A NOTE ON THE VOIGT FUNCTION

J. F. Monaghan

(Received 1971 January 19)

SUMMARY

A simple method for the evaluation of the Voigt function is proposed. Differential equations are used.

Several authors have proposed methods for the evaluation of the Voigt function, which is defined here as

$$U \equiv U(a, x) = \frac{1}{\pi} \int_{0}^{\infty} e^{-t^{2}/4 - at} \cos xt \, dt.$$  \hspace{1cm} (1)

The most recent such proposals have been due to Hummer (1965), who gives numerous references, and Chiarella & Reichel (1966). Hummer proceeds by expanding $U$ as a power series in $a$, the coefficients being calculated by means of a recurrence relation. The disadvantage with this method is that up to four guarding decimal places must be employed in order to counteract severe cancellation in the series. A separate, and very accurate tabulation of a function is also required. Chiarella and Reichel also use a series expansion. Again very accurate arithmetic is required to offset the cancellation of terms in the series.

The method proposed here is based on the use of differential equations. None of the numerical difficulties associated with the use of series expansions appears.

Defining

$$J = \frac{1}{\pi} \int_{0}^{\infty} e^{-t^{2}/4 - at} \sin xt \, dt$$  \hspace{1cm} (2)

we find, using integration by parts, that

$$\frac{dU}{da} = -\frac{2}{\pi} + 2aU + 2xJ,$$  \hspace{1cm} (3)

and

$$\frac{dJ}{da} = 2aJ - 2xU.$$  \hspace{1cm} (4)

Eliminating $J$ from (3) and (4) and defining

$$V = U \exp (-a^{2})$$  \hspace{1cm} (5)

we find

$$\frac{d^{2}V}{da^{2}} + 4x^{2}V = \frac{4d}{\pi} \exp (-a^{2}).$$  \hspace{1cm} (6)

To solve (6) numerically by a step by step method we need $V$ at $a = 0$ and $a = \Delta$ where $\Delta$ is the step length. From (1) and (5) we find

$$V(0) = U(0, x) = \frac{1}{\sqrt{\pi}} \exp (-x^{2}).$$
To find $V$ at $a = \Delta$, we can use a Taylor series expansion noting that

$$V'(0) = U'(0, x),$$

where $'$ stands for $d/da$ and

$$U'(0, x) = -\frac{1}{\pi} \int_{0}^{\infty} te^{-t^2/4} \cos xt \, dt. \quad (7)$$

Once $V'$ is calculated all the other derivatives may be found using (6).

To evaluate (7) we again use a differential equation. Defining $I$ by the relation

$$I = \int_{0}^{\infty} te^{-t^2/4} \cos xt \, dt, \quad (8)$$

one can show, using integration by parts, that

$$\frac{dI}{dx} = -\frac{2I}{x} - \frac{1}{2x} \frac{d^2I}{dx^2}.$$

Or, on setting

$$W = I \exp (x^2/2) \quad (9)$$

that

$$\frac{d^2W}{dx^2} + W(3 - x^2) = 0. \quad (10)$$

Equation (10) may be solved using a step by step process noting

$$W(0) = 2, \quad W''(0) = -6, \quad W^{(4)}(0) = 10$$

with the odd derivatives with respect to $x$ vanishing. The evaluation of the Voigt function therefore requires nothing more than the solution of two second-order, ordinary differential equations using a step by step method.

Tests have been carried out using the following algorithm for second-order differential equations without first derivatives. If

$$\frac{d^2y}{dx^2} = f(x, y),$$

then

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12} (f_{n+1} + 10f_n + f_{n-1})$$

where $h$ is the integration interval and $y_n$ is $y$ evaluated at the $n$th step while $f_n$ is $f$ evaluated at the $n$th step. The error in this algorithm is $\delta y_n/240$ neglecting smaller terms.

For the tests an interval of $0.01$ was used for both (6) and (10). The solution was started using the first five terms in the series expansion. The results were found to agree, to one unit in the eighth decimal place, with those found by Hummer. It would be trivial to obtain higher accuracy by starting with more terms in the starting expansion and reducing the integration interval. As an alternative to reducing the integration interval, the difference correction could be included in the manner suggested in Modern Computing Methods (1961).

A differential equation for $U$, using $x$ as the independent variable may also be derived. Further, $U$ satisfies Laplace's equation in $a, x$ space. However,
numerical procedures based on these equations seem to have no advantages over those discussed in detail in this note.

Monash University, Clayton, Victoria 3168, Australia

REFERENCES