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Integro-differential equations to model generalized Voigt profiles: a fractional diffusion approach

Gianni Pagnini, Francesco Mainardi

CRS4, Polaris Bldg. 1, I-09010 Pula (CA), Italy
E-mail: pagnini@crs4.it
Department of Physics, University of Bologna, and INFN,
via Irnerio 46, I-40126 Bologna, Italy
E-mail: mainardi@bo.infn.it URL: www.fracalmo.org

Summary. In molecular spectroscopy and atmospheric radiative transfer, the combined effects of Doppler and pressure broadenings lead to the Voigt profile function, which turns out to be the convolution of the Gaussian (due to the Doppler broadening) and the Lorentzian (due to the pressure broadening) distributions. Here we are interested to study the Voigt profile function when the widths are not constant but depending on a scale-factor with a power law. Since in probability theory the Gaussian and the Lorentzian distributions are known to belong to the class of symmetric Lévy stable distributions, in this framework we propose to generalize the Voigt function by adopting the convolution of two arbitrary symmetric Lévy distributions. Moreover, we provide the integro-differential equations with respect to the scale-factor satisfied by the generalized Voigt profiles. These evolution equations can be interpreted as space-fractional diffusion equations of double order.

Key words: Voigt profile function, Lévy stable distributions, integro-differential equations, Riesz space-fractional derivative, Mellin-Barnes integrals

1 Introduction

In the present paper some mathematical aspects of the Voigt profile are discussed. This function emerges as a profile spectrum in molecular spectroscopy and atmospheric radiative transfer due to the combined effects of Doppler and pressure broadenings and it turns out to be the convolution of the Gaussian (due to the Doppler broadening) and the Lorentzian (due to the pressure broadening) probability densities.

Noting that the Gaussian and the Lorentzian distributions belong to the symmetric class of Lévy stable distributions, after a short review of classical and new representations, we introduce a probabilistic generalization of the Voigt profile in terms of the Lévy distributions.

Generally, the widths of distributions are assumed with a constant value fixed by the process. Here we are interested to study the ordinary and generalized Voigt profile function when the density widths are not constant but depending on a scale factor with a power law.

Physically, the one-dimensional variable of the Voigt function is a wavenumber (or frequency) and then this permits to take into account spatial inhomogeneity or temporal non-stationarity when the scale factor is the distance from an origin or the elapsed time, respectively. To this purpose, we derive the integro-differential equations in respect of the scale factor satisfied by the ordinary and the generalized Voigt profiles. These integro-differential equations can be classified as space-fractional diffusion equations of double order. A further generalization can be obtained considering space-fractional diffusion equations of distributed order [4, 43].

The rest of the paper is organized as follows. In section 2 the basic definitions of the Voigt profile and some classical and recent representations are given. In section 3 the connection with the Lévy stable distribution class is introduced and in section 4 the ordinary and the generalized Voigt functions are analyzed considering the scale factor and the associated integro-differential equations are introduced. In section 5 the limits of low and high scale factor values are considered. Finally, in section 6 the summary and conclusions are given.

2 The Voigt profile function

2.1 Literature

The computation of the Voigt profile is an old issue in literature and many efforts are directed to evaluate it with different techniques. In fact, an analytical explicit representation does not exist and it can be considered a special function itself. It turns out to be related to a number of special function as, for example, the confluent hypergeometric function, the complex complementary error function, the Dawson function, the parabolic cylinder function and the Whittaker function, see e.g. [3, 10, 11, 17, 40, 41, 50] and also to the plasma dispersion function [12]. Its mathematical properties and numerical algorithms are largely studied, e.g. [2, 3, 5, 6, 9, 14, 15, 16, 18, 24, 30, 32, 35, 37, 38, 42, 46, 50, 51, 52, 53] and [1, 7, 8, 21, 22, 23, 27, 28, 29, 36, 40, 41, 48], respectively, and references therein.

It remains up to nowadays a mathematically and computationally interesting problem because computing profiles with high accuracy is still an expensive task.

2.2 Basic definitions

The Gaussian $G(x)$ and the Lorentzian $N(x)$ profiles are defined as

$$G(x) = \frac{1}{\sqrt{\pi}\omega_G} \exp\left[-\left(\frac{x}{\omega_G}\right)^2\right], \quad N(x) = \frac{1}{\pi\omega_L} \frac{\omega_L^2}{x^2 + \omega_L^2}, \tag{1}$$

where ω_G and ω_L are the corresponding widths. From their convolution we have the ordinary Voigt profile $V(x)$

$$V(x) = \int_{-\infty}^{+\infty} N(x-\xi) G(\xi)\, d\xi = \frac{\omega_L/\omega_G}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{\mathrm{e}^{-(\xi/\omega_G)^2}}{(x-\xi)^2 + \omega_L^2}\, d\xi. \tag{2}$$

The main parameter of the Voigt function is the weight-parameter a defined as

$$a = \frac{\omega_L}{\omega_G}. \tag{3}$$

The weight-parameter a is the ratio of the Lorentzian to Gaussian width and then a measure of the relative importance between their influence on the properties of the process. Generally, the $a < 1$ case is important in astrophysics while $a > 1$ in spectroscopy of cold and dense plasmas [6]. In particular, two limits can be considered: $i)$ $a \to 0$; $ii)$ $a \to \infty$. In the first case, the Lorentzian contribution is negligible in respect of the Gaussian one, in other words, $\omega_L \to 0$ so that the Lorentzian profile tends to a Dirac δ-function and the Voigt profile to a Gaussian one. In the second case, the Gaussian contribution is negligible, $\omega_G \to 0$, and the Gaussian profile tends to a Dirac δ-function and the Voigt function to a Lorentzian distribution.

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

$$\widehat{f}(\kappa) = \int_{-\infty}^{+\infty} \mathrm{e}^{+i\kappa x} f(x)\, dx, \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{-i\kappa x} \widehat{f}(\kappa)\, d\kappa, \tag{4}$$

then

$$\widehat{V}(\kappa) = \widehat{G}(\kappa)\widehat{N}(\kappa) = \mathrm{e}^{-\omega_G^2\kappa^2/4}\, \mathrm{e}^{-\omega_L|\kappa|}, \tag{5}$$

and

$$V(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{-i\kappa x} \mathrm{e}^{-\omega_G^2\kappa^2/4 - \omega_L|\kappa|}\, d\kappa = \frac{1}{\pi} \int_0^{+\infty} \mathrm{e}^{-\omega_L\kappa - \omega_G^2\kappa^2/4} \cos(\kappa x) d\kappa. \tag{6}$$

2.3 The differential equations of the Voigt profile function

Consider dimensionless variable $x \to x/\omega_G$, the Voigt function can be re-arranged in the form

$$V(x) = \frac{1}{\sqrt{\pi}\omega_G} H(x), \quad H(x,a) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{e}^{-\xi^2}}{(x-\xi)^2 + a^2} d\xi, \tag{7}$$

and from (6) we have

$$H(x,a) = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} \mathrm{e}^{-a\xi - \xi^2/4} \cos(x\xi)\, d\xi. \tag{8}$$

The differential equations of the Voigt profile function (7) were stated in 1978 by T. Andersen [2]. It is possible to show that the following three differential equations

$$\frac{\partial^2 H}{\partial a^2}+\frac{\partial^2 H}{\partial x^2}=0\,, \tag{9}$$

$$\frac{\partial^2 H}{\partial a^2}-4a\frac{\partial H}{\partial a}+(4a^2+4x^2-2)H=\frac{4a}{\sqrt{\pi}}\,, \tag{10}$$

$$\frac{\partial^2 H}{\partial x^2}+4x\frac{\partial H}{\partial x}+(4a^2+4x^2+2)H=\frac{4a}{\sqrt{\pi}}\,, \tag{11}$$

are solved by substitution using (8). The combination of (9-11) yields the first-order partial differential equation

$$x\frac{\partial H}{\partial x}-a\frac{\partial H}{\partial a}+2(a^2+x^2)H=\frac{2a}{\sqrt{\pi}}\,. \tag{12}$$

2.4 Further representations

The Voigt function has not yet an analytical explicit representation and several alternative representations of (2) were given in literature, e.g. formula (8). The following classical representations can be found in [3, 40, 41, 50].

Combining x and a in the complex variable $z=x-ia$, the function $H(x,a)$ (7) is

$$H(x,a)=Re[W(z)]\,,\quad W(z)=\frac{i}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{e}^{-\xi^2}}{z-\xi}\,d\xi\,, \tag{13}$$

where $W(z)$ is strongly related to the plasma dispersion function [12]. Moreover, the relation of $W(z)$ with the complex complementary error function $\mathrm{erfc}\{-\mathrm{iz}\}$ and the Dawson function $F(z)=\mathrm{e}^{-z^2}\int_0^z \mathrm{e}^{\xi^2}d\xi$ can be used to obtain

$$H(x,a)=Re[W(z)]\,,\quad W(z)=\mathrm{e}^{-z^2}\mathrm{erfc}\{-iz\}\,,\quad a>0\,, \tag{14}$$

$$H(x,a)=Re[W(z)]\,,\quad W(z)=\mathrm{e}^{-z^2}+\frac{2i}{\sqrt{\pi}}F(z)\,. \tag{15}$$

Further representations are given in terms of special functions, see for example the one involving the confluent hypergeometric function ${}_1F_1$ [17, 11]

$$\begin{aligned}K(x,y)=\mathrm{e}^{(y^2-x^2)}\cos(2xy)-\frac{1}{\sqrt{\pi}}\left\{(y+ix)\,{}_1F_1(1;3/2;(y+ix)^2)+\right.\\ \left.(y-ix)\,{}_1F_1(1;3/2;(y-ix)^2)\right\}\,,\end{aligned} \tag{16}$$

and others involving the Whittaker function $W_{k,m}$, the erfc$-$function and the parabolic cylinder function [50, formulae (17,13,16)]

$$\begin{aligned}K(x,y)=\frac{1}{2\sqrt{\pi}}\Big\{(y-ix)^{-1/2}\,\mathrm{e}^{(y-ix)^2/2}\,W_{-1/4,-1/4}((y-ix)^2)+\\ (y+ix)^{-1/2}\,\mathrm{e}^{(y+ix)^2/2}\,W_{-1/4,-1/4}((y+ix)^2)\Big\}\,,\end{aligned} \tag{17}$$

$$K(x,y) = \frac{1}{2}\left\{ \mathrm{e}^{(y-ix)^2}\,\mathrm{erfc(y-ix)} + \mathrm{e}^{\mathrm{(y+ix)}^2}\,\mathrm{erfc(y+ix)} \right\}, \tag{18}$$

$$K(x,y) = \frac{\mathrm{e}^{(y^2-x^2)/2}}{\sqrt{2\pi}}\left\{ \mathrm{e}^{-ixy} D_{-1}[\sqrt{2}(y-ix)] + \mathrm{e}^{+ixy} D_{-1}[\sqrt{2}(y+ix)] \right\}. \tag{19}$$

More recent representations are those derived in 2001 by Di Rocco *et al.*[6] and in 2007 by Zaghloul [51] "completing" a previous formula published in 2005 by Roston & Obaid [35]. Di Rocco *et al.* [6] derived

$$H(x) = \sum_{n=0}^{\infty} (-1)^n \times \left\{ \frac{1}{\Gamma(n+1)} M\left(\frac{2n+1}{2}, \frac{1}{2}; a^2\right) - \frac{2a}{\Gamma\left(\frac{2n+1}{2}\right)} M\left(n+1, \frac{3}{2}; a^2\right) \right\} x^{2n}, \tag{20}$$

where $M(\alpha,\beta;z)$ is the confluent hypergeometric function. Roston & Obaid [35] derived the following representation

$$H(x,a) = [1-\mathrm{erf(a)}]\,\mathrm{e}^{(-\mathrm{x}^2+\mathrm{a}^2)}\cos(2\mathrm{xa}) - \frac{2\mathrm{e}^{-x^2}}{\sqrt{\pi}}\left[\cos(2xa)\int_0^x \mathrm{e}^{\xi^2}\sin(2\xi a)\,d\xi - \sin(2xa)\int_0^x \mathrm{e}^{\xi^2}\cos(2\xi a)\,d\xi\right],$$

that was re-written as a single proper integral with a damped sine integrand by Zaghloul [51]

$$H(x,a) = [1-\mathrm{erf(a)}]\,\mathrm{e}^{(-\mathrm{x}^2+\mathrm{a}^2)}\cos(2\mathrm{xa}) + \frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{(-x^2+\xi^2)}\sin[2a(x-\xi)]\,d\xi. \tag{21}$$

Recently, He & Zhang [16] 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 this representation assumes negative value in contrast with the non negative character of the Voigt function. For this reason that result has to be considered wrong. A different and less direct argoument is used in [53] to show the falsity of He & Zhang claim.

3 The Voigt profile function generalization via Lévy stable distributions

3.1 The probabilistic generalization of the Voigt profile function

It is well known that if X_1 and X_2 are two independent random variables with probability density function (PDF) q_1 and q_2, respectively, then the PDF $p(z)$ of the random variable $Z = X_1 + X_2$ is given by the convolution integral

$$p(z) = \int_{-\infty}^{+\infty} q_1(z-x_2)\,q_2(x_2)\,dx_2. \tag{22}$$

From (2) and (22), the Voigt profile can be seen as the resulting PDF of the sum of two independent random variables, one with Gaussian PDF and the other with Lorentzian PDF.

The Voigt function has been generalized in literature in different ways, e.g. on physical ground considering self-broadening [33], or as a mathematical generalization: in [44, 45] the cosine function in (6) is replaced by the Bessel function and by the Wright function, respectively, in [19] the generalization in [44, 45] is further generalized to multi-variables, in [37] the integrand function in formula (6) is multiplied by a polynomial.

In this paper we propose a probabilistic generalization in the framework of Lévy distributions. It is well known that the Gaussian and the Lorentzian distributions are two special cases of the class $\{L_\alpha(x)\}$ of the symmetric Lévy stable distributions, where α, $0 < \alpha \le 2$, is called characteristic exponent. A straightforward generalization in the probabilistic sense is then introduced as the sum of two independent random variables with symmetric stable densities. Mathematically, this corresponds to the convolution of two arbitrary symmetric Lévy densities of characteristic exponents α_1 and α_2. Denoting with $\mathcal{V}(x)$ the generalized Voigt function, without considering any width factor, its integral representation and its characteristic function $\widehat{\mathcal{V}}(\kappa)$ are

$$\mathcal{V}(x) = \int_{-\infty}^{+\infty} L_{\alpha_1}(x-\xi) L_{\alpha_2}(\xi)\, d\xi\,, \quad \widehat{\mathcal{V}}(\kappa) = \mathrm{e}^{-|\kappa|^{\alpha_1} - |\kappa|^{\alpha_2}}\,. \tag{23}$$

The plots of $\mathcal{V}(x)$ are shown in Fig. 1 for different pairs of (α_1, α_2).

Looking at (23) a further generalization of the Voigt function can be stated. In fact, the sum of two addenda, in the argoument of the exponential function, can be replace by a sum of an arbitrary number of addenda each of them with a weight w_j, $j = 1, \ldots, n$, i.e.

$$\widehat{\mathcal{V}}_d(\kappa) = \mathrm{e}^{-\sum_{j=1}^{n} w_j |\kappa|^{\alpha_j}}\,,$$

or by a continuum distribution with a weight function $w(\alpha)$

$$\widehat{\mathcal{V}}_c(\kappa) = \mathrm{e}^{-\int_0^2 w(\alpha)|\kappa|^{\alpha} d\alpha}\,. \tag{24}$$

4 The scale factor and the parametric equations

4.1 From the weight-parameter to the scale factor

In the previous sections the widths ω_G and ω_L are considered constants and the weight-parameter a fixed. However, differently from previous papers on the topic, we would like to know what happens when the widths ω_G and ω_L changes in space or time with a power law in respect of a scale factor. This is the inhomogeneous or not stationary case if the scale factor corresponds to the distance from an origin or the elapsed time, respectively. Conversely, constant values of widths can be considered for homogeneous and stationary case. In the present section we consider the Voigt profile in terms of a scale factor τ common for both spatial inhomogeneity and temporal non-stationarity.

It is well known that the Lévy density functions $L_\alpha(x,\tau)$ are the fundamental solutions of the space-fractional diffusion equation, see e.g. [4, 13, 25, 43, 47],

$$\frac{\partial L_\alpha(x,\tau)}{\partial \tau} = {}_xD^\alpha L_\alpha(x,\tau)\,, \quad L_\alpha(x,0) = \delta(x)\,, \quad 0 < \alpha \le 2\,, \tag{25}$$

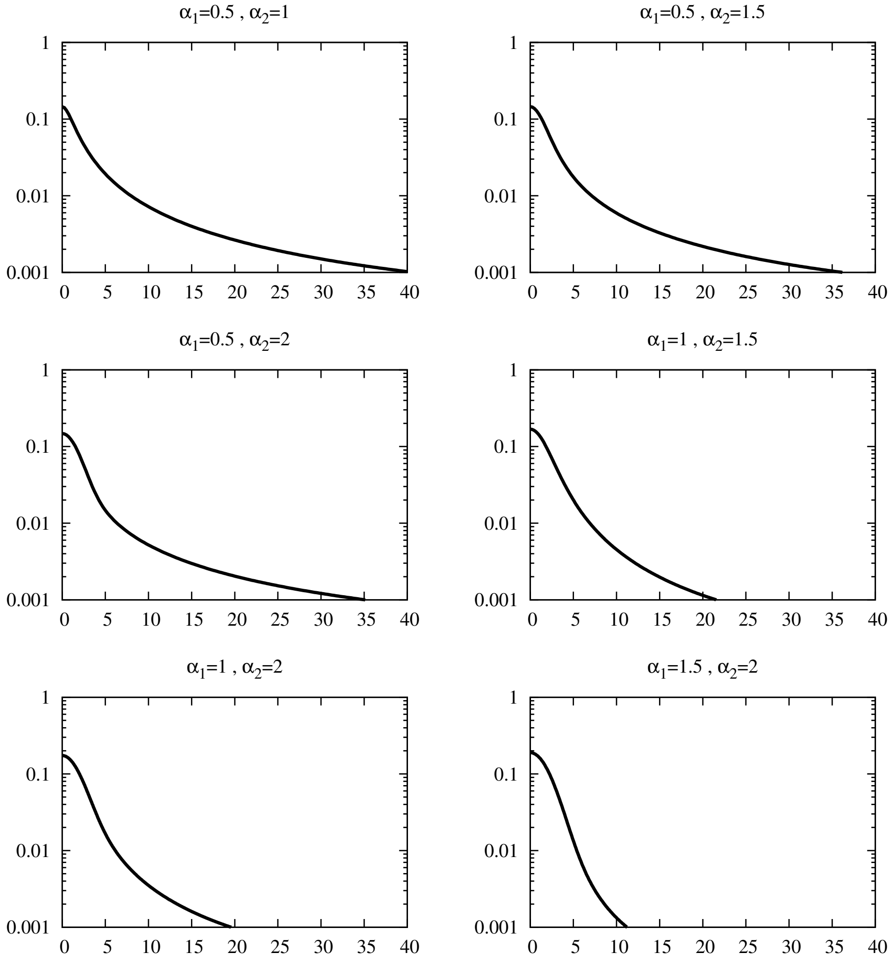

Fig. 1 Plots of the generalized Voigt function $\mathcal{V}(x)$, for symmetry reasons on the positive semi-axis, for the pairs $(\alpha_1, \alpha_2) = \{(0.5,1),(0.5,1.5),(0.5,2),(1,1.5),(1,2),(1.5,2)\}$.

where ${}_xD^\alpha$ is the Riesz space-fractional derivative of order α. The pseudo-differential operator ${}_xD^\alpha$ is defined in terms of its Fourier transform $-|\kappa|^\alpha$. The Fourier transform of ${}_xD^\alpha f(x)$ is $-|\kappa|^\alpha \widehat{f}(\kappa)$, and it admits the explicit representation

$$
{}_xD^\alpha f(x) = \begin{cases} \dfrac{\Gamma(1+\alpha)}{\pi} \sin\left(\dfrac{\alpha\pi}{2}\right) \displaystyle\int_0^{+\infty} \dfrac{f(x+\xi) - 2f(x) + f(x-\xi)}{\xi^{1+\alpha}} \, d\xi \,, & \alpha \neq 1 \,, \\ -\dfrac{1}{\pi} \dfrac{d}{dx} \displaystyle\int_{-\infty}^{+\infty} \dfrac{f(\xi)}{x-\xi} \, d\xi \,, & \alpha = 1 \,, \end{cases} \tag{26}
$$

and the limit ${}_xD^\alpha f(x) = d^2 f/dx^2$ when $\alpha = 2$. The reader acquainted with integral transforms can recognize that ${}_xD^1 f(x)$ is related to the Hilbert transform. For more details on fractional derivatives the interested reader is referred to texts on fractional calculus, see e.g. [20, 34, 39].

Solutions of (25) have the following power law scaling:

$$L_\alpha(x,\tau) = \tau^{-1/\alpha} L_\alpha\left(\frac{x}{\tau^{1/\alpha}}\right). \tag{27}$$

We observe that the processes defined in (27) are self-similar and they obey to the same power law scaling for any value of the scale factor τ. In particular, for $\alpha = 2$ and $\alpha = 1$ the Gaussian and the Lorentzian densities are recovered, respectively, and from (27) we have that

$$\omega_G \propto \tau^{1/2} \quad \text{and} \quad \omega_L \propto \tau. \tag{28}$$

4.2 The ordinary Voigt function case

From scaling (27), the ordinary Voigt function is

$$V(x,\tau) = \int_{-\infty}^{+\infty} L_1(x-\xi,\tau) L_2(\xi,\tau)\, d\xi = \tau^{-3/2} \int_{-\infty}^{+\infty} N\left(\frac{x-\xi}{\tau}\right) G\left(\frac{\xi}{\tau^{1/2}}\right) d\xi.$$

In this case, from (4), the characteristic function of $V(x,\tau)$ is

$$\widehat{V}(\kappa,\tau) = \mathrm{e}^{-|\kappa|\tau - \kappa^2\tau}, \quad \widehat{V}(\kappa,0) = 1. \tag{29}$$

It is possible to show that the Voigt function $V(x,\tau)$ is the solution of the following integro-differential equation

$$\frac{\partial V}{\partial \tau} = \frac{\partial^2 V}{\partial x^2} + {}_xD^1 V(x,\tau), \quad V(x,0) = \delta(x), \tag{30}$$

or in explicit form

$$\frac{\partial V}{\partial \tau} = \frac{\partial^2 V}{\partial x^2} - \frac{1}{\pi}\frac{\partial}{\partial x}\int_{-\infty}^{+\infty} \frac{V(\xi,\tau)}{x-\xi} d\xi, \quad V(x,0) = \delta(x).$$

In fact, applying the Fourier transform (4), Eq. (30) becomes

$$\frac{\partial \widehat{V}}{\partial \tau} = -\kappa^2 \widehat{V}(\kappa,\tau) - |\kappa| \widehat{V}(\kappa,\tau),$$

which is solved by (29).

4.3 The generalized Voigt function case

Following scaling (27), the generalized Voigt function is

$$\mathcal{V}(x,\tau) = \tau^{-1/\alpha_1 - 1/\alpha_2} \int_{-\infty}^{+\infty} L_{\alpha_1}\left(\frac{x-\xi}{\tau^{1/\alpha_1}}\right) L_{\alpha_2}\left(\frac{\xi}{\tau^{1/\alpha_2}}\right) d\xi, \tag{31}$$

and its characteristic function is

$$\widehat{\mathcal{V}}(\kappa,\tau) = \mathrm{e}^{-|\kappa|^{\alpha_1}\tau-|\kappa|^{\alpha_2}\tau}, \quad \widehat{\mathcal{V}}(\kappa,0) = 1\,. \tag{32}$$

In this case, it possible to show that formula (31) is the solution of the following integro-differential equation

$$\frac{\partial \mathcal{V}}{\partial \tau} = {}_xD^{\alpha_1}\mathcal{V}(x,\tau) + {}_xD^{\alpha_2}\mathcal{V}(x,\tau)\,, \quad \mathcal{V}(x,0) = \delta(x)\,. \tag{33}$$

In fact, after the Fourier transformation, Eq. (33) becomes

$$\frac{\partial \widehat{\mathcal{V}}}{\partial \tau} = -|\kappa|^{\alpha_1}\widehat{\mathcal{V}}(\kappa,\tau) - |\kappa|^{\alpha_2}\widehat{\mathcal{V}}(\kappa,\tau)\,,$$

which is solved by (32). When $\alpha_1 = 1$ and $\alpha_2 = 2$ the integro-differential equation (33) reduces to Eq. (30) and the ordinary Voigt function is recovered, i.e. $\mathcal{V}(x,\tau) \equiv V(x,\tau)$. The evolution of $\mathcal{V}(x,\tau)$ for different pairs of (α_1,α_2) with $\tau = 0.1, 1, 10$ is shown in Fig. 2.

The integro-differential equation (33), as (30), can be classified as *space-fractional diffusion equation of double order*. The generalization stated in (24) is the solution of the following integro-differential equation, which results to be the *space-fractional diffusion equation of distributed order* [4, 43],

$$\frac{\partial \widehat{\mathcal{V}}}{\partial t} = \int_0^2 {}_xD^{\alpha}\widehat{\mathcal{V}}(x,\tau)\, w(\alpha)\, d\alpha\,, \quad \mathcal{V}(x,0) = \delta(x)\,. \tag{34}$$

Applying the Fourier transformation (4) in (34), the characteristic function of the solution of (34) is

$$\widehat{\mathcal{V}}(\kappa,\tau) = \mathrm{e}^{-\tau\int_0^2 |\kappa|^{\alpha}\, w(\alpha)\, d\alpha}, \quad \widehat{\mathcal{V}}(\kappa,0) = 1\,.$$

Equation (33) is recovered when $w(\alpha) = \delta(\alpha-\alpha_1) + \delta(\alpha-\alpha_2)$ and Eq. (30) when $w(\alpha) = \delta(\alpha-1) + \delta(\alpha-2)$.

5 The asymptotic scaling laws for low and high scale-factor

The Voigt (2) and the generalized Voigt (23) profiles are derived from the convolutions of two self-similar processes with different scaling laws and, as a consequence, the similarity is lost. However, we ask which are the scaling laws of the Voigt functions in the limits of low and high values of the scale-factor τ.

Since for Lévy stable densities with $\alpha \neq 2$ the mean square displacement diverges, the same occurs for the ordinary and the generalized Voigt functions then, to analyze the scaling laws when $\tau \to 0$ and $\tau \to \infty$, the variance $\langle x^2 \rangle$ cannot be used. However, West & Seshadri [49] introduced for the Lévy densities $L_\alpha(x)$ the q-th fractional modulo moment $\langle |x^q| \rangle$ when $q < \alpha$. Then, the characteristic scaling of Lévy process can be study by mean the quantity $\langle |x^q| \rangle^{1/q}$. In this respect, Zolotarev [54] derived the following formula that holds for a generic probability density $f(x)$

$$\langle |x|^q \rangle = \frac{2}{\pi}\Gamma(1+q)\sin\left(\frac{\pi q}{2}\right)\int_0^{+\infty}(1 - Re[\widehat{f}(\kappa)])\kappa^{-q-1}\, d\kappa\,.$$

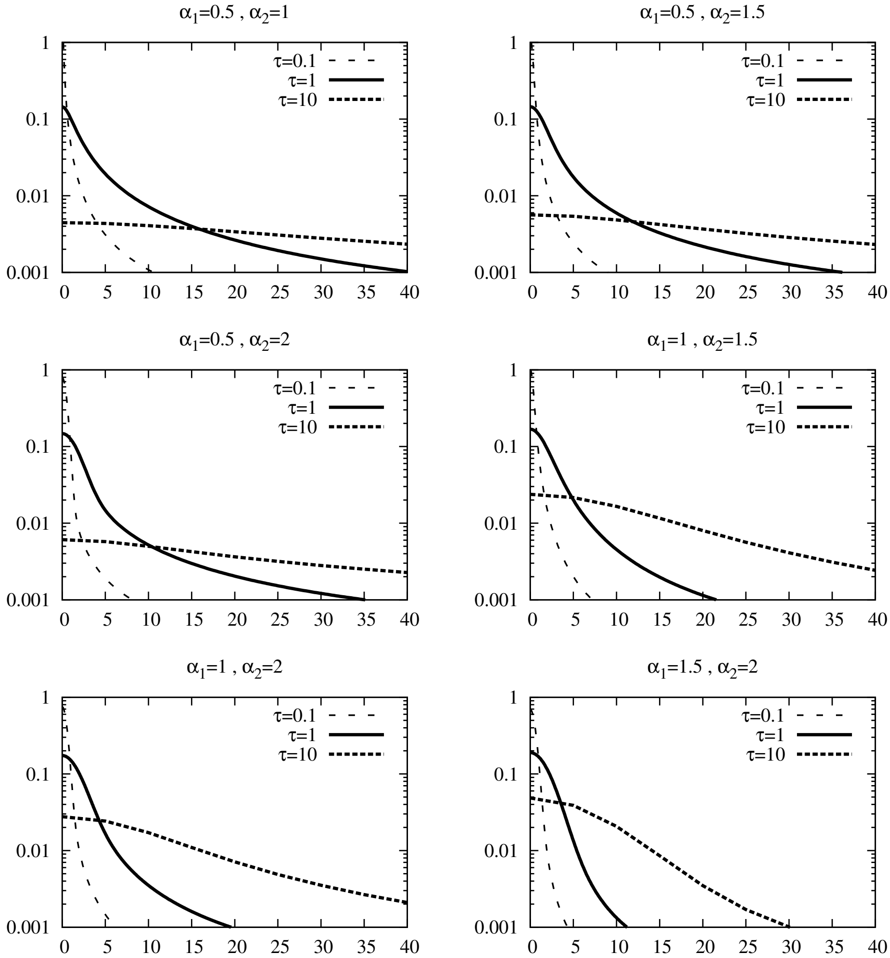

Fig. 2 The evolution of the generalized Voigt function $\mathcal{V}(x,\tau)$, for symmetry reasons on the positive semi-axis, for the pairs $(\alpha_1,\alpha_2) = \{(0.5,2),(1.5,2),(0.5,1.5),(1,1.5)\}$ with $\tau = 0.1,1,10$.

In our case $\widehat{f}(\kappa)$ is replaced by $\widehat{\mathcal{V}}(\kappa,\tau)$ and $q < \min\{\alpha_1,\alpha_2\}$. In papers [4, 43] the limits $(\tau \to 0\,, \tau \to \infty)$ are computed using the Zolotarev formula for the case of convolution of two Lévy densities.

Here, in order to study the asymptotic scaling laws, the Mellin transform is used. In fact

$$\langle |x|^q \rangle = 2\int_0^{+\infty} x^q \mathcal{V}(x,\tau)\,dx = 2\,\mathcal{V}^*(q+1,\tau)\,, \quad 0 < q < \min\{\alpha_1,\alpha_2\}\,, \tag{35}$$

where $\mathcal{V}^*(s)$ is the Mellin transform of $\mathcal{V}(x)$, $x > 0$, defined as [31]

$$\mathcal{V}^*(s) = \int_0^{+\infty} \mathcal{V}(x) x^{s-1}\,dx\,, \qquad \mathcal{V}(x) = \frac{1}{2\pi i}\int_{c-\infty i}^{c+\infty i} \mathcal{V}^*(s) x^{-s}\,ds\,. \tag{36}$$

Without loss in generality, let us state $\alpha_1 < \alpha_2$. Starting from (23) and following [26, 30], the Mellin-Barnes integral representation of the generalized Voigt function $\mathcal{V}(x)$ is

$$\begin{aligned}\mathcal{V}(x,\tau) = \frac{\tau^{-1/\alpha_2}}{\alpha_2\pi}\frac{1}{2\pi i}\int_{\mathcal{L}_0}\frac{1}{2\pi i}\int_{\mathcal{L}_1}\Gamma(s_0)\Gamma(s_1)\Gamma\left(\frac{1-s_0-\alpha_1 s_1}{\alpha_2}\right)\\ \times\quad \tau^{s_0/\alpha_2+(\alpha_1/\alpha_2-1)s_1}\cos(s_0\pi/2)x^{-s_0}\,ds_0 ds_1\,.\end{aligned} \tag{37}$$

Hence its Mellin transform is

$$\begin{aligned}\mathcal{V}^*(s_1,\tau) = &\frac{\tau^{(s_0-1)/\alpha_2}}{\alpha_2\pi}\Gamma(s_0)\cos(s_0\pi/2)\\ &\times\quad \frac{1}{2\pi i}\int_{\mathcal{L}_1}\Gamma(s_1)\Gamma\left(\frac{1-s_0-\alpha_1 s_1}{\alpha_2}\right)\tau^{(\alpha_1/\alpha_2-1)s_1}ds_1\,,\end{aligned} \tag{38}$$

and finally,

$$\begin{aligned}\langle|x|^q\rangle &= 2\mathcal{V}^*(q+1,\tau)\\ &= -\frac{2\,\tau^{q/\alpha_2}}{\alpha_2\pi}\Gamma(q+1)\sin(q\pi/2)\frac{1}{2\pi i}\int_{\mathcal{L}_1}\Gamma(s_1)\Gamma\left(\frac{-q-\alpha_1 s_1}{\alpha_2}\right)\tau^{(\alpha_1/\alpha_2-1)s_1}ds_1\,.\end{aligned} \tag{39}$$

Applying the residue theorem to $\Gamma\left(\frac{-q-\alpha_1 s_1}{\alpha_2}\right)$, we obtain the convergent series for $\tau\to\infty$,

$$\langle|x|^q\rangle = -\frac{2\tau^{q/\alpha_1}}{\alpha_1\pi}\Gamma(q+1)\sin(q\pi/2)\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Gamma\left(\frac{\alpha_2 n-q}{\alpha_1}\right)\tau^{-n(\alpha_2/\alpha_1-1)}\,. \tag{40}$$

Applying the residue theorem to $\Gamma(s_1)$, we obtain the convergent series for $\tau\to 0$,

$$\langle|x|^q\rangle = -\frac{2\tau^{q/\alpha_2}}{\alpha_2\pi}\Gamma(q+1)\sin(q\pi/2)\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Gamma\left(\frac{\alpha_1 n-q}{\alpha_2}\right)\tau^{n(1-\alpha_1/\alpha_2)}\,. \tag{41}$$

Then the two limits under consideration give

$$\begin{cases}\langle x^q\rangle^{1/q}\propto\tau^{1/\alpha_2}\,,\ \ \tau\to 0\,;\\ \langle x^q\rangle^{1/q}\propto\tau^{1/\alpha_1}\,,\ \tau\to\infty\,.\end{cases} \tag{42}$$

To conclude, the ordinary and generalized Voigt profile functions are not self-similar and their power law scaling depends on the limit of the scale factor considered. This occurs even if the two Lévy densities convoluted are self-similar. In the limit $\tau\to 0$, the corresponding scaling law of the generalized Voigt profile is governed by the Lévy densities with a higher value of the characteristic exponent, while in the limit $\tau\to\infty$ by that with a lower value. In particular, for the ordinary Voigt profile $(\alpha_1 = 1\,,\alpha_2 = 2)$ the process scales as $\tau^{1/2}$ and τ for low and high values of the scale factor, respectively.

This means that if the power law represent inhomogeneity, or not stationarity, the resulting profile is approximated by a Gaussian for small distances from an origin, or small elapsed times, and it is approximated by a Lorentzian for large distances, or large elapsed times. This result is consistent with the usual limits $a\to 0$ and $a\to\infty$, see Fig. 1.

6 Conclusion

In the present paper we have considered the Voigt profile function. It is an interesting function that emerges from molecular spectroscopy and atmospheric radiative transfer as the combined effects of Doppler and pressure broadenings. The Voigt function is the convolution of the Gaussian (due to the Doppler broadening) and the Lorentzian (due to the pressure broadening) densities.

The Gaussian and the Lorentzian densities belong to the symmetric class of the Lévy stable densities so a straightforward generalization of their convolution is obtained by the convolution of two arbitrary symmetric Lévy densities.

Generally, Voigt profile characteristics are studied with respect to a weight-parameter a that is the ratio of Lorentzian to Gaussian widths, $a = \omega_L/\omega_G$, and it is assumed to be a constant property of the process. Differently, here we have considered both widths depending on a scale factor τ that can be representative of inhomogeneity or not stationarity. We have introduced parametric integro-differential equations for the ordinary and the generalized Voigt functions. These integro-differential equations can be classified as *space-fractional diffusion equations of double order* because they include two Riesz space-fractional derivatives. Further generalization can be obtained considering *space-fractional diffusion equations of distributed order*.

Finally, the limits of the Voigt function for low and high values of the scale factor are considered. In this respect, the Voigt function turns out to be not self similar, even if it is expressed as the convolution of two self similar Lévy processes. In fact, the Voigt profile has not a single power law scaling for each values of the scale factor, as it is for self similar processes, but its scaling law is governed by the Lévy density with the higher value of the characteristic exponent when $\tau \to 0$ and by the Lévy density with the lower value of the characteristic exponent when $\tau \to \infty$. In the ordinary case, it means by the Guassian density when $\tau \to 0$ and by the Lorentzian density when $\tau \to \infty$. These results are not in opposition with previous studied limits $a \to 0$ and $a \to \infty$, but here they are obtained as consequence of two different power law scalings for the Doppler and the pressure broadenings and not by variation of the relative weight of density widths.

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