NOTES AND CORRESPONDENCE

Comments on "A Common Misunderstanding about the Voigt Line Profile"

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ABSTRACT

In a recent paper, it was argued that some of the illustrations in popular textbooks comparing the Lorentz and Gaussian profiles with the "corresponding" Voigt profile are incorrect. These "misunderstandings" are shown to be a result of ambiguous specifications of the Voigt profile (i.e., there is no unique corresponding Voigt profile). Additionally, some comments on half-widths, numerics, and visualization are given.

1. Introduction

The convolution of a Lorentz and a Gauss profile, commonly known as the Voigt profile, is important in many branches of physics (e.g., atomic and molecular spectroscopy and atmospheric radiative transfer; Armstrong 1967). Basic definitions and properties are presented in many physics textbooks, and mathematical properties, relations to other special functions, and numerical methods are discussed in numerous papers. In a recent paper, Huang and Yung (2004) discussed "a common misunderstanding about the Voigt line profile." In this note we continue this discussion on some of the points raised in this paper.

2. Definitions

For the infrared and microwave spectral region, the combined effect of pressure (collision) broadening corresponding to a Lorentzian line shape

$$g_L(\nu - \hat{\nu}, \gamma_L) = \frac{\gamma_L/\pi}{(\nu - \hat{\nu})^2 + \gamma_L^2}, \qquad (1)$$

(with a half-width proportional to pressure, $\gamma_L \sim p$) and Doppler broadening corresponding to a Gaussian line shape

$$g_D(\nu - \hat{\nu}, \gamma_D) = \frac{1}{\gamma_D} \left(\frac{\ln 2}{\pi}\right)^{1/2} \exp\left[-\ln 2 \left(\frac{\nu - \hat{\nu}}{\gamma_D}\right)^2\right] \quad (2)$$

(with a half-width depending on line position $\hat{\nu}$ and temperature $\gamma_D \sim \hat{\nu}\sqrt{T}$) can be modeled by convolution (i.e., a Voigt line profile):

$$g_V(\nu - \hat{\nu}, \gamma_L, \gamma_D) \equiv g_L \otimes g_D$$
$$= \int_{-\infty}^{\infty} d\nu' g_L(\nu - \gamma; \gamma_L) \times g_D(\nu' - \hat{\nu}; \gamma_D). \qquad (3)$$

In the case of infrared spectroscopy, ν is the wavenumber (typically in units of inverse centimeters), although frequencies (in MHz or GHz) are more customary in the microwave regime; $\hat{\nu}$ denotes the line center position. Note that these profiles are normalized to 1; that is, $\int_{-\infty}^{\infty} g(\nu) \, d\nu = 1$.

It is convenient to define the Voigt function $K(x, y)$ normalized to $\sqrt{\pi}$,

$$g_V = \frac{1}{\gamma_D} \left(\frac{\ln 2}{\pi}\right)^{1/2} K(x,y), \qquad (4)$$

$$K(x,y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{(x - t)^2 + y^2} dt, \qquad (5)$$

where $K(x, y)$ is the real part of the complex error function (Abramowitz and Stegun 1964)

$$w(z) \equiv K(x,y) + iL(x,y) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t} dt \quad \text{with} \quad z = x + iy$$
$$(6)$$

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and the dimensionless variables x and y are defined in terms of the distance from the center position, $\nu - \hat{\nu}$, and the Lorentzian and Gaussian half-widths γ_L and γ_D:

$$x = (\ln 2)^{1/2} \frac{\nu - \hat{\nu}}{\gamma_D} \quad \text{and} \quad y = (\ln 2)^{1/2} \frac{\gamma_L}{\gamma_D}. \quad (7)$$

3. Half-widths

For all profiles, a half-width at half-maximum (HWHM) defined by $g(\hat{\nu} \pm \gamma) = g\hat{\nu}/2$ has been used, whereas Huang and Yung (2004) use an $1/e$ half-width for the Gaussian profile:

$$\alpha_D = \gamma_D (\ln 2)^{-1/2} \quad (8)$$

but

$$\alpha_L \equiv \gamma_L. \quad (9)$$

Neglecting self-broadening, the half-width of the Lorentzian is given by

$$\gamma_L(p, T) = \gamma_{\text{ref}}^{(\text{air})} \left(\frac{p}{p_{\text{ref}}} \right) \left(\frac{T_{\text{ref}}}{T} \right)^n. \quad (10)$$

Typical air broadening half-widths for $p_{\text{ref}} = 1013.25$ hPa and $T_{\text{ref}} = 296$ K are on the order of about 0.1 cm^{-1}, with the exponent $n = 1/2$ according to simple kinetic theory [see, e.g., Table 6 in Rothman et al. (2003)—a discussion of the HITRAN 2000 database—for actual values]. The half-width of the Gaussian (2) is given by

$$\gamma_D = \hat{\nu} \left(\frac{2 \ln 2 \, kT}{mc^2} \right)^{1/2}. \quad (11)$$

For typical atmospheric molecules [$m \approx 36$ atomic mass units (amu)], one has $\gamma_D \approx 6 \times 10^{-8} \hat{\nu} \sqrt{T(\text{K})}$.

Several empirical approximations for the half-width of a Voigt line have been developed (Olivero and Longbothum 1977; see also Belafhal 2000; Zdunkowski et al. 2007). For the approximation

$$\gamma_V(\gamma_L, \gamma_D) = \frac{1}{2} [c_1 \gamma_L + (c_2 \gamma_L^2 + 4\gamma_D^2)^{1/2}]$$
$$\text{with} \quad c_1 = 1.0692, \ c_2 = 0.86639, \quad (12)$$

an accuracy of 0.02% has been specified; with $c_1 = c_2 = 1$ the accuracy is on the order of 1%. A comparison of Lorentzian, Gaussian, and Voigt half-widths for atmospheric conditions is given in Fig. 1. Although Huang and Yung do not specify units for frequencies (wavenumbers) and half-widths, it should be clear from this figure that half-widths of about 1 (used in their Figs. 2 and 3) are not realistic for infrared atmospheric spec-

troscopy with wavenumber units, whereas $\gamma_D \approx 1$ MHz is reasonable for lines around $\hat{\nu} \approx 1$ THz ≈ 33 cm^{-1}.

4. The Voigt profile for equal Lorentz and Gauss widths

Textbooks on atmospheric radiation (Liou 1980; Andrews et al. 1987; Goody and Yung 1995; Salby 1996; Thomas and Stamnes 1999; López-Puertas and Taylor 2001; Zdunkowski et al. 2007) introducing the Voigt profile frequently compare the Lorentz and Gauss profiles with the "corresponding" Voigt profile for equal half-widths. Huang and Yung (2004) argue that some of the figures illustrating these profiles are incorrect or misleading; in particular, they say that the "impression that, for Lorentz and Doppler profiles with the same half-widths, the corresponding Voigt profile is steeper than the Lorentz profile and flatter than the Doppler profile in the line core ... is found to be incorrect" (p. 1630).

Equation (5) clearly shows that the shape of the Voigt function K is essentially determined by the ratio of the widths; however, because of the horizontal and vertical scaling [cf. (7) and (4)], the shape of the Voigt profile g_V is determined by both γ_L and γ_D. As a consequence, the notion of a corresponding Voigt profile is ambiguous even for $y = 1$.

According to Eq. (12), the Voigt profile arising from the convolution of a Lorentzian and Gaussian with equal widths is indeed wider; that is, $\gamma_V > \gamma_L, \gamma_D$. However, the corresponding Voigt profile might just as well be defined by $\gamma_V = 1$. (In fact, a figure caption saying "The Lorentz, Doppler, and Voigt profiles with the same half-width" could easily be interpreted as g_L for $\gamma_L = 1$, g_D for $\gamma_D = 1$, and g_V for $\gamma_V = 1$). For $\alpha_L = \alpha_D$ or $y = 1.0$ this corresponds to $\alpha_L = 2/[1 + (1 + 4\ln 2)^{1/2}] = 0.6797$, whereas for $\gamma_L = \gamma_D$ or $y = (\ln 2)^{1/2}$ this corresponds to $\gamma_L = 2/(1 + 5^{1/2}) = 0.6180$. A comparison of these profiles shown in Fig. 2 also indicates that—in contrast to Huang and Yung's expectations—in the line wings the Voigt profile can be intermediate between those of the Lorentz and Doppler profiles.

These findings can be easily checked using the values at the line center (cf. Table 1):

$$g_V(\nu = \hat{\nu}, \gamma_L, \gamma_D) = \frac{1}{\gamma_D} \left(\frac{\ln 2}{\pi} \right)^{1/2} K(0, y)$$

$$= \frac{1}{\gamma_D} \left(\frac{\ln 2}{\pi} \right)^{1/2} \text{erfce}(y), \quad (13)$$

$$g_D(\nu = \hat{\nu}, \gamma_D) = \frac{1}{\gamma_D} \left(\frac{\ln 2}{\pi} \right)^{1/2}, \quad (14)$$
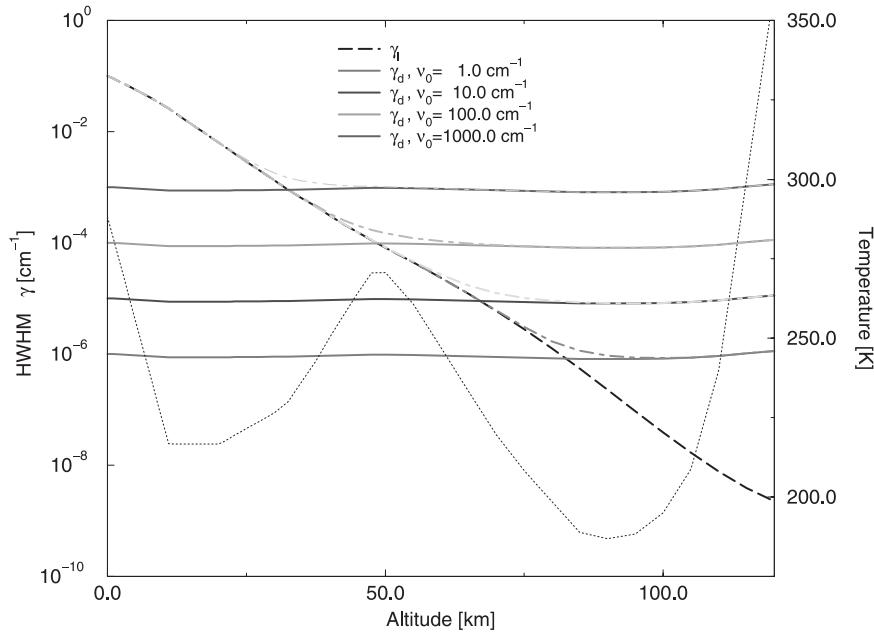
FIG. 1. Half-widths for Lorentz, Gauss, and Voigt profiles as a funtion of altitude for a variety of line positions ν. The dotted line indicates atmospheric temperature. (Pressure and temperature based on the U.S. Standard Atmosphere model; molecular mass 36 amu.)

$$g_L(\nu = \hat{\nu}, \gamma_L) = \frac{1}{\pi \gamma_L}. \tag{15}$$

Because of $\mathrm{erfce}(y) \equiv e^{y^2} \, \mathrm{erfc}(y) \leq 1$, it follows that $g_V(\nu = \hat{\nu}, \gamma_L, \gamma_D) \leq g_D(\nu = \hat{\nu}, \gamma_D)$. Furthermore, $e^{y^2} \, \mathrm{erfc}(y) \approx \pi^{-1/2}/y$ for $y \gg 1$. Note that the exponentially scaled error function is decreasing monotonically with y.

5. Numerics

Huang and Yung (2004, 1630–1631) verify their arguments by "numerically computing the Voigt profile ... with the approximate formula given by Humliček (1982); they also "calculate the Voigt profile by numerical integration ... using the trapezoidal rule." The
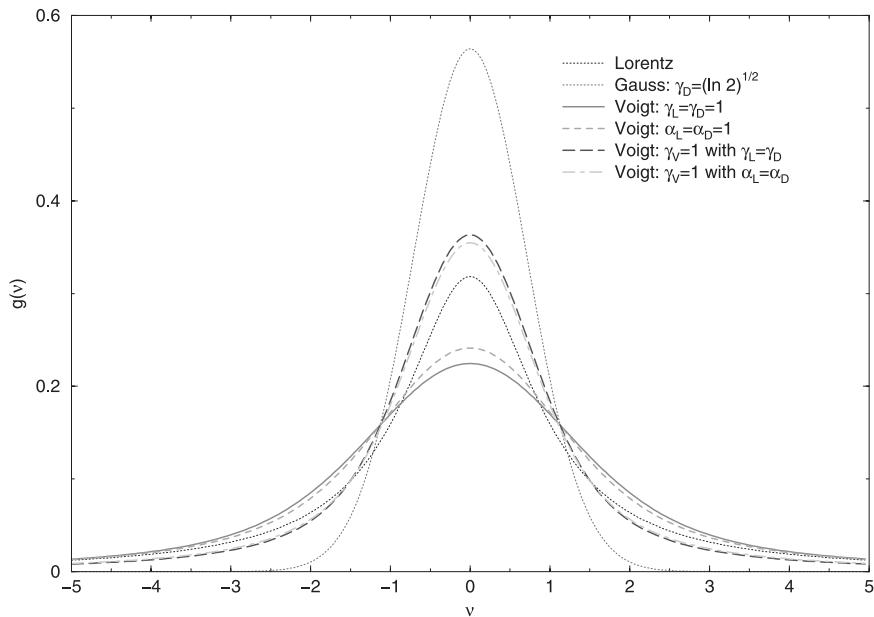

FIG. 2. Lorentz and Gauss profiles with unit half widths compared with corresponding Voigt profiles.

TABLE 1. A comparison of "corresponding" Voigt profiles. In the last three rows, values for the limiting cases of Lorentz and Gaussian line profiles are given. [The Voigt profile center values in the last column have been obtained using the Weideman (1994) algorithm for the Voigt function. Using the rational approximation (7.1.25) of Abramowitz and Stegun (1964) gives erfce(1.) = 0.427 44 and erfce ($\sqrt{\ln 2}$) = 0.478 02].

γ_L	γ_D	γ_V	y	$g_V(0)$
1.0	1.0	$\dfrac{1 + \sqrt{5}}{2}$	$\sqrt{\ln 2}$	0.224 56
$1/\sqrt{\ln 2}$	1.0	$\dfrac{1 + \sqrt{1 + 4\ln 2}}{2\sqrt{\ln 2}}$	1.0	0.200 84
1.0	$\sqrt{\ln 2}$	$\dfrac{1 + \sqrt{1 + 4\ln 2}}{2}$	1.0	0.241 24
$\dfrac{2}{1 + \sqrt{5}}$	$\dfrac{2}{1 + \sqrt{5}}$		1.0	$\sqrt{\ln 2}$ 0.363 34
$\dfrac{2}{1 + \sqrt{1 + 4\ln 2}}$	$\dfrac{2\sqrt{\ln 2}}{1 + \sqrt{1 + 4\ln 2}}$		1.0	1.0 0.354 90
1.0				0.318 31
	1.0			0.469 72
	$\sqrt{\ln 2}$			0.564 19

stated difference of the two approaches is less than 0.05% and corresponds to the accuracy claimed by Humliček.

It should be emphasized that the integrals (3) and (5) cannot be solved analytically; that is, numerical approximations have to be used. However, a direct evaluation of the integral (3) by numerical quadrature (Trapez, Gauss-Hermite, etc.) cannot be recommended in general and is only justified numerically for $y \gtrsim 1$.

Numerous algorithms have been developed for the Voigt function (5) [cf. the review of Armstrong (1967) or the comparisons by Twitty et al. (1980), Klim (1981), Schreier (1992), and Thompson (1993)]. Most modern algorithms evaluate the complex error function (6); in particular, rational approximations (Ralston and Rabinowitz 2001) have been proven to be an efficient and accurate approach (e.g., Hui et al. 1978; Humliček 1979, 1982; Weideman 1994). Further optimizations of the Hui et al. and Humliček algorithms have been presented by Schreier (1992), Shippony and Read (1993, 2003), Kuntz (1997), Ruyten (2004), Wells (1999), and Schreier and Kohlert (2008).

6. Choice of abscissa

For graphical illustrations of the line profiles, Huang and Yung (2004) as well as some of the cited textbooks use wavenumber or frequency scaled by the Gaussian width as the abscissa. Clearly, usage of x [Eq. (7)] is convenient from a mathematical point of view [cf. (5)].

However, from a physics point of view (emphasized by Huang and Yung), wavenumber or frequency is relevant, for example for the transmission $\mathcal{T}(\nu)$. Furthermore, dividing the independent variable by a constant without multiplying the dependent variable simultaneously destroys the normalization properties.

7. Summary and conclusions

The concerns of Huang and Yung (2004) about incorrect interpretations of the Voigt line profile in popular textbooks on atmospheric physics have been discussed. The reason for these supposed misinterpretations have been demonstrated to be due to imprecise usage of the half-width parameters. In comparisons with the Lorentz and Gaussian profiles, the notion of a "corrresponding" Voigt profile has been shown to be ambiguous.

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CORRIGENDUM

Several press errors appeared in "Comments on 'A Common Misunderstanding about the Voigt Line Profile'" by Franz Schreier, which was published in the *Journal of the Atmospheric Sciences,* Vol. 66, No. 6, 1860–1864. Equation (3) should read

$$g_V(\nu - \hat{\nu}, \gamma_L, \gamma_D) \equiv g_L \otimes g_D$$

$$= \int_{-\infty}^{\infty} d\nu' \, g_L(\nu - \nu', \gamma_L) \times g_D(\nu' - \hat{\nu}, \gamma_D). \quad (3)$$

The definition of half widths given at the beginning of section 3 should be $g(\hat{\nu} \pm \gamma) = g(\hat{\nu})/2$. The numerical estimate for the Gaussian half-width given after Eq. (11) should be $\gamma_D \approx 6 \times 10^{-8} \hat{\nu} \sqrt{T}$ with line position $\hat{\nu}$ in cm^{-1} and temperature T in kelvins.

Furthermore, the two figures were printed in black and white instead of color. They appear below as they were meant to appear originally.
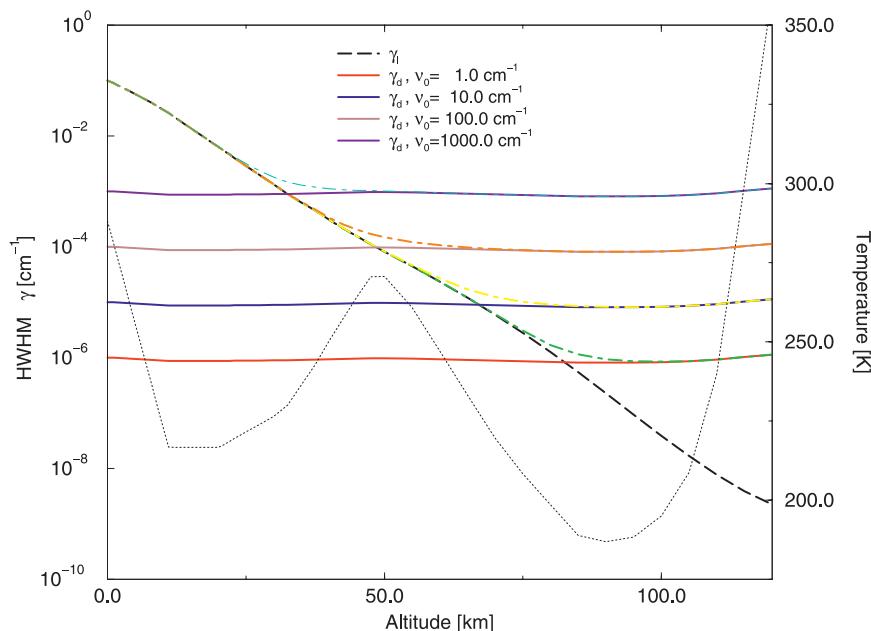
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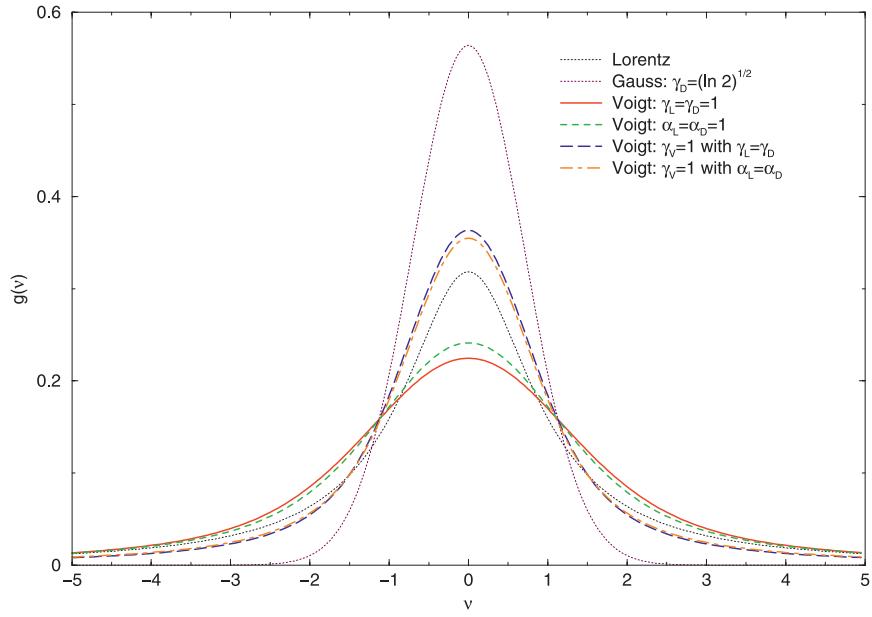
FIG. 2. Lorentz and Gauss profiles with unit half-widths compared with the corresponding Voigt profiles.