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Journal of Quantitative Spectroscopy & Radiative Transfer

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Generalized Voigt functions and their derivatives

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Received 5 May 2006; received in revised form 19 August 2006; accepted 22 August 2006

Abstract

This paper deals with a special class of functions called generalized Voigt functions $H^{(n)}(x,a)$ and $G^{(n)}(x,a)$ and their partial derivatives, which are useful in the theory of polarized spectral line formation in stochastic media. For $n=0$ they reduce to the usual Voigt and Faraday–Voigt functions $H(x,a)$ and $G(x,a)$. A detailed study is made of these new functions. Simple recurrence relations are established and employed for the calculation of the functions themselves and of their partial derivatives. Asymptotic expansions are given for large values of x and a. They are used to examine the range of applicability of the recurrence relations and to construct a numerical algorithm for the calculation of the generalized Voigt functions and of their derivatives valid in a large (x,a) domain. It is also shown that the partial derivatives of the usual $H(x,a)$ and $G(x,a)$ can be expressed in terms of $H^{(n)}(x,a)$ and $G^{(n)}(x,a)$.

Keywords: Line shapes; Voigt function; Dispersion function; Recurrence relations; Partial derivatives

1. Introduction

The Voigt function $H(x,a)=H^{(0)}(x,a)$ is widely used to represent spectral line shapes in many fields of physics such as astrophysics, atmospheric spectroscopy, plasma physics, etc. wherever measurements and theory of spectral line profiles are involved. The quantity x is the non-dimensional frequency and a is the damping parameter, both expressed in Doppler width units. In the presence of a magnetic field, the medium becomes anisotropic, causing differential absorption/refraction for different states of polarization. The absorption of radiation is described by the imaginary part of the complex refractive index of the medium. The real part describes the dispersive effects, also called magneto-optical effects, when the anisotropy is caused by the presence of a magnetic field. The dispersive or magneto-optical effects involve a line shape function called "anomalous dispersion function" $G(x,a)=G^{(0)}(x,a)$ (also denoted by $K(x,a)$, or $F(x,a)$, or $L(x,a)$ in literature). These functions $H^{(0)}(x,a)$ and $G^{(0)}(x,a)$ together have been traditionally employed in the theory of Zeeman line formation, which involves absorption and emission of photons between the Zeeman sub-states of an atom.

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0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2006.08.011

Please cite this article as: M. Sampoorna et al., Generalized Voigt functions and their derivatives, Journal of Quantitative Spectroscopy & Radiative Transfer (2006), doi:10.1016/j.jqsrt.2006.08.011

Magnetic fields met in astrophysics, say stellar atmospheres, will have in general random fluctuations and the line formation theory has to be extended to account for the randomness of the field. When the characteristic scale of the fluctuations is much smaller than the photon mean free path, randomness of the field can be taken into account by locally averaging (convolving) the Zeeman "propagation matrix" with a given vector magnetic field probability distribution function (see [1–4], and references cited therein). In some cases the averaging process can be performed analytically, for example, when the distribution function of the magnetic field is an isotropic Gaussian. Then one encounters integrals of the type

$$\int_{-\infty}^{+\infty} \mathrm{e}^{-(y-y_0)^2} F(x - x_0 y, a)\, P(y)\, \mathrm{d}y, \tag{1}$$

where F is either $H^{(0)}$ or $G^{(0)}$ and $P(y)$ is a polynomial (see [2,5,6]). Here y and y_0 are the magnitude of the random magnetic field and of its mean value, in units of the RMS value about the mean field, and $x_0 y$ the Zeeman shift by the random field in Doppler width units. These integrals can be expressed in terms of a new class of functions $H^{(n)}(x,a)$ and $G^{(n)}(x,a)$ introduced in Dolginov and Pavlov [5] (see Eqs. (2) and (3) below). They appeared first in the theory of the turbulent Zeeman effect, but may be of interest in other related fields. This has motivated us to study them in detail. Hereafter, for convenience, we drop the arguments (x,a) on these functions.

Non-linear least square fitting algorithms require higher-order partial derivatives of $H^{(0)}$ and $G^{(0)}$ in extracting physical parameters from the polarized spectral line data (see [1,7,8]). Rapid approximations to compute the derivatives of $H^{(0)}$ and $G^{(0)}$ have been developed by Heinzel [9] and Wells ([10], see also references cited therein). In this paper we discuss $H^{(n)}$ and $G^{(n)}$ for $n \geqslant 1$, and also their mth order partial derivatives. They will be essential for the development of inversion techniques employing Zeeman line formation theory in turbulent media [2,3,5,6].

In Section 2 we define $H^{(n)}$ and $G^{(n)}$ and introduce a new function $W^{(n)}(z)$, where z is complex. Starting from this function $W^{(n)}(z)$ we derive recurrence relations for $H^{(n)}$ and $G^{(n)}$. We show that $G^{(n)}$ can be expressed in terms of the real Dawson's function for the special case of $a = 0$. In this section 2, we also graphically present the $H^{(n)}$ and $G^{(n)}$ up to seventh order, for different values of a, and discuss the properties of these functions as well as computational aspects. A method for obtaining simple recurrence relations for the partial derivatives of $H^{(n)}$ and $G^{(n)}$ with respect to x and a is presented in Section 3, along with the computational details. In Section 4, we show that partial derivatives of the conventional Voigt and Faraday–Voigt functions $H^{(0)}$ and $G^{(0)}$ can be expressed in terms of $H^{(n)}$ and $G^{(n)}$.

2. Generalized Voigt functions $H^{(n)}$ and $G^{(n)}$

2.1. Definitions and recurrence relations

The functional form of $H^{(n)}$ and $G^{(n)}$ is

$$H^{(n)}(x,a) = \frac{a}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{u^n \mathrm{e}^{-u^2}\, \mathrm{d}u}{(x-u)^2 + a^2} \tag{2}$$

and

$$G^{(n)}(x,a) = \frac{1}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{u^n (x-u) \mathrm{e}^{-u^2}\, \mathrm{d}u}{(x-u)^2 + a^2}. \tag{3}$$

We know that for $n = 0$, the usual $H^{(0)}$ and $G^{(0)}$ functions are the real and imaginary parts of the function $W^{(0)}(z)$, known as the complex probability function or Faddyeva function (see for e.g. [11–13]). In a similar way $H^{(n)}$ and $G^{(n)}$ are the real and imaginary parts of a complex-valued function defined in Frisch et al. [2] as

$$W^{(n)}(z) = \frac{\mathrm{i}}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{u^n \mathrm{e}^{-u^2}\, \mathrm{d}u}{z - u}, \quad \Im(z) > 0, \tag{4}$$

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where $z = x + \mathrm{i}a$, with x and a being real and $a > 0$. The function $W^{(n)}$ is analytic in the upper-half of the complex plane. It has a branch cut along the real axis. The limit $a \to 0$ can be taken in the definitions of $H^{(n)}(x, a)$ and $G^{(n)}(x, a)$. When $a \to 0$, the Lorentzian in Eq. (2) becomes a delta function and the integral can be calculated exactly. The $H^{(n)}(x, 0)$ are modified Gaussian functions (see Eq. (9)). As for the $G^{(n)}(x, 0)$ functions, they can be expressed in terms of the real Dawson function (see Eq. (12)).

The $W^{(n)}$ satisfy a recurrence formula which in turn leads to simple recurrence relations for $H^{(n)}$ and $G^{(n)}$ and enable us to propose a method of calculation. In the numerator of Eq. (4), we can write $u^n = u^{n-1}(u - z + z)$ and immediately obtain

$$W^{(n)}(z) = zW^{(n-1)}(z) - \frac{\mathrm{i}}{\pi^{3/2}} \int_{-\infty}^{+\infty} u^{n-1} \mathrm{e}^{-u^2} \, \mathrm{d}u, \quad n \geqslant 1. \tag{5}$$

Separating the real and imaginary parts, we find the two recurrence relations

$$H^{(n)}(x, a) = xH^{(n-1)}(x, a) - aG^{(n-1)}(x, a), \tag{6}$$

$$G^{(n)}(x, a) = xG^{(n-1)}(x, a) + aH^{(n-1)}(x, a) - \frac{1}{\pi} c^{(n-1)}, \tag{7}$$

where $c^{(n-1)}$ is a constant which is zero when n is even. When n is odd, say $n = 2k + 1$, with k a positive integer, we have

$$c^{(2k)} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} u^{2k} \mathrm{e}^{-u^2} \, \mathrm{d}u = \frac{1.3 \ldots (2k-1)}{2^k}. \tag{8}$$

The recurrence relations take very simple forms when the Voigt parameter $a = 0$. For $H^{(n)}$, we obtain from the recurrence relation, or directly from Eq. (2),

$$H^{(n)}(x, 0) = \frac{1}{\sqrt{\pi}} x^n \mathrm{e}^{-x^2}. \tag{9}$$

For $G^{(n)}$ we have two different expressions depending on the parity of n. For odd values of n ($n = 2k + 1$),

$$G^{(2k+1)}(x, 0) = xG^{(2k)}(x, 0) - \frac{1}{\pi} c^{(2k)}, \tag{10}$$

and for even values of n ($n = 2k$),

$$G^{(2k)}(x, 0) = xG^{(2k-1)}(x, 0). \tag{11}$$

$G^{(0)}(x, 0)$ can be simply expressed in terms of the real Dawson's function, $D(x)$, as shown in Heinzel [9]. The recurrence relations (10) and (11) yield higher-order $G^{(n)}(x, 0)$ ($n \geqslant 1$). We list below the first four $G^{(n)}(x, 0)$ for convenience:

$$\begin{aligned}
G^{(0)}(x, 0) &= \frac{2}{\pi} D(x), \\
G^{(1)}(x, 0) &= \frac{1}{\pi}[-1 + 2xD(x)], \\
G^{(2)}(x, 0) &= \frac{x}{\pi}[-1 + 2xD(x)], \\
G^{(3)}(x, 0) &= \frac{1}{\pi}\left[-\frac{1}{2} - x^2 + 2x^3 D(x)\right],
\end{aligned} \tag{12}$$

where the real Dawson's function is defined (see, for example, [11]) as

$$D(x) = \mathrm{e}^{-x^2} \int_0^x \mathrm{e}^{t^2} \, \mathrm{d}t = \frac{1}{2} \int_0^{\infty} \mathrm{e}^{-t^2/4} \sin(xt) \, \mathrm{d}t. \tag{13}$$

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2.2. Some properties of the generalized Voigt functions

We have calculated the $H^{(n)}$ and $G^{(n)}$ with recurrence relations given above. They have to be initialized with the values of $H^{(0)}$, $G^{(0)}$, and $D(x)$. For the calculations of the latter we have used the algorithm given in Matta and Reichel [14] (see also [15]). Recently an efficient algorithm has been proposed by Wells [10]. We have compared graphically the results presented in [10] (see his Figs. 1, 2, 11 and 12) for $H^{(0)}$, $G^{(0)}$ and first partial derivative of $H^{(0)}$, with the results of the Matta and Reichel algorithm. We have found that the latter has a comparable accuracy and have retained it for its simplicity. Actually many algorithms are available for computation of $H^{(0)}$ and $G^{(0)}$. They have been introduced for studies in atmospheric physics or astrophysics. Schreier [16] has made a comparative study of some of them based on the accuracy and computational speed (see also [10]). Unfortunately these studies do not include the algorithm of Matta and Reichel [14] but they show, for example, that algorithms by Humlíček [13] and Wells [10] provide a greater accuracy in the computation of $H^{(0)}$ and $G^{(0)}$ over a larger domain in x and a than that of Hui et al. [17].[2] In Section 2.3 we give some details on the Matta and Reichel algorithm and discuss accuracy problems, but first we show the overall behavior of $H^{(n)}$ and $G^{(n)}$ around the line center. They are displayed in Figs. 1 and 2, respectively, for $n = 0$–7 and several damping parameter values ($a = 0, 0.1, 0.5, 1.0, 2.0$). For computing $H^{(n)}(x,0)$, we use recurrence relation (6), although Eq. (9) can also be employed. Similarly, for computing $G^{(0)}(x,0)$, the first one among the set of Eqs. (12) is used, and for $n \geqslant 1$, recurrence relation (Eq. (7)) is used.

We now discuss Fig. 1. The first obvious remark is that for even n the $H^{(n)}$ are even functions of x, and, for odd n, odd functions of x. For $a = 0$, we can easily find the position and amplitudes of the maxima. Taking the derivative of Eq. (9) with respect to x, we get

$$x_{\max}^{(n)} = \pm\sqrt{n/2}, \tag{14}$$

and hence the value of $H^{(n)}$ at $x_{\max}$ is

$$|H^{(n)}(x_{\max}^{(n)}, 0)| = \frac{1}{\sqrt{\pi}}\left(\frac{n}{2}\right)^{n/2} \mathrm{e}^{-n/2}. \tag{15}$$

We note that the absolute value of $H^{(n)}$ at maxima decreases from $n = 0$ to 2, but then increases for $n > 2$ as $\exp[n/2(\ln(n/2) - 1)]$. When $a \neq 0$, we observe a broadening of the peaks and a decrease in their amplitudes. For even n, the broadening of the individual peaks causes a superposition, resulting in profiles with a single peak at line center.

We now turn to Fig. 2. The definition of $G^{(n)}$ shows immediately that the $G^{(n)}$ are odd functions of x for even n and even functions of x for odd n. For $a = 0$, the recurrence relations (10) and (11), and the explicit expressions given in Eq. (12) allow one to understand the qualitative behavior of the $G^{(n)}$. The function $G^{(0)}$ is an odd function of x, which is zero at $x = 0$ and has two symmetric peaks around $|x| = 1$ (the maximum of the Dawson's integral is at $x = 0.924$ and has a value 0.541, Abramowitz and Stegun [11], pp. 298, 319). To go from $G^{(0)}$ to $G^{(1)}$ there is multiplication by x which transforms the odd function into an even function. Further, a subtraction of the term $1/\pi$ then yields the result shown in Fig. 2. To go from $G^{(1)}$ to $G^{(2)}$, there is only a multiplication by x. The central dip in $G^{(1)}$ gives rise to a sine-shaped curve around $x = 0$ in $G^{(2)}$ and the two maxima around $|x| = 1$ get transformed into a maximum about $x = +1$ and a minimum about $x = -1$. The sine-shaped curve around $x = 0$ in $G^{(2)}$ will lead to a w-shaped minimum around $x = 0$ in $G^{(3)}$. For $n \geqslant 4$, we have similar patterns. All the $G^{(n)}$ with odd values of n are similar to $G^{(3)}$ and all the $G^{(n)}$ with even values of n are similar to $G^{(2)}$. We observe a small shift of the extrema away from $x = 0$, when n increases together with an increase in the absolute values of extrema. The reason for this behavior, common to $H^{(n)}$ and $G^{(n)}$, is given above (see discussion following Eq. (15)).

When the damping parameter is not zero, the curves keep the same shapes but we can observe a flattening of the peaks with increasing values of a due to the factor a^2 in the denominator of Eq. (3).

[2]In Frisch et al. [2], Appendix D, the calculations of the $H^{(n)}$ and $G^{(n)}$ functions have also been performed with the Matta and Reichel algorithm and it was incorrectly stated that Hui et al. [17] algorithm is more accurate.

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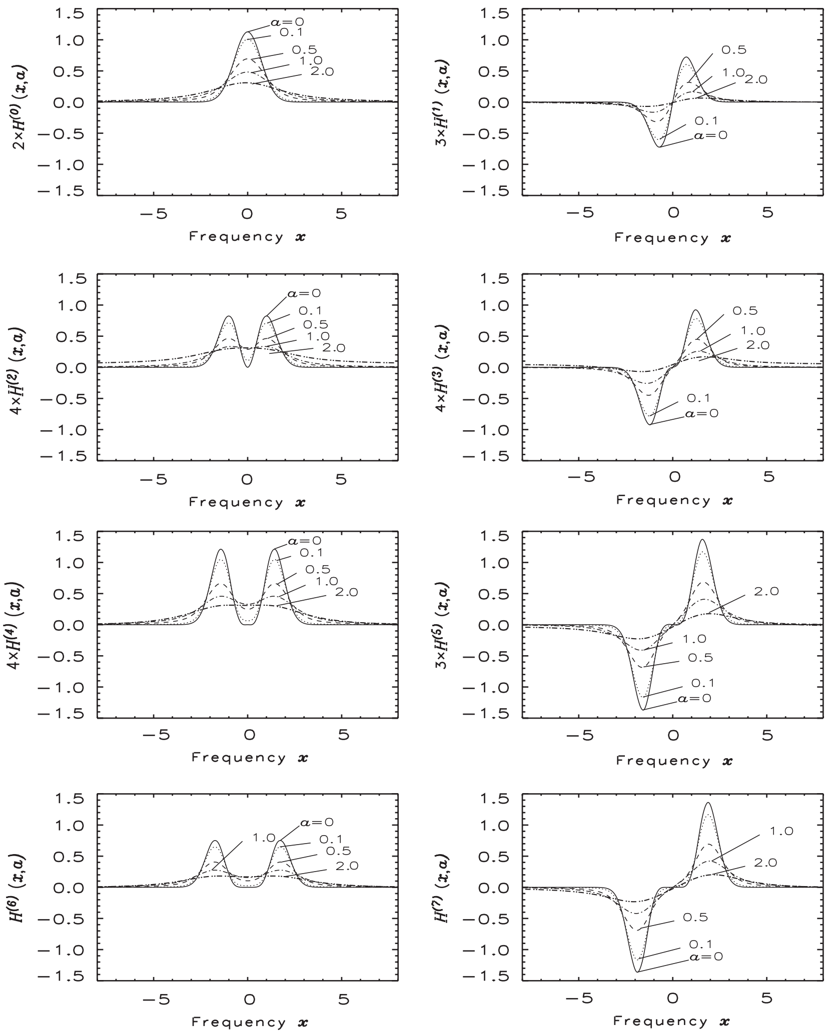

Fig. 1. $H^{(n)}$ functions for $n = 0$–7. Various line types refer to different values of the damping parameter a. All the functions are expressed in same scale for the sake of comparison. $H^{(n)}$ $(n = 1, 3, 5, 7 \ldots)$ have positive and negative maxima, while $H^{(n)}$ $(n = 2, 4, 6 \ldots)$ are entirely positive-valued functions.

The $H^{(n)}$ and $G^{(n)}$ functions have simple asymptotic behaviors for $|x|$ and a going to infinity which can be deduced from Eq. (4). In the limit $z \to \infty$, we can write

$$W^{(n)}(z) \simeq \frac{\mathrm{i}}{\pi^{3/2}} \frac{1}{z} \int_{-\infty}^{+\infty} u^n \mathrm{e}^{-u^2} \left[1 + \frac{u}{z} + \text{h.o.t.} \right] \mathrm{d}u, \tag{16}$$

where h.o.t. stands for higher-order terms. Thus, when n is even, say $n = 2k$, we have to the leading order

$$W^{(2k)}(z) \simeq \frac{\mathrm{i}}{\pi} \frac{c^{(2k)}}{z}, \tag{17}$$

where $c^{(2k)}$ is the constant already introduced in Eq. (8). Thus, to the leading order

$$H^{(2k)}(x,a) \simeq \frac{1}{\pi} \frac{a}{x^2 + a^2} c^{(2k)}, \quad a \neq 0, \tag{18}$$

$$G^{(2k)}(x,a) \simeq \frac{1}{\pi} \frac{x}{x^2 + a^2} c^{(2k)}. \tag{19}$$

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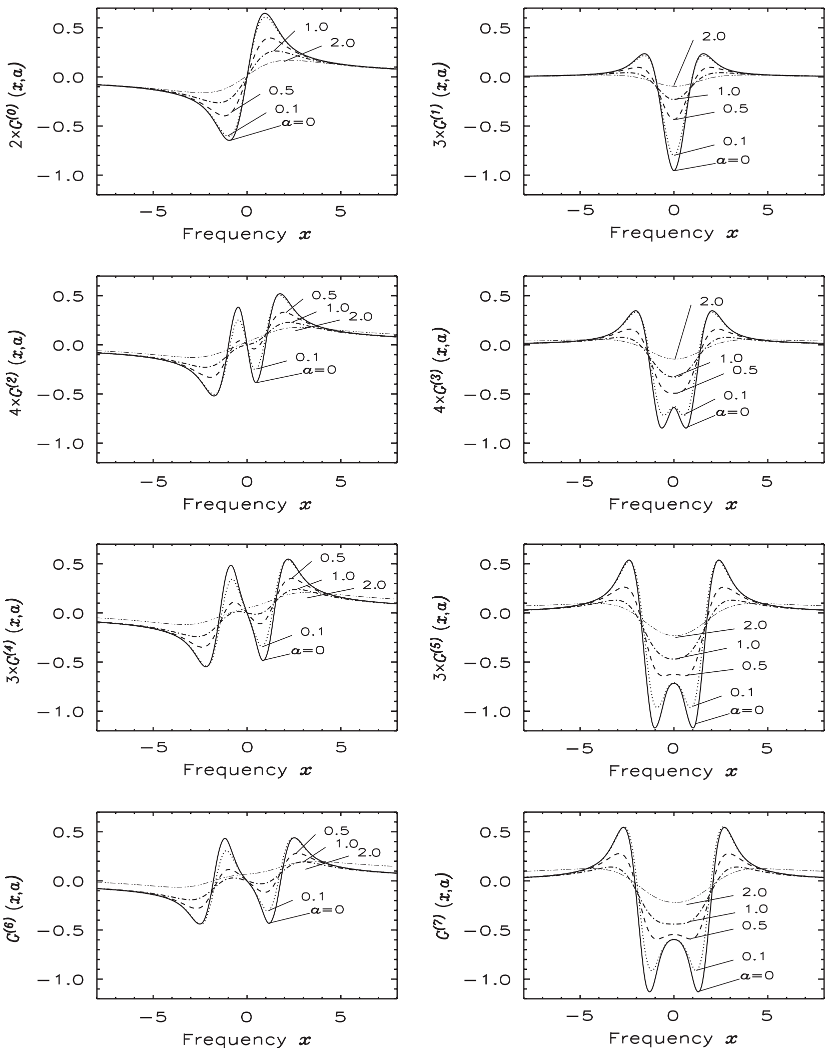

Fig. 2. Same as Fig. 1, but for $G^{(n)}$ functions. Notice that all the functions have positive and negative values.

When n is odd, say $2k+1$, the leading term comes from the second term in the square bracket of Eq. (16). We thus obtain

$$W^{(2k+1)}(z) \simeq \frac{\mathrm{i}}{\pi}\frac{c^{(2k+2)}}{z^2}, \tag{20}$$

from which we deduce

$$H^{(2k+1)}(x,a) \simeq \frac{1}{\pi}\frac{2ax}{(x^2+a^2)^2}c^{(2k+2)}, \quad a\neq 0, \tag{21}$$

$$G^{(2k+1)}(x,a) \simeq \frac{1}{\pi}\frac{x^2-a^2}{(x^2+a^2)^2}c^{(2k+2)}. \tag{22}$$

When $a=0$, the $H^{(n)}(x,0)$ decrease exponentially at large $|x|$ as already pointed out above (see Eq. (9)).

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For $|x|$ going to infinity and a small or order of unity, Eqs. (18)–(22) simplify to

$$H^{(2k)}(x,a) \simeq \frac{1}{\pi}\frac{a}{x^2}\,c^{(2k)}; \quad G^{(2k)}(x,a) \simeq \frac{1}{\pi}\frac{1}{x}\,c^{(2k)}, \tag{23}$$

$$H^{(2k+1)}(x,a) \simeq \frac{1}{\pi}\frac{2a}{x^3}\,c^{(2k+2)}; \quad G^{(2k+1)}(x,a) \simeq \frac{1}{\pi}\frac{1}{x^2}\,c^{(2k+2)}. \tag{24}$$

For a smaller than unity, this asymptotic behavior holds for $|x| \gg \sqrt{-\ln a}$. One can observe in Figs. 1 and 2 that the $H^{(n)}$ and $G^{(n)}$ of odd order have less extended wings than the corresponding functions of even order. We stress that the asymptotic behavior of $G^{(n)}$ is independent of a. Thus, even for $a = 0$, the $G^{(n)}$ has slowly decreasing wings. In Fig. 3, we can clearly observe that the wings of the $G^{(n)}$ functions are independent of a, for say $x > 5$. The asymptotic behavior of the $G^{(n)}$ can also be deduced from the asymptotic behavior of the Dawson's integral (see [11]):

$$D(x) \simeq \frac{1}{2x}\left(1 + \sum_{k=1}^{\infty} \frac{1.3\ldots(2k-1)}{2^k x^{2k}}\right), \quad x \to \infty. \tag{25}$$

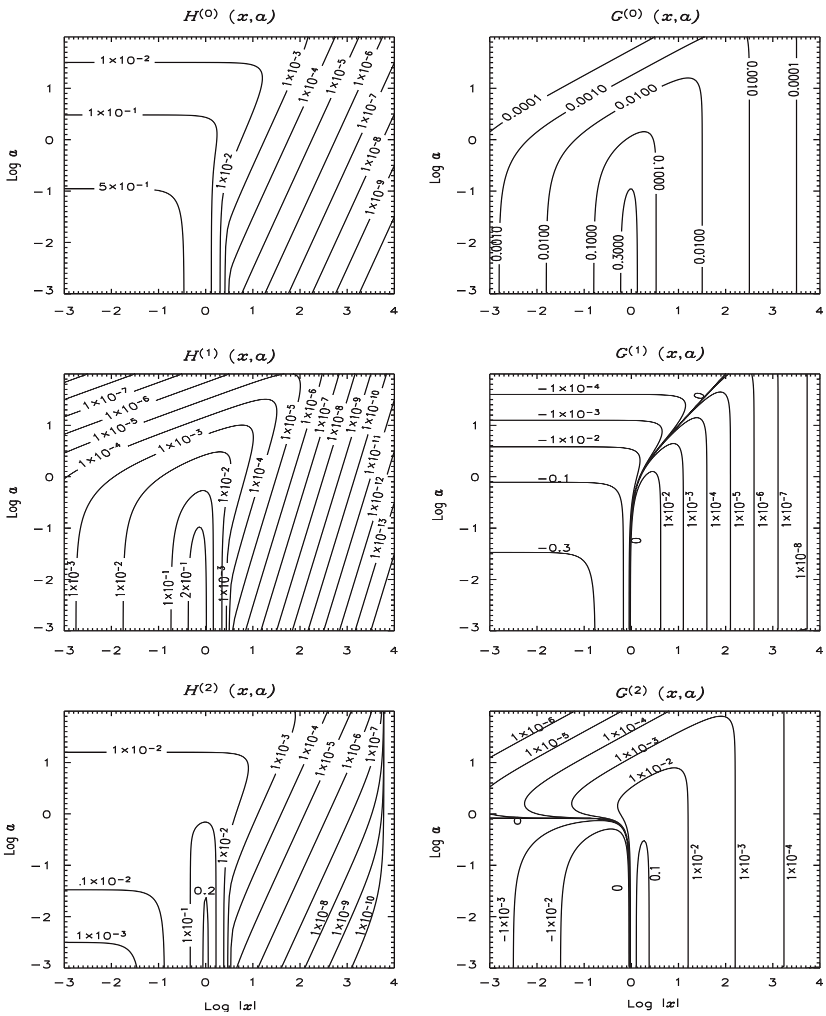

Fig. 3. Higher-order generalized Voigt functions in the $(|x|, a)$ plane. Notice a departure from the correct asymptotic regime (large $|x|$ and large a) visible through the change of slope in the panel for $H^{(2)}$.

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When $|x|$ is small and a large, Eqs. (18)–(22) yield

$$H^{(2k)}(x,a) \simeq \frac{1}{\pi}\frac{1}{a}c^{(2k)}; \quad G^{(2k)}(x,a) \simeq \frac{1}{\pi}\frac{x}{a^2}c^{(2k)}, \tag{26}$$

$$H^{(2k+1)}(x,a) \simeq \frac{1}{\pi}\frac{2x}{a^3}\,c^{(2k+2)}; \quad G^{(2k+1)}(x,a) \simeq -\frac{1}{\pi}\frac{1}{a^2}\,c^{(2k+2)}. \tag{27}$$

These asymptotic behaviors can be observed in contour plots shown in Fig. 3.

2.3. Computational aspects regarding the calculation of H^n and $G^{(n)}$

In this section we discuss details of computation of the generalized Voigt functions. All the calculations have been performed in double precision. For computing $H^{(0)}$ and $G^{(0)}$, we employ algorithm of Matta and Reichel [14], where $H^{(0)}$ and $G^{(0)}$ are represented as a series in terms of an expansion parameter h. The exact values are recovered when h goes to zero. The errors due to the finite value of h can be expressed in terms of a function $E(h)$ that goes to zero with h. They vary like $aE(h)$ for $H^{(0)}$ and like $xE(h)$ for $G^{(0)}$. Here we use $h = 0.5$ and 12 terms in the series expansion. For this choice, Matta and Reichel give $E(h)$ around 10^{-15} and errors around 10^{-15} in the summation due to truncation of the series. The $H^{(n)}$ and $G^{(n)}$ functions are computed with the recurrence relations given in Eqs. (6) and (7). In Figs. 1 and 2 we have shown these functions up to $n = 7$ for values of a and x typical of local thermodynamic equilibrium (LTE), and non-LTE astrophysical problems. These figures clearly show that an asymptotic regime is reached for $|x| > 4$.

In Fig. 3 we present $H^{(0,1,2)}$ and $G^{(0,1,2)}$, computed on a logarithmic grid of damping parameters ($10^{-3} \leqslant a \leqslant 10^2$) and frequencies ($10^{-3} \leqslant |x| \leqslant 10^4$), both with a resolution of 51 points per decade. We have chosen this very wide parameter range as considered in previous works on the numerical calculations of the function $H^{(0)}$ and its derivative (see [10]) to examine the applicability of our recurrence relations in the asymptotic regime.

Since we are using recurrence relations to calculate the functions $H^{(n)}$ and $G^{(n)}$, errors contained within the initial $n = 0$ solution will propagate in the generalized Voigt functions of higher order, due to additions and subtractions of terms involved in these relations. The nature of these numerical errors are similar to those discussed by Wells [10], with reference to the use of recurrence formula. Also, since the functions of order $(n-1)$ in the RHS of Eqs. (6) and (7) are multiplied by factors x and a, one can expect the errors to increase with the value of these variables. This phenomenon can indeed be detected in the contour plots shown in Fig. 3. In the regime of large $|x|$ the functions $H^{(n)}$ and $G^{(n)}$ become straight lines in the $(\log|x|, \log a)$ plane since they vary algebraically with a and $|x|$ (see the asymptotic behavior given in Eqs. (23) and (24)). When errors become significant, this asymptotic behavior is destroyed. In Fig. 3, panel with $H^{(2)}$, we see that the straight lines start bending for large $|x|$ values (see the contours for function values $< 10^{-7}$). For $G^{(2)}$, the asymptotic behavior is preserved, presumably because there are less rounding errors, $G^{(2)}$ decreasing more slowly than $H^{(2)}$. The region of $(|x|, a)$ plane in which $H^{(n)}$ and $G^{(n)}$ functions are computed to acceptable accuracy gradually shrinks as n increases. Figs. 1 and 2 are computed for values of x, a and n ($x < 20$, $a < 3$, $n \leqslant 7$) for which the recurrence relations yield numerically reliable results. That the recurrence relations may have some problems in the asymptotic regime of large $|x|$ can be guessed by inserting the leading terms of the asymptotic behaviors of $H^{(n-1)}$ and $G^{(n-1)}$ in the RHS of Eqs. (6) and (7). For n even, one correctly recovers the leading terms in the asymptotic behaviors of $H^{(n)}$ and $G^{(n)}$, but for odd values of n, the leading terms cancel each other, and it becomes necessary to go to higher-order terms in the asymptotic expansion. In the asymptotic regimes of large $|x|$ and/or a, the best strategy is to use asymptotic formulae rather than recurrence relations. This strategy is recommended by Wells [10] for the calculation of the functions $H^{(0)}$ and $G^{(0)}$ and is carried out in Section 3.4 to calculate the partial derivatives of $H^{(n)}$ and $G^{(n)}$.

3. Partial derivatives of generalized Voigt functions

Closed form expressions to evaluate partial derivatives of $H^{(0)}$ and $G^{(0)}$ are presented in Heinzel [9]. We have adapted Heinzel's approach to obtain the partial derivatives of $H^{(n)}$ and $G^{(n)}$ to all orders m. We first re-express $W^{(n)}(z)$ in a form more suitable for the construction of recurrence relations for these partial derivatives. Following the same method as for $H^{(0)}$ (see [18]), we set $z = x + \mathrm{i}a$ in Eq. (4) and recognize that we can write

$$\frac{\mathrm{i}}{x - u + \mathrm{i}a} = \int_0^{\infty} \mathrm{e}^{-ay} \mathrm{e}^{\mathrm{i}(x-u)y} \, \mathrm{d}y. \tag{28}$$

The function $W^{(n)}(x, a)$ can thus be rewritten as

$$W^{(n)}(x, a) = \frac{1}{\pi^{3/2}} \int_{-\infty}^{+\infty} u^n \mathrm{e}^{-u^2} \int_0^{\infty} \mathrm{e}^{-ay} \mathrm{e}^{\mathrm{i}(x-u)y} \, \mathrm{d}y \, \mathrm{d}u. \tag{29}$$

Introducing the nth derivative of $\mathrm{e}^{-\mathrm{i}uy}$ with respect to y, and then calculating the integral over u we obtain

$$W^{(n)}(t) = \frac{\mathrm{i}^n}{\pi} \int_0^{\infty} \mathrm{e}^{-ty} \frac{\mathrm{d}^n}{\mathrm{d}y^n} (\mathrm{e}^{-y^2/4}) \, \mathrm{d}y, \tag{30}$$

where $t = a - \mathrm{i}x$. The function $W^{(n)}(t)$ is analytic in the right-hand part of the complex plane defined by $\Re(t) > 0$.

We remark that for $a \neq 0$, it is possible to construct series expansions in powers of a in the form $H^{(n)}(x, a) = \sum_k a^k H_k^{(n)}(x)$ with a technique inspired from the method described in Mihalas [18]. This is achieved by expanding e^{-ay} in Eq. (29) in power series of a. This method is interesting when $a \ll 1$ and may provide $H^{(n)}$ with a greater accuracy than the method based on recurrence relations. As recalled in Wells [10], the calculation of $H^{(0)}$ for a very small is a numerical challenge. Similar series expansions can be constructed for the $G^{(n)}$ and for the partial derivatives of $H^{(n)}$ and $G^{(n)}$.

Differentiating Eq. (30) m times with respect to t, we obtain

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m} W^{(n)} = \frac{(-1)^m \mathrm{i}^n}{\pi} \int_0^{\infty} y^m \mathrm{e}^{-ty} \frac{\mathrm{d}^n}{\mathrm{d}y^n} (\mathrm{e}^{-y^2/4}) \, \mathrm{d}y. \tag{31}$$

For $n = 0$, the above equation is the same as Eq. (3.1) in Heinzel [9]. For simplicity we introduce the notations

$$\mathrm{d}_t^m W^{(n)} = \frac{\mathrm{d}^m}{\mathrm{d}t^m} W^{(n)}, \quad \partial_x^m F^{(n)} = \frac{\partial^m F^{(n)}}{\partial x^m}, \quad \partial_a^m F^{(n)} = \frac{\partial^m F^{(n)}}{\partial a^m},$$

where F stands for any of the functions W, H and G. The analyticity of $W^{(n)}$ (see e.g. Eq. (31)) yields for any m, the two important relations:

$$\mathrm{d}_t^m W^{(n)} = \partial_a^m W^{(n)} = \partial_a^m H^{(n)} + \mathrm{i}\partial_a^m G^{(n)}, \tag{32}$$

$$\mathrm{d}_t^m W^{(n)} = \mathrm{i}^m \partial_x^m W^{(n)} = \mathrm{i}^m (\partial_x^m H^{(n)} + \mathrm{i}\partial_x^m G^{(n)}), \tag{33}$$

which are the consequence of the regularity (differentiability) of $W^{(n)}$. Equating the RHS and taking the real and imaginary parts, we obtain Cauchy–Riemann conditions for the partial derivatives of $H^{(n)}$ and $G^{(n)}$ with respect to x and a (see for e.g. [19]). For even values of m, they may be written as

$$\partial_a^m H^{(n)} = (-1)^{m/2} \partial_x^m H^{(n)}, \tag{34}$$

with a similar expression for $\partial_a^m G^{(n)}$. For odd values of m,

$$\partial_a^m H^{(n)} = (-1)^{(m+1)/2} \partial_x^m G^{(n)}, \quad \partial_a^m G^{(n)} = (-1)^{(m-1)/2} \partial_x^m H^{(n)}. \tag{35}$$

In the next section we show how to calculate the partial derivatives with respect to x of $H^{(n)}$ and $G^{(n)}$ of any order m. Using the Cauchy–Riemann conditions one can then get their partial derivatives with respect to a.

3.1. Recurrence relations

To compute $\mathrm{d}_t^m W^{(n)}$ for all possible n and m, a direct recurrence formula is most convenient. Such a formula can be derived from Eq. (31). Following Heinzel [9] we integrate Eq. (31) by parts and thus obtain

$$\mathrm{d}_t^m W^{(n)} = \frac{(-1)^{m+1} \mathrm{i}^n}{\pi} \int_0^{\infty} \frac{y^{(m+1)}}{m+1} \mathrm{e}^{-ty} \left[-t \frac{\mathrm{d}^n}{\mathrm{d}y^n} + \frac{\mathrm{d}^{(n+1)}}{\mathrm{d}y^{(n+1)}} \right] (\mathrm{e}^{-y^2/4}) \, \mathrm{d}y. \tag{36}$$

Changing $m \to m-1$ and $n \to n-1$ in the above equation, we obtain the recurrence relation

$$\mathrm{d}_t^m W^{(n)} = \mathrm{i}m\mathrm{d}_t^{m-1} W^{(n-1)} + \mathrm{i}t\mathrm{d}_t^m W^{(n-1)}, \quad (n,m) \geqslant 1. \tag{37}$$

However, the above relation holds only for $n \geqslant 1$. To get recurrence relation for $n=0$, we start from Eq. (31) with $n=0$. An integration by parts yields

$$\mathrm{d}_t^m W^{(0)} = 2t\mathrm{d}_t^{m-1} W^{(0)} + 2(m-1)\mathrm{d}_t^{m-2} W^{(0)}, \quad m \geqslant 2. \tag{38}$$

We note that our symbols $W^{(0)}$, t, and x correspond to, respectively, $D(w)$, w, and u of Heinzel [9] and that our Eq. (38) is Heinzel's Eq. (4.1).

Using Eqs. (32) and (33), we can write the recurrence relations for the partial derivatives of $W^{(n)}$ as

$$\partial_x^m W^{(n)} = (x+\mathrm{i}a)\partial_x^m W^{(n-1)} + m\partial_x^{m-1} W^{(n-1)}, \tag{39}$$

$$\partial_a^m W^{(n)} = (x+\mathrm{i}a)\partial_a^m W^{(n-1)} + \mathrm{i}m\partial_a^{m-1} W^{(n-1)}, \quad (m,n) \geqslant 1. \tag{40}$$

With Eq. (39), as we now show, it is possible to construct separate recurrence relations for the partial derivatives of $H^{(n)}$ and $G^{(n)}$ with respect to x. Taking the real and imaginary parts of Eq. (39), we obtain

$$\Re\{\partial_x^m W^{(n)} - m\partial_x^{m-1} W^{(n-1)} - x\partial_x^m W^{(n-1)}\} = -a\,\Im\{\partial_x^m W^{(n-1)}\}, \tag{41}$$

$$\Im\{\partial_x^m W^{(n)} - m\partial_x^{m-1} W^{(n-1)} - x\partial_x^m W^{(n-1)}\} = a\,\Re\{\partial_x^m W^{(n-1)}\}. \tag{42}$$

To obtain a recurrence relation for, say, $\Re\{\partial_x^m W^{(n)}\} = \partial_x^m H^{(n)}$, we extract from the RHS of Eq. (41) the three terms which appear in the LHS of Eq. (42). For this purpose we write Eq. (41) for the three sets (m,n), $(m,n-1)$ (Eq. (41) itself), and $(m-1,n)$. Exchanging the roles of Eqs. (41) and (42), we obtain a recurrence relation for $\Im\{\partial_x^m W^{(n)}\} = \partial_x^m G^{(n)}$. It is actually the same as the recurrence relation for $\partial_x^m H^{(n)}$. They can be written as

$$\begin{aligned}&\partial_x^m F^{(n)} - 2x\partial_x^m F^{(n-1)} + (x^2+a^2)\partial_x^m F^{(n-2)} - 2m\partial_x^{m-1} F^{(n-1)}\\ &\quad + 2mx\partial_x^{m-1} F^{(n-2)} + m(m-1)\partial_x^{m-2} F^{(n-2)} = 0; \quad (n,m) \geqslant 2,\end{aligned} \tag{43}$$

where $F^{(n)}$ stands for $H^{(n)}$ or $G^{(n)}$.

The partial derivatives with respect to a can be deduced from the partial derivatives with respect to x by making use of the Cauchy–Riemann conditions written in Eqs. (34) and (35). We remark here that the procedure applied to Eq. (39) to obtain recurrence relations for the partial derivatives with respect to x does not work with Eq. (40). The real and imaginary parts of Eq. (40) yield a set of equations similar to (41) and (42) but they cannot be combined to obtain recurrence relations separately for the partial derivatives of $H^{(n)}$ and $G^{(n)}$ with respect to a.

3.2. Initialization of the recurrence relations

In order to apply the recurrence formula given in Eq. (43) to the computation of the partial derivatives with respect to x, it is necessary to know all the mth derivatives of $H^{(0)}$, $G^{(0)}$, $H^{(1)}$ and $G^{(1)}$, and the first derivatives with respect to x of all the $H^{(n)}$ and $G^{(n)}$. The mth derivatives of $H^{(0)}$ and $G^{(0)}$ are given in Heinzel [9] (see also Eq. (60)). The mth derivatives of $H^{(1)}$ and $G^{(1)}$ can be related to the mth derivatives of $H^{(0)}$ and $G^{(0)}$. Starting from the definition of $H^{(0)}$ and $G^{(0)}$, making the change of variable $x-u=v$, and using

$$\frac{\mathrm{d}^m}{\mathrm{d}v^m}[\mathrm{e}^{-(x-v)^2}] = -2\frac{\mathrm{d}^{m-1}}{\mathrm{d}v^{m-1}}[(x-v)\mathrm{e}^{-(x-v)^2}], \tag{44}$$

we immediately obtain

$$\partial_x^m F^{(1)} = -\tfrac{1}{2}\partial_x^{m+1} F^{(0)}, \quad m \geqslant 1, \tag{45}$$

where F stands for H or G. The first derivative with respect to x of all the $H^{(n)}$ and $G^{(n)}$ can be obtained with the same procedure. Starting from the definition of $H^{(n)}$ (or $G^{(n)}$), we find

$$\partial_x^1 F^{(n)} = nF^{(n-1)} - 2F^{(n+1)}, \tag{46}$$

where again F stands for H or G.

3.3. Asymptotic behavior of the partial derivatives

The partial derivatives of $H^{(n)}$ and $G^{(n)}$ have simple asymptotic behaviors for $|x|$ and a going to infinity which can be deduced from Eq. (4). In the limit $z \to \infty$, we can write

$$\frac{\mathrm{d}^m W^{(n)}}{\mathrm{d}z^m}(z) \simeq (-1)^m \frac{\mathrm{i}}{\pi^{3/2}} \frac{m!}{z^{m+1}} \int_{-\infty}^{+\infty} u^n \mathrm{e}^{-u^2} \left[1 + (m+1)\frac{u}{z} + \text{h.o.t.}\right] \mathrm{d}u. \tag{47}$$

We thus obtain up to the first-order sub-leading term

$$\frac{\mathrm{d}^m W^{(2k)}}{\mathrm{d}z^m}(z) \simeq (-1)^m \frac{\mathrm{i}}{\pi} \frac{m!}{z^{m+1}} c^{(2k)} \left[1 + \frac{(2k+1)}{4} \frac{(m+2)(m+1)}{z^2}\right], \tag{48}$$

$$\frac{\mathrm{d}^m W^{(2k+1)}}{\mathrm{d}z^m}(z) \simeq (-1)^m \frac{\mathrm{i}}{\pi} \frac{(m+1)!}{z^{m+2}} c^{(2k+2)} \left[1 + \frac{(2k+3)}{12} \frac{(m+3)(m+2)}{z^2}\right], \tag{49}$$

where k is a positive integer and the constant $c^{(n)}$, n even, has been introduced in Eq. (8). For example $c^{(0)} = 1$, $c^{(2)} = \frac{1}{2}$, $c^{(4)} = \frac{3}{4}$. Separating real and imaginary parts, one readily obtains the partial derivatives with respect to x or a of $H^{(n)}$ and $G^{(n)}$ of any order m. The asymptotic formulae for the first two partial derivatives of $H^{(0,1)}$ are

$$\frac{\partial H^{(0)}}{\partial x} \simeq -\frac{1}{\pi} \frac{2ax}{(x^2+a^2)^2} \left[1 + \frac{3(x^2-a^2)}{(x^2+a^2)^2}\right], \tag{50}$$

$$\frac{\partial^2 H^{(0)}}{\partial x^2} \simeq \frac{2}{\pi} \frac{a(3x^2-a^2)}{(x^2+a^2)^3} \left[1 + \frac{3(5x^4+a^4-10x^2a^2)}{(3x^2-a^2)(x^2+a^2)^2}\right], \tag{51}$$

$$\frac{\partial H^{(1)}}{\partial x} \simeq -\frac{1}{\pi} \frac{a(3x^2-a^2)}{(x^2+a^2)^3} \left[1 + \frac{3(5x^4+a^4-10x^2a^2)}{(3x^2-a^2)(x^2+a^2)^2}\right], \tag{52}$$

$$\frac{\partial^2 H^{(1)}}{\partial x^2} \simeq \frac{12}{\pi} \frac{ax(x^2-a^2)}{(x^2+a^2)^4} \left[1 + \frac{5}{2} \frac{(3x^4+3a^4-10x^2a^2)}{(x^2-a^2)(x^2+a^2)^2}\right]. \tag{53}$$

The corresponding formulae for $G^{(0,1)}$ are

$$\frac{\partial G^{(0)}}{\partial x} \simeq -\frac{1}{\pi} \frac{(x^2-a^2)}{(x^2+a^2)^2} \left[1 + \frac{3}{2} \frac{(x^4+a^4-6x^2a^2)}{(x^2-a^2)(x^2+a^2)^2}\right], \tag{54}$$

$$\frac{\partial^2 G^{(0)}}{\partial x^2} \simeq \frac{2}{\pi} \frac{x(x^2-3a^2)}{(x^2+a^2)^3} \left[1 + \frac{3(x^4+5a^4-10x^2a^2)}{(x^2-3a^2)(x^2+a^2)^2}\right], \tag{55}$$

$$\frac{\partial G^{(1)}}{\partial x} \simeq -\frac{1}{\pi} \frac{x(x^2-3a^2)}{(x^2+a^2)^3} \left[1 + \frac{3(x^4+5a^4-10x^2a^2)}{(x^2-3a^2)(x^2+a^2)^2}\right], \tag{56}$$

$$\frac{\partial^2 G^{(1)}}{\partial x^2} \simeq \frac{3}{\pi} \frac{(x^4+a^4-6x^2a^2)}{(x^2+a^2)^4} \left[1 + \frac{5[x^6-a^6-15x^2a^2(x^2-a^2)]}{(x^4+a^4-6x^2a^2)(x^2+a^2)^2}\right]. \tag{57}$$

The first and second partial derivatives of $H^{(2)}$ and $G^{(2)}$ can be easily deduced from the corresponding derivatives of $H^{(0)}$ and $G^{(0)}$. It suffices to multiply the leading terms by $c^{(2)}/c^{(0)} = 1/2$ and the sub-leading term by $c^{(4)}/c^{(2)} = 3/2$. We stress that the asymptotic expansions for the first derivatives of $H^{(1)}$ and $G^{(1)}$ satisfy the exact relation in Eq. (45) which yields $\partial_x^m H^{(1)}$ in terms of $\partial_x^{m+1} H^{(0)}$ and similarly for $G^{(1)}$.

For $|x|$ going to infinity and small a, the expressions given above simplify. We note that the leading terms can be recovered in a straightforward way by taking partial derivatives with respect to x of the leading terms of $H^{(n)}$ and $G^{(n)}$ given in Eqs. (23) and (24).

3.4. Computation of the derivatives of $H^{(n)}$ and $G^{(n)}$

We have used the recurrence relations given in Eqs. (43), (45) and (46) to calculate the $m = 1$ and 2 partial derivatives of $H^{(1,2)}$ and $G^{(1,2)}$ with respect to x. All the partial derivatives entering in Eqs. (43) and (45) have been expressed in terms of $H^{(n)}$ and $G^{(n)}$ using the results in Table 1. In Fig. 4 left-side panels show $\partial_x^1 H^{(1)}$, $\partial_x^1 H^{(2)}$, $\partial_x^2 H^{(1)}$, $\partial_x^2 H^{(2)}$ as functions of x for different values of a and right-side panels show the corresponding quantities for $G^{(n)}$. In addition to the obvious symmetries, this figure shows that an asymptotic regime is reached for $|x|>4$ and in some cases even for $|x|>3$. For small values of a (say, $a<0.5$), the derivatives show a strong frequency dependence in the line center region ($|x|<4$). For larger values of a, these derivatives weakly depend on frequency and approach an asymptotic regime with respect to a also. When $|x|$ and a take large values, in the hundreds or thousands, the recurrence relations fail to reproduce the correct asymptotic

Table 1
First three partial derivatives of $H^{(0)}$ and $G^{(0)}$ in terms of $H^{(n)}$ and $G^{(n)}$

$\partial_x^1 H^{(0)} = -2H^{(1)}$	$\partial_a^1 H^{(0)} = 2G^{(1)}$	$\partial_a^1 G^{(0)} = -2H^{(1)}$
$\partial_x^2 H^{(0)} = -2H^{(0)} + 4H^{(2)}$	$\partial_a^2 H^{(0)} = 2H^{(0)} - 4H^{(2)}$	$\partial_a^2 G^{(0)} = 2G^{(0)} - 4G^{(2)}$
$\partial_x^3 H^{(0)} = 12H^{(1)} - 8H^{(3)}$	$\partial_a^3 H^{(0)} = 12G^{(1)} - 8G^{(3)}$	$\partial_a^3 G^{(0)} = -12H^{(1)} + 8H^{(3)}$

The partial derivatives of $G^{(0)}$ with respect to x have the same form as that for $H^{(0)}$, but with $H^{(n)}$ replaced by $G^{(n)}$.

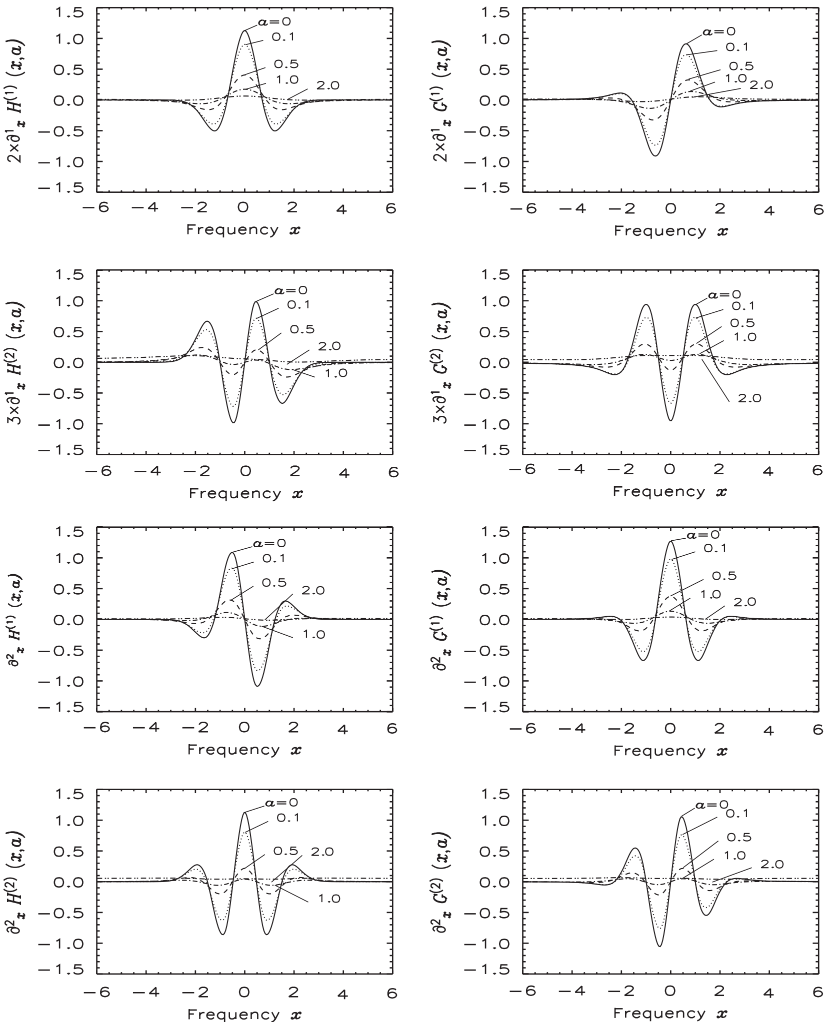

Fig. 4. Partial derivatives first- and second-order ($m \leqslant 2$) generalized Voigt functions. Notice the onset of the asymptotic regime for $|x| \sim 5$ and $a \geqslant 2$.

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behavior. We have encountered similar numerical problems when computing the $H^{(n)}$ and $G^{(n)}$ functions for $n \geqslant 2$ (see Fig. 3). They are due to cancellation effects and rounding errors. The accuracy problem is accentuated for larger n and m, and also larger values of $|x|$ and a. For the partial derivatives considered here ($m \leqslant 2$, $n \leqslant 2$) the applicability domain of the recurrence relations is $|x| \leqslant 11$, $a \leqslant 11$. It will be larger for lower-order derivatives and smaller for higher ones. For the asymptotic expansions, it is clear that they are valid if $|x|$ and/or a are sufficiently large. We have found by trial and error, comparing values given by the asymptotic expansions and the recurrence relations, that they give identical results in the region $6 < |x| \leqslant 11$ and $6 < a \leqslant 11$. To obtain matching solution in this domain, the asymptotic expansion had to be pushed to the first-order sub-leading term. Keeping only the leading term was not sufficient. In contrast to the upper bound of the matching domain, the lower bound for the validity of the asymptotic expansion will be essentially independent of the values of n and m (see Figs. 1 and 2 for $H^{(n)}$ and $G^{(n)}$).

We show in Fig. 5 contour plots corresponding to Fig. 4. They are computed using the recurrence relations inside the domain ($|x|, a \leqslant 6$) and the asymptotic formulae outside this domain. In Fig. 5, the region of ($|x|, a$) plane computed using asymptotic formulae is shaded gray. One can note a perfect matching between the two sets of values. We stress that the same cut-off between the asymptotic domain and the recurrence relations should be applied to all the functions occuring in the recurrence relation (43). In computing Fig. 5 we employ a grid resolution of 51 points per decade in both $|x|$ and a variables. For the practical range of parameters that we encounter in Solar line formation theory, namely a smaller than unity and x a few Doppler widths, the recurrence relations are applicable.

The computer program to evaluate the $H^{(n)}$ and $G^{(n)}$ functions and their derivatives can be obtained from the authors on request.

4. Derivatives of $H^{(0)}$ and $G^{(0)}$ in terms of $H^{(n)}$ and $G^{(n)}$

The partial derivatives of $H^{(0)}$ and $G^{(0)}$ have been expressed in terms of $H^{(0)}$ and $G^{(0)}$ themselves in Heinzel [9]. In this section, we show that it is possible to write the partial derivatives of $H^{(0)}$ and $G^{(0)}$ in terms of the $H^{(n)}$ and $G^{(n)}$. Setting $n = 0$ and $x - u = v$ in Eqs. (2) and (3), we see that the calculation of the mth partial derivative of $H^{(0)}$ with respect to x requires the mth derivative of $\mathrm{e}^{-(x-v)^2}$. As recognized in Luque et al. [20], they can be expressed in terms of Hermite polynomial $\mathscr{H}_m$ (see [11, p. 785]). Indeed we have

$$\frac{\mathrm{d}^m}{\mathrm{d}x^m}[\mathrm{e}^{-x^2}] = (-1)^m \, \mathrm{e}^{-x^2} \mathscr{H}_m(x). \tag{58}$$

The Hermite polynomial can be written as a power series in x (see [11, p. 775])

$$\mathscr{H}_m(x) = m! \sum_{k=0}^{[m/2]} \frac{(-1)^k}{k!(m-2k)!} \, (2x)^{(m-2k)}, \tag{59}$$

where $[m/2]$ means $m/2$ for even m and $(m-1)/2$ for odd m. Using the definition of $H^{(n)}$, we obtain the general formula

$$\partial_x^m H^{(0)} = (-1)^m \, m! \sum_{k=0}^{[m/2]} \frac{(-1)^k}{k!(m-2k)!} \, 2^{(m-2k)} \, H^{(m-2k)}. \tag{60}$$

For the $\partial_x^m G^{(0)}$ we have an expression similar to the above with $H^{(m-2k)}$ replaced by $G^{(m-2k)}$. With this general formula one can determine the partial derivatives of $H^{(0)}$ for any given m, in terms of $H^{(n)}$ functions, which in turn can be easily computed using the recurrence relations (6) and (7). We note that mth partial derivatives of $H^{(1)}$ and $G^{(1)}$ with respect to x can also be expressed in terms of $H^{(n)}$ and $G^{(n)}$, by combining Eqs. (45) and (60).

The derivatives of $H^{(0)}$ and $G^{(0)}$ with respect to the damping parameter a can also be expressed in terms of $H^{(n)}$ and $G^{(n)}$. Using for $n = 0$ the Cauchy–Riemann conditions given in Eqs. (34) and (35), we obtain

$$\partial_a^m H^{(0)} = (-1)^{3m/2} m! \sum_{k=0}^{m/2} \frac{(-1)^k}{k!(m-2k)!} \, 2^{(m-2k)} \, H^{(m-2k)}, \tag{61}$$

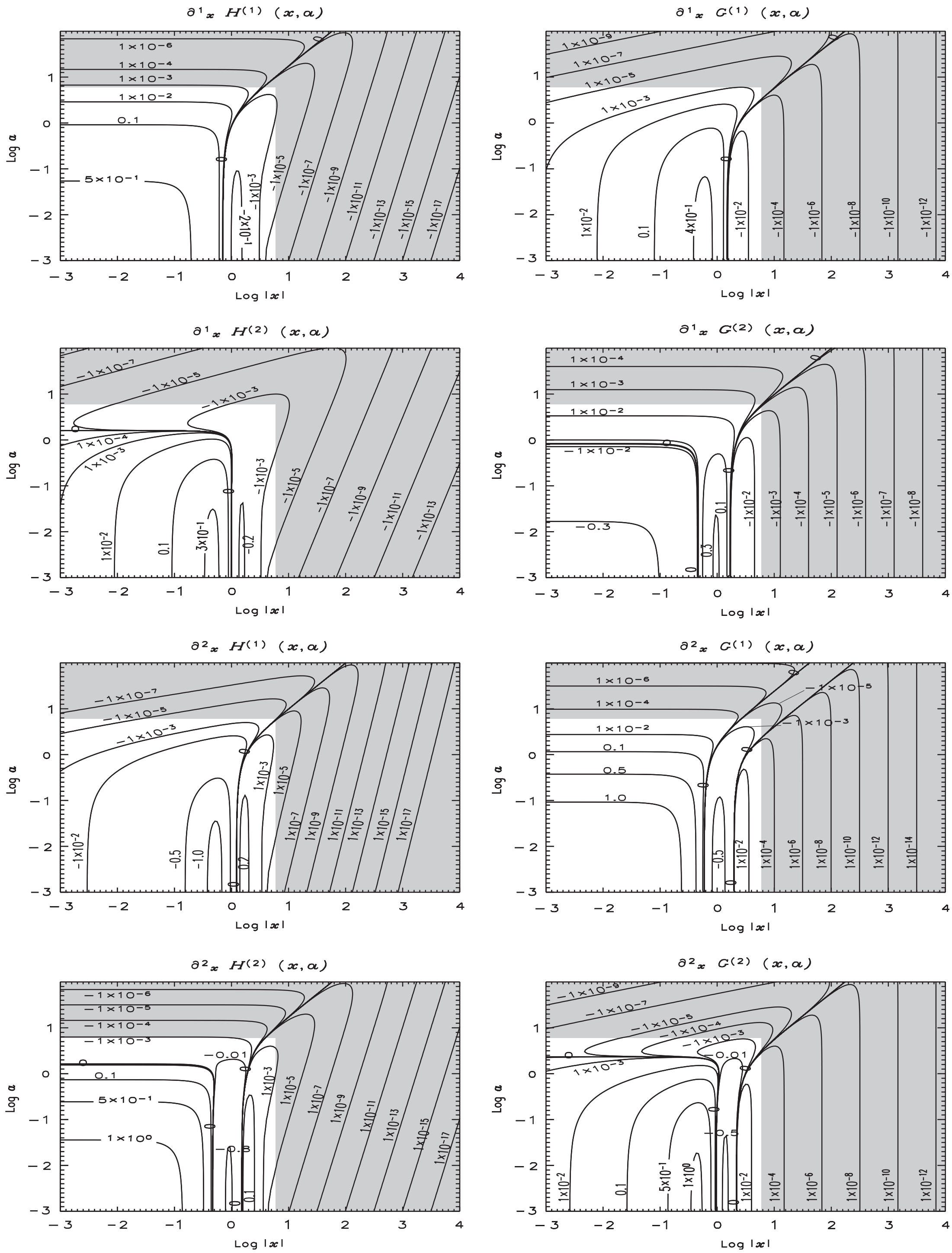

Fig. 5. Contour plots of partial derivatives of $H^{(n)}$ and $G^{(n)}$ functions, in the $(|x|, a)$ plane. For $|x| \leqslant 6$ and $a \leqslant 6$ recurrence relations are used. Outside this domain asymptotic formulae are used, as the recurrence relations become less accurate.

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for even values of m, and a similar expression for $\partial_a^m G^{(0)}$. For odd values of m

$$\partial_a^m H^{(0)} = (-1)^{(3m+1)/2} m! \sum_{k=0}^{(m-1)/2} \frac{(-1)^k}{k!(m-2k)!} 2^{(m-2k)} G^{(m-2k)}, \tag{62}$$

$$\partial_a^m G^{(0)} = (-1)^{(3m-1)/2} m! \sum_{k=0}^{(m-1)/2} \frac{(-1)^k}{k!(m-2k)!} 2^{(m-2k)} H^{(m-2k)}. \tag{63}$$

In Table 1 we list the first three partial derivatives of $H^{(0)}$ with respect to x, calculated using Eq. (60). The partial derivatives of $G^{(0)}$ satisfy the same relation. We also list $\partial_a^m H^{(0)}$ and $\partial_a^m G^{(0)}$, for $m = 1, 2, 3$, calculated using Eqs. (61)–(63). If we use the recurrence relations given in Eqs. (6) and (7) for $H^{(n)}$ and $G^{(n)}$, we recover the expressions given in Table 1 of Heinzel [9], where the derivatives are expressed in terms of $H^{(0)}$ and $G^{(0)}$ and polynomials in a and x.

Acknowledgment

M.S. is financially supported by Council of Scientific and Industrial Research (CSIR), through a SRF (Grant No: 9/890(01)/2004-EMR-I), which is gratefully acknowledged. She is grateful to the Indo-French *Sandwich Thesis Program* for making possible a visit to the Observatoire de la Côte d'Azur (OCA). K.N.N. and M.S. are also grateful to OCA and Laboratoire Cassiopée (CNRS) for providing research facilities and financial support for a visit to Nice in 2005, during which part of this work was completed. We appreciate very useful comments and suggestions by a referee, which helped in improving the paper. We appreciate the help from Dr. B.A. Varghese in making the illustrations.

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