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Asymptotic forms of convolved line profiles

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Abstract. Analytical properties of the convolution integral of a Lorentzian profile with a quasi-static Van der Waals profile are derived from a result due to Stormberg. It is shown that far from line centre the sum of the individual line profiles is a good approximation to the convolution integral. The conditions under which this result is true for general line profiles are also derived. A comparison of the convolution integral with the average of the line profiles is also made, and a specific example of physical interest is given.

1. Introduction

In this paper we derive certain analytical properties of integrals which arise from the convolution of line profiles of spectroscopic interest. Convolution integrals have received much attention in a variety of contexts and, in particular, the convolution of two Lorentzians is a well known analytical result. In general, convolution integrals require numerical evaluation (for example, the Voigt profile (Kuhn 1969)). Recently, Stormberg (1980) has obtained an analytical expression for the convolution integral of a Lorentzian and a quasi-static Van der Waals profile. In § 2 of this paper we discuss the asymptotic form of his result, and show that far from line centre the convolution integral has the same dominant behaviour and magnitude as the sum of the two individual line profiles. In § 3 we discuss the conditions under which the summation of *general* line profiles is a good approximation to their convolution integral far from line centre. A specific example is given in § 4.

2. Asymptotic expansion of Stormberg's result

We begin with a Lorentzian profile of the form

$$\beta/(\beta^2+\beta^2\sigma^2), \tag{1}$$

where β is the semi-half-width, and $\beta\sigma = \nu_0 - \nu$, ν_0 being the frequency at line centre; σ is therefore a non-dimensional measure of a typical position ν from line centre. Normalising (1) to unit area, we have

$$L_1 = 1/\pi(1+\sigma^2). \tag{2}$$

For the quasi-static form of the Van der Waals profile relating to pressure broadening

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due to foreign neutral atoms, we have (Sobel'man 1972)

$$\begin{cases} \exp(-\alpha/\beta\sigma)/(\beta\sigma)^{3/2}, & \sigma \geqslant 0, \\ 0, & \sigma \leqslant 0, \end{cases} \tag{3}$$

where α is a constant proportional to the Van der Waals constant. We note that this profile is not symmetrical and that the effect acts only on the red side of line centre for which $\beta\sigma = \nu_0 - \nu \geqslant 0$. Normalising (3) to unit area, we find

$$L_2 = \begin{cases} \left(\dfrac{\alpha}{\beta\pi}\right)^{1/2} \dfrac{\exp(-\alpha/\beta\sigma)}{\sigma^{3/2}}, & \sigma \geqslant 0, \\ 0, & \sigma \leqslant 0. \end{cases} \tag{4}$$

The convolution integral of these two normalised line profiles, L_1 and L_2 (itself a normalised function), is

$$C(\sigma) = \int_{-\infty}^{\infty} L_2(\sigma - \sigma')L_1(\sigma')\,\mathrm{d}\sigma' \tag{5}$$

$$= \frac{1}{\pi^{3/2}}\left(\frac{\alpha}{\beta}\right)^{1/2} \int_{-\infty}^{\sigma} \frac{\exp[-\alpha/\beta(\sigma-\sigma')]}{(\sigma-\sigma')^{3/2}(1+\sigma'^2)}\,\mathrm{d}\sigma', \tag{6}$$

where the upper limit of integration is σ since the Van der Waals profile is zero for $\sigma' > \sigma$. Writing $\sigma - \sigma' = 1/y$ and $\varepsilon = \alpha/\beta$, (6) becomes

$$C(\sigma) = \frac{\varepsilon^{1/2}}{\pi^{3/2}} \int_0^{\infty} \frac{y^{3/2}\,\mathrm{e}^{-\varepsilon y}}{y^2 + (1-\sigma y)^2}\,\mathrm{d}y. \tag{7}$$

Stormberg (1980) has evaluated this integral (expressed in slightly different notation) by writing it as the sum of inverse Laplace transforms of known functions, and obtained the result which, in our notation, is

$$C(\sigma) = \frac{1}{\pi(1+\sigma^2)} - \frac{\mathrm{i}}{2}\left(\frac{\varepsilon}{\pi}\right)^{1/2} [z_1^{3/2}\,\mathrm{e}^{\varepsilon z_1}\,\mathrm{erfc}(\varepsilon z_1)^{1/2} - z_2^{3/2}\,\mathrm{e}^{\varepsilon z_2}\,\mathrm{erfc}(\varepsilon z_2)^{1/2}], \tag{8}$$

where

$$z_1 = \frac{-\sigma - \mathrm{i}}{1+\sigma^2}, \qquad z_2 = \frac{-\sigma + \mathrm{i}}{1+\sigma^2}. \tag{9}$$

For $\sigma > 0$, we expand all terms in (8) in powers of $1/\sigma$, using (9). Ensuring that the correct arguments of the complex square roots are taken when expanding the complementary error functions (see Copson 1971, p 84), we find

$$C(\sigma) \sim \frac{1}{\pi\sigma^2} + \left(\frac{\varepsilon}{\pi}\right)^{1/2} \frac{1}{\sigma^{3/2}} + \mathrm{O}\left(\frac{1}{\sigma^{5/2}}\right). \tag{10}$$

Similarly, when $\sigma < 0$, an expansion in powers of $1/|\sigma|$ gives

$$C(\sigma) \sim 1/\pi\sigma^2 + \mathrm{O}(1/|\sigma|^{5/2}). \tag{11}$$

From (2) and (4), it is seen that the asymptotic forms of $L_1 + L_2$ for $\sigma \to \infty$ and $\sigma \to -\infty$ are (10) and (11) respectively. Hence for $|\sigma| \to \infty$,

$$|C(\sigma) - L_1(\sigma) - L_2(\sigma)| = \mathrm{O}(1/|\sigma|^{5/2}). \tag{12}$$

3. Asymptotic behaviour of convolution integrals

We now give a rigorous derivation of the result that for large $|\sigma|$, $C(\sigma) \sim L_1(\sigma) + L_2(\sigma)$ for a wide class of profiles L_1 and L_2.

We consider profiles for which

$$L_1(\sigma) \leqslant K_1|\sigma|^{-a-1}, \qquad L_2(\sigma) \leqslant K_2|\sigma|^{-b-1} \tag{13}$$

and

$$|L_1'(\sigma)| \leqslant M_1|\sigma|^{-a-2}, \qquad |L_2'(\sigma)| \leqslant M_2|\sigma|^{-b-2} \tag{14}$$

for $|\sigma| \geqslant 1$, say, where a, b, K_1, K_2, M_1 and M_2 are positive constants. We now split the range of integration in (5) into

$$C(\sigma) = \left(\int_{-\infty}^{-\sigma/2} + \int_{-\sigma/2}^{\sigma/2} + \int_{\sigma/2}^{3\sigma/2} + \int_{3\sigma/2}^{\infty}\right) L_1(\sigma')L_2(\sigma - \sigma')\,\mathrm{d}\sigma', \tag{15}$$

taking $\sigma > 0$, so that

$$\begin{aligned}
&|C(\sigma) - L_1(\sigma) - L_2(\sigma)| \\
&\quad = \Bigg| -L_2(\sigma)\int_{-\infty}^{-\sigma/2} L_1(\sigma')\,\mathrm{d}\sigma' - L_2(\sigma)\int_{\sigma/2}^{\infty} L_1(\sigma')\,\mathrm{d}\sigma' \\
&\quad + \left(\int_{-\sigma/2}^{-1} + \int_{-1}^{1} + \int_{1}^{\sigma/2}\right) L_1(\sigma')[L_2(\sigma - \sigma') - L_2(\sigma)]\,\mathrm{d}\sigma' \\
&\quad + \int_{-\infty}^{-\sigma/2} L_1(\sigma')L_2(\sigma - \sigma')\,\mathrm{d}\sigma' - L_1(\sigma)\int_{-\infty}^{-\sigma/2} L_2(-K)\,\mathrm{d}K \\
&\quad - L_1(\sigma)\int_{\sigma/2}^{\infty} L_2(-K)\,\mathrm{d}K + \left(\int_{-\sigma/2}^{-1} + \int_{-1}^{1} + \int_{1}^{\sigma/2}\right) L_2(-K) \\
&\quad \times [L_1(K + \sigma) - L_1(\sigma)]\,\mathrm{d}K + \int_{3\sigma/2}^{\infty} L_1(\sigma')L_2(\sigma - \sigma')\,\mathrm{d}\sigma' \Bigg|,
\end{aligned} \tag{16}$$

where $\sigma' = K + \sigma$ has been substituted in some integrals. Now for σ *large* we insert the forms (13) and (14) in all integrals except those with range $[-1, 1]$, and perform the integrations. Each of these terms is of order $|\sigma|^{-a-b-1}$. Hence

$$\begin{aligned}
&|C(\sigma) - L_1(\sigma) - L_2(\sigma)| \\
&\quad \leqslant \frac{A_1}{|\sigma|^{a+b+1}} + \int_{-1}^{1} L_1(\sigma')|L(\sigma - \sigma') - L_2(\sigma)|\,\mathrm{d}\sigma' \\
&\quad + \int_{-1}^{1} L_2(-K)|L_1(K + \sigma) - L_1(\sigma)|\,\mathrm{d}K.
\end{aligned} \tag{17}$$

Using the mean value theorem

$$L_2(\sigma - \sigma') - L_2(\sigma) = -\sigma' L_2'(\sigma - \theta\sigma') \tag{18}$$

where $0 \leqslant \theta \leqslant 1$, we find that the first integral in (17) may be written

$$\int_{-1}^{1} L_1(\sigma')|\sigma'|\,|L_2'(\sigma - \theta\sigma')|\,\mathrm{d}\sigma'. \tag{19}$$

Substituting the form (14) for $|L_2'(\sigma-\theta\sigma')|$, we find that (19) is of order $|\sigma|^{-b-2}$. Similarly, the second integral in (17) is of order $|\sigma|^{-a-2}$. Hence, for large σ,

$$|C(\sigma)-L_1(\sigma)-L_2(\sigma)| \leq \frac{A_1}{|\sigma|^{a+b+1}}+\frac{A_2}{|\sigma|^{a+2}}+\frac{A_3}{|\sigma|^{b+2}} \tag{20}$$

where A_1, A_2 and A_3 are positive constants. We retain only the leading-order term on the right-hand side of (20) to obtain the bound on $|C(\sigma)-L_1(\sigma)-L_2(\sigma)|$. The profiles (2) and (4) considered in § 2 satisfy $a=1$, $b=\frac{1}{2}$ and we retrieve the result (12) from (20).

4. Comparison of the convolution integral with sums of profiles

Although we have seen in the previous section that $C(\sigma)$ behaves like $L_1(\sigma)+L_2(\sigma)$ far from line centre, it is clearly not appropriate to approximate $C(\sigma)$ by this form over the whole range, since

$$\int_{-\infty}^{\infty} [L_1(\sigma)+L_2(\sigma)]\, d\sigma = 2, \tag{21}$$

whereas $\int_{-\infty}^{\infty} C(\sigma)\, d\sigma = 1$.

In order to obtain a correct integral relationship over the range, we should compare $C(\sigma)$ with $\frac{1}{2}(L_1(\sigma)+L_2(\sigma))$. Clearly, neither $L_1(\sigma)+L_2(\sigma)$ nor $\frac{1}{2}(L_1(\sigma)+L_2(\sigma))$ is a good approximation to $C(\sigma)$ over the whole range, the former being good only in the wings of the profile, the latter giving only normalised areas. As a specific example, we consider the profiles (2) and (4) and calculate numerically $L_1(\sigma)+L_2(\sigma)$, $\frac{1}{2}(L_1(\sigma)+L_2(\sigma))$ and $C(\sigma)$ for the 589 nm sodium D-line under conditions typical of the centre of a high-pressure sodium lamp for which $\varepsilon \simeq 0.005$. We note that the Van der Waals profile (4) has its maximum value of

$$(3/2e)^{3/2}/\varepsilon\pi^{1/2} \tag{22}$$

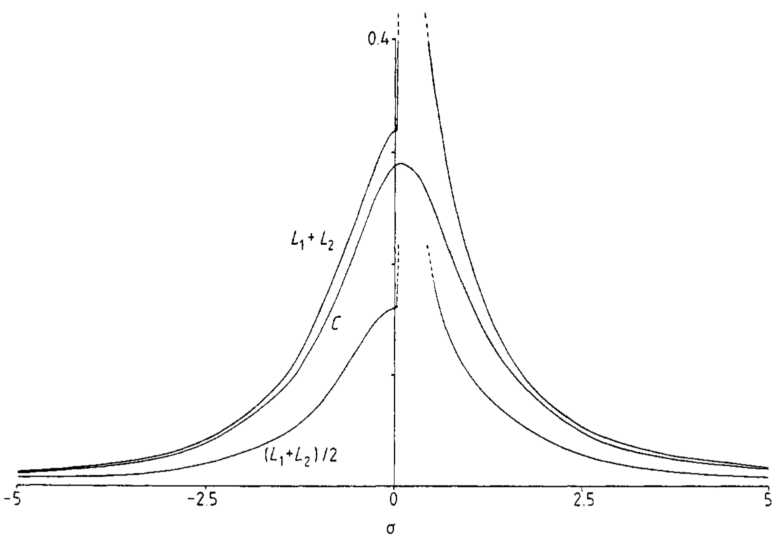

Figure 1. C, L_1+L_2 and $\frac{1}{2}(L_1+L_2)$ plotted against σ for $\varepsilon=0.005$.

at $\sigma = 2\varepsilon/3$. For $\varepsilon = 0.005$ we therefore obtain a maximum value of 46.25 at $\sigma = 0.0033$. This maximum is large compared with the maximum of the Lorentzian (2). Accordingly, both $L_1(\sigma) + L_2(\sigma)$ and $\frac{1}{2}(L_1(\sigma) + L_2(\sigma))$ show a very sharp peak near $\sigma = 0.0033$ as can be seen in figure 1. The convolution integral (7), evaluated numerically using NAG library program DO1AGF, based on the method of Clenshaw and Curtis (1960), does not exhibit a sharp peak. The integral (7) has been tabulated also for a wide range of ε-values (Radmore and Froment, unpublished), and from these results the value of σ beyond which $L_1(\sigma) + L_2(\sigma)$ is a good approximation to $C(\sigma)$ may be readily determined.

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