10.9: Appendix A- Convolution of Gaussian and Lorentzian Functions

Equation 10.5.6 is

$$G(x)=G_1(x)*G_2(x)=\frac{1}{g_1g_2}\frac{\ln 2}{\pi}\int_{-\infty}^{\infty}\exp\left(-\frac{\xi^2\ln 2}{g_1^2}\right)\exp\left(-\frac{(\xi-x)^2\ln 2}{g_2^2}\right)d\xi. \tag{10.A.1}$$

The integration is straightforward, if taken slowly and carefully, provided you know the integral $\int_{-\infty}^{\infty}\exp(-kx^2)dx=\sqrt{\frac{\pi}{k}}$. It goes thus:

$$G(x)=\frac{1}{g_1g_2}\frac{\ln 2}{\pi}\int_{-\infty}^{\infty}\exp[-(a\xi^2+b\xi+c)]d\xi, \tag{10.A.2}$$

where

$$a=\frac{\left(g_1^2+g_2^2\right)\ln 2}{g_1^2g_2^2},\quad b=-\frac{x\ln 4}{g_2^2},\quad c=\frac{x^2\ln 2}{g_2^2}.$$

$$G(x)=\frac{1}{g_1g_2}\frac{\ln 2}{\pi}\int_{-\infty}^{\infty}\exp[-a(\xi^2+2B\xi+C)]d\xi, \tag{10.A.3}$$

where

$$B=b/(2a),\quad C=c/a. \tag{10.9.1}$$

$$\begin{aligned}G(x)&=\frac{1}{g_1g_2}\frac{\ln 2}{\pi}\int_{-\infty}^{\infty}\exp[-a\{(\xi+B)^2+C-B^2\}]d\xi &(10.A.4)\\ &=\frac{1}{g_1g_2}\frac{\ln 2}{\pi}\int_{-\infty}^{\infty}\exp[-a(\zeta^2+C-B^2)]d\zeta &(10.A.5)\\ &=\frac{K\ln 2}{\pi g_1g_2}\int_{-\infty}^{\infty}\exp\left(-a\zeta^2\right)d\zeta=\frac{K\ln 2}{g_1g_2\sqrt{\pi a}}, &(10.A.6)\end{aligned}$$

where

$$K=\exp[-a(C-B^2)]. \tag{10.9.2}$$

We have now completed the integration, except that we now have to remember what a, C and B were. When we do this, after a bit more careful algebra we arrive at the result

$$G(x)=G_1(x)*G_2(x)=\frac{1}{g}\cdot\sqrt{\frac{\ln 2}{\pi}}\exp\left(-\frac{x^2\ln 2}{g^2}\right). \tag{10.A.7}$$

In a similar manner, equation 10.5.10 is

$$L(x)=L_1(x)*L_2(x)=\frac{l_1l_2}{\pi^2}\int_{-\infty}^{\infty}\frac{1}{\xi^2+l_1^2}\frac{1}{(\xi-x)^2+l_2^2}d\xi. \tag{10.A.8}$$

Resolve the integrand into partial fractions:

$$\frac{1}{\xi^2+l_1^2}\frac{1}{(\xi-x)^2+l_2^2}=\frac{A\xi}{\xi^2+l_1^2}+\frac{B}{\xi^2+l_1^2}+\frac{C(\xi-x)}{(\xi-x)^2+l_2^2}+\frac{D}{(\xi-x)^2+l_2^2}. \tag{10.A.9}$$

Evaluation of the constants is straightforward, if slightly tedious, by the usual method of partial fractions:

$$\begin{aligned}&A=-C=2x\alpha, &(10.A.10)\\ &B=(x^2+l_2^2-l_1^2)\alpha, &(10.9.3)\\ &D=(x^2-l_2^2+l_1^2)\alpha, &(10.9.4)\\ &\text{where } \alpha=1/[(x^2+l_2^2+l_1^2)^2-4l_1^2l_2^2]. &(10.9.5)\end{aligned}$$

Now

$$L(x)=\frac{l_1 l_2}{\pi^2}\left(A\int_{-\infty}^{\infty}\frac{\xi d\xi}{\xi^2+l_1^2}+B\int_{-\infty}^{\infty}\frac{d\xi}{\xi^2+l_1^2}+C\int_{-\infty}^{\infty}\frac{(\xi-x)d\xi}{(\xi-x)^2+l_2^2}+D\int_{-\infty}^{\infty}\frac{d\xi}{(\xi-x)^2+l_2^2}\right). \tag{10.A.11}$$

From symmetry considerations, this is:

$$L(x)=\frac{2l_1 l_2}{\pi^2}\left(B\int_0^{\infty}\frac{d\xi}{\xi^2+l_1^2}+D\int_0^{\infty}\frac{d\xi}{\xi^2+l_2^2}\right). \tag{10.A.12}$$

$$L(x)=\frac{2l_1 l_2}{\pi^2}\left(\frac{\pi B}{2l_1}+\frac{\pi D}{2l_2}\right)=(l_2 B+l_1 D)/\pi. \tag{10.A.13}$$

We have now completed the integration, except that we now have to remember what B and D were. When we do this, after a bit more careful algebra we arrive at the result

$$L(x)=\frac{l}{\pi}\cdot\frac{1}{x^2+l^2}, \tag{10.A.14}$$

where

$$l=l_1+l_2. \tag{10.9.6}$$

The Voigt profile is given by equation 10.5.14:

$$V(x)=\frac{l}{g}\sqrt{\frac{\ln 2}{\pi^2}}\int_{-\infty}^{\infty}\frac{\exp\left(-[(\xi-x)^2\ln 2]/g^2\right)}{\xi^2+l^2}d\xi. \tag{10.A.15}$$

For short, I am going to write the ratio l/g as a. The relation between this ratio and the gaussian fraction $k_{\rm G}$ is $a=(1-k_{\rm G})/k_{\rm G},\ k_{\rm G}=1/(1+a)$. In the above equation, $x=\lambda-\lambda_0$, and I am going to choose a wavelength scale such that $g=1$; in other words wavelength interval is to be expressed in units of g. Thus I shall write the equation as

$$V(x)=a\sqrt{\frac{\ln 2}{\pi^3}}\int_{-\infty}^{\infty}\frac{\exp\left(-(\xi-x)^2\ln 2\right)}{\xi^2+a^2}d\xi. \tag{10.A.16}$$

The integration has to be done numerically, and there is a problem in that the limits are infinite. We can deal with this with the change of variable $\xi=a\tan\theta$, when the integral becomes

$$V(x)=\sqrt{\frac{\ln 2}{\pi^3}}\int_{-\pi/2}^{\pi/2}\exp[-(a\tan\theta-x)^2\ln 2]d\theta. \tag{10.A.17}$$

The limits are now finite, and the integrand is zero at each limit. Computing time will be much diminished by the further substitution $t=\tan\frac{1}{2}\theta$, when the expression becomes

$$V(x)=\sqrt{\frac{\ln 16}{\pi^3}}\int_{-1}^{1}\frac{\exp[-\{2at/(1-t^2)-x\}^2\ln 2]}{1+t^2}dt \tag{10.A.18}$$

This is faster than the previous expression because one avoids having to compute the trigonometric function tan. It could also have been arrived at in one step by means of the substitution $\xi=\frac{2at}{1-t^2}$, though such a substitution may not have been immediately obvious. Like the previous expression, the limits are finite, and the integrand is zero at each end. Numerical integration would now seem to be straightforward, although there may yet be some difficulty. Suppose one is integrating, for example, by Simpson's method. A question might arise as to how many intervals should be used. Simpson's method is often very effective with a remarkably small number of intervals, but, for high precision, one may nevertheless wish to use a fine interval. If one uses a fine interval, however, as one approaches either limit, the expression $t/(1-t^2)$ becomes very large, and, even though the integrand then becomes small, a computer may be reluctant to return a value for the exp function, and it may deliver an error message. The best way to deal with that difficulty is to set the integrand equal to zero whenever the absolute value of the argument of the exp function exceeds some value below which the computer is happy.

One might be tempted to reduce the amount of computation by saying that $\int_{-1}^{1}=2\int_0^1$, but this is not correct, for, while the Voigt profile is symmetric about $x=1$, the integrand is not symmetric about $t=0$. However, if

$$V(x) = \int_{-1}^{1}, \text{ and } V_1(x) = \int_{-1}^{0}, \text{ and } V_2(x) = \int_{0}^{1}, \tag{10.9.7}$$

it is true that $V(x) = V_1(x) + V_2(x)$ and $V_1(x) = V_2(-x)$, and hence that $V(x) = V_1(x) + V_1(-x)$ and this can be used to economise to a small extent. It is still necessary to calculate $V_1(x)$ for all values of x, both positive and negative, but the number of integration steps for each point can be halved.