Line Breadths and Voigt Profiles

Hulst, H.C. van de; Reesinck, J.J.M.

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H. C. van de Hulst and J. J. M. Reesinck
Yerkes Observatory and Utrecht Observatory
Received April 1, 1947

ABSTRACT

Voigt functions are useful approximations for the intensity distribution in spectral lines. A table of these functions is given, and its use in computations on instrumental distortion is explained. Some mathematical properties of the Voigt functions are mentioned.

1. It is well known that the intensity distribution in a spectral line broadened by two independent effects is expressed by the equation

$$f(x) = \int_{-\infty}^{+\infty} f'(x-y)\, f''(y)\, dy\,. \tag{1}$$

Here $f'(x)$ and $f''(x)$ are the profiles that the line would assume if only one of the broadening effects was present. All functions f, f', and f'' denote intensities, and x is the distance from the center of the line in terms of either wave-length or frequency units.

Often the functions $f(x)$ and $f'(x)$ are known, and $f''(x)$ has to be found from equation (1). Such is the case, for instance, if the observed profile of a spectral line and the instrumental function are known and the true profile is sought. Numerous methods for solving the integral equation (1) have been applied.[1] However, all the general methods are very laborious. This is not unexpected, since even the direct integration of equation (1) when $f'(x)$ and $f''(x)$ are given is laborious. A separate integration is then needed for each value of x, so that the construction of a *single* line profile, $f(x)$, requires a large number of integrations.

A short way of solving either problem is to approximate the profiles by analytic functions. One of us has shown that Voigt functions are very suitable for this purpose.[2] Convenient tables of these functions are not available. We shall accordingly present here a table and a graph which we have found to be useful in practice. With their use the method can be applied to other problems without any effort.

2. The prototype of a method using simple analytic functions as approximations is the "half-breadth method." The profiles are supposed to agree with functions of the Gaussian type:

$$f(x) = c\, e^{-x^2/\beta_2^2}\,,$$

where c and β_2 are constants. If in equation (1) the functions $f'(x)$ and $f''(x)$ are of this type, then so is $f(x)$, and the parameters β_2 are related by

$$\beta_2^2 = \beta_2'^2 + \beta_2''^2\,. \tag{2}$$

The half-breadths, which for Gaussian functions are equal to $1.665\beta_2$, satisfy a similar relation. Therefore, the two operations to which equation (1) gives rise consist of simple addition, or subtraction, of the squares of the half-breadths.

This widely practiced method may be good for frequency functions in mathematical

[1] Cf. H. C. van de Hulst, *B.A.N.*, **10**, 75, 1946. [2] *Ibid.*, p. 79.

statistics, but it is unsatisfactory for spectral lines. The reason is that *most* profiles have *extended wings*, in which the intensity decreases proportionally to x^{-2}. Such wings are present in the profiles of lines broadened by collision damping or by radiation damping. They are also present in the instrumental curves of most spectrographs (compare sec. 6). The classical example of profiles with very strong wings is provided by functions of the dispersion type,

$$f(x) = \frac{c}{1 + x^2/\beta_1^2},$$

where c and β_1 are constants. These functions also have the property that two functions of this type define by means of equation (1) a third function of the same type. The parameters β_1 are connected by the relation

$$\beta_1 = \beta_1' + \beta_1'' . \quad (3)$$

The half-breadths, which for dispersion functions are equal to $2\beta_1$, must also be added linearly.

As an example, we consider the case of an observed spectral line having a profile of the dispersion type with half-width $h = 2.0$ A, while the instrumental profile is also known to be of the dispersion type, with $h' = 1.6$ A. Since we have to subtract linearly, we obtain $h'' = 0.4$ A for the true half-width of the line. If, instead, we had applied the usual quadratic subtraction, we should have found the value $h'' = 1.2$ A, which is three times too large. This example shows how much the common half-breadth method may be systematically in error when applied to spectral lines.

Voigt functions[3] are a more general type of function, including, as extreme cases, the two types mentioned above. They originate as functions $f(x)$ in equation (1) if $f'(x)$ is a Gaussian function and $f''(x)$ is a dispersion function. Thus they are characterized by two parameters, β_1 and β_2, and show more or less strong wings, dependent on the ratio β_1/β_2.

An important theorem (see sec. 5) is: *If in equation* (1) f′(x) *and* f″(x) *are Voigt functions, then* f(x) *is also a Voigt function. Their parameters satisfy the relations*

$$\left.\begin{aligned} \beta_1 &= \beta_1' + \beta_1'' , \\ \beta_2^2 &= \beta_2'^2 + \beta_2''^2 . \end{aligned}\right\} \quad (4)$$

Using this theorem, we can perform the operation (1) and its inverse process very rapidly. Only a little more effort is required than in the common half-breadth method, and the systematic errors of that method are avoided. In fact, we have found that the profiles of most spectral lines which show no asymmetry, fine structure, or strong self-absorption are very nearly Voigt profiles. Generally, therefore, equation (1) can be solved by the new method as accurately as the observations will permit.

3. For practical use of this method a set of standard Voigt functions is needed. Table 1 gives such a complete set. It is based on existing tables. If we denote by A the area

$$A = \int_{-\infty}^{+\infty} f(x)\, dx , \quad (5)$$

[3] First studied by W. Voigt, *Münch. Ber.*, *1912*, p. 603.

a Voigt function $f(x)$ is completely determined by the parameters A, β_1, and β_2. Numerically computed tables have been published for the following cases:

$$\text{Born}^4\colon A = \pi ,\quad \beta_1 = 1 ,\quad \beta_2 = \eta ,$$

$$\text{for } \eta = 0,\ 0.1,\ 0.5,\ 1,\ \text{and } 2 ;$$

$$\text{Hjerting}^5\colon A = \sqrt{\pi} ,\quad \beta_1 = a ,\quad \beta_2 = 1 ,$$

$$\text{for } a = 0, \ldots, (0.01), \ldots, 0.2,\ 0.3,\ 0.4,\ \text{and } 0.5 .$$

TABLE 1

STANDARD VOIGT PROFILES

PARAMETERS					ORDINATES IN TERMS OF CENTRAL ORDINATE										
					0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.05	0.02	0.01
β_1/h	β_1/β_2	β_2/h	β_2^2/h^2	p	Widths in Terms of Half-width										
0.000	0.00	0.60	0.36	1.06	0.57	0.72	0.86	1.00	1.15	1.32	1.52	1.82	2.08	2.38	2.58
.025	0.04	.59	.34	1.08	.56	.72	.86	1.00	1.15	1.33	1.53	1.84	2.12	2.49	2.82
.050	0.09	.57	.32	1.11	.56	.71	.86	1.00	1.15	1.33	1.54	1.87	2.19	2.63	3.13
.075	0.14	.55	.31	1.13	.56	.71	.86	1.00	1.16	1.33	1.56	1.90	2.25	2.79	3.56
.100	0.19	.54	.29	1.16	.56	.71	.86	1.00	1.16	1.34	1.57	1.94	2.34	3.00	4.08
.125	0.24	.52	.27	1.18	.56	.71	.86	1.00	1.17	1.34	1.59	1.98	2.42	3.24	4.58
.150	0.30	.50	.25	1.20	.55	.71	.85	1.00	1.17	1.35	1.60	2.02	2.54	3.52	5.05
.175	0.36	.48	.23	1.23	.55	.70	.85	1.00	1.17	1.36	1.62	2.06	2.64	3.80	5.50
.200	0.43	.46	.21	1.25	.55	.70	.85	1.00	1.18	1.37	1.64	2.10	2.75	4.14	5.96
.225	0.51	.44	.20	1.28	.54	.70	.85	1.00	1.18	1.38	1.66	2.15	2.87	4.44	6.40
.250	0.59	.42	.18	1.30	.54	.70	.84	1.00	1.18	1.39	1.68	2.19	2.98	4.73	6.78
.275	0.69	.40	.16	1.33	.53	.69	.84	1.00	1.19	1.40	1.71	2.24	3.12	5.03	7.15
.300	0.79	.38	.14	1.35	.53	.69	.84	1.00	1.19	1.41	1.74	2.29	3.26	5.32	7.52
.325	0.92	.35	.12	1.38	.53	.68	.84	1.00	1.19	1.42	1.77	2.34	3.39	5.57	7.86
.350	1.07	.33	.11	1.40	.52	.68	.84	1.00	1.20	1.44	1.81	2.40	3.54	5.83	8.21
.375	1.26	.30	.09	1.43	.52	.68	.83	1.00	1.20	1.45	1.85	2.46	3.70	6.07	8.55
.400	1.50	.27	.07	1.45	.52	.67	.83	1.00	1.21	1.47	1.88	2.54	3.85	6.30	8.86
.425	1.83	.23	.05	1.48	.51	.67	.83	1.00	1.21	1.48	1.92	2.64	4.00	6.55	9.18
.450	2.38	.19	.04	1.51	.51	.66	.82	1.00	1.22	1.50	1.96	2.74	4.13	6.76	9.50
.475	3.54	.13	.02	1.54	.51	.66	.82	1.00	1.22	1.52	1.98	2.87	4.25	6.92	9.77
0.500	∞	0.00	0.00	1.57	0.50	0.66	0.82	1.00	1.22	1.53	2.00	3.00	4.36	7.00	9.95

The values of the central ordinate, c, and of the total half-breadth, h, were found for each tabulated function. All ordinates were then divided by c and all abscissae by h, and the resulting functions were plotted. Born's and Hjerting's tables are complementary; together they cover the complete range of positive values of β_1/β_2. For the case $\beta_1/\beta_2 = 0.5$, which they have in common, the results were found to be in good agreement. As a further check, the values of the half-breadths in the entire range were compared with those computed by Minkowski and Bruck;[6] the differences were less than

[4] M. Born, *Optik* (Berlin: Julius Springer, 1933), pp. 482–86.

[5] F. Hjerting, *Ap. J.*, **88**, 508, 1938.

[6] R. Minkowski and H. Bruck, *Zs. f. Phys.*, **95**, 299, 1935.

Now if the subscripts g and d denote functions of Gaussian and dispersion types, respectively, the symbolical product of two Voigt functions may be reduced as follows:

$$f_1 \cdot f_2 = f_{1g} \cdot f_{1d} \cdot f_{2g} \cdot f_{2d} = f_{1g} \cdot f_{2g} \cdot f_{1d} \cdot f_{2d} = f_{3g} \cdot f_{3d} = f_3 .$$

This proves the theorem stated in section 2 and the correctness of equations (4).

b) Let the Fourier integral of any symmetrical function $f(x)$ be denoted by

$$\varphi(t) = \int_{-\infty}^{+\infty} \cos xt\, f(x)\, dx ; \tag{9}$$

then, as is well known, the symbolical multiplication in equation (8) corresponds to an ordinary multiplication,

$$\varphi(t) = \varphi'(t) \cdot \varphi''(t) . \tag{10}$$

By means of these equations we find that the Fourier integral of a Voigt function has the form

$$\varphi(t) = A\, e^{-\beta_1 t - \beta_2^2 t^2/4} , \tag{11}$$

as was first derived by Reiche.[8]

c) If a profile is *not* a Voigt profile, its Fourier integral will often admit of the expansion

$$\log \varphi(t) = \log A - \beta_1 t - \tfrac{1}{4}\, \beta_2^2 t^2 - \beta_3^3 t^3 \ldots . \tag{12}$$

By neglecting the third- and higher-order terms in equation (12), we approximate the given profile by a Voigt profile. We call β_1 and β_2 its "Voigt parameters."

d) If functions of the type (12) act together with other Voigt functions or non-Voigt functions according to equation (1), the third-order terms lose importance relative to the first- and second-order terms. In particular, if many such functions act together, the Fourier integral, $\varphi(t)$, of the resulting function is practically zero at the values of t where the third-order terms would become important. Thus the combination of many independent broadening effects *tends to yield a Voigt profile.*

Theorems closely corresponding to the points mentioned are found in the theory of probability distributions.[9] In that case, however, the emphasis is on distribution functions that possess one or more finite momenta, whereas all momenta of the functions discussed above are infinite (unless $\beta_1 = 0$). In particular, if the functions mentioned in section *d* are supposed to have no extended wings, i.e., to have $\beta_1 = 0$, one obtains the well-known theorem of statistics that many independent sources of error yield a Gaussian distribution function.

6. For some frequently occurring profiles we list the values of the parameters below:

a) *Doppler broadening.*—A pure Voigt profile with $\beta_1 = 0$ and $\beta_2^2 = (2kT/mc^2)\lambda^2$; β_2 is expressed in wave-length units and the symbols have the usual meanings.

b) *Damping profile.*—A pure Voigt profile with $\beta_2 = 0$; $\beta_1 = 1/t$, expressed in angular-frequency units. Here t is either the time in which the intensity is damped to $1/e$ of its original value or the average time between two collisions. The usual damping constant, γ, equals $2\beta_1$. To convert into wave-length units, multiply by $\lambda^2/2\pi c$.

[8] A. C. G. Mitchell and M. W. Zemansky, *Resonance Radiation and Excited Atoms* (Cambridge Cambridge University Press, 1934), pp. 319 ff.

[9] S. Chandrasekhar, *Rev. Mod. Phys.*, **15**, 1, Appen. IV, 1943.

By combining these three steps several kinds of operations may be performed. If many broadening effects have to be combined, or disentangled, it is convenient to represent the results graphically as vectors in a (β_1, β_2^2) diagram. Such a diagram will also help to estimate how uncertainties in the primary data affect the results. For a practical example we may refer to an earlier paper,[2] in which this method was applied to weak lines in the Utrecht *Photometric Atlas* of the solar spectrum.

5. We may, finally, add some remarks on the mathematical properties of the Voigt functions.

a) The relation (1) can be written symbolically as

$$f = f' \cdot f'' , \tag{8}$$

and the symbolical product thus defined has all the properties of common products.

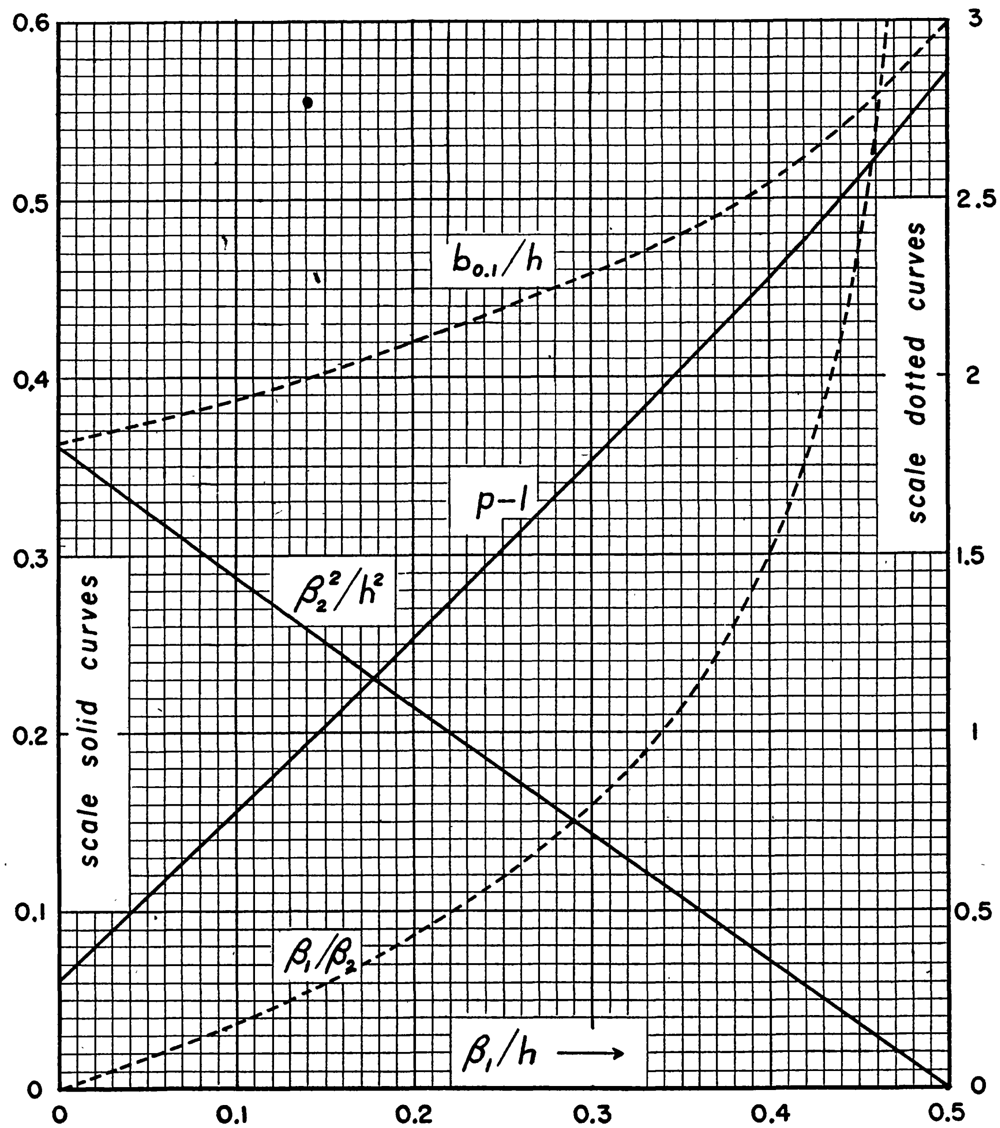

FIG. 2.—Working graph of the parameters

1 per cent. Finally, the values given in our Table 1 were obtained by graphical interpolation.

Arrangement of the table.—Since most of the values needed are approximately linear functions of β_1/h, the table was arranged with equal intervals of this argument. The upper line, with $\beta_1/h = 0$, gives data on a Gaussian function; the bottom line, with $\beta_1/h = 0.50$, gives data on a dispersion function; any intermediate line gives data on a particular Voigt function. The first four columns contain the parameters defined above. The parameter p, given in the fifth column, is defined by the relation

$$A = phc\,. \tag{6}$$

The further columns show to what breadth the line extends at a given fraction of the central intensity. In addition to h ($\equiv b_{0.5}$), we use, in particular, the value $b_{0.1}$. Figure 1 illustrates the shape of the line in the two extreme cases and in one intermediate case.

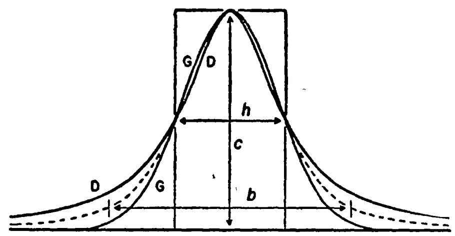

FIG. 1.—Voigt profiles. G = Gaussian type, D = dispersion type, and the intermediate case of $\beta_1/h = 0.25$ (*dotted curve*).

The values in the table are believed to have errors smaller than one unit in the last decimal, with the exception of the values in the last three columns, which may have larger errors. This accuracy may be sufficient for all cases in which the approximation of line profiles by Voigt functions is suitable.

4. We shall now describe what calculations can be performed by means of this table and the graph in Figure 2.

a) *To find the parameters for a given profile.*—Read the central ordinate, c, the breadth, h, of the line at half this ordinate, and the breadth, $b_{0.1}$, at one-tenth of this ordinate. Take the ratio $b_{0.1}/h$ and read the corresponding values of β_1/h, β_2^2/h^2, and p from Figure 2. Find β_1 and β_2^2 by substituting the value of h. In order to check whether the approximation is good, the breadth at ordinates other than $0.5c$ and $0.1c$ as found from the table may be compared with the observed widths. As a further check the area may be determined by planimetering and by means of formula (6).

b) *To solve the integral equation* (1).—Determine the parameters β_1, β_2^2, and A for both known profiles. Find the parameters for the unknown profile by means of subtraction or addition according to equation (4). Find its area from[7]

$$A = A' \cdot A''\,. \tag{7}$$

c) *To construct the profile for given parameters.*—Find the value of β_1/β_2 and the corresponding value of β_1/h from Figure 2. Compute h from β_1 and β_1/h; find c from equation (6); and multiply the tabulated ordinates and breadths of the standard profile by the factors c and h, respectively.

[7] In most cases, where one of the functions is a simple broadening function with the area 1 per definition, the rule used is that the area does not change by broadening or narrowing the line.

c) *Straight slit.*—The profile is a rectangular function of breadth, s. The Fourier integral is

$$\varphi(t) = A \frac{2 \sin \frac{st}{2}}{st},$$

from which we find the Voigt parameters $\beta_1 = 0$ and $\beta_2 = 0.408s$ by means of equation (12).

d) *Diffraction pattern of straight slit.*—The instrumental profile of a perfect spectrograph is determined by the limited size of prism or grating. If the limiting edges are a distance s apart, the instrumental function is $\{\sin(\pi s x/\lambda)/(\pi s x/\lambda)\}^2$, where x is expressed in radians. Its Fourier integral is a triangular function:

$$\varphi(t) = A\left(1 - \frac{t\lambda}{2\pi s}\right) \quad \text{for } t < \frac{2\pi s}{\lambda}$$

and 0 for $t \geq 2\pi s/\lambda$. By means of equation (12) we find that the best-approximating Voigt profile has the parameters $\beta_1 = \lambda/2\pi s$ and $\beta_2^2 = 2(\lambda/2\pi s)^2$, both β_1 and β_2 being expressed in radians.