

A Simpler Formula for Certain Integrals in the Theory of the Mössbauer Line Shape

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It is shown that the integrals Q_m which occur in the problem of the Mössbauer thick-absorber line shape can be expressed as the real part of a polynomial of degree m .

In their work on the Mössbauer thick-absorber line shape, HEBERLE and FRANCO^{1,2} have shown that the integral which gives the fractional absorption of the recoil-free radiation can be evaluated by means of an infinite series

$$\varepsilon(x) = 1 - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\exp\{-\gamma^2 s / (z^2 + \gamma^2)\}}{1 + (z-x)^2} dz$$

$$= - \sum_{m=1}^{\infty} \frac{(-s)^m}{m!} Q_m(\gamma, x), \quad (1)$$

where

$$Q_m(\gamma, x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(\frac{\gamma^2}{z^2 + \gamma^2} \right)^m \frac{dz}{1 + (z-x)^2}. \quad (2)$$

For the definitions of the various symbols, the reader is referred to Ref. 1. The integral Q_m has been expressed as [see Eqs. (2.6) and (10.10) of Ref. 2]

$$Q_m(\gamma, x) = \left(\frac{\gamma(\gamma+1)}{x^2 + (\gamma+1)^2} \right)^m$$

$$+ \frac{m}{[4(\gamma+1)]^m} \sum_{l=1}^{m-1} \left(\frac{\gamma(\gamma+1)^2}{x^2 + (\gamma+1)^2} \right)^l \frac{1}{m-l} \sum_{i=1}^{m-l} \binom{2m-2l}{i-1}$$

$$\binom{2m-l-i}{m} \gamma^{i-1}. \quad (3)$$

It is the purpose of this note to present a formula for Q_m that is considerably simpler than Equation (3).

We begin by using the identity

$$1/[1 + (z-x)^2] = \text{Re}[i/(z-x+i)]$$

in Equation (2). For an integral of a real variable it is possible to commute integration and taking the real part. Thus, if we define the complex function

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¹ J. HEBERLE and S. FRANCO, Z. Naturforsch. 23 a, 1439 [1968].

$$U_m(\gamma, x) = \frac{i\gamma^{2m}}{\pi} \int_{-\infty}^{\infty} \frac{dz}{(z-x+i)(z+i\gamma)^m(z-i\gamma)^m} \quad (4)$$

then it is apparent that

$$Q_m = \text{Re}(U_m).$$

In the upper half of the complex plane, the only singularity of the integrand in (4) is a pole of order m at $z = i\gamma$. Applying the residue theorem, we have

$$U_m = - \frac{2\gamma^{2m}}{(m-1)!} \lim_{z \rightarrow i\gamma} \left\{ \frac{d^{m-1}}{dz^{m-1}} \left[\frac{1}{(z-x+i)(z+i\gamma)^m} \right] \right\}. \quad (5)$$

The derivative can be evaluated by means of Leibniz's theorem³

$$D_n(z) \equiv \frac{d^n}{dz^n} \left[\frac{1}{(z-x+i)(z+i\gamma)^{n+1}} \right] = \sum_{l=0}^n \binom{n}{l} \left[\frac{d^{n-l}}{dz^{n-l}} \frac{1}{z-x+i} \right] \left[\frac{d^l}{dz^l} \frac{1}{(z+i\gamma)^{n+1}} \right].$$

The derivatives in D_n can be obtained by use of the relation (valid when k is a positive integer and c is independent of x),

$$\frac{d^j}{dx^j} (x+c)^{-k} = (-1)^j \frac{(k+j-1)!}{(k-1)!} (x+c)^{-(k+j)}.$$

We evaluate D_n at $z = i\gamma$ and obtain

$$D_n(i\gamma) = - \sum_{l=0}^n \frac{(n+l)!}{l!} (2\gamma)^{-(n+1+l)} (\gamma+1+i\gamma)^{-(n+1-l)}.$$

Equation (5) then becomes

$$U_m(\gamma, x) = \frac{2}{4m} \sum_{l=0}^{m-1} \binom{m-1+l}{l} \left(\frac{2\gamma}{\gamma+1+i\gamma} \right)^{m-l}. \quad (6)$$

If we define $\alpha = 2\gamma/(\gamma+1+i\gamma)$, then we have the result that Q_m is the real part of a polynomial of degree m with constant coefficients

$$Q_m(\gamma, x) = \frac{2}{4m} \text{Re} \left\{ \sum_{l=0}^{m-1} \binom{m-1+l}{l} \alpha^{m-l} \right\}. \quad (7)$$

The calculation of ε by the series in Eq. (1) can be performed considerably faster by use of Eq. (7) than with Equation (3).

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² S. FRANCO and J. HEBERLE, Z. Naturforsch. 25 a, 134 [1970].

³ See, for instance, Handbook of Mathematical Functions, ed. M. ABRAMOWITZ and I. A. STEGUN, Dover, New York 1965, Eq. (3.3.8).



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