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On Mellin–Barnes integral representation of Voigt profile function

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Abstract

Voigt profile function emerges in several physical investigations (e.g., atmospheric radiative transfer, astrophysical spectroscopy, plasma waves and acoustics) and it turns out to be the convolution of Gaussian and Lorentzian densities. Its relation

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with a number of special functions has been widely derived in literature starting from its Fourier type integral representation. Here, starting from the Mellin–Barnes integral representation, Voigt function is expressed in terms of Fox H-function which includes expressions in terms of Meijer G-function and previously well-known expressions with other special functions. Voigt function emerges to be representable as the sum of two special functions of the same type but with complex conjugate argouments, as well as, for example, trigonometric functions, J_ν and Y_ν Bessel functions, but, differently from these functions, and in general from a large number of special functions, Voigt profile is not representable with a single Mellin–Barnes integral. When a single integral representation in the complex plane is derived it turns out not to be a Mellin–Barnes integral.

Keywords: Voigt profile function; Mellin–Barnes integral; H-function.
MSC2010: 33-XX; 30E20; 33E20; 33C60.

1 Introduction

In the present paper we analyze the Mellin–Barnes integral representation of Voigt profile and it emerges that this function cannot be expressed by a single Mellin–Barnes integral.

The Mellin–Barnes integral representation of a function has more freedom in the parameters, as well as in the variables, in comparison to the series definition. Then, the results based on the representation in terms of Mellin–Barnes integrals, namely in terms of the H- and G-functions, are more general than those in terms of the series definition.

The Mellin–Barnes integrals are a family of integrals in the complex plane whose integrand is given by the ratio of products of Gamma functions. Despite of the name, the Mellin–Barnes integrals were initially studied in 1888 by the Italian mathematician S. Pincherle [22, 33] in a couple of papers on the duality principle between linear differential equations and linear difference equations with rational coefficients. The Mellin–Barnes integrals are strongly related with Mellin transform, in particular with the inverse transformation. As shown by O.I. Marichev [25], the problem to evaluate integrals can be successfully faced with a powerful method mainly based on their reduction to functions whose Mellin transform is the ratio of product of Gamma functions and then, after the inversion, the problem consists in the evaluation of Mellin–Barnes integrals. Moreover, they are also the essential tools for treating higher transcendental functions as Fox H-function and Meijer G-function and a useful representation to compute asymptotic behaviour of functions [29, 31].

Voigt profile function emerges in several physical investigations as atmospheric radiative transfer, astrophysical spectroscopy, plasma waves and acoustics and molecular spectroscopy in general. Mathematically, it turns out to be the convolution of Gaussian and Lorentzian densities. Here we study the ordinary Voigt function and not its mathematical generalizations, e.g., [5, 15, 37, 41, 43]. The computation of Voigt profile is an old issue in literature and many efforts are directed to evaluate this function with different techniques. In fact, an analytical explicit representation in terms of elementary functions does not exist and it can be considered a special function itself. Moreover it is strictly related to the plasma dispersion function [12] and to a number of special functions as, for example, the confluent hypergeometric function, the complex complementary error function, the Dawson function, the parabolic cylinder function and the Whittaker function, see for example [4, 7, 10, 11, 16, 38, 40, 45]. All previous representations are derived starting from the integral formula due to F. Reiche in 1913 [34] that is a Fourier type integral. The Voigt profile function remains nowadays a mathematically and computationally interesting problem because computing profiles with high accuracy is still an expensive task. The actual interest on this topic is proved by several recent papers on mathematical (e.g., [8, 14, 21, 30, 32, 37, 44, 46]) and numerical aspects (e.g., [1, 2, 3, 19, 20, 24, 27, 39, 48]).

Mellin–Barnes integral representation can be considered a useful tool to obtain new analytical results that in the future can lead to efficient numerical algorithms for the Voigt function. A successful application of such approach has been shown in [29]. There the parametric evolution equation of Voigt function (and its probabilistic generalization) is derived, it turns out to be a space-fractional diffusion equation of double order, and the scaling laws in the asymptotic regimes, with respect to the parameter, are computed using the Mellin–Barnes integral representation.

During the recent past, representations of the Voigt profile function in terms of special functions have been discussed, see for example [10, 11, 13, 16, 17, 36]. By these studies it emerges that the Voigt function can be expressed as the sum of two special functions of the same type and complex and conjugate argouments, as for example trigonometric functions sine and cosine or the Bessel functions J_ν and Y_ν. In the present paper we continue those researches deriving, by the Mellin–Barnes integral representation, the expression in terms of Fox H-function, which includes previously well-known results. However, also in this general case, the Voigt function is given by two equal Mellin–Barnes integrals (or H-functions) but with complex and conjugate variables. An important consequence of this analysis is that, differently from sine, cosine, J_ν and Y_ν, and in general from a large number of special functions, the Voigt function is not representable with a single Mellin–Barnes integral (or H-function). When a single integral representation in the complex plane is derived it turns out not to be a Mellin–Barnes integral.

The rest of the paper is organized as follows. In section 2 the basic definition of Voigt profile function is given and some *classical* and recent representations are reviewed. In section 3 the Mellin–Barnes integral representation of Voigt profile is derived and the impossibility to express the Voigt function with a single Mellin–Barnes integral shown. In section 4, first the Voigt function is expressed in terms of Fox H-function and later, in cascade, the representation with Meijer G-function and other special functions are obtained. Finally in section 5 summary and conclusions are given.

2 The Voigt profile function

2.1 Basic definition

Gaussian $G(x)$ and Lorentzian $L(x)$ profiles are defined as

$$
\begin{aligned}
G(x) &= \frac{1}{\sqrt{\pi}\omega_G} \exp\left[-\left(\frac{x}{\omega_G}\right)^2\right] \\
L(x) &= \frac{1}{\pi\omega_L} \frac{\omega_L^2}{x^2+\omega_L^2}\,,
\end{aligned}
\tag{1}
$$

where ω_G and ω_L are the corresponding widths. The variable x is a wave-number and then its physical dimension is a length raised up to -1. The Voigt profile $V(x)$ is obtained by the convolution of $G(x)$ and $L(x)$

$$
\begin{aligned}
V(x) &= \int\limits_{-\infty}^{+\infty} L(x-\xi)G(\xi)\,\mathrm{d}\xi \\
&= \frac{\omega_L/\omega_G}{\pi^{3/2}} \int\limits_{-\infty}^{+\infty} \frac{\mathrm{e}^{-(\xi/\omega_G)^2}}{(x-\xi)^2+\omega_L^2}\,\mathrm{d}\xi\,.
\end{aligned} \tag{2}
$$

Let $\widehat{f}(\kappa)$ be the Fourier transform of $f(x)$ so that

$$
\begin{aligned}
\widehat{f}(\kappa) &= \int\limits_{-\infty}^{+\infty} \mathrm{e}^{+i\kappa x} f(x)\,\mathrm{d}x \\
f(x) &= \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} \mathrm{e}^{-i\kappa x} \widehat{f}(\kappa)\,\mathrm{d}\kappa\,,
\end{aligned} \tag{3}
$$

then

$$
\begin{aligned}
\widehat{V}(\kappa) &= \widehat{G}(\kappa) \\
\widehat{L}(\kappa) &= \mathrm{e}^{-\omega_G^2\kappa^2/4}\,\mathrm{e}^{-\omega_L|\kappa|}\,,
\end{aligned} \tag{4}
$$

and

$$
\begin{aligned}
V(x) &= \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} \exp\{-i\kappa x - \omega_G^2\kappa^2/4 - \omega_L|\kappa|\}\,\mathrm{d}\kappa \\
&= \frac{1}{\pi} \int\limits_{0}^{+\infty} \exp\{-\omega_L\kappa - \omega_G^2\kappa^2/4\}\cos(\kappa x)\,\mathrm{d}\kappa\,.
\end{aligned} \tag{5}
$$

Formula (5) is the integral representation due to F. Reiche [34].

2.2 Some *classical* and recent representations

Let x' be the dimensionless variable $x' = x/\omega_G$. Then the Voigt function can be re-arranged in the form

$$
\text{(6)} \qquad
\begin{aligned}
V(x') &= \frac{1}{\sqrt{\pi}\,\omega_G} K(x', y) \\
K(x, y) &= \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-\xi^2}}{(x-\xi)^2 + y^2}\, d\xi
\end{aligned}
$$

where $y = \omega_L/\omega_G$ and from (3) it follows that

$$
\text{(7)} \qquad K(x, y) = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-y\xi - \xi^2/4} \cos(x\xi)\, d\xi \,.
$$

Voigt function does not possess an explicit representation in terms of elementary functions and several alternatives to (2) have been given in literature, mainly with the intention to obtain a more efficient numerical computation.

Combining x and y in the complex variable $z = x - iy$, function $K(x, y)$ in (6) reads

$$
\text{(8)} \qquad
\begin{aligned}
K(x, y) &= Re[W(z)] \\
W(z) &= \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-\xi^2}}{z - \xi}\, d\xi
\end{aligned}
$$

where $W(z)$ is strongly related to the plasma dispersion function [12] and some *classical* representations can be found, see for example [4, 38, 40]. In fact, from the relation of $W(z)$ with the complex complementary error function $\mathrm{erfc}(-iz)$ and with the Dawson function $F(z) = \exp(-z^2)\int_0^z \exp(\xi^2) d\xi$, it follows that

$$
\text{(9)} \qquad
\begin{aligned}
K(x, y) &= Re[W(z)] \\
W(z) &= e^{-z^2} \mathrm{erfc}(-iz) \quad y > 0 \,,
\end{aligned}
$$

$$
\text{(10)} \quad K(x, y) = Re[W(z)], \quad W(z) = e^{-z^2} + \frac{2i}{\sqrt{\pi}} F(z).
$$

More recent representations are, for example, those derived in 2001 by H.O. Di Rocco *et al.* [6]

$$K(x,y) = \sum_{n=0}^{\infty}(-1)^n \left\{ \frac{1}{\Gamma(n+1)} {}_1F_1\left(\frac{2n+1}{2}, \frac{1}{2}; y^2\right) - \frac{2y}{\Gamma\left(\frac{2n+1}{2}\right)} {}_1F_1\left(n+1, \frac{3}{2}; y^2\right) \right\} x^{2n}, \tag{11}$$

where ${}_1F_1(\alpha,\beta;z)$ is the confluent hypergeometric function, in 2007 by M.R. Zaghloul [46], which "completed" a previous formula given by G.D. Roston & F.S. Obaid [35],

$$\begin{aligned} K(x,y) &= [1-\mathrm{erf}(y)]\exp\{-x^2+y^2\}\cos(2xy) \\ &\quad + \frac{2}{\sqrt{\pi}}\int_0^x \exp\{-x^2+\xi^2\}\sin[2y(x-\xi)]\,\mathrm{d}\xi \end{aligned} \tag{12}$$

in 2008 by S.P. Limandri and co-authors [21]

$$\begin{aligned} K(x,y) = \exp\{-x^2+y^2\}\{&\mathrm{erfc}(y)\cos(2xy) \\ &+ \cos(2xy)[\mathrm{erf}(y) - \mathrm{Re}(\mathrm{erf}(y+ix))] \\ &+ \sin(2xy)[\mathrm{Im}(\mathrm{erf}(y+ix))]\} \end{aligned} \tag{13}$$

and in 2011 by D.A.P. Palma and co-authors [30]

$$\begin{aligned} K(x,y) &= \exp\{-x^2+y^2\}\cos(2xy) \\ &\times \{1+\mathrm{Re}[\mathrm{erf}(ix-y)] + \tan(2xy)\,\mathrm{Im}[\mathrm{erf}(ix-y)]\}. \end{aligned} \tag{14}$$

J. He & Q. Zhang [14] claimed to have derived an exact calculation of the Voigt profile that is proportional to the product of an exponential and a cosine function. However, as it is stated in [28], this representation assumes negative values in contrast with the non-negativity of the Voigt function and then this result is not correct. In [47] a different and less direct argourment is used to prove the falsity of J. He & Q. Zhang claim.

Further representations are given in terms of special functions, see for example the one involving the confluent hypergeometric function ${}_1F_1$ [16, 11]

$$
\begin{aligned}
K(x,y) &= e^{(y^2-x^2)}\cos(2xy) \\
&- \frac{1}{\sqrt{\pi}}\Big\{(y+ix)\,{}_1F_1(1;3/2;(y+ix)^2) \\
&\quad + (y-ix)\,{}_1F_1(1;3/2;(y-ix)^2)\Big\},
\end{aligned} \tag{15}
$$

and others involving the Whittaker function $W_{k,m}$, the erfc–function and the parabolic cylinder function [45, formulae (17,13,16)]

$$
\begin{aligned}
K(x,y) &= \frac{1}{2\sqrt{\pi}} \\
&\cdot\Big\{(y-ix)^{-1/2}\,e^{(y-ix)^2/2}\,W_{-1/4,-1/4}((y-ix)^2) \\
&+ (y+ix)^{-1/2}\,e^{(y+ix)^2/2}\,W_{-1/4,-1/4}((y+ix)^2)\Big\},
\end{aligned} \tag{16}
$$

$$
\begin{aligned}
K(x,y) &= \\
&\frac{1}{2}\Big\{e^{(y-ix)^2}\,\mathrm{erfc}(y-ix) + e^{(y+ix)^2}\,\mathrm{erfc}(y+ix)\Big\},
\end{aligned} \tag{17}
$$

$$
\begin{aligned}
K(x,y) &= \frac{1}{\sqrt{2\pi}} \\
&\Big\{e^{(y-ix)^2/2}\,D_{-1}[\sqrt{2}(y-ix)] \\
&+ e^{(y+ix)^2/2}\,D_{-1}[\sqrt{2}(y+ix)]\Big\}.
\end{aligned} \tag{18}
$$

Looking at formulae (15-18), one can observes that Voigt function is given by expressions of the type

$f(z) + f(\overline{z})$ where $\overline{z}$ is the complex conjugate of z. The same type of expression can be find for other functions, the most simplest are the trigonometric functions $2i\sin(\xi) = \mathrm{e}^{i\xi} - \mathrm{e}^{-i\xi}$, $2\cos(\xi) = \mathrm{e}^{i\xi} + \mathrm{e}^{-i\xi}$, or Bessel functions J_ν and Y_ν, of first and second kind respectively, [45]

$$J_\nu(\xi) = (2\xi)^{-1/2}\pi^{1/2} \left\{ \exp\left[\left(\frac{\nu}{2} + \frac{1}{2} + \frac{1}{4}\right)\pi i\right] W_{0,\nu}(2i\xi) + \exp\left[-\left(\frac{\nu}{2} + \frac{1}{2} + \frac{1}{4}\right)\pi i\right] W_{0,\nu}(-2i\xi) \right\},$$

$$Y_\nu(\xi) = (2\xi\pi)^{-1/2} \left\{ \exp\left[\left(\frac{\nu}{2} + \frac{1}{2} - \frac{1}{4}\right)\pi i\right] W_{0,\nu}(2i\xi) + \exp\left[-\left(\frac{\nu}{2} + \frac{1}{2} - \frac{1}{4}\right)\pi i\right] W_{0,\nu}(-2i\xi) \right\}.$$

However, as it will be shown later, differently from these functions, and in general from a large number of special functions, Voigt profile cannot be expressed by a single Mellin–Barnes integral.

3 The Mellin–Barnes integral representation

Let us consider again dimensional variables and the Gauss, Lorentz and Voigt functions defined as in (1-2). From (4) we have

$$V(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\{-i\kappa x - \omega_G^2 \kappa^2/4 - \omega_L|\kappa|\} \, \mathrm{d}\kappa$$

$$(19) \qquad = \frac{1}{2\pi} \Big\{ I_+(x) + I_-(x) \Big\},$$

where

$$(20) \qquad I_\pm(x) = \int_0^{+\infty} \exp\{-(\omega_L \pm ix)\kappa - \omega_G^2 \kappa^2/4\} \, \mathrm{d}\kappa \, .$$

Following [31, 23], the Mellin–Barnes integral representations of $I_\pm(x)$ can be obtained from the definition of the Gamma function

$$(21) \qquad \Gamma(z) = \int_0^{+\infty} \xi^{z-1} \mathrm{e}^{-\xi} \, \mathrm{d}\xi \, , \quad Re(z) > 0 \, ,$$

and the Mellin–Barnes integral representation of e^{-z} $(z \neq 0)$

$$(22) \qquad \mathrm{e}^{-z} = \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s) z^{-s} \, \mathrm{d}s = \sum\nolimits_{n=0}^{\infty} \frac{(-1)^n}{n!} z^n \, ,$$

where $\mathcal{L}$ denotes a loop in the complex s plane which encircles the poles of $\Gamma(s)$ (in the positive sense) with endpoints at infinity in $Re(s) < 0$ and with no restrictions on $\arg z$ [31]. The functions $I_\pm(x)$ have the following Mellin–Barnes integral repre-

sentations
(23)

$$I_{\pm}(x) = \int_0^{+\infty} \mathrm{e}^{-\omega_G^2\kappa^2/4} \left\{ \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s)[(\omega_L \pm ix)\kappa]^{-s}\,\mathrm{d}s \right\} \mathrm{d}\kappa$$

$$= \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s) \left\{ \int_0^{+\infty} \mathrm{e}^{-\omega_G^2\kappa^2/4} \kappa^{-s}\,\mathrm{d}\kappa \right\} (\omega_L \pm ix)^{-s}\,\mathrm{d}s,\ Re(s) < 1$$

$$= \frac{1}{\omega_G} \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s)\Gamma\left(\frac{1}{2} - \frac{s}{2}\right) \left[\frac{2}{\omega_G}(\omega_L \pm ix) \right]^{-s} \mathrm{d}s.$$

Hence the Mellin–Barnes integral representation of Voigt function is given by [23]

$$V(x) = \frac{1}{2\pi\omega_G} \left\{ \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s)\Gamma\left(\frac{1}{2} - \frac{s}{2}\right) \left[\frac{2}{\omega_G}(\omega_L + ix) \right]^{-s} \mathrm{d}s \right. \\ \left. + \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(s)\Gamma\left(\frac{1}{2} - \frac{s}{2}\right) \left[\frac{2}{\omega_G}(\omega_L - ix) \right]^{-s} \mathrm{d}s \right\}. \tag{24}$$

However, we note that for a complex number $z = |z|e^{i\theta}$, $\theta = \arctan(Im(z)/Re(z))$, the following rule holds

$$\begin{aligned} z^n + \bar{z}^n &= |z|^n \mathrm{e}^{in\theta} + |z|^n \mathrm{e}^{-in\theta} \\ &= |z|^n (\mathrm{e}^{in\theta} + \mathrm{e}^{-in\theta}) \\ &= 2|z|^n \cos(n\theta) \\ &= 2|z|^n \cos(n \arctan(Im(z)/Re(z))), \end{aligned} \tag{25}$$

and formula (24) becomes

$$(26)\quad V(x) = \frac{1}{\pi\omega_G}\frac{1}{2\pi i}$$

$$\int_{\mathcal{L}} \Gamma(s)\Gamma\left(\frac{1}{2}-\frac{s}{2}\right)\cos\left[s\arctan\left(\frac{x}{\omega_L}\right)\right]\left(4\frac{\omega_L^2+x^2}{\omega_G^2}\right)^{-s/2} \mathrm{d}s.$$

Consider again (23), changing $s \to -s$ and taking the corresponding integration path $\mathcal{L}$ as a loop in the complex plane that encircles the poles of $\Gamma(-s)$, an other Mellin–Barnes integral representation of the Voigt function equivalent to (24) is

(27)

$$V(x) = \frac{1}{2\pi\omega_G}\left\{\frac{1}{2\pi i}\int_{\mathcal{L}} \Gamma(-s)\Gamma\left(\frac{1}{2}+\frac{s}{2}\right)\left[\frac{2}{\omega_G}(\omega_L+ix)\right]^s \mathrm{d}s\right.$$

$$\left.+\frac{1}{2\pi i}\int_{\mathcal{L}} \Gamma(-s)\Gamma\left(\frac{1}{2}+\frac{s}{2}\right)\left[\frac{2}{\omega_G}(\omega_L-ix)\right]^s \mathrm{d}s\right\},$$

and in more compact form

$$(28)\quad V(x) = \frac{1}{\pi\omega_G}\frac{1}{2\pi i}$$

$$\int_{\mathcal{L}} \Gamma(-s)\Gamma\left(\frac{1}{2}+\frac{s}{2}\right)\cos\left[s\arctan\left(\frac{x}{\omega_L}\right)\right]\left(4\frac{\omega_L^2+x^2}{\omega_G^2}\right)^{s/2} \mathrm{d}s.$$

Formulae (26) and (28) show the main property of the Voigt function derived here. In fact, since (26) and (28) are not Mellin–Barnes integrals this means that Voigt function cannot be expressed by a single Mellin–Barnes integral, but only by the sum of two equal Mellin–Barnes integrals with complex and conjugate variables as it is shown in (24) and (27). Differently from other function representable with two functions of the same type but complex conjugate variables, as trigonometric functions sine and cosine or J_ν and Y_ν, and in general from a large number of special functions, that can be represented by a single Mellin–Barnes integral [25, 26, 42].

4 The Fox H- and Meijer G-function representations

4.1 The Fox H-function representation

Voigt function can be represented in terms of well-known special functions, see §2.2, but its representation in terms of Fox H-function is still not known. The expression in terms of Fox H-function is important because it is the most modern representation method and, actually, it is the most compact form to represent higher transcendental functions [18]. The definition of Fox H-function is given in Appendix.

For ω_G and ω_L fixed, $2(\omega_L+ix)/\omega_G \neq 0$ and $2(\omega_L-ix)/\omega_G \neq 0$, from (27) and (24) we have, respectively,

(29)

$$V(x) = \frac{1}{2\pi\omega_G}\left\{H_{11}^{11}\left[\frac{2}{\omega_G}(\omega_L+ix)\,\middle|\,\begin{matrix}(1/2,1/2)\\(0,1)\end{matrix}\right] + H_{11}^{11}\left[\frac{2}{\omega_G}(\omega_L-ix)\,\middle|\,\begin{matrix}(1/2,1/2)\\(0,1)\end{matrix}\right]\right\},$$

(30)
$$V(x) = \frac{1}{2\pi\omega_G}\left\{H_{11}^{11}\left[\frac{\omega_G}{2(\omega_L+ix)}\,\middle|\,\begin{matrix}(1,1)\\(1/2,1/2)\end{matrix}\right] + H_{11}^{11}\left[\frac{\omega_G}{2(\omega_L-ix)}\,\middle|\,\begin{matrix}(1,1)\\(1/2,1/2)\end{matrix}\right]\right\},$$

As a consequence of the fact that this is the most comprehensive representation, in cascade, the others with less general functions can be obtained.

4.2 The Meijer G-function representation

The first H-function in (29) can be rewritten in terms of Meijer G-function. Setting $Z = 2(\omega_L + ix)/\omega_G$, we have

$$
\begin{aligned}
& H_{11}^{11}\left[Z \,\middle|\, \begin{matrix} (1/2, 1/2) \\ (0,1) \end{matrix}\right] \\
& = \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(-s)\Gamma\left(\frac{1}{2} + \frac{s}{2}\right) Z^s \, \mathrm{d}s \\
& = \frac{2}{2\pi i} \int_{\mathcal{L}} \Gamma(-2s)\Gamma\left(\frac{1}{2} + s\right) Z^{2s} \, \mathrm{d}s \\
& = \frac{1}{\sqrt{\pi}} \frac{1}{2\pi i} \int_{\mathcal{L}} \Gamma(-s)\Gamma\left(\frac{1}{2} - s\right)\Gamma\left(\frac{1}{2} + s\right)\left(\frac{Z^2}{4}\right)^s \mathrm{d}s \\
& = \frac{1}{\sqrt{\pi}} G_{12}^{21}\left[\frac{Z^2}{4} \,\middle|\, \begin{matrix} 1/2 \\ 0, 1/2 \end{matrix}\right],
\end{aligned}
\tag{31}
$$

where the change of variable $s \to 2s$ and the duplication rule for the Gamma function, $\Gamma(2z) = \Gamma(z)\Gamma(1/2+z)2^{2z-1}\pi^{-1/2}$, are applied. The second H-function in (29) follows from the first with $\bar{Z} = 2(\omega_L - ix)/\omega_G$. Finally, the Voigt function in terms of Meijer G-function is given by

$$
\begin{aligned}
V(x) = & \frac{1}{2\pi^{3/2}\omega_G} \\
& \left\{ G_{12}^{21}\left[\frac{Z^2}{4} \,\middle|\, \begin{matrix} 1/2 \\ 0, 1/2 \end{matrix}\right] + G_{12}^{21}\left[\frac{\bar{Z}^2}{4} \,\middle|\, \begin{matrix} 1/2 \\ 0, 1/2 \end{matrix}\right] \right\}.
\end{aligned}
\tag{32}
$$

Meijer G-function can be reduced to other special functions and, for example, representations given in (16,17,18) are straightforwardly recovered.

In fact, the Meijer G-function and the Whittaker function $W_{k,m}$ are related by the formula [9, p. 435]

$$
G^{21}_{12}\left[z\,\middle|\,\begin{matrix} a \\ b,c \end{matrix}\right] = \Gamma(b-a+1)\Gamma(c-a+1)z^{(b+c-1)/2}\mathrm{e}^{z/2}W_{k,m}(k), \tag{33}
$$

where $k = a-(b+c+1)/2$ and $m = (b-c)/2$. Thus the G-functions in (32) are expressed in terms of Whittaker function as

$$
G^{21}_{12}\left[\frac{Z^2}{4}\,\middle|\,\begin{matrix} 1/2 \\ 0,1/2 \end{matrix}\right] = \sqrt{\pi}\left(\frac{Z}{2}\right)^{-1/2}\mathrm{e}^{Z^2/8}\,W_{-1/4,-1/4}(Z^2/4). \tag{34}
$$

Hence, Voigt function in terms of Whittaker function is

$$
V(x) = \frac{1}{2\pi\omega_G}\left\{\left(\frac{Z}{2}\right)^{-1/2}\mathrm{e}^{Z^2/8}\,W_{-1/4,-1/4}(Z^2/4 + \left(\frac{\bar{Z}}{2}\right)^{-1/2}\mathrm{e}^{\bar{Z}^2/8}\,W_{-1/4,-1/4}(\bar{Z}^2/4)\right\}. \tag{35}
$$

Moreover, from the identity

$$
G^{21}_{12}\left[\frac{Z^2}{4}\,\middle|\,\begin{matrix} 1/2 \\ 0,1/2 \end{matrix}\right] = \pi\,\mathrm{e}^{Z^2/4}\,\mathrm{erfc}(Z/2), \tag{36}
$$

we have

$$(37)\quad V(x)=\frac{1}{2\sqrt{\pi}\,\omega_G}\left\{e^{Z^2/4}\,\mathrm{erfc}(Z/2)+e^{\bar{Z}^2/4}\,\mathrm{erfc}(\bar{Z}/2)\right\},$$

and from

$$(38)\quad G^{21}_{12}\left[\frac{Z^2}{4}\,\middle|\,\begin{array}{c}1/2\\0,1/2\end{array}\right]=\sqrt{2\pi}\,e^{Z^2/8}\,D_{-1}(Z/\sqrt{2}),$$

we have

$$(39)\quad V(x)=\frac{1}{\sqrt{2}\pi\omega_G}\left\{e^{Z^2/8}\,D_{-1}(Z/\sqrt{2})+e^{\bar{Z}^2/8}\,D_{-1}(\bar{Z}/\sqrt{2})\right\}.$$

Setting $\omega_G = 1$ in (35,37,39) formulae (16,17,18) are recovered, respectively.

5 Summary and conclusions

In the present paper the Mellin–Barnes integral representation of Voigt profile function is derived and it emerges that, differently from a large number of special functions, Voigt function cannot be expressed by a single Mellin–Barnes integral. When the Mellin–Barnes integrals are used, the Voigt function emerges to be expressed by the sum of two Mellin–Barnes integrals that represent the sum of two functions of the same type but with complex and conjugate variables.

Mellin–Barnes integral representation of a function has more freedom in the parameters as well as in the variables in comparison to its series definition. This means that the results based on the representation in terms of Mellin–Barnes integrals, that is in terms of the H- and G-functions, are more general than those in terms of the series definition. Moreover, Mellin–Barnes integral representation is a useful tool to have new analytical and numerical results.

Starting from this, Voigt function has been expressed in terms of Fox H-function, which is the most comprehensive representation, in cascade, the expression in terms of Meijer G-function is obtained and the previous well-known representations with the Whittaker, the complementary error and the parabolic cylinder functions are recovered.

Appendix: The Fox H- and the Meijer G- functions

Fox H-function is defined as [26, 42, 18]

$$H_{pq}^{mn}\left[z\left|\begin{array}{c}(a_1,A_1),\cdots,(a_p,A_p)\\(b_1,B_1),\cdots,(b_q,B_q)\end{array}\right.\right]= \frac{1}{2\pi i}\int_{\mathcal{L}} h(s)z^s\,\mathrm{d}s, \tag{40}$$

where

$$h(s)=\frac{\prod_{j=1}^{m}\Gamma(b_j-B_js)\prod_{j=1}^{n}\Gamma(1-a_j+A_js)}{\prod_{j=m+1}^{q}\Gamma(1-b_j+B_js)\prod_{j=n+1}^{p}\Gamma(a_j-A_js)}, \tag{41}$$

an empty product is interpreted as unity, $\{m,n,p,q\}$ are non negative integers so that $0\le m\le q$, $0\le n\le p$, $\{A_j,B_j\}$ are positive numbers and $\{a_j,b_j\}$ complex numbers.

Making the assumption that

$$A_j(b_h+\nu)\neq B_h(a_j-\lambda-1) \tag{42}$$

for $\nu, \lambda = 0, 1, \ldots,\ h = 1, \ldots, m$ and $j = 1, \ldots, n$, the integration path $\mathcal{L}$ is the contour that separates the points

$$s = \left(\frac{b_j + \nu}{B_j}\right), \quad j = 1, \ldots, m, \quad \nu = 0, 1, \ldots, \tag{43}$$

which are the poles of $\Gamma(b_j - B_j s)$ $(j = 1, \ldots, m)$, from the points

$$s = \left(\frac{a_j - \nu - 1}{A_j}\right), \quad j = 1, \ldots, n, \quad \nu = 0, 1, \ldots, \tag{44}$$

which are the poles of $\Gamma(1 - a_j + A_j s)$ $(j = 1, \ldots, n)$.

The H-function is an analytic function of z and makes sense if [26, 42]

$$\begin{array}{lll} i) & \forall z \neq 0, & \mu > 0 \\ ii) & 0 < |z| < \beta^{-1}, & \mu = 0 \end{array}, \tag{45}$$

where

$$\begin{aligned} \mu &= \sum\nolimits_{j=1}^{q} B_j - \sum\nolimits_{j=1}^{p} A_j \\ \beta &= \prod\nolimits_{j=1}^{p} A_j^{A_j} \prod\nolimits_{j=1}^{q} B_j^{-B_j}. \end{aligned} \tag{46}$$

The Meijer G-function corresponds to the special case $A_j = B_k = 1$ $(j = 1, \ldots, p; k = 1, \ldots, q)$

$$H_{pq}^{mn}\left[z \left| \begin{array}{c} (a_1, 1), \cdots, (a_p, 1) \\ (b_1, 1), \cdots, (b_q, 1) \end{array} \right.\right] = G_{pq}^{mn}\left[z \left| \begin{array}{c} a_1, \cdots, a_p \\ b_1, \cdots, b_q \end{array} \right.\right]. \tag{47}$$

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