An algorithm for calculating the contour Voigt and its improvement and refinement for some ranges of parameters

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Abstract. We present an approximation Voigt contour for some parameters intervals such as the interval with y less than 0.02 and absolute value x less than 1.6 gives a simple formula for calculating and relative error less than 0.1%, and for some of the intervals suggetsted to use Hermite quadrature.

In [1] was presented the method for calculating the Voigt contour, in this, it refined and improved. Voigt profile contour used for calculations of the absorption lines and takes into account the effect of Doppler broadening and collision effects [2], this intractable integral with infinite boundaries of integration:

$$\chi(\nu)=\frac{x_0 y}{\pi}\int_{-\infty}^{\infty}\frac{\exp\left(-t^2\right)}{y^2+\left(x-t\right)^2}dt\,, \tag{1}$$

where x, $y\geq 0$ - parameters of Voigt conotour depending on wavelength and broadening effects, $x_0=\frac{S}{\gamma_D}\left(\frac{\ln 2}{\pi}\right)^{1/2}$, $y=\frac{\gamma_L}{\gamma_D}(\ln 2)^{1/2}$, $x=\frac{\nu-\nu_0}{\gamma_D}(\ln 2)^{1/2}$, γ_D,γ_L - Doppler and Laurence half width, $\gamma_D=\frac{\gamma_0}{c}\left(\frac{2kT}{m}\ln 2\right)^{1/2}$, T - temperature, m - molecular mass, k - Boltzmann constant, ν_0 - absorption line frequency.

Different algorithmic approaches to calculate the integral in (1) are used, some of them described in [3-7]. Here it offers improved relative error for $|x|<1.6$ and $y<0.02$ range with an error of less than 0.1% compared with the error <0.5% at first algorithm realization and for $y<0.001$ less than 0.001% by approximation given:

$$f(x,y)=\frac{\exp\left(\frac{-x^2}{y+1}\right)}{(0.351y+0.3183)y-\left(1.4x^4-0.38x^2\right)y^2 0.093} \tag{2}$$

It approximate following function:

$$\varphi(x,y)=\int_{-\infty}^{\infty}\frac{\exp\left(-t^2\right)}{y^2+(x-t)^2}dt \tag{3}$$

Relative errors estimated for different parameter y are presented at figure 1, to determine the coefficients of the approximation formula and its type used a genetic algorithm [8].

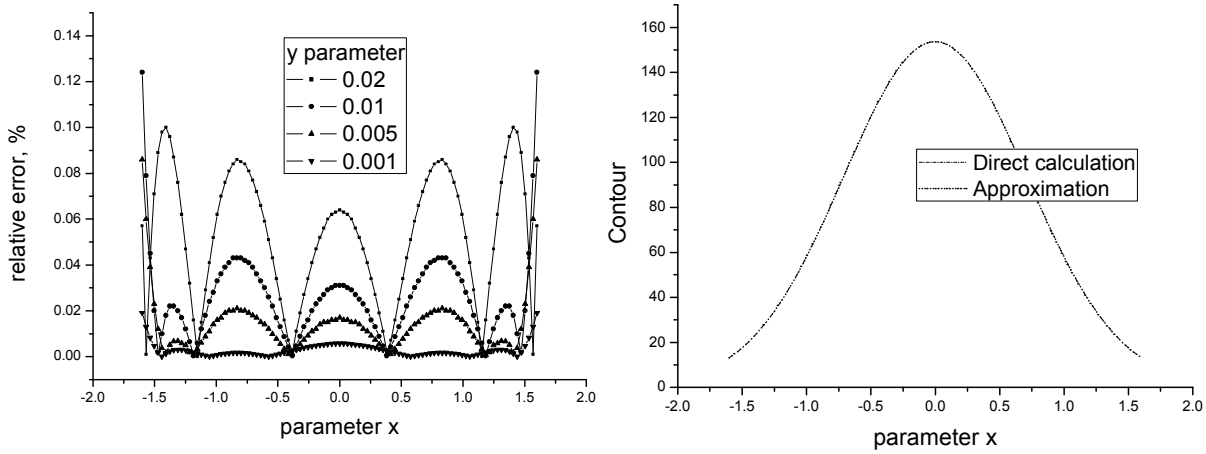

Figure 1. – Relative errors of contour approximation for $|x|<1.6$ and $y<0.02$

Approximation based on orthogonal polynomials Hermite:

$$f(x,y)=\sum_{i=1}^{10}\frac{A_i}{y^2+(x-Ax_i)^2},\quad (y\geq 1.0)\vee(|x|>3.55\wedge y>0.01)\vee|x|>5.000001 \tag{4}$$

where $A_i.Ax_i$ - precalculated weight Hermite quadrature, values listed in Table 1.

Table 1. precalculated weight Hermite quadrature values

Index number	*Ax*	*A*
1	3.4361583	7.641e-6
2	2.5327307	1.344e-3
3	1.7566830	0.034
4	1.0366104	0.240
5	0.3429013	0.611
6	-0.3429013	0.611
7	-1.0366104	0.240
8	-1.7566830	0.034
9	-2.5327307	1.344e-3
10	-3.4361583	7.641e-6

For $|x|>5.000001$ error is less than 0.001%, for $y\geq 0.7$ and $y\leq 1.0$ and $|x|<3.55$ error less than 0.5%, for $y\geq 1.0$ and $|x|<3.55$ less than 0.1%, and for $|x|>3.55$ less than 0.01% (figure 2).

For the intervals $y<0.01$ and $|x|>3.55$ and $|x|<5.000001$ is recommended to use direct calculation using recursive procedure dividing each grid spacing if necessary and check the relative error of calculation in the division of the interval for calculating the integral for 2, 4 and 8 parts, or use another methods [4-7], unfortunately this algorithm with a small stack size for small y<0.000001 can not enough memory, this range has features in which, for example, a standard Mathcad integration algorithm is not working properly.

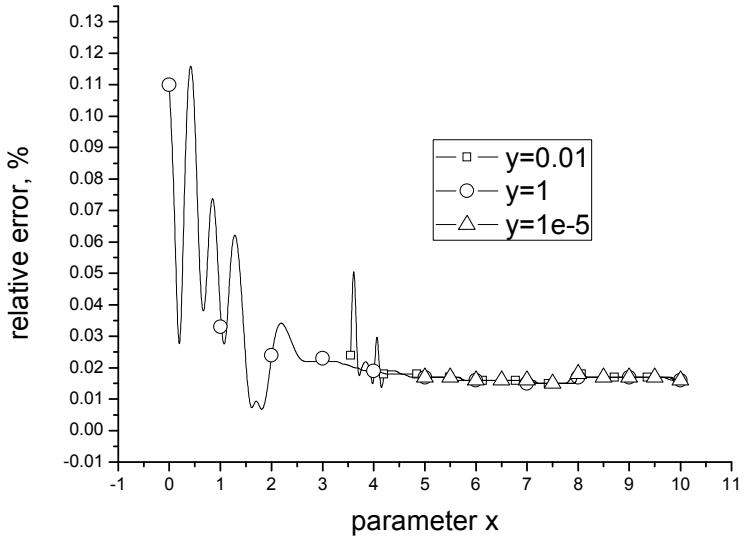

Figure 2. Relative errors of contour approximation for $|x| > 5.000001$, for $y = 0.01$ and $x \geq 3.55$, for $y = 1.0$ and $|x| > 0$

It is suggested to use a linear approximation of integral in expression (1) on a uniform x and y grid for another cases, the accuracy will depend on the amount of memory allocated for the approximation coefficients. Computation speed does not depend on grid spacing, as the respective numbers of coefficients are linear based on it, but it requires estimation and preservation of the approximation coefficients and a large amount of memory for them (for example if $|x| < 1.6$ and $y > 0.02$ and $y < 0.7$ it is need more 100 points for x and more than 2000 points for y with relative error <0.01%).

References

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