The Voigt Profile as a Sum of a Gaussian and a Lorentzian Functions, when the Weight Coefficient Depends Only on the Widths Ratio

H.O. Di Rocco[a,b,*] and A. Cruzado[c,d]

[a]Instituto de Física Arroyo Seco (IFAS), Universidad Nacional del Centro de la Pcia. de Buenos Aires
Pinto 399, 7000 Tandil, Buenos Aires, Argentina

[b]Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET)
Rivadavia 1917, C1033AAJ Buenos Aires, Argentina

[c]Facultad de Ciencias Astronómicas y Geofísicas, Universidad Nacional de La Plata, Paseo del Bosque s/n
1900 La Plata, Buenos Aires, Argentina

[d]Instituto de Astrofísica de La Plata (IALP-CONICET), Paseo del Bosque s/n
1900 La Plata, Buenos Aires, Argentina

(Received December 20, 2011; revised version March 6, 2012; in final form May 24, 2012)

Assuming that $V(x) \approx (1-\mu)\, G_1(x) + \mu L_1(x)$ is a very good approximation of the Voigt function, in this work we *analytically* find μ from mathematical properties of $V(x)$. $G_1(x)$ and $L_1(x)$ represent a Gaussian and a Lorentzian function, respectively, with the same height and HWHM as $V(x)$, the Voigt function, x being the distance from the function center. μ is obtained as a function of a, a being the ratio of the Lorentz width to the Gaussian width. We find that, the Voigt function calculated with the expression we have obtained for μ, deviates from the exact value less than 0.5% with respect to the peak value.

PACS: 32.70.−n, 32.70.Jz

1. Introduction

As it is well known, the convolution of a Gaussian and a Lorentzian function is a Voigt profile. Calling $\gamma_{\rm G}$ and $\gamma_{\rm L}$ the HWHM of the Gaussian and the Lorentzian profile, respectively, these functions normalized to unity are expressed as

$$G(x) = \frac{1}{\sqrt{\pi} w_{\rm G}} \exp\left(-(x/w_{\rm G})^2\right) \quad \text{with} \quad w_{\rm G} = \gamma_{\rm G}/\sqrt{\ln 2}, \tag{1}$$

$$L(x) = \frac{1}{\pi w_{\rm L}} \frac{w_{\rm L}^2}{(x^2 + w_{\rm L}^2)} \quad \text{with} \quad w_{\rm L} = \gamma_{\rm L}, \tag{2}$$

and

$$V_a(x) \equiv V(a,x) = \frac{a}{\pi^{3/2}} \int_{-\infty}^{\infty} \frac{{\rm e}^{-(x'/w_{\rm G})^2}}{(x-x')^2 + w_{\rm L}^2} \, {\rm d}x' \tag{3}$$

with $a = w_{\rm L}/w_{\rm G}$.

There are very powerful programs, written, both, in compiled languages (i.e.: Fortran or C) and in C.A.S (i.e.: Maple), that permit $V(x)$ to be evaluated with amazing precision. However, in many applications such a high precision is not much needed. In some cases, the Voigt function is only an approximation in modeling the line profile[†]. In other cases, it makes no sense to fit a measured noisy profile with a theoretical one so precisely calculated. Also, for the calculation of the optical thickness, a lower precision can be accepted. In all these cases, $V(a,x)$ can be written in a very good approximate form as

$$V_a(x) \approx (1-\mu) G_1(x) + \mu L_1(x), \tag{4}$$

$G_1(x)$ and $L_1(x)$ being a Gaussian and a Lorentzian functions with the same height and width at half-maximum as $V(x)$, and $0 \le \mu \le 1$. $G_1(x)$ and $L_1(x)$ are, therefore, totally different from those that would generate $V(x)$ except when $\mu = 0$ and when $\mu = 1$, being in these cases $V(x) = G_1(x) = G(x)$ and $V(x) = L_1(x) = L(x)$, respectively.

The Voigt function expressed as a weighted sum of a Lorentzian and a Gaussian functions, as the expression (4) is, has been proposed by Kielkopf [1] and ana-

* corresponding author; e-mail: hdirocco@exa.unicen.edu.ar

† For example, in the case of dense and cold plasmas, the spectral profile is a Voigt one only when the ionic contribution is neglected.

lyzed by Liu et al. [2], among other authors. Since $V(x)$ is between $G_1(x)$ and $L_1(x)$ for all values of x except for $x = 0$ and $x = \pm\gamma_V$, where the three functions are coincident, this choice is fully justified.

The above cited authors, based on purely numerical considerations, have found mathematical expressions for the μ parameter by fitting the approximated calculation to exact values from numerical integration of the expression (3). They claim a 0.6% agreement between V as calculated with Eq. (4) and V calculated by the corresponding convolution.

The purpose of this work is to deduce, from mathematical properties of $V(x)$, an analytical expression for μ so that the sum given by Eq. (4) makes sense.

We organize this paper as follows: in Sect. 2 we do some general considerations that justify the way we handle the problem. In Sect. 3 we pose the theoretical mathematical expressions that allow us to find the analytical expression for μ we are looking for. In Sect. 4 we illustrate our results and discuss about the accuracy of our calculations.

2. Some previous general considerations

We may intend to calculate μ from Eq. (4) as

$$\mu(a,x) = \frac{V(a,x) - G_1(x)}{L_1(x) - G_1(x)}. \tag{5}$$

Immediately, several difficulties would become evident. First of all, $\mu(a,x)$ depends, not only on a, but also on x. Secondly, expression (5) cannot be calculated at $x = 0$ nor $x = \pm\gamma_V$. At these values of x, the numerator and denominator of (5) are zero (we will discuss this point in a second paper of this series). Finally, Eq. (5) cannot be written in a simple analytical form, even by using series expansions (and/or asymptotic development) of the three functions, since it also depends on the a value.

However, in the second paper of this series, we will see that an analytical expression, easily programmable, that excellently fits the exact values far from the peak profiles, can be achieved.

In this paper we do not calculate $\mu(a,x)$ from Eq. (5). Instead of that, we use analytical properties of $V(x)$ in order to obtain $\mu(a)$, as we explain in the following sections.

3. μ analytical deduction using the property of the normalized area

In this section, and according to which is stated in §1, we build first of all $G_1(x)$ and $L_1(x)$ with the same height, $V(a,0)$, and HWHM, γ_V, as $V(x)$, so that they verify Eq. (4).

In order to find $V(a,0)$ and γ_V we use, on the one hand, the well known expression

$$V_a(0) \equiv V(a,0) = \frac{e^{a^2}\,\Phi_c(a)}{\sqrt{\pi}w_G}, \tag{6}$$

where $\Phi_c(a) = 1 - \mathrm{erf}(a)$.

On the other hand, we consider the relation between γ_V and w_G which is exactly given by

$$\gamma_V = \gamma_V(a) = w_G b_{1/2}(a),$$

being

$$b_{1/2}(a) = a + \sqrt{\ln 2}\exp\big(-0.6055a + 0.0718a^2 - 0.0049a^3 + 0.000136a^4\big),$$

as can be found in [3]. From the properties of $b_{1/2}(a)$:

$$b_{1/2}(0) = \sqrt{\ln(2)}, \quad \lim_{a\to\infty} b_{1/2}(a) = a,$$

the limit values of γ_V

$$\gamma_V(0) = \gamma_G, \quad \lim_{a\to\infty} \gamma_V(a) = \gamma_L$$

can be found.

Therefore, using $w_G = \gamma_V/b_{1/2}(a)$, we write Eq. (6) as

$$V_a(0) = \frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)}{\sqrt{\pi}\gamma_V}, \tag{7}$$

always with the area normalized to unity

$$\int_{-\infty}^{\infty} V(x)\,dx = 1. \tag{8}$$

In order to $G_1(x)$ and $L_1(x)$ meet the above conditions, it must be

$$G_1(x) = \frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)\exp\big(-\ln(2)(x/\gamma_V)^2\big)}{\sqrt{\pi}\gamma_V} \tag{9}$$

and

$$L_1(x) = \frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)\gamma_V}{\sqrt{\pi}(x^2+\gamma_V^2)}. \tag{10}$$

$G_1(x)$ and $L_1(x)$ are not normalized to unity, but

$$A_G \equiv \int_{-\infty}^{\infty} G_1(x)\,dx = \frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)}{\sqrt{\ln(2)}}, \tag{11}$$

and

$$A_L \equiv \int_{-\infty}^{\infty} L_1(x)\,dx = \sqrt{\pi}b_{1/2}(a)\,e^{a^2}\,\Phi_c(a). \tag{12}$$

By integrating both members of Eq. (4), and taking into account Eqs. (8), (11), and (12), it holds that

$$(1-\mu)A_G + \mu A_L = (1-\mu)\frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)}{\sqrt{\ln(2)}} + \mu\sqrt{\pi}b_{1/2}(a)\,e^{a^2}\,\Phi_c(a) = 1, \tag{13}$$

and therefore

$$\mu_a = \frac{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a) - \sqrt{\ln(2)}}{b_{1/2}(a)\,e^{a^2}\,\Phi_c(a)\Big(1 - \sqrt{\pi\ln(2)}\Big)}, \tag{14}$$

where μ depends only on a. Taking into account Eq. (7), expression (14) can be written as

$$\mu_a = \frac{\pi^{1/2}V_a(0)\gamma_V - \sqrt{\ln(2)}}{\pi^{1/2}V_a(0)\gamma_V\Big(1 - \sqrt{\pi\ln(2)}\Big)}, \tag{15}$$

where both, $V_a(0)$ as γ_V, can be determined from the experimental data. Therefore, in this case

$$V(\mu_a, x) \approx (1-\mu_a)G_1(x) + \mu_a L_1(x). \tag{16}$$

4. Results and discussion

In order to illustrate the expression (4), a Gaussian, a Lorentzian, and a Voigt profiles, all of them with an intensity normalized to $V(0)$ and with the same value of HWHM, are shown in Fig. 1.

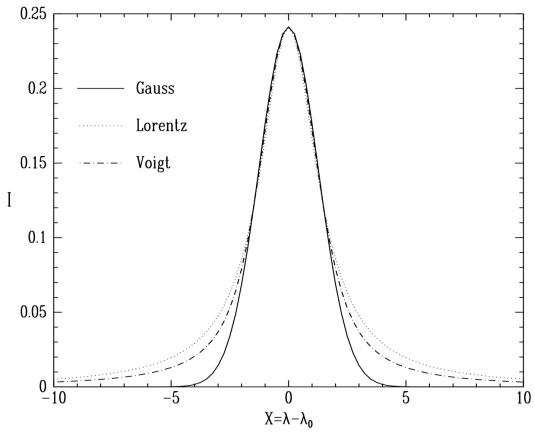

Fig. 1. A Gaussian, a Lorentzian, and a Voigt profiles, all of them with an intensity normalized to $V(0)$ and with the same value of HWHM.

Figure 2 shows $\mu(a)$ as a function of a, according to Eq. (14), ranging from 0 to 1, as expected. The same function obtained empirically by Kielkopf [1] is also shown for comparison. As can be seen in the drawing scale, our results are almost indistinguishable from those obtained by Kielkopf [1]. Therefore, a priori, the same quality of adjustment is expected. The advantage of our results rests on that they were obtained on theoretical bases, whereas Kielkopf [1] has reached his results applying numerical arguments.

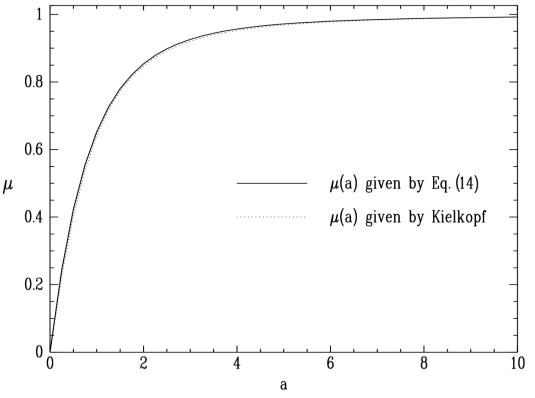

Fig. 2. μ as a function of a. $\mu(a)$ as it is obtained with Eq. (14) and $\mu(a)$ obtained empirically by Kielkopf.

We can test the quality of our fit by normalizing the deviation of $V(\mu_a, x)$ from the exact value
a) to the peak value, $V_a(0)$

$$\Delta_1 = \frac{V_a(x) - V(\mu_a, x)}{V_a(0)} \quad \text{or}$$

b) to the value at x, $V_a(x)$

$$\Delta_2 = \frac{V_a(x) - V(\mu_a, x)}{V_a(x)}.$$

It is important to point out that both, Kielkopf [1] and Liu et al. [2], have applied the criterion (a) to test their fit. They, as well us, have obtained $\Delta_1 \leq 1\%$. Using criterion (b), higher relative deviations are obtained.

Figures 3 and 4 display, as a function on x, Δ_1 and Δ_2, respectively. Both figures have been obtained assuming $a = 1$; for other a values the behavior is completely similar. As it is shown in these figures, our calculations as well as the Kielkopf [1] and Liu et al. [2] calculations, give, all of them, good and comparable fitting for $|x| \approx 4$–5. But, our fitting and Kielkopf [1] fitting are both better than that of Liu et al. [2] for $|x|$ values higher than ≈ 5, as it is clear from Fig. 4. Our adjustment is usually better than Kielkopf's [1] for $|x|$ values lower than ≈ 5, as it is seen in the figures. A correction factor introduced by Kielkopf [1] for $|x| \gtrsim 5$ allows the author to get better results than ours in that range (we will do something similar in the second paper of this series).

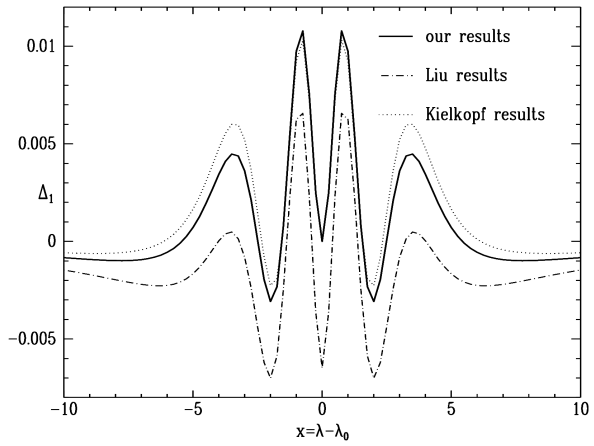

Fig. 3. Δ_1 as a function of x (see text).

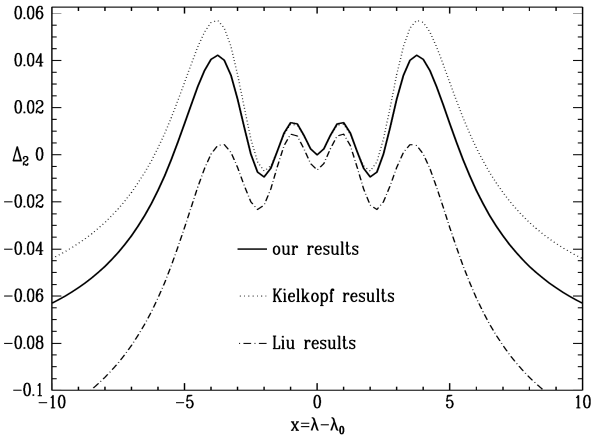

Fig. 4. Δ_2 as a function of x (see text).

Depending on the specific physical parameter we are interested on, criterium (a) or (b) will be suitable to test the goodness of our fit. Usually, criterium (a) is the right

choice if the optical thickness is calculated. To calculate other parameters instead, the parameter a for example, criterium (a) is not sufficient and criterium (b) has to be adopted. Indeed, Di Rocco et al. [3] have shown that, to reduce the difficulties caused by experimental noise, it is appropriate to normalize the area under the curve to the unit and consider the product

$$V_a(0)\gamma_{\mathrm{V}} = \frac{b_{1/2}(a)\,\mathrm{e}^{a^2}\,\Phi_{\mathrm{c}}(a)}{\sqrt{\pi}}$$

with Gaussian and Lorentzian limits 0.4697 and 0.3183, respectively.

In this paper, we do not intend to give a method to calculate $V(x)$ with a comparable accuracy to the numerical methods. This work gives, instead, an analytical base to the empirical approximations used by Kielkopf [1] and by Liu et al. [2], giving also an idea of their capabilities and limitations.

In order to show that the formula we have proposed is suitable for practical applications, we present an example. For a Voigt profile obtained assuming $w_{\mathrm{G}} = 1$ and $a = 1$, Eq. (15) gives us $\mu = 0.6525$. However, in fitting such a profile with the expression (4) (with a correlation coefficient $R^2 = 0.99993$), we obtain $\mu = 0.737$, which implies $a \approx 1.29$. Then, the relative error in a, is $\Delta a \approx 29\%$. Since the error in calculating the quotient $W_{\mathrm{G}}/W_{\mathrm{L}}$ verifies $\Delta(W_{\mathrm{G}}/W_{\mathrm{L}}) = \Delta W_{\mathrm{G}} + \Delta W_{\mathrm{L}}$, assuming that errors in calculating w_{G} and w_{L} are not very different from each other, the relative errors in calculating each of them are therefore about 15%. This enables us to say that our approximation correctly recovers the parameters of the Voigt function.

In short, raising our approximation in the form (4), based on the observation that the Voigt distribution is intermediate between the Gaussian and the Lorentzian distributions, and using the property of the normalization of the areas, we obtain a mathematical expression for μ as a function of a that deviates very little from that obtained previously by other authors, with the advantage of being theoretically justified.

However, we do not forget that in general μ depends not only on a but also on x. This will be addressed by us in the next paper of this series.

Acknowledgments

We wish to thank the Referees for their valuable suggestions that allowed us to significantly improve our article.

References

[1] J.L. Kielkopf, *J. Opt. Soc. Am.* **63**, 987 (1973).

[2] Y. Liu, J. Lin, G. Huang, Y. Guo, C. Duan, *J. Opt. Soc. Am. B* **18**, 666 (2001).

[3] H.O. Di Rocco, D.I. Iriarte, J.A. Pomarico, *Appl. Spectrosc.* **55**, 822 (2001).