NUCLEAR SCIENCE AND ENGINEERING: **20**, 547-550 (1964)

Letters to the Editors

On The Evaluation of Doppler-Broadened Cross-Section Functions

The functions

$$\psi(x,\xi) = \frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{+\infty} \frac{\exp\left[-\frac{1}{4}\xi^2(x-y)^2\right]dy}{1+y^2} \qquad (1)$$

and

$$\phi(x,\xi) = \frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{+\infty} \frac{\exp\left[-\frac{1}{4}\xi^2(x-y)^2\right]y\,dy}{1+y^2} \qquad (2)$$

may be rapidly evaluated using an expansion of the function $\psi(x,\xi) + i\phi(x,\xi)$ in Hermite Polynomials and separating real and imaginary parts. The resulting simple routine is as follows:

Let $K = \frac{\xi^2}{4+\xi^2}$, and let

$$I_0 = \psi(0, 2K^{\frac{1}{2}}) = \sqrt{\pi}\sqrt{K}\,e^K \operatorname{erfc}\sqrt{K}$$

(i.e., the peak value of Eq. (1) with ξ replaced by $2K^{\frac{1}{2}}$). Then form

$$I_1 = 2K\left[1 - I_0\right]$$

$$I_{n+1} = 2K\left[(-1)^{n+1} I_n - nI_{n-1}\right]$$

for $n = 1, 2, 3, \ldots\ldots$.

Let

$$J_n(x) = \frac{H_n(x)}{2^n n!}$$

where $H_n(x)$ are Hermite Polynomials, and we have

$$J_0 = 1, \qquad J_1 = x$$

$$J_{n+1}(x) = \frac{1}{2(n+1)}\left[2xJ_n(x) - J_{n-1}(x)\right]$$

for $n = 1,2,3, \ldots\ldots$.

Then

$$\psi(x,\xi) = I_0J_0 + I_2J_2 + I_4J_4 + \ldots . \qquad (3)$$

$$\phi(x,\xi) = I_1J_1 + I_3J_3 + I_5J_5 + \ldots . . \qquad (4)$$

The series (3), (4) can be terminated on specification of the desired accuracy (say 10^{-7}). The series may be found alternatively as a special case of Hermite Polynomial expansions of certain convolution integrals given in a paper to be published[1].

For x larger than $\frac{7}{\xi}$ it has been found economic to switch to the well known asymptotic developments of $\psi(x,\xi)$ and $\phi(x,\xi)$ or to the following:

$$\psi(x,\xi) \simeq \frac{1}{x^2} + \frac{\frac{6}{\xi^2} - 1}{x^4} + \frac{\frac{60}{\xi^4} - \frac{20}{\xi^2} + 1}{x^6} + \frac{\frac{840}{\xi^6} - \frac{420}{\xi^4} + \frac{42}{\xi^2} - 1}{x^8} + \ldots$$

$$\phi(x,\xi) \simeq \frac{1}{x} + \frac{\frac{2}{\xi^2} - 1}{x^3} + \frac{\frac{12}{\xi^4} - \frac{12}{\xi^2} + 1}{x^5} + \frac{\frac{120}{\xi^6} - \frac{180}{\xi^4} + \frac{30}{\xi^2} - 1}{x^7} + \ldots$$

Hastings[2] gives a simple computer routine for the function

$$e^{x^2} \operatorname{erfc} x = e^{x^2} \frac{2}{\sqrt{\pi}}\int_x^{\infty} e^{-u^2}\,du .$$

Alex Reichel

The University of Sydney
Sydney, N.S.W.
Australia

Received March 10, 1964
Revised July 27, 1964

---

[1] A. REICHEL, "Voigt Profile Functions in the Complex Domain," *J. Aust. Math. Soc.* (to appear).

[2] C. HASTINGS, Jr., *Approximation for the Digital Computer*, p. 169, Princeton University, N. J. (1955).