[Gaussian Broadening]
(Chapter 2.3.2 in *Elements*)
We have worked out a Gaussian broadening in relation to the resolution of a pulsed-source chopper spectrometer (Loong et al. 1987).

The result is the convolution of the Ikeda-Carpenter (I-C) function with the instrument response function (broadening function), a Gaussian,

$$i_G(t) = \int_{-t}^{\infty} i(t+\tau)g(\tau)d\tau, \tag{1}$$

where

$$g(t) = \sqrt{\frac{\gamma}{\pi}}\exp\left(-\gamma t^2\right), \tag{2}$$

in which $\gamma = \dfrac{1}{2\sigma^2(E)}$ (for later simplification of the algebra, we express in terms of the parameter γ), and $\sigma^2(E)$ is the variance of the broadening function. Then, after somewhat arduous calculation, three forms arise in the broadened I-C function that modify the unbroadened function, with the result

$$\begin{aligned} i_G(t) = \frac{2}{a}\Big\{ & \Big[(1-R)a^2t^2 - \frac{a^2\beta R}{(a-\beta)^3}\Big(1+(a-\beta)t+\frac{1}{2}(a-\beta)^2t^2\Big)\Big]\exp(-at)f_o(a,\gamma,t) + \\ & + \frac{a^2\beta R}{(a-\beta)^3}\exp(-\beta t)f_o(\beta,\gamma,t) + \\ & + \left[2(1-R)a^2t - \frac{a^2\beta R}{(a-\beta)^2}\big(1+(a-\beta)t\big)\right]\exp(-at)f_1(a,\gamma,t) + \\ & + \left[(1-R)a^2 - \frac{1}{2}\frac{a^2\beta R}{(a-\beta)}\right]\exp(-at)f_2(a,\gamma,t)\Big\} \ . \end{aligned} \tag{3}$$

The functions $f_o(x,\gamma,t)$, $f_1(x,\gamma,t)$, and $f_2(x,\gamma,t)$ might be calculated by *integration by parts*, a well-known procedure described in most elementary calculus texts. However, a slicker method is that of *differentiation on imbedded parameters*, by which the higher order functions emerge easily from the lowest-order one (a defensible procedure because the integrand is well behaved),

$$f_o(x,\gamma,t) = \int_{-t}^{\infty} \exp(-x\tau)\exp(-\gamma\tau^2)d\tau = \frac{2}{\sqrt{\pi\gamma}}\exp\left(\frac{x^2}{4\gamma}\right)\text{erfc}\left(\frac{x}{2\sqrt{\gamma}} - \sqrt{\gamma}t\right) \ , \tag{4}$$

where

$$\text{erfc}(y) = \frac{2}{\sqrt{\pi}}\int_{y}^{\infty} \exp(-u^2)du \tag{5}$$

is the *complementary error function* and

$$\frac{d\,\text{erfc}(y)}{dy} = -\frac{2}{\sqrt{\pi}}\exp(-y^2) \ . \tag{6}$$

Then

$$f_1(x,\gamma,t) = \int_{-t}^{\infty} \tau \exp\left(-x\tau\right)\exp\left(-\gamma\tau^2\right)d\tau = -\frac{\partial}{\partial x} f_o(x,\gamma,t) \tag{7}$$

and

$$f_2(x,\gamma,t) = \int_{-t}^{\infty} \tau^2 \exp\left(-x\tau\right)\exp\left(-\gamma\tau^2\right)d\tau = -\frac{\partial}{\partial \gamma} f_o(x,\gamma,t), \tag{8}$$

and we have

$$f_1(x,\gamma,t) = \frac{2}{\pi\gamma}\exp\left(\frac{x^2}{4\gamma}\right)\left[\exp\left(-\gamma\left(t-\frac{x}{2\sqrt{\gamma}}\right)^2\right) - \frac{x}{2}\sqrt{\frac{\pi}{\gamma}}\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\gamma}} - \sqrt{\gamma}\right)\right] \tag{9}$$

and

$$f_2(x,\gamma,t) = \frac{2}{\sqrt{\pi\gamma}}\exp\left(\frac{x^2}{4\gamma}\right)\left[\left(1+\frac{x^2}{2\gamma}\right)\mathrm{erfc}\left(\frac{x}{2\sqrt{\gamma}} - \sqrt{\gamma}\right) - \frac{1}{\sqrt{\pi\gamma}}\left(\frac{x}{2\gamma} - t\right)\exp\left(-\gamma\left(t-\frac{x}{2\sqrt{\gamma}}\right)^2\right)\right] . \tag{10}$$

Laplace transform methods are inappropriate here because the Gaussian function is finite (though small at the extremes) on the full range $-\infty < t < \infty$ rather than the finite range required in the Laplace transform. (The resolution broadening function is actually nonzero in a finite range, and the Gaussian approximation is good only around the maximum point.) The results are similar to those derived for the resolution of pulsed-source chopper spectrometers in Loong et al. (1987), but for some reason, the integrals involved are not explicitly found in standard handbooks. However, consult the *Handbook of Mathematical Functions*, AMS-55.

In application the time t usually is offset by a delay time, $t \rightarrow t - t_o$. If parameters of the broadened I-C function are to be fitted to data, then a, β, t_o, γ, and a normalization factor are the only adjustable parameters. Because the Gaussian is a symmetric function of t, the mean value of the Gaussian-broadened I-C function is the same as before,

$$t_e = \frac{3}{a} + \frac{R}{\beta}, \tag{11}$$

and because the variance of the Gaussian is $\sigma^2_{Gaussian}$ and variances of convoluted distributions add, the variance of the Gaussian-broadened I-C function is

$$\sigma^2_{Gaussian-broadened} = \frac{3}{a^2} + \frac{\left(2R - R^2\right)}{\beta^2} + \sigma^2_{Gaussian} \quad , \tag{12}$$

in which all variables may be functions of the energy, E.