BULLETIN OF THE ASTRONOMICAL INSTITUTES OF THE NETHERLANDS

1941 August 8

Volume IX

No. 342

COMMUNICATIONS FROM THE OBSERVATORY AT UTRECHT

The determination of the true profile of a spectral line, by H. C. van de Hulst.

1. In order to determine accurately the true profile of a spectral line, it is necessary to take into account the deforming influence of the spectral apparatus. This influence is characterized by the instrumental curve, i.e. the profile of an ideal narrow spectral line, shown by the imperfect instrument. We denote this profile by A(x), x being an arbitrary measure for wavelength or frequency; this function

must be normalized so that $\int_{-\infty}^{+\infty} A(x) dx = 1$.

If a line has itself a finite width, each ordinate will be obliterated in the same way, so that not the true profile T(x), but an apparent one O(x)

 $\int_{-\infty}^{+\infty} T(y) A(x-y) dy \text{ is observed. This integral-operation}$

means the obliteration of T by A. For simplicity we shall in the following denote O, T and A, and similar functions, by heavy types. For this integral-operation we shall use the abridged notation O = T.A, and call this ,,the multiplication of T by A. This convention can be more or less justified by the validity of the relations: A.B = B.A, A.(B.C) = (A.B).C and A.(B+C) = A.B + A.C, which can easily be proved.

2. The problem set by practice is: Determine T, when O and A are given profiles. In this article a method is developed for solving this problem in a rather simple way; besides it will be possible to make an estimate of the accuracy reached.

The obvious and not new solution of the problem is: Find an operating-function B, of such a nature that, multiplied by O, it gives T. One property, which B must necessarily possess, can be seen at once: beside positive values it must also assume negative ones, otherwise it would obliterate O still further. B must likewise be normalized to 1.

Using the properties mentioned of the multiplication, and introducing the *unity-function* 1, an extremely narrow peak normalized to one, our ideal should

be to find such a function B, that

$$0.B = (T.A).B = T.(A.B) = T.1 = T.$$

This, however, requires the solution of the integralequation A.B = 1, which is theoretically impossible. We have always to deal with the operation:

O.B = (T.A).B = T.(A.B) = T.A' = O' where $A' \neq 1$, and $O' \neq T$. This is the fundamental formula for any operation on a line-profile. The operation of any B on O always yields a new profile O', that may be also conceived to result from a direct registration of T by another apparatus having the instrumental profile A' = A.B. The bearing of this statement is that, as regards the choice of B, we need not take into account the particular spectral line, which we want to correct, but that we only have to reckon with the resulting A'. This can never become the unity-function itself, but it should sufficiently closely resemble 1, i.e. be sufficiently narrow.

3. Before proceeding to the different methods for choosing a suitable operating-function **B**, we have to fill up a gap in the former reasoning. The extremely narrow peak normalized to one is, mathematically, not yet completely defined. This may be accomplished by forming from each profile-function, e.g.

A(x), the "integral-function" $\alpha(x) = \int_{-\infty}^{x} A(y) dy$. This

 $\alpha(x)$ increases continuously, from o for $x = -\infty$ to 1 for $x = +\infty$. The integral-function of the unity peak has now the values:

$$\alpha(x) = 0$$
 for $x < 0$
 $\alpha(x) = 1$ for $x > 0$
discontinuity for $x = 0$.

In this way innumerable new profile-functions, having an integral-function with points of discontinuity, may be defined. If the integral-function changes its value only in these points, the profile-function consists of discrete peaks only, whence we shall call it a "peak-function". We shall choose our

B more particularly from this group of functions. One may still remark, that this new group of functions makes a new definition of multiplication necessary; $\alpha(x)$, $\beta(x)$, $\gamma(x)$ being the integral-functions

of **A**, **B** and **C**, this definition is
$$\alpha(x) = \int_{-\infty}^{+\infty} \beta(x) d\gamma(x)$$
.

The integral is a STIELTJES-integral. In the case of continuous profile-functions it is reduced to the former definition; in the case of peak-functions it means a simple summation of a number of products $b_k c_k^{-1}$).

4. The first method to choose an operatingfunction B, has been given by Burger and VAN CITTERT 2). They choose a series of possible functions

 B_n , equal to the development of $\frac{1}{A} = \frac{1}{1 - (1 - A)}$,

broken off at the n-th term.

 $B_n=1+(1-A)+(1-A)^2+\ldots+(1-A)^n$; e.g. $B_0=1$; $B_1=2-A$; $B_2=3-3A+A^2$. Generally speaking, B_n consists of a central peak n, and a continuous function, which in the central part is negative, but in the wings of alternating sign; Burger and van Cittert call this function \mathfrak{A}_n . The result reached may be judged by $A'_n=B_n$. $A=1-(1-A)^{n+1}$. For further details the reader is referred to the publications.

One may observe that $A.B_n \rightarrow 1$, therefore $0.B_n \rightarrow T$ converge indeed for $n \rightarrow \infty$, but that B_n itself has no definite function as a limit. For that reason we have in any case to resort to an approximation.

5. It would seem now, that, using this method, we can compute T within any degree of accuracy that may be desired. This, however, is not true. Beside the practical drawback that each operation $A.A = A^2$, $A^2.A = A^3$, etc. takes much time, there is another essential objection. The random measuring-or reading-errors of O are, by the operation O, first multiplied by O, and then increased and decreased by several terms; the random errors resulting in O will therefore be much greater than the original ones in O. This objection is peculiar to all O's, whichever we choose. The narrower we make O's, the more enlarged the random errors of O will enter into O'. This is not astonishing, for otherwise it would be possible to perform very accurate measurements with

an instrument of very low dispersion. In practice one must decide on a compromise between the errors caused by the finite width of A', and the random errors in O'. The result will be most favourable, when both errors are of the same order. We observe, by-the-way, that the place of this optimum does indeed depend on the profiles operated upon. For the flat line wings an operation is superfluous and even obnoxious owing to the enlarged random errors. On the other hand in the narrow cores we will readily permit some larger random errors, in order to make A' narrow enough, i.e. the profile O' pure enough.

6. Our method is to use as operating-function a suitable peak-function. We shall briefly indicate its advantages. First, the important advantage is that it is easy to operate with. For, when **B** consists of n, e.g. 10 peaks, each integral for the computation of one point of 0' = B.0 is now reduced to a simple summation of n products, e.g.:

$$O'_0 = \sum b_k O_k$$
.

Herein the b_k 's are the heights of **B**'s peaks, and the O_k 's are the ordinates of **0** at the corresponding abscissae. In numerical as well as in mechanical computing this means an important simplification. One obtains a particularly simple survey of the computation, when all distances between the peaks are chosen equal to one "peak-distance" d, or simple multiples of it. In the choice of **B** we have confined ourselves to this kind of "equidistant peak-functions".

Beside the operations with **B** the convenience of computing **B** itself must be taken into account. Our method is wholly unlike that of Burger and van Citter, which provides a series of approximations. Once having chosen the peak-distance d, on which parameter the width of the resulting **A'** and consequently the enlarging factor of the random errors depends, our purpose is to choose the best **B** directly. It would be advisable to have some **B's** with different parameters in store for one and the same apparatus, and to use one for very narrow lines, an other for less narrow lines, etc. Considering that for one instrumental curve such a **B** would have to be computed only once for all, some amount of labour would certainly be worthwhile.

As to the appropriateness of this method one might remark that, operating with such a peak-function only a very small part of the data is used in computing an ordinate of $\mathbf{0}'$, e.g. its central intensity; it appears difficult to believe that the accuracy is equal to that, reached by using a continuous operating-function. Though it seems impossible to give a complete elucidation of this question, we shall show the way of solving it. Suppose that we had found a

¹⁾ The method, by which von Neumann joins wave mechanics and quantum mechanics in a single strictly mathematical system is, more-dimensionally, essentially the same. J. v. Neumann, *Die Grundlagen der Quantenmechanik*, Berlin 1932.

²⁾ H. C. BURGER und P. H. VAN CITTERT, "Wahre und scheinbare Intensitätsverteilung in Spektrallinien", Zs. f. Phys. 79, 722, 1932; 81, 428, 1933.

satisfactory continuous B, e.g. by the method of B.-v.C.; then A' = A.B would still have a finite width, from which it follows that all details in T, within such a width w, would be almost completely obliterated in O'. Foreseeing this we can, without making O' much worse, take the drastic measure to divide B into strips of width w and then contract each of these into a peak, making B a peak-function with peak-distance d = w. Comparing now this peak B with the former continuous B, we may draw the conclusion that the above remark is wrong; for either:

- 1. **0** is completely smooth between the points used. Then there is no objection to use only these points, or:
- 2. 0 has some unexpected details between these points; this can only be caused by T having such details, narrower than d. In this case the resulting profile O' will not be the true one. But then this is due to the insufficient narrowness of A', and not to the fact that a peak-function is used instead of a continuous operating-function 1). This is only a short indication of the nature of the problem, which will suffice for the time being.

7. The determination of B.

The possibility just touched upon of contracting the strips of a continuous \mathbf{B} has of course no practical meaning. In practice we can determine \mathbf{B} by two methods.

a) By way of trial.

This is done graphically. In the centre A is drawn and two reduced replicas of A, placed at a distance d to the left and to the right, are subtracted, so as to suppress the wings of A as completely as possible. **B** has now a positive central peak and two negative peaks near it. This kind of operatingfunction has first been used by VAN ALBADA 2). By further negative or positive peaks the wings may be still more completely suppressed. In order to be used as an operating-function, the peak-function found in this way must be normalized to 1. This graphical determination may be carried out with the original instrumental curve or with its integralfunction. We recommend the last, lest a considerable area in the far wings would remain uncorrected. This trial method, which is very helpful to suppress the wings of the instrumental curve, grows troublesome, when one wants a narrower core for it. Then it is difficult to find the right reducing coefficients, and an other method is needed.

b) By solution of a system of linear equations.

We shall illustrate this method, which leaves a considerable freedom for modification, by a numerical example, the result of which may be interesting our readers too. In the new *Photometric Atlas of the Solar Spectrum*, edited by the Utrecht Observatory ¹), the profiles of the Fraunhofer lines have still an appreciable instrumental obliteration. It would be very useful to eliminate this in a correct way. This indeed was the reason why this subject, first by Dr. P. KREMER, was entered upon.

8. The instrumental curve for exposures in the second order near λ 6000 is given. The peak-distance is chosen equal to d = 30 mÅ, i.e. 0.6 mm in the registrograms. First A is divided from the centre into strips of width d, the areas of which are:

To the left: 472, 181, 62, 24, 12, 19, 9, 10, 9, 6, 4, 4, 4, 3, 2.

To the right: 472, 181, 70, 45, 35, 22, 15, 11, 8, 7, 6, 6, 4, 3, 2.

In total: to the left 813, to the right 887, together 1700 (measured arbitrarily with abscissa-unit = 5 mÅ, ordinate-unit = 1/100 of max. ordinate). Next we symmetrize the curve:

To the left \(\)\(\)\(\)\(472, \)\(181, \)\(66, \)\(35, \)\(24, \)\(16, \)\(12, \)\(11, \)\(9, \)\(\)\(16, \)\(5, \)\(5, \)\(4, \)\(3, \)\(1. \)

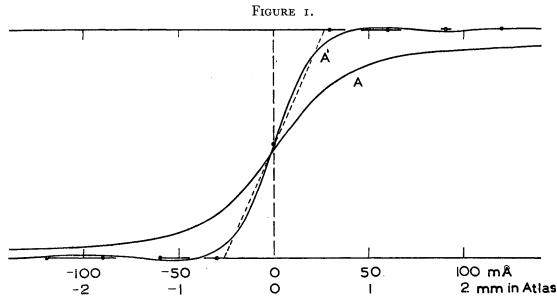
Now, for a while, we imagine these strips contracted to peaks at distances $\frac{1}{2}$ d, $l_{\frac{1}{2}}$ d, $l_{\frac{1}{2}}$ d, etc. from the centre. Then we require that this peak-instrumental curve \mathbf{A}_{p} , multiplied by \mathbf{B} , shall yield a peak-function \mathbf{A}_{p} . B consisting of only two peaks of height 850, $\frac{1}{2}$ d apart from the centre. This requirement, which appears the most efficient one, is equivalent to fixing the points $\frac{1}{2}$ (= 850) in the centre, o at distance -d, -2d, etc. from the centre, and 1 (= 1700)at distances +d, +2d, etc. from the centre, of the integral-function of the resulting instrumental curve A.B, as may be easily shown. This requirement can strictly be complied with mathematically. The B defined in this way consists of a central peak b_0 , and peaks b_1 , b_2 , b_3 etc. at distances d, 2d, 3d, etc. to the left and to the right. These unknown quantities satisfy the equations:

¹⁾ Here too an analogy with quantum mechanics may be observed: The matrixelements, though apparently containing less than the wave functions, actually contain no fewer physical data.

²⁾ B.A.N. No. 301, 8, 179, 1937.

¹⁾ MINNAERT, HOUTGAST and MULDERS: Photometric Atlas of the Solar Spectrum, Amsterdam 1940.

228 UTRECHT B. A. N. 342



Integral curves of A, original instrumental curve, and A.B = A', resulting instrumental curve after operation by B; it is equivalent to a slit with a width of 52 mA (dotted line). The points of A' fixed beforehand (black dots) are not quite reached by the curve, owing to the graphical corrections applied afterwards.

In order to solve them approximately, we cut the system beyond the ninth equation and the ninth a satisfactory definition unknown quantity b_8 ; then by a method analogous to the method used by Gauss for solving normal equations, the unknown quantities b_8 , b_7 , b_6 , b_5 , b_4 , The result was:

$$\frac{1}{2}$$
 b_0 b_1 b_2 b_3 b_4 1.46 -0.80 -0.03 0 -0.05

The sum ought to be exactly equal to $\frac{1}{2}$.

Taking this solution as a starting point, no further difficulty is met with, in using the graphical method described sub a). In this way the errors due to the

Distance from the centre 0 d 2d 4d 7d 12d Total Peaks
$$\begin{cases} \text{to the left} \\ \text{to the right} \end{cases}$$
 + 2.82 $\begin{cases} -0.80 & -0.04 & -0.02^5 & -0.01^5 \\ -0.80 & -0.04 & -0.06 & -0.02^5 & -0.01^5 \end{cases}$ 1.00

In order to keep the operation with B simple the peaks in the far wings have been contracted as far as was possible without spoiling the satisfactory shape of A'.

9. It may be of some use to have numerical values for the accuracy reached. To this end one can define the effective width w of A' in a way shown in the figure, where it is 52 mA, so that the disturbing influence of A' in the resulting spectrum is fairly equal to that of a slit of width

 b_3 , b_2 , b_1 are successively eliminated ¹). In this way a satisfactory determination, more in particular of the central peaks b_0 , b_1 , b_2 is obtained, without complications arising from our rounding-off method. The result was:

$$b_5$$
 b_6 b_7 b_8 Sum -0.01 0 0 -0.02 0.55

cutting of the system, and some computing errors can be corrected, while, starting from the original instrumental profile, also the asymmetry is taken into account. The operating-function **B** is finally chosen:

50 mÅ. The enlarging of the random errors too, can be expressed by a numerical factor, e.g.
$$\beta = \text{root}$$
 of the sum of the squares of B's peaks. For our operating-function $\beta = 3$ 1. This means that all random errors in $\mathbf{0}$ enter three times enlarged into $\mathbf{0}'$.

For computing a suitable operating-function in practical cases the following data may be a guide for the choice of d and the accuracy to be reached $(h = \text{half-width of } \mathbf{A}, \text{ i.e. total width at 50% of maximum height)}.$

Chosen
$$d = h$$
 0.7 h 0.5 h 0.4 h 0.3 h
gives $\begin{cases} w = 1.5 h & h & 0.8 h & 0.7 h & 0.5 h \\ \beta = 1\frac{1}{2} & 2 & 3 & 5 & 12 \end{cases}$

Finally, I wish to thank Prof. MINNAERT for his stimulating interest and helpful discussions.

Taking $b_0 + b_1$, $b_1 + b_2$, $b_2 + b_3$ etc. as unknown quantities, one obtains a symmetrical system to which the Gaussian methods are directly applicable.

B. A. N. 367 UTRECHT 79

is a solution of the integral equation (1) with Gaussian apparatus function. The proof is essentially the same as in the first variant. This variant may be regarded as a generalization of Seeliger's method, which results from it if only $a_{\circ} = 0$. Still other variations are certainly possible and may easily be constructed.

6. Practical application.

This paper about the solution of the integral equation (1) is mainly meant as a contribution to the better and easier understanding of some methods already used in literature. Some extensions and generalizations were the natural result of a new derivation of these methods. As to the question whether they are very useful in *practical* application to the material now

available, we are, however, not quite optimistic. In most applications of stellar and mathematical statistics only one or two correction terms are used. But even these are often very uncertain, owing to the scanty and inhomogeneous material and the uncertainty of the "apparatus function". In spectral optics conditions are quite different. The line profiles may be measured accurately and the apparatus function is certainly reproducible. But in this very case the method of expansion in a power series is theoretically not justified, as was pointed out in section 3. So we have to look for future progress in the accuracy of statistical research or to other fields of application in order to see the above formulae applied to their full extent.

It is a pleasure to me to thank Prof. MINNAERT and Prof. Oort for their kind interest and helpful advice.

Instrumental distortion of weak spectral lines, by H. C. van de Hulst.

The profiles are approximated by Voict profiles. Mutual obliteration consists in adding β_r and β_2 separately. Application to the photometric atlas of the solar spectrum. The apparatus function appears to be narrower than the function given in the Atlas. Figure 1 shows all results.

Statement of the problem.

In systematic work by the joint workers of the Utrecht Observatory on the photometric atlas of the solar spectrum, we wanted to revise the apparatus function. This can only be deduced from the false profile of a narrow spectral line, on the true profile of which we have reliable information.

True profile, false profile and apparatus function are related by an integral equation. Among the well known methods of solution 1) no convenient method for our purpose is found. On account of the weakness of the lines we can characterize each profile sufficiently by a few parameters. The widely used method, however, of characterizing each profile by one parameter — the halfwidth — only, is certainly too rough. We now have tried to approximate the three functions involved by *Voigt profiles* with two parameters β_1 and β_2 .

Mutual obliteration of Voigt profiles.

A symmetrical profile has a Fourier integral, defined by

$$\varphi(t) = \int_{-\infty}^{\infty} \cos xt \ f(x) \ dx \tag{1}$$

where x = distance from the centre of the line, f(x) = intensity or depression, c = f(o) = central intensity or central depression, h = halfwidth = total width at height $\frac{1}{2}c$, $S = \varphi(o) = p$ h c = area or equivalent width. We expand $\log \varphi(t)$ in a power series and cut

off beyond the second term:

$$\varphi(t) = S \cdot \exp(-\beta_1 t - \beta_2^2 t^2 / 4)$$
 (2)

Thus the profile f(x) is approximated by a function of well known type that we shall call a *Voigt profile*, having two parameters β_1 and β_2 . Two particular forms are

$$\varphi(t) = S \cdot e^{-\beta_1 t}$$
 , $f(x) = S \cdot \frac{\beta_1}{\pi (\beta_1^2 + x^2)}$ (3a)

$$\varphi(t) = S \cdot e^{-\beta_2 t^2/4}, f(x) = S \cdot \frac{1}{\beta_2 \sqrt{\pi}} e^{-x^2/\beta_2 t^2}$$
 (3b)

The first one is a dispersion profile, having extended wings; the second one is a Gaussian profile. Up to now the Voigt profiles have been formulated as obliterations of a dispersion profile and a Gaussian profile. We now observe that mutual obliteration of two Voigt profiles always yields a new Voigt profile. In mutual obliterations of arbitrary functions the Fourier integrals are multiplied. Hence according to (2), in order to obliterate a Voigt profile by another Voigt profile, we must multiply both areas S, add both parameters β_1 and add both squares β_2 . The reverse process consists in a division and two subtractions. The processes can be graphically represented by addition and subtraction of the vectors (β_1, β_2^2) .

Voigt profiles 1) and their halfwidths 2) have been computed for a number of values of β_1/β_2 ranging

¹⁾ Cf. section 3 of the preceding article.

F. Hjerting, Ap. J. 88, 508, 1938, giving references.
 R. Minkowski & H. Brück, Z. f. Physik, 95, 299, 1935.

TABLE 1.

Profiles in second order of the photometric atlas, unit = 10^{-6} k; primary data from measurements or from theory are shown by *.

						•		
	h	β_{1}	eta_{2^2}	β_2	β_1/β_2	p	source	
O' false profile O true profile O abs. coeff. mean values for Six O ₂ -lines near λ6300	10.20* 3.05 5.35	3.67 1.48 1.16*	12.2 0.1 0.0*	3°50 0°25 0°00	1.02* 2.8 ∞	1'41 1'56 1'57	measured from O _o Allen's	
A apparatus function At theoretical apparatus function	8·42 6·40	2°19 1°07*	12°1 9'7*	3.48 3.11	o 63 o 34	1'31 1'22	= O'-O theory	
Ne' false profile Neon emission- Ne true profile line λ5852	12.20* . 7.30	o.86	26.5 14.4	5°14 3°78	oʻ59* oʻ23	1.30	measured = Ne'-A	
Ti' false profile Ti true profile Ti _o abs. coeff. mean values for six Ti-lines near λ5900	16·80* 13·15 12·50	2.23 0.33 0.33	70'7 58'6 53'0	8·40 7·65 7·30	0'30* 0'04 0'04	1.08 1.08	measured = Ti'-A from Ti	

from o to ∞ . In addition to the halfwidths h and central ordinates c, we computed the factor p = S/hc, introduced by Allen 1). This factor ranges from 1.06 for a purely Gaussian profile to 1.57 for a purely dispersion profile.

Application to the atlas of the solar spectrum.

Some lines near \(\lambda 6000 \) in the second order were investigated. The results are shown in Table 1 and in Figure 1. For the different lines observed, analysis of profiles by several numerical, graphical and analytical methods gave consistent values of β_{r} and β_2 , indicating that the approximation by Voigt profiles is a good one. All breadths β_1 , β_2 and h are expressed in micro wavelengths (unit = $10^{-6} \lambda$), in order to make lines of slightly different wavelengths intercomparable. One more decimal than warranted is written. The probable error of h is 0.6 micro wavelengths = 0.08 mm in the tracings of the atlas.

The course of the computations follows the scheme given above. A reliable true profile of the atmospheric oxygen lines is known from theory. This compared to the false profile then yields the apparatus function, which, finally, is used for finding true profiles of the Ne and Ti-lines. A few further remarks will elucidate the meaning of Table 1.

The lines, though weak, already diverge from the linear curve of growth. This fact is accounted for by the slight differences between O and O_o, Ti and Ti_o.

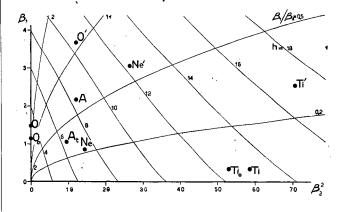
The atmospheric oxygen lines, which are basic to all results, will be treated in another paper. Allen's theory 2), though not wholly correct, will do for our purpose. On each level the absorption coefficient is a combination of damping (β_{τ}) and Doppler effect (β_2) . We assumed $\beta_r = b_0 = 2.32$ on Mt Wilson level. Integration over the height of the atmosphere reduces β_{r} to $\frac{1}{2}$ b_o and β_{r} to nearly zero.

The resulting apparatus function is much broader than the theoretical function A_t of an ideal grating spectrograph. But it is considerably narrower than the function given in the preface of the atlas, having h = 10.2.

The profile of the Neon emission line photographed by Mulders in order to derive the apparatus function can now be unterstood 1). The true profile appears to have a considerable width as was already stated by Allen 2). Experimental evidence shows that the Neon lines are very sensitive to the mode of excitation of the tube. The value h = 7.3 now found is consistent with the h = 5.8 for moderate current 3).

It was very satisfactory to find the absorption coefficient of the solar titanium lines to be of nearly

FIGURE 1. Obliteration by vector addition.



¹⁾ We used the original profile, not the narrowed profile

C. W. Allen, Ap. J. 85, 165, 1937.
 C. W. Allen, Ap. J. 85, 156, 1937.

reproduced in the atlas.

2) C. W. Allen, Ap. J. 85, 165, 1937.

3) G. Balaise & R. Ghislain, Acad. Roy. Belg., Cl. d. sci.