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LETTER TO THE EDITOR

Voigt lineshape function as a series of confluent hypergeometric functions

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Abstract. A new series of confluent hypergeometric functions is investigated. It is shown to have the Voigt lineshape function as its sum. Kummer transformation is applied on this series to obtain a much faster converging series for the Voigt lineshape function. The well known asymptotic behaviour of confluent hypergeometric functions is made use of to also obtain an asymptotic series for the Voigt lineshape function.

Confluent hypergeometric functions have important applications in a wide range of physical problems. Extensive discussion of their mathematical properties can be found in many of the standard reference books (Erdélyi 1953, Slater 1960, Abramowitz and Stegun 1970, Magnus *et al* 1966). However investigations on series of confluent hypergeometric functions are rather limited and most of the well known series are listed by Erdélyi (1953) and Hansen (1975). On the other hand, the Voigt lineshape function also occurs in a wide variety of fields such as the study of radiative transfer in stellar atmospheres, laser optics, plasma studies, nuclear physics and reactor physics. As is well known, evaluation of this function is not easy and a large number of papers have appeared in the literature devoted to the study of its mathematical properties useful not only for purposes of numerical computation but also for theoretical studies, see e.g. the review by Armstrong (1967). Analytic approximations to this function are still of interest (Németh *et al* 1981). In this paper we investigate a new series of confluent hypergeometric functions. We show that this series is convergent and has the Voigt lineshape function as its sum. Application of Kummer transformation on the series gives a transformed series which converges much faster than the original one. We also obtain, making use of the known asymptotic behaviour of the confluent hypergeometric functions, an asymptotic series for the Voigt lineshape function. We show how this asymptotic series reduces, under certain approximations, to the one found in the earlier literature (Dresner 1960).

We start with the confluent hypergeometric function of the second kind, $U(a, b, z)$ given (see e.g. Slater 1960) by

$$U(a,b,z)=\frac{\pi}{\sin \pi b}\left(\frac{{}_1F_1(a;b;z)}{\Gamma(1+a-b)\Gamma(b)}-z^{1-b}\frac{{}_1F_1(1+a-b;\ 2-b;z)}{\Gamma(a)\Gamma(2-b)}\right). \tag{1}$$

This is related to the Whittaker function $W_{\kappa,\mu}$ through

$$W_{\kappa,\mu}(z)=\mathrm{e}^{-z/2}z^{1/2+\mu}U(\tfrac{1}{2}+\mu-\kappa,\ 1+2\mu,\ z). \tag{2}$$

We take z to be a real quantity which we denote by R. We also write, for later convenience,

$$R=\tfrac{1}{4}(u^2+\theta^2) \tag{3}$$

and also set $a=2n+1$, $b=n+\tfrac{3}{2}$. The integral representation of this U function is

$$U(2n+1, n+\tfrac{3}{2}, R)=R^{-1/2-n}U(\tfrac{1}{2}+n, \tfrac{1}{2}-n, R) \tag{4a}$$

$$=\frac{R^{-1/2-n}}{\Gamma(n+\frac{1}{2})}\int_0^\infty \mathrm{e}^{-Rt}t^{n-1/2}(1+t)^{-2n-1}\,\mathrm{d}t \tag{4b}$$

$$=\frac{2}{\Gamma(n+\frac{1}{2})}\int_0^\infty \frac{\mathrm{e}^{-t^2}}{t^2+R}\frac{t^{2n}}{(t^2+R)^{2n}}\,\mathrm{d}t \tag{4c}$$

the relation (4a) being a Kummer transformation. We now consider the series

$$S=\tfrac{1}{2}\sum_{n=0}^{\infty} u^{2n}\Gamma(n+\tfrac{1}{2})U(2n+1, n+\tfrac{3}{2}, R). \tag{5}$$

The convergence of the series can be seen as follows. Using (4c) we have

$$\tfrac{1}{2}u^{2n}\Gamma(n+\tfrac{1}{2})U(2n+1, n+\tfrac{3}{2}, R)<u^{2n}\int_0^\infty \frac{t^{2n}}{(t^2+R)^{2n+1}}\,\mathrm{d}t \tag{6a}$$

$$=\frac{\sqrt{\pi}}{2\sqrt{R}}\left(\frac{u^2}{u^2+\theta^2}\right)^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}. \tag{6b}$$

Therefore

$$S<\frac{\sqrt{\pi}}{2\sqrt{R}}\sum_{n=0}^{\infty}\left(\frac{u^2}{u^2+\theta^2}\right)^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}$$

$$=\frac{\pi}{2\sqrt{R}}\sum_{n=0}^{\infty}\left(\frac{u^2}{4(u^2+\theta^2)}\right)^n\frac{2n!}{(n!)^2}. \tag{7}$$

Since $u^2/(u^2+\theta^2)<1$, the series on the RHS sums up to $\sqrt{u^2+\theta^2}/\theta$ (Lebedev 1972, Hansen 1975) and we have the inequality

$$S<\pi/\theta \tag{8}$$

and hence the series (5) under investigation is convergent.

We will now show that the series (5) sums up to the Voigt lineshape function which is just the real part of the complex probability function $w(u+\mathrm{i}\theta)$. Explicitly,

$$S=\tfrac{1}{2}\sum u^{2n}\Gamma(n+\tfrac{1}{2})U(2n+1, n+\tfrac{3}{2}, R)$$

$$=\int_0^\infty \mathrm{d}t\frac{\mathrm{e}^{-t^2}}{t^2+R}\sum_{n=0}^{\infty}\left(\frac{u^2t^2}{(t^2+R)^2}\right)^n. \tag{9}$$

It should be noted now that the maximum value of the function

$$f(t)=u^2t^2/(t^2+R)^2 \qquad 0\leqslant t<\infty \tag{10}$$

obtained from

$$(\mathrm{d}f/\mathrm{d}t)_{t=t_m}=0$$

is

$$f_m=u^2/(u^2+\theta^2)<1 \qquad t_m=\sqrt{R}. \tag{11}$$

That this is really the maximum in the range $0 \leq t < \infty$ can also be seen through

$$f(t_m+\delta) = \frac{u^2}{u^2+\theta^2+\delta^2(\delta+2t_m)^2/(\delta+t_m)^2} \leq f_m \tag{12}$$

where δ is an arbitrary number such that $0 \leq t_m + \delta < \infty$. This function $f(t)$ is plotted in figure 1. Therefore

$$\begin{aligned} S &= \int_0^\infty \frac{e^{-t^2}}{(t^2+R)}\left(1-\frac{u^2t^2}{(t^2+R)^2}\right)^{-1} dt \\ &= \tfrac{1}{2}\int_0^\infty e^{-t^2}\left(\frac{1}{t^2+R-ut}+\frac{1}{t^2+R+ut}\right) dt \\ &= \tfrac{1}{2}\int_{-\infty}^{+\infty} \frac{e^{-t^2}}{(\frac{1}{2}u-t)^2+\frac{1}{4}\theta^2}\, dt. \end{aligned} \tag{13}$$

One can easily recognise this integral as the real part of the complex probability function except for a constant factor. Thus we have the result

$$\frac{\theta}{2\pi}\sum_{n=0}^{\infty} u^{2n}\Gamma(n+\tfrac{1}{2})U(2n+1, n+\tfrac{3}{2}, R) = \mathrm{Re}\, w(\tfrac{1}{2}u+\mathrm{i}\tfrac{1}{2}\theta). \tag{14}$$

where $\mathrm{Re}\, w(\frac{1}{2}u+\mathrm{i}\frac{1}{2}\theta)$ represents the real part of the complex probability function, $w(\frac{1}{2}u+\mathrm{i}\ \frac{1}{2}\theta)$. The series (14) has been obtained for the first time to our knowledge. The Voigt lineshape function, in the notation of Armstrong (1967), is

$$K(\tfrac{1}{2}u, \tfrac{1}{2}\theta) \equiv \mathrm{Re}\, w(\tfrac{1}{2}u+\mathrm{i}\tfrac{1}{2}\theta). \tag{14'}$$

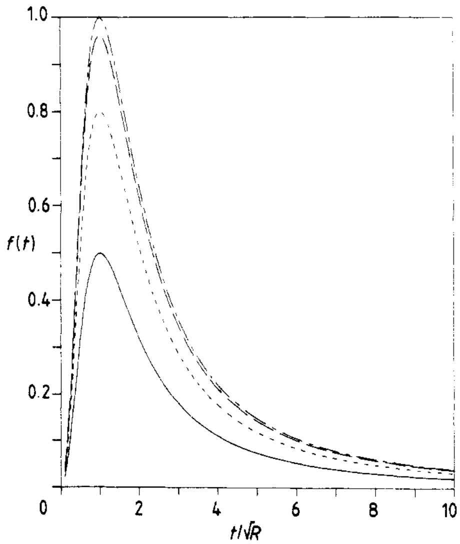

Figure 1. The function $f(t)$ for various values of x (——, $x = 1.0$; - - -, $x = 2.0$; — —, $x = 5.0$, — · —, $x = 100.0$). The parameter x is defined through (15c).

The Doppler broadening functions ψ and χ which are used in reactor physics calculations and also by experimentalists doing neutronic resonance reactions, are

$$\psi(x,\theta)\equiv\sqrt{\pi}\ \tfrac{1}{2}\theta\ \mathrm{Re}\ w(\tfrac{1}{2}u+\mathrm{i}\tfrac{1}{2}\theta) \tag{15a}$$

$$\chi(x,\theta)\equiv\sqrt{\pi}\tfrac{1}{2}\theta\ \mathrm{Im}\ w(\tfrac{1}{2}u+\mathrm{i}\tfrac{1}{2}\theta)$$

$$=2x\psi(x,\theta)+\frac{4}{\theta^2}\frac{\partial\psi}{\partial x}. \tag{15b}$$

Here

$$u=x\theta=(E-E_0)\theta/\tfrac{1}{2}\Gamma \qquad \theta=\Gamma/\Delta \qquad \Delta=(4kTE_0/A)^{1/2} \tag{15c}$$

where E_0 represents the resonance energy E, the energy at which the broadening functions are to be calculated, Γ is the width of the resonance which gets broadened due to thermal motion of the target atoms and Δ is the Doppler width for the nucleus (A being its mass number) at temperature T. The series (14) gives for $\psi(x,\theta)$ at $x=0$

$$\psi(0,\theta)=\sqrt{\pi}\tfrac{1}{2}\theta\ \mathrm{e}^{\theta^2/4}\ \mathrm{erfc}\ \tfrac{1}{2}\theta \tag{15d}$$

in agreement with earlier results (Dresner 1960, Armstrong 1967).

The series (14) would be more useful as an analytical expansion for the Voigt lineshape function if it could be transformed into a faster converging one through a series transformation. We make use of one of the earliest known transformations, due to Kummer, for this purpose. To apply this transformation, we need to know the behaviour of s_k, the kth term of the series (14) as $k\to\infty$. This can be written as

$$s_k=(\theta/2\pi)u^{2k}\Gamma(k+\tfrac{1}{2})U(2k+1,k+\tfrac{3}{2},R)$$

$$=\frac{\theta}{\pi}\left(\frac{u^2}{u^2+\theta^2}\right)^k\int_0^\infty\frac{\mathrm{e}^{-t^2}}{(t^2+R)}g(t)^k\,\mathrm{d}t \tag{16}$$

where

$$g(t)=((u^2+\theta^2)/u^2)f(t). \tag{16'}$$

The function $f(t)$ has already been defined through (10) and is plotted in figure 1. The function $g(t)$ has the same shape as $f(t)$ but has the maximum value one. It is clear that higher powers of $g(t)$ become sharper and sharper and we can write

$$\lim_{k\to\infty}s_k\simeq\frac{\theta}{\pi}\left(\frac{u^2}{u^2+\theta^2}\right)^k\frac{\mathrm{e}^{-R}}{2R}\int_0^\infty g(t)^k\,\mathrm{d}t \tag{17a}$$

$$=\frac{\theta}{\pi}\frac{\mathrm{e}^{-R}}{2R}\sqrt{\pi R}\left(\frac{u^2}{4R}\right)^k\frac{\Gamma(k-\frac{1}{2})}{\Gamma(k)} \tag{17b}$$

$$\simeq\frac{\theta}{2\sqrt{\pi R}}\mathrm{e}^{-R}\left(\frac{u^2}{u^2+\theta^2}\right)^k\frac{\Gamma(k+\frac{1}{2})}{\Gamma(k+1)}. \tag{17c}$$

We now consider a comparison series as given by the RHS of equation (7), namely

$$1=\frac{\theta}{2\sqrt{\pi R}}\sum_{n\mp}^{\infty}\left(\frac{u^2}{u^2+\theta^2}\right)^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}. \tag{18a}$$

The kth term of this series is

$$c_k=\frac{\theta}{2\sqrt{\pi R}}\left(\frac{u^2}{u^2+\theta^2}\right)^k\frac{\Gamma(k+\frac{1}{2})}{\Gamma(k+1)}. \tag{18b}$$

We therefore have

$$\lim_{k\to\infty} s_k/c_k = \mathrm{e}^{-R} \tag{19}$$

a quantity independent of k. Thus we obtain, by Kummer transformation of series (14), the result

$$K(\tfrac{1}{2}u, \tfrac{1}{2}\theta) \equiv \mathrm{Re}\ w(\tfrac{1}{2}u + \mathrm{i}\tfrac{1}{2}\theta)$$

$$= \mathrm{e}^{-R} + \sum_{n=0}^{\infty} (s_n - \mathrm{e}^{-R}c_n). \tag{20}$$

This series converges much faster than the original one. For the $n=0$ term in (20), we have

$$K^{n=0}(u, \theta) = \mathrm{e}^{-u^2-\theta^2} + \frac{\theta}{(u^2+\theta^2)^{1/2}}[\mathrm{e}^{u^2+\theta^2}\,\mathrm{erfc}(u^2+\theta^2)^{1/2} - \mathrm{e}^{-u^2-\theta^2}]. \tag{21}$$

This expression for the $n=0$ term only is plotted in figure 2 (broken curve) along with some actual values of $K(u, \theta)$ (Abramowitz and Stegun 1970) for comparison. In many physical problems the cases where θ is small are of more practical importance. In reactor physics problems, for example, the important range for θ is $\sim 10^{-3}$–10^{-1}. In such cases, as is indicated by figure 2, one may use the simple form

$$\psi(x, \theta) \approx \sqrt{\pi}\tfrac{1}{2}\theta\left(\mathrm{e}^{-R} + \frac{1}{\sqrt{1+x^2}}(\mathrm{e}^{R}\,\mathrm{erfc}(\sqrt{R}) - \mathrm{e}^{-R})\right) \tag{22}$$

for approximate calculations. As $x\to\infty$ (i.e. $R\to\infty$), since

$$\mathrm{erfc}(\sqrt{R}) \sim \frac{\mathrm{e}^{-R}}{\sqrt{\pi R}} = \frac{\mathrm{e}^{-R}}{\sqrt{\pi}\tfrac{1}{2}\theta\sqrt{1+x^2}} \tag{23}$$

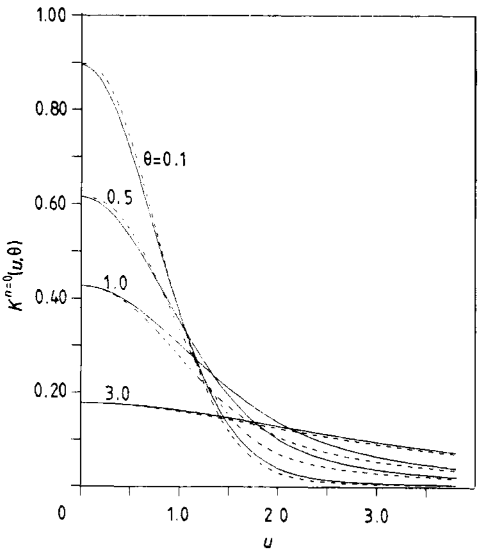

Figure 2. Comparison of $K^{n=0}(u, \theta)$ (- - -) calculated using expression (21) with the actual values (——) (taken from Abramowitz and Stegun 1970) of the Voigt lineshape function.

we find again

$$\psi_{x\to\infty}(x, \theta) \sim 1/(1+x^2) \tag{24}$$

the well known Lorentzian behaviour of $\psi(x, \theta)$ (Dresner 1960) as $x \to \infty$.

Two well known properties of the confluent hypergeometric function U prove to be quite useful in this context:

$$\text{(i)}\ \ U_{R\to 0}(2n+1, n+\tfrac{3}{2}, R) = \frac{\Gamma(n+\frac{1}{2})}{\Gamma(2n+1)} R^{-n-1/2} + \mathrm{O}(R^{n-1/2}) \tag{25}$$

$$\text{(ii)}\ \ U_{R\to\infty}(2n+1, n+\tfrac{3}{2}, R) = R^{-2n-1}\left(\sum_{r=0}^{N-1} \frac{(2n+1)_r(n+\frac{1}{2})_r}{r!}(-R)^{-r} + \mathrm{O}(R^{-N})\right). \tag{26}$$

This asymptotic expansion (ii) for the U function leads us to an asymptotic series for $\psi(x, \theta)$:

$$\psi(x, \theta) \sim \frac{\theta^2}{4\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{u^{2n}\Gamma(n+\frac{1}{2})}{R^{2n+1}} \sum_r (-1)^r \frac{(2n+1)_r(n+\frac{1}{2})_r}{R^r}. \tag{27a}$$

If we retain the $r=0$ term only in this expansion, we have

$$\psi(x, \theta) \sim \frac{\theta^2}{4\sqrt{\pi}} \sum_n \frac{\Gamma(n+\frac{1}{2})}{R^{2n+1}} u^{2n}. \tag{27b}$$

It is interesting to note here that if we retain the $(n=0, r=0)$, $(n=0, r=1)$ and $(n=1, r=0)$ terms in (27a) only, then

$$\psi(x, \theta) \sim \frac{\theta^2}{4\sqrt{\pi}}\left[\frac{\Gamma(\frac{1}{2})}{R}\left(1-\frac{1}{2R}\right) + u^2\frac{\Gamma(\frac{3}{2})}{R^3}\right] + \dots$$

$$= \frac{\theta^2}{u^2+\theta^2}\left(1+\frac{2}{(u^2+\theta^2)^2}(3u^2-\theta^2)\right) + \dots$$

which may also be written as

$$\psi(x, \theta) \sim \frac{1}{1+x^2}\left(1+\frac{1}{\theta^2(1+x^2)^2}(6x^2-2)\right) + \dots. \tag{27c}$$

This expression is well known (Dresner 1960) and is used in many cross section processing codes in reactor physics.

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