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Statistical Uncertainty in Line Shift and Width Interpretation

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Abstract

Elementary but general statistical analyses determine the uncertainty arising from photon statistics in measuring a line shift and width. Account is taken of a background as well as the required signal.

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1 Introduction

In many spectroscopic situations, the shift and width of a spectral line is desired. The shift is most often wanted as a measure of the mean velocity of the emitters in the line of sight, and the width as their Doppler temperature. The statistical uncertainty of such a measurement can be written down extremely simply, provided the problem is approached in the right way.

If there is present, in addition to the line signal of interest, a background signal, which is to be subtracted from the signal, this complicates the problem somewhat. Nevertheless, a simple result is obtained. The way that the instrumental spectral line shape affects the result can also be trivially included.

Although the statistical analysis set forth here is elementary, it does not appear in a usable form, to the author's knowledge, in the standard textbook discussions of uncertainty. Nor are most students or researchers familiar with it. Therefore it seems useful to set it forth in a pedagogic style. The required mathematical results will be cited from an introductory text book[1] as references to its numbered theorems.

Classical statistics (uncorrelated photons) rather than Bose-Einstein statistics will be assumed throughout, as is an excellent approximation in most experimental situations.

2 Line Shift

2.1 Perfect Spectrometer, Zero Background

We suppose initially that a perfect spectrometer is available, which measures the exact wavelength λ of every photon arriving. The line shape is taken to have the form $I(\lambda)$, where I is the probability distribution function of photon wavelength. That is, the probability of any photon having wavelength in the range $(\lambda, \lambda + d\lambda)$, in the limit of small $d\lambda$, is $I(\lambda)d\lambda$.

A measurement consists of collecting photons for a certain time interval. We shall approximate this as being to collect a fixed *total number* of photons. Provided the number of photons in the sample, N , is large, this will introduce negligible error, at least in the line position. The formulation of our problem of determining the uncertainty in a line-shift measurement is then to determine what is the probability distribution (or at least its width) for the line position deduced from the sample of N independent photons. There are, of course, many complicated possible ways of determining the line position of the photon sample. However, provided that these methods are not able to take advantage of important *a priori* information about line shifts, they will have no intrinsic advantage over the simplest measure of line position, namely the *centroid* of the photon wavelength distribution:

$$\mu_k = \frac{1}{N} \sum_{i=1}^N \lambda_i. \quad (1)$$

The index k here is used to refer to the k th measurement (or sample), and i refers to the photon number within that sample.

The advantage of using the centroid as the line position metric, is that the distribution of μ_k is the subject of the Central Limit Theorem of statistics ([1] theorem 12.1), which states that if the standard deviation of the population $I(\lambda)$ from which the sample is drawn is σ_I , then in the limit of large N , the values of μ are distributed with normal (Gaussian) distribution, with standard deviation

$$\sigma_\mu = \sigma_I / \sqrt{N}. \quad (2)$$

Note that this result is regardless of the shape of the original distribution $I(\lambda)$.

Equation (2) gives the required uncertainty in the measured line-shift. It is the width of the line to be measured divided by the square root of the number of photons in the sample. Moreover the Central Limit Theorem also tells us the bonus that the distribution of μ is Gaussian.

2.2 Perfect Spectrometer, Background Subtraction

Now we consider a situation in which we know that there are, in addition to the photons we care about, background photons, which we will have to subtract from our spectrum. Suppose the background spectrum to be given by a probability distribution $B(\lambda)$ (so that $\int B(\lambda)d\lambda = 1$), having a standard deviation (spectral width) σ_B and a centroid μ_B .

A measurement consists of obtaining a large number of photons, each of whose wavelength is measured. Of those photons, N_I are the signal photons, and N_B are the background photons, $N = N_I + N_B$. We don't know which photon is which, but for purposes of reference, we will suppose them to be ordered such that the first N_I are the signal photons. We will assume initially that the numbers N_I and N_B are known and fixed.

Our best estimate of the background is that its spectral photon density is $N_B B(\lambda)$, so that the background contribution to the centroid sum $\sum \lambda$ is on average $N_B \mu_B$. We will subtract this background from the spectrum and then obtain the centroid of the remaining "signal". Therefore the estimate we should use for the signal photons' centroid is

$$\mu_{Ik} = \frac{1}{N_I} \left(\sum_{i=1}^N \lambda_i - N_B \mu_B \right) = \frac{1}{N_I} \left(\sum_{i=1}^{N_I} \lambda_i + \sum_{i=N_I+1}^N \lambda_i - N_B \mu_B \right). \quad (3)$$

The second equality in eq (3) is written to show that if we had a perfect knowledge of the background contribution, the last two terms exactly cancel, returning us to our original form (1).

However, the two terms do not exactly cancel, even if our knowledge of $B(\lambda)$ is perfect, because of the statistics of the background photons. We know that the centroid of the background photons in the sample,

$$\mu_{Bk} = \frac{1}{N_B} \sum_{i=N_I+1}^N \lambda_i, \quad (4)$$

is distributed with Gaussian probability distribution with mean μ_B and standard deviation $\sigma_B/\sqrt{N_B}$. Therefore our line position estimate is the sum of three terms. The first is the centroid of the signal photons in the sample, distributed with standard deviation $\sigma_I/\sqrt{N_I}$. The second is the centroid of the background photons in the sample, μ_{Bk} times N_B/N_I ; and the last is a constant, which we chose to annihilate the mean of μ_{Bk} .

Utilizing the theorem that a random variable that is the sum of two other independent random variables has a distribution whose mean is the sum of the means ([1] Property 7.4), and whose variance (standard deviation squared) is the sum of the variances (Property 7.9), we can immediately deduce that the distribution of our line shift estimate μ_k has mean equal to the centroid of $I(\lambda)$ and standard deviation:

$$\sigma_\mu = \sqrt{\frac{\sigma_I^2}{N_I} + \frac{\sigma_B^2 N_B}{N_I^2}}. \quad (5)$$

This important result shows how rapidly a background can come to dominate the uncertainty in the measurement of line shift. If $\sigma_I \sim \sigma_B$, then as soon as $N_B > N_I$ it is the second term, coming from statistics of the background photons, that determines the shift uncertainty.

Notice also, that if the background spectrum is broad, for example flat, in the vicinity of the signal line, then the effective σ_B is determined purely by the spectral band chosen over

which to sum the photons. To minimize this width we should choose a spectral band that is just wide enough to encompass the signal line, but no wider. In that case, the background width will be wider than the actual line spread by roughly a factor of 2 or 3, depending on the exact band width chosen.

In the contrasting case where the background line mimics the signal line in width so that $\sigma_I = \sigma_B$, the resultant uncertainty is

$$\sigma_\mu = \frac{\sigma_B}{\sqrt{N_I}} \sqrt{1 + N_B/N_I}. \quad (6)$$

Either way, when $N_B \gg N_I$, the uncertainty becomes

$$\sigma_\mu \approx \frac{\sigma_B \sqrt{N_B}}{N_I}. \quad (7)$$

Since both of the random contributions to μ_k are normally distributed (by the Central Limit Theorem), and the distribution of a sum of normally distributed random variables is normally distributed ([1] Theorem 10.6), μ_k itself is also normally distributed.

2.3 Offset Background: Background-fraction Fluctuations.

If the background distribution is substantially shifted in its mean from the mean of the signal, an additional effect may be non-negligible. We must account for the statistical uncertainty in the fraction of sample photons that is actually background, rather than signal. In other words, although we will assume we know the average number of signal and background photons, N_I and N_B , we do not know the actual numbers for any specific sample, N_{Ik} and N_{Bk} . Therefore, our expression for the estimate of the signal mean, eq (3), must more precisely be written

$$\mu_{Ik} = \frac{1}{N_I} \left(\sum_{i=1}^N \lambda_i - N_B \mu_B \right) = \frac{1}{N_I} \left(\sum_{i=1}^{N_{Ik}} \lambda_{Ii} + \sum_{i=N_{Ik}+1}^N \lambda_{Bi} - N_B \mu_B \right), \quad (8)$$

where we explicitly denote with a subscript those photons that are signal and background. Grouping terms appropriately we then write

$$\mu_{Ik} = \frac{1}{N_I} \left(\sum_{i=1}^{N_I} \lambda_{Ii} + \sum_{i=N_I+1}^{N_{Ik}} \lambda_{Ii} - \sum_{i=N_I+1}^{N_{Ik}} \lambda_{Bi} + \sum_{i=N_I+1}^N \lambda_{Bi} - N_B \mu_B \right), \quad (9)$$

which is precisely the previous expression, eq (3), *plus* the combination

$$\frac{1}{N_I} \left(\sum_{i=N_I+1}^{N_{Ik}} \lambda_{Ii} - \sum_{i=N_I+1}^{N_{Ik}} \lambda_{Bi} \right). \quad (10)$$

This expression is zero if $N_{Ik} = N_I$, but for fixed difference $N_{Ik} - N_I$ has expectation $(N_{Ik} - N_I)(\mu_I - \mu_B)/N_I$. To lowest order in $1/N$, this additional term is therefore distributed

as $\mu_I - \mu_B$ times the fractional deviation of N_{Ik} from N_I . The standard deviation of N_{Ik}/N is $\sqrt{N_I N_B / N^3}$. So the additional term has standard deviation $(\mu_I - \mu_B) \sqrt{N_B / (N_I N)}$.

Consequently the standard deviation of the estimate of the line position (eq 5) is generalized to

$$\sigma_\mu = \sqrt{\frac{\sigma_I^2}{N_I} + \frac{(\mu_I - \mu_B)^2 N_B}{N_I N} + \frac{\sigma_B^2 N_B}{N_I^2}}. \quad (11)$$

Recalling the considerations in the previous subsection, the wavelength collection region must be chosen approximately centered on μ_I and with (half) width no more than 2 to 3 times σ_I . As a result the mean collected background photon wavelength cannot deviate more than 2 to 3 times σ_I from μ_I : $|\mu_I - \mu_B| \lesssim 2\sigma_I$. The additional (center) term in eq (11) is most significant when $N_B \sim N_I$ because if $N_B \ll N_I$, it is negligible compared with the first term and if $N_I \ll N_B$ it is negligible compared with the last. Thus the worst case is that the extra term increases the uncertainty arising from the signal width term by about a factor of 2. More typically, $|\mu_I - \mu_B| < \sigma_I$, in which case the additional term is essentially negligible.

2.4 Imperfect Spectrometer or Complex Line Shape

In practice a spectrometer has a finite instrumental line width. Its effects can often be described by an instrument line shape $S(\lambda)$, such that the observed spectrum is the *convolution* of $S(\lambda)$ with the incident spectrum. Consequently a perfectly monochromatic line, $I(\lambda) = \delta(\lambda - \lambda_0)$, acquires the instrumental shape $S(\lambda - \lambda_0)$. Because the instrument shape can be taken to have zero centroid shift, the convolution introduces no systematic shift of the line, nor, more importantly, any random shift. What it does, however, is to broaden the width of the observed line, relative to what would otherwise have been observed.

From the point of view of statistics, all of the previous arguments still apply. But they apply to the *instrumentally broadened* observed line rather than to the original line shapes. In particular all of the foregoing formulas will still apply if the σ factors are taken as the widths of the lines after convolving with the instrumental function. In other words, if the observed widths are used.

By the same token, if the lines being examined have complex line shape due, for example, to a multiplet structure, then all of the foregoing formulas *still* apply. But the width of the lines is then perhaps dominated by the multiplet structure rather than the other broadening mechanisms.

2.5 Finite-width Wavelength Bins

A situation of importance for modern spectrometers, is when the instrument does *not* simply produce a convolution of the line with an instrumental line-shape. Instead, one might have a series of bins of finite-width into which the photons are sorted. This will occur, for example, with a multi-element detector when each of the different elements corresponds to a different wavelength bin. It is clear that if the bin width is much less than the observed width of the

line, then the binning will amount simply to a discrete approximation to the integrals and sums invoked above.

However, if the bin size is larger than the line width, then strongly non-linear effects on the shift will be introduced. For example, as a narrow line moves across a wider bin, no detectable change in the spectrum occurs until the line approaches the boundary between bins. Then as it crosses the bin boundary, a step in apparent position of the photons occurs from one bin to the next.

If the bins are of equal width, perhaps the best way to see the effect of the bins is as follows. We deduce the centroid by assigning each photon in a bin a wavelength equal to the center of the bin; this is the most reasonable unbiased estimate. Let the center of the j^{th} bin be at wavelength $\lambda_j = j\Delta\lambda$ (measured from a convenient zero). Then the error in the centroid for a photon at position λ lying in the j^{th} bin is $\lambda - \lambda_j$, which is a linear ramp. If the photon lies in the next bin $j + 1$, the error has an identical ramp ($\lambda - \lambda_{j+1}$). Therefore the error function has the form of a *sawtooth*:

$$\mathcal{E}(\lambda) = \lambda - \lambda_j, \quad \text{for } (\lambda_j + \lambda_{j-1})/2 < \lambda \leq (\lambda_{j+1} + \lambda_j)/2 . \quad (12)$$

And a line shape $I(\lambda)$ acquires an error

$$\int I(\lambda)\mathcal{E}(\lambda)d\lambda . \quad (13)$$

Now \mathcal{E} is a periodic function, and can thus be expressed as a Fourier series

$$\mathcal{E} = \sum_{m=1}^{\infty} A_m \sin(2\pi m\lambda/\Delta\lambda) . \quad (14)$$

When this is substituted into eq (13), we see immediately that the error arising from a line shape $I(\lambda)$ can be written as a weighted sum of the Fourier transform of $I(\lambda)$ evaluated at the (spatial) frequencies $2\pi m/\Delta\lambda$. The most important error will arise from the fundamental $m = 1$, both because A_m is a decreasing function of m and because the Fourier transform will be a decreasing function of frequency. Indeed if $I(\lambda)$ is a Gaussian, then its Fourier transform is also a Gaussian, whose width is $\sim 1/\sigma_I$. Provided that $2\pi/\Delta\lambda$ is substantially larger than this width, the binning error will become negligibly small. This condition is equivalent to the requirement that there be more than a few bins covering the width of the line.

Thus, somewhat counter-intuitively, if we have a binned spectrum, it is advantageous, from the viewpoint of line position measurement, that the effective line-shape (the convolution of the received line with the instrument function) should be significantly *broader* than the bin width. It is actually a substantial *disadvantage* to have a line narrower than approximately the bin width. For that reason, a detector array ought always to be spaced closer than the instrumental resolution.

Moreover, the naive idea that the bin size represents a minimum resolution, and thus a minimum line-shift resolution, is *false*. For a Gaussian line, the Fourier transform decays so rapidly at a few times its width that it becomes completely negligible. When that occurs, if there are enough photons in the line, the uncertainty given by eq (5) may be far smaller than the bin width.

3 Line Width

3.1 Line Width, Zero Background

Generally speaking, the line width can be analysed in a way comparable to the shift. However, the elementary statistical theorems are not quite as general.

The line width can be defined in terms of the second moment of the sample. The usual unbiased statistical estimate for the width (σ_I) of the population, based on a sample of size N , is S_k , the square root of the sample variance given by:

$$S_k^2 = \frac{1}{N-1} \sum_{i=1}^N (\lambda_i - \mu_k)^2 \quad (15)$$

If $I(\lambda)$ is a Gaussian distribution, then by Theorem 10.8[1], the variable $u = S^2(N-1)/\sigma_I^2$, which is the sum of N independent normally distributed variables, has a chi-squared distribution of N degrees of freedom. In other words, its probability distribution function is

$$\frac{1}{2^{N/2}} \Gamma(N/2) u^{N/2-1} e^{-u/2} \quad (16)$$

In particular, since that chi-squared distribution has mean N and variance $2N$, the variance of S^2 is $2N \times [\sigma_I^2/N]^2 = \sigma_I^4 2/N$, and the standard deviation of S^2 is $\sigma_I^2 \sqrt{2/N}$.

For large N (by [1] Theorem 9.2) if u is distributed as a chi-squared distribution of N degrees of freedom, then the variable $\sqrt{2u}$ has approximately a normal distribution of mean $\sqrt{2N-1}$ and variance unity. Thus for large N the distribution of S is Gaussian with mean

$$\mu_S = \sigma_I \sqrt{\frac{2N-1}{2(N-1)}} \approx \sigma_I, \quad (17)$$

and standard deviation

$$\sigma_S = \frac{\sigma_I}{\sqrt{2(N-1)}}. \quad (18)$$

The value σ_S , eq (18), can be considered the uncertainty in determination of the line width, when the width is evaluated by using the second moment of the line shape. As before, it should be applied to the observed line width (including instrumental broadening).

3.2 Line Width, Background Subtraction

The natural unbiased estimate of the line width in the presence of background photons is S_k , where

$$S_k^2 = \frac{1}{N_I - 1} \left[\sum_{i=1}^N (\lambda_i - \mu_{Ik})^2 - N_B \{ \sigma_B^2 + (\mu_{Ik} - \mu_B)^2 \} \right] \quad (19)$$

where μ_{Ik} is given by eq (3). This can be written

$$\begin{aligned}
S_k^2 &= \frac{1}{N_I - 1} \left[\sum_{i=1}^{N_I} (\lambda_i - \mu_{Ik})^2 + \sum_{N_{I+1}}^N (\lambda_i - \mu_B)^2 - \sum_{N_{I+1}}^N 2\lambda_i(\mu_{Ik} - \mu_B) + N_B(\mu_{Ik}^2 - \mu_B^2) \right. \\
&\quad \left. - N_B\{\sigma_B^2 + (\mu_{Ik} - \mu_B)^2\} \right] \\
&= \frac{1}{N_I - 1} \left[\sum_{i=1}^{N_I} (\lambda_i - \mu_{Ik})^2 + \sum_{N_{I+1}}^N \{(\lambda_i - \mu_B)^2 - \sigma_B^2\} + 2(\mu_B - \mu_{Ik}) \sum_{N_{I+1}}^N (\lambda_i - \mu_B) \right]
\end{aligned} \tag{20}$$

The second and third sums in this expression come from the statistics of the background photons. The variances of these two expressions are given by:

$$\text{Var}\left(\frac{1}{N_B - 1} \sum_{N_{I+1}}^N \{(\lambda_i - \mu_B)^2 - \sigma_B^2\}\right) = \frac{2\sigma_B^4}{N_B - 1} \tag{21}$$

and

$$\text{Var}\left(\frac{2(\mu_B - \mu_{Ik})}{N_B - 1} \sum_{N_{I+1}}^N (\lambda_i - \mu_B)\right) = \frac{4(\mu_B - \mu_{Ik})^2 \sigma_B^2}{N_B - 1}. \tag{22}$$

Assuming that the variance of S^2 can be written as the sum of the variances of these three terms (which is not obvious since they aren't independent) we get

$$\text{Var}(S_k^2) = \frac{2\sigma_I^4}{N_I - 1} + \left(\frac{2\sigma_B^4}{N_B - 1} + \frac{4(\mu_B - \mu_{Ik})^2 \sigma_B^2}{N_B - 1} \right) \left(\frac{N_B - 1}{N_I - 1} \right)^2 \tag{23}$$

Let us drop the irrelevant small distinction between $N - 1$ and N . Then this expression shows that the background terms will dominate if $(N_B/N_I)\sigma_B^4 > \sigma_I^4$. The third term will give an additional contribution unless we can arrange that the background spectrum is centered on the signal line to better than σ_B ; but that should be easy to accomplish; so we will ignore the third term. Then

$$\text{Var}(S_k^2) = \frac{2\sigma_I^4}{N_I} + \frac{2\sigma_B^4 N_B}{N_I^2} \tag{24}$$

And of course the expectation (mean) of S^2 is σ_I^2 .

Provided the distribution of S_k^2 is narrow, we can regard its distribution as centered at μ_{S^2} with a much smaller width σ_{S^2} . Then the square-root variable S , can be expanded schematically as

$$S = \sqrt{S^2} = \sqrt{\mu_{S^2} + \sigma_{S^2}} \approx \sqrt{\mu_{S^2}} \left(1 + \frac{1}{2} \sigma_{S^2} / \mu_{S^2}\right) \tag{25}$$

which shows that the mean of S is $\sqrt{\mu_{S^2}}$ but the standard deviation of S is $\approx \frac{1}{2} \sigma_{S^2} / \sqrt{\mu_{S^2}}$. Applying this to the result of eq (24), we find that the standard deviation of our estimate S of the line width is

$$\sigma_S \approx \frac{1}{2\sigma_I} \sqrt{\frac{2\sigma_I^4}{N_I} + \frac{2\sigma_B^4 N_B}{N_I^2}} = \frac{\sigma_I}{\sqrt{2N_I}} \sqrt{1 + \frac{\sigma_B^4 N_B}{\sigma_I^4 N_I}}. \tag{26}$$

This result is consistent with eq (18), which was obtained using more specific distribution assumptions, but without the approximations made here.

4 Summary

When line shift and width are measured using a large sample of N_I signal photons from a line whose width is σ_I in the presence of N_B background photons from a population centered on the signal line but with width σ_B , the photon statistical uncertainties in the shift and width of the signal line, deduced from the moments of the distribution, are respectively:

$$\sigma_\mu = \frac{\sigma_I}{\sqrt{N_I}} \sqrt{1 + \frac{\sigma_B^2 N_B}{\sigma_I^2 N_I}} \quad (27)$$

and

$$\sigma_S = \frac{\sigma_I}{\sqrt{2N_I}} \sqrt{1 + \frac{\sigma_B^4 N_B}{\sigma_I^4 N_I}}. \quad (28)$$

In these expressions, the observed widths of the line and background, including instrumental or multiplet broadening effects, should be used.

References

- [1] Paul L Meyer. *Introductory Probability and Statistical Applications*. Addison Wesley, Reading, MA, 1966.