NUMERICAL EVALUATION OF THE LINE BROADENING FUNCTION $H(a, v)$

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Abstract. We present a procedure for the numerical evaluation of $H(a, v)$ which is found to work quickly and leads to accurate results.

It is shown that the improper integral defining $H(a, v)$ may be conveniently reduced to a definite integral over the interval $[-6, +6]$ with a small bound residual error; this is particularly interesting since it allows the use of the Gaussian quadrature formulae for most values of $a$ and $v$, which achieves a higher accuracy than Hermite’s quadrature formula for improper integrals. In addition, the use of the Gaussian formula for the evaluation of definite integrals in this paper results in a substantial reduction of computation time over other numerical approaches to this problem. However, for $a \leq 0.01$ and $|v| < +6$ it was found more convenient to calculate $H(a, v)$ using a series expansion in $a$.

The number of correct significant figures obtained for $H(a, v)$ as a function of $a$ and $v$ is discussed.

1. Introduction

The mathematical expression of the Voigt function is given by

$$H(a, v) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-x^2)}{a^2 + (v - x)^2} \, dx,$$

where $a$ is the ratio of the damping broadening constant $\Gamma$ to $4\pi$ times the Doppler width $\Delta \nu_0$, and $v$ is the frequency departure from the center of the line in units of the Doppler width, i.e., $a = \Gamma/4\pi\Delta \nu_0$ and $v = \Delta \nu/\Delta \nu_0$.

Extensive calculations and tabulations of $H(a, v)$ have been given by Finn and Mugglestone (1965) and by Hummer (1965) (references to earlier investigations may be found in these papers), and although accurate methods exist for its evaluation (Hummer, 1987) some work is still devoted to this problem in the recent literature (e.g., Drummond and Steckner, 1985; Jie-Hai, 1986), while in other cases, the evaluation of $H(a, v)$ is made in a rather simplified way (Carlsson, 1986).

We here present an alternative, efficient, and accurate method for evaluating $H(a, v)$, which was found to perform correctly in large as well as in small computers; use is made of the Gauss quadrature formulae for definite integrals, which offer a number of advantages. In the following sections the numerical methods are worked out in detail and the results discussed.

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2. Reduction of the Improper Integral

For the evaluation of Hjerting's function we have made use of the approximation

$$H(a, v) = \int_{-\infty}^{\infty} h(x) \, dx \approx \int_{-A}^{A} h(x) \, dx$$

(2)

(where $A$ is a real number), with an error $\Delta(A)$ given by

$$\Delta(A) = \int_{-A}^{A} h(x) \, dx + \int_{-\infty}^{-A} h(x) \, dx.$$  

The choice of an appropriate value for $A$ so that (2) may hold requires only order-of-magnitude estimates of $\Delta(A)$ and of the right-hand side of Equation (2); both of these expressions may, therefore, be evaluated approximately for this purpose. Adopting $A = 6$ and using a Gauss-Laguerre formula of 15th order for $\Delta(A)$ we obtained the results presented in Table I.

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$I = \int_{-A}^{A} h(x) \, dx$; $II = \Delta(6)$.

It is seen that for $10^{-6} \leq a \leq 1$ and $0 \leq v \leq 10^{10}$, $\Delta(6)$ is at least 16 orders of magnitude smaller than (2) so that, if the definite integral between $-6$ and $+6$ is evaluated with care, $H(a, v)$ is obtained with an accuracy of no less than 15 significant figures.

If larger values of $A$ are adopted for the integral in (2), the estimates of the error term are naturally reduced, though this seems at all unnecessary.

3. Evaluation of $H(a, v)$

All definite integrals in this work have been numerically evaluated by means of the 24-point Gaussian quadrature formula; abscissas and weight factors to the required