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The integral width of the convolution of a Gaussian and a Cauchy distribution. By W. Ruland, *Union Carbide European Research Associates, S.A.*, 95, *rue Gatti de Gamond, Bruxelles* 18, *Belgium*

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The correction of a line width for instrumental broadening leads to simple expressions only when the true line profile and the 'measure distribution' representing the instrumental broadening are both of the Gaussian or both of the Cauchy type. In the latter case, the resulting width is the sum, in the former the square root of the sum of the squares of the true line width and the width due to instrumental broadening (Warren, 1941). In the general case the problem has to be solved by a deconvolution (Stokes, 1948) but this procedure is time-consuming and, for practical purposes, only of interest when a line profile analysis is required.

Alexander (1950) has found that the instrumental broadening of counter diffractometers can in most of the cases be represented by a Gaussian distribution, whereas the true line profiles are nearer to a Cauchy distribution.

The purpose of this note is to show that an analytical expression exists for the integral width of the convolution of a Gaussian and a Cauchy distribution.

Taking $h_1 = \exp(-\pi s^2/B_1^2)$ and $h_2 = 1/(1+\pi^2 s^2/B_2^2)$ with integral width B_1 and B_2 defined by $\int_{-\infty}^{\infty} h\,ds/h(0)$, one finds for the width of the convolution of h_1 and h_2

$$B = \frac{\int_{-\infty}^{\infty} h_1 * h_2\,ds}{(h_1 * h_2)_{(0)}},$$

and by Fourier transformation

$$B = \frac{H_{1(0)} \cdot H_{2(0)}}{\int_{-\infty}^{\infty} H_1 \cdot H_2\,dr}$$

where H_1 and H_2 are the Fourier transforms of h_1 and h_2, respectively. This yields

$$B = \frac{1}{2\int_0^{\infty} \exp(-\pi B_1^2 r^2 - 2B_2 r)\,dr}$$

$$= B_1 \frac{\exp[-(B_2/B_1)^2/\pi]}{1 - 2\,\mathrm{erf}\,(\sqrt{(2/\pi)} \cdot B_2/B_1)},$$

where the error function erf (x) is defined by

$$\frac{1}{\sqrt{(2\pi)}} \int_0^x \exp(-t^2/2)\,dt.$$

From observed values of B and B_1 the value of B_2 can be computed from this equation by numerical methods.

Using appropriate series developments for erf (x) and $1-2$ erf (x), one finds the following approximations:

$$\frac{B_2}{B} \simeq \frac{\pi}{2}\left(1 - \frac{B_1}{B}\right) \quad \text{for } B_2 < B_1,$$

and

$$\frac{B_2}{B} \simeq 1 - \frac{\pi}{2}\left(\frac{B_1}{B}\right)^2 \quad \text{for } B_2 > B_1.$$

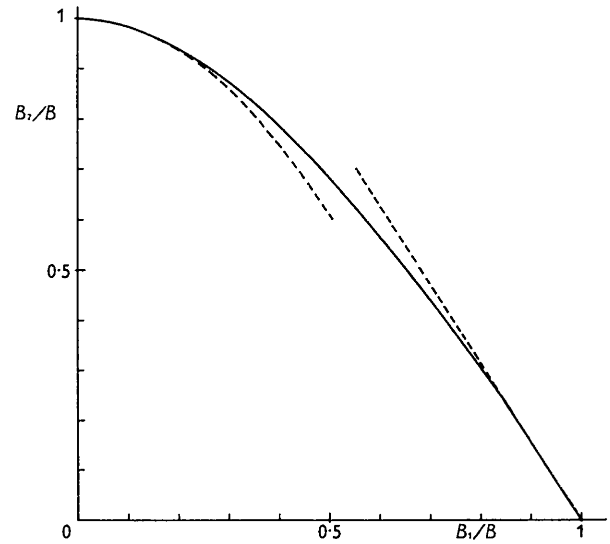

Fig. 1. B_2/B as a function of B_1/B.
——— exact curve - - - - - limiting cases.

Fig. 1 gives B_2/B as a function of B_1/B; the curves for the limiting cases are also drawn and show that their range of validity is fairly large, extending nearly to $B_1 = B_2$.

References

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