Contents

1 Intoduction

The routines of the file gpg_22nuclear.f90 is the core of all nuclear scattering programs. The quantum-mechanical solution of the general case of multipol transitions is taken from the article M. Blume and O.C. Kistner [1] 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.

These outlines shall help to understand the structure of the two subroutines th_hdeq() and the more detailed th_hdeqf() including an anistropic Lamb-Mossbauer factor and texture.
Further the input/fit parameters mg/cm2xf (effective thickness) and the Poincaré vector used for the programs of synchrotron scattering are described.

2 Classical index of refraction

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

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

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

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

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

$$\begin{aligned} I(z) &= \sum_j \mathbf{E}_j \mathbf{E}_j^\dagger \\ &= \sum_j \sum_\alpha (e^{inkz})_{j\alpha} \mathbf{E_{0\alpha}} \cdot \sum_\beta \mathbf{E}^*_{\mathbf{0}\beta} (e^{-in^\dagger kz})_{\beta j} \\ &= |\mathbf{E_0}|^2 \sum_{j\alpha,\beta} (e^{inkz})_{j\alpha} \rho_{\alpha,\beta} (e^{-in^\dagger kz})_{\beta j} \end{aligned} \tag{7}$$

with the density matrix $\rho_{\alpha,\beta} = \mathbf{E_{0\alpha}} \mathbf{E^*_{0\beta}} / |\mathbf{E_0}|^2$. The sum is written as the trace of a density matrix dependent on z

$$\begin{aligned} \rho(\omega, z) &= e^{i\mathbf{n}kz} \rho e^{-i\mathbf{n}^\dagger kz} \\ I(z) &= |\mathbf{E_0}|^2 Tr(e^{i\mathbf{n}kz} \rho e^{-i\mathbf{n}^\dagger kz}) \end{aligned} \tag{8}$$

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

$$\mathbf{n} = \underline{1} - \frac{\sigma f(\mathbf{k})}{2k} \sum_j N_j \sum_i r_i^j \cdot \frac{\Gamma/2}{E - E_i^j - i\Gamma/2} \tag{9}$$

f depends on the direction of propagation **k**. Γ is the natural linewidth. The first sum collects N_j scatteres of type j and the second sum runs over alltransitions of site j. r_i^j are the density matrices of the transitions i with transition energies E_i^j.

3 Index of refraction for multipole transitions

Following the article of M. Blume and O.C. Kistner [1] the index of refraction (M. Lax [2]) is the first equation

$$\mathbf{n} = \underline{1} + \frac{2\pi}{k^2} NF \tag{10}$$

The solution for the forward scattering matrix F_{pq} of Eq. 19 in [1] the index of refraction (M. Lax [2]) is the first equation is rewritten by the tensor quantities (introduced in [3])

$$V_{LM}^{\alpha\beta} = \left(\frac{2L+1}{2I_e+1} \right)^{\frac{1}{2}} \sum_{m_e m_g} (e_\alpha^{m_e})^* g_\beta^{m_g} C(I_g\, L\, I_e, m_g M m_e) \tag{11}$$

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) in Eq. 19 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

$$\begin{aligned} x_p^{\alpha\beta}(mag.\ L-pol) &= V_{Lp}^{\alpha\beta} M_L - p V_{L+1p}^{\alpha\beta} E_{L+1} \\ x_p^{\alpha\beta}(elect.\ L-pol) &= -p V_{Lp}^{\alpha\beta} E_L + V_{L+1p}^{\alpha\beta} M_{L+1} \end{aligned} \tag{12}$$

the forward scattering matrix F of Eq. 19 in [1] reads

$$F_{pq}^{\alpha\beta} = -2\pi f(\mathbf{k})\frac{2I_e+1}{2I_g+1}\,\frac{x_p^{\alpha\beta}x_q^{\alpha\beta *}}{E-(E_\alpha-E_\beta)+i\Gamma/2} \tag{13}$$

M_L and E_L are reduced matrix elements

$$\begin{aligned} M_L &= \langle I_e||\frac{1}{c}\sum_i j(r_i)A_L(m)||I_g\rangle \\ E_L &= \langle I_e||\frac{1}{c}\sum_i j(r_i)A_L(e)||I_g\rangle \end{aligned} \tag{14}$$

The partial width for γ-emission of the excited nuclear state $\langle I_e|$ is expressed by the reduced matrix elements (see Appendix in [1])

$$\begin{aligned} \Gamma_\gamma(mag.L-pol) &= 8\pi k(|M_L|^2+|E_{L+1}|^2) \\ \Gamma_\gamma(elect.L-pol) &= 8\pi k(|E_L|^2+|M_{L+1}|^2) \end{aligned} \tag{15}$$

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 [1]), so that δ is real.
Redefining the amplitudes to a_p

$$\begin{aligned} a_p^{\alpha\beta}(mag.\ L-pol) &= V_{Lp}^{\alpha\beta} - pV_{L+1p}^{\alpha\beta}\delta_m \\ a_p^{\alpha\beta}(elect.\ L-pol) &= -pV_{Lp}^{\alpha\beta} + V_{L+1p}^{\alpha\beta}\delta_e \end{aligned} \tag{16}$$

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

$$\begin{aligned} \sigma_0 &= \frac{2\pi}{k^2}\,\frac{2I_e+1}{2I_g+1}\,\frac{\Gamma_\gamma}{\Gamma} \\ \frac{1}{1+\delta_m^2} &= |M_L|^2/(|M_L|^2+|E_{L+1}|^2)^{\frac{1}{2}} \\ \frac{1}{1+\delta_e^2} &= |E_L|^2/(|E_L|^2+|M_{L+1}|^2)^{\frac{1}{2}} \end{aligned} \tag{17}$$

the forward scattering matrix F of Eq. 19 in [1] now reads

$$F_{pq}^{\alpha\beta} = -\frac{k}{4\pi}f(\mathbf{k})\sigma_0\frac{1}{1+\delta^2}\,a_p^{\alpha\beta}a_q^{\alpha\beta *}\,\frac{\Gamma/2}{E-(E_\alpha-E_\beta)+i\Gamma/2} \tag{18}$$

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

$$n_{pq} = \delta_{pq} - \frac{f(\mathbf{k})\sigma_0}{k}N\sum_{\alpha\beta}\frac{1}{2}r_{pq}^{\alpha\beta}\,\frac{\Gamma/2}{E-(E_\alpha-E_\beta)+i\Gamma/2} \tag{19}$$

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

$$\sum_{\alpha\beta} r_{pq}^{\alpha\beta} = \delta_{pq} \tag{20}$$

4 The density matrix of photons

According the Eq. 8 the calculation of the intensity or even the polarization of the beam traveling throug an absober of thickness z the density matrix ρ of the incoming beam has to be known. For a single line Mossbauer source ρ is 1/2 of the 2x2 unit matrix. In case of a split source $\rho(E)$ depends on energy and its polarization degree varies with E. The synchrotran beam has a linear polarization in the horizontal plane which will be the x-direction $\mathbf{e}_x$ in a coordinate system with $\mathbf{e}_z$ parallel the γ-direction and $\mathbf{e}_y$ pointing upwards.

ρ depends on the basis, which should be the same as used for the forward scattering matrix F_{pq}. Two spherical bases are in use. In the textbook of Rose [5] (Elementary Theory of Angular Momentum) the vector potential of the elektromagnetic field $\mathbf{A} = \mathbf{u}_p exp(i\mathbf{k}\cdot\mathbf{r})$ uses the definition

$$\begin{aligned} \boldsymbol{\xi}_1 &= -\frac{1}{\sqrt{2}}(\mathbf{e}_x + i\mathbf{e}_y) \\ \boldsymbol{\xi}_0 &= \mathbf{e}_z \\ \boldsymbol{\xi}_{-1} &= \frac{1}{\sqrt{2}}(\mathbf{e}_x - i\mathbf{e}_y) \\ \mathbf{u}_p &= -p\boldsymbol{\xi}_p \end{aligned} \tag{21}$$

The textbook of Brink and Satchler [6] (Angular Momentum) use the basis $\boldsymbol{\xi}_p$ itself instead of -p$\boldsymbol{\xi}_p$. Their choice does not exclude from the beginning fields which have also longitudinal components (p=0). The forward scattering matrix F_{pq} of section 3 uses the basis $\mathbf{u}_p$. The E_p components expressed by the carthesian components of electric vector $\mathbf{E} = E_x\mathbf{e}_x + E_y\mathbf{e}_y$ (orthonormal to $\mathbf{e}_z$) reads

$$\begin{aligned} E_p &= \mathbf{E}^* \cdot \mathbf{u}_p \\ &= \frac{1}{\sqrt{2}}(E_x + ipE_y) \end{aligned} \tag{22}$$

such that $\sum_p E_p^* \mathbf{u}_p = \mathbf{E}$. In optics $\mathbf{u}_1$ defines a left circular and $\mathbf{u}_{-1}$ a right circular polarization. The density matrices $\rho_{\alpha\beta} = E_\alpha E_\beta^*/E^2$

$$\rho = \begin{pmatrix} E_1E_1^* & E_1E_{-1}^* \\ E_{-1}E_1^* & E_{-1}E_{-1}^* \end{pmatrix} / E^2 \tag{23}$$

are in case of left ($E_1 \neq 0, E_{-1} = 0$), and right ($E_1 = 0, E_{-1} \neq 0$) circular polarisation

$$\rho(left) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \rho(right) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Inserting $E_p = \frac{1}{\sqrt{2}}E_x$ or $E_p = \frac{1}{\sqrt{2}}ipE_y$ the ρ matrices for an electric field in x/y-direction are obtained:

$$\rho(E_x) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}/2 \qquad \rho(E_y) = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}/2 \tag{24}$$

The linear polarisation with $E_x = Ecos\varphi$ and $E_y = Esin\varphi$ gives the density matrix ($E_p = \frac{E}{\sqrt{2}}e^{ip\varphi}$)

$$\rho(E_\varphi) = \begin{pmatrix} 1 & e^{i2\varphi} \\ e^{-i2\varphi} & 1 \end{pmatrix}/2 \tag{25}$$

Starting with the basis $\boldsymbol{\xi}$= -p $\mathbf{u}$ Eq. 22 reads

$$\begin{aligned} E_p &= \mathbf{E}^* \cdot \boldsymbol{\xi}_p \\ &= \frac{-p}{\sqrt{2}}(E_x + ipE_y) \end{aligned} \tag{26}$$

and the linear polarization in direction φ is calculated from $E_p = -p\frac{E}{\sqrt{2}}e^{ip\varphi}$:

$$\rho(E_\varphi) = \begin{pmatrix} 1 & -e^{i2\varphi} \\ -e^{-i2\varphi} & 1 \end{pmatrix}/2 \tag{27}$$

The offdiagonal elements get opposite signs. The transition amplitudes of Eq. 16 according to Brink and Satchler [6] are

$$\begin{aligned} a_p^{\alpha\beta}(mag.\ L-pol) &= -pV_{Lp}^{\alpha\beta} + V_{L+1p}^{\alpha\beta}\delta_m \\ &= -pa_p^{\alpha\beta}(mag.\ L-pol, Rose) \end{aligned} \tag{28}$$

and give absorber matrices which also have opposite signs of the offdiagonal elements. So the results at the end are independent of the bases.

Where come this basis change from? In the contribution of Karl Blum "Density Matrix Theory and Applications" in - Springer Series on Atomic, Optical, and Plasma Physics 64 (2012) - is stated: "Note that in the terminology of classical optics the opposite convention is usually adopted: Light of positive (negative) helicity is called left-handed (right-handed) circularly polarized. We will always use the helicity state notation in order to avoid this ambiguity".
The ± 1 indices of the basis components of $\boldsymbol{\xi}$ are conform with the helicity $\lambda = \pm 1$.

5 Poincaré vector

The Poincaré vector components are used to describe the density matrix ρ of the synchrotron beam. The Poincaré representation decomposes ρ

$$\rho = \frac{1}{2}(\mathbf{1}_2 + \mathbf{P} \cdot \boldsymbol{\sigma}) \tag{29}$$

$\mathbf{1}_2$ is the 2x2 unit matrix and $\boldsymbol{\sigma}$ represents the three Pauli matrices.

$$\sigma_\xi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_\eta = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_\zeta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{30}$$

The routines of the file gpg_22nuclear.f90 follow the article of Blume and Kistner [1] with the $\mathbf{u}_p$-basis with the density matrix of Eq. 25

$$\rho(E_\varphi) = \begin{pmatrix} 1 & e^{i2\varphi} \\ e^{-i2\varphi} & 1 \end{pmatrix} /2 \tag{31}$$

The Poincaré vector components for linear polarization become

$$P_\xi = cos\, 2\varphi, \qquad P_\eta = sin\, 2\varphi, \qquad P_\zeta = 0 \tag{32}$$

The synchrotran beam with its linear polarization in the horizontal plane choosen as the x-direction $\mathbf{e}_x$ in a coordinate system with $\mathbf{e}_z$ parallel the γ-direction and $\mathbf{e}_y$ pointing upwards has the Poincaré vector $\mathbf{P} = (1, 0, 0)$.

6 Miscellaneous

6.1 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

$$\begin{aligned} Fe\_uthick\_w &= \sigma_0 \cdot N_{Avogadro}/G_{atomicweight} \cdot abundance \\ &= 2.56\,10^{-18} cm^2 \cdot 6.022\,10^{23}/55.85g \cdot 0.0214 \\ &= 0.5907 \cdot (mg/cm^2)^{-1} \end{aligned} \tag{33}$$

The fitted number for the parameter mg/cm2*f is multiplied by $0.5907 \cdot (mg/cm^2)^{-1}$ giving a 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.

6.2 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

$$\begin{aligned} I^{L,\alpha\beta}_{MM'} &= V^{\alpha\beta}_{LM} V^{\alpha\beta *}_{LM'} \\ J^{L,\alpha\beta}_{MM'} &= V^{\alpha\beta}_{LM} V^{\alpha\beta *}_{L+1M'} \end{aligned} \tag{34}$$

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

$$Tr(I^{L,\alpha\beta})\delta_{pq} \quad = \quad (2L+1)\frac{1}{\Omega}\int_{\Omega} d\Omega D^L_{pM}(\Omega) I^{L,\alpha\beta}_{MM'} D^L_{M'q}(\Omega) \tag{35}$$

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

References

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