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NOTE

CALCULATION OF THE ABSORPTION COEFFICIENT FOR LINES WITH COMBINED DOPPLER AND LORENTZ BROADENING

CHARLES YOUNG

High Altitude Engineering Laboratory, Department of Aeronautical and Astronautical Engineering, University of Michigan, Ann Arbor, Michigan, U.S.A.

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Abstract—Methods are described for calculating the spectral absorption coefficient for lines with combined Doppler and Lorentz broadening.

RADIATIVE transfer calculations involving gases at low pressures require values for the absorption coefficient incorporating Doppler and collisional broadening. The appropriate absorption coefficient can be written (cf. PENNER[1]),

$$k_\nu = \frac{k_0 y}{\pi} \int_{-\infty}^{\infty} \frac{\exp[-t^2]}{y^2 + (x-t)^2}\, dt \tag{1}$$

where

$$k_0 = \frac{S}{\alpha_D}\left(\frac{\ln 2}{\pi}\right)^{1/2}$$

$$y = \frac{\alpha_L}{\alpha_D}(\ln 2)^{1/2}$$

$$x = \frac{\nu - \nu_0}{\alpha_D}(\ln 2)^{1/2}$$

S = the line strength

$$\alpha_D = \frac{\nu_0}{c}\left(\frac{2kT \ln 2}{m}\right)^{1/2}, \text{ the Doppler half-width}$$

α_L = Lorentz half-width

ν_0 = wave number of the line center

ν = wave number at which k_ν is to be evaluated.

Unfortunately (1) is not easy to integrate for the range of x and y which would apply to a planetary atmosphere. PENNER[1] discusses and references some methods for evaluating (1) which are rather restricted in their range of applicability and accuracy. Some recent tabulations are given by POSENER,[2] FADDEEVA and TERENTEV[3] and FRIED and

CONTE.[4] Tables are not particularly convenient if radiative transfer calculations are being performed on a digital computer. SHVED and TSARITSYNA[5] detail a procedure for calculating (1); their method, however, appears inefficient for routine use on a digital computer. The method used by FADDEEVA and TERENTEV[3] to generate their tables is not readily adaptable for computer use. FRIED and CONTE,[4] on the other hand, generated their tables using a digital computer and a rather elegant method. A variation of their method was used to evaluate (1) over part of the range of interest.

The integral appearing in (1) is related to the probability integral for complex argument,

$$w(z) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp[-t^2]}{t-z}\,dt \tag{2}$$

where

$$z = (x+iy);\ w(z) = u(x,y) + iv(x,y)$$

It is easy to show (cf. FADDEEVA and TERENTEV[3]) that

$$\frac{k_\nu}{k_0} = \frac{v(x,y)}{\sqrt{\pi}}$$

Equation (2) may also be expressed as a differential equation

$$w'(z) + 2zw(z) + 2i = 0 \tag{3}$$

with the initial condition $w(0) = i\sqrt{\pi}$. Equation (3) may be alternatively written in the form

$$\begin{aligned} &\frac{\partial u}{\partial x} + 2xu - 2yv + 2 = 0 \\ &\frac{\partial v}{\partial x} + 2xv + 2yu = 0 \end{aligned} \tag{4}$$

with initial conditions

$$u(0,0) = 0, \qquad v(0,0) = \sqrt{\pi}$$

Integrating (4) along the y-axis allows $u(0,y)$ and $v(0,y)$ to be determined while integrating along the x-axis gives $u(x,0)$ and $v(x,0)$. The values obtained are

$$u(0,y) = 0, \quad v(0,y) = \sqrt{(\pi)}\exp[y^2](1-\operatorname{erf}(y))$$

and

$$u(x,0) = -2\exp[-x^2]\int_0^x \exp[t^2]\,dt, \quad v(x,0) = \sqrt{(\pi)}\exp[-x^2]$$

To evaluate (2) for $y \leqslant 1$, FRIED and CONTE[4] solved the differential equations (4) using a numerical technique. Knowing $u(0,y)$ and $v(0,y)$ they integrated in the x-direction until the desired value of x was reached. The integrating step size was 0·01. This method is satisfactory for producing a set of tables but on a routine basis it would involve a large amount of computer time for even moderately large values of x. Also round-off error is increased if a large number of integrating steps are used. The method adopted was to integrate in the y-direction using $u(x,0)$ and $v(x,0)$ as initial values. Since y will not be

greater than unity reasonably few iterations are required. It was determined that a step size of 0·02 gave six significant figure accuracy if a fourth order Runge–Kutta procedure was used. The value $v(x,0)$ is readily calculated but $u(x,0)$ is somewhat more difficult. For values of $x \geqslant 4{\cdot}5$ an asymptotic expansion (ERDELYI *et al.*[6]) was used,

$$\exp[-x^2]\int_0^x \exp[t^2]\,\mathrm{d}t = \frac{1}{2}\left[\sum_{m=0}^{M}\frac{(\tfrac{1}{2})_m}{x^{2m+1}}\right]$$

where

$$(a)_n = a(a+1)\ldots(a+n-1),\quad n = 1,2,3,\ldots$$

$$(a)_0 = 1$$

The number of terms needed to obtain seven significant figure accuracy is given approximately by $2+40/x$. For $2{\cdot}0 < x < 4{\cdot}5$ an expansion in terms of Chebyshev polynomials given by HUMMER[7] was used. This expansion is very accurate, fourteen significant figure accuracy being obtained if all the terms are included. Seven significant figure accuracy being obtained by taking the first 21 terms. For values of $x \leqslant 2{\cdot}0$ a convergent series expansion (ERDÉLYI *et al.*[6]) was used,

$$\exp[-x^2]\int_0^x \exp[t^2]\,\mathrm{d}t = \sum_{n=0}^{\infty}\frac{(-1)^n x^{2n+1}}{(\tfrac{3}{2})_n}$$

The number of terms required for seven significant figure accuracy is approximately $(12+5x^2)$. Both of the above series were evaluated by nesting the sums to reduce round-off error.

FRIED and CONTE[4] give a continued fraction expansion for (2), derived using the quotient difference algorithm, applicable for $y > 0$. It can be written

$$w(z) = \lim_{n\to\infty}\frac{A_n}{B_n}$$

where

$$A_{n+1} = b_{n+1}A_n + a_{n+1}A_{n-1}$$

$$B_{n+1} = b_{n+1}B_n + a_{n+1}B_{n-1}$$

$$A_{-1} = 1 : A_0 = 0 : B_{-1} = 0 : B_0 = 1$$

$$a_{n+1} = -n(2n-1)/2,\quad n = 1,2,\ldots$$

$$a_1 = z$$

$$b_{n+1} = -z^2 + \tfrac{1}{2} + 2n,\quad n = 0,1,2,\ldots$$

The continued fraction expansion converges slowly for $y \leqslant 1$ but rapid convergence is obtained for $y > 1$. For example for $y = 10{\cdot}0$, $x = 10{\cdot}0$ only three terms are required for six significant figure accuracy and only six terms are required for the same accuracy for $y = 2{\cdot}0$, $x = 0{\cdot}5$. The continued fraction expansion was used for $y > 1{\cdot}0$.

It was determined that the Runge–Kutta method became unstable for $x > 50{\cdot}0$. However, equation (1) is in a form suitable for integration using Hermite–Gauss quadrature (cf. HILDEBRAND[8]). Unfortunately Hermite–Gauss quadrature is satisfactory only for fairly large x or y due to the very sharp peak in the curve $\exp[-t^2]/(y^2-(x-t)^2)$ vs. t for small x and y. It was found that for $x > 10{\cdot}0$, $y \geqslant 0$, 20-point Hermite–Gauss quadrature gave results comparable to the Runge–Kutta and continued fraction expansion. The disagreement varied from 2 to 5 in the sixth significant figure except for small values of y ($y < 0{\cdot}01$) and large x ($x > 20$) when the disagreement became larger, up to 3 in the fifth significant figure. In these cases k_v/k_0 was in the range 10^{-5} to 10^{-7} so this error was considered negligible.

The results obtained were compared with the values given by FADDEEVA and TERENTEV[3] and FRIED and CONTE.[4] Complete agreement was obtained. Needless to say when the above procedure was being developed the three methods used to evaluate (1) were checked by overlapping the regions they covered, excellent agreement was obtained.

To sum up, equation (1) was evaluated for

$y \leqslant 1{\cdot}0$, $x < 10{\cdot}0$ using Runge–Kutta method

$y > 1{\cdot}0$, $x < 10{\cdot}0$ using continued fraction expansion

$y \geqslant 0$, $x \geqslant 10{\cdot}0$, using 20-point Hermite–Gauss quadrature.

A Fortran program and tabulations of the integral in (1) for selected values of x and y can be obtained by contacting the author.

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* MAD–Michigan Alogorithm Decoder, a programming language similar to Fortran.

† UMAP–University of Michigan Assembly Program, an assembly language similar to FAP.