Conclusions

Using the method of moments, which was applied for the solution of the integral equations (3) and (48), the ground-state energy and the excitation spectrum of a one dimensional N particle system, interacting in a $\delta(x_i - x_j)$ potential, have been calculated.

The same method has been applied for the solution of Hulthen's equation (65) from which the ground-state energy and the magnetization of the system have been calculated for the Hamiltonian (61) and for $\Delta = -1$.

The expressions (23) and (30) corresponding to the zero approximation of the moments method can be used for all values of parameter γ and λ except for the case $\gamma = 0$, which must be studied separately.

The approximate results (55) and (56) are valid for all values of the parameter $S \geqq 1$. For large and small values of λ and for $S \approx 1$ we arrive at the well-known results of Lieb.

The most important result is the determination of magnetization expression (82). This expression corresponds to the zero approximation but is valid for all values of λ and in addition gives the actual magnetization curve.

If the above magnitudes are calculated by the use of higher order approximations the real solution of the problems are obtained. This can easily be done since the system of coefficients is linear.

Transmission of a Lorentzian Spectral Line Through a Layer of Lorentzian Absorbers. Part II

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The formalism presented in Part I has been developed further. By analytical methods we have derived a formula for the linewidth

$$W = (\Gamma_S + \Gamma_A)\{1 + \gamma\, T[1 + \gamma\, T/2! - (\gamma+1)^2\, T^2/3! - (7\gamma^3 + 6\gamma^2 - 2)\, T^3/4! + \tfrac{1}{3}(31\gamma^4 + 120\gamma^3 + 156\gamma^2 + 72\gamma + 6)\, T^4/5! + \ldots]\}$$

where $\gamma = \Gamma_A/\Gamma_S$ and T is a new dimensionless parameter which is proportional to the absorber thickness. The application to Mössbauer spectroscopy is discussed. The results are valid for environmental broadening of the Lorentzian type.

8. Summary of Results Obtained in Part I

In Part I of this investigation [15], we considered the total intensity – of an originally Lorentzian line – that is transmitted through a layer of Lorentzian absorbers. This transmitted intensity is given by

$$P(\Delta E) = P(\infty)\, \mathrm{tran}(\gamma, s; x)$$

where the *transmission function* is defined by

$$\mathrm{tran}(\gamma, s; x) = \frac{1}{\pi} \int \frac{\exp\{-s/[1+(z/\gamma)^2]\}}{1+(z+x)^2}\, dz\,.$$

For the definitions of the various symbols, the reader is referred to Sections 1 and 2. We continue to employ the convention, adopted in Section 2, that the limits of an integral are $-\infty$ and $+\infty$ when they are not indicated explicitly.

Our main result was that the transmission function can also be represented by a series,

$$\mathrm{tran}(\gamma, s; x) = \sum_{m=0}^{\nu-1} \frac{(-s)^m}{m!} Q_m(\gamma, x) + \frac{1}{2}\frac{(-s)^\nu}{\nu!} Q_\nu(\gamma, x) \pm \frac{1}{2}\frac{s^\nu}{\nu!} Q_\nu(\gamma, x) \quad \text{for} \quad \nu \geqq s\,. \tag{8.1}$$

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[15] Part I appeared in Z. Naturforsch. **23 a**, 1439 [1968]. Sections, equations and references of Part II are numbered consecutively after those of Part I.

In Section 5 it was stated, erroneously, that a sufficient condition for the validity of Eq. (8.1) is that $\nu \geqq s-1$; upon reconsideration we conclude that a sufficient condition is simply $\nu \geqq s$.

The functions Q_m are related to the polynomials G_{lm} by

$$Q_m(\gamma, x) = \sum_{l=1}^{m} (\gamma/X)^l \, G_{lm}(\gamma) \qquad (2.6)$$

where $X = x^2 + (\gamma+1)^2$ and

$$G_{lm}(\gamma) = \frac{1}{4^{m-l}} \sum_{k=1}^{l+1} a(k, l, m)\, \gamma^{k-1}. \qquad (2.8)$$

The numerical coefficients $a(k, l, m)$ can be generated by the recursive formulas (2.9), beginning with

$$a(1,1,1) = a(2,1,1) = 1 .$$

In Section 4 various special cases were discussed in terms of the *fractional absorption* defined by

$$\varepsilon(\gamma, s; x) = 1 - \mathrm{tran}(\gamma, s; x). \qquad (8.2)$$

In Section 6 we have answered the question: What kind of environmental broadening preserves the Lorentzian form of the cros section as a function of energy?

9. Introduction to Part II

In Part I we raised the question whether or not the coefficients $a(k, l, m)$ are integers for all values of the indices. In Section 10 we present a proof that all these coefficients are indeed integers. In the course of this proof, we derive direct formulas for the polynomials G_{lm}, so that we are now able to compute the G_{lm} without having to resort to recursion formulas.

If the transmitted intensity P is plotted as a function of ΔE with the parameters γ and s being kept constant, the curve thus obtained is called a *resonance curve*. A quantity of interest is the *width* W of the resonance, defined by the equation

$$\varepsilon(\gamma, s; W/\Gamma_S) = \tfrac{1}{2}\, \varepsilon(\gamma, s; 0). \qquad (9.1)$$

One way to deal with Eq. (9.1) is to solve it numerically [11] by use of the Newton-Raphson method. This approach requires a knowledge of the derivative $\partial\varepsilon/\partial x$. Section 11 is devoted to the calculation of this derivative.

In Section 13 we solve Eq. (9.1) by analytical methods and obtain for W a power series in T, a new dimensionless variable which is proportional to s. The range of validity of this formula for W is treated in Section 14 by comparison with exact values. Section 15 deals with the application to Mössbauer spectroscopy.

10. Direct Evaluation of G_{lm}

The results of Section 3 suggest that the polynomial G_{lm} can be written in the form

$$G_{lm}(\gamma) = \frac{(\gamma+1)^{2l-m}}{4^{m-l}}\, g_{m-l,\,m}(\gamma). \qquad (10.1)$$

In particular, since $G_{mm} = (\gamma+1)^m$, we have

$$g_{0,\,m} = 1 . \qquad (10.2)$$

Furthermore, from (3.1) we obtain

$$g_{m,\,m+1} = \frac{(2\,m)\,!}{(m!)^2}\,(\gamma+1)^{m-1} = \binom{2\,m}{m} \sum_{i=1}^{m} \binom{m-1}{i-1} \gamma^{i-1}. \qquad (10.3)$$

In general, $g_{m-l,\,m}$ is a polynomial of degree $m-l-1$ in γ,

$$g_{jm} = \sum_{i=1}^{j} \alpha(i, j, m)\, \gamma^{i-1}. \qquad (10.4)$$

Here we have introduced the subscript $j \equiv m-l$, which ranges from 1 to $m-1$.

From Eq. (2.7a) we obtain a recursion relation for g_{jm}:

$$g_{j+1,\,m+1} = \frac{1}{m}\Big[2(3\,j\,\gamma + m + j) + (m-j-1)\, g_{j+1,\,m} - 2\,\gamma(\gamma+1)\,\frac{\mathrm{d}}{\mathrm{d}\gamma}\, g_{jm} \Big]. \qquad (10.5)$$

By applying the method of mathematical induction to (10.5), we have proved the following equations

$$g_{1,\,m} = m\,,$$
$$g_{2,\,m} = m[\tfrac{1}{2}\,(m+1) + 2\,\gamma],$$
$$g_{3,\,m} = m[\tfrac{1}{6}\,(m+1)\,(m+2) + 2(m+1)\,\gamma + 5\,\gamma^2],$$
$$g_{4,\,m} = m[\tfrac{1}{24}\,(m+1)\,(m+2)\,(m+3) + (m+1)\,(m+2)\,\gamma + 7(m+1)\,\gamma^2 + 14\,\gamma^3],$$
$$g_{5,\,m} = m[\tfrac{1}{120}\,(m+1)\,(m+2)\,(m+3)\,(m+4) + \tfrac{1}{3}\,(m+1)\,(m+2)\,(m+3)\,\gamma + \tfrac{9}{2}\,(m+1)\,(m+2)\,\gamma^2 + 24(m+1)\,\gamma^3 + 42\,\gamma^4]\,.$$

It looks as if the coefficient $\alpha(i, j, m)$ can be written as the product of two factors

$$\alpha(i, j, m) = \beta(i, j) \binom{m+j-i}{m-1} \qquad (10.6)$$

where $\beta(i, j)$ does not depend on m. This is clearly true for $1 \leqq j \leqq 5$. Now we need to prove that (10.6) is true for al values of j.

By inserting (10.4) into (10.5) and then equating the coefficients of like powers of γ, we are led to

$$\alpha(1, j+1, m+1) = \frac{1}{m} [(m-j-1)\, \alpha(1, j+1, m) + 2(m+j)\, \alpha(1, j, m)],$$

$$\alpha(i, j+1, m+1) = \frac{1}{m} \{(m-j-1)\, \alpha(i, j+1, m) + 2[(3j-i+2)\alpha(i-1, j, m) + (m+j-i+1)\, \alpha(i, j, m)]\},$$

where it is understood that $\alpha(i, j, m) = 0$ if $i > j$. We substitute (10.6) in these recursive formulas and obtain

$$\beta(1, j+1) = \beta(1, j),$$

$$\beta(i, j+1) = \frac{2}{2j-i+3} [(3j-i+2)\, \beta(i-1, j) + (j-i+2)\, \beta(i, j)]\,. \tag{10.7a}$$

Since $g_{1,m} = \alpha(1, 1, m) = m$, it follows that $\beta(1, 1) = 1$, and therefore

$$\beta(1, j) = 1\,. \tag{10.7b}$$

The formulas (10.7) are independent of m. This proves that our assumption (10.6) is valid for *all* values of the indices.

Now we can evaluate $\beta(i, j)$ by considering the case $m = j+1$. From (10.3) we have

$$\alpha(i, j, j+1) = \frac{(2j)!}{(j!)^2} \binom{j-1}{i-1}.$$

But according to (10.6)

$$\alpha(i, j, j+1) = \beta(i, j) \binom{2j+1-i}{j}.$$

Comparison of the last two equations leads to a direct formula for $\beta(i, j)$, namely

$$\beta(i, j) = \frac{j-i+1}{j} \binom{2j}{i-1}. \tag{10.8}$$

By substituting (10.8) back into (10.6), we obtain a direct formula also for $\alpha(i, j, m)$

$$\alpha(i, j, m) = \frac{j-i+1}{j} \binom{2j}{i-1} \binom{m+j-i}{m-1} = \frac{m}{j} \binom{2j}{i-1} \binom{m+j-i}{m} \tag{10.9}$$

which is valid for all values of the indices

$$1 \leqq i \leqq j \leqq m\,.$$

The last result allows us to write the following expressions for G_{lm}

$$G_{lm} = \frac{(\gamma+1)^{2l-m}}{4^{m-l}} \frac{m}{m-l} \sum_{i=1}^{m-l} \binom{2m-2l}{i-1} \binom{2m-l-i}{m} \gamma^{i-1}$$

$$\text{for} \quad m > 1,\ l < m\,, \tag{10.10}$$

$$G_{mm} = (\gamma+1)^m \quad \text{for} \quad m \geqq 1\,.$$

With Eq. (10.10) one can perform the direct computation of any G_{lm}, without having to go through the computation of the G_{lm} of lower index, as required when using recursion formulas. However we want to point out that, when a sufficiently large number of the G_{lm} needs to be computed, then the recursive fomulas may turn out to be more efficient than the direct formulas.

Our next task is to prove that the $a(k, l, m)$ are integers. First we show that the $\alpha(i, j, m)$ are integers. For $i = 1$ we have

$$\alpha(1, j, m) = \binom{m+j-1}{m-1}$$

which is an integer because all binomial coefficients are integers. For $i > 1$, it is easily verified with the aid of Eq. (10.9) that

$$\alpha(i, j, m) = \left[\binom{2j}{i-1} - 2\binom{2j-i}{i-2}\right] \binom{m+j-i}{m-1}$$

which is clearly also an integer. From (2.8), (10.1) and (10.4), we obtain

$$\sum_{k=1}^{l+1} a(k, l, m)\, \gamma^{k-1} = (\gamma+1)^{2l-m} \sum_{i=1}^{m-l} \alpha(i, m-l, m)\, \gamma^{i-1}\,.$$

In general, if a polynomial with non-integral coefficients is multiplied by $\gamma+1$, the resulting polynomial also contains non-integral coefficients. On the other hand, if a polynomial with only integral coefficients is multiplied by $\gamma+1$, the new polynomial has only integral coefficients. It follows that the $a(k, l, m)$ are integers.

11. Slope of Resonance Curve

The slope $\partial P/\partial(\Delta E)$ of the resonance curve is proportional to the derivative $\partial\varepsilon/\partial x$

$$\frac{\partial P}{\partial(\Delta E)} = -\pi A_0 \frac{\partial \varepsilon}{\partial x}\,.$$

This derivative is given by

$$\frac{\partial \varepsilon}{\partial x} = \frac{2x}{X} \sum_{m=1}^{\infty} \frac{(-s)^m}{m!} Q_m^1(\gamma, x) \tag{11.1}$$

where

$$Q_m^1 = -\frac{X}{2x}\frac{\partial}{\partial x} Q_m = \sum_{l=l}^{m} l\left(\frac{\gamma}{X}\right)^l G_{lm}. \qquad (11.2)$$

In order to become able to investigate the convergence of the series in (11.1), we must find an upper limit to the ratio Q_{m+1}^1/Q_m^1. We begin by changing the variable of integration in (2.3b) to $y=z+x$, and we obtain

$$Q_m = \frac{1}{\pi}\int\left[\frac{\gamma^2}{(y-x)^2+\gamma^2}\right]^m \frac{dy}{1+y^2}.$$

Now

$$\frac{\partial Q_m}{\partial x} = \frac{2m}{\gamma^2\pi}\int\left[\frac{\gamma^2}{(y-x)^2+\gamma^2}\right]^{m+1}\frac{(y-x)\,dy}{1+y^2}.$$

After changing back to z and making use of (11.2), we obtain

$$Q_m^1(\gamma,x) = -\frac{mX}{\gamma^2\pi x}\int\left(\frac{\gamma^2}{z^2+\gamma^2}\right)^{m+1}\frac{z\,dz}{1+(z+x)^2}. \qquad (11.3)$$

From (11.2) it is obvious that Q_m^1 is an even function of x. Therefore we have also

$$Q_m^1(\gamma,x) = \frac{mX}{\gamma^2\pi x}\int\left(\frac{\gamma^2}{z^2+\gamma^2}\right)^{m+1}\frac{z\,dz}{1+(z-x)^2}. \qquad (11.4)$$

We add (11.3) to (11.4) and then divide by 2, thus obtaining

$$Q_m^1 = \frac{2mX}{\gamma^2\pi}\int\left(\frac{\gamma^2}{z^2+\gamma^2}\right)^{m+1}\frac{z^2\,dz}{[1+(z+x)^2][1+(z-x)^2]}.$$

By inspection of the last equation, we perceive that

$$Q_{m+1}^1/(m+1) < Q_m^1/m$$

or

$$Q_{m+1}^1/Q_m^1 < (m+1)/m. \qquad (11.5)$$

Let us now rewrite Eq. (11.1) as

$$\frac{\partial\varepsilon}{\partial x} = \frac{2x}{X}\left[\sum_{m=1}^{\nu-1}\frac{(-s)^m}{m!}Q_m^1 + \sum_{m=\nu}^{\infty}\frac{(-s)^m}{m!}Q_m^1\right]$$

where ν is to be chosen so that the absolute value of the term with $m=\nu$ is less than that of the preceding term; furthermore in the second summation the absolute values of the terms must decrease with increasing m. This condition requires that

$$\frac{Q_{m+1}^1}{Q_m^1}\frac{s}{m+1} < 1 \qquad for \quad m \geqq \nu-1. \qquad (11.6)$$

In view of the inequality (11.5), a sufficient condition for (11.6) is

$$\nu \geqq s+1.$$

Now we can write

$$\frac{\partial\varepsilon}{\partial x} = \frac{2x}{X}\left[\sum_{m=1}^{\nu-1}\frac{(-s)^m}{m!}Q_m^1 + \frac{1}{2}\frac{(-s)^\nu}{\nu!}Q_\nu^1 \pm E_\nu^1\right], \qquad (11.7)$$

where the error E_ν^1 is given by

$$E_\nu^1\ (s^\nu/\nu!)\ Q_\nu^1\ (\gamma,x).$$

By comparing (11.2) with (2.6), we find that

$$Q_\nu^1 \leqq \nu\, Q_\nu,$$

which leads to

$$E_\nu^1 \leqq \nu\, E_\nu,$$

where E_ν may be estimated by means of (5.3).

At times it may be useful to have a simple estimate for the upper limit of $\partial\varepsilon/\partial x$. We differentiate both sides of Eq. (2.2a) with respect to x

$$\frac{\partial\varepsilon}{\partial x} = -\frac{2}{\pi}\int\frac{z+x}{[1+(z+x)^2]^2}\exp\left\{\frac{-\gamma^2 s}{z^2+\gamma^2}\right\}dz.$$

Next we apply the Cauchy-Schwarz inequality (see Section 5) and obtain

$$\left(\frac{\partial\varepsilon}{\partial x}\right)^2 \leqq \left(\frac{2}{\pi}\right)^2\int\left[\frac{z+x}{1+(z+x)^2}\right]^2 dz \cdot \int\left[\frac{\exp\{-\gamma^2 s/(z^2+\gamma^2)\}}{1+(z+x)^2}\right]^2 dz.$$

But

$$\frac{1}{\pi}\int\left[\frac{z+x}{1+(z+x)^2}\right]^2 dz = \frac{1}{\pi}\int\frac{y^2\,dy}{(1+y^2)^2} = Q_0(1,0) - Q_1(1,0) = \tfrac{1}{2}$$

and

$$\frac{1}{\pi}\int\left[\frac{\exp\{-\gamma^2 s/(z^2+\gamma^2)\}}{1+(z+x)^2}\right]^2 dz < \frac{1}{\pi}\int\frac{\exp\{-\gamma^2 s/(z^2+\gamma^2)\}}{1+(z+x)^2}dz = 1-\varepsilon,$$

so that

$$(\partial\varepsilon/\partial x)^2 < 2(1-\varepsilon). \qquad (11.8)$$

12. New Variables

It turns out that the algebraic labor of calculating the width will be reduced, if we replace s and x by a new pair of dimensionless variables

$$T = s/[4(\gamma+1)] \quad \text{and} \quad \xi = x/(\gamma+1).$$

Furthermore we define

$$q_m(\xi) = [4(\gamma+1)]^m Q_m(\gamma,x)$$

which assumes the rather simple form

$$q_m(\xi) = \sum_{l=1}^{m}\left(\frac{4\gamma}{1+\xi^2}\right)^l g_{m-l,m}(\gamma). \qquad (12.1)$$

Thus

$$q_1 = \frac{4\gamma}{1+\xi^2}, \qquad q_2 = \frac{8\gamma}{1+\xi^2}\left(1+\frac{2\gamma}{1+\xi^2}\right),$$

$$q_3 = \frac{24\gamma(\gamma+1)}{1+\xi^2} + 3\left(\frac{4\gamma}{1+\xi^2}\right)^2 + \left(\frac{4\gamma}{1+\xi^2}\right)^3.$$

Another useful quantity is defined by

$$q_m^n(\xi) = \sum_{l=1}^{m} l^n \left(\frac{4\gamma}{1+\xi^2}\right)^l g_{m-l,m}(\gamma), \qquad (12.2)$$

which is a generalization of q_m since $q_m = q_m^0$. This quantity satisfies a recursion relation

$$\frac{\partial}{\partial\xi} q_m^n = -\frac{2\xi}{1+\xi^2} q_m^{n+1}. \qquad (12.3)$$

Finally we introduce the function

$$\lambda(\xi, T) = \frac{\varepsilon(\gamma, s; x) - \frac{1}{2}\varepsilon(\gamma, s; 0)}{2\gamma T}.$$

We have not indicated explicitly that q_m and λ are also functions of γ because in Section 13 the quantity γ will play only the role of a constant parameter. After appropriate substitutions, we obtain the more explicit formula

$$\lambda(\xi, T) = \frac{1}{2\gamma} \sum_{m=1}^{\infty} \frac{(-T)^{m-1}}{m!} r_m(\xi) \qquad (12.4)$$

where $\quad r_m(\xi) \equiv q_m(\xi) - \frac{1}{2} q_m(0).$

For certain values of the partial derivatives of λ, we adopt the notation

$$\lambda_{hk} = \left[\frac{\partial^{h+k}}{\partial\xi^h \, \partial T^k} \lambda(\xi, T)\right]_{\xi=1,\, T=0}. \qquad (12.5)$$

13. Width of Resonance

In terms of the new variables, Eq. (9.1) becomes

$$\lambda(w, T) = \frac{1}{2\gamma} \sum_{m=1}^{\infty} \frac{(-T)^{m-1}}{m!} r_m(w) = 0 \qquad (13.1a)$$

where we have set

$$W = w(\gamma + 1)\,\Gamma_S. \qquad (13.1b)$$

We regard w as a function of T that is defined [16] implicitly by Eq. (13.1a). We denote the derivatives of $w(T)$ as

$$w^{(k)}(T) = \frac{d^k}{dT^k} w(T).$$

Also we abbreviate

$$w_0 = w(0).$$

In order to solve Eq. (13.1a), we expand $w(T)$ in a Maclaurin series

$$w = w_0 + \sum_{k=1}^{\infty} w^{(k)}(0) \cdot T^k/k!. \qquad (13.1c)$$

[16] The present definition of w is different from that employed earlier by HEBERLE [11].

The value of w_0 is found by letting $T \to 0$ in Eq. (13.1a). This leads to

$$(1/2\gamma)\, r_1(w_0) = 0 \quad \text{or} \quad 1/(1 + w_0^2) = 1.$$

Thus we obtain

$$w_0 = 1.$$

The other coefficients $w^{(k)}(0)$ will be evaluated by repeated differentiations of Eq. (13.1a) with respect to T and then letting T approach zero. Since the function λ depends on T explicitly and also implicitly through w, the first differentiation yields

$$\left(\frac{dw}{dT}\frac{\partial}{\partial w} + \frac{\partial}{\partial T}\right)\lambda(w, T) = 0, \qquad (13.2)$$

and $\quad w^{(1)}(0) = -\lambda_{01}/\lambda_{10}.$

We obtain these partial derivatives by differentiating (12.4)

$$\frac{\partial}{\partial T}\lambda(w, T) = -\frac{1}{2\gamma}\sum_{m=2}^{\infty}\frac{(m-1)(-T)^{m-2}}{m!} r_m(w), \qquad (13.3a)$$

$$\frac{\partial}{\partial w}\lambda(w, T) = \frac{1}{2\gamma}\sum_{m=1}^{\infty}\frac{(-T)^{m-1}}{m!}\frac{d}{dw} q_m(w). \qquad (13.3b)$$

As $T \to 0$, $w \to w_0 = 1$, and we have

$$\lambda_{01} = -(1/4\gamma)\, r_2(w_0) = \gamma$$

and $\quad \lambda_{10} = (1/2\gamma)\,(dq_1/dw)_{w=1} = -1,$

so that

$$w^{(1)}(0) = \gamma.$$

We are now equipped to calculate $w^{(2)}(0)$ by differentiating (13.2) with respect to T

$$\left[\frac{d^2w}{dT^2}\frac{\partial}{\partial w} + \left(\frac{dw}{dT}\right)^2\frac{\partial^2}{\partial w^2} + 2\frac{dw}{dT}\frac{\partial^2}{\partial w\,\partial T} + \frac{\partial^2}{\partial T^2}\right]\lambda(w, T) = 0. \qquad (13.4)$$

Letting $T \to 0$ in (13.4), we obtain

$$w^{(2)}(0) = -\{[w^{(1)}(0)]^2\lambda_{20} + 2\,w^{(1)}(0)\,\lambda_{11} + \lambda_{02}\}/\lambda_{10}.$$

The three required partial derivatives are calculated by differentiating (13.3),

$$\frac{\partial^2\lambda}{\partial w^2} = \frac{1}{2\gamma}\sum_{m=1}^{\infty}\frac{(-T)^{m-1}}{m!}\frac{d}{dw}\left[-\frac{2w}{1+w^2}q_n^1(w)\right] \qquad (13.5a)$$

$$= \frac{1}{\gamma}\sum_{m=1}^{\infty}\frac{(-T)^{m-1}}{m!}\frac{1}{(1+w^2)^2}\left[(w^2-1)\,q_m^1 + 2\,w^2\,q_m^2\right],$$

$$\frac{\partial^2\lambda}{\partial w\,\partial T} = \frac{1}{\gamma}\sum_{m=2}^{\infty}(m-1)\frac{(-T)^{m-2}}{m!}\frac{w}{1+w^2}q_m^1, \qquad (13.5b)$$

$$\frac{\partial^2 \lambda}{\partial T^2} = \frac{1}{2\gamma} \sum_{m=3}^{\infty} (m-2)(m-1) \frac{(-T)^{m-3}}{m!} r_m(w). \tag{13.5c}$$

Setting $T=0$ and $w=w_0=1$ in (13.5), we obtain

$$\lambda_{20} = (1/2\gamma)\, q_1{}^2(w_0) = 1,$$
$$\lambda_{11} = (1/4\gamma)\, q_2^1(w_0) = 1+2\gamma,$$
$$\lambda_{02} = (1/6\gamma)\, r_3(w_0) = -2\gamma(1+2\gamma),$$

and

$$w^{(2)}(0) = \gamma^2.$$

In general, after n differentiations of (13.1a) with respect to T, we have

$$\left(\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\partial}{\partial w} + \frac{\partial}{\partial T}\right)^n \lambda(w,T) = 0. \tag{13.6}$$

This equation, for $T=0$, consists of terms that are linear in λ_{hk}, where h and k are non-negative integers that satisfy the condition $h+k \leqq n$. From (12.4) one can see that, for $h>0$,

$$\lambda_{hk} = \frac{(-1)^k}{2(k+1)\gamma}\left[\frac{\partial^h}{\partial w^h} q_{k+1}(w)\right]_{w=w_0}. \tag{13.7a}$$

On the other hand, for $h=0$, we have

$$\lambda_{0,k} = \frac{(-1)^k}{2(k+1)\gamma} r_{k+1}(w_0) \tag{13.7b}$$
$$= \frac{(-1)^{k+1}}{k+1} \sum_{l=2}^{k+1} (2^{l-1}-1)(2\gamma)^{l-1} g_{k+1-l,k+1}.$$

The last step was performed with the aid of (12.1).

By considering Eq. (12.2), it is not difficult to convince oneself that the following formula is valid

$$\left[\frac{\partial^h}{\partial w^h} q_m^n(w)\right]_{w=w_0} = \sum_{l=1}^{m} l^{n+1} p_{h-1}(l)(2\gamma)^l g_{m-l,m} \tag{13.7c}$$

where $p_{h-1}(l)$ is a polynomial of degree $h-1$. By applying the recursion relation (12.3), we have evaluated the first four of these polynomials

$$p=-1, \quad p_1 = l, \quad p_2 = -(l+1)(l-1),$$
$$p_3 = (l+1)(l^2-l-3).$$

For $h=5$, we obtain

$$\frac{\partial^5}{\partial w^5} q_m^n = 8\Big[-\frac{15\,w}{(1+w^2)^3}(2\,q_m^{n+1}+3\,q_m^{n+2}+q_m^{n+3}) + \frac{20\,w^3}{(1+w^2)^4}(6\,q_m^{n+1}+11\,q_m^{n+2}+6\,q_m^{n+3}+q_m^{n+4})$$
$$-4\left(\frac{w}{1+w^2}\right)^5 (24\,q_m^{n+1}+50\,q_m^{n+2}+35\,q_m^{n+3}+10\,q_m^{n+4}+q_m^{n+5})\Big], \tag{13.8}$$

which leads to

$$p_4 = -(l+1)(l+2)(l^2-3l-3).$$

By using these results together with the formulas (13.7), we have calculated all the partial derivatives contained in (13.6) for $n \leqq 5$. These derivatives, evaluated for $w=1$ and $T=0$, are listed in the appendix of Part II.

Proceeding in the same manner as above in the case of $n=1$ and $n=2$, we obtain

$$w^{(3)}(0) = \gamma(\gamma+1)^2 \quad \text{and} \quad w^{(4)}(0) = -\gamma(7\gamma^3+6\gamma^2-2).$$

For $n=5$, Eq. (13.6) becomes

$$\Big\{\frac{\mathrm{d}^5 w}{\mathrm{d}T^5}\frac{\partial}{\partial w} + 5\left[\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\mathrm{d}^4 w}{\mathrm{d}T^4} + 2\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\frac{\mathrm{d}^3 w}{\mathrm{d}T^3}\right]\frac{\partial^2}{\partial w^2} + 5\frac{\mathrm{d}^4 w}{\mathrm{d}T^4}\frac{\partial^2}{\partial w\,\partial T} + 5\frac{\mathrm{d}w}{\mathrm{d}T}\left[2\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\mathrm{d}^3 w}{\mathrm{d}T^3} + 3\left(\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\right)^2\right]\frac{\mathrm{d}T^3}{\mathrm{d}^3 w}$$
$$+10\frac{\mathrm{d}^3 w}{\mathrm{d}T^3}\frac{\partial^3}{\partial w\,\partial T^2} + 5\left[3\left(\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\right)^2 + 4\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\partial w^3}{\partial^3}\right]\frac{\partial^3}{\partial w^2\,\partial T} + 10\left(\frac{\mathrm{d}w}{\mathrm{d}T}\right)^3\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\frac{\partial^4}{\partial w^4} + 30\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\left[\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\partial^4}{\partial w^3\,\partial T} + \frac{\partial^4}{\partial w^2\,\partial T^2}\right]$$
$$+10\frac{\mathrm{d}^2 w}{\mathrm{d}T^2}\frac{\partial^4}{\partial w\,\partial T^3} + \left(\frac{\mathrm{d}w}{\mathrm{d}T}\right)^5\frac{\partial^5}{\partial w^5} + 5\left(\frac{\mathrm{d}w}{\mathrm{d}T}\right)^2\left[\left(\frac{\mathrm{d}w}{\mathrm{d}T}\right)^2\frac{\partial^5}{\partial w^4\,\partial T} + 2\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\partial^5}{\partial w^3\,\partial T^2} + 2\frac{\partial^5}{\partial w^2\,\partial \mathrm{T}^3}\right] \tag{13.9}$$
$$+5\frac{\mathrm{d}w}{\mathrm{d}T}\frac{\partial^5}{\partial w\,\partial T^4} + \frac{\partial^5}{\partial T^5}\Big\}\lambda(w,T) = 0.$$

By using the results listed in the appendix, we obtain from Eq. (13.9)

$$w^{(5)}(0) = (\gamma/3)(31\gamma^4+120\gamma^3+156\gamma^2+72\gamma+6).$$

Thus the first six terms of the series (13.1c) are

$$w_5 = 1+\gamma T\left[1+\frac{T}{2!}\gamma - \frac{T^2}{3!}(\gamma+1)^2 - \frac{T^3}{4!}(7\gamma^3+6\gamma^2-2) + \frac{T^4}{5!}\frac{31\gamma^4+120\gamma^3+156\gamma^2+72\gamma+6}{3}\right]. \tag{13.10}$$

We have presented Eqs. (13.8) and (13.9) as a starting point for anyone who may wish to carry this calculation to higher values of n.

14. Accuracy of Width Formula

The series (13.1c) can be made as accurate as one wants by taking a sufficiently large number of terms. We have seen, however, that in practice the algebraic labor of calculating $w^{(k)}(0)$ increases rapidly with k. Therefore the question arises how accurate our formula is when it is terminated as in (13.10).

An obvious method of estimating the error incurred is to use Taylor's formula with remainder. Thus we can write

$$w(T) = w_n(T) + R_{n+1}(T),$$

where

$$w_n = w_0 + \sum_{k=1}^{n} w^{(k)}(0)\,\frac{T^k}{k!} \qquad (14.1)$$

and

$$R_{n+1} = w^{(n+1)}(\Theta T)\,\frac{T^{n+1}}{(n+1)!}, \quad 0<\Theta<1.$$

Although this is the ideal way to treat the problem of accuracy, we cannot apply it readily because it is very difficult to estimate the sixth derivative of $w(T)$ for $T>0$.

A direct way of ascertaining the accuracy of (13.10) is to compute exact values of w and to compare them with the corresponding values of w_5. What range of γ should be covered by such computations? To answer this equation, we remember that the main area of application is in Mössbauer spectroscopy. Therefore the range of γ should be chosen so as to cover the cases of interest in this area. As it was discussed in Section 6, $\gamma \neq 1$ indicates the presence of environmental broadening. Our entire formalism is valid only if (see Section 6) the environmental broadening is such that the average cross section has a Lorentzian dependence on energy

$$\langle \sigma(E) \rangle = \frac{f_A\,\sigma_{res}}{1+[(E-E_A)/\frac{1}{2}\varkappa_A \Gamma]^2}. \qquad (14.2)$$

We expect Eq. (14.2) to be a good approximation only for values of $\varkappa_A$ close to unity. Similarly, in considering the environmental broadening in the source, we conclude that our formalism is likely to be valid only for values of $\varkappa_S$ in the neighborhood of unity. Thus it appears that only values of γ in the vicinity of $\gamma=1$ are of immediate interest. Therefore we have chosen $\gamma=0.5$, 1.0, and 2.0 for our investigation of the accuracy.

Values of w were computed by the Newton-Raphson method in two ways:

(1) The equation

$$\varepsilon(\gamma, s; w_x) - \tfrac{1}{2}\varepsilon(\gamma, s; 0 = 0$$

was solved for w_x. The function ε and the derivative $\partial\varepsilon/\partial w_x$ were evaluated by numerical integration, as in the work of HEBERLE[11] for the case $\gamma=1$. Then

$$w = w_x/(\gamma+1).$$

(2) We solved Eq. (13.1a) for w. The derivative $\partial\lambda/\partial w$ was also computed as a series by making use of the results of Section 11. Thus numerical integrations were avoided entirely.

Satisfactory agreement was achieved between the results that were obtained by two so different methods; this constitutes a check on the correctness of our mathematical developments.

T	γ 0.5	1.0	2.0
0.001	1.0005	1.0010	1.0020
0.05	1.0253	1.0512	1.1046
0.10	1.0511	1.1043	1.2165
0.20	1.1035	1.2143	1.4505
0.30	1.1564	1.3258	1.6821
0.40	1.2089	1.4360	1.9007
0.50	1.2605	1.5426	2.1034
0.60	1.3108	1.6448	2.2908
0.80	1.4068	1.8354	2.6272
1.0	1.4965	2.0089	2.9247
1.2	1.5804	2.1681	
1.4	1.6592	2.3155	
1.6	1.7336		
1.8	1.8041		
2.0	1.8714		

Table 1. Computed values of the width w for various values of T, and for three different values of γ. The last digit in w is uncertain by ± 1, or less.

The values of w are listed in Table 1. (In the case of $\gamma=1.0$, values of w_x are available in graphical form[17] for $0 \leqq t \leqq 29$.) The case of $\gamma=2.0$ and $T=1.0$ required the largest number of terms in Eq. (13.1a); it was necessary to include the term $m=37$ in order to achieve the desired accuracy. A comparison of the values of w with those of w_5 is presented in Fig. 1. The result of the comparison may be epitomized by stating, somewhat conservatively, that for these three values of γ the deviation $|w_5 - w|$ is less than 2.0% of w for $s \leqq 5.0$. In looking at Fig. 1, one may wonder why so many terms are required to describe curves that look almost like straight lines.

[17] L. D. ROBERTS and J. O. THOMSON, Phys. Rev. **129**, 664 [1963]; see also D. W. HAFEMEISTER and E. B. SHERA, Nucl. Instr. Methods **41**, 133 [1966].

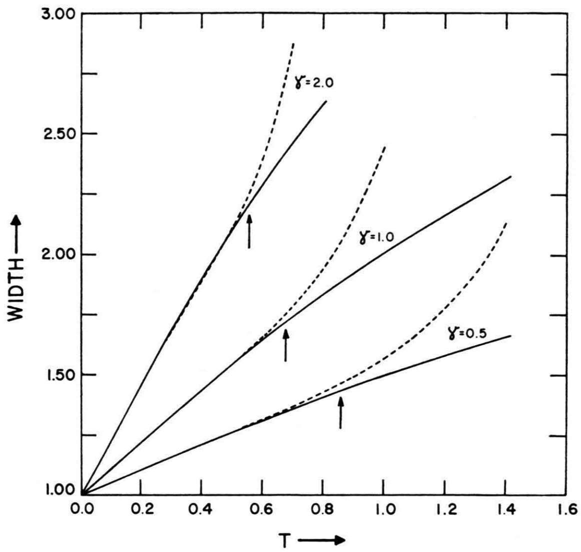

Fig. 1. Dimensionless width as a function of the thickness parameter T. The solid curves represent the exact values of w, whereas the dashed curves represent the approximate values w_5. The arrows indicate where w and w_5 differ by 2.0%.

It turns out that w_3 is also a good approximation of w, and that it is true also for w_3 that its accuracy is better than 2.0% for $s \leqq 5.0$. Of course, for small values of T, the accuracy of w_5 is much better than that of w_3.

15. Application to Mössbauer Spectroscopy

In terms of the quantities introduced in Section 6, we have

$$T = \frac{\varkappa_S}{\varkappa_A(\varkappa_S+\varkappa_A)}\,(t/4)\,. \qquad (15.1)$$

Then, according to (13.10), the observed width is given by

$$W = \Gamma \Big\{ (\varkappa_S+\varkappa_A) + t/4 + \frac{(t/4)^2}{2!\,(\varkappa_S+\varkappa_A)} - \frac{(t/4)^3}{3!\,\varkappa_A^2} - \frac{(t/4)^4}{4!\,(\varkappa_S+\varkappa_A)^3}\left[7+6\left(\frac{\varkappa_S}{\varkappa_A}\right)-2\left(\frac{\varkappa_S}{\varkappa_A}\right)^3\right] + \frac{(t/4)^5}{5!\,3\,(\varkappa_S+\varkappa_A)^4}\left[31+120\left(\frac{\varkappa_S}{\varkappa_A}\right)+156\left(\frac{\varkappa_S}{\varkappa_A}\right)^2 + 72\left(\frac{\varkappa_S}{\varkappa_A}\right)^3+6\left(\frac{\varkappa_S}{\varkappa_A}\right)^4\right] + \dots \Big\}\,. \qquad (15.2)$$

For a vanishingly thin absorber, W becomes

$$W_0 = (\varkappa_S+\varkappa_A)\,\Gamma = \Gamma_S + \Gamma_A\,,$$

in agreement with the result of Section 4a. We rewrite Eq. (15.2) in terms of Γ_S, Γ_A and W_0

$$W = W_0 + \Gamma(t/4) + \frac{\Gamma^2}{2!\,W_0}(t/4)^2 - \frac{\Gamma^3}{3!\,\Gamma_A^2}(t/4)^3 + \dots \qquad (15.3)$$

and we note that, to the second order in t, W is a function of W_0 but does not depend on either Γ_S or Γ_A separately.

A frequent experimental problem is to measure f_A and to determine the extent of environmental broadening by measuring W_0. In Section 6 it was stated that

$$t = n\,f_A\,\sigma_{res}\,, \qquad (15.4)$$

where n is the number of nuclei of the resonant isotope per unit area of the absorber. By measuring W for various values of n and then fitting these data with a suitable formula, it is possible to determine f_A and W_0. This procedure has been used by BRYUKHANOV et al. [18] for Mg_2Sn^{119}, by HAFEMEISTER et al. [19] for compounds of I^{129}, and by PERLOW [20] for compounds of Xe^{129}.

We suggest that our width formula, as it is written in (15.2) or (15.3), is perhaps more suitable for this purpose than the previously used formulas.

16. Further Remarks

If a digital computer is used to compute ε according to the method outlined in Section 8, it appears necessary to create a three-dimensional array for storing the coefficients $a(k,l,m)$. The improved formulation presented in Section 10 offers the advantage that, according to Eq. (10.10), only a two-dimensional array of binomial coefficients is required. Thus a considerable saving in memory can be effected.

It should not be thought that the new variables T and ξ, which were introduced in Section 12, are always superior to s and x. It seems to us that the new variables are better suited to the series, whereas the various integrals have a simpler form if expressed in terms of the old variables s and x.

Among our reasons for listing the values of w in Table 1 is their usefulness in testing a program for computing ε. This can be done by computing ε for $x=0$ and for $x=(\gamma+1)\,w$ and checking whether or not Eq. (9.1) is satisfied by these values of ε.

[18] V. A. BRYUKHANOV, N. N. DELYAGIN, and R. N. KUZ'MIN, Zh. Eksp. Teor. Fiz. **46**, 137 [1964].

[19] D. W. HAFEMEISTER, G. DEPASQUALI, and H. DE WAARD, Phys. Rev. **135**, B 1089 [1964].

[20] G. J. PERLOW, in: Chemical Applications of Mössbauer Spectroscopy, edited by V. I. GOLDANSKII and R. H. HERBER, Academic Press, New York 1968, p. 394 ff.

From the results of Section 10, one can obtain a formula for a definite integral that is not listed in the standard tables

$$\int_{-\infty}^{+\infty}\left(\frac{a^2}{z^2+a^2}\right)^m \frac{dz}{1+(z+x)^2}=\pi\left\{\left[\frac{a(a+1)}{x^2+(a+1)^2}\right]^m+m\sum_{l=1}^{m-1}\frac{1}{l[4(a+1)]^l}\left[\frac{a(a+1)}{x^2+(a+1)^2}\right]^{m-l}\sum_{k=1}^{l}\binom{2l}{k-1}\binom{m+l-k}{m}a^{k-1}\right\}.$$

Similarly, from Eqs. (10.10), (11.2) and (11.3), we obtain

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

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

In both formulas it is assumed that $a \geqq 0$.

These two articles have dealt with the behavior of ε and w in the case of absorbing layers of small thickness. An open question remains as to how these quantities behave for large values of s and T.

Acknowledgements

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Appendix

We list here the partial derivatives of $\lambda(\xi, T)$ evaluated at $\xi=1$ and $T=0$. The notation is defined by Eq. (12.5).

$\lambda_{01}=\gamma$, $\lambda_{02}=-2\gamma(2\gamma+1)$,

$\lambda_{03}=\gamma(14\gamma^2+16\gamma+5)$,

$\lambda_{04}=-2\gamma(24\gamma^3+45\gamma^2+30\gamma+7)$,

$\lambda_{05}=(2\gamma/3)(248\gamma^4+660\gamma^3+693\gamma^2+336\gamma+63)$,

$\lambda_{10}=-1$, $\lambda_{11}=2\gamma+1$,

$\lambda_{12}=-2(\gamma+1)(2\gamma+1)$,

$\lambda_{13}=8\gamma^3+25\gamma^2+20\gamma+5$,

$\lambda_{14}=-2(8\gamma^4+45\gamma^3+63\gamma^2+35\gamma+7)$,

$\lambda_{20}=1$, $\lambda_{21}=-(4\gamma+1)$,

$\lambda_{22}=2(6\gamma^2+5\gamma+1)$,

$\lambda_{23}=-(\gamma+1)(32\gamma^2+25\gamma+5)$,

$\lambda_{30}=0$, $\lambda_{31}=6\gamma$,

$\lambda_{32}=-4\gamma(8\gamma+3)$, $\lambda_{40}=-6$,

$\lambda_{41}=6(\gamma+1)$, $\lambda_{50}=30$.