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

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

where

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

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

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

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,

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

Consider the contour integral

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

taken around the rectangle $-R \leqq x \leqq +R$, $-\pi/h \leqq y \leqq \pi/h$, 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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$$I = h \sum_{n=-\infty}^{+\infty} f(nh)U_0(nh, t)$$

$$(5) \qquad + 2\pi i \sum_k \lim_{z \to z_k} \left\{ \frac{(z - z_k)f(z)}{1 - e^{-2\pi iz/h}} \cdot U_0(z, t) \right\}$$

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

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

Also, allowing $R \to \infty$,

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

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

$$(7) \qquad \oint_\Gamma f(z)U_0(x, t) = \frac{+i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \pi i f(u - i) \exp[-u^2/4t]du + 2\pi i \sum_k \lim_{z \to z_{lk}} \{(z - z_{lk})f(z)U_0(z, t)\}$$

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

$$(8) \qquad \int_{-\infty - i\pi/h}^{+\infty - i\pi/h} f(x)U_0(x, t)dx = \int_{-\infty}^{+\infty} f(x)U_0(x, t)dx + \frac{i}{(4\pi t)^{1/2}} \int_{-\infty}^{+\infty} \exp[-u^2/4t]\pi i f(u - i)du + 2\pi i \sum_k \lim_{z \to z_{lk}} \{(z - z_{lk})f(z)U_0(z, t)\}.$$

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

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

$$(10) \qquad E_2(h) = 2\pi i \sum_k \lim_{z \to z_{lk}} \{(z - z_{lk})f(z)U_0(z, t)\} - 2\pi i \sum_k \lim_{z \to z_k} \left\{ \frac{(z - z_k)f(z)U_0(z, t)}{1 - e^{-2\pi iz/h}} \right\}$$

and

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

Now

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

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

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

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

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

and for $y > +1$

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

where

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

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

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

$$U_0(u - i\pi/h, t) = U_0(-u + i\pi/h)$$

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

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

$$\int_{-\infty}^{+\infty} e^{-ipx} U_0(x, t)dx = \pi \exp\left[-|p| - p^2 t\right],$$

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

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

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

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),

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

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

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

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

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

For $h = 1$ and $t = 4$, $E_1(h) \doteqdot 0.0026$. Since $z_{lk} = -i$, $z_k = -i, +i$, 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 $h = 1$, $t = 4$, $E_2(h) \doteqdot 0.0016$.

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