SOME NEW RESULTS IN MÖSSBAUER RELAXATION THEORY
F. Hartmann-Boutron

To cite this version:
F. Hartmann-Boutron. SOME NEW RESULTS IN MÖSSBAUER RELAXATION THEORY. Journal de Physique Colloques, 1980, 41 (C1), pp.C1-223-C1-224. 10.1051/jphyscol:1980171. jpa-00219740

HAL Id: jpa-00219740
https://hal.archives-ouvertes.fr/jpa-00219740
Submitted on 1 Jan 1980

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
SOME NEW RESULTS IN MOSSBAUER RELAXATION THEORY

F. Hartmann-Boutron

Laboratoire de Spectrométrie Physique, B.P. 53 X, 38041 GRENOBLE-CEDEX (France).

Abstract.- We discuss the validity of the perturbation treatments and we derive some expressions for the Mössbauer lineshape both without and with the noise approximation.

VALIDITY RANGE AND COMPARISON OF VARIOUS TREATMENTS

The problem of relaxation effects in Mössbauer spectra has given rise to several approaches based on a) stochastic models b) the relaxation equation for the density matrix c) the resolvent method following Fano. All three approaches use Liouville formalism and lead to relaxation supermatrices which enter the Mössbauer lineshape. Methods b) and c) have been compared in great detail in Ref 11: we summarize here the conclusions of this study.

Both b) and c) are perturbation methods. It can be shown that if the "white noise approximation" (WNA) is valid they can describe the whole range of relaxation effects in the Mössbauer spectra (small, intermediate or large compared with the distance between lines). On the contrary if the WNA is not valid, they are only valid for small relaxation effects (and then one can apply the "secular approximation"). This last result solves the ambiguities met in p. 301 of [2] (nota), in p. 307 of [2] (top of first column) and in p. 2117 of [2] (the spurious third order terms always cancel out when the theory applies).

Method b) leads to relaxation supermatrices and when it is valid it can be shown that the matrix elements of and which control the broadening of a given Mössbauer line become identical at the top of that line, i.e., line profiles obtained with both methods are very similar, although c) is slightly better.

EXPRESSIONS FOR THE MOSSBAUER LINESHAPE WHEN THE WNA IS NOT VALID

I/ Lineshape in the isotropic case. In Ref. [1] we used the tensor operator method in order to compute the Mössbauer lineshape for an ion with a hyperfine coupling in the excited state and in the ground state. When its electronic spin is submitted to a coupling with a random field whose fluctuations are isotropic and are characterized by a correlation function:

\[ I(\omega) = \langle \psi | \hat{H}_B^{2} | \psi \rangle \int_{0}^{\infty} dt e^{i\omega t} \langle H_{2}(t) H_{2}(t) > \tag{1} \]

(this is a high temperature calculation : \( k_B T \gg A, A_g \)).

Here we will not give the general formulas obtained in [1] but only their application to the Mössbauer lineshape of \( \text{Yb}^{170} \) in the electronic doublet state \( \Gamma_B \) or \( \Gamma_g \) of cubic symmetry (effective electronic spin \( S = 1/2 \)). \( \text{Yb}^{170} \) has an excited nuclear state \( \Gamma = 2 \), whence two hyperfine states \( F=5/2 \) with \( E_F = A \) and \( F=3/2 \) with \( E_F = -3/2 \) \( A \), and a ground state \( \Gamma = 0 \) with no h.f.s. Let us define:

\[ X = I(\omega+3/2 \ h \ + 1 \ \Gamma/2) \quad \text{and} \quad Y = I(\omega-A/M + 1 \ \Gamma/2) \]

(where \( I(\omega) \) is defined above: Eq (1)). The Mössbauer lineshape of \( \text{Yb}^{170} \) is found to be (\( p=5/2-i\omega \)):

\[ I(\omega) = \frac{X + \omega Y}{\omega^2 + \omega + 1} \]

I/ Lineshape in the anisotropic case.
A formula equivalent to this one has been derived by Afanasev et al.\footnote{AFANASEV A.M. et al Sov. Phys. JETP 47 (1978) 585. Phys. Rev. Lett. 40 (1978) 816.} When the WNA is valid, Eq\(2\) reduces to Eq\(3\) of \cite{BRADFORD583} with \(X+Y-1/15\).

2/ Lineshape of \((\text{Yb}^{170})_{3+}\) in uniaxial symmetry. Assume that state \(I=2\) has a hyperfine structure:

\[
\mathcal{H}_0 = A/I^2 S_z^2 + a(I^2-2) \text{ with } S = 1/2, \text{ and that } \frac{\partial}{\partial t} S \text{ is submitted to a fluctuating field } \mathcal{H} = g_i / \mu_B H_z(t) \\
\times S_z + \mu_B H_z(t) S_z, \text{ i being the eigenvalue of } \text{... (Eq VI, 42) of 121 with } k = L1.
\]

We want to compute \(\delta\).

(\text{ewla}~e^{-(1/2m/2+a(m^2-2)2)} - (W_\mu)^2.
\]

When the WNA is valid, \(W_\mu = W_{\mu L}\) and this expression reduces to Eq\(79\) of 161.

WNA VALID : ANALOG FOR THE M.E. OF ABRAGAM-POUND COEFFICIENTS FOR PERTURBED ANGULAR CORRELATIONS

When relaxation is very fast the spectrum reduces to a single broadened line \(\mathcal{J}(\omega) = \text{Re}[1/(\pm i \omega + \Gamma / 2 + \delta)]\).

We want to compute \(\delta\).

\(1/\text{Paramagnetic case.}\) Assume a Mössbauer transition with multipolarity \(L\) and a fluctuating Hamiltonian \(A I^2 S_z(t)\) or \(A I^2 \pm \Delta S(t)\) with correlation time \(\tau_{1S}\) (electronic relaxation time). Tensor operator methods lead to:

\[
\delta = \frac{S(I+1)}{3h^2} \tau_{1S} \left\{ A^2 I(I+1)^2 - \frac{A^2}{2} I^2(I+1)(I+1) - \frac{A^2}{2} I(I+1) - L(L+1) \right\} \text{ (4)}
\]

As a check, when \(I = 3/2, I = 1/2\) and \(L = 1\) (\text{Fe}) we recover the Bradford Marshall result \(\delta\) for b/R of \(1/3\).

\[
\delta = \frac{S(I+1)}{3h^2} \tau_{1S} \left\{ A^2 I(I+1)^2 + \frac{A^2}{2} I^2(I+1)(I+1) - \frac{A^2}{2} I(I+1) - L(L+1) \right\} \text{ (5)}
\]

On the other hand, when \(A = A_g, I = I_g\) we recover the PAC result for the damping coefficient of the multipole of order \(L\) (Eq\(79\) of 2\) with \(k = L\).