DOPPLER BROADENED CONTOUR FUNCTIONS IN THE COMPLEX DOMAIN

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Abstract

The definitions of the functions used to describe Doppler broadened Breit Wigner contours are extended to the complex domain. The properties of the analytic functions are then used to evaluate a number of integrals by the theory of residues.

1. Introduction

The Doppler broadened contour functions, otherwise known as Voigt profiles, can be defined for a real variable x in terms of integrals, as:

$$
(1) \qquad \begin{aligned} \psi(x, t) &= \frac{1}{2\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\{-(x-u)^2/4t\} \frac{du}{1+u^2} \\ \phi(x, t) &= \frac{1}{2\sqrt{(\pi t)}} \int_{-\infty}^{\infty} \exp\{-(x-u)^2/4t\} \frac{udu}{1+u^2} \end{aligned}
$$

where t is a parameter. These functions were investigated in the early part of the century in connection with the anomalous dispersion of light and have been the subject of intensive study in recent years because of their importance in the estimation of the temperature coefficients of reactivity of reactor systems. The functions also make their appearance in the investigation of certain astrophysical problems. A review of the literature related to the functions particularly as they apply to the resonance absorption of neutrons has been given by Dresner ([4]; 1960).

Born ([1]; 1933) considered the function

$$
\chi(x, t) = \psi(x, t) + i\phi(x, t),
$$

and discussed some of its properties as a complex function of the real variable x. Using as a variable the complex quantity $w = 1-ix$ he was able to perform the integration in Equation (1) and express $\chi(x, t)$ in terms of the complex error function. He also derived the asymptotic expansion valid for large $|1-ix|$. More recently Cook ([3]; 1958) drew at-

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tention to this work of Born and considered the integral of $\chi^n(x, t)$ over the real axis. Without giving a valid proof he stated the correct value of the integral.

Buckler and Pull ([2]; 1962) have introduced the function

$$F(w) = \int_0^\infty \exp(-u^2) \frac{w du}{u^2+w^2},$$

which is proportional to and provides an alternative expression for the function $\chi(x, t)$ as given by Born. They have used this equation to define $F(w)$ when w is a complex variable. This definition is not completely satisfactory since the integral is undefined for Re $(w) = 0$ and furthermore it is implied that ψ and ϕ are not analytic but are the real and imaginary parts of $F(w)$.

It is perhaps most convenient to extend the Doppler broadened contour functions over the complex domain by defining them as the solutions of a pair of first order differential equations. This approach is adopted in the next section where the properties of the functions are described. In the final section the extended definition of these functions is used in applying the theory of residues to the evaluation of a number of integrals on the real axis.

2. The functions ψ and ϕ in the complex plane

It is well known that for real values of z the functions ψ and ϕ defined in Equation (1) satisfy the pair of first order differential equations:

$$\begin{aligned} 2t\frac{d\psi}{dz} &= \phi - z\psi, \\ 2t\frac{d\phi}{dz} &= 1-\psi-z\phi \end{aligned} \tag{2}$$

with the initial conditions:

$$\begin{aligned} \psi(0, t) &= \tfrac{1}{2}\sqrt{(\pi/t)} \exp(1/4t) \operatorname{erfc}(1/2\sqrt{t}) \\ \phi(0, t) &= 0. \end{aligned} \tag{3}$$

We will use the equations (2) and (3) to define $\psi(z, t)$ and $\phi(z, t)$ in the complex z-plane.

Introducing $\chi(z, t) = \psi(z, t)+i\phi(z, t)$, it is seen to satisfy the equation

$$2t\frac{d\chi}{dz} + (z+i)\chi = i,$$

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which has no singular points in the z-plane and can be solved readily with the aid of an integration factor to give:

$$\chi(z, t) = \tfrac{1}{2}\sqrt{(\pi/t)} \exp \{(1-iz)^2/4t\} \operatorname{erfc} \{(1-iz)/2\sqrt{t}\}.$$

This equation was obtained by Born ([1]; 1933) for real z by an alternative method. Straightforward manipulation leads to the simpler expression

$$\chi(z, t) = \int_0^\infty \exp(-p^2t-p+ipz)dp, \tag{4}$$

showing that $\chi(z, t)$ is a solution of the partial differential equation

$$\frac{\partial^2\chi}{\partial z^2} = \frac{\partial\chi}{\partial t}.$$

It is immediately deducible from Equation (4) that $\chi(z, t)$ is an integral function of the complex variable z and consequently has an isolated essential singularity at infinity. In the range $5\pi/4 < \arg(z+i) < 7\pi/4$ the function is unbounded while, provided $-\pi/4 < \arg(z+i) < 5\pi/4$ it tends asymptotically to $1/(1-iz)$ for large $|z|$. The asymptotic expansions in these two regions are easily obtained from the integral in Equation (4) as:

$$\chi(z, t) \cong \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dz^{2n}} \frac{1}{1-iz}, \quad -\pi/4 < \arg(z+i) < 5\pi/4 \tag{5}$$

$$\begin{gathered}\chi(z, t) \cong \sqrt{(\pi/t)} \exp\{(1-iz)^2/4t\} + \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dz^{2n}} \frac{1}{1-iz}, \\ 5\pi/4 < \arg(z+i) < 7\pi/4.\end{gathered} \tag{6}$$

Outside the region $5\pi/4 < \arg(z+i) < 7\pi/4$ in the lower half plane, the exponential term in Equation (6) is of lesser order than any other term. Hence the expansion (6) is valid over the whole of the lower half plane.

The unbounded behaviour of $\chi(z)$ in the region $5\pi/4 < \arg(z+i) < 7\pi/4$ is clearly seen if z is replaced by $x+iy$ in the integrand of Equation (4) when it may be shown that:

$$\begin{aligned}\chi(z, t) &= \frac{1}{1+y}\chi\left(\frac{x}{1+y}, \frac{t}{(1+y)^2}\right), && y > -1 \\ &= \tfrac{1}{2}\sqrt{(\pi/t)} \exp(-x^2/4t) \operatorname{erfc}(-ix/2\sqrt{t}), && y = -1 \\ &= \frac{1}{1+y}\chi\left(\frac{x}{1+y}, \frac{t}{(1+y)^2}\right) + \sqrt{(\pi/t)} \exp\{(1+y-ix)^2/4t\}, && y < -1.\end{aligned}$$

From these equations the real and imaginary part of $\chi(z, t)$ may be obtained. In particular, when z is a pure imaginary, that is, $z = iy$, then $\chi(z, t)$ is real, and

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$$
\begin{aligned}
\chi(iy, t) &= \frac{1}{1+y}\,\psi\left(0, \frac{t}{(1+y)^2}\right), && y > -1 \\
&= \tfrac{1}{2}\sqrt{(\pi/t)}, && y = -1 \\
&= \frac{1}{1+y}\,\psi\left(0, \frac{t}{(1+y)^2}\right) + \sqrt{(\pi/t)} \exp\{(1+y)^2/4t\}, && y < -1.
\end{aligned} \tag{7}
$$

Alternatively, on starting from Equations (2) and (3) we could have defined a function $\mathscr{S}(z, t) = \psi(z, t) - i\phi(z, t)$ and followed through a similar argument to obtain in place of Equation (4),

$$
\mathscr{S}(z, t) = \int_0^\infty \exp\,(-p^2t - p - ipz)\,dp. \tag{8}
$$

Comparing Equations (8) and (4) it is obvious that $\mathscr{S}(z, t) = \chi(-z, t)$, so that

$$
\chi(-z, t) = \psi(z, t) - i\phi(z, t). \tag{9}
$$

It is now possible to obtain the Doppler broadened contour functions $\psi(z, t)$ and $\phi(z, t)$ from the relations:

$$
\begin{aligned}
2\psi(z, t) &= \chi(z, t) + \chi(-z, t), \\
2i\phi(z, t) &= \chi(z, t) - \chi(-z, t),
\end{aligned}
$$

which, combined with Equation (4) give:

$$
\begin{aligned}
\psi(z, t) &= \int_0^\infty \exp\,(-p - p^2t) \cos pz\, dp \\
\phi(z, t) &= \int_0^\infty \exp\,(-p - p^2t) \sin pz\, dp.
\end{aligned} \tag{10}
$$

Thus $\psi(z, t)$ is an even function of z while $\phi(z, t)$ is odd.

In view of the asymptotic behaviour of the function $\chi(z, t)$ it is evident that both $\psi(z, t)$ and $\phi(z, t)$ are unbounded for $\pi/4 < \arg\,(z-i) < 3\pi/4$ and $5\pi/4 < \arg\,(z+i) < 7\pi/4$. Their asymptotic expansions in the upper half plane are:

$$
\begin{aligned}
\psi(z, t) &\simeq \tfrac{1}{2}\sqrt{(\pi/t)} \exp\{(1+iz)^2/4t\} + \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dz^{2n}} \frac{1}{1+z^2} \\
\phi(z, t) &\simeq \tfrac{i}{2}\sqrt{(\pi/t)} \exp\{(1+iz)^2/4t\} + \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dz^{2n}} \frac{z}{1+z^2},
\end{aligned} \tag{11}
$$

while in the lower half plane:

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$$\psi(z,t) \cong \tfrac{1}{2}\sqrt{(\pi/t)}\exp\{(1-iz)^2/4t\} + \sum_{0}^{\infty} \frac{t^n}{n!}\frac{d^{2n}}{dz^{2n}}\frac{1}{1+z^2}$$
(12)
$$\phi(z,t) \cong -\tfrac{i}{2}\sqrt{(\pi/t)}\exp\{(1-iz)^2/4t\} + \sum_{n=0}^{\infty} \frac{t^n}{n!}\frac{d^{2n}}{dz^{2n}}\frac{z}{1+z^2}.$$

3. General theorems

The extension of the range of definition of the Doppler broadened contour functions to the whole complex plane leads to the possibility of using Cauchy Residue Theory for the evaluation of integrals involving the functions. In the present section a number of general theorems are developed which can be used to evaluate a variety of such integrals involving products of the contour functions with themselves and with other elementary functions.

In proving the theorems we integrate around a contour C consisting of the real axis from $-R$ to R and the semi-circle Γ of radius R in the upper half plane with this axis as diameter. In the limit as R tends to infinity this allows conversion of an integral along the real axis to another integral around the semicircle Γ in which the integrand may be replaced by the leading term in its asymptotic expansion.

THEOREM 1.

$$\int_{-\infty}^{\infty} \{\psi(x,t)+i\phi(x,t)\}^n dx = \begin{cases} \pi, & n=1 \\ 0, & n>1. \end{cases} \tag{13}$$

PROOF. Consider $\oint_C \chi^n(z,t)dz$ where n is an integer. Since $\chi(z,t)$ is analytic in the upper half plane we have:

$$\int_{-\infty}^{\infty} \chi^n(z,t)dz = -\lim_{R\to\infty}\int_\Gamma \chi^n(z,t)dz$$
$$= -\lim_{R\to\infty}\int_\Gamma \frac{dz}{(1-iz)^n}.$$

On the semicircle Γ, $z = Re^{i\theta}$, so that:

$$\lim_{R\to\infty}\int_\Gamma \frac{dz}{(1-iz)^n} = \lim_{R\to\infty}\int_0^\pi \frac{iRe^{i\theta}}{(1-iRe^{i\theta})^n}d\theta$$
$$= \begin{cases} -\pi & \text{if} \quad n=1, \\ 0 & \text{if} \quad n>1, \end{cases}$$

which proves the theorem.

The trend of the proof is not altered if the integrand in Equation (13) is multiplied by any function of the complex variable z which is analytic

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in the upper half plane. This allows us to generalise the theorem in a number of ways of which two are:

$$(14)\qquad \int_{-\infty}^{\infty} x^k\{\psi(x,t)+i\phi(x,t)\}^n dx = \begin{cases} i^{n-1}\pi, & n = k+1 \\ 0, & n > k+1, \end{cases}$$

and

$$(15)\qquad \int_{-\infty}^{\infty} \{\psi(x,t)+i\phi(x,t)\}^n\{\psi(x,\tau)+i\phi(x,\tau)\}^m dx = 0, \qquad n+m > 1.$$

Equations (13), (14), and (15) provide a large number of equalities between integrals involving powers of ψ and ϕ of which two particular examples are:

$$\int_{-\infty}^{\infty} x^2\psi^3(x,t)dx = 3\int_{-\infty}^{\infty} x^2\psi(x,t)\phi^2(x,t)dx-\pi,$$

and

$$\int_{-\infty}^{\infty} \frac{\psi(x,t)}{(1+x^2)}\,dx = 3\int_{-\infty}^{\infty} \frac{x\phi(x,t)}{(1+x^2)}\,dx.$$

THEOREM 2.

$$(16)\qquad \int_{-\infty}^{\infty} [\chi(-x,t)-\sqrt{(\pi/t)}\exp\{(1+ix)^2/4t\}]^n dx = \begin{cases} -\pi, & n = 1 \\ 0, & n > 1. \end{cases}$$

PROOF. Although $\chi(-z,t)$ is unbounded in the upper half plane it follows from Equation (6) that in this region the function $\chi(-z,t)-\sqrt{(\pi/t)}\exp\{(1+iz)^2/4t\}$ will be bounded and well behaved, tending asymptotically to $1/(1+iz)$ for large $|z|$. Hence by considering the integral

$$\oint_C [\chi(-z,t)-\sqrt{(\pi/t)}\exp\{(1+iz)^2/4t\}]^n dz$$

we obtain

$$\int_{-\infty}^{\infty} [\chi(-x,t)-\sqrt{(\pi/t)}\exp\{(1+iz)^2/4t\}]^n dx = -\lim_{R\to\infty}\int_\Gamma \frac{dz}{(1+iz)^n}.$$

Since $z = Re^{i\theta}$ on the semicircle Γ the result follows as in Theorem 1.

By a slight extension of the above argument we obtain:

$$(17)\qquad \int_{-\infty}^{\infty} \chi^n(x,\tau)[\chi(-x,t)-\sqrt{(\pi/t)}\exp\{(1+ix)^2/4t\}]^m dx = 0, \text{ if } n+m > 1,$$

and

$$(18)\qquad \int_{-\infty}^{\infty} [\psi(x,t)-\tfrac{1}{2}\sqrt{(\pi/t)}\exp\{(1+ix)^2/4t\}]^n dx = 0, \text{ if } n > 0.$$

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Particular results which may be deduced from this theorem are:

$$\int_{-\infty}^{\infty} \chi(-x, t) \exp\{(1+ix)^2/4t\}dx = \tfrac{1}{2}\sqrt{(\pi/t)} \int_{-\infty}^{\infty} \exp\{(1+ix)^2/2t\}dx$$
$$= \pi/\sqrt{2},$$

and

$$\int_{-\infty}^{\infty} [\psi^2(x, t)+\phi^2(x, t)]\,dx = \int_{-\infty}^{\infty} \chi(x, t)\sqrt{(\pi/t)} \exp\{(1+ix)^2/4t\}dx$$
$$= 2\pi\chi(i, 2t)$$
$$= \pi\psi(0, t/2).$$

THEOREM 3.

$$(19) \qquad {}^*\!\!\int_{-\infty}^{\infty} \frac{[\psi(x, t)+i\phi(x, t)]^n}{x-a}\,dx = \pi i[\psi(a, t)+i\phi(a, t)]^n, \qquad n > 0,$$

where $^*\!\!\int$ *denotes a Cauchy Principal Value.*

PROOF. The function $\chi^n(z, t)/(z-a)$ has a simple pole at $z = a$, so that:

$$^*\!\!\int_{-\infty}^{\infty} \frac{(\psi+i\phi)^n}{x-a}\,dx = -\lim_{R\to\infty} \int_{\Gamma} \frac{\chi^n(z, t)}{z-a}\,dz + \pi i \text{ [Residue at } z = a].$$

Since

$$\lim_{R\to\infty} \int_{\Gamma} \frac{\chi^n(z, t)}{z-a}\,dz = \lim_{R\to\infty} \int_{0}^{\pi} \frac{iRe^{i\theta}\,d\theta}{(Re^{i\theta}-a)(1-iRe^{i\theta})^n}$$
$$= 0, \quad \text{for} \quad n > 0,$$

and

$$\lim_{z\to a}\,(z-a)\,\frac{\chi^n(z, t)}{z-a} = \chi^n(a, t),$$

the result follows.

In particular when $n = 1$ the theorem gives:

$$\frac{1}{\pi}\, {}^*\!\!\int_{-\infty}^{\infty} \frac{\psi(x, t)}{x-a}\,dx = -\phi(a, t),$$

(20) and

$$\frac{1}{\pi}\, {}^*\!\!\int_{-\infty}^{\infty} \frac{\phi(x, t)}{x-a}\,dx = \psi(a, t),$$

showing that the functions $\psi(x, t)$ and $\phi(x, t)$ are a Hilbert transform pair. This result could alternatively have been deduced from the fact that $\chi(z, t)$ is analytic in the upper half plane (see for example Tricomi ([5]; 1957)).

Using a combination of the proofs of Theorems (2) and (3) we obtain the further result:

$$(21)\quad {}^{*}\!\!\int_{-\infty}^{\infty} [\chi(-x,t)-\sqrt{(\pi/t)}\exp\{(1+ix)^2/4t\}]\frac{dx}{x-a} = \pi i[\psi(a,t)-i\phi(a,t)-\sqrt{(\pi/t)}\exp\{(1+ia)^2/4t\}]^n,$$

giving, when $n = 1$,

$${}^{*}\!\!\int_{-\infty}^{\infty} [\sqrt{(\pi/t)}\exp\{(1+ix)^2/4t\}\frac{dx}{x-a} = \pi i[\sqrt{(\pi/t)}\exp\{(1+ia)^2/4t\}-2\chi(-a,t)].$$

This provides alternative expressions for $\psi(x, t)$ and $\phi(x, t)$.

Theorem 4.

$$(22)\quad \int_{-\infty}^{\infty}\frac{[\psi(x,t)+i\phi(x,t)]^n}{x^2+a^2}dx = \frac{\pi}{a(1+a)^n}\psi^n\left(0,\frac{t}{(1+a)^2}\right), \qquad n>0.$$

Proof. If we consider $\oint_C \chi^n(z, t)/(z^2+a^2)dz$ which has a simple pole at $z = ia$ within the contour C, then we obtain:

$$\int_{-\infty}^{\infty}\frac{\chi^n(x,t)}{x^2+a^2}dx = -\lim_{R\to\infty}\int_\Gamma\frac{dz}{(z^2+a^2)(1-iz)^n} + 2\pi i\ [\text{Residue at } z = ia].$$

The integral around Γ vanishes and the residue at $z = ia$ is given by:

$$\lim_{z\to ia}(z-ia)\frac{\chi^n(z,t)}{z^2+a^2} = \frac{1}{2ia}\chi^n(ia,t),$$

which produces the required result on employing Equation (7).

Since the first term of the asymptotic expansion of $\chi(z, t)$ in the upper half plane is $1/(1-iz)$ and is thus independent of t, all the above theorems may be generalised by replacing $\chi^n(x, t)$ by the product $\prod_k \chi(x, t_k)$. A similar remark applies to theorems involving

$$[\chi(-z,t)-\sqrt{(\pi/t)}\exp\{(1+iz)^2/4t\}]^n.$$

A complementary set of theorems can be obtained by considering integrals around the semicircle in the lower half plane, while extension to integrals containing additional poles is obvious. The method is not restricted to integrands containing only positive powers of $\chi(z, t)$ but may be generalised to obtain the values of a variety of integrals involving functions of $\chi(z, t)$.

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