High-accuracy approximation of the Voigt function based on Fourier expansion of exponential multiplier

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Abstract A rapidly convergent series, based on Fourier expansion of the exponential multiplier, is presented for highly accurate approximation of the Voigt function (VF). The computational test reveals that with only the first 33 terms Fourier expansion of the exponential multiplier, this approximation provides accuracy better than $5.5383 \times 10^{-19}$ in the domain of practical interest $0 < x < 40,000$ and $10^{-4} < y < 10^{2}$ that is needed for applications using the HITRAN molecular spectroscopic database. Compared with the typical approximation algorithms, the proposed approximation still available even if $y$ is very small and the accuracy in the narrow band domain $0 < x < 40,000 \cap 10^{-10} < y < 10^{-4}$ remains high and better than $5.5385 \times 10^{-13}$.

Key words Voigt function, Fourier series, High-accuracy approximation, Boundary-free

1. Introduction

The Voigt function (VF) describes emission and absorption properties of the gas molecules in the atmosphere, and, consequently, it is widely used in many scientific disciplines\cite{1-4}. Mathematically, the VF can be expressed in terms of the real part of the Faddeeva function or complex error function

$$w(z) = \exp(-z^2)\text{erfc}(-iz), \quad (1)$$

where $z = x + iy$ and $y > 0$. In common representation, the VF is given by the following integral

$$K(x, y) = \frac{1}{\pi} \int_{0}^{\infty} \exp(-t^2) \exp(-t^2) \cos(\alpha t) dt, \quad (2)$$

where $y = \sqrt{2} \alpha_L / \alpha_G$, $x = \sqrt{2}(v - v_0)/\alpha_G$, $v$ is the frequency spanning from the line center $v_0$, $\alpha_L$ and $\alpha_G$ are Lorentz and Doppler HWHM, respectively.

Applying the Fourier transform, the Eq. (2) can be rewritten in the following form\cite{45}

$$K(x, y) = \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} \exp(-z^2) \exp(-yt) \cos(zt) dt. \quad (3)$$

None of the integrals above have analytical solutions, thus many modern “state-of-the-art” algorithms for evaluating the VF utilizing sophisticated numerical techniques have been discussed in numerous papers. An efficient algorithm on the basis of a modified Humlicek algorithm\cite{6} was developed by Wells\cite{7} with relative error chosen between $10^{-2}$ and $10^{-5}$. Although the Wells algorithm is sufficient for the most practical tasks, the more accurate calculation of the VF may also be required.

Recently, Abrarov et al.\cite{8-10} proposed two similar algorithms based on exponential series approximation for the rapid and high-accuracy calculation of the VF. Abrarov algorithm I\cite{8-9} which based on Fourier expansion of the exponential multiplier is more accurate than $10^{-9}$ in the Humlicek regions 3 and 4\cite{6}. Abrarov algorithm II\cite{10} which based on rational approximation of the exponential multiplier provides accuracy better than $10^{-9}$ over a wide domain of practical interest for applications using the HITRAN molecular spectroscopic database. However
the accuracy of Abrarov algorithm I or II deteriorates further with decreasing \( y \). Different approaches have been implemented to overcome this problem\[5\]. For example, the Chiarella and Reichel approximation (equation (15) in \[11\]), the Weideman’s rational approximation (equation (38-I) in \[12\]), the exponential series approximation (equation (14) in \[13\]) and the rational approximation (equation (14) in \[10\]) that provide highly accurate and rapid calculation for the VF within narrow band domain \( 0 \leq x \leq 15 \) and \( 10^{-6} \leq y \leq 15 \). However the accuracy of these algorithms deteriorates significantly while \( y \) is small than \( 10^{-6} \). Abrarov and Quine\[14\] presented two approximations for the VF with small \( y \) (\( y \leq 10^{-6} \)), however these two approximations need to calculate Dawson’s integral which has no analytical solution. Therefore, The highly accurate and simultaneously rapid computation of VF at \( 0 < y << 1 \) still remains problematic\[15\] and the high-accuracy approximation with boundary-free may also be required.

In this work we propose a new approximation for the VF based on the Fourier expansion of the exponential multiplier for efficient computation and the availability of the algorithm over a wide domain \((10^{-4} \leq x \leq 40,000 \) and \(10^{-10} \leq y \leq 10^2\)\) is verified by computational test. This algorithm is based on elementary functions that are freely available in a standard library of most programming languages. We applied MATLAB R2014a supporting array programming features. A typical desktop computer Intel(R) Quad CPU with RAM 4.00 GB was utilized.

2. Approximation methods

2.1 Truncation approximation of the Voigt function

In the Abrarov algorithm II, the upper integration limit \( \infty \) in Eq. (3) was replaced by \( T \) as sufficient for high-accuracy calculation since the exponential multiplier decays very rapidly with increasing \( t \). Here we discuss the error caused by this truncation through numerical calculation in detail.

The truncation approximation of the VF is defined as

\[
K_T(x, y) = \frac{1}{\sqrt{\pi}} \int_0^T \exp\left(-\frac{t^2}{4}\right) \exp(-yt) \cos(\pi t) dt,
\]

(4)

(where \( T \) is a real number), with a relative error given by

\[
\Delta_T = \left| \frac{K_T(x, y) - K(x, y)}{K(x, y)} \right|.
\]

Fig. 1 show the logarithm relative error \( \log_{10}\Delta_T \) of the truncation approximation in the domain \( 0 \leq x \leq 15 \) and \( 10^{-10} \leq y \leq 15 \) (this domain is the most difficult for rapid and accurate computation of the VF, Ref\[10\]) at \( T = 10, 12, 14, \) and \( 16 \) respectively.
Fig. 1. Contour plot of $\log_{10} \Delta T$ for domain $0 \leq x \leq 15$ and $10^{-10} \leq y \leq 15$ at (a) $T = 10$, (b) $T = 12$, (c) $T = 14$ and (d) $T = 16$ respectively. The parameter $y$ is using logarithmic axes.

As we can see from Fig. 1a, the relative error of the truncation approximation is less than $10^{-5}$ in the region $y \geq 10^4$ and the relative error increases rapidly to 0.25 with decreasing $y$ at $T = 10$. Figs. 1b, 1c and 1d illustrate that the maximum relative error is decreases significantly with the increase of $T$. For example, the maximum relative error still less than $10^{-17}$ even if $y$ is very small ($y \geq 10^{-10}$) at $T = 16$.

2.2 Approximation of exponential multiplier in arbitrary interval

The exponential multiplier $\exp(-1/4t^2)$ can be approximated by Fourier series within a certain integration domain $[-\tau, \tau]$ as

$$\exp(-\frac{t^2}{4}) \approx \sum_{n=0}^{N} a_n \cos\left(\frac{\pi n}{\tau}t\right),$$

(6)

with a relative error given by

$$\delta(t) = \left|\exp(-\frac{t^2}{4}) - \sum_{n=0}^{N} a_n \cos\left(\frac{\pi n}{\tau}t\right)\right| / \exp(-\frac{t^2}{4}).$$

(7)

where the corresponding expansion coefficients are

$$a_n = \frac{1}{(1 + \delta_0)\tau} \int_{-\tau}^{\tau} \exp(-\frac{1}{2}t^2) \cos\left(\frac{\pi n}{\tau}t\right) dt.$$  

(8)

Fig. 2. The relative error $\delta(t)$ at $N = 23$ within the integration domain $t \in [0, \tau]$, where $\tau = 12$. 
Fig. 2 illustrates the relative error $\delta(t)$ at $N = 23$ within the integration domain $t \in [0, \tau]$, where $\tau = 12$. As we can see the accuracy of Eq. (6) is better than $10^{-16}$ in the smaller domain $t \in [0, 4]$, however the accuracy deteriorates further with decreasing $y$. This fact explains that the accuracy of Abrarov algorithm I is two orders lower than the truncation approximation ($T = 12$) of the VF.

In order to achieve the high accuracy of the exponential multiplier in a larger interval, the number of terms of Eq. (6) needs to be greatly increased, which will significantly reduce the computational efficiency of VF. In this work, piecewise function method is used to approximate the exponential multiplier in arbitrary interval with high accuracy as following

$$
\exp(-\frac{t^2}{4}) = \exp\left[-\frac{(2m+1)^2 T_0^2}{4}\right] \exp\left[-\frac{(t-(2m+1)T_0)^2}{4}\right]
$$

$$
\approx \exp\left[-\frac{(2m+1)^2 T_0^2}{4}\right] \exp\left[-\frac{(t-(2m+1)T_0)^2}{4}\right] \sum_{n=0}^N a_n \cos\left(\frac{\pi n}{\tau} (t-(2m+1)T_0)\right) \quad 2mT_0 \leq t < 2(m+1)T_0, m = 0, 1, \ldots,
$$

where $T_0$ is smaller than $\tau$ to ensure higher accuracy of exponential multiplier. The accuracy of Eq. (9) is determined by the maximum relative error of Eq. (6) in the subdomain $t \in [0, T_0]$, for example, the maximum relative error of Eq. (9) is less than $10^{-16}$ in arbitrary interval while $N = 23$, $\tau = 12$ and $T_0 = 4$.

### 2.3 Approximations expressions of Voigt function

By substituting Eq. (9) into Eq. (3), the following approximations expressions of VF in analytic form is yielded (Appendix A)

$$
K_p(x, y) = \sum_{m=0}^{N} \frac{1}{\sqrt{\pi}} \exp\left[-y(2m+1)T_0 - \frac{(2m+1)^2 T_0^2}{4}\right] I_m(x, y),
$$

where $2MT_0$ is the upper integration limit of the truncation approximation of the VF, and

$$
I_m = \sum_{n=0}^N a_n \left[ \frac{e^{a_n T_0}}{\alpha_m^2 + \beta_m^2} \left( \alpha_m \cos(\beta_n T_0 + \gamma_m) + \beta_n \sin(\beta_n T_0 + \gamma_m) \right) 
- \frac{e^{-a_n T_0}}{\alpha_m^2 + \beta_m^2} \left( \alpha_m \cos(-\beta_n T_0 + \gamma_m) + \beta_n \sin(-\beta_n T_0 + \gamma_m) \right) 
+ \frac{e^{a_n T_0}}{\alpha_m^2 + \beta_m^2} \left( \alpha_m \cos(\beta_n T_0 + \gamma_m) + \beta_n \sin(\beta_n T_0 + \gamma_m) \right) 
- \frac{e^{-a_n T_0}}{\alpha_m^2 + \beta_m^2} \left( \alpha_m \cos(-\beta_n T_0 + \gamma_m) + \beta_n \sin(-\beta_n T_0 + \gamma_m) \right) \right],
$$

and the coefficients in Eq.(11) is defined as follows

$$
\alpha_m = -y \frac{(2m+1)T_0}{2},
\beta_m = x + \frac{\pi n}{\tau},
\beta_m = x - \frac{\pi n}{\tau},
\gamma_m = (2m+1)T_0 x.
$$

### 3. Results and discussion

#### 3.1 Error Analysis

In order to quantify accuracy of the series approximation (10), it is convenient to define the relative error as
\[
\Delta_p = \left| \frac{K_p(x, y) - K(x, y)}{K(x, y)} \right|
\]  

(13)

where the highly accurate reference values of \(K(x, y)\) can be obtained according to Eq. (1) by using the MATLAB that supports error function of complex argument.

Figures 3a and 3b show the logarithm \(\log_{10}\Delta_p\) of the relative error of the series approximation (10) at \(N=33\), \(M = 1\), \(T_0 = 4.1515\), and \(\tau = 14.3417\) (the corresponding expansion coefficients \(a_n\) with 32-bit significant number are shown in Appendix B). The domain required for coverage of the HITRAN molecular spectroscopic database is \(0 < x < 40,000\) and \(10^{-4} < y < 10^2\)\(^{[16]}\) while the domain \(y << 1\) is the most difficult for accurate and rapid computation of the Voigt function. Therefore, we will consider the accuracy behavior within the HITRAN domain and narrow band domain \(10^{-4} \leq x \leq 40,000 \cap 10^{-4} \leq y \leq 10^2\) and \(10^{-4} \leq x \leq 40,000 \cap 10^{-10} \leq y \leq 10^{-4}\) separately as shown in Figs. 2a and 2b, respectively.

As we can see from Fig. 3a, within the HITRAN domain the accuracy of the series approximation is better than \(10^{-23}\) over most of this area. The worst accuracies occurs in the HITRAN subdomain \(3 \leq x \leq 40,000 \cap 10^{-4} \leq y \leq 10^{-2}\), and remains high and better than \(5.5383 \times 10^{-19}\). In the narrow band shown in the Fig. 2b, the accuracy deteriorates further with decreasing \(y\). However, it still remains high and better than \(10^{-15}\) over most of this area. The worst accuracies occurs in the narrow band subdomain \(3 \leq x \leq 40,000 \cap 10^{-10} \leq y \leq 10^{-8}\), and remains high and better than \(5.5385 \times 10^{-13}\). The increase of \(\log_{10}\Delta_p\) can be explained from the fact that the decay rate of the multiplier \(\exp(-yt)\) in Eq. (3) decelerates when \(y \rightarrow 0\).

### 3.2 Parameter optimization

Since higher accuracy is unnecessary in some cases, for example, the accuracy of the Voigt function should be better than \(10^{-6}\) in modern applications requiring the HITRAN molecular spectroscopic database, we may select the optimal parameters to minimize the number of terms in the series approximation (10) in order to gain computational acceleration. By numerical calculation, the optimal parameters under different accuracy levels are shown in Table 1.

<table>
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<tr>
<th>(N)</th>
<th>(M)</th>
<th>(T_0)</th>
<th>(\tau)</th>
<th>((M+1)\times N)</th>
<th>(\Delta^4)</th>
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<td>6.6882</td>
<td>14</td>
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<td>66</td>
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*Δ* represents the worst accuracy within the HITRAN domain $0 < x < 40,000$ and $10^{-4} \leq y \leq 10^{2}$.

### 4. Conclusion

A analytical approximation expressions for rapid and accurate computation of the Voigt function is presented. The computational test reveals that with only the first 33 terms Fourier expansion of the exponential multiplier, the proposed approximation provides accuracy better than $5.5383 \times 10^{-19}$ in the domain of practical interest $0 < x < 40,000$ and $10^{-4} < y < 10^{2}$ that is needed for applications using the HITRAN molecular spectroscopic database. Compared with the typical approximation algorithms, the proposed approximation still available even if $y$ is very small and the accuracy in the narrow band domain $0 < x < 40,000 \cap 10^{-10} < y < 10^{-4}$ remains high and better than $5.5385 \times 10^{-13}$. Since the approximations Eq. (10) is a general expressions, the desired accuracy can be easily achieved by choosing reasonable parameters. In particular, the optimal parameters under different accuracy levels from $10^{-2}$ to $10^{-19}$ are given in Table 1 in order to gain computational acceleration.

### Appendix A

The infinite integral interval in Eq. (3) can be rewritten in the following form

$$K(x, y) = \sum_{n=0}^{\infty} \frac{1}{\sqrt{\pi}} K_{m}(x, y), \quad (A-1)$$

where $K_{m}(x, y)$ is defined as

$$K_{m}(x, y) = \int_{2mT_{0}}^{2(m+1)T_{0}} \exp(-\frac{r^{2}}{4}) \exp(-yr) \cos(xr)dr. \quad (A-2)$$

By substituting Eq. (9) into Eq. (A-2) and using the product to sum formulas for cosine functions, the $K_{m}(x, y)$ can be approximated in the following form

$$K_{m}(x, y) \approx \frac{1}{2} \exp[-y((2m+1)T_{0}) - \frac{(2m+1)^{2}T_{0}^{2}}{4}] \sum_{n=0}^{N} \alpha_{n} [I_{mn1}(x, y) + I_{mn2}(x, y)], \quad (A-3)$$

where $I_{mn1}(x, y)$ and $I_{mn2}(x, y)$ are defined as

$$I_{mn1}(x, y) = \int_{-\infty}^{\infty} \exp[-(y + \frac{2(2m+1)T_{0}}{4})r] \cos[(x + \frac{\pi n}{r_{m}})r + (2m+1)xT_{0}]dr, \quad (A-4)$$
\[ I_{\text{max}}(x, y) = \int_{-\infty}^{\infty} \exp\left[-\left(y + \frac{2(2m+1)T_0}{\tau}\right)t\right] \cos\left((x - \frac{\pi n}{\tau})t + (2m+1)xT_0\right) dt. \]  

(A-5)

The exact solutions of integral (A-4) and (A-5) can be found analytically by using the following formula

\[ \int e^{ax} \cos bx dx = e^{ax} \frac{a \cos bx + b \sin bx}{a^2 + b^2}, \]

(A-4)

\[ \int e^{ax} \sin bx dx = e^{ax} \frac{a \sin bx - b \cos bx}{a^2 + b^2}. \]

(A-5)

Thus the approximations expressions of VF in analytic form is yielded by taking the first \( M \) terms of Eq. (A-1).

**Appendix B**

Table B-1. The corresponding expansion coefficients \( a_n \) with 32-bit significant number (\( \tau = 14.3417 \)).

<table>
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<th>values</th>
<th>( a_n )</th>
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