Derivation for the rational approximation of the Voigt function

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The Voigt function is defined as [1, 2]

$$K(x,y) = \frac{y}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{y^2 + (x-t)^2}\,dt\,. \tag{1}$$

It cannot be represented in a closed form and, therefore, requires a numerical solution. The Voigt function is closely related to the complex error function, also known as the Faddeeva function [1, 2]

$$w(x,y) = e^{-(x+iy)^2}\left[1 - \operatorname{erf}\left(-i(x+iy)\right)\right] = \frac{1}{\sqrt{\pi}}\int_0^{\infty} \exp\left(-t^2/4\right)\exp(-yt)\exp(ixt)\,dt\,. \tag{2}$$

Specifically, we can write [1, 2]

$$K(x,y) = \operatorname{Re}\left[w(x,y)\right] = \frac{1}{\sqrt{\pi}}\int_0^{\infty} \exp\left(-t^2/4\right)\exp(-yt)\cos(xt)\,dt\,, \quad y \ge 0\,. \tag{3}$$

By changing the variable $x \to -x$ in the equation (3) we can see that

$$\operatorname{Re}\left[w(x,y)\right] = \operatorname{Re}\left[w(-x,y)\right]$$

or

$$K(x,y) = K(-x,y)\,.$$

Consequently, we can write

$$K(x,y) = \operatorname{Re}\left[w(x,y)\right] = \left[w(x,y) + w(-x,y)\right]/2\,. \tag{4}$$

It is interesting to note that substituting identity (4) into equation (2) leads to an identity for real part of the error function of complex argument

$$\operatorname{Re}\left[\operatorname{erf}(x+iy)\right] = \frac{\operatorname{erf}(x+iy) + \operatorname{erf}(x-iy)}{2}\,.$$

Using the same procedure for imaginary part of the complex error function

$$\mathrm{Im}\left[w(x,y)\right]=\frac{1}{\sqrt{\pi}}\int_0^\infty \exp\left(-t^2/4\right)\exp\left(-yt\right)\sin\left(xt\right)dt$$

we can also find that

$$\mathrm{Im}\left[\mathrm{erf}\,(x+iy)\right]=\frac{\mathrm{erf}\,(x+iy)-\mathrm{erf}\,(x-iy)}{2i}.$$

From equation (3) it follows that

$$\mathrm{Re}\left[w(x,y=0)\right]=K(x,y=0)=\frac{1}{\sqrt{\pi}}\int_0^\infty \exp\left(-t^2/4\right)\cos\left(xt\right)dt\equiv\exp\left(-x^2\right).$$

Consequently, using identity (4) we obtain

$$\exp\left(-x^2\right)=\left[K(x,y=0)+K(-x,y=0)\right]/2. \tag{5}$$

Further we will use the notation for the complex variable $z=x+iy$ and imply that $\mathrm{Im}[z]\geq 0$.

Recently we have shown that a sampling methodology based on incomplete expansion of the sinc function results in the following approximation [3]

$$w(z)\approx\sum_{m=1}^{2^{M-1}}\frac{A_m+(z+i\varsigma/2)B_m}{C_m^2-(z+i\varsigma/2)^2}, \tag{6}$$

where

$$A_m=\frac{\sqrt{\pi}(2m-1)}{2^{2M}h}\sum_{n=-N}^{N}e^{\varsigma^2/4-n^2h^2}\sin\left(\frac{\pi(2m-1)(nh+\varsigma/2)}{2^M h}\right),$$

$$B_m=-\frac{i}{2^{M-1}\sqrt{\pi}}\sum_{n=-N}^{N}e^{\varsigma^2/4-n^2h^2}\cos\left(\frac{\pi(2m-1)(nh+\varsigma/2)}{2^M h}\right),$$

$$C_m=\frac{\pi(2m-1)}{2^{M+1}h}$$

and $\varsigma=2.75$, $h=0.25$, $M=5$, $N=23$. Change of the upper limit integer in the series approximation (6) as $2^{M-1}\to m_{\max}$ yields

$$w(z)=\sum_{m=1}^{m_{\max}}\frac{A_m+(z+i\varsigma/2)B_m}{C_m^2-(z+i\varsigma/2)^2}, \tag{7}$$

where the coefficients are rewritten now as

$$A_m = \frac{\sqrt{\pi}\left(m-1/2\right)}{2m_{\max}^2 h}\sum_{n=-N}^{N} e^{\varsigma^2/4-n^2h^2}\sin\left(\frac{\pi\left(m-1/2\right)\left(nh+\varsigma/2\right)}{m_{\max}h}\right),$$

$$B_m = -\frac{i}{m_{\max}\sqrt{\pi}}\sum_{n=-N}^{N} e^{\varsigma^2/4-n^2h^2}\cos\left(\frac{\pi\left(m-1/2\right)\left(nh+\varsigma/2\right)}{m_{\max}h}\right),$$

$$C_m = \frac{\pi\left(m-1/2\right)}{2m_{\max}h}.$$

Taking $y=0$ in the series approximation (7) and applying identity (5) results in the following approximation of the exponential function

$$\exp\left(-x^2\right) \approx \frac{1}{2}\sum_{m=1}^{m_{\max}}\left[\frac{A_m+\left(x+i\varsigma/2\right)B_m}{C_m^2-\left(x+i\varsigma/2\right)^2}+\frac{A_m+\left(-x+i\varsigma/2\right)B_m}{C_m^2-\left(-x+i\varsigma/2\right)^2}\right]. \tag{8}$$

Substituting approximation (8) into equation (1) leads to

$$K\left(x,y\right) \approx \frac{y}{2\pi}\int_{-\infty}^{\infty}\frac{1}{y^2+\left(x-t\right)^2}\sum_{m=1}^{m_{\max}}\left[\frac{A_m+\left(t+i\varsigma/2\right)B_m}{C_m^2-\left(t+i\varsigma/2\right)^2}+\frac{A_m+\left(-t+i\varsigma/2\right)B_m}{C_m^2-\left(-t+i\varsigma/2\right)^2}\right]dt, \tag{9}$$

We can apply a contour integral on the upper-half complex plane as a semicircle C_{ccw} with infinite radius in counterclockwise (CCW) direction. Substituting $1+2m_{\max}$ isolated points located inside domain enclosed by contour C_{ccw}:

$$t_r = \left\{x+iy, -C_m+i\varsigma/2, C_m+i\varsigma/2\right\}, \quad m\in\left\{1,2,3,\ldots m_{\max}\right\}$$

into the Residue Theorem's formula

$$\frac{1}{2\pi i}\oint_{C_{ccw}} f\left(t\right)dt = \sum_{r=1}^{1+2m_{\max}}\operatorname{Res}\left[f\left(t\right),t_r\right],$$

where $f\left(t\right)$ is the integrand of integral (9), we obtain

$$K\left(x,y\right) \approx$$
$$\sum_{m=1}^{m_{\max}}\frac{A_m\left[C_m^2-x^2+\left(y+\varsigma/2\right)^2\right]+iB_m\left(y+\varsigma/2\right)\left[C_m^2+x^2+\left(y+\varsigma/2\right)^2\right]}{\left[C_m+x-i\left(y+\varsigma/2\right)\right]\left[C_m-x+i\left(y+\varsigma/2\right)\right]\left[C_m^2-\left(x+i\left(y+\varsigma/2\right)\right)^2\right]}$$

or

$$
\begin{aligned}
\kappa(x,y) &\triangleq \sum_{m=1}^{m_{\max}} \frac{\alpha_m\left(\beta_m + y^2 - x^2\right) + \gamma_m y\left(\beta_m + x^2 + y^2\right)}{\beta_m^2 + 2\beta_m\left(y^2 - x^2\right) + \left(x^2 + y^2\right)^2} \\
&\Rightarrow K(x,y) \approx \kappa(x, y + \varsigma/2),
\end{aligned}
\tag{10}
$$

where the corresponding coefficients are $\alpha_m = A_m$, $\beta_m = C_m^2$ and $\gamma_m = iB_m$.

The computational testing we performed with arbitrary variables x and y shows that within domain of practical interest $0 < x < 40,000$ and $10^{-4} < y < 10^4$ required for applications using the HITRAN molecular spectroscopic database, the proposed rational approximation provides average accuracy 10^{-14}. The detailed description of the rational approximation (10) for efficient computation of the Voigt function will be shown in our publication [4].

References

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