AN EMPIRICAL APPROXIMATION TO THE VOIGT PROFILE

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Abstract—A closed-form approximation to the Voigt profile is developed from an examination of Voigt profile calculations. This approximation matches the Voigt profile within 5 per cent at worst and is generally within 3 per cent or less. In radiant energy transport calculations this approximation is shown to closely reproduce the curves of growth given by use of the Voigt profile expression.

INTRODUCTION

THE WELL-KNOWN Voigt profile is an often-used approximation to the thin-gas intensity distribution within an atomic line or a molecular rotational line when both thermal broadening and broadening due to natural, pressure, and Stark mechanisms are encountered. The exact Voigt profile\(^{(1)}\) can be expressed in wavelength terms as

\[
I_{\lambda} = \frac{2}{\pi} \frac{\lambda_q}{w_1} I_{\lambda q} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{2.772 \lambda_q^2 (v/c)^2}{w_q^2 (c)}\right]}{1 + \frac{4}{w_1^2} \left[\lambda_q - \lambda (v/c)\right]^2} \, dv \, d\lambda
\]

where most of the symbols are defined in Fig. 1, and \(I_{\lambda q}\) is a fictitious peak line intensity corresponding to pure thermal broadening, \(c\) is the speed of light, and \(v\) is integrated over all molecular velocities that may contribute to the line intensity at \(\lambda\).
The application of the exact Voigt profile to radiation computations, such as computing a synthetic spectrum or computing energy transport through a radiating gas, requires that the integral in equation (1) be evaluated at every wavelength. This is a very difficult and time-consuming task. To facilitate the use of this expression, several tables of \( I_\lambda \) of high accuracy have been compiled. However, even with these tables the use of the exact Voigt profile is a time-consuming process for extensive computations. This fact discourages the use of the Voigt profile and recourse is often made to the less accurate Gaussian or Lorentzian line profile expressions, which can be written in closed form. For convenience and later reference these expressions are listed below.

**Gaussian profile**

\[
I_\lambda = I_{\lambda_0} \exp \left(-2.772(\lambda - \lambda_0)^2/w_0^2\right). \tag{2}
\]

**Lorentzian profile**

\[
I_\lambda = \frac{1}{1 + 4(\lambda - \lambda_0/w_0)^2} \tag{3}
\]

Other more accurate approximations to the Voigt profile are discussed in Refs. 1 and 5. However, most of these approximations are limited to special regions of applicability or are themselves complex expressions.

The above discussion indicates a need for a simple closed-form approximation to the Voigt profile that is valid over a useful range of parameters and yields reasonably accurate results. The purpose of this paper is to discuss an empirical approximation that meets these criteria. The resulting expression matches the exact Voigt profile within 5 per cent at worst and is generally within 3 per cent or less and reproduces the curve-of-growth with adequate accuracy.

**DEVELOPMENT OF APPROXIMATION**

The analysis is based primarily on the numerical computations tabulated by Posener in Ref. 2. The correspondence between his notation and that used herein is given below:

<table>
<thead>
<tr>
<th>This paper</th>
<th>Ref. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intensity at line center</td>
<td>( I_{\lambda_0} )</td>
</tr>
<tr>
<td>Normalized line intensity</td>
<td>( I_\lambda/I_{\lambda_0} )</td>
</tr>
<tr>
<td>Normalized wavelength</td>
<td>( (\lambda - \lambda_0)/w_v )</td>
</tr>
<tr>
<td>Lorentz width at half-height</td>
<td>( w_l )</td>
</tr>
<tr>
<td>Gauss width at half-height</td>
<td>( w_g )</td>
</tr>
<tr>
<td>Voigt width at half-height</td>
<td>( w_v )</td>
</tr>
<tr>
<td>Ratio of Lorentz width to Voigt width</td>
<td>( w_l/w_v )</td>
</tr>
</tbody>
</table>

The basis of the approximation was found by plotting \( I_\lambda/I_{\lambda_0} \) from Ref. 2 as a function of \( w_l/w_v \) for various values of \( (\lambda - \lambda_0)/w_v \). Representative curves from these plots are shown in Fig. 2. Clearly, \( I_\lambda/I_{\lambda_0} \) varies nearly linearly with \( w_l/w_v \) from the Gaussian value \((w_l/w_v = 0)\) to the Lorentzian value \((w_l/w_v = 1.0)\).
The nearly linear behavior of $I_\lambda/I_{\lambda Q}$ with $w_\lambda/w_\nu$ suggests that the Voigt profile should be reasonably approximated by

$$I_\lambda/I_{\lambda Q} = \left[1 - \frac{w_\lambda}{w_\nu}\right] \exp\left[-2\cdot772\left(\frac{\lambda - \lambda Q}{w_\nu}\right)^2\right] + \left[\frac{w_\lambda}{w_\nu}\right]\frac{1}{1 + 4(\lambda - \lambda Q/w_\nu)^2}.$$  

(4)

Note that the Voigt line width, $w_\nu$, is used in both the Gaussian and Lorentzian terms. When $w_\lambda/w_\nu = 0$, equation (4) reduces to the Gaussian profile and when $w_\lambda/w_\nu = 1$, it reduces to the Lorentzian profile. Hence, this approximate expression is exact at those limits. It is also exact when $(\lambda - \lambda Q)/w_\nu = 0$ and $1/4$. For the remainder of this report equation (4) is identified as the first approximation. Its accuracy is demonstrated in Fig. 3, by comparison with the numerical computations for the exact Voigt profile from Ref. 2.

Dashed lines are used when the number of significant digits in Ref. 2 is limited and the curves are uncertain.

Generally the accuracy of the first approximation is reasonable except in the far wings of the line profile near the Gaussian limit. A large percentage error is present in this region.
but the absolute error, as indicated in Fig. 2, is quite small. Therefore, the usefulness of the
first approximation depends on the particular application intended. For those applications
requiring high percentage accuracy in the far wings a more accurate approximation is
needed.

A second approximation to give better accuracy in the far wings was developed by
correcting for most of the error in the first approximation at \( w_l/w_v = 0.5 \) and applying a
quadratic variation of this correction between the end points \( w_l/w_v = 0 \) and \( w_l/w_v = 1.0 \).
The second approximation is given by

\[
\frac{I_\lambda}{I_{\lambda t}} = \left[1 - \frac{w_l}{w_v}\right] \exp\left[-2.772\left(\frac{\lambda - \lambda_q}{w_v}\right)^2\right] + \left[\frac{w_l}{w_v}\right] \frac{1}{1 + 4(\lambda - \lambda_q/w_v)^2}
+ 0.016 \left[1 - \frac{w_l}{w_v}\right] \left[\frac{w_l}{w_v}\right] \left\{\exp\left[-0.4\left(\frac{\lambda - \lambda_q}{w_v}\right)^2\right] - \frac{10}{10 + (\lambda - \lambda_q/w_v)^2}\right\}.
\]

The accuracy of the second approximation is shown in Fig. 4. This approximation is
also exact for either pure Gaussian or pure Lorentzian profiles and is nearly exact when

\[\frac{\lambda - \lambda_q}{w_v} = 0 \text{ and } \frac{1}{2}. \]

The accuracy has been examined extensively out to \((\lambda - \lambda_q)/w_v = 10\) (the limit of the values given in Ref. 2) and the extreme values shown in Fig. 4, -5 and
+2.5 per cent, are maximum errors.

To gain a better feeling for the accuracy of the first and second approximations, a plot
of some representative line profiles is given in Fig. 5. The lower curve is the pure Gaussian
profile and the upper curve is the pure Lorentzian profile. Two intermediate cases at \( w_l/w_v \)
of 0.11 and 0.5, selected from Fig. 4 to illustrate nearly maximum errors, are also shown.
As noted above, the first approximation is somewhat high in the far wings whereas the
second approximation matches the exact Voigt profile very closely.

A more meaningful test of these approximations, for many applications involving
radiant energy transport, is the accuracy with which the curves-of-growth can be repro-
duced. Curve-of-growth calculations using the exact Voigt profile have been made by
several persons and a convenient plot is given in Fig. 4–6 of Ref. 1. For comparison pur-
poses that figure is reproduced herein in Fig. 6. Also shown in Fig. 6 are curve-of-growth

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**Fig. 4. Accuracy of second approximation to Voigt profile.**
An empirical approximation to the Voigt profile

FIG. 5. Comparison of first and second approximations to exact Voigt profile from Ref. 2.

FIG. 6. Comparison of curves-of-growth computed from first and second approximations with those computed from exact Voigt profile. (Notation from Ref. 1.)

computed using the first and second approximations. The lower curve \((a = 0)\) is for a pure Gaussian profile and the upper curve \((a = 10)\) is for an almost purely Lorentzian profile \((a \to \infty)\). As expected, at these limits both the first and second approximations agree almost precisely with the result for the exact Voigt profile. The comparison for intermediate curves is not as close, but even here the second approximation gives nearly exact results, and the first approximation has a maximum error of only about 20 per cent.

An additional point of interest is that the approximations were developed from calculations that only extended 10 times \(w_e\) from the line center, whereas the calculations shown in Fig. 6 were carried out much further. For example, the highest point on the curve for \(a = 0.5\) was carried out to 3240 times \(w_e\).

The above comparisons demonstrate that the normalized Voigt profile is reasonably represented by equation (5). However, to be useful in computations \(w_e\) and \(I_{\lambda B}^e\) must also be specified. \(w_e\) is of course related to \(w_t\) and \(w_l\) and if these line widths are known, \(w_e\) can be found. The following simple approximation to \(w_e\) was found by fitting the plotted results
The accuracy of this equation is shown in Fig. 7 (lower curve) to be about 1 per cent. Equation (6) is a more accurate expression than the approximations listed in Ref. 2.

Again, on the basis of the plotted values in Ref. 3, the following equation was found for $I_{\lambda q}$.

$$I_{\lambda q} = \frac{I}{w'_v[1.065 + 0.447(w'_v/w_v) + 0.058(w'_v/w_v)^2]}$$  \hspace{1cm} (7)

where $I$ is the integrated line intensity (see Fig. 1). Expressions for $I$ can be found in several texts, for example, Refs. 6 and 7. The accuracy of equation (7) is also shown in Fig. 7. Clearly the small error in equation (7) is produced almost entirely by the error in $w_v$. From this figure it is obvious that a quadratic correction term applied to the equation for $w_v$ would make both $w_v$ and $I_{\lambda q}$ nearly exact. However, the present accuracy seems sufficient considering the error present in $I/w_{\lambda q}$.

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REFERENCES