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Application of the Scherer-Blume Theory to the Intermediate Ionization Regime†

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Abstract

Blume's formula for the time differential attenuation coefficients for the hyperfine perturbation of ions recoiling in gas is rewritten in a form convenient for numerical solution when the number of precession frequencies is large. Asymptotic expressions for the behaviour of the solutions for very short, and very long correlation time are given. Approximate condition for the existence of a minimum in the pressure dependence of the time differential coefficients, as well as the position and depth of such a minimum, are also derived, and compared with the results of calculations for various physical systems.

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1. Introduction

Measurements of the hyperfine perturbation experienced by excited nuclei recoiling into gas are used extensively for the determination of magnetic moments of short-lived nuclear levels. In several cases (e.g. when the hard-core attenuation coefficient is nearly equal to unity) the attenuation due to the static perturbation in vacuum is very small, while in a recoil-into-gas experiment it may be possible to obtain appreciable attenuations which can be readily observed.

Given the static perturbation, and within certain limiting assumptions, the attenuation coefficients for a certain correlation time τ_c are given by the Scherer-Blume theory.[1,2]

The actual calculation of the coefficients involves the solution of a polynomial equation whose degree is determined by the number of the hyperfine frequencies. In simple cases, such as hydrogen-like and helium-like ions, the number of frequencies is small and the solution of the equation does not pose any particular problem. In other physical circumstances, the observed attenuation has been shown [3-7] to be well accounted for by a model which considers statistical population of a large number of electronic configurations. The number of frequencies resulting from the model, which is sometimes referred to as the Intermediate Ionization Model, is large and the degree of the corresponding polynomial may be well over a hundred. The ordinary methods for solving polynomials are no longer useful in these cases.

In the following, we present equivalent forms of Blume's formula, which can be easily solved numerically, along with first approximations to the solutions which ensure rapid convergence to all the different roots over the whole range of correlation times. Results of such calculations for various physical systems are also presented.

A well-known feature of the solutions of Blume's formula is the minimum in the pressure dependence of the attenuation coefficients. Approximate expressions, concerning the position of the minimum, the value of the attenuation coefficient at that pressure and the values of the time at which such a minimum can be obtained are derived.

2. Results and Discussion

The attenuation coefficients for the angular distribution of gamma-rays emitted by excited nuclei recoiling into vacuum and experiencing static hyperfine perturbation is given by

$$G_k^o(t) = \sum_{i=-N}^{N} C_i e^{i\omega_i t} \qquad (1)$$

The frequencies ω_i are given by $\omega_i \equiv \omega_{FF'} = (E_F - E_{F'})/\hbar$, where E_F and $E_{F'}$ are the eigenvalues of the hyperfine interaction Hamiltonian

$$\omega_{-i} = -\omega_i \quad ; \quad \omega_o = 0.$$

The coefficients C_i are products of a geometrical term, depending on F,F', k and on the nuclear and electronic spins, and a statistical term, specifying the charge state distribution and the probability of occupying a certain configuration within this charge state.[3] They are real numbers, satisfying $C_{-i} = C_i$, and the normalization condition $\sum_i C_i = 1$. Considering a stochastic model for the perturbation in gas, Blume[2] obtained the following expression for the Laplace transform of the attenuation coefficient

$$\tilde{G}_k(\lambda,p) = \frac{\tilde{G}_k^o(\lambda+p)}{1-\lambda\tilde{G}_k^o(\lambda+p)} \tag{2}$$

where:

$\lambda = 1/\tau_c$ and τ_c is the correlation time, and

$$\tilde{G}_k^o(p) = \sum_i \frac{C_i}{p-i\omega_i} \tag{3}$$

is the **Laplace transform** of $G_k^o(t)$.

Using (3), eq. (2) can be written in the following form:

$$\tilde{G}_k(\lambda,p) = \frac{\sum_i C_i \prod_{j\neq i}(\lambda+p-i\,\omega_j)}{\prod_i(\lambda+p-i\omega_i) - \lambda\sum_i C_i \prod_{j\neq i}(\lambda+p-i\,\omega_j)} \tag{4}$$

As we shall see, the denominator of (4), which is a polynomial of degree 2N+1 in p, has only simple roots, and therefore the inverse transform of (4) is

$$G_k(\lambda,t) = \sum_{i=-N}^{N} A_i\; e^{\alpha_i t} \tag{5}$$

where α_i are the roots of the polynomial, and A_i are given by:

$$A_i = \frac{\lambda+\alpha_i-i\omega_i}{\lambda}\prod_{j\neq i}\left[\frac{\lambda+\alpha_i-i\,\omega_j}{\alpha_i-\alpha_j}\right] \quad \text{(the residue of (4) at } p=\alpha_i) \tag{6}$$

The problem reduces, therefore, to the solution of the equation

$$\prod_i(\lambda+\alpha-i\,\omega_i) - \lambda\sum_i C_i\prod_{j\neq i}(\lambda+\alpha-i\,\omega_j) = 0. \tag{7}$$

When the number of frequencies is large, we have to deal with a polynomial of high degree, and therefore it is inconvenient to solve the problem in its polynomial form. Equation (7) can, however, be rewritten as

$$\sum_{i=-N}^{N} \frac{\lambda C_i}{\lambda+\alpha-i\,\omega_i} = 1 \,, \tag{8}$$

and this equation (or trivial transformations of it), can be easily solved numerically.

Eq. (8) has 2N+1 roots, and we must find all of them. Therefore, we need good first approximations to the numerical solutions in order to ensure convergence for all the different roots. It is expedient in this context to study the properties of the solutions in the limiting cases $\lambda \to 0$ and $\lambda \to \infty$.

For $\lambda \to 0$ we obtain

$$\alpha_j = i\omega_j - (1-C_j)\lambda + iC_j \sum_{i\neq j} \frac{C_i}{\omega_i-\omega_j}\lambda^2 + [-C_j(\sum_{i\neq j}\frac{C_i}{\omega_i-\omega_j})^2 + C_j^2 \sum_{i\neq j}\frac{C_i}{(\omega_i-\omega_j)^2}]\lambda^3 + O(\lambda^4) \tag{9}$$

For the real solution α_o , eq. (9) reduces to:

$$\alpha_o = -(1-C_o)\lambda + C_o^2 \sum_{i\neq 0} \frac{C_i}{\omega_i^2}\ \lambda^3 + O(\lambda^5) \tag{10}$$

For $\lambda \to \infty$ the behaviour of the real solution is no longer similar to that of the complex solutions:

$$\alpha_o = -\frac{\sum C_i\omega_i^2}{\lambda} + 1/\lambda^3\ [\sum C_i\omega_i^4 - 2(\sum C_i\omega_i^2)^2] + O(1/\lambda^5) \tag{11}$$

The first term is the Abragam-Pound expression for the attenuation coefficient at high gas pressures.

The complex solutions have the form

$$\alpha_{j\neq o} = -\lambda + i\,\beta_j + \frac{\gamma_j}{\lambda} + O(1/\lambda^2) \tag{12}$$

where β_j are the solutions of

$$\sum_{i=-N}^{N} \frac{C_i}{\omega_i^2 - \beta^2} = 0 \quad , \tag{13}$$

and therefore satisfy $|\omega_{j-1}| < |\beta_j| < |\omega_j|$

and γ_j are given by

$$\gamma_j = [\sum_i \frac{C_i}{(\beta_j - \omega_i)^2}]^{-1} \tag{14}$$

The following relations, which turn out to be useful in obtaining approximate expression for A_o can be derived

$$\sum_i C_i \ \omega_i^2 = \sum_i (\omega_i^2 - \beta_i^2)/2 = \sum_i \gamma_i \tag{15}$$

Having obtained expressions for the frequencies α_i , we can now use (6) to calculate the coefficients A_i .

For A_o we have

$$A_o \underset{\lambda \to o}{=\!=} C_o(1+\lambda^2 \left\{ \sum_{i \neq 0} \frac{C_i}{\omega_i^2} [(2C_o - C_i/2 \ ) - \omega_i \sum_{j \neq i} \frac{C_j}{\omega_j - \omega_i}] \right\} + O(\lambda^3)) \tag{16}$$

and

$$A_o \underset{\lambda \to \infty}{=\!=} 1 + 1/\lambda^2 \left\{ \sum_i \gamma_i - \sum_i C_i \omega_i^2 + \sum_i (\omega_i^2 - \beta_i^2)/2 \right\} + O(1/\lambda^4)$$

which reduces, by (15) to

$$A_o \underset{\lambda \to \infty}{=\!=} 1 + \frac{\sum C_i \omega_i^2}{\lambda^2} + O(\frac{1}{\lambda^4}) \quad . \tag{17}$$

In the same manner we obtain

$A_j \underset{\lambda \to o}{\longrightarrow} C_j$; $A_j \underset{\lambda \to \infty}{\longrightarrow} 0$, and A_i also satisfy $\sum_i A_i = 1$ and $A_{-i} = A_i^*$.

We can now return to the problem of the numerical solution. In the intermediate ionization regime, the coefficients C_i are small numbers for all $i \neq 0$, usually of the order 1% or less. Therefore, in both limits we see from (9) and (12) that the real part of the complex solutions is very nearly equal to $-\lambda$. From (15) we see that $\frac{\omega_i^2 - \beta_i^2}{\omega_i^2}$ is of the order of C_i, and therefore we find again from (9) and (12) that the imaginary part of α_j is approximately ω_j

$$\alpha_{j\neq o} \approx -\lambda + i\omega_j \quad \text{for all} \quad \lambda . \tag{18}$$

With (18) as a first approximation, and rewriting (8) as

$$\sum_{i\neq j} \lambda C_i \frac{\lambda+\alpha-i\omega_j}{\lambda+\alpha-i\omega_i} + \lambda (C_j-1) - \alpha + i\omega_j = 0 ,$$

one obtains rapid convergence with the Newton-Raphson method. For small λ, the real solution α_o can also be found in this method, however, when λ becomes larger, it is better to write (8) as

$$\sum_i C_i \frac{\alpha(\lambda+\alpha) + \omega_i^2}{(\lambda+\alpha)^2 + \omega_i^2} = 0, \quad \text{and use} \quad \alpha_o = -\frac{\sum C_i \omega_i^2}{\lambda}$$ as a first approximation.

Some typical results are presented in Figs. 1-2. We consider two gamma transitions in nuclei recoiling into gas with velocity $v/c = 0.011$ which is appropriate for the intermediate ionization regime. Fig. 1 represents attenuation coefficients of the decay of the 6.13 MeV 3^- state of ^{16}O while Fig. 2 represents those of the 197 keV $5/2^+ \rightarrow 1/2^+$ transition in ^{19}F. The various G_k are given in each case for t=30 ps, 60 ps, 150 ps in the whole range of λ.

The different pressure dependence at the same value of t for the two levels is due mainly to differences in the values of the hyperfine frequencies. Indeed, it can be seen from (5) and (7) that any change in the frequency scale (e.g. by changing the value of the g factor), should be followed by a change in both λ and $1/t$ by the same factor if we are to leave the form of the attenuation curve $G_k(\lambda, t)$ invariant.

The dominant feature of these curves is the minimum, which becomes shallower if either t or the value of the hyperfine fields becomes smaller. In order to understand this behaviour, and to have estimates of the position and depth of the minimum, we use again the approximate relation (18) to solve the equation $\frac{\partial G_k}{\partial \lambda} = 0$.

$$\frac{\partial G_k}{\partial \lambda} = \sum \frac{\partial A_i}{\partial \lambda} e^{\alpha_i t} + t \sum A_i \frac{\partial \alpha_i}{\partial \lambda} e^{\alpha_i t} . \qquad (19)$$

From (18) $\frac{\partial \alpha_i}{\partial \lambda} \approx -1$ for all $i \neq 0$.

Thus we can write:

$$\frac{1}{t} \frac{\partial A_o}{\partial \lambda} + A_o \frac{\partial \alpha_o}{\partial \lambda} \approx \sum_{i \neq o} (A_i - \frac{1}{t} \frac{\partial A_i}{\partial \lambda}) e^{(\alpha_i - \alpha_o)t} \approx e^{-(\lambda+\alpha_o)t} \sum_{i \neq o} (A_i - \frac{1}{t} \frac{\partial A_i}{\partial \lambda}) e^{i\omega_i t} . \qquad (20)$$

For large enough t, the different precession angles $\omega_i t$ get out of phase, and the right-hand side of (20), which is even further reduced by the damping exponential, can be neglected. The approximation is expected to hold for $\bar{\omega} t > \pi$, where $\bar{\omega}$ is an average frequency, to be defined in the following.

Eq. (20) can be written now as

$$\frac{\partial \alpha_o}{\partial \lambda} = - \frac{1}{t} \frac{\partial (\ln A_o)}{\partial \lambda} \qquad (21)$$

We note that as $t \to \infty$, the position of the minimum becomes independent of time and is determined by the condition

$$\left. \frac{\partial \alpha_o}{\partial \lambda} \right/_{\lambda_{min}} = 0 \qquad (22)$$

Taking the leading terms in (10) and (11) we have:

$$\alpha_o \underset{\lambda \to o}{\approx} -(1 - C_o)\lambda \qquad ; \qquad \alpha_o \underset{\lambda \to \infty}{\approx} - \frac{\sum C_i \omega_i^2}{\lambda}$$

We may connect the two limiting expressions by writing

$$\alpha_o = -\frac{(1 - C_o)\lambda}{1+\lambda^2/\bar{\omega}^2} \tag{23}$$

with
$$\bar{\omega}^2 = \frac{\sum C_i\omega_i^2}{1-C_o} = \frac{\sum_{i\neq o} C_i\omega_i^2}{\sum_{i\neq o} C_i} . \tag{24}$$

Eq. (23) has the correct asymptotic behaviour at both limits, and it has been verified numerically that it provides a good approximation for α_o, also for intermediate values of λ.

The solution of (22) is therefore:

$$\lambda_{min} = \bar{\omega} \quad , \qquad \text{or} \qquad \bar{\omega}\tau_{c\ min} = 1. \tag{25}$$

As t decreases, λ_{min} decreases too, the minimum becomes shallower until it disappears completely.

The condition for the existence of a minimum is $\bar{\omega}t > \pi$, which has been mentioned above as the criterion for the validity of (21). Under these conditions $G_k(\lambda_{min},t) \approx A_o e^{\alpha_o t}$, and to a good approximation $A_o \approx 1$, so from (23) and (25) we have

$$G_k(\lambda_{min},t) \approx e^{-\frac{1-C_o}{2}\bar{\omega}t} . \tag{26}$$

We may compare these results with the calculated curves of Figs. 1 and 2. In Fig. 1 we see that the 60 ps curve of G_6 exhibits a minimum, which disappears in the corresponding curves for G_2 and G_4, since the condition $\bar{\omega}t > \pi$ is no longer satisfied. There are large differences in the depth of the minima for different k. This behaviour can be understood as follows. It can be shown(8) that $\sum_{i=-N}^{N} C_i\omega_i^2 \propto k(k+1)$. Therefore, the k dependence of the exponent of eq. (26) is given by $(1-C_o)\bar{\omega} \propto \sqrt{(1-C_o)k(k+1)}$ and the last expression increases with k since $(1-C_o)$ also increases with k.

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Figure Captions

Fig. 1. Attenuation coefficients $G_k(\lambda,t)$ calculated for the 6.13 MeV $3^- \rightarrow 0^+$ decay in ^{16}O, with $\lambda = 1/\tau_c$. The mean frequencies $\bar{\omega}$ are given for every k. The three curves for each k correspond to t = 30 ps (broken line) t = 60 ps (dotted line) and t = 150 ps (solid line).

Fig. 2. Attenuation coefficients $G_k(\lambda,t)$ calculated for the 197 keV $5/2^+ \rightarrow 1/2^+$ decay in ^{19}F, with $\lambda = 1/\tau_c$. The mean frequencies $\bar{\omega}$ are given for every k. The three curves for each k correspond to t = 30 ps (broken line) t = 60 ps (dotted line) and t = 150 ps (solid line).

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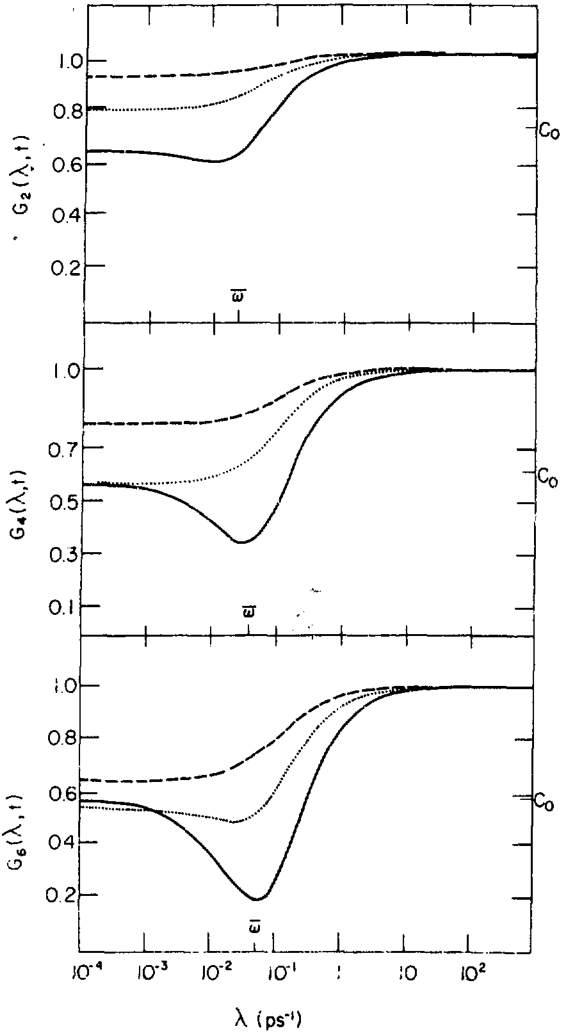
1.0
0.8
0.6
0.4
0.2
$G_2(\lambda, t)$
$\bar{\omega}$
C_0
1.0
0.7
0.5
0.3
0.1
$G_4(\lambda, t)$
$\bar{\omega}$
C_0
1.0
0.8
0.6
0.4
0.2
$G_6(\lambda, t)$
$\bar{\omega}$
C_0
10^{-4}
10^{-3}
10^{-2}
10^{-1}
1
10
10^{2}
λ (ps^{-1})

Figure 1

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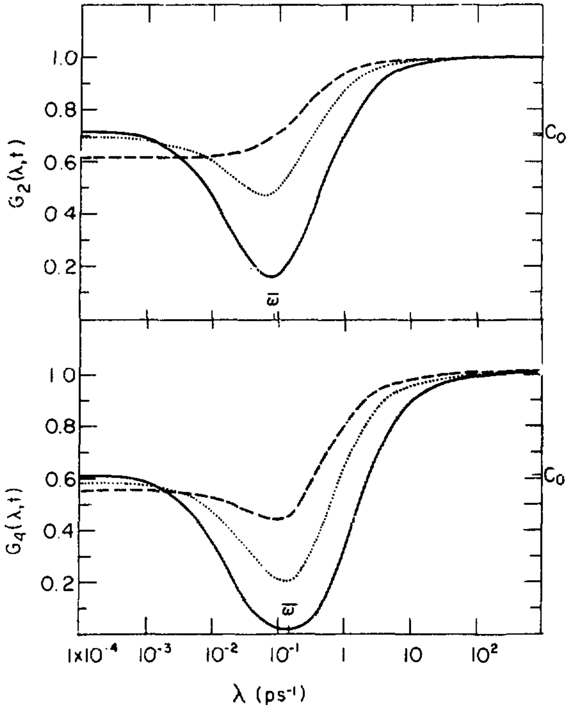

1.0
0.8
0.6
0.4
0.2
$G_2(\lambda,t)$
C_0
$\bar{\omega}$
1.0
0.8
0.6
0.4
0.2
$G_4(\lambda,t)$
C_0
$\bar{\omega}$
1×10^{-4} 10^{-3} 10^{-2} 10^{-1} 1 10 10^2
λ (ps^{-1})

Figure 2