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

BRUCE T. CLEVELAND

Department of Physics and Astronomy
State University of New York at Buffalo
Buffalo, New York, USA

(Z. Naturforsch. 27 a, 370 [1972]; received 10 January 1972)

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

$$\varepsilon(x) = 1 - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\exp\{-\gamma^2 s/(z^2+\gamma^2)\}}{1+(z-x)^2}\,\mathrm{d}z = -\sum_{m=1}^{\infty} \frac{(-s)^m}{m!} Q_m(\gamma, x), \quad (1)$$

where

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

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

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

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

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

then it is apparent that

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

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

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

The derivative can be evaluated by means of Leibniz's theorem [3]

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

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),

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

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

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

Equation (5) then becomes

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

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

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

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

The author is grateful to the Research Foundation of the State University of New York for the award of a Faculty Research Fellowship.

Reprint requests to Dr. B. T. CLEVELAND, Dept. of Physics, SUNY at Buffalo, *Buffalo*, New York 14 214, USA.

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

[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).