# TRANSPORT OF PHOTONS INCLUDING POLARIZATION EFFECTS

- adds polarization effects to the scalair theory

## PHYSICAL MODEL

- infinite thickness target
- collimated beams of incidence and take-off
- monochromatic excitation
- polarized or non-polarized source

## APPLICATION

- Synchrotoon radiation X-Ray spectrometry
- appropriate description of photon transport from polarized and non-polarized sources
- multiple scattering computations offer the possibility of spectrum build-up giving the state of polarization of the emitted x-rays.

POLARIZATION STATE → WAVE NATURE OF PHOTONS

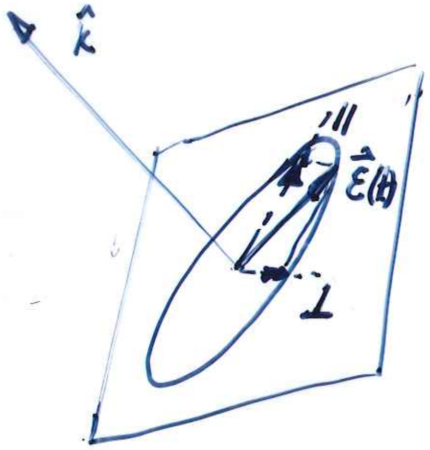
## FACTS

- Photons obey polarization dependent interactions.
- The models describing photon transport usually ignore polarization or treat it in incomplete way

## QUESTIONS

- Are different the intensities predicted with a vector model and with a scalar model?
- Which is the extent of the difference?
- How it depends on the polarization of the source?
- How it depends on the type and the number of collisions involved?

# REPRESENTATION OF POLARIZED LIGHT



components of the electric vector

$$\begin{cases} \mathcal{E}_{\parallel}(t) = \mathcal{E}^0_{\parallel} \sin(\omega t - \delta_{\parallel}) \\ \mathcal{E}_{\perp}(t) = \mathcal{E}^0_{\perp} \sin(\omega t - \delta_{\perp}) \end{cases}$$

$\omega$ the frequency

Since the intensity is proportional to the square of the electric field, then we can choose

$$\boxed{I = (\mathcal{E}^0_{\parallel})^2 + (\mathcal{E}^0_{\perp})^2 = I_{\parallel} + I_{\perp}}$$

$$I \propto \mathcal{E}^2(t)$$

By averaging in one period we get

$$\int_0^T dt\, I \propto \int_0^T dt \left[\mathcal{E}^2_{\parallel}(t) + \mathcal{E}^2_{\perp}(t)\right]$$

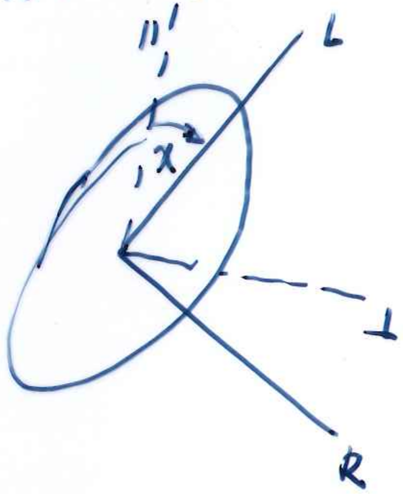
By eliminating the time variable in the above equations we obtain

$$\boxed{\left(\frac{\mathcal{E}_{\parallel}(t)}{\mathcal{E}^0_{\parallel}}\right)^2 - 2\cos(\delta_{\parallel} - \delta_{\perp}) \frac{\mathcal{E}_{\parallel}(t)\,\mathcal{E}_{\perp}(t)}{\mathcal{E}^0_{\parallel}\,\mathcal{E}^0_{\perp}} + \left(\frac{\mathcal{E}_{\perp}(t)}{\mathcal{E}^0_{\perp}}\right)^2 = \sin^2(\delta_{\parallel} - \delta_{\perp})}$$

(equation of an ellipse)

In general, the axes of this ellipse do not coincide with those ∥ and ⊥. This is expressed by the cross term, which is different from zero. This is expressed by the cross term, which is different from zero.

To find the axes of the ellipse we should perform a rotation $\chi$



$$\mathcal{E}_{\parallel} = \mathcal{E}_L \cos\chi - \mathcal{E}_R \sin\chi$$
$$\mathcal{E}_{\perp} = \mathcal{E}_L \sin\chi + \mathcal{E}_R \cos\chi$$

By replacing into the cross product term we get

$$\left[\frac{1}{\mathcal{E}_{\perp}^{o\,2}} - \frac{1}{\mathcal{E}_{\parallel}^{o\,2}}\right] \sin 2\chi - 2\,\frac{\cos(\delta_{\parallel}-\delta_{\perp})}{\mathcal{E}_{\parallel}^{o}\,\mathcal{E}_{\perp}^{o}} \cos 2\chi = 0$$

from which

$$\boxed{tg\, 2\chi = \frac{2\,\mathcal{E}_{\perp}^{o}\,\mathcal{E}_{\parallel}^{o}\cos(\delta_{\parallel}-\delta_{\perp})}{(\mathcal{E}_{\parallel}^{o})^2 - (\mathcal{E}_{\perp}^{o})^2}}$$

The other quantity of interest is the ellipticity, i.e. the ratio of the axes of the ellipse

From the substitution in the ellipse equation, we get

$$tg^2\rho = \frac{\dfrac{\cos^2\chi}{(\mathcal{E}_{\parallel}^{o})^2} - \dfrac{\sin 2\chi}{\mathcal{E}_{\parallel}^{o}\,\mathcal{E}_{\perp}^{o}}\cos(\mathcal{E}_{\parallel}-\mathcal{E}_{\perp}) + \dfrac{\sin^2\chi}{(\mathcal{E}_{\perp}^{o})^2}}{\dfrac{\sin^2\chi}{(\mathcal{E}_{\parallel}^{o})^2} + \dfrac{\sin 2\chi}{\mathcal{E}_{\parallel}^{o}\,\mathcal{E}_{\perp}^{o}}\cos(\mathcal{E}_{\parallel}-\mathcal{E}_{\perp}) + \dfrac{\cos^2\chi}{(\mathcal{E}_{\perp}^{o})^2}}$$

and after some algebra

$$\boxed{\sin 2\beta = \pm \frac{2\,\varepsilon^0_{\parallel}\,\varepsilon^0_{\perp}\sin(\delta_{\parallel}-\delta_{\perp})}{(\varepsilon^0_{\parallel})^2+(\varepsilon^0_{\perp})^2}}$$

The Stokes parameters are defined as

$$I = (\varepsilon^0_{\parallel})^2+(\varepsilon^0_{\perp})^2 = I_{\parallel}+I_{\perp}$$

$$Q = (\varepsilon^0_{\parallel}) - (\varepsilon^0_{\perp})^2 = I_{\parallel}-I_{\perp}$$

$$U = 2\,\varepsilon^0_{\parallel}\,\varepsilon^0_{\perp}\cos(\delta_{\parallel}-\delta_{\perp})$$

$$V = 2\,\varepsilon^0_{\parallel}\,\varepsilon^0_{\perp}\sin(\delta_{\parallel}-\delta_{\perp})$$

From the above equations

$$\cos 2\beta = \pm\frac{\left\{\left[(\varepsilon^0_{\parallel})^2-(\varepsilon^0_{\perp})^2\right]^2+4\,\varepsilon^{0\,2}_{\parallel}\varepsilon^{0\,2}_{\perp}\cos^2(\delta_{\parallel}-\delta_{\perp})\right\}^{1/2}}{(\varepsilon^0_{\parallel})^2+(\varepsilon^0_{\perp})^2}$$

$$\sin 2\chi = \pm\frac{2\,\varepsilon^0_{\parallel}\,\varepsilon^0_{\perp}\cos(\delta_{\parallel}-\delta_{\perp})}{\left\{\left[(\varepsilon^0_{\parallel})^2-(\varepsilon^0_{\perp})^2\right]^2+4\,\varepsilon^{0\,2}_{\parallel}\varepsilon^{0\,2}_{\perp}\cos^2(\delta_{\parallel}-\delta_{\perp})\right\}^{1/2}}$$

$$\cos 2\chi = \pm\frac{(\varepsilon^0_{\parallel})^2-(\varepsilon^0_{\perp})^2}{\left\{\left[(\varepsilon^0_{\parallel})^2-(\varepsilon^0_{\perp})^2\right]^2+4\,\varepsilon^{0\,2}_{\parallel}\varepsilon^{0\,2}_{\perp}\cos(\delta_{\parallel}-\delta_{\perp})\right\}^{1/2}}$$

by replacing above, the Stokes parameters become

$$\boxed{\begin{aligned} Q &= I\cos 2\beta\cos 2\chi \\ U &= I\cos 2\beta\sin 2\chi \\ V &= I\sin 2\beta \end{aligned}}$$

# REPRESENTATION OF POLARIZED RADIATION (SUMMARY)

four parameters {
STOKES parameters: $(I, Q, U, V)$ "(S) system"

Scattering parameters: $(I_{\parallel}, I_{\perp}, U, V)$ "$\parallel(\perp)$ system"

$$\boxed{\begin{aligned} I &= I_{\parallel} + I_{\perp} \\ Q &= I_{\parallel} - I_{\perp} \end{aligned}}$$

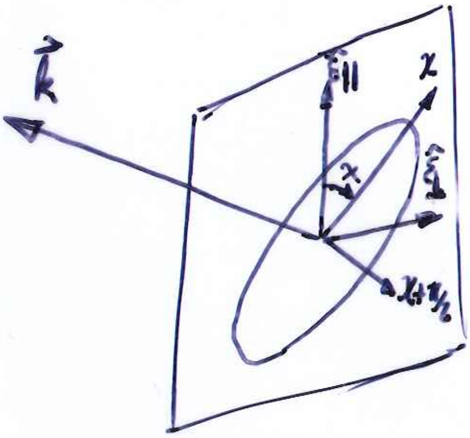
to specify {
the intensity
the degree of polarization
the orientation of the ellipse of polarization
the ellipticity

$$I = (E_{\parallel}^{0})^2 + (E_{\perp}^{0})^2$$

$$Q = (E_{\parallel}^{0})^2 - (E_{\perp}^{0})^2$$

$$U = 2\, E_{\parallel}^{0} E_{\perp}^{0} \cos(\delta_{\parallel} - \delta_{\perp})$$

$$V = 2\, E_{\parallel}^{0} E_{\perp}^{0} \sin(\delta_{\parallel} - \delta_{\perp})$$



$$Q = I \cos 2\beta \cos 2\chi$$

$$U = I \cos 2\beta \sin 2\chi$$

$$V = I \sin 2\beta$$

$I$ represents the whole intensity

$\chi$ gives the rotation of the ellipse major axis about the coordinate system $\hat{\varepsilon}_{\parallel}, \hat{\varepsilon}_{\perp}$

$\beta$ gives the ellipticity (major/minor axis ratio)

## FULL ELLIPTICAL POLARIZATION

$$\sin 2\beta = \frac{I_V}{I_I}$$

$$tg\, 2\chi = \frac{I_U}{I_Q}$$

and

$$I_I^2 = I_Q^2 + I_u^2 + I_V^2$$

## PARTIAL ELLIPTICAL POLARIZATION

$$I_I^2 \geq I_Q^2 + I_u^2 + I_V^2$$

## UNPOLARIZED BEAM

$$I_Q = I_U = I_V = 0$$

## GENERAL BEAM

$$\sin 2\beta = \frac{I_V}{(I_Q^2 + I_u^2 + I_V^2)^{1/2}}$$

$$tg\, 2\chi = \frac{I_U}{I_Q}$$

$$P = \frac{(I_Q^2 + I_u^2 + I_V^2)^{1/2}}{I_I}$$

$$\begin{pmatrix} I_I \\ I_Q \\ I_U \\ I_V \end{pmatrix} = I_I (1-P) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + I_I P \begin{pmatrix} 1 \\ \cos 2\chi \cos 2\beta \\ \sin 2\chi \cos 2\beta \\ \sin 2\beta \end{pmatrix}$$

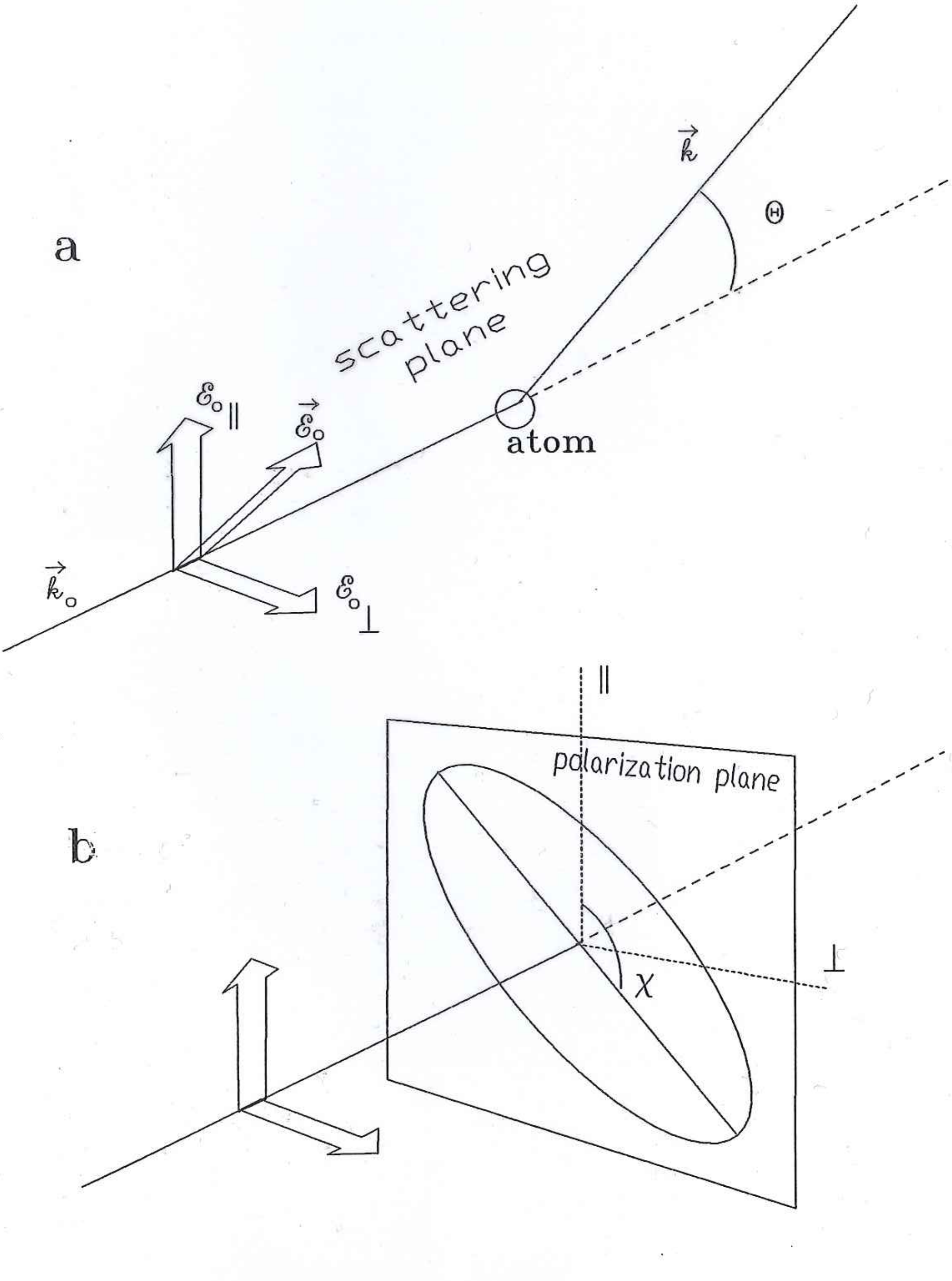

a
$\vec{k}$
$\Theta$
scattering plane
$\mathcal{E}_o \parallel$
$\vec{\mathcal{E}}_o$
atom
$\vec{k}_o$
$\mathcal{E}_o \perp$
b
$\parallel$
polarization plane
$\chi$
$\perp$

TABLE I.

Some characteristic states of polarization are shown using the set of parameters S, normalized to an unitary total intensity. $\chi$ denotes the orientation of the line of polarization with respect to the intersection of the polarization plane with the scattering plane.

| Polarization state | Set S (I,Q,U.V) |
|---|---|
| Unpolarized | (1,0,0,0) |
| Linear (generic) | $(1, \cos 2\chi, \sin 2\chi, 0)$ |
| Linear (∥) (parallel) | (1,1,0,0) |
| Linear (⊥) (perpendicular) | (1,-1,0,0) |
| Linear ($45^\circ$) | (1,0,1,0) |
| Circular | (1,0,0,1) |

# BOLTZMANN TRANSPORT EQUATION FOR POLARIZED PHOTONS

(Chandrasekhar)

$$\vec{\omega}\cdot\nabla\vec{f}(\vec{r},\vec{\omega},\lambda) = -\mu(\vec{r},\lambda)\,\vec{f}(\vec{r},\vec{\omega},\lambda)$$

$$+\int_0^\infty d\lambda'\int_{4\pi} d\vec{\omega}'\,\mathbb{H}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\,\vec{f}(\vec{r},\vec{\omega}',\lambda')$$

$$+\vec{S}(\vec{r},\vec{\omega},\lambda)$$

where

$$\vec{f} = \begin{pmatrix} f_I \\ f_Q \\ f_U \\ f_V \end{pmatrix} \qquad \vec{S} = \begin{pmatrix} S_I \\ S_Q \\ S_U \\ S_V \end{pmatrix}$$

$$\mathbb{H}(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \mathbb{L}(\pi-\psi)\,\underbrace{\mathbb{K}(\omega,\lambda,\vec{\omega}';\lambda')}_{\text{scattering matrix}}\,\mathbb{L}(-\psi')$$

$$\cos\psi = \frac{\eta'\sqrt{1-\eta^2} - \eta\sqrt{1-\eta'^2}\cos(\varphi-\varphi')}{\left[1-(\vec{\omega}'\cdot\vec{\omega})^2\right]^{1/2}}$$

$$\cos\psi' = \frac{\eta\sqrt{1-\eta'^2} - \eta'\sqrt{1-\eta^2}\cos(\varphi-\varphi')}{\left[1-(\vec{\omega}'\cdot\vec{\omega})^2\right]^{1/2}}$$

$$\mathbb{L}(\varphi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\varphi & \sin 2\varphi & 0 \\ 0 & -\sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Fig 2
ernández/Hubbell/Hanson/Spencer

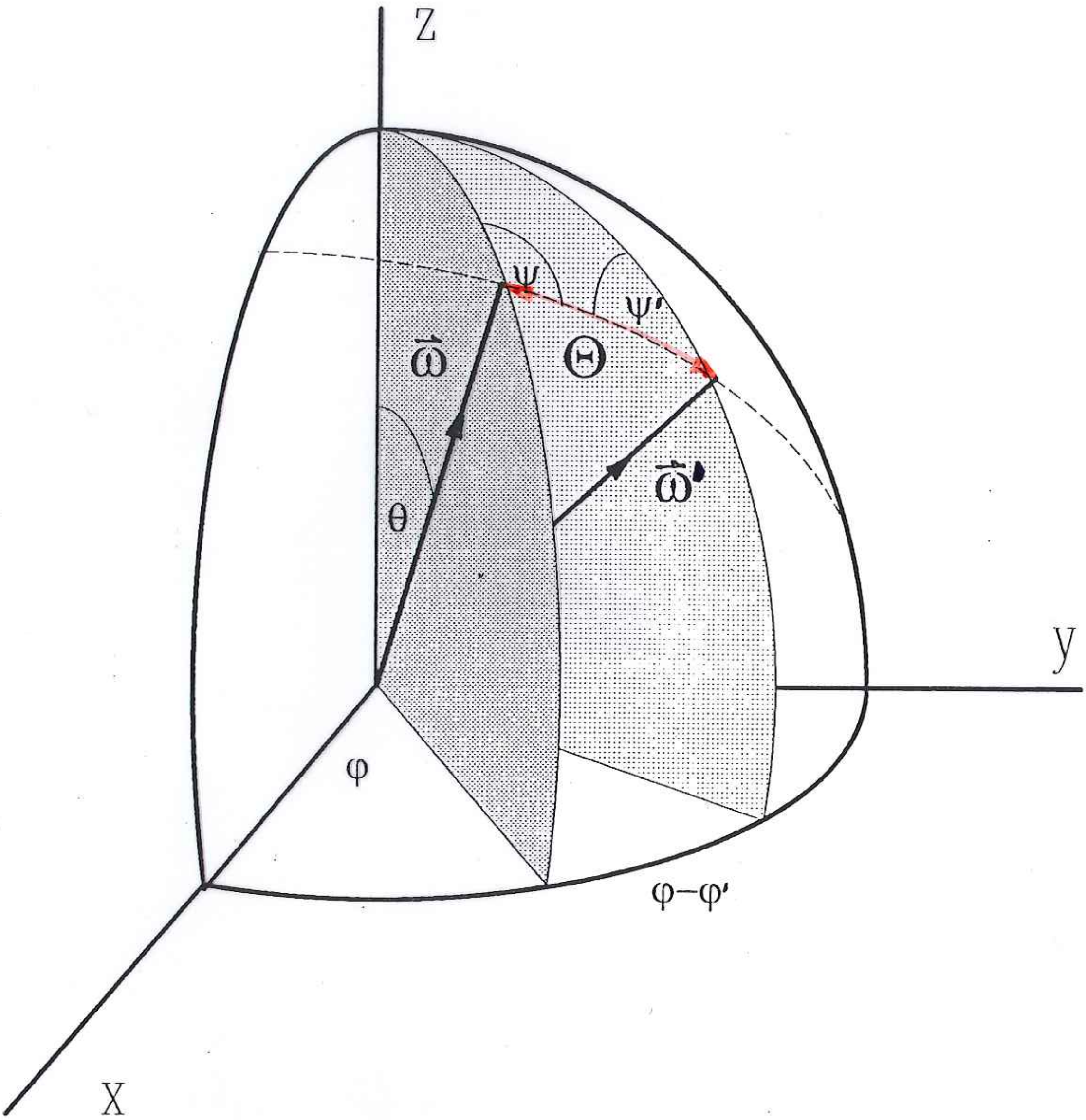


Figure 2. Transformation between the plane of scattering and the meridian plane.

WE CAN WRITE THE BOLTZMANN EQUATION FOR THE SINGLE COMPONENTS :

$$\vec{\omega}\cdot\nabla f_i(\vec{r},\vec{\omega},\lambda) = -\mu(\vec{r},\lambda) f_i(\vec{r},\vec{\omega},\lambda)$$

$$+ \int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}' \sum_j H_{ij}(\vec{\omega},\lambda,\vec{\omega}';\lambda') f_j(\vec{r},\vec{\omega}';\lambda')$$

$$+ S_i(\vec{r},\vec{\omega},\lambda) \qquad \text{for } i,j = I, Q, U, V$$

H introduces coupling between the components of $\vec{f}$ if it is non-diagonal

WE SOLVE, AS USUALLY, IN ORDERS-OF-INTERACTION USING THE DEVELOPMENT

K DENOTES NUMBER OF COLLISION

$$f_i(\vec{r},\vec{\omega},\lambda) = \sum_{K=0}^{\infty} f_i^{(K)}(\vec{r},\vec{\omega},\lambda) \qquad (i = I, Q, U, V)$$

# VECTOR TRANSPORT EQUATION

$$\eta \frac{\partial}{\partial z} \vec{f}^{(S)}(z,\vec{\omega},\lambda) = -\mu(\lambda)\,\vec{f}^{(S)}(z,\vec{\omega},\lambda) +$$

$$+\ \mathcal{U}(z)\int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}'\ \mathbb{H}^{(S)}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\,\vec{f}^{(S)}(z,\vec{\omega}';\lambda')$$

$$+\ \underbrace{\delta(z)}_{\text{(plane source at } z=0\text{)}}\ \vec{S}(\vec{\omega},\lambda)$$

IS A LINEAR EQUATI

where
$$\mathbb{H}^{(S)}(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \mathbb{L}^{(S)}(\pi-\psi)\ \underbrace{\mathbb{K}^{(S)}(\vec{\omega},\lambda,\vec{\omega}';\lambda')}_{\text{INTERACTION KERNEL}}\ \mathbb{L}^{(S)}(-\psi')$$

and

$$\cos\psi = \frac{\eta'\sqrt{1-\eta^2} - \eta\sqrt{1-\eta'^2}\cos(\phi-\phi')}{[1-(\vec{\omega}'\cdot\vec{\omega})^2]^{1/2}}$$

$$\cos\psi' = \frac{\eta\sqrt{1-\eta'^2} - \eta'\sqrt{1-\eta^2}\cos(\phi-\phi')}{[1-(\vec{\omega}'\cdot\vec{\omega})^2]^{1/2}}$$

$$\mathbb{L}^{(S)}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\phi & \sin 2\phi & 0 \\ 0 & -\sin 2\phi & \cos 2\phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$f^{(S)} = \begin{pmatrix} f_I \\ f_Q \\ f_U \\ f_V \end{pmatrix}$$

THE VECTOR EQUATION REPRESENTS AN EQUATION SYSTEM:

$$\eta \frac{\partial}{\partial z} f_i^{(S)}(z, \vec{w}, \lambda) = -\mu(\lambda) f_i^{(S)}(z, \vec{w}, \lambda) +$$

$$+ \mathcal{U}(z) \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}' \sum_j \underbrace{H_{ij}^{(S)}(\vec{w}, \lambda, \vec{w}'; \lambda') f_j^{(S)}(z, \vec{w}'; \lambda')}_{\text{coupled terms}}$$

$$+ \delta(z)\, S_i(\vec{w}, \lambda)$$

$$(i, j = I, Q, U, V)$$

Let us write the equation for the $I$ component of the flux:

$$\eta \frac{\partial}{\partial z} f_I(z, \vec{w}, \lambda) = -\mu(\lambda) f_I(z, \vec{w}, \lambda) +$$

$$+ \mathcal{U}(z) \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}' \left\{ K_{11} f_I(z, \vec{w}'; \lambda') + K_{12} \left[ f_Q(z, \vec{w}, \lambda) \cos 2\psi' - f_U(z, \vec{w}, \lambda) \sin 2\psi' \right] \right\}$$

$$+ \delta(z)\, S_I(\vec{w}, \lambda)$$

where $K_{11} = k(\vec{w}, \lambda, \vec{w}'; \lambda')$

and $K_{12} = k(\vec{w}, \lambda, \vec{w}'; \lambda')\, a_{12}(\vec{w}, \lambda, \vec{w}'; \lambda')$

assuming that:

$$\mathbb{K} = \begin{pmatrix} K_{11} & K_{12} & 0 & 0 \\ K_{21} & K_{22} & 0 & 0 \\ 0 & 0 & K_{33} & 0 \\ 0 & 0 & 0 & K_{44} \end{pmatrix} = k(\vec{w}, \lambda, \vec{w}'; \lambda') \begin{pmatrix} 1 & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & 0 \\ 0 & 0 & 0 & a_{44} \end{pmatrix}$$

MULTIPLE SCATTERING SOLUTION:

$$f_i^{(0)}(z, \vec{w}, \lambda) = \frac{1}{2|\eta|} S_i(\vec{w}, \lambda)\, e^{-\frac{\mu|z|}{|\eta|}} (1 + \operatorname{sgn}\eta \operatorname{sgn} z)$$

$$f_i^{(n)}(z, \vec{w}, \lambda) = \frac{1}{2|\eta|} \int_0^\infty d\tau\, e^{-\frac{|z-\tau|\mu}{|\eta|}} (1 + \operatorname{sgn}\eta \operatorname{sgn}(z-\tau))$$

$$\int_0^\infty d\lambda' \int_{4\pi} d\vec{w}' \sum_j H_{ij}(\vec{w}, \lambda, \vec{w}'; \lambda')\, f_j^{(n-1)}(\tau, \vec{w}'; \lambda')$$

$$(i,j = I, Q, U, V)$$

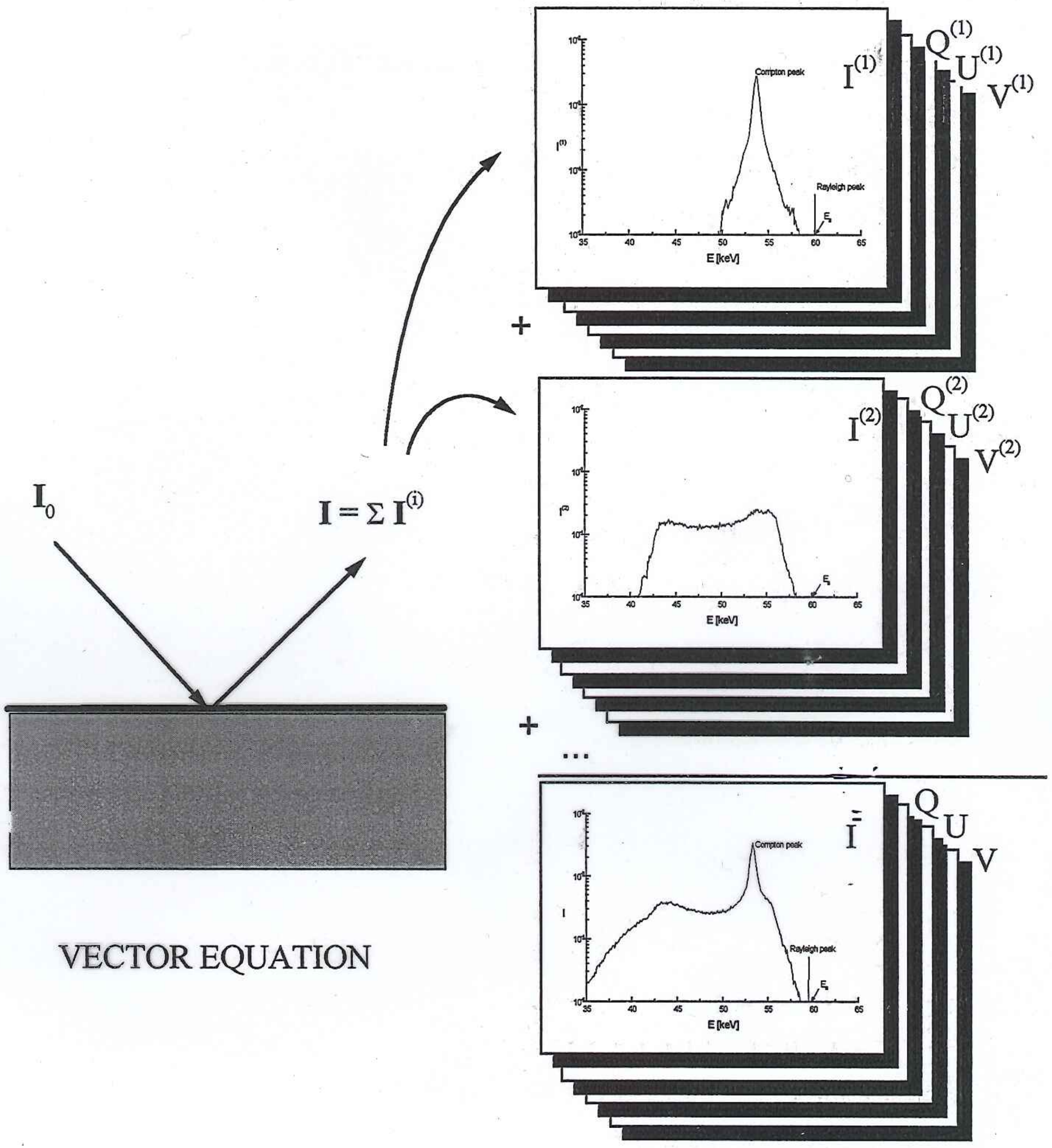
the solution for the n-th flux can be splitted according to the sign of $(z-\tau)$, i.e.

$$f_i^{(n)}(z, \vec{w}, \lambda) = \frac{1}{|\eta|} \Bigg\{ \left(\frac{1+\operatorname{sgn}\eta}{2}\right) e^{-\frac{\mu z}{|\eta|}} \int_0^z d\tau\, e^{\frac{\mu\tau}{|\eta|}} \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}' \sum_j H_{ij}(\vec{w}, \lambda, \vec{w}; \lambda')\, f_j^{(n-1)}(\tau, \vec{w}'; \lambda')$$

$$+ \left(\frac{1-\operatorname{sgn}\eta}{2}\right) \int_0^\infty d\tau\, e^{-\frac{\mu\tau}{|\eta|}} \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}' \sum_j H_{ij}(\vec{w}, \lambda, \vec{w}; \lambda')\, f_j^{(n-1)}(\tau + z, \vec{w}; \lambda') \Bigg\}$$

The intensity is given, as usually, by

$$I_i^{(n)}(\vec{w}, \lambda) = |\eta| \underbrace{f_i^{(n)}(0, \vec{w}, \lambda)}_{\text{albedo flux}}$$



VECTOR EQUATION

# FIRST TWO ORDERS OF THE INTENSITY

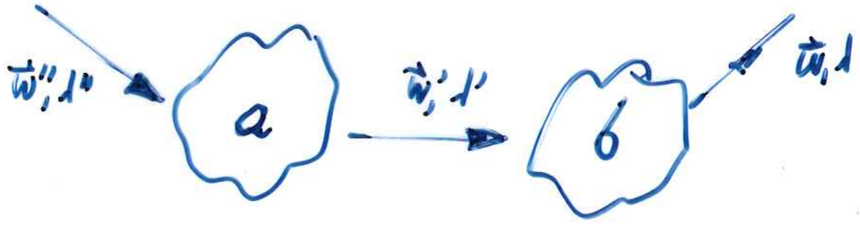
$$I^{(1)}_{(a)i}(\vec{\omega},\lambda) = \left(\frac{1-\operatorname{sgn}\zeta}{2}\right)\int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}' \left(\frac{1+\operatorname{sgn}\zeta'}{2}\right)\frac{1}{|\zeta'|}\;\frac{1}{\frac{\mu}{|\zeta|}+\frac{\mu'}{|\zeta'|}}$$

$$\sum_j H_{(a)ij}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\, S_j(\vec{\omega}';\lambda')$$

$$I^{(2)}_{(a,b)i}(\vec{\omega},\lambda) = \left(\frac{1-\operatorname{sgn}\zeta}{2}\right)\int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}'\,\frac{1}{|\zeta'|}$$

$$\sum_j\sum_k\Bigg\{\left(\frac{1+\operatorname{sgn}\zeta'}{2}\right)\int_0^\infty d\lambda''\int_{4\pi} d\vec{\omega}''\left(\frac{1+\operatorname{sgn}\zeta''}{2}\right)\frac{H^{b}_{ij}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\,H^{a}_{jk}(\vec{\omega}';\lambda';\vec{\omega}'';\lambda'')\,S_k(\vec{\omega}'';\lambda'')}{|\zeta''|\left(\frac{\mu}{|\zeta|}+\frac{\mu'}{|\zeta'|}\right)\left(\frac{\mu}{|\zeta|}+\frac{\mu''}{|\zeta''|}\right)}$$

$$+\left(\frac{1-\operatorname{sgn}\zeta'}{2}\right)\int_0^\infty d\lambda''\int_{4\pi} d\vec{\omega}''\left(\frac{1+\operatorname{sgn}\zeta''}{2}\right)\frac{H^{b}_{ij}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\,H^{a}_{jk}(\vec{\omega}';\lambda';\vec{\omega}'';\lambda'')\,S_k(\vec{\omega}'';\lambda'')}{|\zeta''|\left(\frac{\mu''}{|\zeta''|}+\frac{\mu'}{|\zeta'|}\right)\left(\frac{\mu}{|\zeta|}+\frac{\mu''}{|\zeta''|}\right)}\Bigg\}$$

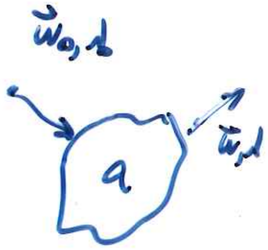


$(i,j,k = I, Q, U, V)$

# UNPOLARIZED EXCITATION

$$I^{(1)(5)}_{(a)_I}(\vec{\omega},\lambda) = A(\zeta_0,\lambda_0,\zeta,\lambda)\,k_{(a)}(\vec{\omega},\lambda,\vec{\omega}_0,\lambda_0)$$

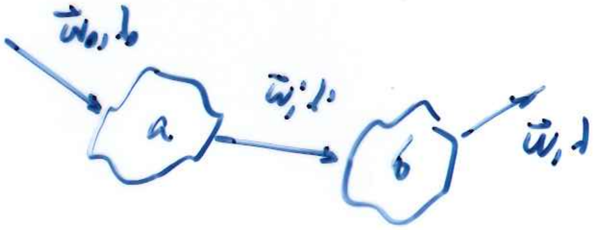
$$= \underbrace{I^{(1)}_{(a)}(\vec{\omega},\lambda)}_{\text{first-order intensity from scalar equation}}$$



$$I^{(2)(5)}_{(a,b)_I}(\vec{\omega},\lambda) = A(\zeta_0,\lambda_0,\zeta,\lambda)\int_0^\infty d\lambda'\int_{4\pi} d\vec{\omega}'\,\frac{1}{|\zeta'|}$$

$$\left\{\left(\frac{1+\operatorname{sgn}\zeta'}{2}\right)\frac{k_{(b)}(\vec{\omega},\lambda,\vec{\omega}',\lambda')\,k_{(a)}(\vec{\omega}',\lambda';\vec{\omega}_0,\lambda_0)}{\frac{\mu}{|\zeta|}+\frac{\mu'}{|\zeta'|}}\Big[1+\underbrace{\mathcal{G}_{ab}(\vec{\omega},\lambda,\vec{\omega}',\lambda';\vec{\omega}_0,\lambda_0)}_{\text{corrective factors}}\Big]\right.$$

$$\left.+\left(\frac{1-\operatorname{sgn}\zeta'}{2}\right)\frac{k_{(b)}(\vec{\omega},\lambda,\vec{\omega}',\lambda')\,k_{(a)}(\vec{\omega}',\lambda';\vec{\omega}_0,\lambda_0)}{\frac{\mu_0}{|\zeta_0|}+\frac{\mu'}{|\zeta'|}}\Big[1+\mathcal{G}_{ab}(\vec{\omega},\lambda,\vec{\omega}',\lambda';\vec{\omega}_0,\lambda_0)\Big]\right\}$$



$$\mathcal{G}_{ab}(\vec{\omega},\lambda,\vec{\omega}',\lambda';\vec{\omega}_0,\lambda_0) = \underbrace{P_b(\vec{\omega},\lambda,\vec{\omega}',\lambda')\;P_a(\vec{\omega},\lambda,\vec{\omega}',\lambda')}_{\text{degrees of polarization for interactions a and b}}\cos 2(\psi_a+\psi_b')$$

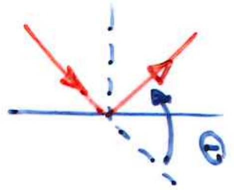
$$A(\zeta_1,\lambda_1,\zeta_2,\lambda_2) = \left(\frac{1+\operatorname{sgn}\zeta_1}{2}\right)\left(\frac{1-\operatorname{sgn}\zeta_2}{2}\right)\frac{I_0}{|\zeta_1|}\,\frac{1}{\frac{\mu_1}{|\zeta_1|}+\frac{\mu_2}{|\zeta_2|}}$$

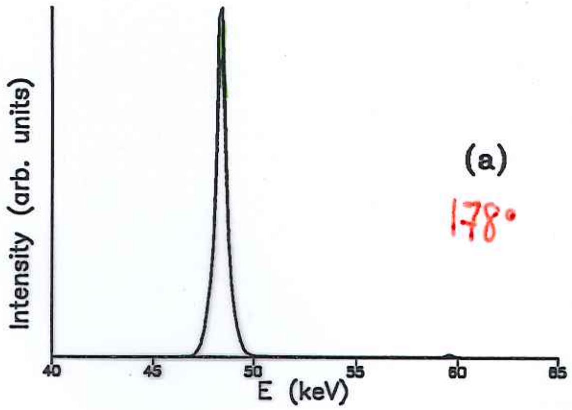
$$\boxed{\text{If } P_a=0 \text{ or } P_b=0 \text{ then } \mathcal{G}_{ab}\equiv 0}$$

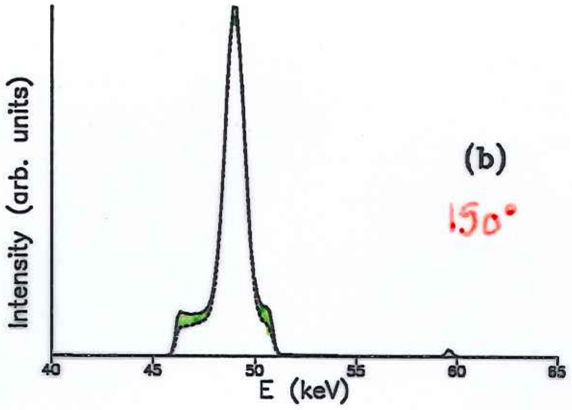
This is true for all collisions involving photoelectric effect!

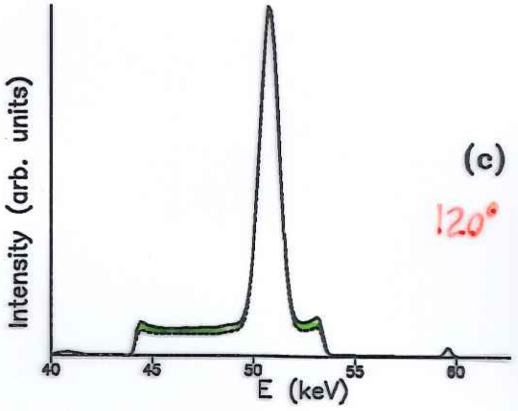
WATER $E_0 = 59.54$ keV

DIFFERENT SCATTERING ANGLES

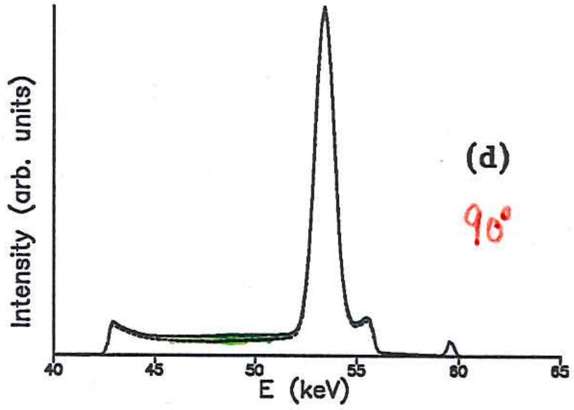


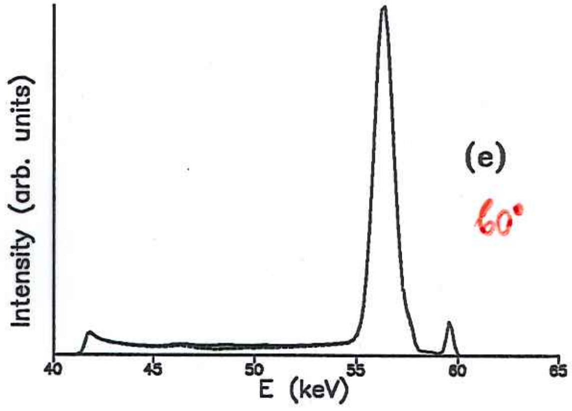






COMPARISON BETWEEN SPECTRA BUILT WITH THE SCALAR AND THE VECTOR MODEL. (SOURCE: UNPOLARIZED)





## COMPARISON BETWEEN THE SCALAR AND VECTOR EQUATIONS (INTENSITY TERM)

FOR UNPOLARIZED EXCITATION $S_I(\vec{w},\lambda) = I_0\,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$

then the equation for the intensity component becomes

$$\eta\frac{\partial}{\partial z} f_I(z,\vec{w},\lambda) = -\mu(\lambda)\, f_I(z,\vec{w},\lambda) +$$

$$+\,\mathcal{U}(z)\int_0^\infty d\lambda'\int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}',\lambda')\, f_I(z,\vec{w},\lambda')$$

COUPLING

$$\boxed{+\,\mathcal{U}(z)\int_0^\infty d\lambda'\int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}',\lambda')\left[q_{12} f_Q \cos 2\phi' - q_{12} f_U \sin 2\phi'\right]}$$

$$+\, I_0\,\delta(z)\,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$$

**NON-LINEAR EQ.**

Comparing with the scalar equation

$$\eta\frac{\partial}{\partial z} f(z,\vec{w},\lambda) = -\mu(\lambda)\, f(z,w,\lambda) +$$

$$+\,\mathcal{U}(z)\int_0^\infty d\lambda'\int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}',\lambda')\, f(z,\vec{w}',\lambda')$$

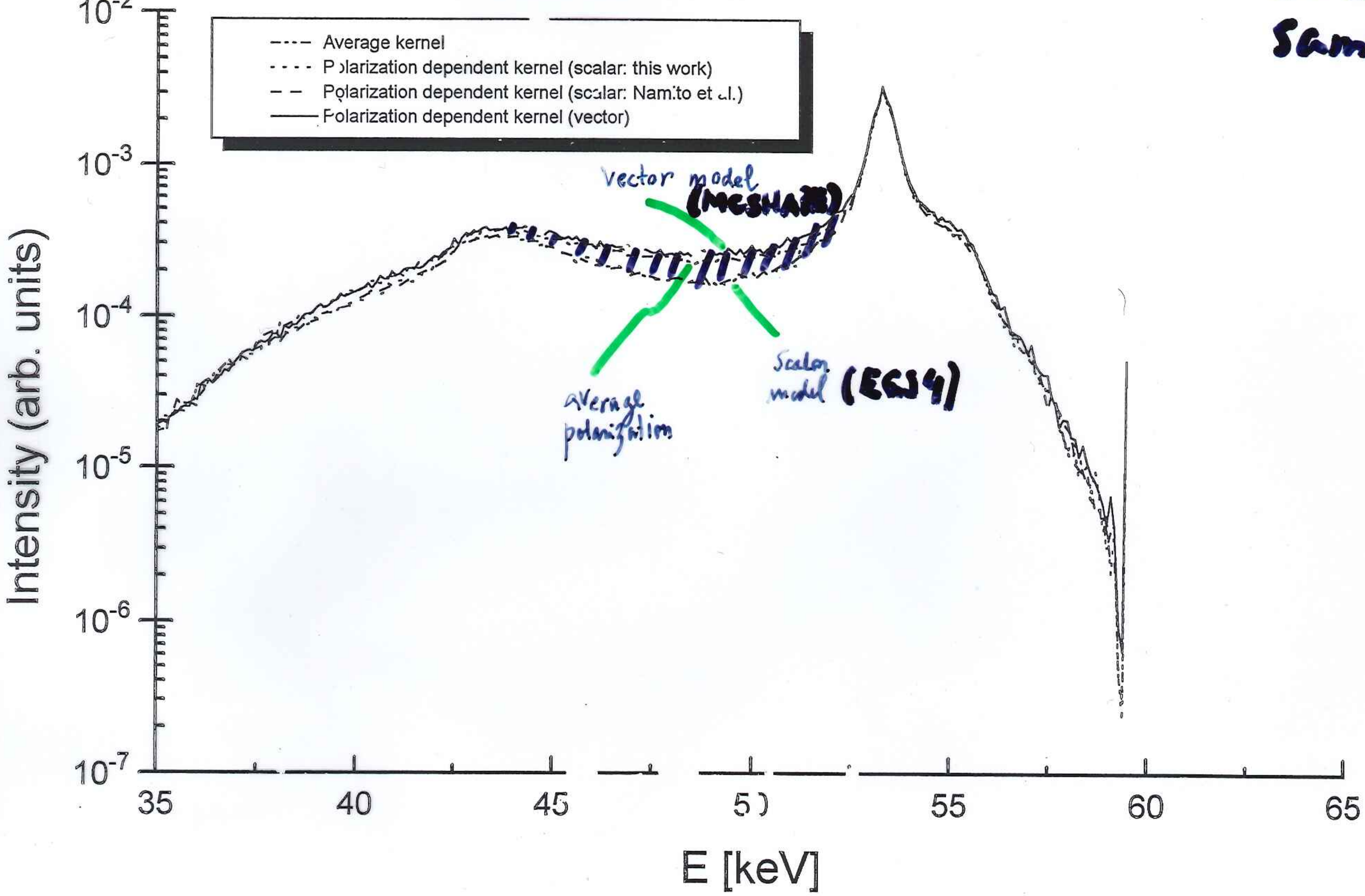
$$+\, I_0\,\delta(z)\,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$$

**LINEAR EQ.**

we see that the non-linearity is due to the coupling term

**Infinite thickness sample**

Comparison between spectra computed with scalar (dashed lines) and vector (solid lines) codes for Carbon. Only the first 4 terms where considered. All the MC simulations used 100000 histories.



## PHOTOELECTRIC EFFECT

$K_\alpha, K_\beta, L_\beta, L_\gamma$ DO NOT DEPEND ON POLARIZATION

$L_\ell, L_\alpha$ DEPEND ON POLARIZATION

Theory
FLÜGGE et al. (1972

Exp.
Kahlon et al. (1991)

- WE ASSUME THAT PHOTOELECTRIC EFFECT DOES NOT DEPEND ON POLARIZATION

## RAYLEIGH SCATTERING

STRONGLY DEPENDS ON POLARIZATION

## COMPTON SCATTERING

STRONGLY DEPENDS ON POLARIZATION

# PHOTOELECTRIC EFFECT

$$\mathbb{K}^{(S)}_{p_{\lambda_i}}(\vec{\omega},\lambda,\vec{\omega}';\lambda') = k_{p_{\lambda_i}}(\vec{\omega},\lambda,\vec{\omega}';\lambda')\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}$$

$$k_{p_{\lambda_i}}(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \frac{1}{4\pi}\,Q_{\lambda_i}(\lambda')\,\delta(\lambda-\lambda_i)\,[1-\mathcal{U}(\lambda'-\lambda_{e_i})]$$

$$Q_{\lambda_i}(\lambda') = \tau_s(\lambda')\begin{cases}\left(1-\frac{1}{J_K}\right)\omega_K\,\Gamma_{\lambda_i}, & \lambda_i \in \text{serie } K\\[4pt] \left(1-\frac{1}{J_{L_1}}\right)\omega_{L_1}\,\Gamma_{\lambda_i}, & \lambda_i \in L_1\\[4pt] \left[\left(1-\frac{1}{J_{L_2}}\right)+f_{12}\left(1-\frac{1}{J_{L_1}}\right)\right]\omega_{L_2}\,\Gamma_{\lambda_i}, & \lambda_i \in L_2\\[4pt] \left[\left(1-\frac{1}{J_{L_3}}\right)+f_{23}\left(1-\frac{1}{J_{L_2}}\right)+(f_{13}+f_{12}f_{23})\left(1-\frac{1}{J_{L_1}}\right)\right]\omega_{L_3}\,\Gamma_{\lambda_i} & \\ & \lambda_i \in L_3\end{cases}$$

$$k_p(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \sum_i k_{p_{\lambda_i}}(\vec{\omega},\lambda,\vec{\omega}';\lambda')$$

takes into account all lines

# RAYLEIGH SCATTERING

$$\mathbb{K}_R^{(S)}(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \frac{k_R(\vec{\omega},\lambda,\vec{\omega}';\lambda')}{1+(\bar{\omega}\cdot\bar{\omega}')^2}\begin{pmatrix} 1+(\bar{\omega}\cdot\bar{\omega}')^2 & (\bar{\omega}\cdot\bar{\omega}')^2-1 & 0 & 0 \\ (\bar{\omega}\cdot\bar{\omega}')^2-1 & (\bar{\omega}\cdot\bar{\omega}')^2+1 & 0 & 0 \\ 0 & 0 & 2\,\bar{\omega}\cdot\bar{\omega}' & 0 \\ 0 & 0 & 0 & 2\,\bar{\omega}\cdot\bar{\omega}' \end{pmatrix}$$

$$k_R(\vec{\omega},\lambda,\vec{\omega}';\lambda') = \sigma\,\delta(\lambda-\lambda')\left(1+(\bar{\omega}\cdot\bar{\omega}')^2\right)\frac{F^2(\lambda',\bar{\omega}\cdot\bar{\omega}',Z)}{Z}$$

# COMPTON SCATTERING

$$\mathbb{K}_c^{(S)}(\omega,\lambda,\vec{\omega}';\lambda') = \frac{\sigma}{\lambda_c}\left(\frac{\lambda'}{\lambda}\right)^2 \delta\left(1-\vec{\omega}\cdot\vec{\omega}' + \frac{\lambda-\lambda'}{\lambda_c}\right)$$

term for electric charge distribution

$$\Bigg[\Bigg\{ S(\lambda';\vec{\omega}\cdot\vec{\omega}';Z)\begin{pmatrix} a+b(b-2) & b(b-2) & 0 & 0 \\ b(b-2) & 2+b(b-2) & 0 & 0 \\ 0 & 0 & 2(1-b) & 0 \\ 0 & 0 & 0 & a(1-b) \end{pmatrix} +$$

term for magnetization distribution

$$\Bigg[ + \frac{F^M(\lambda';\vec{\omega}\cdot\vec{\omega}';Z)}{Z}\begin{pmatrix} 0 & 0 & 0 & b((1-b)c'\vec{n}'+c\vec{n})\cdot\hat{B} \\ 0 & 0 & 0 & bc'\vec{n}\times\vec{n}'\cdot\vec{n}'\times\hat{B} \\ 0 & 0 & 0 & bc\vec{n}\times\vec{n}'\cdot\hat{B} \\ b((1-b)c\vec{n}+c'\vec{n}')\cdot\hat{B} & bc\,\vec{n}'\times\vec{n}\cdot\vec{n}\times\hat{B} & bc'\vec{n}'\times\vec{n}\cdot\hat{B} & 0 \end{pmatrix}\Bigg\}$$

where

$$\underbrace{F^M(\vec{K})}_{\text{magnetic form factor}} = \frac{1}{2\mu_B}\left|\int d^3r\, e^{i\vec{K}\cdot\vec{r}}\underbrace{\vec{M}_S(\vec{r})}_{\text{spin density}}\right| \qquad \vec{K} = \underbrace{\vec{k}-\vec{k}'}_{\text{momentum transfer}}$$

$$a = \frac{\lambda}{\lambda'}+\frac{\lambda'}{\lambda} \qquad b = \frac{\lambda-\lambda'}{\lambda_c} = 1-\vec{\omega}\cdot\vec{\omega}'$$

$$c = \frac{\lambda_c}{\lambda} \qquad c' = \frac{\lambda_c}{\lambda'}$$

$$n = \frac{\vec{k}}{k} \qquad \vec{n}' = \frac{\vec{k}'}{k'}$$

Ratio of the terms:

$$\frac{\text{magnetic intensity}}{\text{charge intensity}} \sim \frac{F^M(\lambda';\vec{\omega}\cdot\vec{\omega}';Z)}{\underbrace{Z\,S(\lambda';\vec{\omega}\cdot\vec{\omega}';Z)}_{\in[0,1]}}\boxed{\frac{\lambda_c}{\lambda'}} \rightarrow \frac{E'}{mc^2}$$

# KERNEL MATRICES

## PHOTOELECTRIC EFFECT:

$$K_{P_{\lambda i}}(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') = k_{P_{\lambda i}}(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') \times \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}$$

$$k_{P_{\lambda i}}(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') = \frac{1}{4\pi} Q_{\lambda_i}(\lambda')\delta(\lambda-\lambda_i)\times\left[1-U(\lambda'-\lambda_{ei})\right]$$

$$Q_{\lambda i}(\lambda') = \tau_s(\lambda')\left(1-1/J_{\lambda i}\right)\omega_{\lambda i}\,\Gamma_{\lambda i}$$

## RAYLEIGH SCATTERING:

$$k_R(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') = \sigma\delta(\lambda-\lambda')\left(1+(\overline{\varpi}\cdot\overline{\varpi}')^2\right)\frac{F^2(\lambda',\overline{\varpi}\cdot\overline{\varpi}',Z)}{Z}$$

$$K_R = \frac{k_R(\overline{\varpi},\lambda,\overline{\varpi}',\lambda')}{1+(\overline{\varpi}\cdot\overline{\varpi}')^2} * \begin{vmatrix} 1+(\overline{\varpi}\cdot\overline{\varpi}')^2 & \left[(\overline{\varpi}\cdot\overline{\varpi}')^2-1\right] & 0 & 0 \\ \left[(\overline{\varpi}\cdot\overline{\varpi}')^2-1\right] & 1+(\overline{\varpi}\cdot\overline{\varpi}')^2 & 0 & 0 \\ 0 & 0 & 2(\overline{\varpi}\cdot\overline{\varpi}') & 0 \\ 0 & 0 & 0 & 2(\overline{\varpi}\cdot\overline{\varpi}') \end{vmatrix}$$

## COMPTON SCATTERING (without Doppler):

$$k_C(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') = \sigma\,K_{KN}(\lambda,\lambda')S(\lambda',\overline{\varpi}\cdot\overline{\varpi}',Z)\frac{1}{\lambda_C}\delta\left(1-\overline{\varpi}\cdot\overline{\varpi}'+\frac{\lambda'-\lambda}{\lambda_C}\right)$$

$$K_{KN}(\lambda,\lambda') = \left(\frac{\lambda'}{\lambda}\right)^2\left\{\frac{\lambda}{\lambda'}+\frac{\lambda'}{\lambda}+\frac{\lambda-\lambda'}{\lambda_C}\left(\frac{\lambda-\lambda'}{\lambda_C}-2\right)\right\}$$

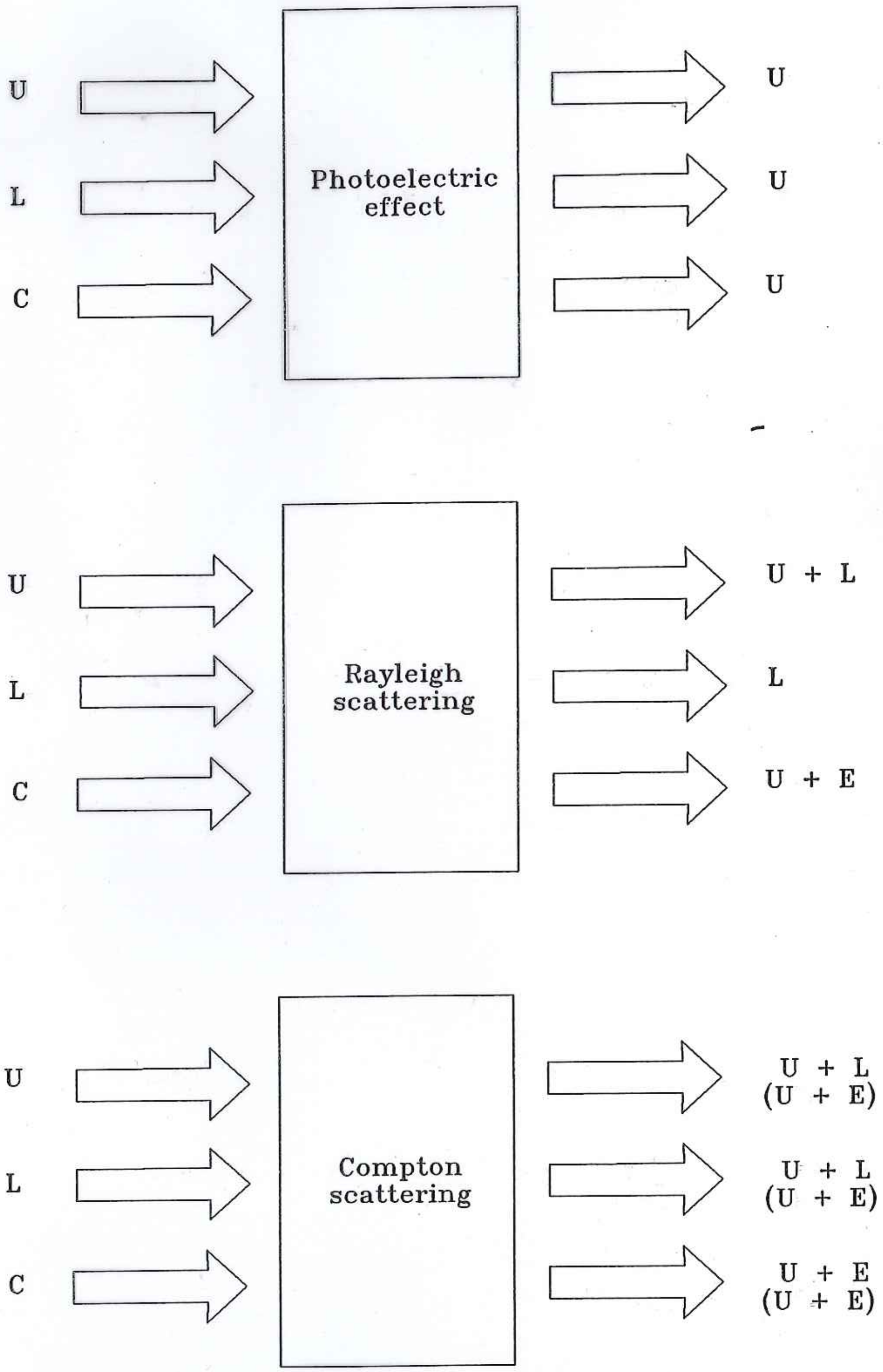
$$K_C(\overline{\varpi},\lambda,\overline{\varpi}',\lambda') = \frac{k_C(\overline{\varpi},\lambda,\overline{\varpi}',\lambda')}{a+b(b-2)} * \begin{vmatrix} a+b(b-2) & b(b-2) & 0 & 0 \\ b(b-2) & \left[2+b(b-2)\right] & 0 & 0 \\ 0 & 0 & (1-b) & 0 \\ 0 & 0 & 0 & a(1-b) \end{vmatrix}$$

with

$$a = \frac{\lambda}{\lambda'}+\frac{\lambda'}{\lambda} = \frac{\left[\lambda'+\lambda_C(1-\overline{\varpi}\cdot\overline{\varpi}')\right]^2+\lambda'^2}{\lambda'\left[\lambda'+\lambda_C(1-\overline{\varpi}\cdot\overline{\varpi}')\right]},$$

$$b = \frac{\lambda-\lambda'}{\lambda_C}$$

# CHANGES IN THE POLARIZATION STATE PRODUCED BY DIFFERENT INTERACTIONS



U: unpolarized; L: linearly polarized;
C: circularly polarized; E: elliptically polarized
Values between parenthesis correspond to an applied external magnetic field.

# Rayleigh Scattering

## Unpolarized source

$$I^{(1)(S)}_{(R)_I}(\boldsymbol{\omega},\lambda) = 2\frac{\sigma}{Z}\delta(\lambda-\lambda_0)A(\eta_0,\lambda_0,\eta,\lambda_0)F^2(\lambda_0,\boldsymbol{\omega}\cdot\boldsymbol{\omega}_0,Z)\boxed{\tfrac{1}{2}(1+\cos^2\Theta)}$$

## Linearly polarized source

$$I^{(1)(S)}_{(R)_I}(\boldsymbol{\omega},\lambda) = 2\frac{\sigma}{Z}\delta(\lambda-\lambda_0)A(\eta_0,\lambda_0,\eta,\lambda_0)F^2(\lambda_0,\boldsymbol{\omega}\cdot\boldsymbol{\omega}_0,Z)\boxed{(1-\sin^2\Theta\cos^2(\psi'+\chi))}$$

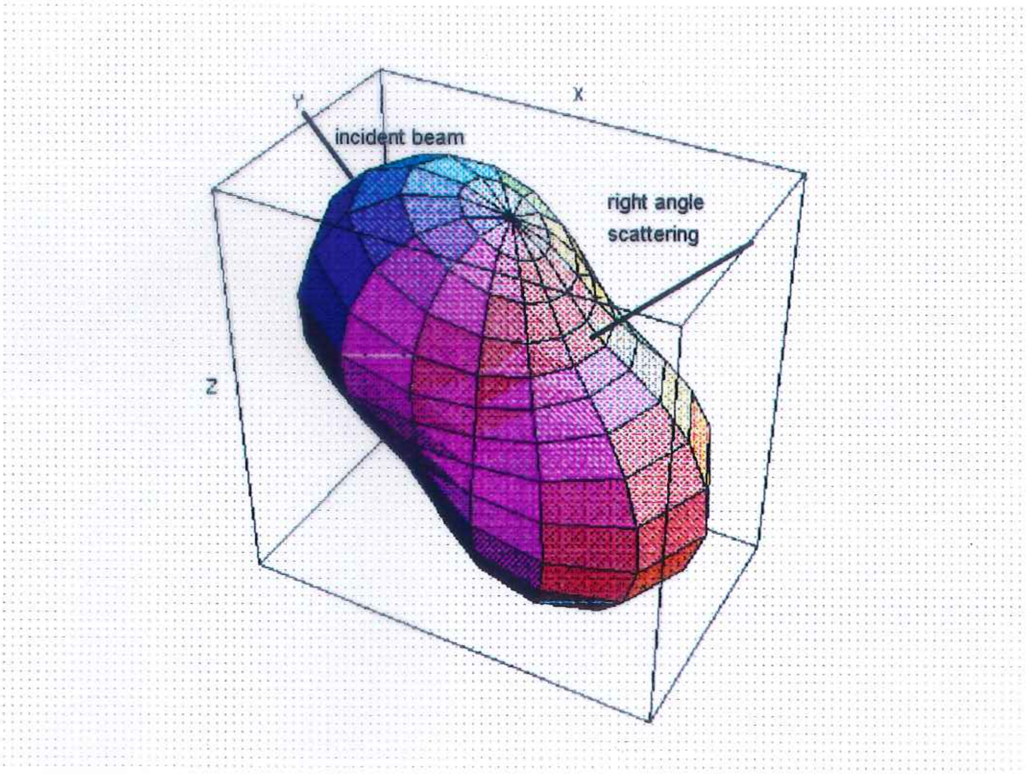
where

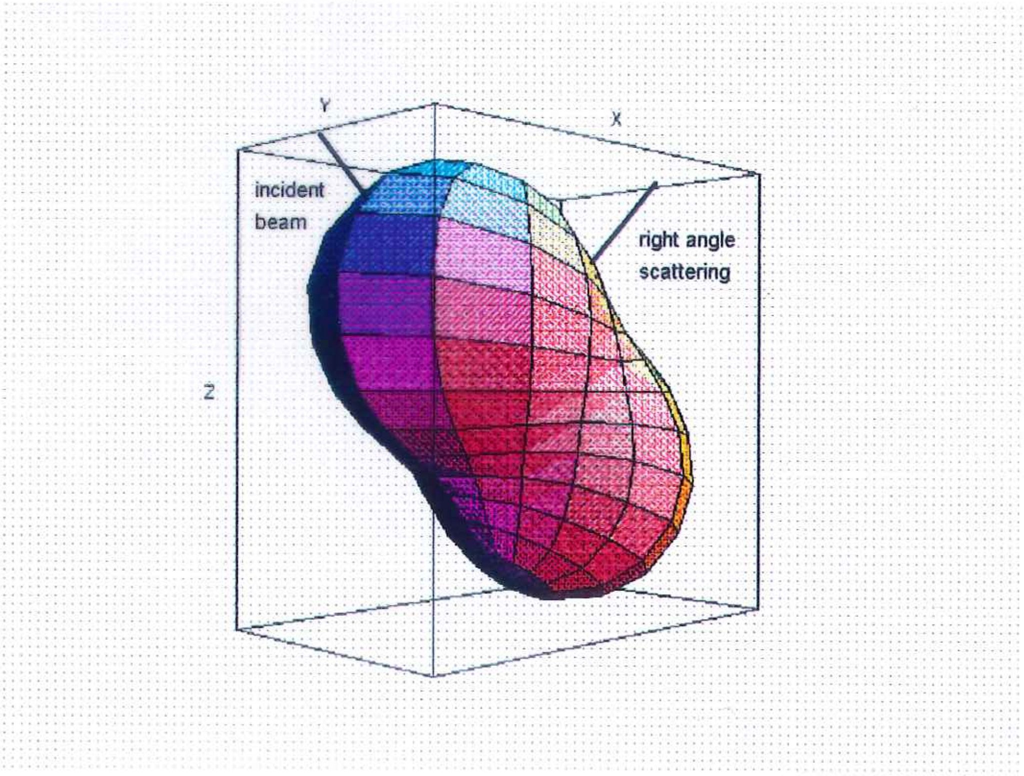
$\Theta$ is the scattering angle,

$\chi$ is the orientation of the polarization line; and

$$\cos\ \psi' = \frac{\eta\sqrt{1-\eta_0^2}\ -\ \eta_0\sqrt{1-\eta^2}\cos(\varphi-\varphi_0)}{\sin^2\Theta}$$

Source : Unpolarized

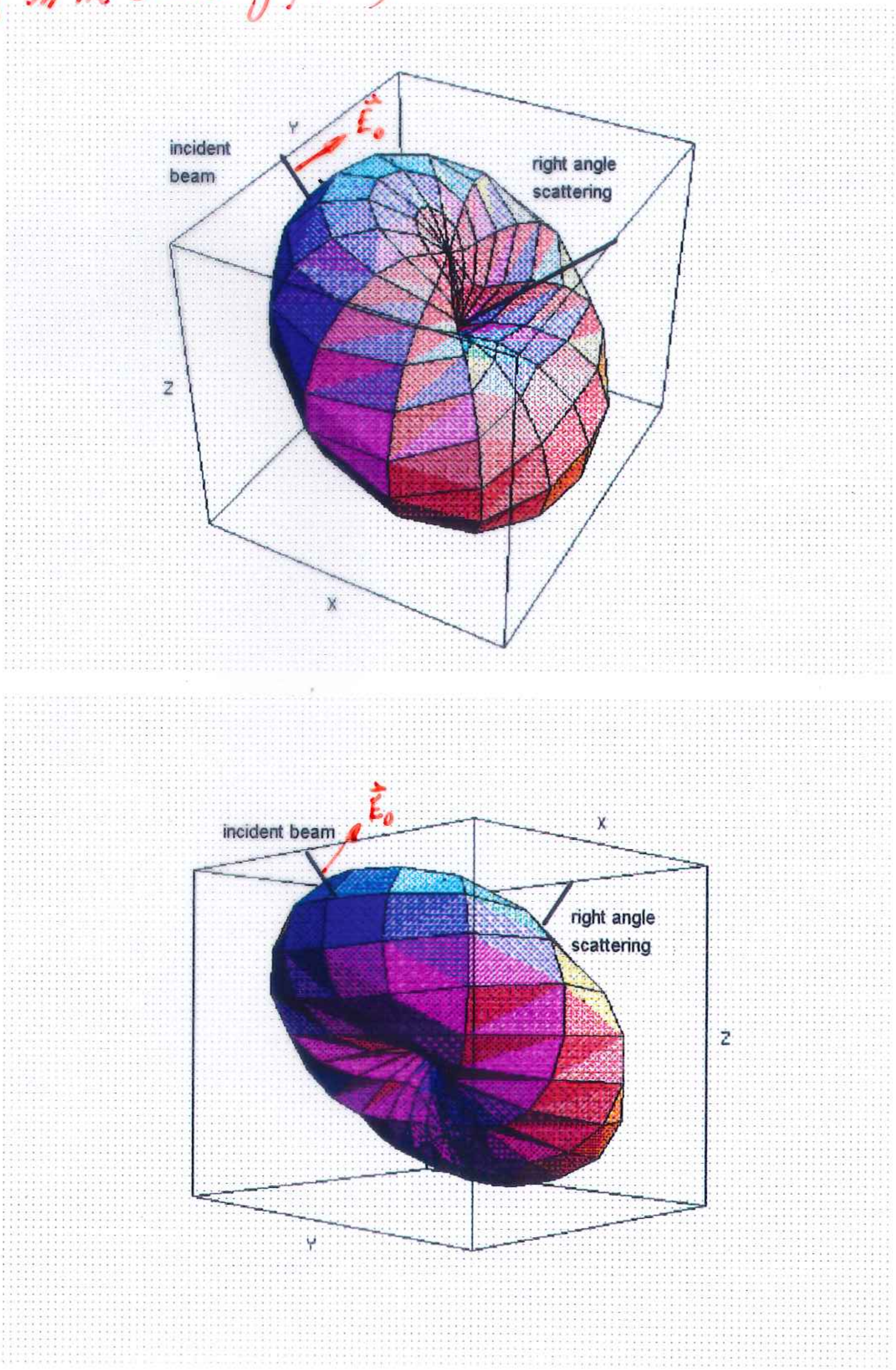




Angular function $\{1 + \cos^2\Theta\}/2$ in the first-order intensity term corresponding to an unpolarized source. The solid line on the left shows the incidence direction, while the solid line on the right illustrates a $90^{\circ}$ scattering direction lying on the plane x-z. The strength of the angular function (here represented by the vector radius to the surface of the solid) is minimum and constant for $90^{\circ}$ scattering in all directions.

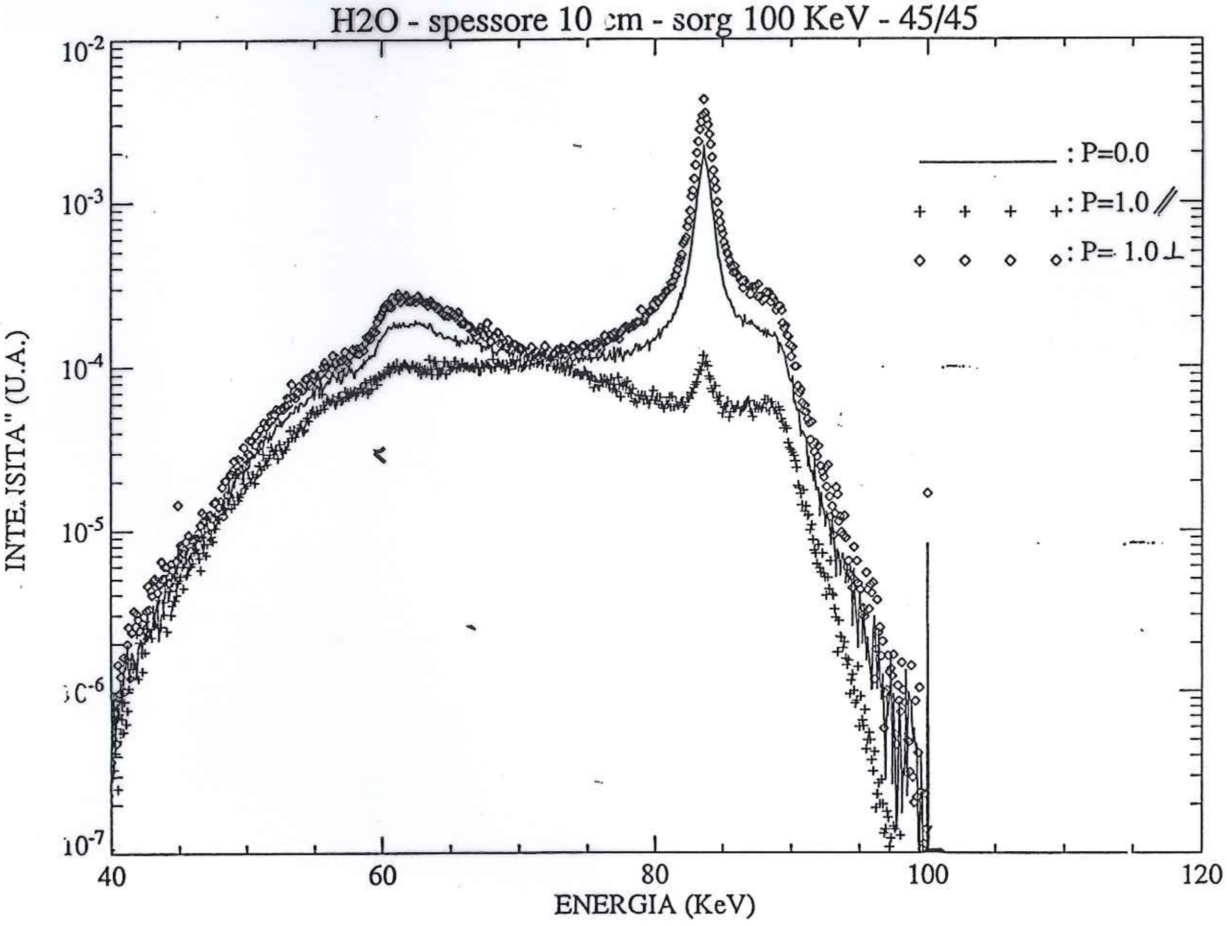
Source = LP

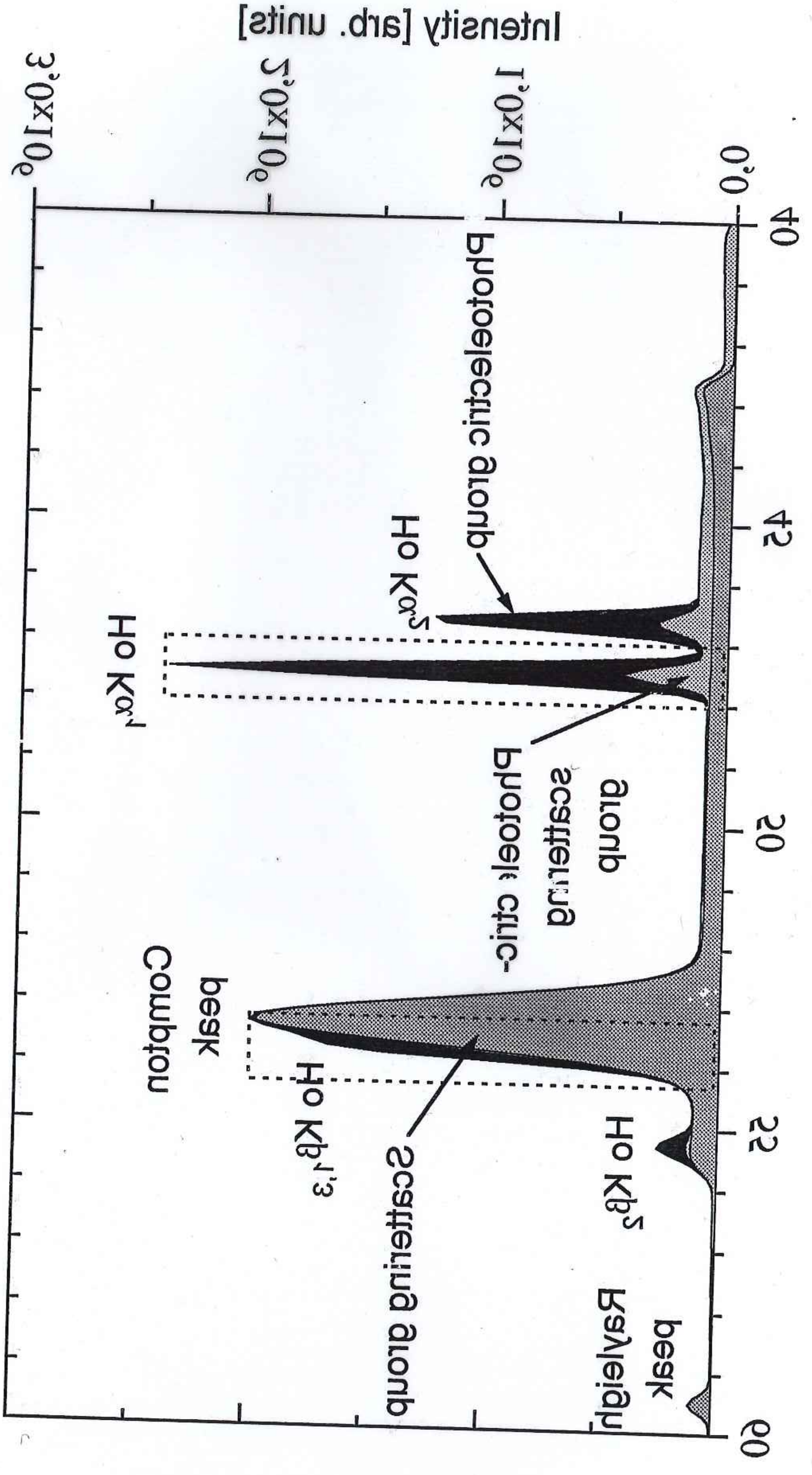
$\chi = 0$ (on the scattering plane)



Angular function $\{1 - \sin^2\Theta \cos^2(\psi' + \chi)\}$ in the first-order intensity term corresponding to a linearly polarized source having the line of polarization oriented along the z-axis (i.e. $\chi = 0$, or the electric vector of the incident beam propagating in the plane x-z). The solid line on the left shows the incidence direction, while the solid line on the right illustrates a 90° scattering direction lying on the plane x-z. The strength of the angular function (here represented by the vector radius to the surface of the solid) is null for this direction. In contrast, it is maximum for the scattering vectors lying on a plane normal to the plane x-z which contains the incidence direction.

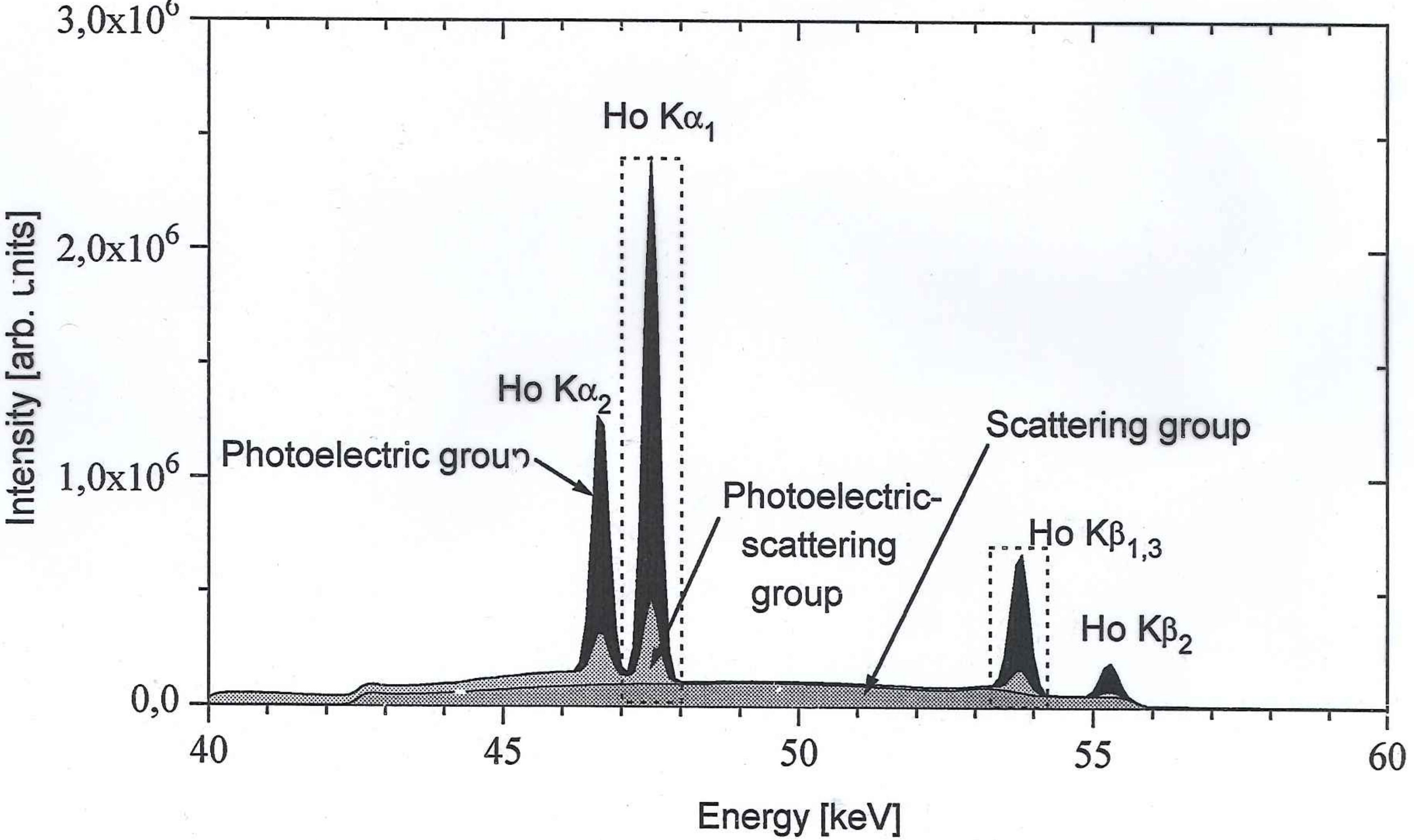
Fig 4: WATER excited with 100 keV photons, α1=α2=45°
with different degree of polarization



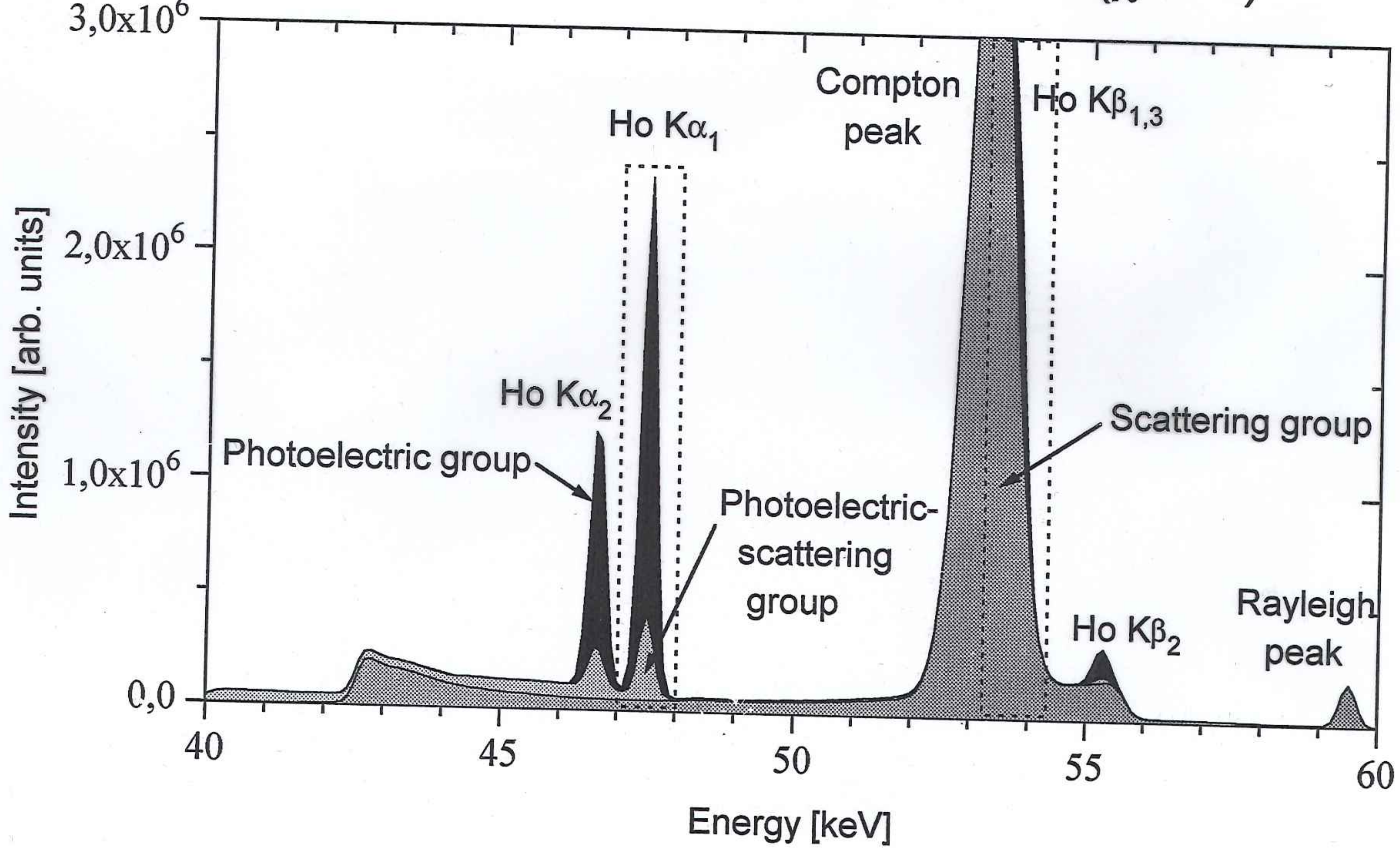


Unpolarized source

# Linearly polarized source ($\chi$=0



## Linearly polarized source ($\chi$=90)



# Linearly polarized source ($\chi$=45)

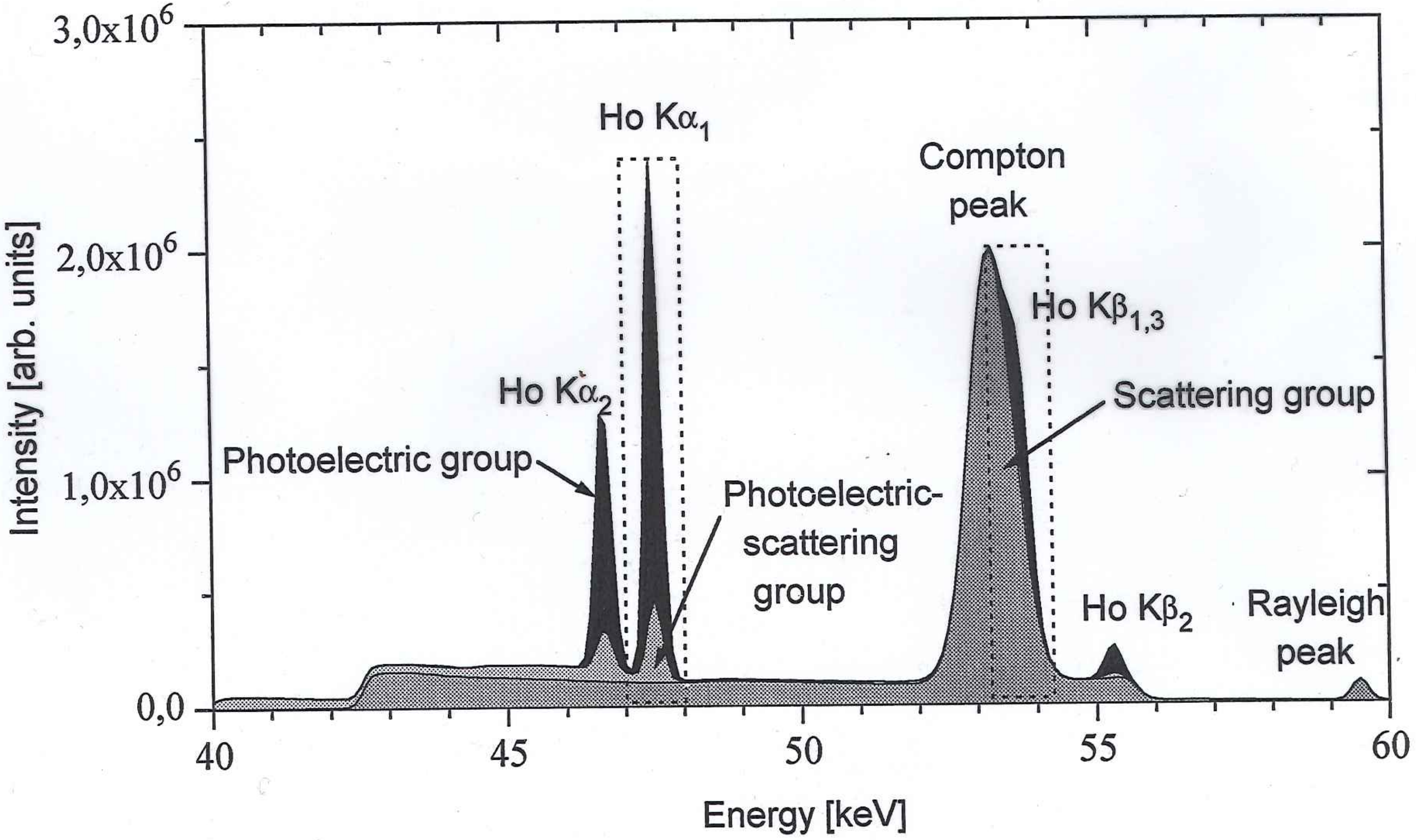


Fig. 23
Fernandez/Hubbell/Hanson/Spencer

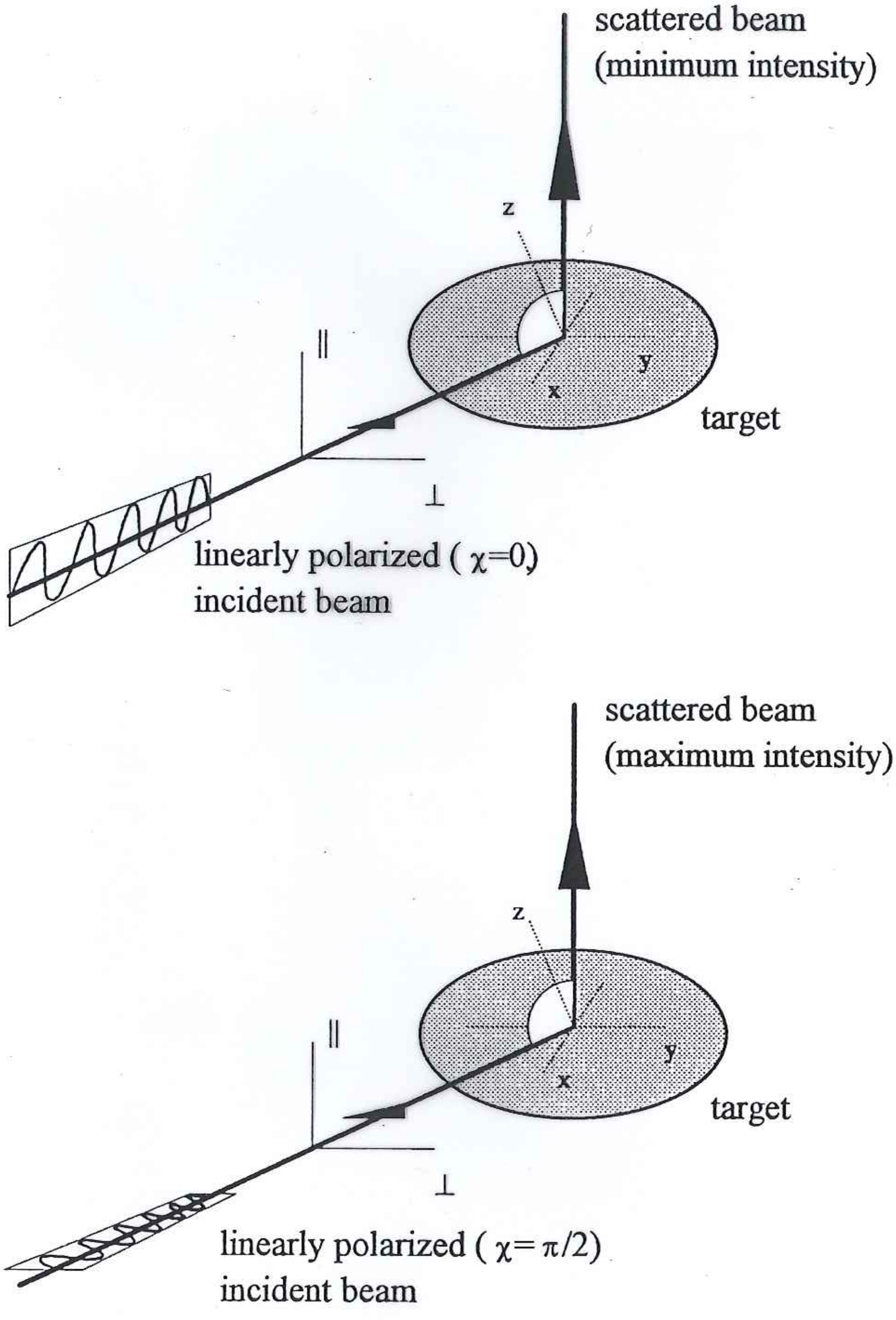
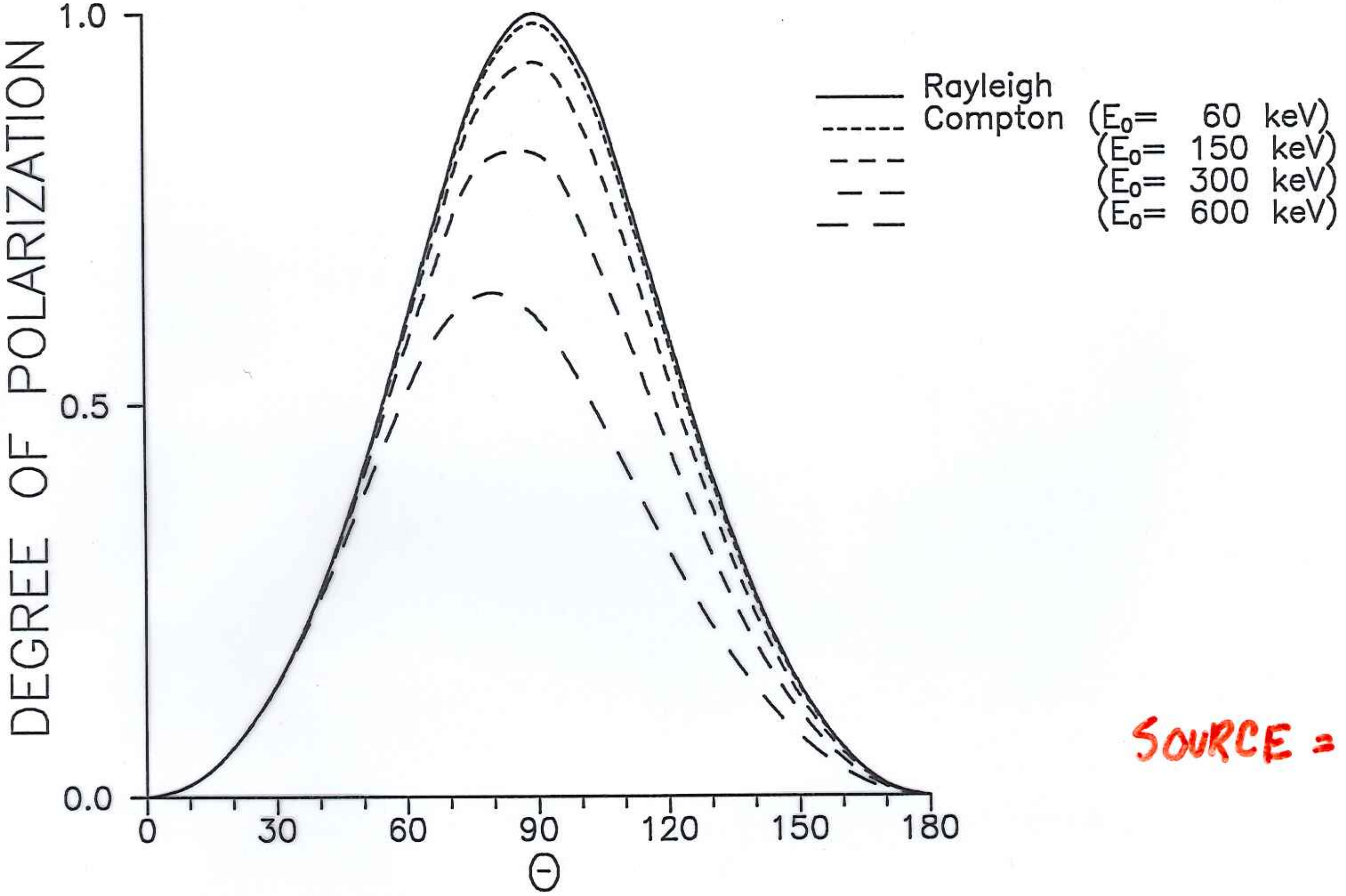
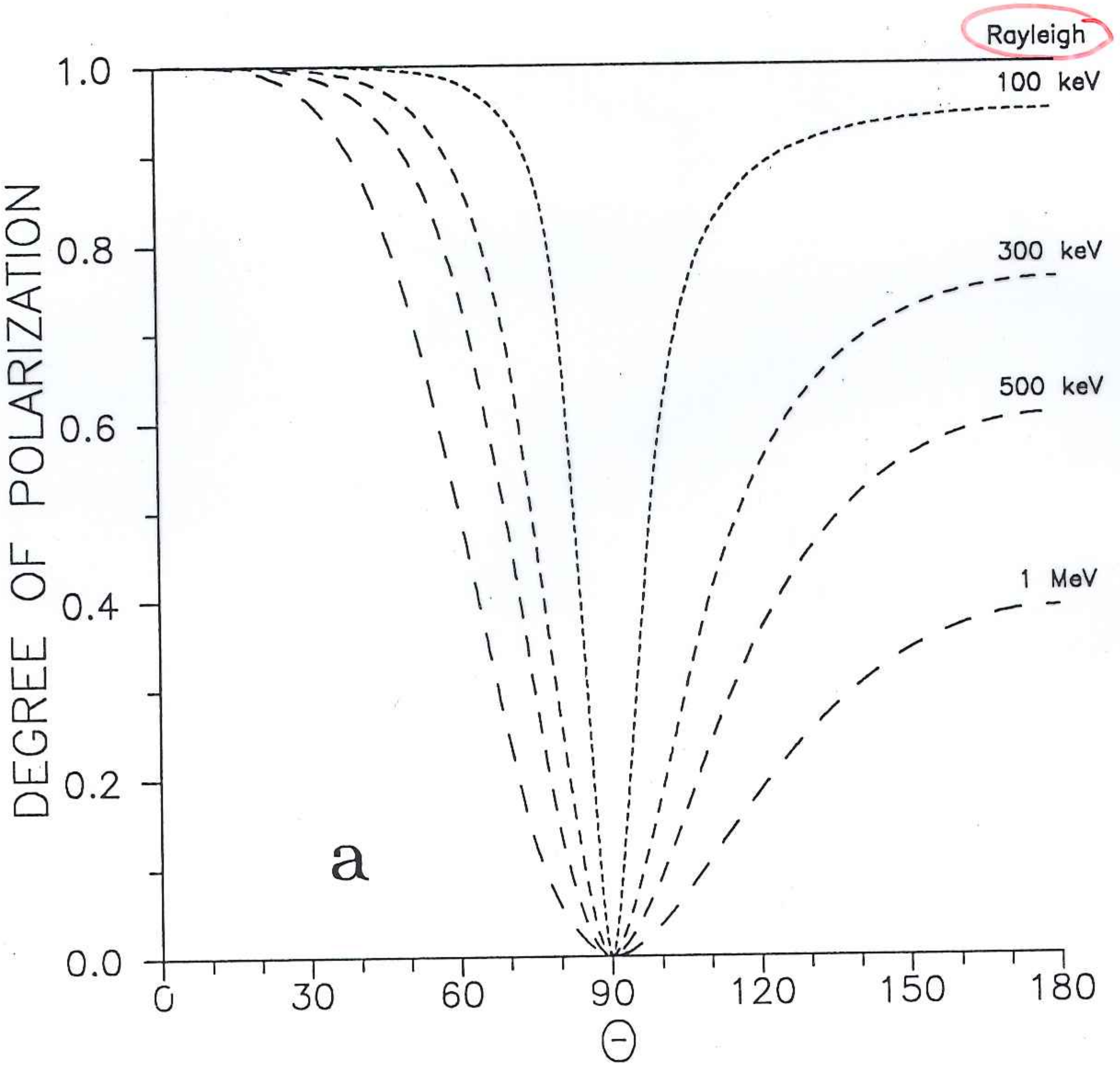


Figure 23. A linearly polarized incident beam with the electric field lying on a plane parallel (perpendicular) to the scattering plane gives minimum (maximum) first-order intensities for 90° Rayleigh and Compton scattering. In this figure, we assume that both directions, incidence and take off, belong to the x-z plane normal to the target surface ($\varphi_0=\varphi=0$).



SOURCE = UNPOLARIZED

Fig 24(a)
Fernández/Hubbell/Hanson/Spencer



Compton

DEPOLARIZES
GRADUALLY
FOR INCREASING
ENERGY

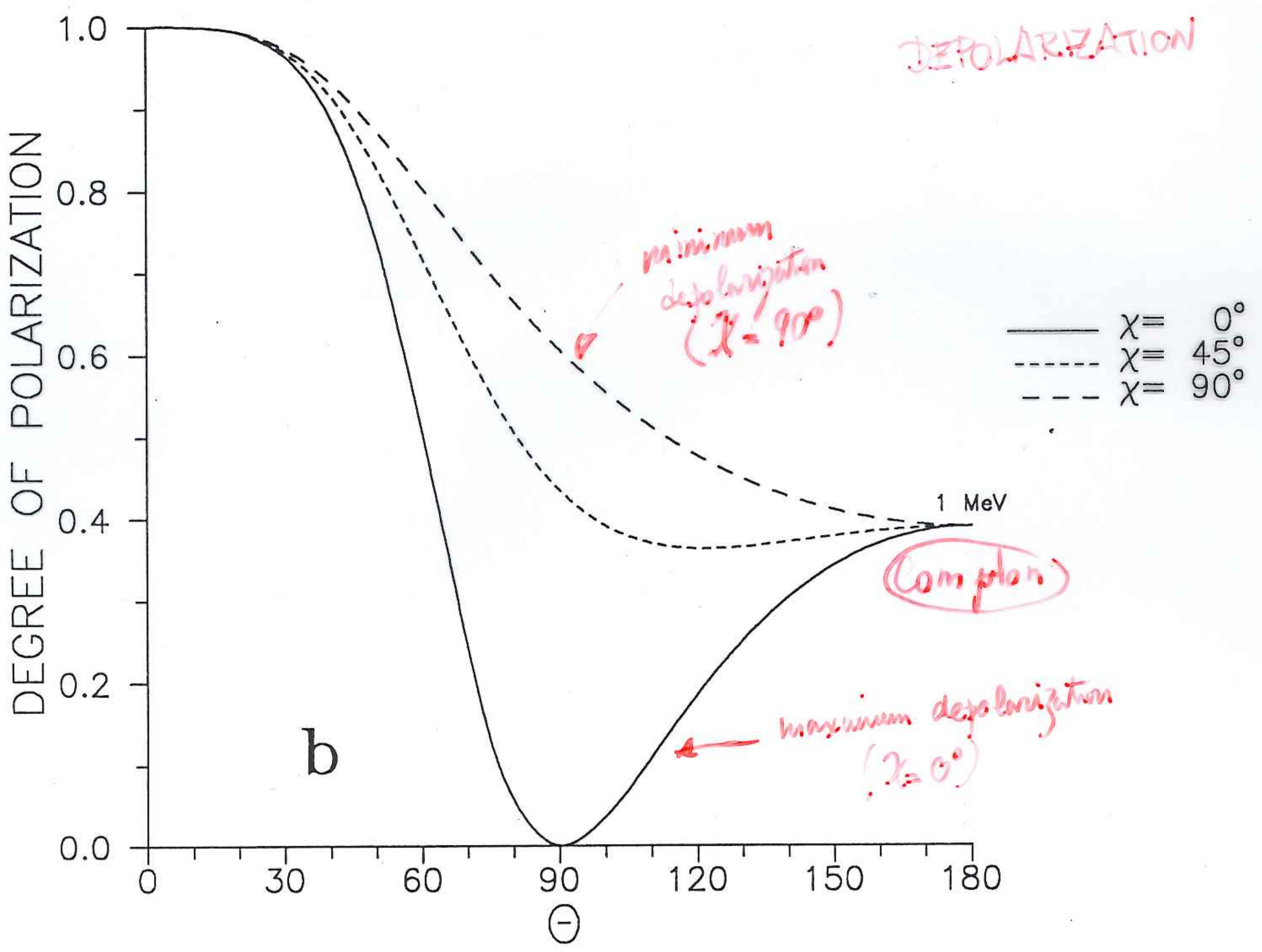
$\chi_0 = 0$ (on the scattering plane!)

Source = LP

Fig. 24(b)
Fernández/Hubbell/Hanson/Spencer

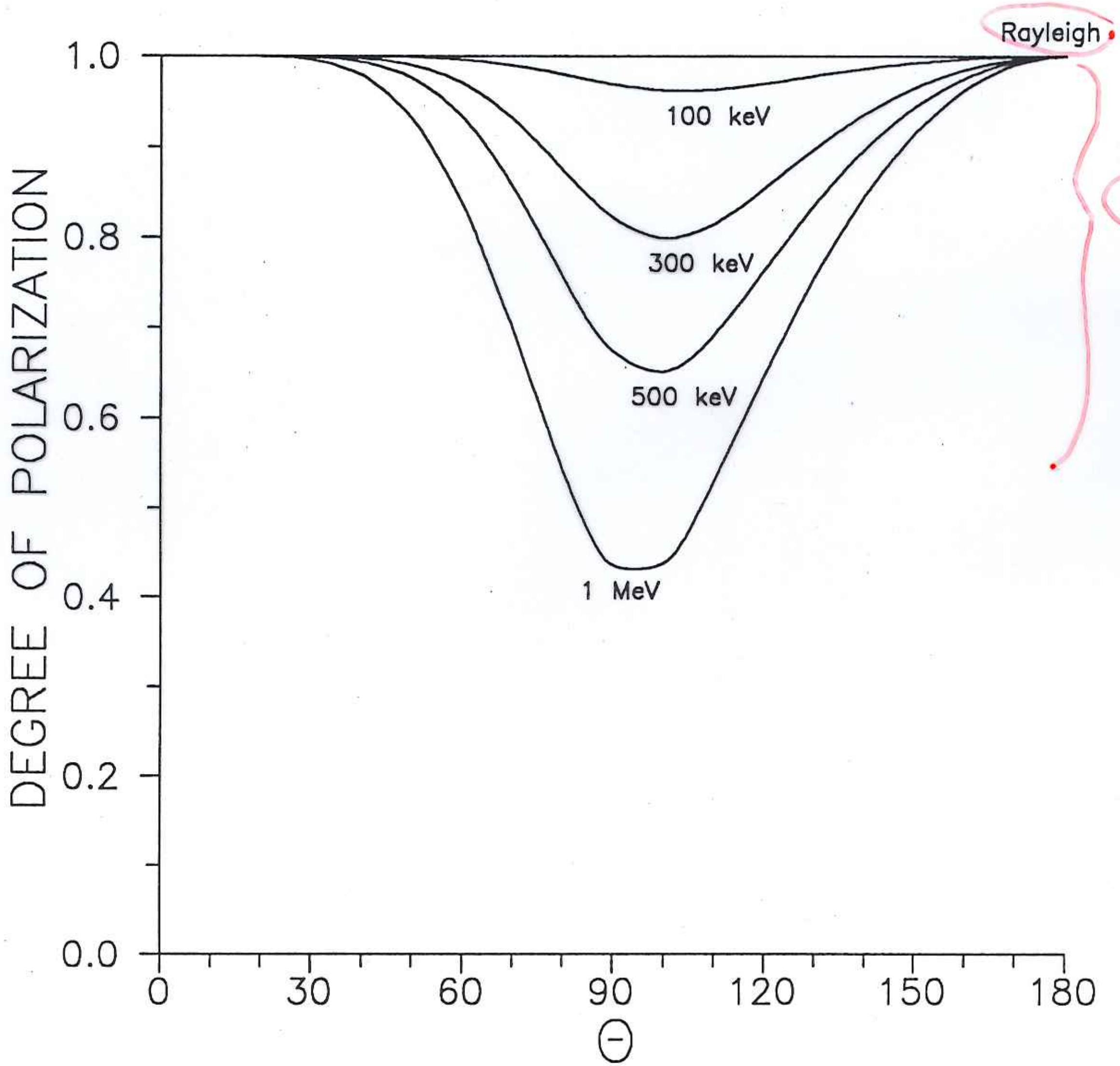
WE HAVE

DEPOLARIZATION



Source = LP

Fig. 27
Fernández / Hubbell / Hanson / Sjaner

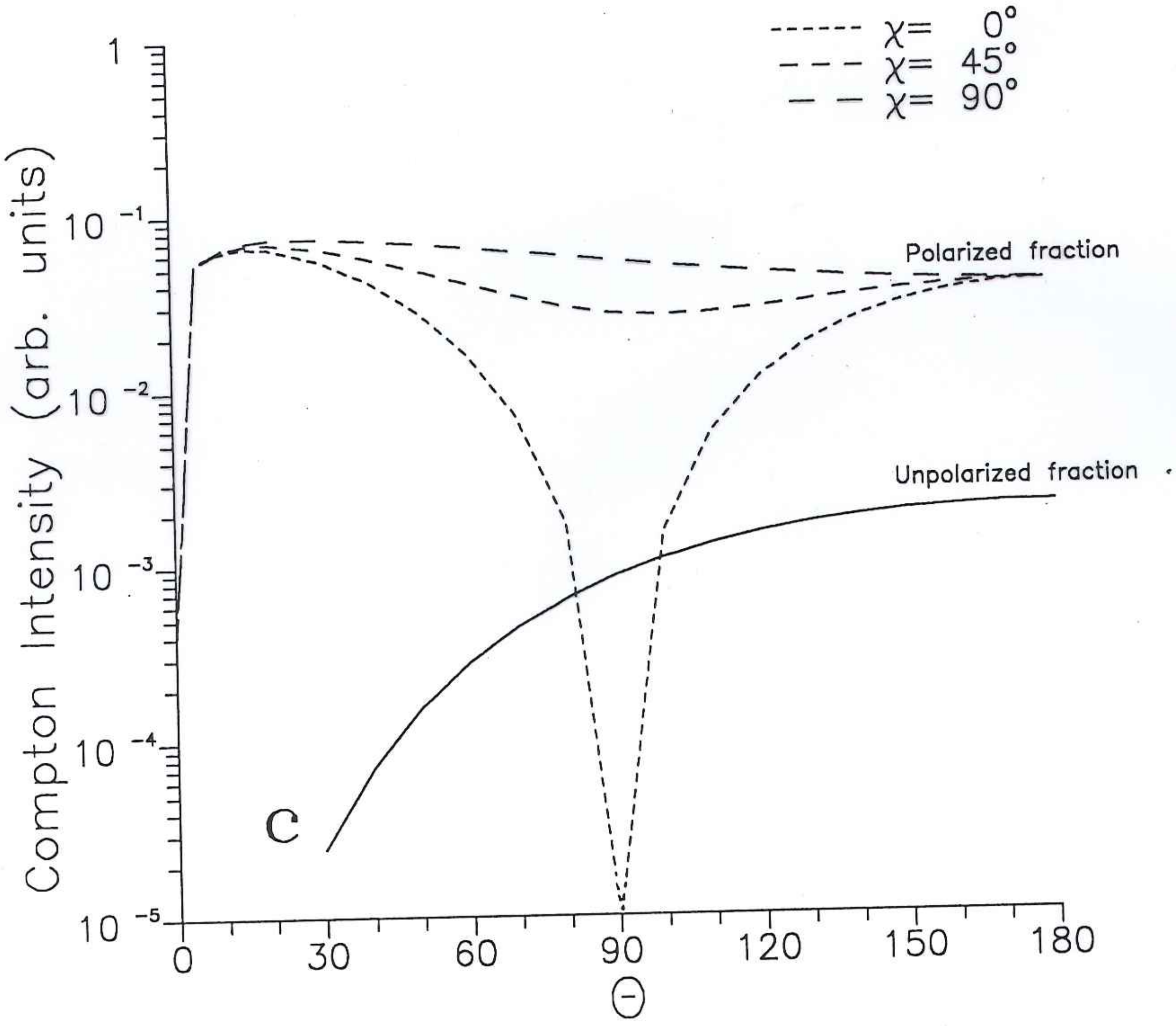


COMPTON

depolarizes gradually for increasing energy

Source = CP

ig 24(c)
ernández / Hubbell / Hanson / Spencer



FIRST-ORDER COMPTON INTENSITY

Source : LP

# POLARIZATION STATE FOR A SINGLE COLLISION CHAIN

$$\vec{I}^{(i)} = \underbrace{I^{(i)}\left(1 - P^{(i)}\right)\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}}_{\text{unpolarized}} + \underbrace{I^{(i)} p^{(i)} \begin{pmatrix} 1 \\ \cos 2\chi^{(i)} \cos 2\beta^{(i)} \\ \sin 2\chi^{(i)} \cos 2\beta^{(i)} \\ \sin 2\beta^{(i)} \end{pmatrix}}_{\text{polarized}}$$

# COMPUTATION OF THE TOTAL POLARIZATION STATE USING SINGLE CHAIN STATE MAGNITUDES

$$I = \sum_i I^{(i)}$$

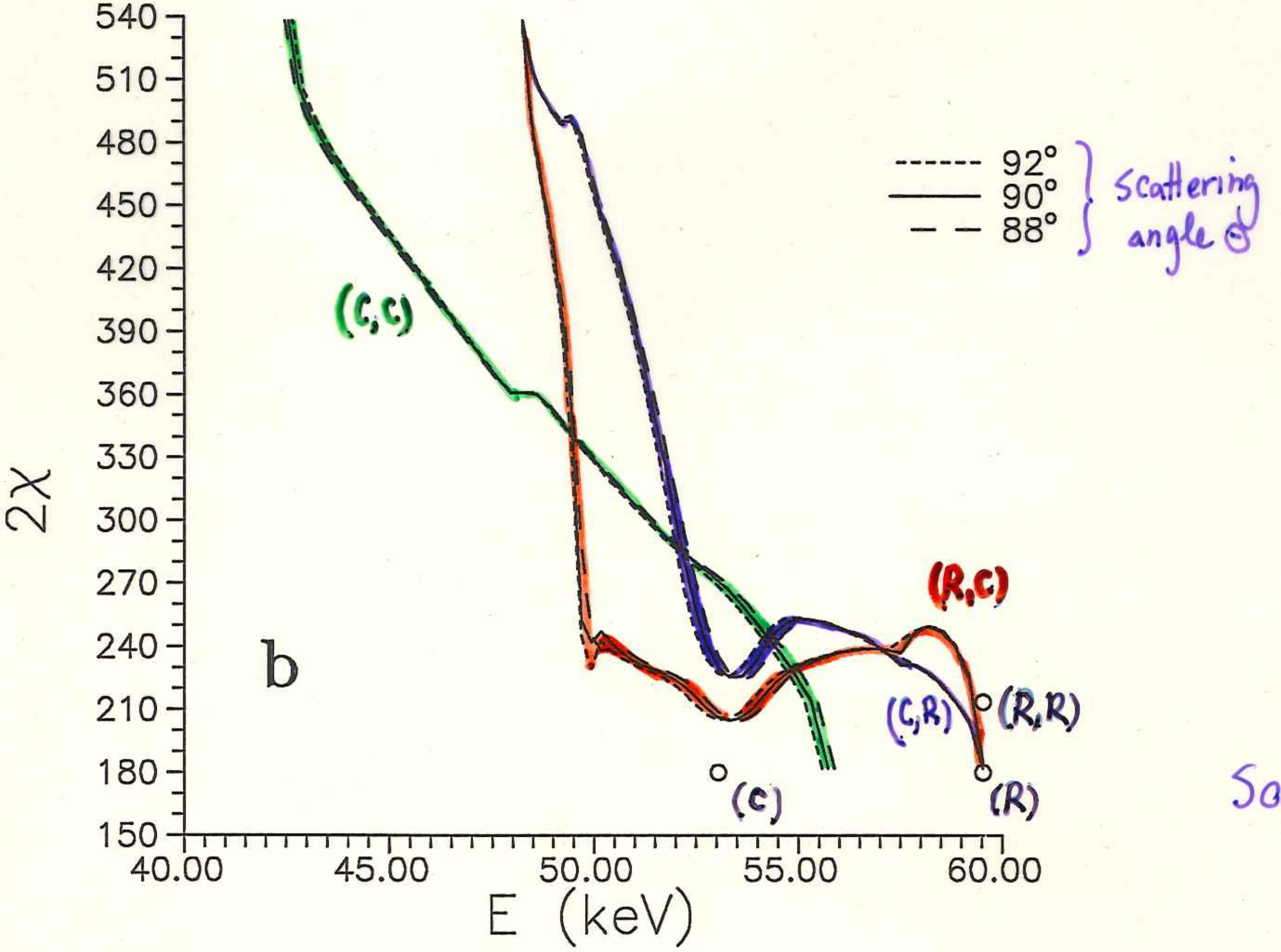
$$P = \frac{\sum_i I^{(i)} p^{(i)}}{\sum_i I^{(i)}}$$

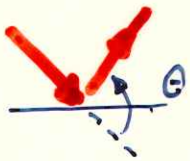
$$tg\, 2\chi = \frac{\sum_i P^{(i)} I^{(i)} \cos 2\chi^{(i)} \cos 2\beta^{(i)}\, tg\, 2\chi^{(i)}}{\sum_i P^{(i)} I^{(i)} \cos 2\chi^{(i)} \cos 2\beta^{(i)}}$$

$$\sin 2\beta = \frac{\sum_i p^{(i)} I^{(i)} \sin 2\beta^{(i)}}{\sum_i P^{(i)} I^{(i)}}$$

Note: index i denotes collision chains

ORIENTATION OF $\vec{E}$ FOR WATER AND FOR SOME SELECTED COLLISION CHAINS

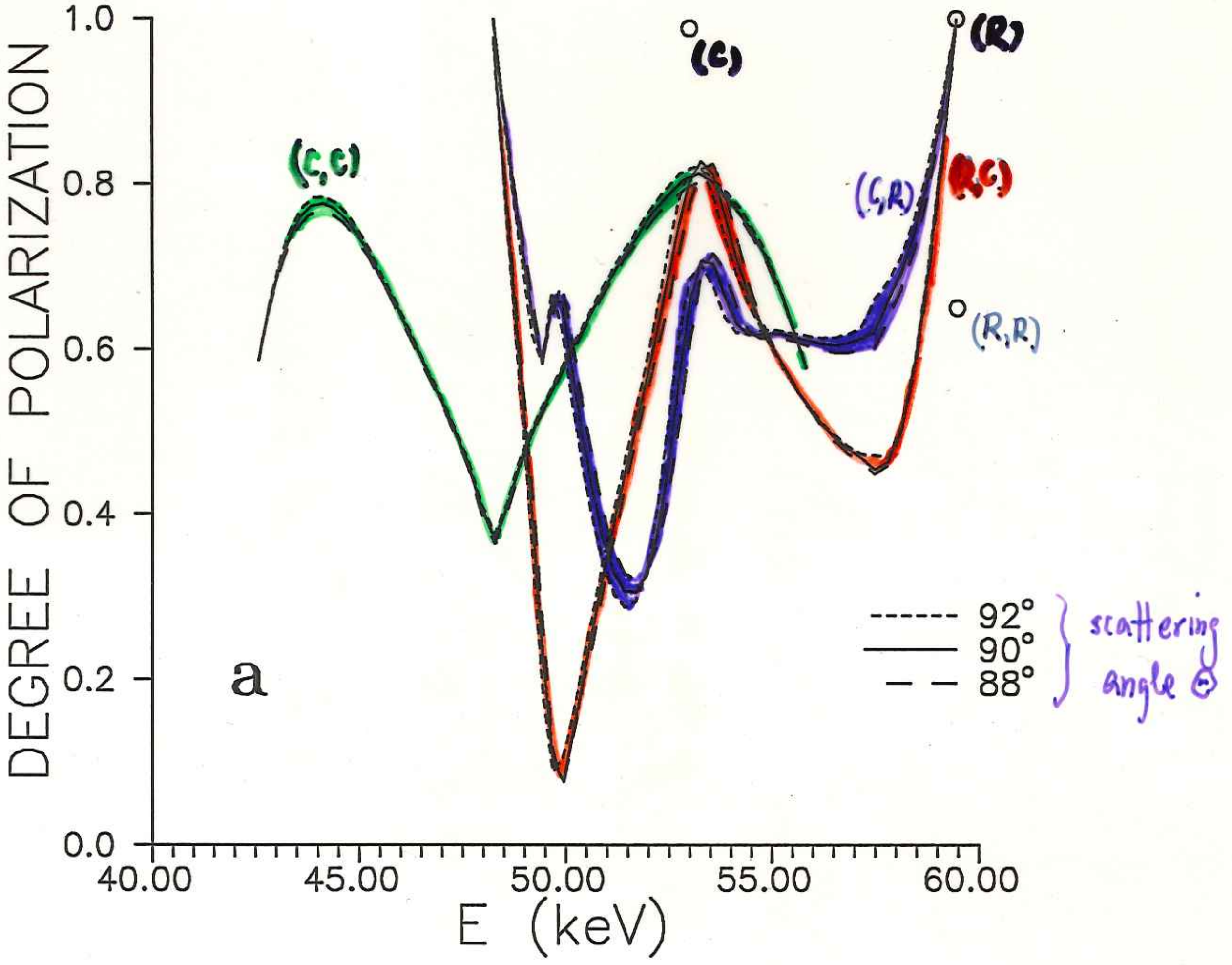


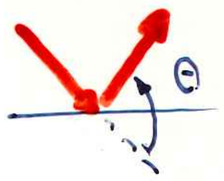


SOURCE: UNPOLARIZED

# DEGREE OF POLARIZATION FOR WATER AND FOR SOME SELECTED COLLISION CHAINS

$E_0 = 59.54$ keV





SOURCE : UNPOLARIZED

# THE TOTAL POLARIZATION STATE IN TERMS OF THE POLARIZATION STATES OF THE CHAINS OF INTERACTIONS

$$\boxed{I} = \sum_i \boxed{I^{(i)}}$$

$$\boxed{P} = \frac{\sum_i I^{(i)} \boxed{P^{(i)}}}{\sum I^{(i)}}$$

$$\boxed{\operatorname{tg} 2\chi} = \frac{\sum_i P^{(i)} I^{(i)} \cos 2\chi^{(i)} \cos 2\beta^{(i)} \boxed{\operatorname{tg} 2\chi^{(i)}}}{\sum_i P^{(i)} I^{(i)} \cos 2\chi^{(i)} \cos 2\beta^{(i)}}$$

$$\boxed{\sin 2\beta} = \frac{\sum_i P^{(i)} I^{(i)} \boxed{\sin 2\beta^{(i)}}}{\sum_i P^{(i)} I^{(i)}}$$

index $^{(i)}$ denotes chain $i$ of interactions

# PROPERTIES OF THE TOTAL POLARIZATION STATE

- ALL THE MAGNITUDES ARE FUNCTIONS OF $E$
- ALL THE WEIGHTS CONTAIN THE FACTOR $I^{(i)}$ (PARTIAL INTENSITY FOR THE CHAIN $i$)
- THE WEIGHTS FOR $tg\, 2\chi$ CAN BE POSITIVE OR NEGATIVE
- ALL THE OTHER WEIGHTS ARE POSITIVE DEFINITE
- THE WEIGHTS ARE NORMALIZED
- WE CAN ANALIZE SEPARATELY EVERY ENERGY BIN FOR INVESTIGATING HOW WAS OBTAINED THE STATE
- FOR A GIVEN ENERGY BIN:
  - a) ONLY CONTRIBUTE THE INTERACTION CHAINS WITH $I^{(i)} \neq 0$
  - b) THE PREVAILING CHAINS RULE THE TOTAL STATE OF POLARIZATION.
- THE COMPUTATION OF THE TOTAL $tg\, 2\chi$ CAN BE AFFECTED BY NUMERICAL CANCELLATION.