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GAUSSIAN AND TOP-HAT BROADENED I-C PULSE SHAPE FUNCTIONS, AND A CONJECTURE

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ABSTRACT

The Ikeda-Carpenter (I-C) function describing the shape of the pulsed-moderator emission time distribution fits well the simulated and observed functions in idealized, well-focused circumstances and for most practical moderator materials. However, in practice, the calculations and observations must include broadening effects due to resolution (approximated in a Gaussian) or source pulse width (approximated in a top-hat function.) I present modifications of the I-C function for the two cases and relate the derivation of the results, which may be useful in characterizing moderators and fitting diffractometer line shapes.

Important exceptions in recent experience are those of para-hydrogen moderators, for which, I conjecture, at least two terms of similar form may be required. A possible reason for this may lie in the unusual total scattering cross section of moderators with high para concentrations, which has a minimum in the range of energies just below 15 meV. In contrast with the most common situations in which the cross section minimum lies in the epithermal range, this may lead to more than one thermal-neutron energy eigenfunction and time eigenvalue that is potentially significant in the energy range near 15 meV.

1. Pulse shapes of pulsed-source moderators

There is no question of the time-dependence of the neutrons emitted from a reactor (or any steady-source) moderator—in principle, neutrons come out in a steady stream. However, the time dependence of the neutrons emitted from pulsed-source moderators is of crucial importance, inasmuch as this determines the resolution of time-of-flight measurements. Consequently, the design and optimization of pulsed-source moderators relates closely to the requirements of instruments using the neutrons. Neutrons, initially a very short pulse at high energy, spend time slowing down in the moderator and diffusing around within before emerging. Neutrons emerge in a time distribution that begins at the time of the primary source pulse, as demanded by causality requirements. Figure 1 shows the emission-time distribution of 0.063-eV neutrons from the same moderator as that of Fig. 1. Times t in the expressions that follow correspond to the times that neutrons cross the moderator surface in the direction of travel, adjusted for the time-of-flight to the detector, and are measured from the time of the primary source pulse.

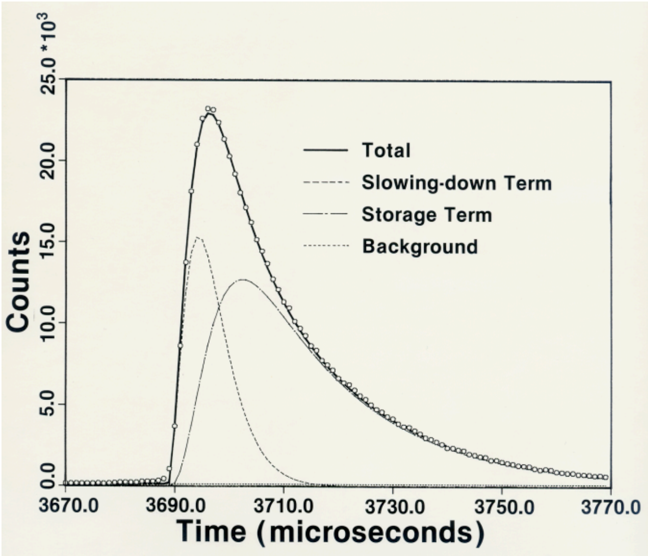

Figure 1. The emission-time distribution of 63.3-meV neutrons of a poisoned room-temperature polyethylene moderator at IPNS. [1,2]

These shapes depend greatly on the wavelength (energy) of the neutrons as well as the details of the moderator. Predominant features of all pulse-source pulse shape functions are the very sharp rising edge and the exponential fall-off at long times. The figure shows a function fitted to the time distribution, which gives an excellent description of the measurement. The function, physics-motivated but basically empirical, normalized to unit area and called the Ikeda-Carpenter (I-C) function, [1,2], is

$$f(E,t) = (1-R(E))f_{SD}(E,t) + R(E)\int_0^t f_{SD}(E,t')\beta\exp(-\beta(t-t')dt' \text{ , (1)}$$

which is the sum of two terms. The first term is a "slowing-down" function $f_{SD}(E,t) = \frac{a}{2}(at)^2\exp(-at)$ with $a(E) = v\Sigma(E)$, where $\Sigma(E)$ is the macroscopic scattering cross section for neutrons of energy E, which is weighted by a factor $(1-R(E))$. The second term is a "storage" term, which represents the decay of the longest-lived eigenfunction of the moderator neutron distribution $\beta\exp(-\beta t)$, a decaying exponential, convoluted with the slowing-down function and weighted by $R(E)$. Explicitly, the function is

$$f_{I-C}(E,t) = \frac{a}{2}\left\{\begin{array}{l}(1-R)(at)^2\exp(-at) + \\ +2R\frac{a^2\beta}{(a-\beta)^3}\left[\exp(-\beta t) - \exp(-at)(1+(a-\beta)t + \frac{1}{2}(a-\beta)^2t^2)\right]\end{array}\right\} \quad (2)$$

This result follows easily from the Laplace transform calculation of $f_{SD}(E,t)$, in which the transform of the convolution product is the product of the transforms of the convoluted functions. Consult any book that tabulates Laplace transform pairs for further information. The Laplace transform method is appropriate here because the functions involved are defined on the half-range, $t > 0$:

$$\tilde{f}(s) \equiv \mathcal{L}\left[f(t)\right] \equiv \int_0^\infty \exp(-st)f(t)dt \ . \ (3)$$

Consulting a table of function-transform pairs, (now suppressing the variable *E*) we find that the transforms are

$$\tilde{f}_{SD}(s) = \mathcal{L}\left[\frac{a}{2}(at)^2 \exp(-at)\right] = \frac{a^3}{(s+a)^3} \ (4)$$

and

$$\tilde{f}_{Storage}(s) = \mathcal{L}\left[\beta \exp(-\beta t)\right] = \frac{\beta}{(s+\beta)} \text{, } (5)$$

so that

$$\tilde{f}_{I-C}(s) = (1-R)\tilde{f}_{SD}(s) + R\tilde{f}_{SD}(s)\tilde{f}_{Storage}(s) = \frac{a^3}{(s+a)^3}\left(1 - R + \frac{\beta R}{(s+\beta)}\right). \ (6)$$

The Laplace transform variable *s* is a complex number.

The I-C function appears complicated but is not when viewed in terms of its basis. The function is entirely tractable as a form for non-linear least squares fitting and for subsequent calculation. The parameters a, R, β, and Σ depend on the energy *E*. In concept, a, β, and Σ are independent of *E* but in terms of the empirical process of fitting can be taken as *E*-dependent, different for the peak for each energy. The times *t* within each peak fitted (as in Figure 1) must be interpreted as $t = t_{obs} - t_o$, in which t_o is also a fitting parameter, which also depends on *E*. Smooth, even physically reasonable, functions can represent the energy variation of these parameters. This enables representing the functions $f(E,t)$ over the entire range of *E* in terms of only a few fitting constants. Although devised to fit one particular measurement, the I-C function has been found, sometimes with elaboration, to fit well the emission-time distributions of a wide variety of moderators. A final reminder is to remember that the I-C function describes the moderator emission time distribution as the response to a delta-function-like source pulse, unbroadened by resolution effects as described in the next subsections.

The function $f_{I-C}(E,t)$ does not represent the variation of $I(E,t)$ as an energy density because it is normalized to an arbitrary area both in theory ($\int_0^\infty f_{I-C}(E,t)dt = 1$) and in measurements, in which an overall normalizing constant is also a fitting parameter.

In time-of-flight applications, the time of arrival at a detector represents the speed (energy, wavelength) of the detected neutron,

$$t = \frac{L}{v} + t_e \,. \; (7)$$

This time represents the time measured from the mean time, as opposed to the starting time of the emission-time distribution, t_e , which for the I-C function is

$$t_e = \frac{3}{a} + \frac{R}{\beta} \cdot (8)$$

When this expression is used to determine the effective flight path length L for instrument wavelength calibration, say, by relating measured times of arrival for known wavelengths, the expression appears indeterminate. This is avoidable if the process is considered as an iterative one, first determining a preliminary length and wavelength, then computing the emission time from the preliminary wavelength, a small correction, then reiterating. The variance of the I-C function is

$$\sigma_t^2 = \frac{(2R - R^2)}{\beta^2} + \frac{3}{a^2} \cdot (9)$$

Although the I-C time distribution assumes a single thermal-neutron eigenfunction, there may be more than one and consequently more than one thermal-neutron eigenfunction represented in each.

2. Broadened Ikeda-Carpenter functions

2.1 Gaussian broadening

When resolution effects broaden the observed function, as in scattering instrument resolution applications, it is frequently the case that many broadening effects convolute together to approximate a Gaussian broadening function (an example of the central limit theorem). To describe the measured emission time distribution then requires a broadened version of the I-C function. We have worked this out [3] in relation to the resolution of a pulsed-source chopper spectrometer. The result is the convolution of the I-C function with the instrument response function (broadening function), a Gaussian function,

$$f_G(t) = \int_{-t}^{\infty} f_{I-C}(t+\tau) g(\tau) d\tau \;, (10)$$

where

$$g(\tau)=\sqrt{\frac{\gamma}{\pi}}\exp(-\gamma t^2) \quad (11)$$

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

$$f_G(t)=\frac{2}{a}\left\{\left[(1-R)a^2t^2-\frac{a^2\beta R}{(a-\beta)^3}(1+(a-\beta)t+\frac{1}{2}(a-\beta)^2t^2)\right]\exp(-at)f_o(a,\gamma,t)+\right.$$
$$+\frac{a^2\beta R}{(a-\beta)^3}\exp(-\beta t)f_o(\beta,\gamma,t)+$$
$$+\left[2(1-R)a^2t-\frac{a^2\beta R}{(a-\beta)^2}\big(1+(a-\beta)t\big)\right]\exp(-at)f_1(a,\gamma,t)+$$
$$\left.+\left[(1-R)a^2-\frac{1}{2}\frac{a^2\beta R}{(a-\beta)}\right]\exp(-at)f_2(a,\gamma,t)\right\}. \quad (12)$$

The functions $f_o(x,y,t)$, $f_1(x,y,t)$, and $f_2(x,y,t)$ might be calculated by integration by parts, but 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),

$$f_o(x,\gamma,t)=\int_{-t}^{\infty}\exp(-x\tau)\exp(-\gamma\tau^2)d\tau=\frac{2}{\sqrt{\pi\gamma}}\exp(\frac{x^2}{4\gamma})\mathrm{erfc}(\frac{x}{2\sqrt{\gamma}}-\sqrt{\gamma}t)\ , (13)$$

where

$$\mathrm{erfc}(y)=\frac{2}{\sqrt{\pi}}\int_{y}^{\infty}\exp(-u^2)du \quad (14)$$

is the complementary error function and

$$\frac{d\mathrm{erfc}(y)}{dy} = -\frac{2}{\sqrt{\pi}}\exp(-y^2)\,. \quad (15)$$

Then

$$f_1(x,\gamma,t) = \int_{-t}^{\infty} \tau \exp(-x\tau)\exp(-\gamma\tau^2)d\tau = -\frac{\delta}{\delta x} f_o(x,\gamma,t) \quad (16)$$

and

$$f_2(x,\gamma,t) = \int_{-t}^{\infty} \tau^2 \exp(-x\tau)\exp(-\gamma\tau^2)d\tau = -\frac{\delta}{\delta \gamma} f_o(x,\gamma,t) \quad (17)$$

so that we have

$$f_1(x,\gamma,t) = \frac{2}{\pi\gamma}\exp(\frac{x^2}{4\gamma})\left[\exp(-\gamma(t-\frac{x}{2\sqrt{\gamma}})^2) - \frac{x}{2}\sqrt{\frac{\pi}{\gamma}}\mathrm{erfc}(\frac{x}{2\sqrt{\gamma}}-\sqrt{\gamma})\right] \quad (18)$$

and

$$f_2(x,\gamma,t) = \frac{1}{\gamma\sqrt{\pi\gamma}}\exp(\frac{x^2}{4\gamma})\times$$

$$\times\left[\left(1+\frac{x^2}{2\gamma}\right)\mathrm{erfc}(\frac{x}{2\sqrt{\gamma}}-t\sqrt{\gamma}) - \frac{2}{\sqrt{\pi}}\left(\frac{x}{2\sqrt{\gamma}}+t\sqrt{\gamma}\right)\exp(-(\frac{x}{2\sqrt{\gamma}}-t\sqrt{\gamma})^2)\right]. \quad (19)$$

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 $0 < t < \infty$ required in the Laplace transform. (The resolution broadening function is actually non-zero 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 [3]. For some reason, the integrals involved are not explicitly found in standard handbooks, however, consult Ref. [4].

In application the time t usually is offset by a delay time, $t \to t - t_o$. If parameters of the Gaussian-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,

$$t_e = \frac{3}{a} + \frac{R}{\beta}, (20)$$

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

$$\sigma^2_{Gaussian\ broadened\ \text{I-C}} = \frac{3}{a^2} + \frac{\left(2R - R^2\right)}{\beta^2} + \sigma^2_{Gaussian}, (21)$$

in which all variables are functions of the energy, E.

2.2 Long-pulse source broadening

When the source pulse is extended in time, as in long-pulse sources, the finite duration of the source pulse broadens the emission time distribution from its form for a delta function source pulse. Representing the source pulse as a step function (Heaviside function) time distribution,

$$H(t) = \begin{cases} \dfrac{1}{T} \text{ for } 0 < t < T \text{ and} \\ 0 \text{ for } t > T \end{cases}, (22)$$

the broadened I-C function is

$$f_H(t) = \int_0^t f_{I-C}(t-\tau)H(\tau)d\tau = \frac{1}{T}\int_{\tau_{\min}}^t f_{I-C}(t-\tau)d\tau \ (23)$$

where $\tau_{\min} = Max(0, t-T)$. Explicitly, collecting terms of equal order in τ, we have

$$f_H(t) = \frac{2}{aT}\int_{\tau_{\min}}^t \left\{ \begin{array}{l} \left[(1-R)a^2 - \dfrac{Ra\beta^2}{(a-\beta)}\right]\tau^2 \exp(-a\tau) - \dfrac{2Ra\beta^2}{(a-\beta)^2}\tau \exp(-a\tau) + \\ + \dfrac{2Ra\beta^2}{(a-\beta)^3}\left(\exp(-\beta\tau) - \exp(-a\tau)\right) \end{array} \right\} d\tau \ (24)$$

Defining functions h_o, h_1, and h_2, which are standard integrals found in the handbooks,

$$h_o(x,t) = x\int_{\tau_{\min}}^{t} \exp(-x\tau)\,d\tau = \exp(-x\tau_{\min}) - \exp(-xt)\,, (25)$$

$$h_1(x,t) = x^2\int_{\tau_{\min}}^{t} \tau\exp(-x\tau)\,d\tau = \left(x\tau_{\min}+1\right)\exp(-x\tau_{\min}) - \left(xt+1\right)\exp(-xt)\,, (26)$$

and

$$h_2(x,t) = x^3\int_{\tau_{\min}}^{t} \tau^2\exp(-x\tau)\,d\tau =$$

$$= (x^2\tau_{\min}^2 + 2x\tau_{\min} + 2)\exp(-x\tau_{\min}) - (x^2t^2 + 2xt + 2)\exp(-xt)\,, (27)$$

we finally have

$$f_H(t) = \frac{a}{2T}\left\{\begin{array}{l}\left[\left(1-R\right)a^2 - \dfrac{Ra\beta^2}{\left(a-\beta\right)^3}\right]\dfrac{h_2(a,t)}{a^2} - \\ -\dfrac{2Ra\beta^2}{\left(a-\beta\right)^2}\dfrac{h_1(a,t)}{a} + \dfrac{2Ra\beta^2}{\left(a-\beta\right)}\left(\dfrac{h_o(a,t)}{a} - \dfrac{h_1(\beta,t)}{\beta}\right)\end{array}\right\} (28)$$

Recall that $\tau_{\min} = Max(0, t-T)$, so that there are three regimes:

$$0 < t < T\text{ , where } \tau_{\min} = 0\,; (29)$$

$$t > T\text{ , where } \tau_{\min} = t - T\,; (30)$$

and

$$t < 0\text{ , where } f_H(t) = 0\,, (31)$$

as it must be because nothing has happened yet for those times.

The mean emission time is

$$t_e = \frac{3}{a} + \frac{R}{\beta} + \frac{T}{2}\,, (32)$$

and the variance of the emission time distribution is

$$\sigma^2_{H-broadened} = \frac{3}{a^2} + \frac{\left(2R - R^2\right)}{\beta^2} + \frac{T^2}{12}, (33)$$

which results follow because the functions are convolutions of the I-C function and the broadening function.

These results will be useful for fitting measured and calculated data and for instrument design simulations. The broaden functions are complicated but explicit, moreover, they introduce only one new parameter into the least-squares scheme, so that, once programmed, there should be no great troubles in view of the great speed of modern computers. Readers interested to derive broadened I-C functions for other forms of sectionally continuous broadening may find useful the very general function-transform pair for rational functions (ratios of polynomials in the transform variable) found, for example, in Ref. [5].

An obvious, needed extension of the present work is to derive expressions for the broadened pulse shape including both gaussian and top-hat broadening in the same form.

3. Conjecture

Important exceptions in recent experience to the single-pulse-shape description for each energy are those of para-hydrogen moderators, for which, I conjecture, at least two terms of similar form may be required. A possible reason for this may lie in the unusual total scattering cross section of moderators with high para concentrations, which has a minimum in the range of energies just below 15 meV. In contrast with the most common situations in which the cross section minimum lies in the epithermal range, this may lead to more than one thermal-neutron energy eigenfunction and time eigenvalue that is potentially significant in the energy range near 15 meV.

References

1. S. Ikeda and J. M. Carpenter, “Wide Energy-Range, High-Resolution Measurements of Neutron Pulse Shapes of Polyethylene Moderators,“ Nucl. Instr. & Methods A, **239**, 536 (1985).

2. J. M. Carpenter and W. B. Yelon. *Neutron Sources*, Chapter 2 in Methods of Experimental Physics, editors-in-chief R. Celotta and J. Levine, Volume 23 Part A, Neutron Scattering, editors K. Sköld and D. L. Price, Academic Press, Inc. (1986). See p. 167.

3. C. K. Loong, J. M. Carpenter, and S. Ikeda, “Resolution Function of a Pulsed-Source Chopper Spectrometer,” Nucl. Instr. & Meth. **A260** p 381 (1987). Also, C. K. Loong, J. M. Carpenter, and S. Ikeda “A Parametric Formulation of the Resolution Function of a Pulsed-Source Chopper Spectrometer,” Proceedings of the XIIth meeting of the International Collaboration on Advanced Neutron Sources, Rutherford-Appleton Laboratory 24-28 May, 1993 (ICANS XII), Rutherford-Appleton Laboratory Report Number 94-025, Volume 1, pp I-320-325.

4. *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun, National Bureau of Standards Applied Mathematics Series, AMS-55, June, 1964, see entry 7.2.3, p 299.

5. *Tables of Integral Transforms, Volume I, the Bateman Manuscript Project*, A. Erdélyi, Editor, W. Magnus, F. Oberhettinger, F. G. Tricomi, Associates, McGraw-Hill Book Company, Inc. (1954). Consult Sect. 5.2, formulas (19, 20, 21), p. 232.