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LINEWIDTH OF MÖSSBAUER ABSORPTION*

J. HEBERLE+

Argonne National Laboratory, Argonne, Illinois and *Clark University, Worcester, Massachusetts, U.S.A.*

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The linewidth W has been computed for various absorber thicknesses. It is assumed that both the source and the absorbing material have the natural linewidth Γ. Then, for an absorber containing n nuclei (of the resonant species) per unit area, the formula $W = 2\Gamma(1+0.1288t + 4.733\times10^{-3}t^2 - 9.21\times10^{-4}t^3 + 3.63\times10^{-5}t^4)$ approximates the computed values, where $t = nf'\sigma_{res}$. The values of W given by this formula are accurate to better than 0.15% for $0 \leqq t \leqq 12$.

1. Introduction

In the usual transmission experiment, the counting rate of photons behind an absorber is measured as a function of the velocity of the source relative to the absorber. Here we are concerned with the case of a single-line absorber illuminated by a single-line source. In order to simplify our discussion, we assume that the chemical and thermal shifts add up to zero, and that all the photons emitted by the source are recoilfree. The reader will realize, however, that formula (5) for the linewidth remains valid when these restrictions are removed. Furthermore, we assume that there is no environmental broadening in either the source or the absorber. (Sect. 3, shows how our result can be extended to a special case of environmental broadening.) A preliminary report of this work has been presented at an earlier occasion[1]).

The cross section of the resonantly absorbing nuclei depends on energy according to the formula

$$\sigma = \sigma_{res}[1+\{(E-E_0)/(\tfrac{1}{2}\Gamma)\}^2]^{-1},$$

where

$$\sigma_{res} = (\lambda^2/2\pi)\{(2J^*+1)/(2J+1)\}(1+\alpha)^{-1}.$$

All symbols, whose meaning is not obvious from the text, are defined in table 1. The energy distribution of the photons from the source is Lorentzian with a maximum at E_0 and the same width Γ. Then the intensity at the detector is

$$I(v) = (I_0/\pi)\int[1+\{E-E_0(1+v/c)\}^2/(\tfrac{1}{2}\Gamma)^2]^{-1}\cdot \cdot\exp[-nf'\sigma_{res}\{1+(E-E_0)^2/(\tfrac{1}{2}\Gamma)^2\}^{-1}]\,dE.$$

The limits of integration must be chosen so that enlarging the range of integration does not increase $I(v)$ significantly.

TABLE 1

Symbols not defined in the text.

c	speed of light
E_0	average energy of photons emitted by the source (at rest)
f'	Mössbauer fraction of the absorber
I_0	intensity far off resonance
J	spin quantum number of the ground state of the resonant nuclei
J^*	spin of the excited state
n	number of nuclei (of the resonant species) per unit area of absorber
v	velocity of the source relative to the absorber
α	internal-conversion coefficient
Γ	natural width in energy of the excited state
λ	wavelength of photons with energy E_0

We introduce the dimensionless variables

$$x = (v/c)E_0/(\tfrac{1}{2}\Gamma);\quad z = (E-E_0)/(\tfrac{1}{2}\Gamma) \text{ and } t = nf'\sigma_{res}$$

and the *fractional absorption* defined by

$$\varepsilon = \{I_0 - I(v)\}/I_0.$$

Then we have

$$\varepsilon(x,t) = 1-\pi^{-1}\int_{-\infty}^{+\infty}\{1+(z-x)^2\}^{-1}\exp\{-t/(1+z^2)\}\,dz. \quad (1)$$

We define the width W of the observed absorption line in the usual way and obtain

$$W = \Gamma w,$$

where w is the solution of the equation

$$\varepsilon(w,t) = \tfrac{1}{2}\varepsilon(0,t). \quad (2)$$

Graphical data for W as a function of t have been given by Margulies and Ehrman[2]) (up to $t = 10$) and later by Ruby and Hicks[3]) (up to $t = 8$). A widely quoted pair of formulas is due to Visscher

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+ Now at Physik-Department, Technische Hochschule, München, Germany, on leave from the State University of New York at Buffalo.

$$W = 2\Gamma(1.00+0.135t) \text{ for } 0 \leqq t \leqq 5, \quad (3a)$$

$$W = 2\Gamma(1.01+0.145t-0.0025t^2) \text{ for } 4 \leqq t \leqq 10. \quad (3b)$$

Visscher's formulas give the width of a Lorentzian that can be used[4]) to approximate the function $\varepsilon(x,t)$.

It is the purpose of this paper to present numerical values of W for a greater range of absorber thicknesses ($0 \leqq t \leqq 12$) and to fit all these values with a single polynomial in t.

2. Computations

We combine eqs. (1) and (2) and obtain

$$F(w) = \pi^{-1}\int_0^\infty [\{1+(z+w)^2\}^{-1}+ + \{1+(z-w)^2\}^{-1}-(1+z^2)^{-1}]\cdot \cdot\exp\{-t/(1+z^2)\}\,dz-\tfrac{1}{2}=0.$$

In order to prepare this equation for numerical integration, we approximate the integral from a to ∞,

$$F(w) \approx \pi^{-1}\int_0^a [\{1+(z+w)^2\}^{-1}+ + \{1+(z-w)^2\}^{-1}-(1+z^2)^{-1}]\cdot \cdot\exp\{-t/(1+z^2)\}\,dz+(\pi a)^{-1}-\tfrac{1}{2}=0, \quad (4)$$

where a is chosen so large as to render the error of approximation small enough.

We have used the Newton-Raphson method[5]) to solve eq. (4) for w with various values of t. The Newton-Raphson method requires an approximate value of the derivative $F'(w)$, which we have computed by means of the formula

$$F'(w) \approx 2\pi^{-1}\int_0^b \{(z-w)[1+(z-w)^2]^{-2}- -(z+w)[1+(z+w)^2]^{-2}\}\cdot \cdot\exp\{-t/(1+z^2)\}\,dz+4w/(\pi b^3).$$

The upper limits a and b in the integrals are chosen so large that w is obtained with the desired accuracy. The solution was carried out by means of a FORTRAN program on the CDC3600 computer. The resulting values of w are listed in table 2.

The next step was to fit a polynomial of fourth degree in t to the values of w in the range $0 \leqq t \leqq 12$. This was accomplished by repeated applications of the least-squares method. The need for repeating the fitting procedure several times arose from our intention to minimize the largest among the deviations (as expressed in percent), whereas the method of least-squares minimizes the sum of the squares of all the deviations. In the first attempt at fitting, all points were weighted equally. In subsequent fittings, we increased the weights of those points, where large deviations had occurred in the preceding fit. In this way the formula (with $t = nf'\sigma_{res}$):

$$W = 2\Gamma(1+0.1288t+4.733\times10^{-3}t^2- -9.21\times10^{-4}t^3+3.63\times10^{-5}t^4) \quad (5)$$

was obtained. The largest deviation occurs at $t = 10.5$ and amounts to 0.14%. For Visscher's formulas, the deviations are somewhat larger, with the largest, 0.48%, occurring at $t = 4.0$.

Table 2

Computed values of the dimensionless linewidth w for various values of absorber thickness. The last digit in w is uncertain by ±1 or less.

t	w	t	w
0.01	2.002 502	3.5	2.952 9
0.05	2.012 5	4.0	3.085 2
0.10	2.025 2	5.0	3.339 4
0.2	2.050 6	6.0	3.579 0
0.4	2.102 33	7.0	3.804 7
0.5	2.128 57	8.0	4.017 8
0.7	2.181 7	9.0	4.219 7
1.0	2.262 87	10.0	4.411 9
1.2	2.317 70	10.5	4.504 6
1.5	2.400 8	11.0	4.595 3
2.0	2.540 21	12.0	4.771 1
2.5	2.679 6	12.5	4.856 3
3.0	2.817 4	20.0	5.978 8

3. Discussion

It often happens that an absorber exhibits a width greater than the natural width Γ because nuclei in different locations within the absorber have slightly different environments. If the nuclear cross section is averaged over all the nuclei in the absorber and the result $\bar{\sigma}$ still depends on energy in a Lorentzian manner, this *environmental broadening* can be described by the factor κ in the equation

$$\bar{\sigma} = (\sigma_{res}/\kappa)[1+\{(E-E_0)/(\tfrac{1}{2}\kappa\Gamma)\}^2]^{-1}.$$

If the source is broadened in the same manner and by the same factor κ, as in the experiment[6]) of Kankeleit et al. on ^{169}Tm, then our formula (5) remains valid if t is replaced by t/κ and Γ by $\kappa\Gamma$ so that

$$W = 2\kappa\Gamma[1+0.1288(t/\kappa)+4.733\times10^{-3}(t/\kappa)^2- -9.21\times10^{-4}(t/\kappa)^3+3.63\times10^{-5}(t/\kappa)^4].$$

It is to be noted that the coefficient of the first-order

term is nearly equal to $\frac{1}{8}$, and that for small values of t the values of w in table 2 are rather accurately represented by

$$w = 2(1 + \tfrac{1}{8}t).$$

This suggests the possibility of expanding w in a Maclaurin series in t by analytic methods. This can indeed by done, to a limited extent, and will be described elsewhere[7]). We wish to point out here that formula (5) is considerably more accurate for $3 \leqq t \leqq 12$ than an analytic formula consisting of only the first five terms of the Maclaurin series. On the other hand, the analytic formula is much more accurate for small values of t. It is clear, however, that the accuracy of formula (5) is sufficient for the purposes of experimentalists.

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