

Error Estimates in Simple Quadrature with Voigt Functions

By Alex Reichel

In a wide range of spectral line computations occurring for example, in astrophysics and reactor physics, it is necessary to compute integrals of the form

$$(1) \quad \int_{-\infty}^{+\infty} f(x)U_0(x, t)dx ,$$

where

$$(2) \quad U_0(x, t) = \frac{1}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \frac{\exp [-(x-y)^2/4t] dy}{1+y^2}$$

is the Voigt or Doppler broadened Breit-Wigner contour. Simple quadrature is often inaccurate due to the occurrence of steep and shifting plateaux in the integrand.

By using a modification of a method suggested by Goodwin [1] for integrals of the form

$$\int_{-\infty}^{+\infty} f(x) \exp [-x^2]dx$$

it is possible to estimate the error $E(h)$ in the quadrature formula

$$(3) \quad \int_{-\infty}^{+\infty} f(x)U_0(x, t)dx = h \sum_{n=-\infty}^{+\infty} f(nh)U_0(nh, t) - E(h)$$

where h is the interval width. Without loss of generality, $f(x)$ may be taken as even.

As shown by the present author [2], for complex z ,

$$(4) \quad U_0(z, t) = \frac{-i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \frac{\exp [-u^2/4t](u-i)du}{(u-i)^2 - z^2} .$$

Consider the contour integral

$$I = \oint \frac{f(z)U_0(z, t)dz}{\{1 - e^{-2\pi iz/h}\}}$$

taken around the rectangle $-R \leq x \leq +R$, $-\pi/h \leq y \leq \pi/h$, where h is sufficiently small as to include the poles of $f(z)$. Thus

$$I = \frac{i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \exp [-u^2/4t](u-i)du \oint \frac{f(z)dz}{[z^2 - (u-i)^2][1 - e^{-2\pi iz/h}]}$$

giving

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$$\begin{aligned}
 I &= h \sum_{n=-\infty}^{+\infty} f(nh)U_0(nh, t) \\
 (5) \quad &+ 2\pi i \sum_k \lim_{z \rightarrow z_k} \left\{ \frac{(z - z_k)f(z)}{1 - e^{-2\pi iz/h}} \cdot U_0(z, t) \right\} \\
 &+ \frac{i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \exp[-u^2/4t] \left\{ \frac{\pi i f(u - i)}{1 - e^{-2\pi iu/h - 2\pi/h}} - \frac{\pi i f(-u + i)}{1 - e^{2\pi iu/h + 2\pi/h}} \right\} du
 \end{aligned}$$

where the z_k are the poles of $f(z)$ within the rectangle.

Also, allowing $R \rightarrow \infty$,

$$\begin{aligned}
 (6) \quad I &= \int_{\infty + i\pi/h}^{-\infty + i\pi/h} \frac{f(x)U_0(x, t)dx}{[1 - e^{-2\pi ix/h}]} + \int_{-\infty - i\pi/h}^{\infty - i\pi/h} f(x)U_0(x, t)dx \\
 &+ \int_{-\infty - i\pi/h}^{\infty - i\pi/h} \frac{f(x)U_0(x, t)e^{-2\pi ix/h}dx}{[1 - e^{-2\pi ix/h}]} .
 \end{aligned}$$

Now, if Γ is the rectangle $-R \leq x \leq R, -(\pi/h) \leq y \leq 0$, we have for sufficiently small h and $R \rightarrow \infty$,

$$\begin{aligned}
 (7) \quad \oint_{\Gamma} f(z)U_0(x, t) &= \frac{+i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \pi i f(u - i) \exp[-u^2/4t] du \\
 &+ 2\pi i \sum_k \lim_{z \rightarrow z_{1k}} \{ (z - z_{1k})f(z)U_0(z, t) \}
 \end{aligned}$$

where z_{1k} are the poles of $f(z)$ in the lower half plane, poles on the x -axis requiring special treatment. Thus,

$$\begin{aligned}
 (8) \quad \int_{-\infty - i\pi/h}^{+\infty - i\pi/h} f(x)U_0(x, t)dx &= \int_{-\infty}^{+\infty} f(x)U_0(x, t)dx \\
 &+ \frac{i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \exp[-u^2/4t] \pi i f(u - i) du \\
 &+ 2\pi i \sum_k \lim_{z \rightarrow z_{1k}} \{ (z - z_{1k})f(z)U_0(z, t) \} .
 \end{aligned}$$

From (5), (6) and (8)

$$\int_{-\infty}^{+\infty} f(x)U_0(x, t)dx = h \sum_{n=-\infty}^{+\infty} f(nh)U_0(nh, t) - E_1(h) - E_2(h) - E_3(h)$$

where

$$(9) \quad E_1(h) = \frac{2\pi}{(4\pi t)^{1/2}} \sum_{r=1}^{\infty} e^{-2r\pi/h} \int_{-\infty}^{+\infty} \exp[-u^2/4t] f(u - i)e^{-2r\pi iu/h} du ,$$

$$\begin{aligned}
 (10) \quad E_2(h) &= 2\pi i \sum_k \lim_{z \rightarrow z_{1k}} \{ (z - z_{1k})f(z)U_0(z, t) \} \\
 &- 2\pi i \sum_k \lim_{z \rightarrow z_k} \left\{ \frac{(z - z_k)f(z)U_0(z, t)}{1 - e^{-2\pi iz/h}} \right\}
 \end{aligned}$$

and

$$\begin{aligned}
 (11) \quad E_3(h) &= \int_{+\infty+i\pi/h}^{-\infty+i\pi/h} \frac{f(x)U_0(x, t)dx}{1 - e^{-2\pi ix/h}} \\
 &+ \int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x)U_0(x, t)e^{-2\pi ix/h}dx}{1 - e^{-2\pi ix/h}}.
 \end{aligned}$$

Now

$$\begin{aligned}
 (12) \quad E_3(h) &= 2 \int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x)U_0(x, t)dx}{e^{+2\pi ix/h} - 1} \\
 &= 2 \sum_{r=1}^{\infty} \exp[-2r\pi^2/h^2] \int_{-\infty}^{+\infty} f(u - i\pi/h)U_0(u - i\pi/h, t)e^{-2r\pi iu/h}du.
 \end{aligned}$$

For a wide class of functions $f(x)$ occurring in practice, the greatest value occurs at the origin, or the function is otherwise bounded within the range of integration.

A reasonable estimate might then be

$$(13) \quad E_3(h) \doteq 2f\left(\frac{i\pi}{h}\right) \sum_{r=1}^{\infty} \exp[-2r\pi^2/h^2] \int_{-\infty}^{+\infty} U_0\left(u - \frac{i\pi}{h}, t\right)e^{-2r\pi iu/h}du.$$

Values of $U_0(z, t)$ for complex z are given in the author's paper [2]. We have for $-1 < y < +1$,

$$\begin{aligned}
 (14) \quad U_0(x + iy, t) &= \frac{1}{2(1 + y)} U_0\left(\frac{x}{1 + y}, \frac{t}{(1 + y)^2}\right) \\
 &+ \frac{1}{2(1 + y)} V_0\left(\frac{x}{1 + y}, \frac{t}{(1 + y)^2}\right) \\
 &+ \frac{1}{2(1 - y)} U_0\left(\frac{x}{1 - y}, \frac{t}{(1 + y)^2}\right) - \frac{i}{2(1 - y)} V_0\left(\frac{x}{1 - y}, \frac{t}{(1 + y)^2}\right)
 \end{aligned}$$

and for $y > +1$

$$\begin{aligned}
 (15) \quad U_0(x + iy, t) &= \frac{1}{2(1 + y)} U_0\left(\frac{x}{1 + y}, \frac{t}{(1 + y)^2}\right) \\
 &+ \frac{i}{2(1 + y)} V_0\left(\frac{x}{1 + y}, \frac{t}{(1 + y)^2}\right) \\
 &- \frac{1}{2(y - 1)} U_0\left(\frac{x}{y - 1}, \frac{t}{(y - 1)^2}\right) \\
 &- \frac{i}{2(y - 1)} V_0\left(\frac{x}{y - 1}, \frac{t}{(y - 1)^2}\right),
 \end{aligned}$$

where

$$(16) \quad V_0(x, t) = \frac{1}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \frac{\exp[-(x - y)^2/4t] y dy}{1 + y^2}$$

is the Hilbert transform of $U_0(x, t)$.

Thus, assuming $\pi/h > 1$,

$$\begin{aligned}
 U_0(u - i\pi/h, t) &= U_0(-u + i\pi/h) \\
 &= \frac{1}{2(1 + \pi/h)} U_0\left(\frac{u}{1 + \pi/h}, \frac{t}{(1 + \pi/h)^2}\right) \\
 &\quad - \frac{i}{2(1 + \pi/h)} V_0\left(\frac{u}{1 + \pi/h}, \frac{t}{(1 + \pi/h)^2}\right) \\
 &\quad - \frac{1}{2(\pi/h - 1)} U_0\left(\frac{u}{\pi/h - 1}, \frac{t}{(\pi/h - 1)^2}\right) \\
 &\quad + \frac{i}{2(\pi/h - 1)} V_0\left(\frac{u}{\pi/h - 1}, \frac{t}{(\pi/h - 1)^2}\right).
 \end{aligned}
 \tag{17}$$

Substituting (17) in (13) and using the results

$$\begin{aligned}
 \int_{-\infty}^{+\infty} e^{-ipx} U_0(x, t) dx &= \pi \exp[-|p| - p^2 t], \\
 \int_{-\infty}^{+\infty} e^{-ipx} V_0(x, t) dx &= \pi i \exp[+p - p^2 t], \quad p < 0, \\
 &= -\pi i \exp[-p - p^2 t], \quad p > 0, \\
 &= 0, \quad p = 0,
 \end{aligned}$$

we find that the contribution to $E_3(h)$ from the first term in (17) for example is

$$2f\left(\frac{i\pi}{h}\right) \sum_{r=1}^{\infty} \exp[-2r\pi^2/h^2] \cdot \frac{\pi}{2} \exp\left[-2r\pi/h\left(1 + \frac{\pi}{h}\right) - \frac{4r^2\pi^2 t}{h^2}\right].$$

For $h < \pi$ and $t > 1$, this term is trivially small. Together with the three remaining terms of (17) in (13) we obtain four terms which cancel in pairs so that the value of $E_3(h)$ on this basis is zero.

For a similar class of functions $f(x)$, we have from (9),

$$E_1(h) \doteq 2\pi f(i) \sum_{r=1}^{\infty} \exp[-2r\pi/h - 4r^2\pi^2 t/h^2].
 \tag{18}$$

Only in special cases is this term important. The term $E_2(h)$ is readily computed using Eqs. (14) and (15). Tables and computer routines for the functions $U_0(x, t)$ and $V_0(x, t)$ are readily available.

Consider for example

$$\int_{-\infty}^{+\infty} \frac{U_0(x, t) dz}{1 + x^2} = \frac{\pi}{2} U_0\left(0, \frac{t}{4}\right).$$

For the special case $t = 4$, the value of the integral is 0.8570 to four places. Using an interval width $h = 1$, we have

$$U_0(0, 4) + \sum_1^{\infty} \frac{2}{1 + n^2} U_0(n, 4) = 0.8612.$$

On account of the singularity in Eq. (18) we must use Eq. (9) to compute $E_1(h)$, and substitute

$$f(u - i) = \frac{1}{u^2 + 4} + \frac{i}{2u} - \frac{iu}{2(u^2 + 4)}.$$

Since

$$\int_{-\infty}^{+\infty} \frac{\exp[-u^2/4t]}{u^2 + 4} e^{-2r\pi iu/h} du < \frac{1}{4} (4\pi t)^{1/2} \exp[-4r^2\pi^2 t/h^2]$$

and

$$i \int_{-\infty}^{+\infty} \frac{\exp[-u^2/4t]u}{u^2 + 4} e^{-2r\pi iu/h} du < -\frac{i}{4} (4\pi t)^{1/2} \exp[-4r^2\pi^2 t/h^2] \operatorname{erf}\left(\frac{i2r\pi\sqrt{t}}{h}\right)$$

both of which are trivially small for $h = 1, t > 1$, we see that

$$E_1(h) \doteq \frac{+\pi^2}{(4\pi t)^{1/2}} \sum_{r=1}^{\infty} e^{-2r\pi/h} \operatorname{erf}\left(\frac{2r\pi\sqrt{t}}{h}\right) \doteq \frac{+\pi^2}{(4\pi t)^{1/2}} \frac{1}{e^{2\pi/h} - 1}.$$

For $h = 1$ and $t = 4$, $E_1(h) \doteq 0.0026$. Since $z_{ik} = -i, z_k = -i, +i$, Eq. (10) gives

$$E_2(h) = \frac{2\pi e^{-2\pi/h}}{1 - e^{-2\pi/h}} U_0(i, t) = \frac{\pi}{2} \frac{U_0(0, t/4)}{e^{2\pi/h} - 1}.$$

For $h = 1, t = 4$, $E_2(h) \doteq 0.0016$.

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