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The numerical computation of the Voigt function by a corrected midpoint quadrature rule for $(-\infty, \infty)$

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Abstract

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This paper presents a method for computing the Voigt function, through the application of a midpoint quadrature rule that has been corrected to accurately integrate a certain class of meromorphic functions.

Keywords: Complex complementary error function, shifted rectangular quadrature rule, meromorphic function, spectral line profile.

1. Introduction

The Voigt function

$$V(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-\lambda^2}}{(x-\lambda)^2 + y^2} \, d\lambda \tag{1.1}$$

is of considerable importance in radiative transfer calculations and is frequently encountered in spectroscopy, where it describes spectral line profiles due to independent Lorentz and Doppler broadening. See [26,27,30].

The Voigt function can also be expressed in terms of the complex complementary error function:

$$V(x, y) = \operatorname{Re}[w(z)]$$

where $z = x + iy$ and

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz)$$
$$= \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-\lambda^2}}{z - \lambda} \, d\lambda, \quad \operatorname{Im} z > 0.$$

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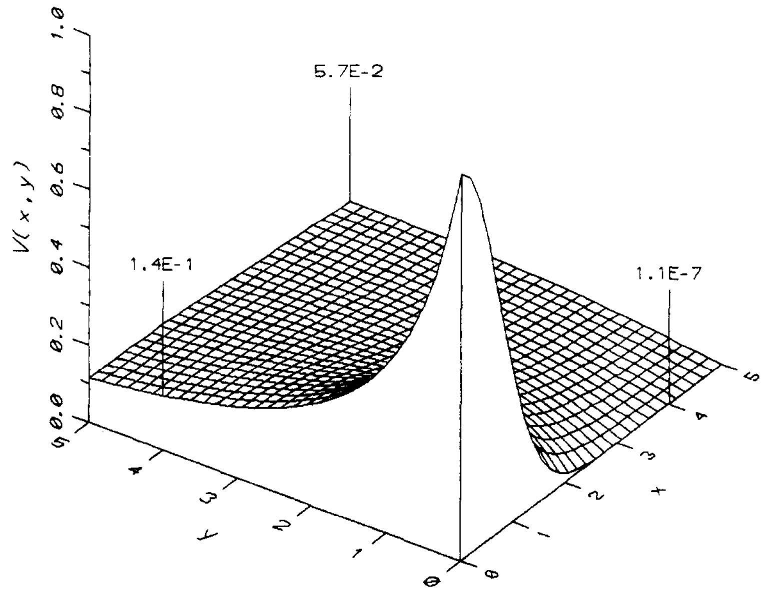

Fig. 1. The Voigt function $V(x, y)$ for $0 \leqslant x, y \leqslant 5$.

In this regard see [9–11,19,21,31,33,35], and the discussion in [38].

No closed-form evaluation for $V(x, y)$ is known except for a few special cases such as

$$V(x, 0) = \exp(-x^2)$$

and

$$V(0, y) = \exp(y^2)\operatorname{erfc}(y) \sim \pi^{-1/2} y^{-1}, \quad y \to \infty.$$

For (x, y) in the first quadrant, it is known that $0 < V(x, y) \leqslant 1$ and for (x, y) bounded away from the x-axis [28]

$$V(x, y) \sim \frac{\pi^{-1/2} y}{(x^2 + y^2)}, \quad x^2 + y^2 \to \infty.$$

These relationships are illustrated in Fig. 1, where annotations such as 5.7E-2 are to be interpreted as 5.7×10^{-2}.

In the following work it will be assumed that x and y are nonnegative, since the Voigt function enjoys the symmetry properties

$$V(-x, y) = V(x, y) \quad \text{and} \quad -V(x, -y) = V(x, y).$$

Considerable effort has been devoted to the numerical calculation of the Voigt function. Much of this work appears in the scientific literature. Notable in this regard is the work of the following authors: Young [39], Hummer [17], Armstrong [2], Harstad [13], Drayson [5], Pierlussi and Vanderwood [29], Karp [20], Hui, Armstrong and Wray [14], Twitty, Rarig and Thompson [37], Klim [22], Sulzmann [36], Drummond and Steckner [6] and Humlicek [15,16]. The approaches of these authors are varied and make use of such techniques as series expansion, rational approximation, and numerical integration.

Many of the published methods for computing $V(x, y)$ partition the first quadrant into two or more zones and use a different mathematical technique on each separate zone. These hybrid algorithms splice together different approximations and have evolved, in part, because the behavior of $V(x, y)$ near the x-axis is radically different from its behavior in the remainder of the first quadrant. These problems concerning the calculation of $V(x, y)$ are not surprising, since the simple poles of the integrand at $x \pm iy$ approach the interval of integration in (1.1) as $y \to 0$. As noted in [2, Section 3.2], the limiting value $V(x, y) \to \exp(-x^2)$ as $y \to 0$ is not obtained by simply setting $y = 0$ in the integral (1.1), and serves as an additional warning that the numerical computation of $V(x, y)$ is difficult when y is small.

For our present purposes it is desirable to make the simple change of variable $\lambda = x - yu$ in (1.1) and express the Voigt function in the form

$$V(x, y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(yu-x)^2}}{u^2+1} du. \tag{1.2}$$

In contrast to (1.1), the integrand in (1.2) has fixed poles at $\pm i$ that do not depend on x and y. The closed forms given above for $V(x, 0)$ and $V(0, y)$ also follow at once from the representation (1.2).

The main purpose of this paper is to show that the Voigt function can be computed accurately from (1.2), through the use of a corrected midpoint quadrature rule that takes the poles at $\pm i$ into account. In particular, the form (1.2) will be used in Result 2.5 of Section 2 to establish the following theorem.

Theorem 1.1. *Let $g(u)$ denote twice the even part of the integrand in* (1.2):

$$g(u) = \frac{e^{-(yu-x)^2}(1 + e^{-4xyu})}{u^2+1}. \tag{1.3}$$

Given $x \geqslant 0$, $y \geqslant 0$ and stepsize $h > 0$, with $hy^2 \neq \pi$, the Voigt function admits the representation

$$V(x, y) = Q(h) + C(h) + E(h) \tag{1.4}$$

where the midpoint quadrature sum

$$Q(h) = \frac{h}{\pi} \sum_{n=0}^{\infty} g(nh + h/2) \tag{1.5}$$

and the correction term

$$C(h) = \begin{cases} \dfrac{2\, e^{y^2-x^2} \cos(2xy)}{1 + e^{2\pi/h}}, & y < (\pi/h)^{1/2}, \\ 0, & y > (\pi/h)^{1/2}. \end{cases} \tag{1.6}$$

The error term E(h) in (1.4) satisfies

$$| E(h) | \leqslant \varphi(h) \tag{1.7}$$

where

$$\varphi(h) = \frac{\pi^{-1/2} y^3}{| y^4 - \pi^2/h^2 |} \operatorname{csch}\left[\pi^2/(hy)^2\right]. \tag{1.8}$$

Table 1
Error bounds (1.8) for $E(h)$

$t = hy$	$y = 0.01$		$y = 2$		$y = 10$	
	h	$\varphi(h)$	h	$\varphi(h)$	h	$\varphi(h)$
1	100	$5.91 \cdot 10^{-8}$	$\frac{1}{2}$	$1.99 \cdot 10^{-5}$	$\frac{1}{10}$	$6.48 \cdot 10^{-6}$
$\frac{1}{2}$	50	$2.05 \cdot 10^{-21}$	$\frac{1}{4}$	$4.55 \cdot 10^{-19}$	$\frac{1}{20}$	$1.33 \cdot 10^{-18}$
$\frac{1}{4}$	25	$1.87 \cdot 10^{-73}$	$\frac{1}{8}$	$3.85 \cdot 10^{-71}$	$\frac{1}{40}$	$5.11 \cdot 10^{-70}$
$\frac{1}{8}$	$\frac{25}{2}$	$8.47 \cdot 10^{-280}$	$\frac{1}{16}$	$1.70 \cdot 10^{-277}$	$\frac{1}{80}$	$1.01 \cdot 10^{-276}$

We note that the choice $y = (\pi/h)^{1/2}$ has been excluded in the correction term (1.6), because $\varphi(h) \to \infty$ as $h \to \pi/y^2$. The error bound (1.7) shows that (1.4) is capable of high accuracy, since $\operatorname{csch}[\pi^2/(hy)^2] \approx 2\exp(-\pi^2/t^2)$, when $t = hy < 1$. In Table 1 we tabulate $\varphi(h)$ for selected values of h and y, the product $t = hy$ being constant in each row of Table 1.

The representation (1.4) is similar to a result of Matta and Reichel [25], who applied a corrected trapezoidal rule to (1.1). By extending a theorem of [24] to include a certain class of meromorphic functions, we can obtain Matta and Reichel's representation for $V(x, y)$ in a direct manner, and thereby compare the merits of (1.4) with their result.

Finally, in Section 3 of this paper we develop an algorithm for computing $V(x, y)$ to a specified absolute error. For a given value of x and y, the algorithm determines both the stepsize h, and the number of terms that must be summed in (1.5) to produce the required accuracy for $V(x, y)$. Some numerical results obtained from FORTRAN and TURBO Pascal implementations of the pseudocode statement of the algorithm are presented.

2. Corrected rectangular quadrature rules for $V(x, y)$

In this section we use quadrature theory to develop an approximation to the Voigt function $V(x, y)$. A family of corrected rectangular quadrature rules is derived for this purpose, and it is shown that $V(x, y)$ can be accurately computed by applying the midpoint rule from this family to the integral representation (1.2).

Consider the numerical approximation of the integral

$$I(f) = \int_{-\infty}^{\infty} f(u)\, \mathrm{d}u$$

by the shifted rectangular approximation [4]

$$I(f) \approx Q(f;\, h, \alpha) \tag{2.1}$$

where the quadrature sum is given by

$$Q(f;\, h, \alpha) = h \sum_{n=-\infty}^{\infty} f(\alpha h + nh)$$

and the shift $\alpha \in [0, 1)$ remains at our disposal.

If $f(u)$ is infinitely differentiable on $(-\infty, \infty)$ and decreases rapidly to zero as $x \to \pm\infty$, then it is well known [4] that $I(f)$ can be computed to a high accuracy by (2.1), even for relatively large values of the stepsize $h > 0$. For example [12], if f is the entire function $f(u) = \exp(-u^2)$, then the absolute error in the approximation (2.1) is $O(\exp(-\pi^2/h^2))$. Further applications and related theory can be found in [8,18,23,32,34].

If (2.1) is applied to a meromorphic function having poles near the interval of integration, then the rate of convergence of the approximation $I(f) \approx Q(f;\ \alpha,\ h)$ is often unsatisfactory when $I(f)$ must be computed to high accuracy. This is the situation for both (1.1) and (1.2), when $y \to 0$. In order to deal with this problem it is helpful to determine a correction term for (2.1), $C(f;\ h,\ \alpha)$, so that the corrected rectangular approximation

$$I(f) \approx Q(f;\ h,\ \alpha) + C(f;\ h,\ \alpha)$$

is more accurate than (2.1) when f is a member of a certain class of meromorphic functions. We also need to understand how the value of the shift α influences the numerical properties of the corrected rectangular approximation. If possible, we would like to choose α so that the quadrature sum and correction term have the same sign, in order to avoid the loss of significant digits through the subtraction of nearly equal numbers on a digital computer.

The following theoretical results can be used to develop approximations to $V(x,\ y)$, and also provide an abstract setting for solving some related problems that we plan to address in a separate paper.

Definition 2.1. Given $s > 0$, let $\mathscr{S}_s$ be the infinite strip

$$\mathscr{S}_s = \{u + \mathrm{i}v: -\infty < u < \infty,\ 0 \leqslant v \leqslant s\}$$

in the top half of the complex $w = u + \mathrm{i}v$ plane. Let $\mathscr{M}_s$ denote the class of all functions $f(w)$ that satisfy the following four conditions:

(a) $f(w)$ is analytic in the strip $\mathscr{S}_s$, except possibly for m poles $w_1,\ w_2, \dots,\ w_m$ in the interior of $\mathscr{S}_s$, with corresponding residues $r_1,\ r_2, \dots,\ r_m$;
(b) $f(w)$ is real-valued when w is real;
(c) the integrals $I[\,|f|\,]$ and $I[\,|f(u + \mathrm{i}s)|\,]$ exist;
(d) $\max_{0 \leqslant v \leqslant s} |f(u + \mathrm{i}v)| \to 0$ as $u \to \pm\infty$.

Note that part (a) of this definition allows for the possibility that $f(w)$ may be analytic in the strip $\mathscr{S}_s$. In this situation we regard m as zero, and interpret the correction term defined in (2.4) below as $C(f;\ h,\ \alpha) = 0$. With this understanding the following theorem extends a result of Martensen [24] for the error in (2.1), to the case when f has $m \geqslant 1$ poles inside the strip $\mathscr{S}_s$.

Theorem 2.2. *Let* $f \in \mathscr{M}_s$ *with* $s > 0$, *and let*

$$\mathscr{K}(w;\ h,\ \alpha) = \frac{2}{1 - \exp[-2\pi\mathrm{i}(w/h - \alpha)]}. \tag{2.2}$$

Then

$$I(f) = Q(f;\ h,\ \alpha) + C(f;\ h,\ \alpha) + E(f;\ h,\ \alpha), \tag{2.3}$$

where the correction term

$$C(f;\ h,\ \alpha) = 2\pi \sum_{k=1}^{m} \mathrm{Re}[\mathrm{i}\mathscr{K}(w_k;\ h,\ \alpha) r_k], \tag{2.4}$$

and the quadrature error

$$E(f;\ h,\ \alpha)=\mathrm{Re}\int_{-\infty+is}^{\infty+is}\mathscr{K}(w;\ h,\ \alpha)f(w)\,\mathrm{d}w \tag{2.5}$$

has the bound

$$|E(f;\ h,\ \alpha)|\leqslant\frac{2\,\mathrm{e}^{-2\pi s/h}}{1-\mathrm{e}^{-2\pi s/h}}M(f;\ s), \tag{2.6}$$

where

$$M(f;\ s)=\int_{-\infty}^{\infty}|f(u+\mathrm{i}s)|\,\mathrm{d}u.$$

Proof. The proof of Theorem 2.2 is analogous to the proof of Martensen's Theorem [24,7], which corresponds to the special case when $\alpha=0$ and $m=0$ in our notation. Accordingly, we only outline the key modifications necessary when $\alpha\in[0,1)$ and $f\in\mathscr{M}_s$, with $m\geqslant 1$. In order to preserve the analogy between the current work and [7, proof of Theorem 3.6.1], it is helpful to note that the kernel function $\mathscr{K}$ in (2.2) can be expressed in the alternate form

$$\mathscr{K}(w;\ h,\ \alpha)=1-\mathrm{i}\cot(\pi w/h-\alpha). \tag{2.7}$$

There are two essential steps in the proof:

(i) the derivation of the corrected quadrature sum representation

$$h\sum_{n=-\infty}^{\infty}f(nh+\alpha h)+2\pi\sum_{k=1}^{m}\mathrm{Re}[r_k\cot(\pi w_k/h-\alpha\pi)]$$
$$=\mathrm{Re}\int_{-\infty+is}^{\infty+is}\mathrm{i}\cot(\pi w/h-\alpha\pi)f(w)\,\mathrm{d}w;$$

(ii) the derivation of the integral representation

$$\int_{-\infty}^{\infty}f(u)\,\mathrm{d}u=\mathrm{Re}\int_{-\infty+is}^{\infty+is}f(w)\,\mathrm{d}w+2\pi\sum_{k=1}^{m}\mathrm{Re}[\mathrm{i}r_k].$$

The representation under (i) is established by applying the residue theorem and the Schwarz reflection principle of complex analysis to the integral of $f(w)\cot(\pi w/h-\alpha\pi)$ about the boundary of the strip

$$\{u+\mathrm{i}v:\ -\infty<u<\infty,\ -s\leqslant v\leqslant s\}$$

obtained by reflecting $\mathscr{S}_s$ about the real axis. In a similar manner the representation under (ii) follows by an application of the residue theorem to the integral of $f(w)$ about both the strip $\mathscr{S}_s$ and its conjugate, as detailed in [7].

Subtracting the representation under (ii) from that of (i) we obtain

$$I(f)=Q(f;\ h,\ \alpha)+2\pi\sum_{k=1}^{m}\mathrm{Re}[\{\mathrm{i}+\cot(\pi w/h-\alpha\pi)\}r_k]$$
$$+\mathrm{Re}\int_{-\infty+is}^{\infty+is}\{1-\mathrm{i}\cot(\pi w/h-\alpha\pi)\}f(w)\,\mathrm{d}w,$$

which is equivalent to (2.3) by the alternate representation for $\mathscr{K}$ given by (2.7).

Finally, the upper bound on E follows directly from (2.2) and (2.5), since the triangle inequality yields

$$|\mathscr{K}(u+\mathrm{i}s;\, h,\, \alpha)| \leqslant \frac{2}{\mathrm{e}^{2\pi s/h}-1}. \qquad \square$$

In order to use (2.3) to compute $V(x, y)$, it is helpful to apply Theorem 2.2 to a particular family of meromorphic functions that contains the integrands in (1.1) and (1.2).

Corollary 2.3. *Let G be an entire function such that $f \in \mathscr{M}_s$, where*

$$f(u) = \frac{G(u)}{(u-a)^2+b^2}, \quad b > 0.$$

Then for $s \neq b$, (2.3) holds with correction term

$$C(f;\, h,\, \alpha) = \begin{cases} \dfrac{2\pi}{b}\mathrm{Re}\left[\dfrac{G(a+b\mathrm{i})}{1-\mathrm{e}^{2\pi b/h - 2\pi(a/h-\alpha)\mathrm{i}}}\right], & s > b, \\ 0, & 0 < s < b, \end{cases}$$

and

$$|E(f;\, h,\, \alpha)| \leqslant \frac{2\mathrm{e}^{-2\pi s/h}}{1-\mathrm{e}^{-2\pi s/h}} \cdot \frac{M(G;\, s)}{|s^2-b^2|}. \tag{2.8}$$

Proof. We first consider the determination of the correction term. If $0 < s < b$, then $m = 0$ and $C(f;\, h,\, \alpha) = 0$. If $s > b$, the desired representation for the correction term follows directly from (2.2) and (2.4), since $m = 1$, $w_1 = a + b\mathrm{i}$, and the residue $r_1 = G(a+b\mathrm{i})/(2b\mathrm{i})$.

To establish the error bound we note that

$$\begin{aligned} |(u-a+\mathrm{i}s)^2+b^2|^2 &= \left[(u-a)^2+s^2+b^2\right]^2 - 4b^2s^2 \\ &\geqslant (s^2+b^2)^2 - 4b^2s^2 = (s^2-b^2)^2 \end{aligned}$$

implies that

$$|(u-a+\mathrm{i}s)^2+b^2| \geqslant |s^2-b^2|.$$

The definition of f in the statement of Corollary 2.3 and the previous inequality yield

$$M(f;\, s) \leqslant \frac{M(G;\, s)}{|s^2-b^2|}.$$

The required upper bound on $E(f;\, h,\, \alpha)$ follows from the previous inequality and (2.6). $\square$

In applications of Corollary 2.3, it is worthwhile to compute $M(G;\, s)$ and then determine a value of s that approximately minimizes the right side of the error bound (2.8). For the integrals (1.1) and (1.2) it turns out that an approximate minimum of (2.8) is obtained when the factor $\exp(-2\pi s/h)M(G;\, s)$ in the numerator is minimized at $s = \pi/h$ and $s = \pi/(hy^2)$, respectively.

For each of the integral representations (1.1) and (1.2), Corollary 2.3 can be used to derive a corrected rectangular rule for the Voigt function of the form

$$V(x,\, y) = Q(f;\, h,\, \alpha) + C(f;\, h,\, \alpha) + E(f;\, h,\, \alpha). \tag{2.9}$$

In view of (2.8), the stepsize h can be chosen so that the approximation, obtained by omitting the error term in (2.9),

$$V(x, y) \approx Q(f;\ h,\ \alpha) + C(f;\ h,\ \alpha) \tag{2.10}$$

has a negligible absolute error. (More on this point and the determination of h will be given in Section 3.)

The following two results give explicit forms for (2.9) when Corollary 2.3 is applied to (1.1) with $s = \pi/h$, and to (1.2) with $s = \pi/(hy^2)$.

Result 2.4. For the integral representation (1.1) we have

$$f(u) = \frac{y}{\pi} \cdot \frac{\exp(-u^2)}{(u-x)^2 + y^2}$$

and the corrected rectangular rule (2.9) has positive quadrature sum

$$Q(f;\ h,\ \alpha) = \frac{hy}{\pi} \sum_{n=-\infty}^{\infty} \frac{\exp\left[-(\alpha h + nh)^2\right]}{(\alpha h + nh - x)^2 + y^2}.$$

In Corollary 2.3, $a = x$, $b = y$, $G(u) = y\pi^{-1}\exp(-u^2)$ and $M(G;\ s) = y\pi^{-1/2}\exp(s^2)$. Taking $s = \pi/h$ in Corollary 2.3 gives for $y \neq \pi/h$ the correction term

$$C(f;\ h,\ \alpha) = \begin{cases} 2\mathrm{e}^{y^2 - x^2}\ \mathrm{Re}\left[\dfrac{\mathrm{e}^{-2xyi}}{1 - \mathrm{e}^{2\pi y/h}\mathrm{e}^{2\pi(\alpha - x/h)i}}\right], & y < \dfrac{\pi}{h}, \\ 0, & y > \dfrac{\pi}{h}, \end{cases}$$

and

$$|E(f;\ h,\ \alpha)| \leqslant \frac{2\pi^{-1/2}y}{|y^2 - \pi^2/h^2|} \cdot \frac{\exp(-\pi^2/h^2)}{1 - \exp(-2\pi^2/h^2)}.$$

For the formulation in Result 2.4, the numerical evaluation of the right side of (2.10) is subject to the loss of significant digits if y is small and $x \approx \alpha h + kh$ for some integer k. In this situation $Q(f;\ h,\ \alpha) \to \infty$ and $C(f;\ h,\ \alpha) \to -\infty$ as $y \to 0$, and an appropriate limiting process must be used to compute

$$\frac{hy}{\pi} \cdot \frac{\mathrm{e}^{-(\alpha h + kh)^2}}{(\alpha h + kh - x)^2 + y^2} + C(f;\ h,\ \alpha).$$

For example, if $\alpha = 0$ and $x = 0$ we must deal with the difference

$$\frac{h}{\pi y} - \frac{2\,\mathrm{e}^{y^2}}{\mathrm{e}^{2\pi y/h} - 1}$$

as $y \to 0$. These subtle numerical difficulties are due to the nature of the integrand in (1.1), and are shared by the approximation given for the Voigt function in [25]. In particular, that approximation for the Voigt function corresponds to the special case when $\alpha = 0$ in Result 2.4. (We remark that the error bound for $E(f;\ h,\ 0)$ given by Result 2.4 depends on y, in contrast to the uniform error bound stated in [25]. However, the derivation of that bound as given in [3, pp. 138, 139] has some apparent technical problems.)

Result 2.5. For the integral representation (1.2) we have

$$f(u)=\frac{1}{\pi}\cdot\frac{\exp\left[-(yu-x)^2\right]}{u^2+1}$$

and the corrected rectangular rule (2.9) has positive quadrature sum

$$Q(f;\ h,\ \alpha)=\frac{h}{\pi}\sum_{n=-\infty}^{\infty}\frac{\mathrm{e}^{-[y(\alpha h+nh)-x]^2}}{(\alpha h+nh)^2+1}.$$

In Corollary 2.3, $a=0$, $b=1$, $G(u)=\pi^{-1}\exp[-(yu-x)^2]$ and $M(G;\ s)=y^{-1}\pi^{-1/2}\exp(y^2s^2)$. Taking $s=\pi/(hy^2)$ in Corollary 2.3 gives for $y\neq(\pi/h)^{1/2}$ the correction term

$$C(f;\ h,\ \alpha)=\begin{cases}2\,\mathrm{e}^{y^2-x^2}\operatorname{Re}\left[\dfrac{\mathrm{e}^{2xyi}}{1-\mathrm{e}^{2\pi/h}\,\mathrm{e}^{2\pi\alpha i}}\right], & y<\left(\dfrac{\pi}{h}\right)^{1/2},\\[2ex] 0, & y>\left(\dfrac{\pi}{h}\right)^{1/2}.\end{cases}$$

The error satisfies

$$|E(f;\ h,\ \alpha)|\leqslant\frac{2\pi^{-1/2}y^3}{|y^4-\pi^2/h^2|}\cdot\frac{\exp\left[-\pi^2/(hy)^2\right]}{1-\exp\left[-2\pi^2/(h^2y^2)\right]}.$$

In Result 2.5 it is possible to select the shift α to avoid the cancellation problems that were encountered in Result 2.4 when computing $Q(f;\ h,\ \alpha)+C(f;\ h,\ \alpha)$ for small y. If we choose $\alpha=\frac{1}{2}$ in Result 2.5, then the corresponding midpoint correction term

$$C(f;\ h,\ \tfrac{1}{2})=\begin{cases}\dfrac{2\,\mathrm{e}^{y^2-x^2}\cos(2xy)}{1+\exp(2\pi/h)}, & y<\left(\dfrac{\pi}{h}\right)^{1/2},\\[2ex] 0, & y>\left(\dfrac{\pi}{h}\right)^{1/2},\end{cases}$$

is positive for the troublesome situation when y is small in (1.2).

We note that Theorem 1.1 provides a convenient way to state the conclusion in Result 2.5 for the important case when $\alpha=\frac{1}{2}$. In Theorem 1.1 we have used the abbreviated notation $Q(h)$, $C(h)$ and $E(h)$ in place of the more explicit $Q(f;\ h,\ \frac{1}{2})$, $C(f;\ h,\ \frac{1}{2})$ and $E(f;\ h,\ \frac{1}{2})$ of this section. The practical application of Theorem 1.1 is considered in the next section.

3. The computation of the Voigt function

This section is concerned with the development of an algorithm for the numerical computation of $V(x,\ y)$, correct to a specified absolute error ε. The algorithm is based on the corrected midpoint representation (1.4), and the theoretical results given in Theorem 1.1. Attention can be restricted to the case $x\geqslant 0$ and $y>0$, since $V(-x,\ y)=V(x,\ y)$, $V(x,\ -y)=-V(x,\ y)$ and $V(x,\ 0)=\exp(-x^2)$.

In order to apply the results of Theorem 1.1 it is convenient to introduce the Nth partial quadrature sum

$$Q_N(h) = \frac{h}{\pi} \sum_{n=0}^{N} g(nh + h/2)$$

and define the corresponding trimming error $T_N(h)$ by

$$T_N(h) = \frac{h}{\pi} \sum_{n=N+1}^{\infty} g(nh + h/2), \tag{3.1}$$

where g is defined by (1.3). With this notation the corrected midpoint representation (1.4) can be written as

$$V(x,\ y) = \left[Q_N(h) + C(h)\right] + T_N(h) + E(h).$$

Given $x \geqslant 0$, $y > 0$ and $\varepsilon > 0$, we wish to determine h and N so that the approximation

$$V(x,\ y) \approx Q_N(h) + C(h)$$

satisfies

$$|V(x,\ y) - \left[Q_N(h) + C(h)\right]| \leqslant \varepsilon.$$

It is sufficient to first determine h so that

$$|E(h)| \leqslant \tfrac{1}{2}\varepsilon \tag{3.2}$$

and then choose N in order that

$$T_N(h) \leqslant \tfrac{1}{2}\varepsilon. \tag{3.3}$$

Consider the requirement (3.2). In view of (1.7) and (1.8) we can satisfy (3.2) if

$$\varphi(h) \leqslant \tfrac{1}{2}\varepsilon$$

or if

$$\psi(t) \leqslant \tfrac{1}{2}\varepsilon \tag{3.4}$$

where $t = hy$ and

$$\psi(t) = \frac{2\pi^{-1/2} y}{|y^2 - \pi^2/t^2|} \cdot \frac{\exp(-\pi^2/t^2)}{1 - \left[\exp(-\pi^2/t^2)\right]^2}. \tag{3.5}$$

Figure 2 is a plot of the level curves

$$-\log \psi(t) = d$$

where the number of decimal digits $d = 0(1)6,\ 8(2)18$. In Fig. 2 the respective horizontal and vertical axes represent t and y, with $0.5 \leqslant t \leqslant 3.5$, $10^{-15} \leqslant y \leqslant 3$. (Due to space limitations near the vertical y-axis in Fig. 2, the last four level curves corresponding to $d = 12(2)18$ are not labeled.)

One way to satisfy (3.4) is to solve numerically for the largest positive root t^*, of the nonlinear equation $\psi(t) = \frac{1}{2}\varepsilon$ and then take $h = t^*/y$. This has the advantage of determining the largest stepsize h satisfying (3.2), and minimizes the number of terms that need to be summed in $Q_N(h)$. We have devised an iterative numerical method for computing t^*, but the resulting algorithm is

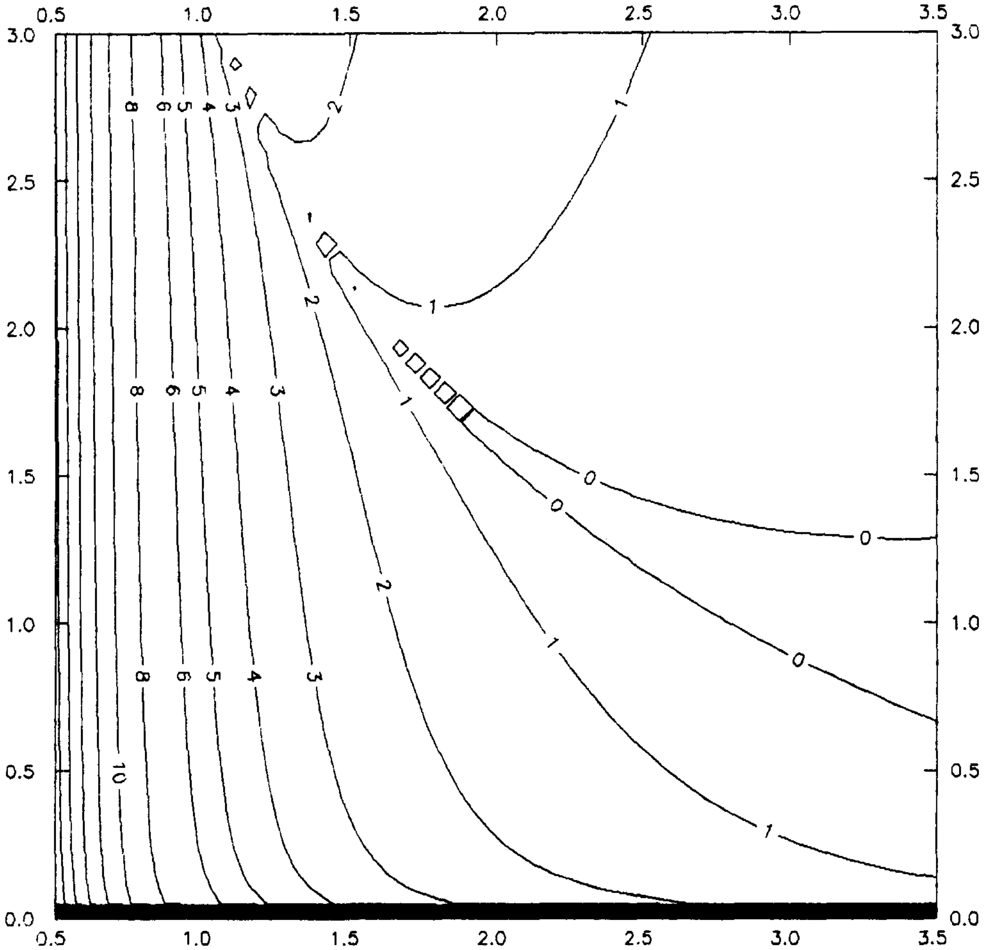

Fig. 2. Level curves for $-\log \psi(t)$, $0.5 \leqslant t \leqslant 3.5$, $10^{-15} \leqslant y \leqslant 3$.

somewhat involved, particularly for the case when y is very small. This is not surprising in view of Fig. 2, due to the nonlinear behavior of $\psi(t)$ near the horizontal t-axis and near the hyperbola $y = \pi/t$.

The following naive approach provides a simple, alternative method for determining an acceptable, but not necessarily optimal value for h. Starting with some initial stepsize h_0 and positive constant $c_1 < 1$, we set $t_0 = h_0 y$ and determine numerically by repeated trials the smallest integer $k \geqslant 0$ such that $\psi(c_1^k t_0) \leqslant \frac{1}{2}\varepsilon$, and then take $h = c_1^k t_0 / y$. In this scheme we have found that a reasonable value for the initial stepsize is $h_0 = b$, where b is given by (3.7) below. It is convenient to take $c_1 = 1/\sqrt{2}$, this particular choice being exploited below for the efficient calculation of $\psi(t)$.

Once h has been determined so that (3.2) is satisfied, the following theorem can be used to determine N so that (3.3) holds.

Theorem 3.1. *Given $x \geqslant 0$, $y > 0$, $h > 0$ and $\varepsilon > 0$, let $\tau > 0$ satisfy the condition*

$$e^{-\tau^2} \leqslant A\tau \tag{3.6}$$

where

$$A = \tfrac{1}{2}\pi\varepsilon y.$$

Set

$$b = \frac{\tau + x}{y}. \tag{3.7}$$

If N is the smallest positive integer satisfying the condition

$$(N + \tfrac{1}{2})h \geqslant b, \tag{3.8}$$

then

$$T_N(h) < \tfrac{1}{2}\varepsilon.$$

Proof. For $u \geqslant x/y$ it is clear from (1.3) that $g(u)$ is positive and decreasing with

$$g(u) \leqslant 2\,\mathrm{e}^{-(yu-x)^2}. \tag{3.9}$$

Since $(N + \frac{1}{2})h \geqslant b \geqslant x/y$, the comparison of

$$T_N(h) = \frac{1}{\pi} \sum_{n=N+1}^{\infty} hg(nh + h/2)$$

with an integral gives

$$T_N(h) \leqslant \frac{1}{\pi} \int_b^{\infty} g(u)\,\mathrm{d}u.$$

By (3.9) we have

$$T_N(h) \leqslant \frac{2}{\pi} \int_b^{\infty} \mathrm{e}^{-(yu-x)^2}\,\mathrm{d}u = \frac{2}{\pi y} \int_{\tau}^{\infty} \mathrm{e}^{-t^2}\,\mathrm{d}t. \tag{3.10}$$

By [1, inequality 7.1.13]

$$\int_{\tau}^{\infty} \mathrm{e}^{-t^2}\,\mathrm{d}t < \frac{\mathrm{e}^{-\tau^2}}{2\tau}$$

and (3.10) yields

$$T_N(h) < \frac{\mathrm{e}^{-\tau^2}}{\pi y \tau} \leqslant \tfrac{1}{2}\varepsilon,$$

the last equality following from (3.6) and the definition of A. □

In order to apply Theorem 3.1 we observe that (3.6) will hold for any $\tau \geqslant \tau_*$, where τ_* is the unique positive root of

$$\mathrm{e}^{-\tau^2} = A\tau.$$

The latter equation can be solved numerically by the following fixed-point iteration scheme:

$$\tau_0 = u^{1/2},$$

$$\tau_{n+1} = F(\tau_n), \quad n = 0, 1, \ldots .$$

Here the iteration function is given by

$$F(\tau) = [-\ln(A\tau)]^{1/2} = u^{1/2}\left[1 - \frac{\ln \tau}{u}\right]^{1/2},$$

where $u = -\ln(A) = -\ln(y) - \ln(\frac{1}{2}\pi\varepsilon)$.

In order to force $\tau_* < \tau_0 = u^{1/2}$, so that (3.6) is satisfied, we make the additional assumption that y satisfies the inequality

$$y \leqslant 2/(\pi\, \mathrm{e}\varepsilon). \tag{3.11}$$

(This constraint on y is not overly restrictive, since $\varepsilon \ll 1$ in practice.) As a consequence of (3.11) we also have $A \leqslant \mathrm{e}^{-1}$ and $u \geqslant 1$. Since $F'(\tau) < 0$ for $\tau > 0$, the fixed-point iterates obey

$$\tau_1 < \tau_3 < \cdots < \tau_* < \cdots < \tau_2 < \tau_0.$$

Therefore, all of the iterates τ_{2m}, $m \geqslant 0$, satisfy (3.6).

```
procedure Voigt(x,y,ε,V,xyOK)
   c0 ← 2/(πe)
   c1 ← 1/√2
   c2 ← 2/√π
   xyOK ← (0 ≤ x) and (0 ≤ y) and (y ≤ c0/ε)
   if not xyOK then
     V ← 0
   else
     if y = 0 then
       V ← exp( − x²)
     else
       c3 ← ln(πε/2)
       τ ← [ − ln(y) − c3]^1/2
       b ← (τ + x)/y
       t ← by
       while {c2y exp( − π²/t²)}/|y² − π²/t²|/{1 − [exp( − π²/t²)]²} > ε/2
         t ← c1t
       end while
       h ← t/y
       N ← trunc(0.5 + b/h)
       S ← 0
       u ← h/2
       for i = 1 to N
         S ← S + {[1+exp( − 4xyu)]exp[ − (yu − x)²]}/(u²+1)
         u ← u + h
       end for
       Q ← hS/π
       if y² < π/h then
         C ← {2 exp(y² − x²)cos(2xy)}/[1+exp(2π/h)]
       else
         C ← 0
       end if
       V ← Q + C
     end if
   end if
end procedure
```

Fig. 3. Pseudocode algorithm for computing $V(x, y)$.

Table 2
Precise values for the Voigt function

x	y	$V(x, y)$
1	10^{-20}	0.36787 94411 71442 32159 63831
10	10^{-4}	$0.57287\ 17561\ 64533\ 22536\ 12329 \cdot 10^{-6}$
10^{-3}	10^{-3}	0.99887 16223 35411 24715 72117
0	0.25	0.77034 65477 30996 74391 67391
1	0.5	0.35490 03328 67577 88392 24455
5	5	$0.56965\ 43988\ 81769\ 78967\ 40047 \cdot 10^{-1}$
1	10	$0.55598\ 31964\ 10553\ 71345\ 93855 \cdot 10^{-1}$

However, for our purposes it is not very beneficial to do any fixed-point iterations beyond the initial guess. Computational experience shows that $\tau_0 = u^{1/2} > \tau_*$ provides a simple, reasonably accurate approximation to τ_*. For example, when $x = 1$, $y = 0.5$ and $\varepsilon = 10^{-10}$ we have $\tau_0 = 4.82$, while $\tau_* = 4.66$. We suggest taking $\tau = \tau_0 = u^{1/2}$ in (3.7). N can then be determined from (3.8), with the certainty that (3.3) holds.

In Fig. 3 we give an informal pseudocode statement of an algorithm for computing $V(x, y)$ to a specified absolute error ε. If the input arguments x and y do not satisfy the requirements $x \geqslant 0$ and $0 \leqslant y \leqslant 2/(\pi\, \mathrm{e}\varepsilon)$, then the algorithm returns zero for V and false for the xy-range status indicator xyOK.

As an aid in verifying the implementation of the pseudocode in a particular computing environment, we list some selected values of $V(x, y)$ in Table 2. The values of $V(x, y)$ in Table 2 are believed to be correct to twenty-five significant digits and were obtained by executing Voigt $(x, y, \varepsilon, V, y\mathrm{OK})$ with $\varepsilon = 0.5 \times 10^{-m}$, $m = 10(10)50$. All of these numerical calculations were done on a VAX 11/785 computer using Version 4.8 of the VAX FORTRAN compiler and REAL*16, quadruple precision, floating-point arithmetic. Quadruple precision on this machine employs (approximately) a 33-decimal digit mantissa, with nonzero numbers having magnitudes in the range 0.84×10^{-4932} to 0.59×10^{4932}.

The algorithm in Fig. 3 was also implemented using TURBO Pascal 5.5 on the Dell 210 PC. For the fixed choice $\varepsilon = 10^{-17}$, we obtained the values listed in Table 3 for the intermediate quantities b, h, N, $Q(h)$ and $C(h)$. The Pascal program utilized the extended data type

Table 3
Parameter values determined by the Voigt function algorithm for $\varepsilon = 10^{-17}$

x	y	b	h	N	$Q(h)$	$C(h)$
1	10^{-20}	$1.02 \cdot 10^{21}$	$1.02 \cdot 10^{21}$	1	$6.10 \cdot 10^{-29}$	$3.68 \cdot 10^{-1}$
10	10^{-4}	$1.69 \cdot 10^{5}$	$5.29 \cdot 10^{3}$	32	$5.73 \cdot 10^{-7}$	$3.72 \cdot 10^{-44}$
10^{-3}	10^{-3}	$6.75 \cdot 10^{3}$	$4.22 \cdot 10^{2}$	16	$6.31 \cdot 10^{-3}$	$9.93 \cdot 10^{-1}$
0	0.25	$2.53 \cdot 10^{1}$	1.58	16	$7.31 \cdot 10^{-1}$	$3.94 \cdot 10^{-2}$
1	0.5	$1.46 \cdot 10^{1}$	$9.09 \cdot 10^{-1}$	16	$3.54 \cdot 10^{-1}$	$5.10 \cdot 10^{-4}$
5	5	2.22	$9.80 \cdot 10^{-2}$	23	$5.70 \cdot 10^{-2}$	$2.80 \cdot 10^{-28}$
1	10	$7.03 \cdot 10^{-1}$	$4.40 \cdot 10^{-2}$	16	$5.56 \cdot 10^{-2}$	0

```
p ← (π/t)²
q ← exp(-p)
r ← q²
while c₂yq/{|y²-p|(1-r)} > ε/2
  t ← c₁t
  p ← 2p
  q ← r
  r ← q²
end while
```

Fig. 4. Replacement pseudocode for efficient while-loop in Fig. 3.

```
α ← exp( - 2h²y²)
β ← exp(2xyh)
γ ← αβ
δ ← 1/β²
G ← 1/β
H ← exp[ - (hy/2 - x)²]
for i = 1 to N
  S ← S + H(1+G)/(u²+1)
  u ← u + h
  G ← δG
  H ← γH
  γ ← αγ
end for
```

Fig. 5. Replacement pseudocode for efficient for-loop in Fig. 3.

supported by the 80287 math coprocessor. Floating-point arithmetic in this computing environment employs (approximately) a 19-decimal digit mantissa, with nonzero numbers having magnitudes in the range from 1.9×10^{-4951} to 1.1×10^{4932}. It should be noted that the noninteger entries in Table 3 have been rounded to the number of places listed. The intermediate values listed in Table 3 may be useful for debugging purposes, if problems are encountered during the computer implementation of the pseudocode.

It is possible to improve the efficiency of the simple algorithm in Fig. 3, by avoiding unnecessary evaluations of the exponential function in the while- and for-loops. This gain in efficiency can be realized by employing the elementary property $\exp(nt) = [\exp(t)]^n$, where n in our applications will be a positive integer. As explained below, the price for this increased efficiency is the somewhat more complicated algorithm obtained by substituting the pseudocode in Figs. 4 and 5, for the respective while-loop and for-loop in Fig. 3.

Consider the evaluations of $\psi(t)$ in the while-loop in Fig. 3. Since $c_1 = 1/\sqrt{2}$, we have $\exp[-\pi^2/(c_1 t)^2] = \{\exp[-\pi^2/t^2]\}^2$. This observation is the basis for replacing the three statements in the while-loop in Fig. 3, by the nine statements in Fig. 4. Only one evaluation of the exponential function is required in Fig. 4 to determine a value of t that satisfies (3.4).

Speeding up the for-loop in Fig. 3 is somewhat more involved. The essential idea is to note that $g(u)$ in (1.3) can be expressed as

$$g(u) = \frac{H(u)[1 + G(u)]}{u^2 + 1}, \tag{3.12}$$

where the functions $H(u) = \exp[-(yu - x)^2]$ and $G(u) = \exp(-4xyu)$ satisfy

$$H(u + h) = \exp(-h^2y^2 - 2hy^2u + 2xyh)H(u)$$

and

$$G(u + h) = \exp(-4xyh)G(u).$$

These later properties yield the recurrence relations

$$H\left[\tfrac{1}{2}(2j + 1)h\right] = \left[\exp(-2h^2y^2)\right]^j \exp(2xyh)H\left[\tfrac{1}{2}(2j - 1)h\right], \quad j = 1, 2, \ldots,$$

and

$$G\left[\tfrac{1}{2}(2j + 1)h\right] = \exp(-4xyh)G\left[\tfrac{1}{2}(2j - 1)h\right], \quad j = 1, 2, \ldots,$$

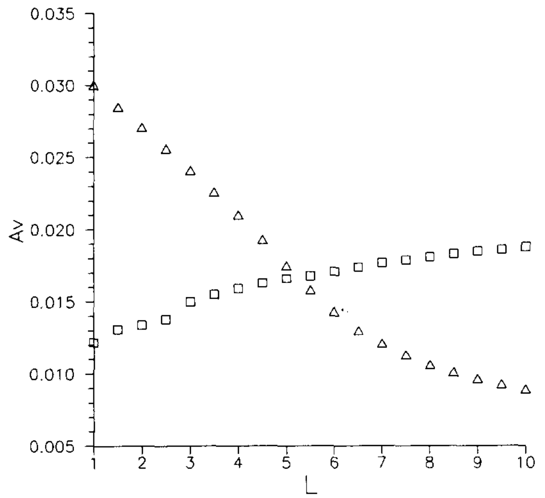

Fig. 6. Average execution times: □ algorithm in Figs. 3–5, △ algorithm in [11].

where $H(\frac{1}{2}h) = \exp[-(\frac{1}{2}hy - x)^2]$ and $G(\frac{1}{2}h) = 1/\exp(2xyh)$. We can compute $H(u)$, $G(u)$, and consequently $g(u)$, at the required midpoints $u = \frac{3}{2}h, \frac{5}{2}h, \ldots$ using only the three seed values $G(\frac{1}{2}h)$, $H(\frac{1}{2}h)$ and $\exp(-2h^2y^2)$, of the exponential function. These observations form the basis for replacing the four statements in the for-loop in Fig. 3, with the thirteen statements in Fig. 5. Unlike Fig 3., only three evaluations of the exponential function are required in Fig. 5 to compute the midpoint sum S in the for-loop, for any value of N.

In order to discuss some timing comparisons, it is convenient to introduce the grid $(x_i, y_j) = (\frac{1}{10}i, \frac{1}{10}j)$, $i, j = 0, 1, \ldots, 10L$, of $(10L+1)^2$ equally spaced points within the square $[0, L] \times [0, L]$. For a fixed value of ε, consider the average execution time $\mathrm{Av}(L)$ required to evaluate $V(x, y)$ over these grid points. In Fig. 6 we plot the average execution times $\mathrm{Av}(L)$, $L = 1(0.5)10$, for both the algorithm specified by Figs. 3–5, with $\varepsilon = 0.5 \times 10^{-10}$, and Gautschi's algorithm [11], with $V(x, y) = \mathrm{Re}\, w(z)$. (This particular value of ε was employed in the timing comparison because Gautschi's algorithm has a absolute accuracy limited to ten decimal digits.) The average execution times shown in Fig. 6 are given in seconds, and were obtained on a Dell 210 PC using TURBO Pascal 5.5 and the extended data type supported by the 80287 match coprocessor. It is interesting to observe that the crossover point in Fig. 6 occurs near $x = 5.33$, where Gautchi's algorithm switches over from a Taylor approximation to a Gauss–Hermite approximation for $w(z)$.

Although the algorithm specified in this paper by Figs. 3–5 is designed to compute $V(x, y)$ to a specified absolute error ε, it can be used in principle to compute $V(x, y)$ to a specified relative error η. To this end we can take $\varepsilon = \eta V_0$, where V_0 is a positive lower bound for $V(x, y)$.

Relative error is more appropriate when x is moderately large and y is very small, since as noted before $V(x, 0) = \exp(-x^2)$. For example, if $(x, y) = (5.4, 10^{-10})$, then Voigt $(x, y, \varepsilon, V, y\mathrm{OK})$ with the ten digit absolute error requirement $\varepsilon = 0.5 \times 10^{-10}$ yields $V \approx 2.3047 \times 10^{-12}$. For ten significant digits we require $\eta = 0.5 \times 10^{-10}$. Taking $V_0 = 2 \times 10^{-12}$ and $\varepsilon = 0.5 \times 10^{-10} V_0 = 10^{-22}$ in Voigt $(x, y, \varepsilon, V, y\mathrm{OK})$ now yields

$$V \approx 2.2608\ 44498\ 419 \times 10^{-12}$$

in comparison with the exact value

$$V = 2.2608\ 44498\ 40791\ 39470\ 84105 \times 10^{-12}.$$

In conjunction with this example it is interesting to note that the double precision complex FORTRAN function ZERFE, for computing $w(z)$ in the IMSL SFUN library, gives the approximation $V \approx 2.0440 \times 10^{-12}$ for $V(x, y) = \text{Re } w(z)$. ZERFE appears to be a translation of Gautschi's algorithm [11] and is accordingly limited to a fixed absolute error $\varepsilon = 0.5 \times 10^{-10}$.

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