = \frac{1}{\sqrt{T}}. \tag{16}$$

The required leading-order results in the limit of large fit window, $\beta \gg 1$, are then obtained from Eqs. (12) and (16),

$$\frac{\mathrm{SD}[\epsilon A_1]}{A_0} = \sqrt{\frac{13 Q_0}{2\pi f_0 T}}, \quad \frac{\mathrm{SD}[\epsilon f_1]}{f_0} = \frac{1}{Q_0}\sqrt{\frac{7 Q_0}{8\pi f_0 T}},$$
$$\frac{\mathrm{SD}[\epsilon Q_1]}{Q_0} = \sqrt{\frac{6 Q_0}{\pi f_0 T}}, \quad \frac{\mathrm{SD}[\epsilon \Pi_1]}{\Pi_0} = \sqrt{\frac{3 Q_0}{2\pi f_0 T}}. \tag{17}$$

These formulas establish that standard deviations of the fit parameters depend on the total duration of the measurement, T, rather than the duration of each subdivision. Standard deviations, and hence uncertainty in the fit parameters, are thus independent of the number of averages, N_{ave}, and decrease as $T^{-1/2}$.

1. Comparison to formula for frequency modulation AFM

The above formula for the uncertainty in the resonant frequency, Eq. (17), is similar in form to the corresponding classical result for frequency modulation AFM (FM-AFM),[24]

$$\frac{\mathrm{SD}[\epsilon f_1]}{f_0} = \frac{1}{Q_0}\sqrt{\frac{Q_0 B}{2\pi f_0}\frac{\langle z^2_{\mathrm{thermal}}\rangle}{\langle z^2_{\mathrm{drive}}\rangle}}, \tag{18}$$

where $\langle z^2_{\mathrm{thermal}}\rangle$ and $\langle z^2_{\mathrm{drive}}\rangle$ are the mean-square displacements due to thermal (Brownian) motion and the self-excited (drive) oscillation of the cantilever, respectively. The measurement bandwidth, B, is often specified in dynamic AFM studies, rather than measurement duration, T; these quantities are reciprocally related.[34]

For FM-AFM, the uncertainty in the resonant frequency decreases with increasing oscillation amplitude, z_{drive}, as discussed above; see Eq. (18). For Brownian motion of the cantilever, the new formula for the uncertainty in the resonant frequency as obtained from a fit to the PSD, Eq. (17), has no

TABLE I. Comparison of relative standard deviations $\mathrm{SD}[X_1]/X_0$ of simulation data (Fig. 1) and Eq. (12), for all fit parameters, for $\beta = 5$ (similar agreement found for $\beta = 2$). Variable X represents specified fit parameters and $\epsilon = 0.001$ has been normalized from the results.

X	Simulation	Eq. (12)
A	0.2627	0.2628
f_R	9.630×10^{-4}	9.636×10^{-4}
Q	0.2534	0.2530
Π	0.1265	0.1264

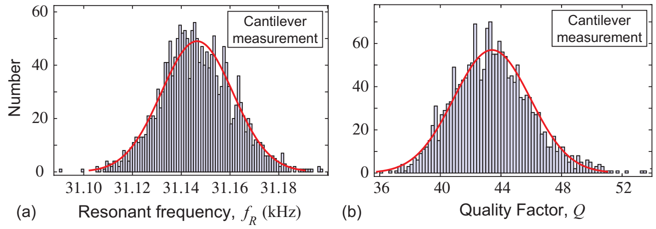

FIG. 2. Histograms of the resonant frequencies, f_R, and quality factors, Q, obtained from fits to measurements of cantilever PSD. Measured means: $f_0 = 31.15$ kHz, $Q_0 = 43.41$. Amplitude histograms affected by thermal drift (not shown). Fits to Gaussian distributions (solid lines).

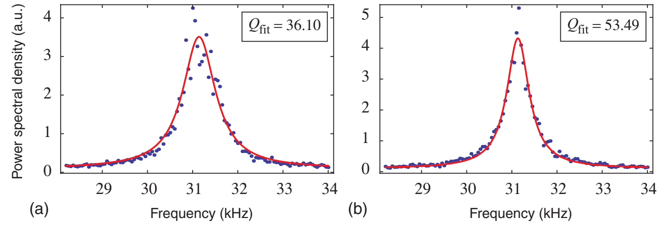

FIG. 3. Averaged periodograms ($N_{ave} = 50$) of the cantilever, with Lorentzian fits (solid lines), for minimum and maximum fitted quality factors: (a) $Q = 36.10$, and (b) $Q = 53.49$. Mean quality factor for the entire sample set is $Q_0 = 43.41$.

dependence on oscillation amplitude. However, for no feedback the displacements in Eq. (18) are identical yielding a similar result to Eq. (17).

2. Comparison to measurements of an AFM cantilever

The predictions of Eq. (17) are now compared to measurements of the stochastic fluctuations of an AFM cantilever in air.[32,35] The PSD of thermal fluctuations of the fundamental mode was measured from a single time series of duration $T = 30$ min (sampling frequency, 100 kHz). This was divided into 1 s intervals, each of which was subdivided into 50 intervals of duration 20 ms. Periodograms of each 20 ms subdivision were computed and averaged together ($N_{ave} = 50$). This gave 1800 estimates of the PSD, which were individually fitted to Lorentzian functions over 14.2 kHz $\leq x \leq$ 48 kHz.

Histograms of the fitted resonant frequencies, f_R, and quality factors, Q, are shown in Fig. 2. These also exhibit Gaussian distributions, in agreement with the foregoing discussion. The standard deviation of the fitted resonant frequency distribution is much smaller than for the quality factor distribution. This is in agreement with the qualitative predictions of Eq. (17), for high Q devices. Table II compares quantitative predictions of Eq. (17) (Ref. 36) to measurements, where excellent agreement is observed. Combined with the results in Table I, these findings illustrate the validity and accuracy of the presented theory.

Histograms of the peak amplitude, A, and area under the Lorentzian, Π, were found to exhibit significant broadening and non-Gaussian response due to (unavoidable) thermal drift; this drift was not quantitatively characterized and these amplitude histograms have thus been omitted from the presentation. This additional systematic uncertainty increased the true standard deviation in measurements of these fit parameters. Since such additional effects are not considered in the present analysis, which only examines the effect of multiplicative noise, the derived formulas must be considered lower bounds to the true uncertainty. Nonetheless, fit parameters that are insensitive to such additional effects, such as the resonant frequency and quality factor, display excellent agreement with the derived theory; see Table II.

TABLE II. Comparison of relative standard deviations $\mathrm{SD}[\epsilon X_1]/X_0$ for resonant frequency, f_R, and quality factor, Q, of cantilever measurements (Fig. 2) and Eq. (17). Variable X represents specified fit parameters.

X	Measurement	Eq. (17)
f_R	4.7×10^{-4}	4.5×10^{-4}
Q	5.8×10^{-2}	5.2×10^{-2}

Results in Fig. 2 highlight the fact that fits to individual PSD measurements can exhibit significant uncertainty: 31.09 kHz $\leq f_R \leq$ 31.20 kHz and $36.10 \leq Q \leq 53.49$. Actual fits to the PSD data are given in Fig. 3 for minimum and maximum values of the fitted quality factors. These values correspond to ~3 and 4 standard deviations away from the mean – the probabilities of attaining values at least at these extremes are ~1/740 and 1/32 000, respectively, according to Eq. (13). Since 1800 samples were used, the observed deviations from the mean are not unexpected.

Significantly, good visual fits to the PSD data are achieved in both cases in Fig. 3, while yielding vastly different fitted quality factors. Fluctuations in the PSD noise conspire to dramatically alter the form of the observed PSD, even though the underlying physical system (the cantilever) is fixed and well-defined. It is thus entirely possible to attain many consecutive repeat measurements with similar fit parameters (and excellent fits to experimental data) that lie many standard deviations away from the true system parameters. The probability of such an event is small but finite, and can lead to quantitative and/or qualitative misinterpretation of stochastic measurements.

This demonstrates that goodness-of-fit may not necessarily provide a measure of uncertainty in ‘single-shot measurements’, as often reported. Proper statistical analysis of repeat measurements is always warranted due to the unavoidable presence of noise, even in such seemingly simple and well-defined physical systems.

IV. CONCLUSIONS

We have presented a rigorous theoretical framework for calculating the uncertainty in least-squares analysis of data subject to multiplicative noise. This has direct applications to modern micro- and nanoscale devices, where the PSD of Brownian fluctuations is often interrogated. The validity of this theory was demonstrated using Monte Carlo simulations of synthetic data and actual measurements of an AFM cantilever – explicit analytical formulas for such Lorentzian processes were derived. Uncertainty in fit parameters derived from a single stochastic process was found to depend on the total measurement time. This study highlights the uncertainty that can result from 'single-shot measurements' with seemingly excellent fits, and provides a framework for optimization and development of robust experimental protocols for least-squares analysis of data containing multiplicative noise.

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