CALCULATION OF THE APPARATUS FUNCTION FOR THE CASE OF A GENERALIZED VOIGT CONTOUR

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The Rayleigh-Bracewell method of finite differences is applied to cases where the apparatus function is either entirely Lorentzian or results from the superposition of Lorentzian and Gaussian components. A first-order correction is calculated, and order of magnitude estimates are given for the remaining terms in the series expansion representing the correction. The method is employed to correct self-reversed contours of spectral lines.

To determine the true contour of a spectral line one has to take into account the influence of the apparatus function upon the measured contour. The problem is complicated when the analytic form of the contour to be measured is not known; in practice, this is the case most frequently encountered. The simplest procedure which makes use of the Rayleigh-Bracewell method of finite differences [1, 2] is applicable only when the apparatus function has a Gaussian form, or some other forms of minor interest. The problem of taking the apparatus function into account has not been solved for the most important cases, i.e., when the apparatus function is Lorentzian, or when it can be represented as a convolution of Lorentzian or Gaussian curves. The latter case, i.e., a Voigt type contour, is the most common one. While the apparatus function of the Fabry-Perot interferometer is Lorentzian, the apparatus functions of other instruments used in diffraction studies, for instance, of the DFS-13 spectrograph, are frequently of the Voigt type. In the latter case, the apparatus function of the diffraction device is nearly Gaussian, but the apparatus function of the photographic plate is exponential in form and resembles a Lorentzian.

However, even in relatively simple cases, it is practically impossible to use the method of finite differences to obtain final results since its solution leads to first-order corrections only.

It is the purpose of the present paper to extend the method of finite differences to cases where the apparatus function is either Lorentzian or of the Voigt type. The terms of higher order are calculated for the general case of an arbitrary shape of the contour to be corrected. The results obtained are employed to determine corrections for the contours of self-reversed spectral lines of unknown analytic form.

The Rayleigh-Bracewell method of finite differences is based on the following procedure. Let \( f(x) \) be the observed contour, \( h(x) \) the apparatus function, and \( \varphi(x) \) the unknown true contour. Fourier analysis then leads to the relation:

\[
\varphi(x) = f(x) + \sum_{n=1}^{\infty} \frac{\mu_n}{(2n+1)!} \lambda_n^2 f(x).
\]

The geometric meaning of the first term of the sum, i.e., the term for \( n = 2 \) (for odd \( n \) the terms are imaginary and make no contribution), is particularly simple. If we retain only the first term of the sum, which makes the largest contribution to the total correction, we find

\[
\varphi(x) = f(x) + \frac{1}{2} \frac{\mu_2}{2} \frac{PQ}{l^2}.
\]

where \( PQ \) is the vertical distance between the curve representing the shape of the measured contour and the chord (see Fig. 1a) and \( 2l \) is the chord span. The relation between \( l \) and \( \mu_2 \) is

\[
\mu_2 l^2 = 2 \int_{-\infty}^{\infty} x^2 h(x) \, dx.
\]

The length \( l \) is arbitrarily chosen. The coefficient \( \mu_2/2 \) is then determined from Eq. (3), while the length \( PQ \) is found by geometric tracing.

Bracewell [2] has given a solution only for the Gaussian form which is just one of the apparatus functions of interest to us. In this case

\[
h(x) = \sqrt{\frac{2}{\pi \sigma^2}} \exp \left( -\frac{x^2}{2\sigma^2} \right) \sqrt{\ln 2}.
\]
for \(2\ell = 2.4\delta, u_2/2 = 0.5\), whence

\[ q(x) = f(x) + 0.5PQ. \]  

We have attempted to determine the first-order correction for a dispersion function (Lorentzian) of the following form

\[ h(x) = \frac{1}{\pi} \frac{1}{x^2 + \delta^2}. \]

But the integral in Eq. (3) turns out to be divergent, and it appears impossible to determine the coefficients in this way. As shown in [3], a Lorentzian apparatus function can, however, be closely approximated by an exponential function of the following form:

\[ h(x) = \frac{\ln 2}{2\delta} \exp\left\{-\frac{\ln 2}{\delta} |x| \right\}. \]

With this exponential function, we obtain for \(2\ell = 2\delta, u_2/2 = 4.2\):

\[ q(x) = f(x) + 4.2PQ. \]

The influence of the remaining terms of the correction series (1) has only been determined for the extremal points of the observed contour, i.e., for the maxima and minima. The influence of the apparatus function is there largest, and it is possible to establish the over-all shape of the contour by making an adjustment at these points only. A semi-empirical method is employed to calculate the remaining terms of the correction series (1). This method is based on a comparison of the ratio \(f(0)/\varphi(0)\), where \(f(0)\) and \(\varphi(0)\) are two known functions representing, respectively, the observed and the true contour, at a point which is either a maximum or a minimum, with the approximate value for this ratio obtained in the evaluation of the first-order correction.

In Fig. 2 curves showing the dependence of the ratio \(f(0)/\varphi(0)\) upon \(\delta/\alpha\) for a Gaussian apparatus function are given; here \(\delta\) is the halfwidth of the apparatus function, and \(\alpha\) the halfwidth of the measured contour. To simplify the calculations, it is assumed that the measured contour is also Gaussian. The halfwidth of the true contour is then determined from the apparatus and observed contours by a quadratic residue calculation in which use is made of the appropriate halfwidths. Curve 2 shows the exact value of the ratio \(f(0)/\varphi(0)\), and curve 1 an approximate value. As can be seen from the figure, the correction is small for small values of \(\delta/\alpha\); in practice, the domain \(\delta/\alpha \approx 0.8-1.0\) is not used. One can introduce a coefficient which takes into account the influence of the remaining terms of the correction series (1). This new corrective coefficient is determined from the ratio of the vertical distances between the horizontal axis AB and the respective points on the curves 2 and 1 for a given value of the ratio \(\delta/\alpha\). In the vicinity of \(\delta/\alpha \approx 0.5\), the value of this coefficient is 1.5. For \(\delta/\alpha > 0.8\), this coefficient deviates from the value 1.5, but, as has been mentioned above, this case is not encountered in practice. When \(\delta/\alpha < 0.5\), the correction is rather small. We can thus take the value 1.5 for the corrective coefficient, and obtain for the total coefficient the value 0.5 \times 1.5 = 0.75 for a Gaussian apparatus function, i.e., in this case.

\[ q(x) = f(x) + 0.75PQ. \]

An analogous relation can be obtained for a Lorentzian apparatus function. The straight line 5 in Fig. 2 corresponds to the case when both the observed contour and the apparatus function are Lorentzian. The halfwidth of the true contour is then obtained by simple subtraction of the corresponding halfwidths. To determine curve 3, the method of finite differences with an exponential apparatus function as starting point has been employed. To determine curve 4, a method due to Eddington [5] has been used, which permits an exact evaluation of the influence of an exponential apparatus function. Comparison of the curves 4 and 5 shows that substitution of an exponential for a Lorentzian apparatus function does not involve a large error; in the domain \(\delta/\alpha \approx 0.3\) to 0.6, curve 4 almost coincides with the straight line 5, but some deviation is noticeable in the domain \(\delta/\alpha < 0.3\). Comparison of the curves 3 and 4, and 3 and 5, respectively, shows that use of the method of finite differences (curve 3) does not lead to large errors. The magnitude of