A Common Misunderstanding about the Voigt Line Profile

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ABSTRACT

In this short note, a misinterpretation of the Voigt line profile is pointed out, which is in several popular textbooks of atmospheric physics. The correct interpretation is given based on mathematical and physical arguments, as well as numerical verification.

The Voigt profile is an important model in molecular spectroscopy and radiative transfer. The Voigt profile describes the combined effect of the Doppler broadening and the pressure broadening and is particularly important in the cases when the Doppler half-width is comparable to the Lorentz half-width. Figure 1 is a plot illustrating the concept of the Voigt profile found in several popular textbooks, such as Fig. 2.9 in *Middle Atmospheric Dynamics* by Andrews et al. (1987, p. 40), Fig. 8.16 in *Introduction to Atmospheric Physics* by Salby (1996, p. 223), and Fig. 3.2 in *Radiative Transfer in the Atmosphere and Ocean* by Thomas and Stamnes (1999, p. 67). Their figures give an 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. In the line wings the Voigt profile is intermediate between those of the Lorentz and Doppler profiles. Figure 1 appears to be reasonable, but after careful examination is found to be incorrect. We also note that in a recently published book, *An Introduction to Atmospheric Physics* by Andrews (2000), there is a figure (Fig. 3.11 in Andrews 2000, p. 73) similar to Fig. 1 but with a different figure caption: ''The Lorentz, Doppler and Voigt profiles with the same half width.'' Given this figure caption, the Voigt profile is correctly plotted in this figure (Fig. 3.11 in Andrews 2000).

The normalized Voigt profile (''normalized'' here means that the area beneath this profile is unity) can be written as

$$f(x) = \frac{\alpha_L}{\alpha_D^2}\frac{1}{\pi^{3/2}}\int_{-\infty}^{+\infty}\frac{e^{-y^2}\,dy}{(x-y)^2+\left(\frac{\alpha_L}{\alpha_D}\right)^2}, \qquad (1)$$

where α_L is the half-width for pressure broadening, α_D is the half-width for Doppler broadening, and $x \equiv (\upsilon - \upsilon_0)/\alpha_D$ with υ_0 being the frequency of the line center. In fact, the normalized Voigt line is just the convolution of the normalized Lorentz profile and the normalized Doppler profile:

$$f(\upsilon) = f_L(\upsilon) \otimes f_D(\upsilon) = \frac{\alpha_L}{\pi}\frac{1}{(\upsilon-\upsilon_0)^2+\alpha_L^2} \otimes \frac{1}{\alpha_D\sqrt{\pi}}\exp\left[-\left(\frac{\upsilon-\upsilon_0}{\alpha_D}\right)^2\right], \qquad (2)$$

where $f_L(\upsilon)$ and $f_D(\upsilon)$ are the normalized Lorentz profile and Doppler profile, respectively. If we look at the line center, $f(\upsilon_0)$ is the weighted average of Lorentz profile over all the frequencies and the weighting factor is the corresponding Doppler profile at each frequency. Since the maximum of the Lorentz profile is at the line center, the weighted average must be smaller than this maximum. This implies that the peak of the normalized Voigt profile should be lower than the peak of the normalized Lorentz profile. Using a similar argument and the fact that the Lorentz profile is monotonically decreasing from the line center to the line wings, we can infer that $f(\upsilon)$ should be smaller than $f_L(\upsilon)$ when υ is near the line center, and larger than $f_L(\upsilon)$ when υ is at the line wings. This is different from the plot in Fig. 1.

This argument can be verified by numerically computing the Voigt profile. Figure 2 shows the normalized

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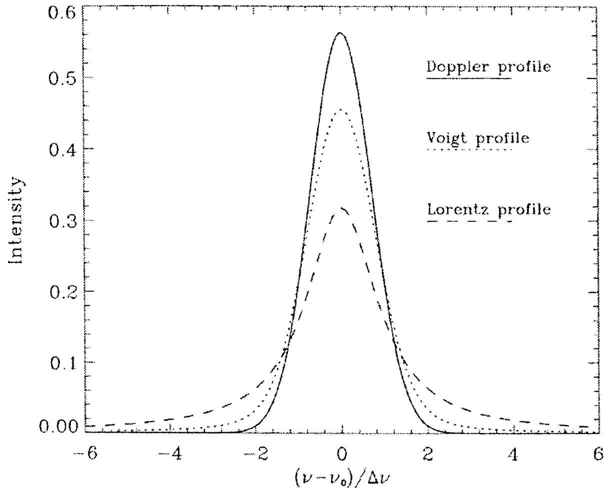

FIG. 1. This is Fig. 3.2 in *Radiative Transfer in the Atmosphere and Ocean* by Thomas and Stamnes (1999). The figure caption reads "Comparison of normalized Lorentz, Voigt and Doppler profiles versus $x = (v - v_0)\Delta v$. Δv is the Doppler width α_D for both Doppler broadening and Voigt broadening and is the Lorentz width α_L for Lorentz broadening. $\alpha = \alpha_L/\alpha_D = 1$ was used for the Voigt profile." (Thomas and Stamnes 1999, reproduced with permission of Cambridge University Press).

Voigt, Lorentz, and Doppler profiles when the Doppler half-width is the same as the Lorentz half-width, the same conditions described for Fig. 1. The Voigt profile is calculated with the approximate formula given by Humlicek (1982). We also calculate the Voigt profile by numerical integration of Eq. (1) from $y = -200$ to $y = 200$ using the trapezoidal rule with interval $\Delta y = 10^{-4}$. The difference between these two calculations is less than 0.05%. From Fig. 2 it can be seen, as described earlier, that the normalized Voigt profile is smaller than the corresponding normalized Lorentz profile in the line core, and larger than the Lorentz profile in the line wings. In the far wings, $f(v)$ is still larger than $f_L(v)$ but the difference is very small. This is because the Doppler profile decreases exponentially away from the center. As a result, the contribution of the line core region to the far wings is very small in this convolution. Therefore, the normalized Voigt profile is flatter than the corresponding normalized Lorentz profile, in contrast to what has been described in the aforementioned textbooks.

From the point of view of physics, the Voigt profile is derived assuming that the pressure broadening and the Doppler broadening are independent of each other. With this assumption, in the time domain the combined effect is simply multiplying the two effects together, and in the frequency domain it is the convolution of the two effects. Therefore, compared with pressure broadening alone, taking Doppler broadening into account would make the profile even broader. Since all line profiles are normalized, the Voigt profile must be flatter than both the corresponding Lorentz and Doppler profiles. Relative to the Voigt profile, the corresponding

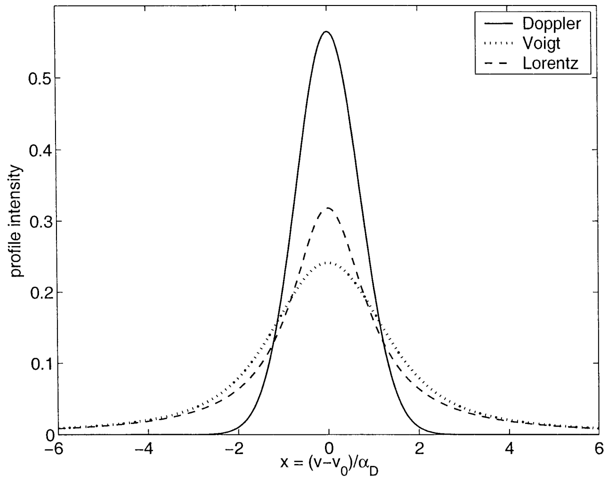

FIG. 2. The Lorentz profile (dashed line) and the Doppler profile (solid line) with the same half-widths ($\alpha_L = \alpha_D = 1$). The dotted line is the corresponding Voigt profile. Here, x is defined as $x \equiv (v - v_0)/\alpha_D$.

Doppler and Lorentz profiles both underestimate the absorption coefficient in the line wings and overestimate it in the line core, as shown in Fig. 2.

Figure 3 shows two cases where the half-width of the Lorentz profile is different from the half-width of the Doppler profile. When α_D is 3 times larger than α_L, the corresponding Voigt profile is significantly different

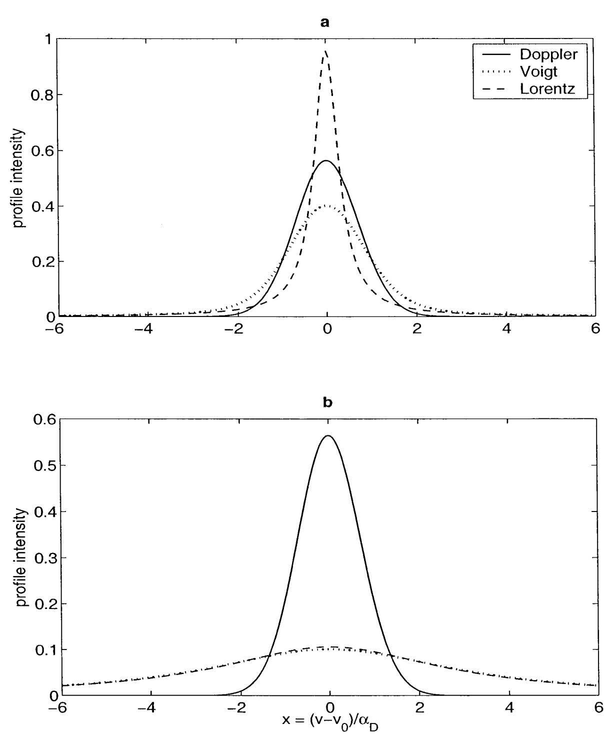

FIG. 3. (a) The Lorentz profile (dashed line) with half-width $\alpha_L = 1/3$, and the Doppler (solid line) with half-width $\alpha_D = 1$. The dotted line is the corresponding Voigt profile. Here, x is defined as $x \equiv (v - v_0)/\alpha_D$. (b) Same as (a), except $\alpha_L = 3$.

from both profiles as shown in Fig. 3a. Inside the full-width of half-maximum (FWHM) of the Doppler profile, the maximum percentage difference between the Doppler profile and the corresponding Voigt profile is 29%. The percentage difference outside the FWHM of the Doppler profile is even larger because of the exponential decay of the Doppler profile. Compared to the Voigt profile, the Doppler profile underestimates the absorption coefficient in the line wings and overestimates the absorption coefficient in the line core. When α_L is 3 times larger than α_D, the corresponding Voigt profile is very close to the Lorentz profile as shown in Fig. 3b, although the Lorentz profile underestimates the absorption coefficient in the line wings and overestimates the absorption coefficient in the line core. The maximum percentage difference between the Lorentz profile and the corresponding Voigt profile inside the FWHM of the Lorentz profile is 4.8%; outside the FWHM of the Lorentz profile, the maximum percentage difference is 3.1%. Therefore, when α_L is a few times larger than α_D, the Lorentz profile would be a reasonable approximation of the corresponding Voigt profile. If α_L is a few times smaller than α_D, neither the Lorentz profile nor the Doppler profile can be a good approximation for the corresponding Voigt profile.

In summary, as far as the understanding of the Voigt profile is concerned, the plots like Fig. 1 can easily mislead the readers. The combined effects of pressure broadening and Doppler broadening will make the Voigt profile broader than the corresponding Lorentz and Doppler profiles.

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