Contents

1 Intoduction

The routines of the file gpg_22nuclear.f90 is the core of all nuclear scattering programms. The quantum-mechanical solution of the general case of multipol transitions is taken from the article M. Blume and O.C. Kistner [3] who follow the concept of the index of refraction for thin media. The classical solution for a dipole transition already shows all characteristics and can be found in any text book of electrodynamics: Theorie of dispersion and absorption of weakly absorbing media.

2 Classical index of refraction

The complex index of refraction of oszillators (electrons) in the limit of infinitely thin medium (the external electric field is the same at all ozillator sites)

$$n^2(\omega) \;=\; 1 + 4\pi\, N \frac{e^2/m}{\omega_0^2 - \omega^2 - i\gamma\omega} \tag{1}$$

with the charge e, mass m, eigen frequency ω_0 and the damping factor $\gamma = \gamma_\gamma + \gamma_\alpha$, the sum of radiation damping and internal friction. γ_α will be identified with the decay channel of internal conversion.
The classical total cross section of an oszillator is given by

$$\begin{aligned} \sigma &= \frac{6\pi\, c^2 \gamma_\gamma \gamma}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \\ \gamma_\gamma &= \frac{2}{3} \cdot \frac{e^2\omega^2}{mc^3} \end{aligned} \tag{2}$$

γ_γ is the damping by radiation of the oszillator. $n^2 \approxeq 1$ differs from 1 only close to resonanz, ω close to ω_0. With the total cross section at resonance ($k_0 \cdot c = \omega_0$)

$$\sigma_0 \;=\; \frac{6\pi\gamma_\gamma}{\gamma k_0^2} \tag{3}$$

the index of refraction can be written as

$$n(\omega) \;=\; 1 - \frac{1}{2k_0}\sigma_0\, N \frac{\gamma/2}{\omega - \omega_0 + i\gamma/2} \tag{4}$$

Since $n^2 \approxeq 1$ the first term of the expansion series of the square root is sufficient and $\omega + \omega_0$ is replaced by $2\omega_0$. In order to model real media an oszillator strength f is intoduced which modifies σ_0 to $f\sigma_0$. For nuclear scattering the cross section is lowered by the Lamb-Mossbauer (Debye-Waller) factor f.

Eq. 4 shall be generalized to different types i of oszillators and polarizabilities different for electric fields in x,y directions (propagation in z-direction). Then the oscillator strength becomes a 2x2 matrix r_i.

$$n(\omega) \;=\; \underline{1} - \frac{1}{2k_0} f\sigma_0 \sum_i N_i r_i \frac{\gamma/2}{\omega - \omega_{0i} + i\gamma/2} \tag{5}$$

Now $n(\omega)$ is a complex 2x2 matrix and $\underline{1}$ the unit matrix.

The electric field vector $\mathbf{E}$ of the plane wave propagating in z-direction develops as

$$\mathbf{E}(\mathbf{z}) \;=\; e^{inkz}\mathbf{E_0} \tag{6}$$

The intensity I(z)=$\mathbf{E}\ \mathbf{E}^\dagger$

$$\begin{aligned} I(z) \;&=\; \sum_j \mathbf{E}_j \mathbf{E}_j^\dagger \qquad (7)\\ &=\; \sum_j \sum_\alpha (e^{inkz})_{j\alpha}\mathbf{E_0}_\alpha \cdot \sum_\beta \mathbf{E}^*_{\mathbf{0}\beta}(e^{-in^\dagger kz})_{\beta j} \\ &=\; \sum_{j\alpha,\beta} (e^{inkz})_{j\alpha}\rho_{\alpha,\beta}(e^{-in^\dagger kz})_{\beta j} \end{aligned}$$

The density matrix $\rho_{\alpha,\beta}(z) = \mathbf{E_0}_\alpha \mathbf{E}^*_{\mathbf{0}\beta}$ at z=0 depends on z

$$\rho(\omega, z) = e^{i\mathbf{n}kz}\rho e^{-i\mathbf{n}^\dagger kz} \tag{8}$$

and the intensity at z is the trace of $\rho(z)$

$$I(z) = Tr(e^{i\mathbf{n}kz}\rho e^{-i\mathbf{n}^\dagger kz}) \tag{9}$$

The index of refraction is readily translated to the case of nuclear scattering

$$\mathbf{n} = \underline{1} - \frac{\sigma f(\mathbf{k})}{2k}\sum_j N_j \sum_i r_i^j \cdot \frac{\Gamma/2}{E - E_i^j - i\Gamma/2} \tag{10}$$

The total intensity, sum over all Lorentzians, is normalized to 1. Γ is the natural linewidth. Since the Lorentz function is real and the density matrix R_i of a transition is hermitian, the diagonal elements of $\rho_r(E)$ are real numbers. f depends on the direction of propagation $\mathbf{k}$.

3 Index of refraction for multipole transitions

Following the article of M. Blume and O.C. Kistner [3] the index of refraction (M. Lax [1]) is the first equation

$$\mathbf{n} = \underline{1} + \frac{2\pi}{k^2}NF \tag{11}$$

The solution for the forward scattering matrix F_{pq} of eq. 19 is rewritten by the tensor quantities (introduced in [2])

$$V_{LM}^{\alpha\beta} = \left(\frac{2L+1}{2I_e+1}\right)^{\frac{1}{2}} \sum_{m_e m_g} (e_\alpha^{m_e})^* g_\beta^{m_g} C(I_g\, L\, I_e, m_g M m_e) \tag{12}$$

where $C(I_g\, L\, I_e, m_g M m_e)$ are the Clebsch-Gordan coefficients, $|I_g g_\beta\rangle = \sum_{m_g}|I_g m_g\rangle$ the ground states and $|I_e e_\alpha\rangle = \sum_{m_e}|I_e m_e\rangle$ the excited states of the nuclear spin-Hamiltonian.
The rotation to another coordinate system (Wigner rotation matrix) can be omitted because the hyperfine fields entering the spin-Hamiltonian are already rotated such that the z-axis is always the γ-direction.
With the amplitudes x_p

$$\begin{aligned} x_p^{\alpha\beta}(mag.\ L-pol) &= V_{Lp}^{\alpha\beta}M_L - pV_{L+1p}^{\alpha\beta}E_{L+1} \\ x_p^{\alpha\beta}(elect.\ L-pol) &= -pV_{Lp}^{\alpha\beta}E_L + V_{L+1p}^{\alpha\beta}M_{L+1} \end{aligned} \tag{13}$$

the forward scattering matrix F of eq. 19 in [3] reads

$$F_{pq}^{\alpha\beta} = -2\pi f(\mathbf{k})\frac{2I_e+1}{2I_g+1}\,\frac{x_p^{\alpha\beta}x_q^{\alpha\beta *}}{E-(E_\alpha-E_\beta)+i\Gamma/2} \tag{14}$$

M_L and E_L are reduced matrix elements

$$\begin{aligned} M_L &= \langle I_e||\frac{1}{c}\sum_i j(r_i)A_L(m)||I_g\rangle \\ E_L &= \langle I_e||\frac{1}{c}\sum_i j(r_i)A_L(e)||I_g\rangle \end{aligned} \tag{15}$$

The partial width for γ-emission of the excited nuclear state $\langle I_e|$ is expressed by the reduced matrix elements (see Appendix in [3])

$$\begin{aligned} \Gamma_\gamma(mag.L-pol) &= 8\pi k(|M_L|^2+|E_{L+1}|^2) \\ \Gamma_\gamma(elect.L-pol) &= 8\pi k(|E_L|^2+|M_{L+1}|^2) \end{aligned} \tag{16}$$

The phase ϵ of the ratios $E_{L+1}/M_L = \delta_m\, e^{i\epsilon}$ and $M_{L+1}/E_L = \delta_e\, e^{i\epsilon}$ should be either 0 or π ([4]) by time-reversal invariance (the topic of [3]), so that δ is real.
Redefining the amplitudes to a_p

$$\begin{aligned} a_p^{\alpha\beta}(mag.\ L-pol) &= V_{Lp}^{\alpha\beta} - pV_{L+1p}^{\alpha\beta}\delta_m \\ a_p^{\alpha\beta}(elect.\ L-pol) &= -pV_{Lp}^{\alpha\beta} + V_{L+1p}^{\alpha\beta}\delta_e \end{aligned} \tag{17}$$

and inserting the cross section at resonance (Γ is the total width factoring in internal conversion)

$$\begin{aligned} \sigma_0 &= \frac{2\pi}{k^2}\,\frac{2I_e+1}{2I_g+1}\,\frac{\Gamma_\gamma}{\Gamma} \\ \frac{1}{1+\delta_m^2} &= |M_L|^2/(|M_L|^2+|E_{L+1}|^2)^{\frac{1}{2}} \\ \frac{1}{1+\delta_e^2} &= |E_L|^2/(|E_L|^2+|M_{L+1}|^2)^{\frac{1}{2}} \end{aligned} \tag{18}$$

the forward scattering matrix F of eq. 19 in [3] now reads

$$F_{pq}^{\alpha\beta} = -\frac{k}{4\pi}f(\mathbf{k})\sigma_0\frac{1}{1+\delta^2}\,a_p^{\alpha\beta}a_q^{\alpha\beta *}\,\frac{\Gamma/2}{E-(E_\alpha-E_\beta)+i\Gamma/2} \tag{19}$$

where δ without index stands for both type of transitions.

The index of refraction n_{pq} for one type of site of the absorber finally is written as

$$n_{pq} = \delta_{pq} - \frac{f(\mathbf{k})\sigma_0}{k} N \sum_{\alpha\beta} \frac{1}{2} r_{pq}^{\alpha\beta} \frac{\Gamma/2}{E - (E_\alpha - E_\beta) + i\Gamma/2} \quad (20)$$

The matrix $r_{pq}^{\alpha\beta} = a_p^{\alpha\beta} a_q^{\alpha\beta *}/(1+\delta^2)$ which shall be called absorber matrix has the property

$$\sum_{\alpha\beta} r_{pq}^{\alpha\beta} = \delta_{pq} \quad (21)$$

4 Miscellaneous

4.1 Effective thickness

The product $\sigma_0 N f$ is called effective thickness of the absorber. The parameter for effective thickness of the Mossbauer routine is named mg/cm2*f. It measures the effective thickness in units of mg of the Mossbauer isotope per cm^2. In case of ^{57}Fe $1mg/cm^2$ of natural iron gives

$$\begin{aligned} Fe\_uthick\_w &= \sigma_0 \cdot N_{Avogadro}/G_{atomicweight} \cdot abundance \quad (22) \\ &= 2.56\,10^{-18} cm^2 \cdot 6.022\,10^{23}/55.85g \cdot 0.0214 \\ &= 0.5907 \cdot (mg/cm^2)^{-1} \end{aligned}$$

The fitted number for the parameter mg/cm2*f is multiplied by $0.5907 \cdot (mg/cm^2)^{-1}$ giving an dimensionless number t, called the effective thickness. The Lamb-Mossbauer factor f is obtained from the fitted parameter mg/cm2*f devided by the amount mg/cm^2 of natural iron contained in the absorber.

4.2 Powder average

The following property of the tensor V_{Lm} is used when calculating intensities of powder samples in the case of an isotropic Lamb-Mossbauer factor. The absorber matrices r_{pq} are elements of the tensor products

$$\begin{aligned} I_{MM'}^{L,\alpha\beta} &= V_{LM}^{\alpha\beta} V_{LM'}^{\alpha\beta *} \quad (23) \\ J_{MM'}^{L,\alpha\beta} &= V_{LM}^{\alpha\beta} V_{L+1M'}^{\alpha\beta *} \end{aligned}$$

The I^L are called intensity matrix. The powder average of an intensity matrix is diagonal for all transitions α, β

$$Tr(I^{L,\alpha\beta})\delta_{pq} \;=\; (2L+1)\frac{1}{\Omega}\int_\Omega d\Omega D^L_{pM}(\Omega) I^{L,\alpha\beta}_{MM'} D^L_{M'q}(\Omega) \qquad (24)$$

The average of the J^L-matrix is zero.

References

[1] Lax M, Rev. Mod. Phys. **23**, 287 (1951).

[2] H. Spiering, In *Mössbauer Spectroscopy Applied to Inorganic Chemistry*, Edited by G.J. (Editor) Long, volume 1, p. 79–169. Plenum (New York), 1984.

[3] M. Blume and O.C. Kistner, Phys. Rev. **171**, 417 (1968).

[4] Lioyd S P, Phys. Rev. **81**, 161 (1951).