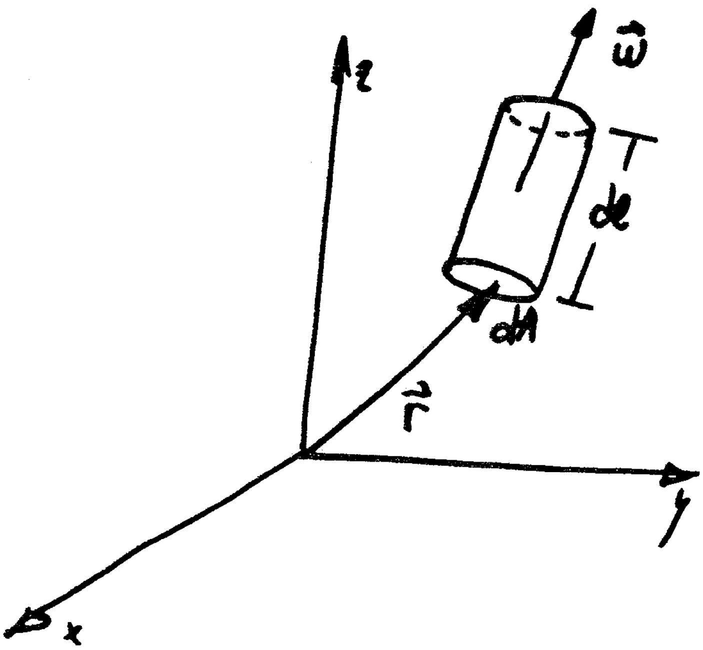
THE BOLTZMANN TRANSPORT EQUATION FOR PHOTONS

- describes the balance between the numbers of photons of given energy and direction entering and leaving an infinitesimal cylinder



- flux $f(\vec{r}, \hat{\omega}, \lambda)\, d\hat{\omega}\, d\lambda$

  the number of photons with wavelengths between λ and $\lambda + d\lambda$ and directions between $\vec{\omega}$ and $\vec{\omega} + d\vec{\omega}$ crossing a unit area per unit time.

- we use λ in place of E (immaterial)
- The net flux with specified direction and λ leaving the cylinder per unit time is

$$f(\vec{r} + \vec{\omega}\, dl, \vec{\omega}, \lambda)\, dA - f(\vec{r}, \vec{\omega}, \lambda)\, dA$$

or

$$\vec{\omega}.\nabla f(\vec{r},\vec{\omega},\lambda)\, dA\, dl$$

in differential form.

- Three factors contribute to this net outflow

(i) "narrow beam" attenuation in the whole volume of the cylinder

$$-\mu(\lambda)\, dl\, dA\, f(\vec{r},\vec{\omega},\lambda)$$

(ii) scattering of photons

$$\vec{\omega}' \rightarrow \vec{\omega}$$
$$\lambda' \rightarrow \lambda$$

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

probability of photon scattering ($\vec{\omega}' \rightarrow \vec{\omega}$, $\lambda' \rightarrow \lambda$) per unit path through the medium and per unit $d\vec{\omega}$ and $d\lambda$

Formerly equivalent to

$$\frac{d\sigma}{d\vec{\omega}\, d\lambda}$$

(iii) The source

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

The density of photons per unit volume, per unit time per steradian and per unit λ.

NEUTRONS (STATIONARY PROBLEM)

$$v\vec{\omega}.\nabla f(\vec{r}, v\vec{\omega}) + \frac{v f}{l_{tot}(v)} =$$

$$= \int \frac{v' \, dv'}{l_{tot}(v')} \iint f(\vec{r}, v'\vec{\Omega}')\, k(v'\vec{\Omega}' \to v\vec{\omega})\, d\vec{\Omega}' + S$$

$f(\vec{r}, v\vec{\omega})\, d\vec{r}\, dv\, d\vec{\omega}$

number of neutrons in d^3r around $\vec{r}$ belonging to $dv\, d\vec{\omega}$ (travelling with speed between v and $v+dv$ in a direction lying within $d\vec{\omega}$ around $\vec{\omega}$.

$v \to E \to \lambda$

$$\frac{1}{l_{tot}} = \Sigma \to \mu$$

THREE-D PHOTON TRANSPORT EQUATION (TIME INDEPENDENT)

$$\vec{\omega}.\nabla f(\vec{r},\vec{\omega},\lambda) = -\mu(\lambda) f(\vec{r},\vec{\omega},\lambda) + $$
$$+ \int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}' \, k(\vec{\omega},\lambda,\vec{\omega}';\lambda') f(\vec{r},\vec{\omega}',\lambda') + S(\vec{r},\vec{\omega},\lambda) \quad (1)$$

ASSUMPTIONS

- the x-ray source is constant in time, and
- is monochromatic and collimated

$$S(\vec{r},\vec{\omega},\lambda) = I_0 \, \delta(\vec{\omega}-\vec{\omega}_0) \, \delta(\lambda-\lambda_0) \, \underline{\delta(\vec{u}.\vec{r} - \vec{u}.\vec{r}_0)}$$

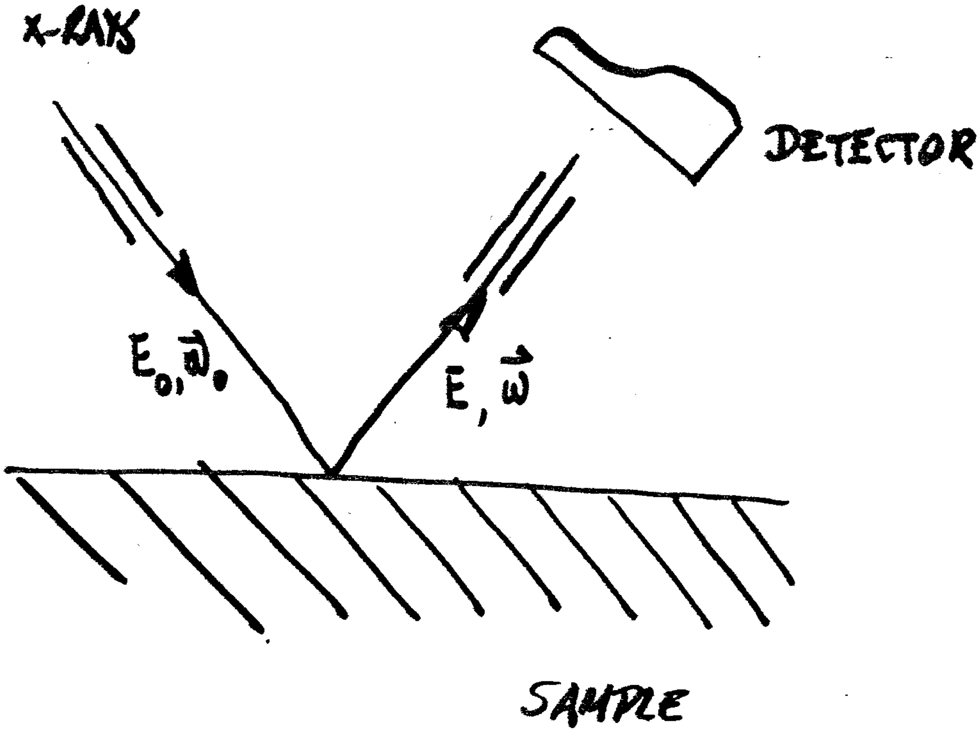
the plane $\vec{u}.\vec{r} = \vec{u}.\vec{r}_0$ defined by the point $\vec{r}_0$ and normal to $\vec{u}$.

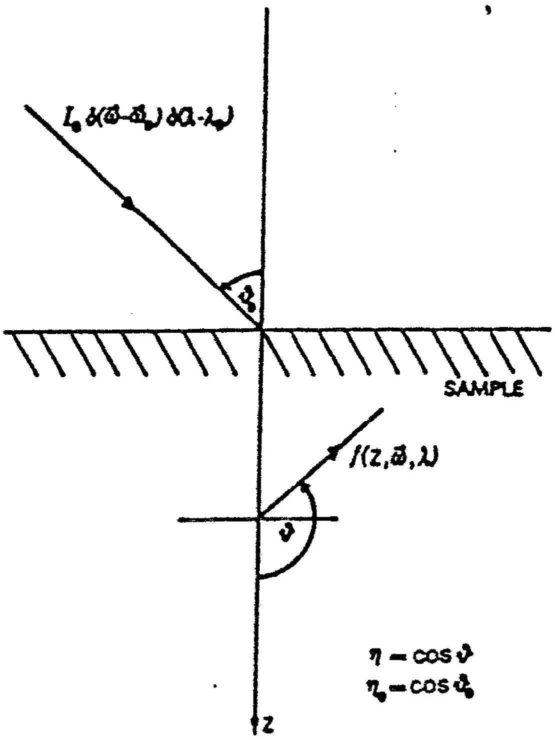
- for an infinite and homogeneous target we get that the source depends on the single space coordinate

$$\vec{r}.\vec{\Omega} \quad (\text{for arbitrary } \vec{\Omega})$$

and the eqn (1) reduces to

$$\eta \frac{\partial f(\vec{r},\vec{\omega},\lambda)}{\partial z} = -\mu(\lambda) f(z,\vec{\omega},\lambda) + $$
$$+ \int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}' \, k(\vec{\omega},\lambda,\vec{\omega}';\lambda') f(z,\vec{\omega}';\lambda') + I_0 \, \delta(z) \, \delta(\vec{\omega}-\vec{\omega}_0) \, \delta(\lambda-\lambda_0)$$





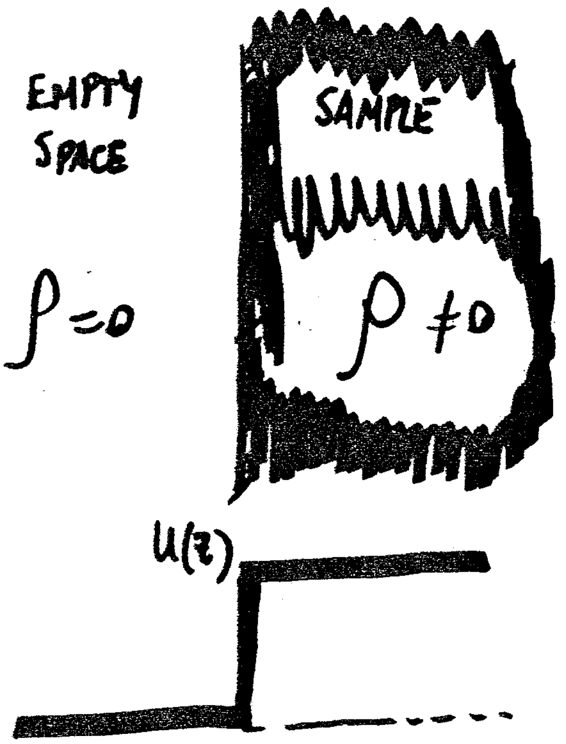
Irradiation arrangement of a homogeneous specimen of infinite thickness under the excitation of a plane monochromatic X-ray source, represented with the photon transport equation (1).

We need to consider a semi-infinite space

$$\eta \frac{\partial f(z,\vec{w},\lambda)}{\partial z} = -\mu(\lambda) f(z,\vec{w},\lambda) + \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, \underline{U(z)}\, k(\vec{w},\lambda,\vec{w}';\lambda')\, f(z,\vec{w}';\lambda') + I_0\, \delta(z)\, \delta(\vec{w}-\vec{w}_0)\, \delta(\lambda-\lambda_0) \tag{2}$$

Heaviside step function

$$U(z) = \begin{cases} 0 & z<0 \\ 1 & z>0 \end{cases}$$

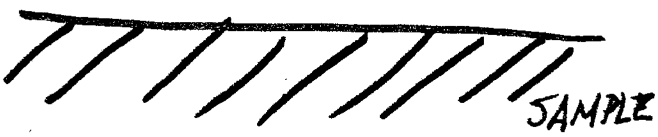


- empty space does not restitute photons (Photons going left does not return.
- Boltzmann Eqn remains unchanged
- $\mu(\lambda)$ remains unchanged

The change in the density ρ <u>is not</u> a requirement.

The properties of the physical model are completely defined by the <u>non-restitution</u> of the upper half-space.

$\rho \neq 0$ only absorbing medium



$\rho \neq 0$ absorbing and interacting medium

Absence of interactions in the upper semi-space prevents the return of photons escaping in that direction.

<u>Advantage</u>: μ <u>does not</u> change

DEVELOPMENT IN ORDERS OF INTERACTION (Neumann Series)

$$f = f^{(0)} + f^{(1)} + f^{(2)} + \dots + f^{(n)} + \dots$$

where

$f^{(n)}$ is the n-th order flux, i.e. the flux due to a chain of n interactions

By substitution in (2) we obtain an equation set

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

$$+ \int_0^\infty d\lambda' \int_{4\pi} d\vec{\omega}'\, k(\vec{\omega},\lambda,\vec{\omega}';\lambda')\, U(z)\, f^{(n-1)}(z,\vec{\omega}';\lambda')\,[1-\delta_{n0}]$$

$$+ I_0\, \delta(z)\, \delta(\vec{\omega}-\vec{\omega}_0)\, \delta(\lambda-\lambda_0)\, \delta_{n0} \qquad (n=0,1,2,\dots) \qquad (3)$$

which is the equation to be solved.

METHOD OF SOLUTION FOR Eq (3)

We split the flux into its <u>even</u> and <u>odd</u> parts

$$f_+(z) = \frac{1}{2}\left(f(z) + f(-z)\right) \quad \text{(even)}$$

$$f_-(z) = \frac{1}{2}\left(f(z) - f(-z)\right) \quad \text{(odd)}$$

In order to do this we write the set of equations (3) for $-z$:

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

$$+ \int_0^\infty d\lambda' \int_{4\pi} d\hat{\omega}'\, k(\vec{\omega},\lambda,\hat{\omega}';\lambda')\, U(-z) f^{(m-1)}(-z,\vec{\omega}';\lambda') \left[1-\delta_{m0}\right]$$

$$+ I_0\, \delta(-z)\, \delta(\vec{\omega}-\vec{\omega}_0)\, \delta(\lambda-\lambda_0)\, \delta_{m0} \qquad (4)$$

By the delta property

$$\delta(ax) = \frac{1}{|a|}\delta(x) \Rightarrow \delta(z) = \delta(-z)$$

and

$$U(z) = \frac{1}{2}(1 + \operatorname{sgn} z)$$

$$\operatorname{sgn} z = \begin{cases} 1 & z > 0 \\ 0 & z = 0 \\ -1 & z < 0 \end{cases}$$

and $\operatorname{sgn}(-z) = -\operatorname{sgn} z$

So

$$U(-z) = \frac{1}{2}\left(1 - \operatorname{sgn} z\right)$$

By adding and substracting Eqns (3) and (4) and using the above properties we get

$(3) + (4) \Rightarrow$

$$\eta \frac{\partial}{\partial z}\left(f^{(m)}(+z) - f^{(m)}(-z)\right) = -\mu(\lambda)\left(f^{(m)}(z) + f^{(m)}(-z)\right) +$$

$$+ \left\{ \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, k(\vec{w}, \lambda, \vec{w}'; \lambda') \frac{\left[f^{(m-1)}(z) + f^{(m-1)}(-z)\right]}{2} + \right.$$

$$\left. + \operatorname{sgn} z \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, k(\vec{w}, \lambda, \vec{w}'; \lambda') \frac{\left[f^{(m-1)}(z) - f^{(m-1)}(-z)\right]}{2} \right\}\left[1 - \delta_{m0}\right]$$

$$+ 2\, I_0\, \delta(z)\, \delta(\vec{w} - \vec{w}_0)\, \delta(\lambda - \lambda_0)\, \delta_{m0}$$

which can be written as

$$\eta \frac{\partial}{\partial z} f_-^{(n)} = -\mu(\lambda) f_+^{(n)} +$$

$$+ \frac{1}{2}\left\{ \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}';\lambda')\, f_+^{(n-1)}(z,\vec{w}';\lambda') + \right.$$

$$\left. + \operatorname{sgn} z \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}';\lambda')\, f_-^{(n-1)}(z,\vec{w}',\lambda') \right\}[1-\delta_{n0}]$$

$$+ I_0\, \delta(z)\, \delta(\vec{w}-\vec{w}_0)\, \delta(\lambda-\lambda_0)\, \delta_{n0}$$

We denote as $\hat{I}$ the <u>operator</u>

$$\hat{I} = \int_0^\infty d\lambda' \int_{4\pi} d\vec{w}'\, k(\vec{w},\lambda,\vec{w}';\lambda')$$

and then we can rewrite the above eqn as follows

$$\eta \frac{\partial}{\partial z} f_-^{(n)} = -\mu(\lambda) f_+^{(n)} +$$

$$+ \left\{ \frac{1}{2} \hat{I} f_+^{(n-1)} + \frac{1}{2} \hat{I} \operatorname{sgn} z\, f_-^{(n-1)} \right\} (1-\delta_{n0})$$

$$+ I_0\, \delta(z)\, \delta(\vec{w}-\vec{w}_0)\, \delta(\lambda-\lambda_0)\, \delta_{n0} \qquad (5.a)$$

Similarly (3)-(4) gives (HOMEWORK)

$$q \frac{\partial f_+^{(n)}}{\partial z} = -\mu(\lambda) f_-^{(n)} +$$

$$+ \left\{ \frac{1}{2} \hat{I} f_-^{(n-1)} + \frac{1}{2} \hat{I} \operatorname{sgn} z \, f_+^{(n-1)} \right\} (1 - \delta_{n0})$$

(5.6)

The operator $\hat{I}$ commutes with functions of z (only)

$$\hat{I} g(z) = g(z) \hat{I}$$

but not with $f_+^{(n)}$ or $f_-^{(n)}$.

We can <u>Fourier transform</u> Eqns (5.a) and (5.5)

Definition

Fourier transform of a function $g(z)$

$$\mathcal{F}(g(z)) = \tilde{g}(q)$$

$$= \int_{-\infty}^{\infty} dz \, e^{-iqz} g(z)$$

Fourier transform gives real and imaginary parts, then

$$\tilde{g}(q) = Re(\tilde{g}) + i \, Im(\tilde{g})$$

$\boxed{Re(\tilde{g}) = \frac{1}{2}\mathcal{F}(g_+)}$ and $\boxed{i\, Im(\tilde{g}) = \frac{1}{2}\mathcal{F}(g_-)}$

to give

$$i q \eta \tilde{f}_-^{(n)} = -\mu(\lambda) \tilde{f}_+^{(n)} +$$

$$+ \left\{ \frac{1}{2} \hat{I} \tilde{f}_+^{(n-1)} + \frac{1}{2} \hat{I} \mathcal{F}\left[\operatorname{sgn} z \, f_-^{(n-1)} \right] \right\} (1 - \delta_{n0})$$

$$+ I_0 \, \delta(\vec{w} - \vec{w}_0) \, \delta(\lambda - \lambda_0) \, \delta_{n0}$$

we have used the properties of the Fourier Transform

$$\mathcal{F}\left(\frac{\partial g}{\partial z} \right) = i q \tilde{g}$$

$$\mathcal{F}(\delta(z)) = 1$$

Still we can use a convolution property (in frequency)

$$\mathcal{F}(g_1(z) \, g_2(z)) = \tilde{g}_1 \otimes \tilde{g}_2$$

$$\equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{g}_1(y) \, \tilde{g}_2(q - y) \, dy$$

in the case of above we get

$$\mathcal{F}\left[\operatorname{sgn} z \, f_-^{(n-1)} \right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{F}(\operatorname{sgn} z) \Big|_{q-y} \, \mathcal{F}\left(f_-^{(n-1)} \right) \Big|_{y} \, dy$$

$$= \frac{1}{\cancel{2}\pi}\int_{-\infty}^{\infty} dy \, \frac{2}{i(q-y)} \, \tilde{f}_-^{(n-1)}$$

$$= -\frac{i}{\pi}\int_{-\infty}^{\infty} dy \, \frac{1}{(q-y)} \, \tilde{f}_-^{(n-1)} \qquad \boxed{\mathcal{F}(\mathrm{sgn}\, z) = \frac{2}{iq}}$$

Fourier transform of (5.a) finally gives

$$iq\eta \, \tilde{f}_-^{(n)} = -\mu(\lambda)\, \tilde{f}_+^{(n)} +$$

$$+\left[\frac{1}{2}\, \hat{I}\, \tilde{f}_+^{(n-1)} - \frac{i}{2}\, \hat{I}\, \hat{k}\, \tilde{f}_-^{(n-1)}\right](1-\delta_{n0})$$

$$+ I_0\, \delta(\vec{w}-\vec{w}_0)\, \delta(\lambda-\lambda_0)\, \delta_{n0} \qquad (6.a)$$

where we have defined

$$\hat{K} = \frac{1}{\pi}\int_{-\infty}^{\infty} dy \, \frac{1}{(q-y)}$$

Transformation of (5.b) gives (HOMEWORK)

$$iq\eta \, \tilde{f}_+^{(n)} = -\mu(\lambda)\, \tilde{f}_-^{(n)} + \left[\frac{1}{2}\, \hat{I}\, \tilde{f}_-^{(n-1)} - \frac{i}{2}\, \hat{I}\, \hat{k}\, \tilde{f}_+^{(n-1)}\right]$$

$$\left[1-\delta_{n0}\right]$$

$$(6.b)$$

For $n=0$ Eqns (6.a) and (6.b) give

$$i q \eta \tilde{f}_-^{(0)} = -\mu(\lambda) \tilde{f}_+^{(0)} + I_0 \,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$$

$$i q \eta \tilde{f}_+^{(0)} = -\mu(\lambda) \tilde{f}_-^{(0)}$$

from which

$$\tilde{f}_+^{(0)} = \frac{\mu}{\mu^2 + q^2\eta^2} I_0 \,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$$

$$\tilde{f}_-^{(0)} = \frac{-iq\eta}{\mu^2 + q^2\eta^2} I_0 \,\delta(\vec{w}-\vec{w}_0)\,\delta(\lambda-\lambda_0)$$

The solution in the physical space is obtained by using the Fourier inversion formula for real functions

since the flux is real!

$$g(z) = \frac{1}{\pi} \mathrm{Re}\left\{ \int_0^\infty dq\, e^{iqz}\, \tilde{g}(q) \right\}$$

is real

Indeed, it can be shown that (HOMEWORK)

$$f^{(0)}(z,\vec{\omega},\lambda) = \frac{I_0}{2|\eta|}\,\delta(\vec{\omega}-\vec{\omega}_0)\,\delta(\lambda-\lambda_0)\,e^{-\frac{\mu|z|}{|\eta|}}$$

$$(1+\operatorname{sgn}\eta\,\operatorname{sgn} z)$$

For $\underline{n>0}$ Eqns (6) give

$$iq\eta\,\tilde{f}_-^{(n)} = -\mu(\lambda)\tilde{f}_+^{(n)} + \frac{1}{2}\hat{I}\tilde{f}_+^{(n-1)} - \frac{i}{2}\hat{I}\hat{k}\tilde{f}_-^{(n-1)}$$
$$iq\eta\,\tilde{f}_+^{(n)} = -\mu(\lambda)\tilde{f}_-^{(n)} + \frac{1}{2}\hat{I}\tilde{f}_-^{(n-1)} - \frac{i}{2}\hat{I}\hat{k}\tilde{f}_+^{(n-1)}$$

in matrix way

$$\underbrace{\begin{pmatrix} iq\eta & \mu \\ \mu & iq\eta \end{pmatrix}}_{\mathbb{A}}\underbrace{\begin{pmatrix} \tilde{f}_-^{(n)} \\ \tilde{f}_+^{(n)} \end{pmatrix}}_{\hat{\mathbb{P}}\tilde{f}^{(n)}} = \frac{\hat{I}}{2}\underbrace{\begin{pmatrix} -i\hat{k} & 1 \\ 1 & -i\hat{k} \end{pmatrix}}_{\mathbb{K}}\underbrace{\begin{pmatrix} \tilde{f}_-^{(n-1)} \\ \tilde{f}_+^{(n-1)} \end{pmatrix}}_{\hat{\mathbb{P}}\tilde{f}^{(n-1)}}$$

$$\Rightarrow \mathbb{A}\hat{\mathbb{P}}\tilde{f}^{n} = \frac{\hat{I}}{2}\mathbb{K}\hat{\mathbb{P}}\tilde{f}^{(n-1)} \qquad (7)$$

where

$$\hat{P}\tilde{f}^{(n)} = \begin{pmatrix} \tilde{f}_-^{(n)} \\ \tilde{f}_+^{(n)} \end{pmatrix}$$

projection on the even and odd parts

From Equ (7) we have

$$\hat{P}\tilde{f}^{(n)} = \mathbb{A}^{-1}\,\frac{\hat{I}}{2}\,\mathbb{K}\,\hat{P}\tilde{f}^{(n-1)}$$

$$= \frac{\hat{I}}{2}\,\mathbb{A}^{-1}\mathbb{K}\,\hat{P}\tilde{f}^{(n-1)} \qquad (8)$$

By using recursively the last equation we found

$$\hat{P}\tilde{f}^{(n)} = 2^{1-n}\left[\mathbb{A}^{-1}\mathbb{K}\,\hat{I}\right]^{n-1}\hat{P}\tilde{f}^{(0)} \qquad (9)$$

and finally we obtain for the total flux

$$\hat{P}\tilde{f} = \sum_{n=1}^{\infty} 2^{1-n}\left[\mathbb{A}^{-1}\mathbb{K}\hat{I}\right]^{n-1}\hat{P}\tilde{f}^{(0)}$$

In the physical space Eqn (9) can be written as

$$\hat{P}f^{(n)} = \frac{\hat{I}}{2} R_e\left(\mathcal{F}^{-1}\left\{\mathbb{A}^{-1}\mathbb{K}\hat{P}\tilde{f}^{(n-1)}\right\}\right)$$

$$= \frac{\hat{I}}{2} R_e\left[\mathcal{F}^{-1}(\mathbb{A}^{-1}) \otimes \mathcal{F}^{-1}(\mathbb{K}\hat{P}\tilde{f}^{(n-1)})\right]$$

$$= \frac{\hat{I}}{2} R_e\left(\mathcal{F}^{-1}(\mathbb{A}^{-1}) \otimes \begin{pmatrix} \operatorname{sgn} z & 1 \\ 1 & \operatorname{sgn} z \end{pmatrix}\hat{P}f^{(n-1)}\right)$$

$\Rightarrow$ (HOMEWORK)

Note that the noncommutability of the matrix operator with the projection operator $\hat{P}$ means that the solution parity cannot be preserved at any order.

$$f^{(n)}(z,\vec{w},\lambda) = \frac{\hat{I}}{2|\eta|}\int_0^{\infty} d\tau\, e^{-\frac{|z-\tau|\mu}{|\eta|}} \times$$

$$\times\left(1+\operatorname{sgn}\eta\,\operatorname{sgn}(z-\tau)\right)f^{(n-1)}(\tau,\vec{w}',\lambda') \qquad (10)$$

We can divide the integral in τ according to the sign of $z-\tau$ which gives different results depending on the sign of z:

POSITIVE z

$$f^{(n)}(z,\vec{\omega},\lambda) = \frac{1}{|\eta|}\left\{ \frac{1+\mathrm{sgn}\,\eta}{2}\, e^{-\frac{z\mu}{|\eta|}} \int_0^z d\tau\, e^{\frac{\tau\mu}{|\eta|}}\, \hat{I} f^{(n-1)}(\tau,\vec{\omega};\lambda') \right.$$

$$\left. + \frac{1-\mathrm{sgn}\,\eta}{2} \int_0^\infty d\tau\, e^{-\frac{\tau\mu}{|\eta|}}\, \hat{I} f^{(n-1)}(\tau+z,\vec{\omega};\lambda') \right\} \tag{11}$$

NEGATIVE z

$$f^{(n)}(z,\vec{\omega},\lambda) = \frac{1}{|\eta|}\, \frac{1-\mathrm{sgn}\,\eta}{2}\, e^{-\frac{|z|\mu}{|\eta|}} \int_0^\infty d\tau\, e^{-\frac{\tau\mu}{|\eta|}}\, \hat{I} f^{(n-1)}(\tau,\vec{\omega};\lambda') \tag{12}$$

For $z \to 0$ the flux given by Eqns (11) and (12) coincide $\longrightarrow$ ALBEDO FLUX

The intensity is given by (12')

$$I^{(n)}(\vec{\omega},\lambda) = |\eta|\, \underbrace{f^{(n)}(0,\vec{\omega},\lambda)}_{\text{albedo flux}}$$

Problem: An analogous problem to the albedo intensity emitted by an infinite thickness target is that of finding the reflected and transmitted intensities through a plane slab of thickness d.

Show that the flux into the slab can be expressed as

$$f(z,\vec{\omega},\lambda) = f^{(0)}(z,\vec{\omega},\lambda) + f^{(1)}(z,\vec{\omega},\lambda) + \dots$$

where

$$f^{(0)}(z,\vec{\omega},\lambda) = \frac{I_0}{2|\eta|}\,\delta(\vec{\omega}-\vec{\omega}_0)\,\delta(\lambda-\lambda_0)\,e^{-\frac{\mu|z|}{|\eta|}}\,(1+\operatorname{sgn}\eta\,\operatorname{sgn} z)$$

and

$$f^{(n)}(z,\vec{\omega},\lambda) = \frac{\hat{I}}{2|\eta|}\int_0^d d\tau\, e^{-\frac{|z-\tau|\mu}{|\eta|}}\,(1+\operatorname{sgn}\eta\,\operatorname{sgn}(z-\tau))\,f^{(n-1)}(\tau,\vec{\omega}',\lambda')$$

for $n>0$.

Find expressions for the first- and second-order (reflected and transmitted) fluxes on the faces of the target.

Hint: Substitute $U(z)$ in the transport equation (2) with $U(z)-U(z-d)$

THE INTERACTIONS

- defined by the kernel $k(\vec{\omega},\lambda,\vec{\omega};\lambda')$
- photon-photon interaction (neglecting electron production)
- $k(\omega,\lambda,\vec{\omega};\lambda') \rightarrow \dfrac{d\sigma}{d\vec{\omega}\, d\lambda}$

Then

$$\sigma(\vec{\omega}';\lambda') = \int d\vec{\omega} \int d\lambda \; k(\vec{\omega},\lambda,\vec{\omega}';\lambda') \qquad (13)$$

is the scattering coefficient for the given process.

- We will consider three types of interaction

photoelectric effect	τ
scattering Rayleigh	σ_R
scattering Compton	σ_C

- For energies between 1 and 100 keV the main interactions are these, therefore

$$\mu = \tau + \sigma_R + \sigma_C$$

μ — total attenuation coefficient

Elementary X-Ray effects

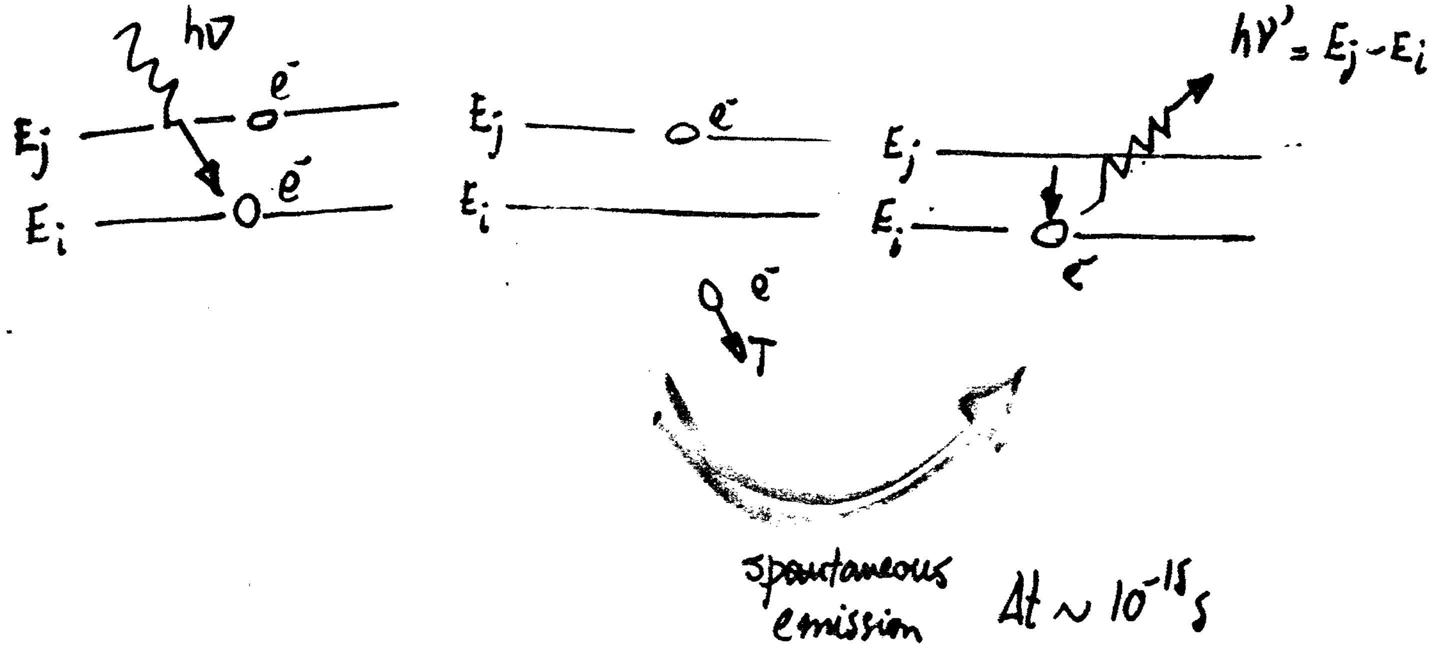
Type of effect / Carrier	Absorption	Scattering: Elastic		Scattering: Inelastic
Atomic electrons	$\boxed{\text{Photoelectric effect}}$	$\boxed{\text{Rayleigh scattering}}$	Anomalous dispersion	$\boxed{\text{Compton scattering}}$
Electron-positron field	Pair production	Delbrück scattering		
Nucleons	Photonuclear (γ,n), (γ,p), etc	(γ,γ) Low energy limit: Thompson scattering		$(\gamma,\gamma)'$
Mesons	Photomeson production	Modified (γ,γ)		

Photoelectric effect

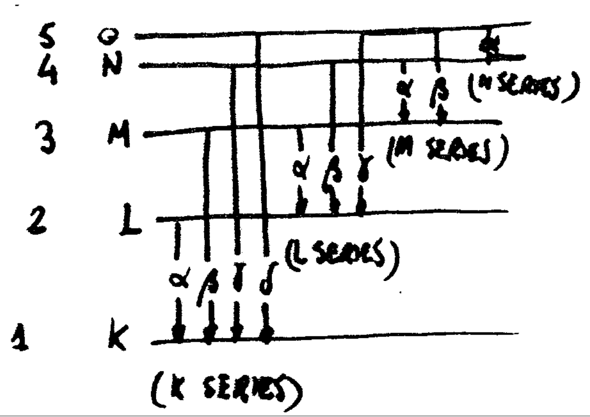
$\boxed{\text{photoelectric effect}}$ produces $\boxed{\text{photon absorption}}$ giving $\begin{cases} e^- \\ \text{Kinetic energy} \end{cases}$

$\boxed{\text{electron emission}}$ produces $\boxed{\text{hole}}$ giving $\boxed{\text{transition from higher energy levels}}$

photon - photon interaction



ELECTRONIC TRANSITIONS



MOSELEY LAW

The energy levels for an hydrogenic atom Z are given by

$$E_n = -R_\infty \, hc \left(\frac{M}{M+m}\right) \frac{Z^2}{n^2} \qquad n = 1, 2, 3, \ldots$$

R_∞ — Rydberg constant

n — the quantum number of the level

$$R_\infty = 2\pi^2 \frac{m e^4}{c h^3} = 13.6 \text{ eV}$$

The energy of a transition from n_i to n_f is

$$h\nu = R_\infty \, hc \left(\frac{M}{M+m_e}\right) Z^2 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad \text{hydrogenic atom}$$

Atom with many electrons

Nuclear charge $\rightarrow (Z - \sigma) e$

σ — screening constant

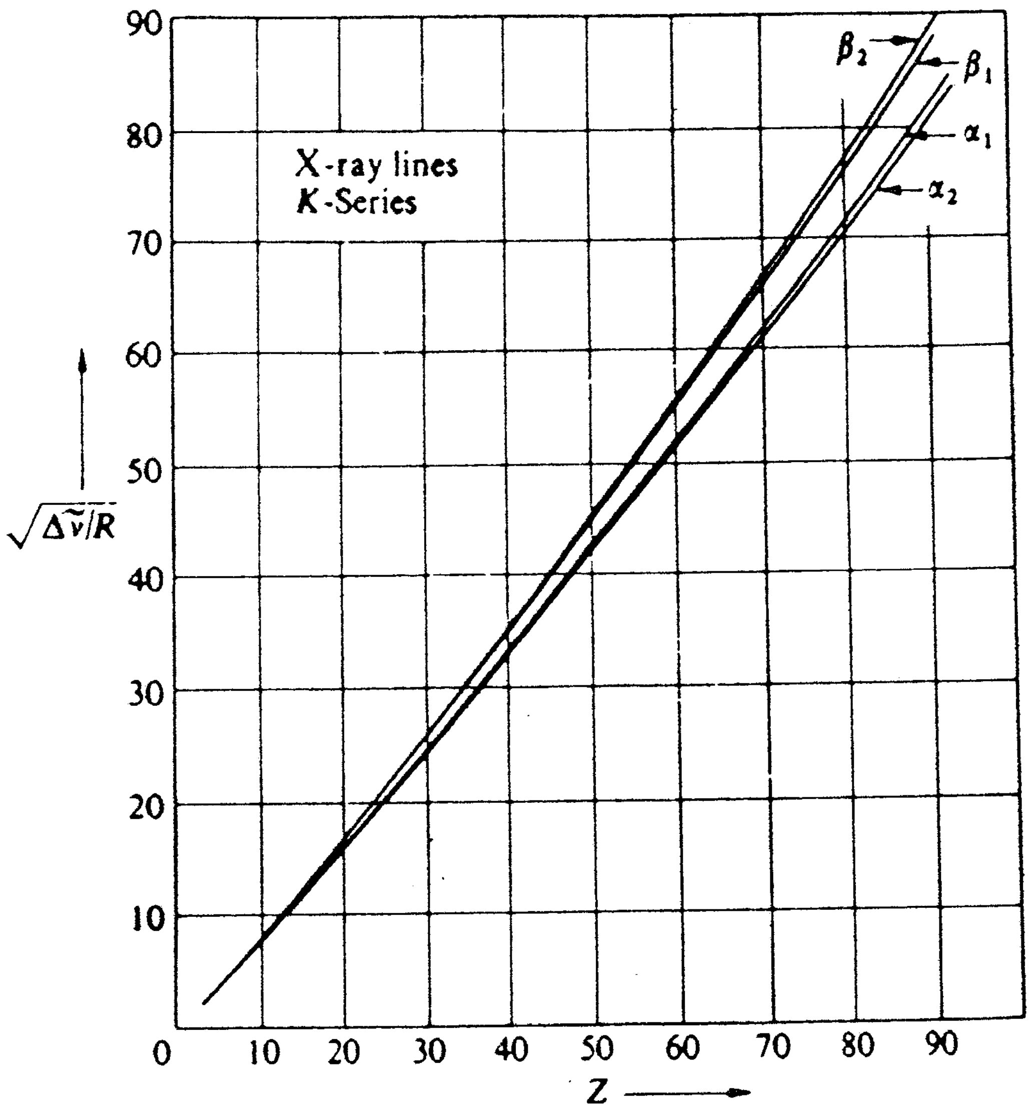
$$h\nu_K \simeq R_\infty \, hc \, (Z - \sigma_K)^2 \left(\frac{1}{1^2} - \frac{1}{2^2}\right) = \frac{3}{4} R_\infty \, hc \, (Z - \sigma_K)^2$$

$$\left(\frac{\nu}{cR}\right)^{1/2}_{K_\alpha} = 0.874 \, (Z - 1.13) \qquad \text{(Moseley law)}$$

$\boxed{\text{stright line}}$

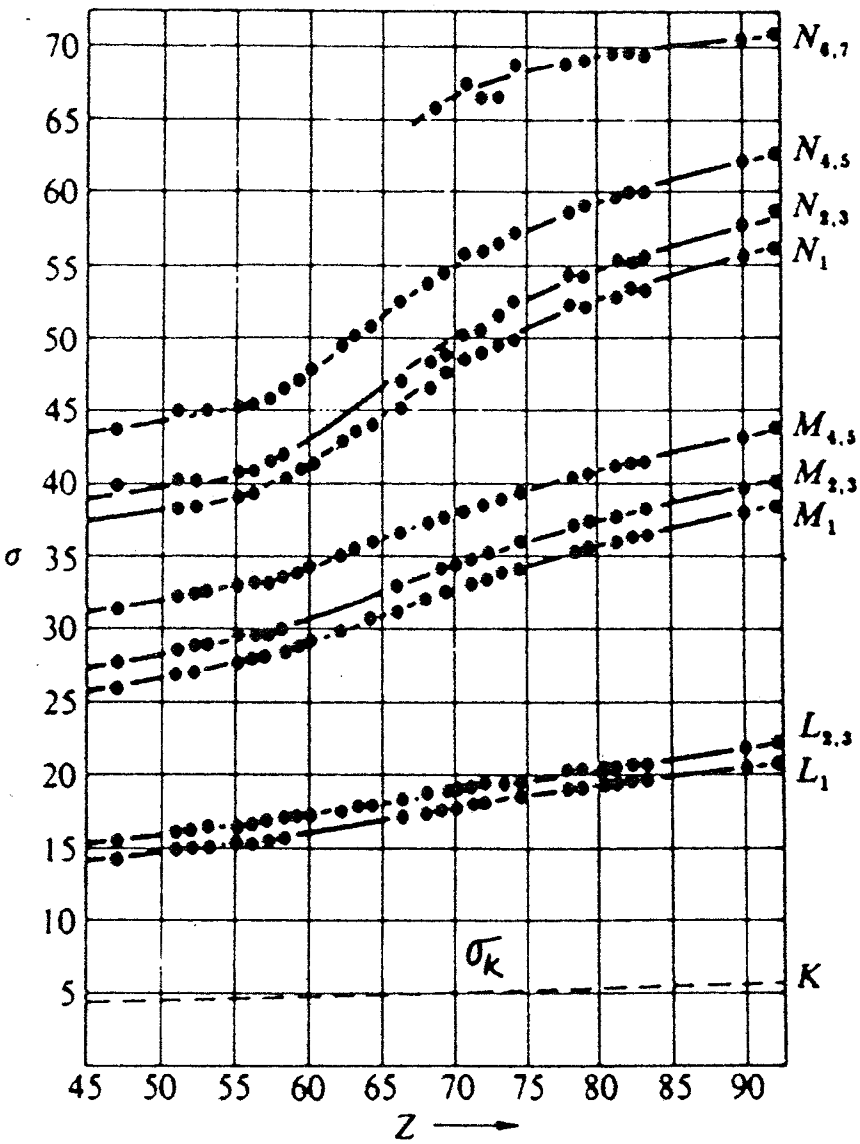
(22J)

Fig. 3.5. K-series lines, illustrating Moseley's law. (White, 1934).



(22-2)

Fig. 3.6. Screening constant σ_s. (After A. Sömmerfeld *Atombau and Spekrallinien*, 1944, Braunschweig: Vieweg. For an English translation of an earlier edition of this text, see Sömmerfeld (1934)).



X-Ray Terms

Wave function for the stationary state of the hydrogen-like atom

$$\psi_{nlmm_s} = R_{nl}(r)\, Y_l(\theta)\, Z_m(\phi)\, \psi_{spin}$$

$n = 1, 2, 3 \ldots$ $\boxed{K, L, M}$ — principal quantum number $\rightarrow$ SHELL and ENERGY

$0 \le l < n$ $\boxed{1, 2, 3, 4, 5 \ldots}$ $\boxed{s, p, d, f, g \ldots}$ — orbital angular momentum $\rightarrow$ SUBSHELL

$-l \le m \le l$ — magnetic quantum number

$m_s = \pm \frac{1}{2}$ — spin orientation

$\boxed{\text{CONFIGURATION}}$

Pauli's exclusion principle: no two electrons in an atom can have the same four quantum numbers

electrons in a subshell $\rightarrow$ $\underbrace{2}_{\text{spin} \uparrow\downarrow}\ \underbrace{(2l+1)}_{\text{different values of } m \text{ corresponding to the subshell } l}$

States with different energy are characterised by n (E_n)

$\Rightarrow$ **degeneracy** (many states ψ_{nlmm_s} have the same energy)

Degeneracy is broken if we consider spin-orbit interaction

$j = l \pm m_s$ — total angular momentum

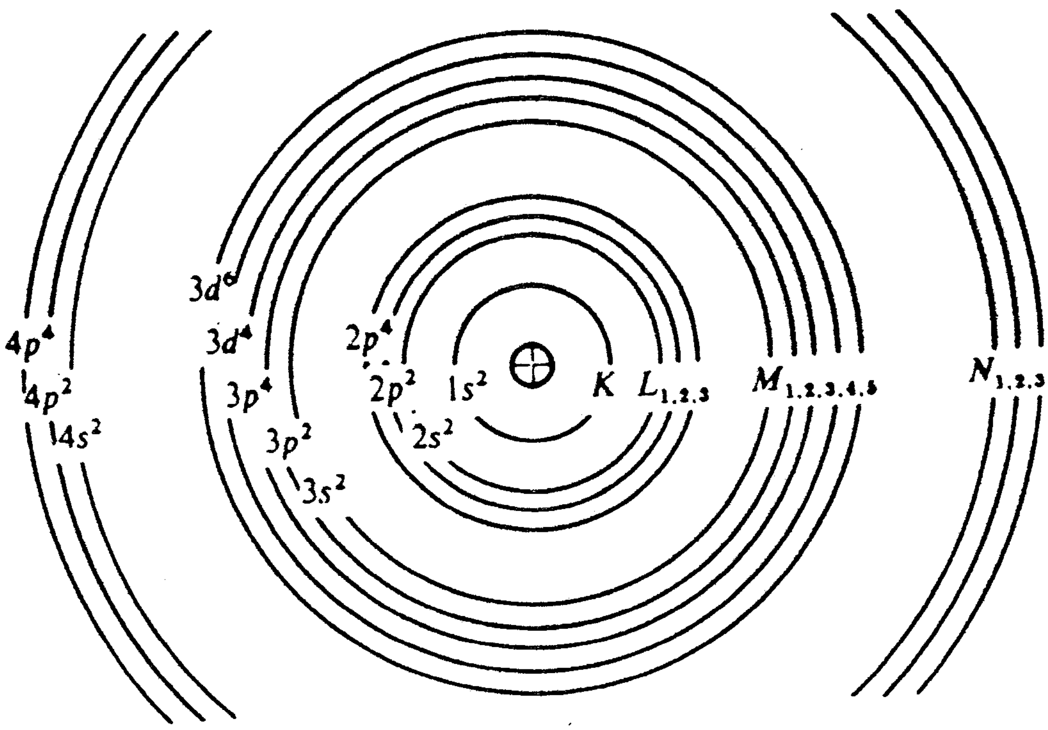
$-j \le m_j \le j$ — $nljm_j$

(23-1)

Table 3.1 *Electronic orbits, with quantum numbers*

n	ℓ	j			
1	0	$\frac{1}{2}$	1s	K	1s
2	0	$\frac{1}{2}$	$2s\frac{1}{2}$	L_1	2s
2	1	$\frac{1}{2}$	$2p\frac{1}{2}$	L_2	2p
2	1	$\frac{3}{2}$	$2p\frac{3}{2}$	L_3	
3	0	$\frac{1}{2}$	$3s\frac{1}{2}$	M_1	3s
3	1	$\frac{1}{2}$	$3p\frac{1}{2}$	M_2	3p
3	1	$\frac{3}{2}$	$3p\frac{3}{2}$	M_3	
3	2	$\frac{3}{2}$	$3d\frac{3}{2}$	M_4	3d
3	2	$\frac{5}{2}$	$3d\frac{5}{2}$	M_5	
4	0	$\frac{1}{2}$	$4s\frac{1}{2}$	N_1	4s
4	1	$\frac{1}{2}, \frac{3}{2}$	$4p\frac{1}{2}, \frac{3}{2}$	$N_{2,3}$	4p
4	2	$\frac{3}{2}, \frac{5}{2}$	$4d\frac{3}{2}, \frac{5}{2}$	$N_{4,5}$	4d
4	3	$\frac{5}{2}, \frac{7}{2}$	$4f\frac{5}{2}, \frac{7}{2}$	$N_{6,7}$	4f

Fig. 3.1. The Bohr atom–shells and sub-shells of krypton. In the designation $3d^6$ (for example), 3 refers to the principal quantum number n, d refers to the angular momentum quantum number ℓ ($\ell = 0, 1, 2, 3, \ldots$ is indicated by the letters $s, p, d, f, \ldots$) and the superscript indicates the number of the electrons in the sub-shell.



Spectroscopic notation

nl_j^{-1} $\longrightarrow$ $1s_{1/2}^{-1}$ K

$2s_{1/2}^{-1}$ L_I $2p_{1/2}^{-1}$ L_{II} $2p_{3/2}^{-1}$ L_{III}

hole or missing electron $3s_{1/2}^{-1}$ M_I $3p_{1/2}^{-1}$ M_{II} $3p_{3/2}^{-1}$ M_{III} $3d_{3/2}^{-1}$ M_{IV} $3d_{5/2}^{-1}$ M_V

x-rays are produced by transitions that fill the holes created by photoelectric effect

Energies of Atomic X-Rays

Non relativistic hamiltonian H_0 (unperturbed)

$$H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

$$H_0 \psi_{nlm} = E_n \psi_{nlm} \quad \text{(Ec. Schrödinger)}$$

$$E_n = - R_\infty hc \frac{Z^2}{n^2} = - \frac{m\alpha^2 c^2}{2} \frac{Z^2}{n^2}$$

Relativistic hamiltonian (perturbation)

$$H = H_0 + H' \qquad H' = -\frac{1}{2mc^2}\left(H_0 + \frac{Ze^2}{r}\right)^2 = -\frac{p^4}{8m^3c^2}$$

$$E_{nl} = E_n + E'_{rel} = E_n\left[1 - (\alpha Z)^2 \frac{1}{n}\left(\frac{3}{4n} - \frac{1}{l+1/2}\right)\right]$$

Removes degeneracy between states with same n and different l

Spin-orbit interaction

$$H = H_0 + H' \qquad H' = \overbrace{\frac{Ze^2\hbar^2}{2m^2c^2}\frac{1}{r^3}}^{\xi(r)} \vec{L}\cdot\vec{S}$$

$$\psi_{nlm m_s} = \psi_{nlm}\,\psi_{spin} = |n l m_l\rangle |m_s\rangle = |n l m_l m_s\rangle$$

$$E'_{spin\text{-}orbit} = \langle nl|\xi(r)|nl\rangle \begin{cases} \dfrac{l}{2} & \text{if } j = l+1/2 \\ -\dfrac{1}{2}(1+l) & \text{if } j = l-1/2 \end{cases}$$

$$\langle nl|\xi(r)|nl\rangle = \frac{R_\infty\, ch\, \alpha^2 Z^4}{n^3\, l(l+1)(l+\frac{1}{2})}$$

Removes $m_l\, m_s$ degeneracy within each configuration (same nl)

$$E_{nlj} = -R_\infty hc \quad \frac{Z^2}{n^2} + \frac{\alpha^2 Z^4}{n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)$$

valid for $j = l+1/2$ and $j = l-1/2$

Screening correction

first term) $\quad Z \to Z - \underbrace{\sigma_1(n,l)}_{\text{total screening constant}}$

second term) $\quad Z \to Z - \underbrace{\sigma_2(n,l)}_{\text{internal screening constant}}$

Atomic x-ray levels

$$\boxed{E_{nlj} = \underbrace{+}_{\text{hole}} R_\infty hc \left\{ \frac{[Z-\sigma_1(n,l)]^2}{n^2} + \frac{\alpha^2[Z-\sigma_2(n,l,j)]^4}{n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right\}}$$

Energy of x-ray lines

X-ray levels
- hole states have positive energy
- neutral atom in its ground state is the zero for energy measurements

X-ray line
- hole transition from a higher level to a lower level on this energy diagram with selection rules

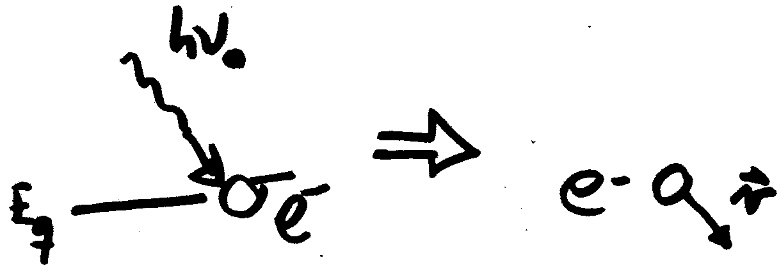
DIAGRAM LINES

$$\begin{cases} \Delta n \neq 0 \\ \Delta l = \pm 1 \\ \Delta j = 0, \pm 1 \end{cases}$$

($\Delta l = \pm 1$, $\Delta j = 0, \pm 1$: electric-dipole selection rules)

suffer further selection depending on parity of the wave function.

Photoelectric effect



$$\underbrace{h\nu_0}_{\text{incident quantum}} = \underbrace{\frac{1}{2} m v^2}_{\text{Kinetic energy of the photoelectrons}} + \underbrace{E_q}_{\text{Binding energy of the electron}}$$

Energy balance of the photoelectric effect

Quantum theory of the photoelectric effect

For a K shell electron

$$E_g = E_k = \frac{1}{2} m c^2 \alpha^2 Z^2 \qquad \text{(unperturbed)}$$

The matrix element for the absorption of a photon is

$$H' = -\frac{e}{m}\left(\frac{\hbar}{V\nu_0}\right)^{1/2} \int \psi_f^* (\vec{p}\cdot\vec{e}_0)\, e^{i\vec{k}_0\cdot\vec{r}}\, \psi_i \, dr$$

volume

momentum operator

polarization Vector

propagation Vector

For K shell electron

$$\psi_i = \left(\frac{a^3}{\pi}\right)^{1/2} e^{-ar} \qquad a = \frac{Z}{a_0} \qquad a_0 = \frac{\hbar^2}{me^2}$$

In Born approximation

$$\psi_f = V^{-1/2}\, e^{i\vec{p}\cdot\vec{r}/\hbar}$$

momentum of free electron

Since ψ_f is an eigenstate of the momentum, we can write

$$\langle f|\, \vec{p}_0\cdot\vec{e}_0\, e^{i\vec{k}_0\cdot\vec{r}}\, |i\rangle = \vec{p}\cdot\vec{e}_0\, \langle f|\, e^{i\vec{k}_0\cdot\vec{r}}\, |i\rangle$$

is a number

then

$$H' = -\frac{e}{mV}\left(\frac{a^3\hbar}{\pi\nu_0}\right)^{1/2}\vec{p}\cdot\vec{e}_0\int_V e^{i\frac{(\vec{k}_0-\vec{p})}{\hbar}\cdot\vec{r}}\,e^{-ar}\,d^3r$$

$$= -\frac{e}{mV}\left(\frac{a^3\hbar}{\pi\nu_0}\right)^{1/2}(\vec{p}\cdot\vec{e}_0)\,\frac{8\pi a}{(a^2+l^2)^2} \qquad \vec{l} = \frac{\vec{k}_0-\vec{p}}{\hbar}$$

The differential cross section is given by

$$d\sigma = \frac{V}{c}\,\frac{2\pi}{\hbar}\,\underline{\rho_f}\,|H'|^2\,d\Omega$$

density of final states $= \dfrac{p\,(mc^2)}{h^3c^2} = \dfrac{mp}{h^3}$

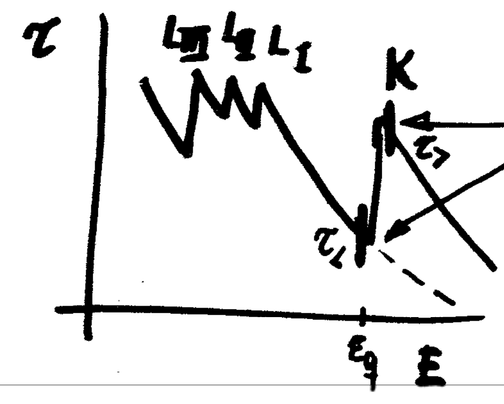
$$\frac{d\sigma}{d\Omega} = \frac{64\,Z^5 a_0^2\,\alpha^8\,(2E/mc^2)^{1/2}\,(\vec{p}\cdot\vec{e}_0)^2}{\left[(\alpha Z)^2 + \frac{2E}{mc^2}\left(1-\frac{v}{c}\,\vec{k}_0\cdot\vec{p}\right)\right]^4}$$

takes into account the photon polarization

Integrated coefficient is

$$\tau_m \propto \nu_0^{-7/2}\,Z^5 \quad \text{as observed}$$

Observed coefficient



two values on either side of the absorption edge at E_q

We define the absorption edge jump

$$r = \frac{\tau_>}{\tau_<} > 1$$

In the region $E > E_k$

$\left(1-\frac{1}{r_k}\right)\tau$ gives the fraction of the total number of photoelectrons that come from the k shell

Ways of filling the vacancy

$\boxed{\text{Radiative}}$

Fluorescence

characteristic lines spectra

$\boxed{\text{Non radiative}}$

Auger effect

an electron is emitted rather than a photon

Coster-Kronig transitions

double ionization giving high energy satellites

Radiative fraction

ω_q fluorescence yield of the q-series

(fraction of radiative transitions in its own series)

Photoelectric kernel

Isotropic (since radiative emission is an spontaneous process separated from photoelectric)

$$k(\omega,\lambda,\bar{\omega};\lambda') = \frac{1}{4\pi}\sum_i Q_{\lambda_i}(\lambda')\,\delta(\lambda-\lambda_i)\left[1-U(\lambda'-\lambda_{e_i})\right]$$

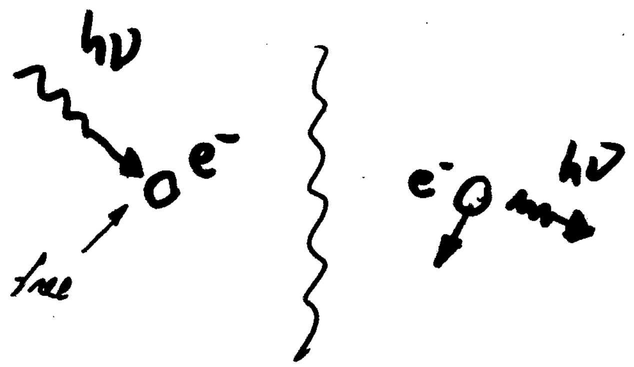
$$Q_{\lambda_i}(\lambda') = \underline{W_s}\,\tau_s(\lambda')\left(1-\frac{1}{r_{\lambda_i}}\right)\omega_{\lambda_i}\,\underline{\Gamma_{\lambda_i}}$$

Weight fraction of element s

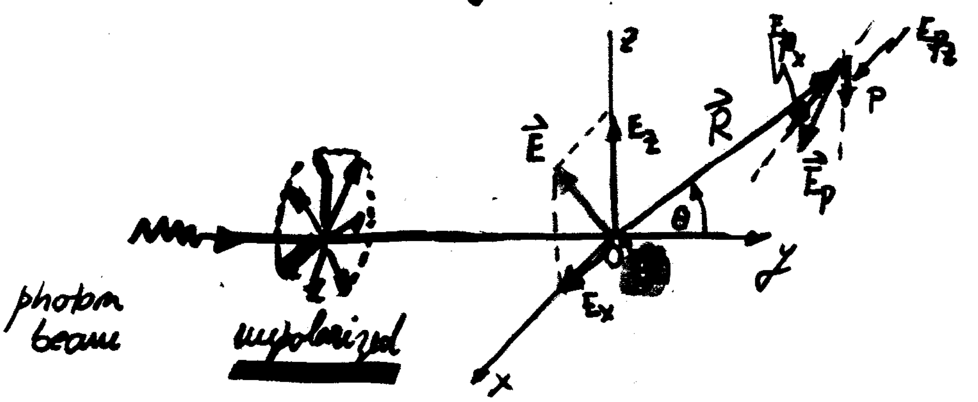
intensity fraction of the line i in its own series

Scattering of x rays

Coherent scattering (Rayleigh)



Classical electrodynamics (THOMPSON)



Electric field of the incident wave at point O (time t): $E = E_0 e^{i\omega t}$

The electron receives an acceleration $\vec{a}$

$$\vec{a} = \frac{e}{m_e}\vec{E}$$ and as an accelerated charge becomes a radiation source (same ω)

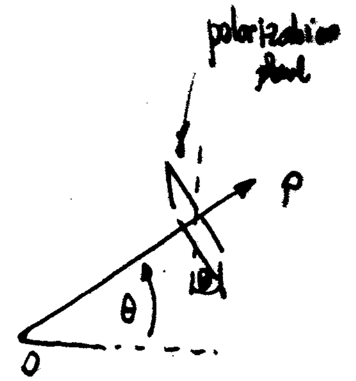
same is nonrelativistic motion

Then there is a scattered wave at point P (at the same t)

$$\vec{E}_P = -\vec{E}\,\frac{e^2}{mc^2 R}\,\sin\theta$$

$$\vec{E} = \vec{E}_0\, e^{i\omega\left(t - \frac{R}{c}\right)}$$

Let P in the plane yz



$$\vec{E}_{p_x} = \frac{e^2}{mc^2 R} \vec{E}_x$$

$$\vec{E}_{p_z} = \frac{e^2}{mc^2 R} \vec{E}_z \cos\theta$$

The ENERGY per unit volume that flows at P is

$$E_p^2 = E_{p_x}^2 + E_{p_z}^2$$

and since $\langle E_x \rangle^2 = \langle E_z \rangle^2 = \frac{\langle E \rangle^2}{2}$ (unpolarized beam)

$$\langle E_p \rangle^2 = \frac{e^4 \langle E \rangle^2}{m^2 c^4 R^2} \left(\frac{1+\cos^2\theta}{2} \right)$$

The INTENSITY $\left(I = \frac{c}{4\pi} |E|^2\right)$ is

$$I = I_0 \frac{r_e^2}{R^2} \left(\frac{1+\cos^2\theta}{2} \right)$$

$r_e = \frac{e^2}{mc^2}$ "classical radius of electron"

The classical differential cross section per electron is

$$\left(\frac{d\sigma_e}{d\Omega} \right)_{\text{Thompson}} = \frac{\text{Energy radiated / unit time / unit solid angle}}{\text{Incident energy flux in energy / unit area / unit time}}$$

$$= \frac{I_e R^2}{I_0} = \frac{r_e^2}{2} (1 + \cos^2\theta)$$

The integrated scattering cross section per electron is

$$\int_{4\pi} d\vec{\omega} \left(\frac{d\sigma_e}{d\vec{\omega}}\right)_{Th} = 2\pi \int_{-1}^{1} d\eta \, \frac{r_e^2}{2}(1+\eta^2) = \underbrace{\boxed{\frac{8\pi}{3} r_e^2}}_{\sigma_{e_{Th}}} = 0.66\ b$$

For an atom with Z electrons $\sigma_{a_{Th}} = Z \frac{8\pi}{3} r_e^2$

and for a pure material of atomic number Z

$$\sigma_{Th} = \frac{N_0 Z}{A} \sigma_{e_{Th}} \left[\frac{cm^2}{g}\right] \simeq 0.2 \ \frac{cm^2}{g}$$ (should be an universal constant)

since $\frac{Z}{A} \simeq 0.5$

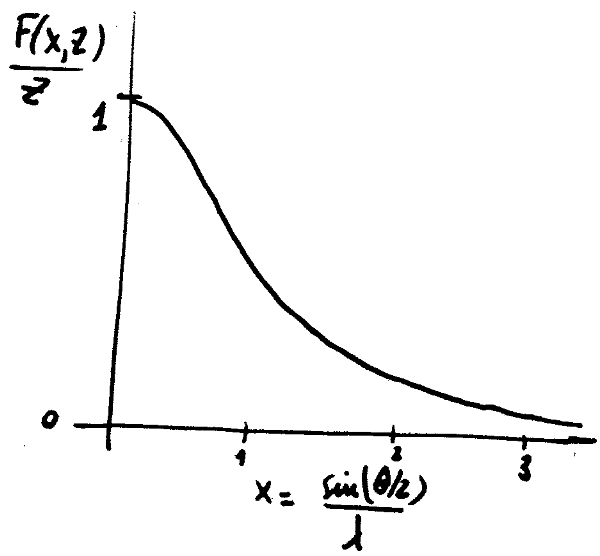
But not all the electrons contribute in the same way to the atomic cross-section because they are bound with different bindings

$$\left(\frac{d\sigma_a}{d\Omega}\right)_{Rayleigh} = \left(\frac{d\sigma_e}{d\Omega}\right)_{Th} \underbrace{F^2(\theta,Z)}_{\text{scattering form factor}}$$

$$F(\theta,Z) = \int \underbrace{\rho(\vec{r})}_{\text{electron density at } \vec{r}} \underbrace{e^{i\vec{q}\cdot\vec{r}}}_{\text{wave contribution from } \vec{r}} d^3r \qquad |\vec{q}| = \frac{2k}{\hbar} \sin\left(\frac{\theta}{2}\right)$$ "momentum transfer"

Rayleigh scattering kernel

$$k(\vec{\omega},\lambda,\vec{\omega}',\lambda') = \underbrace{\delta(\lambda-\lambda')}_{\text{coherence}} \; \underbrace{\frac{r_e^2}{2}\left(1+(\vec{\omega}\cdot\vec{\omega}')^2\right)}_{\text{Thompson differential cross section}} \; \underbrace{F^2(\lambda, \vec{\omega}\cdot\vec{\omega}', Z)}_{\text{form factor (binding)}}$$

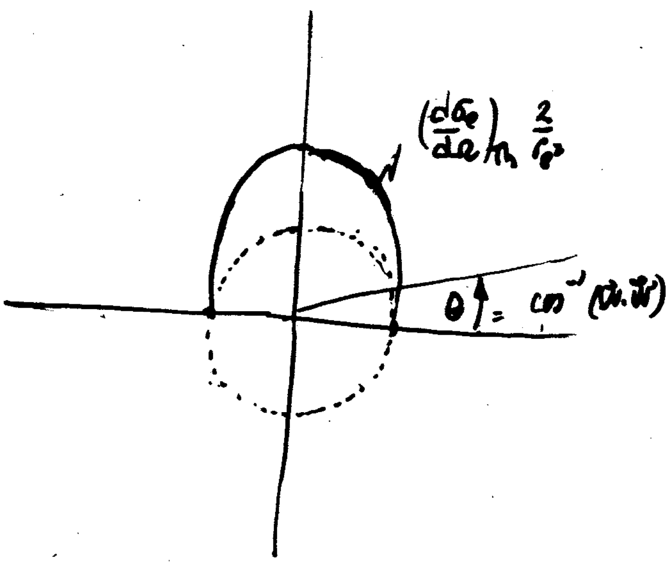


$$\sin\left(\frac{\theta}{2}\right) = \sqrt{\frac{1-\vec{\omega}\cdot\vec{\omega}'}{2}}$$

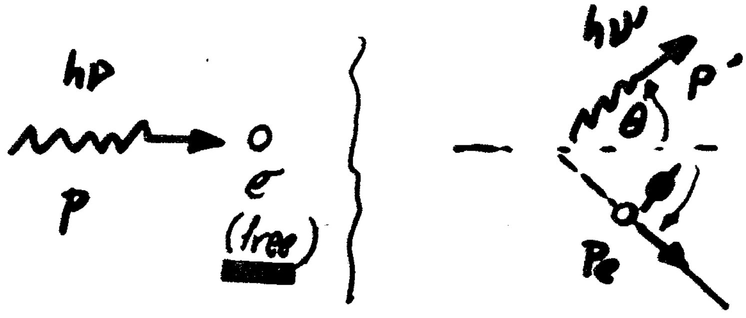
$$E\,[\mathrm{keV}] = \frac{hc}{\lambda} = \frac{12.39}{\lambda\,[\text{Å}]}$$

$$F \to Z \begin{cases} \vec{\omega}\cdot\vec{\omega}' \to 1 \\ \lambda \to \infty \\ (E \to 0) \end{cases}$$

$$F \to 0 \begin{cases} \lambda \to 0 \\ (E \to \infty) \end{cases} \quad \vec{\omega} \neq \vec{\omega}'$$



Incoherent scattering (Compton)



Exchange of energy and momentum

Evidence of the particle nature of the photon

We can analyze energy and momentum conservation in the hit (relativistic particle)

Relativistic energy of a free particle $\sqrt{(pc)^2+(mc^2)^2}$

and momentum is $p = \frac{E}{c}$

For the photon $v=c$ and $mc^2 \equiv 0$ (zero rest mass) then $E = pc$

or $p = \frac{E}{c} = \frac{h\nu}{c}$

Conservation of momentum gives

$$\frac{h\nu}{c} = \left(\frac{h\nu'}{c}\right)\cos\theta + p_e\cos\phi \qquad (C.1)$$

$$0 = \left(\frac{h\nu'}{c}\right)\sin\theta - p_e\sin\phi \qquad (C.2)$$

Conservation of energy gives

$$h\nu + m_e c^2 = h\nu' + \sqrt{P_e^2 c^2 + (m_e c^2)^2} \qquad (C.3)$$

From (C.1) and (C.2)

$$P_e^2 c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu')(h\nu)\cos\theta$$

and from (C.3)

$$P_e^2 c^2 + (m_e c^2)^2 = (h\nu - h\nu')^2 + 2 m_e c^2 (h\nu - h\nu') + (m_e c^2)^2$$

then

$$m_e c^2 (\nu - \nu') = h\nu\nu'(1 - \cos\theta)$$

or

$$\lambda' - \lambda = \underbrace{\boxed{\left(\frac{h}{m_e c}\right)}}_{\lambda_c}(1 - \cos\theta) \qquad \underline{\text{Compton shift}}$$

Compton wavelength

Note that • $\lambda' > \lambda$

• the shift depends only on the scattering angle θ not on the energy of the incident photon

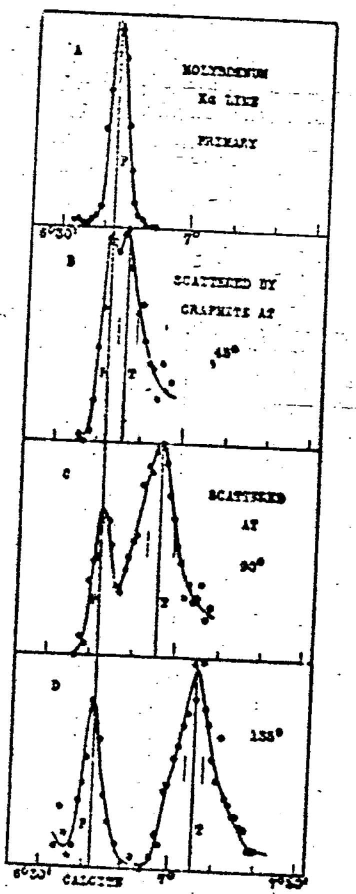


FIGURA 20A. *Questo grafico, tratto dall'articolo di Compton [A. H. Compton, in «Physical Review» 22, 1923, pag. 409], mostra lo spettro della radiazione diffusa in corrispondenza di tre angoli di diffusione differenti. Il grafico superiore mostra la riga della radiazione incidente, di lunghezza d'onda 0,71 Å. L'ascissa è proporzionale alla lunghezza di onda e l'ordinata è una misura dell'intensità. I picchi a sinistra nei tre grafici sottostanti indicano che parte della radiazione diffusa ha la stessa lunghezza di onda della radiazione incidente. I picchi a destra mostrano la radiazione diffusa per effetto Compton, di frequenza spostata. Lo spostamento nella frequenza cresce al crescere dell'angolo di diffusione, secondo la formula di Compton.* (Per gentile concessione di *Physical Review*).

Klein and Nishina computed (Dirac's relativistic theory of electron) the differential cross section for the Compton effect (unpolarized)

$$\left(\frac{d\sigma_e}{d\Omega}\right)_{KN} = \frac{r_e^2}{2}\left[1+\alpha(1-\cos\theta)\right]^{-2}\left[1+\cos^2\theta+\frac{\alpha^2(1-\cos\theta)^2}{1+\alpha(1-\cos\theta)}\right]$$

where $\alpha = \frac{E}{m_e c^2} = \frac{h\nu}{m_e c^2}$

Once more time the electrons contribute differently to the atomic cross section and we must introduce the <u>incoherent scattering function S</u>

$$\frac{d\sigma_a}{d\Omega} = \left(\frac{d\sigma_e}{d\Omega}\right)_{KN} S(\lambda', \theta, Z)$$

S takes into account the binding of electrons with different energies and momenta.

Other processes may occur (they are neglected)

- Distribution of momenta of electrons produces a line broadening.
- Inverse Compton scattering

Compton scattering kernel

$$k(\vec{\omega}, \lambda, \vec{\omega}'; \lambda') = \underbrace{\frac{r_0^2}{2} K_{KN}(\lambda,\lambda')}_{\text{Klein-Nishina electronic differential cross section}} \underbrace{S(\lambda', \hat{\omega}\cdot\hat{\omega}', Z)}_{\text{Scattering function}} \underbrace{\delta\left(\lambda' - \lambda + \lambda_c (1 - \hat{\omega}\cdot\hat{\omega}')\right)}_{\text{Compton shift}}$$

where

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

We can do the check (HOMEWORK)

$$\sigma(\nu') = \int_0^\infty d\nu \int_{4\pi} d\vec{\omega} \; \sigma_{KN}(\nu' \to \nu, \xi)$$

$$= \pi r_0^2 \int_{-1}^{1} d\xi \, \frac{1}{[1 + \alpha'(1-\xi)]^2} \left[1 + \xi^2 + \frac{\alpha'^2 (1-\xi)^2}{1 + \alpha'^2 (1-\xi)} \right]$$

to verify that the integral cross section coincides with the experimental behaviour.

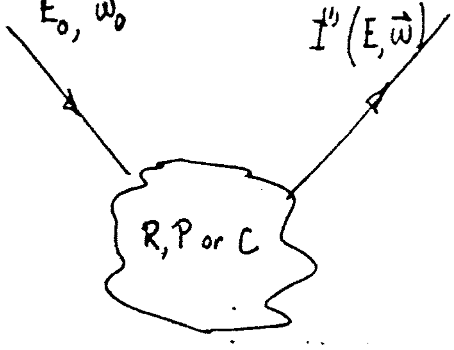
Computation of cross-sections and attenuation coefficients for photon interactions :

CODE: $\boxed{\text{XCOM}}$

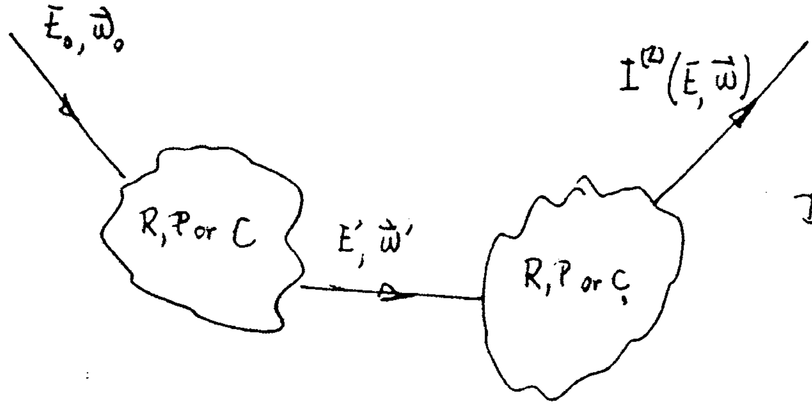
Reference: XCOM : Photon cross sections on a personal computer
Report NBSR-87-3597, National Bureau of Standards (1987)

Author(s): M.J. Berger and J.H. Hubbell

Description: Calculations, with a personal computer, of photon cross-sections and attenuation coefficients for scattering, photoelectric absorption and pair production, in any element, compound or mixture, at energies from 1 keV to 100 GeV



Single interaction process



Double interaction process

a \ b	Photoelectric effect	Coherent (Rayleigh) scattering	Incoherent (Compton) scattering
Photo-electric effect	Secondary XRF intensity[1]	XRF intensity scattered from other scatter centers to the detector[3]	Modification of the symmetry of the XRF line due to the lower energy Compton emiss.[3]
Coherent (Rayleigh) scattering	Coherent scattering enhancement to the XRF intensity[2]	Double scattering Rayleigh[4]	Double scattering Compton (this work)
Incoherent (Compton) scattering	Incoherent scattering enhancement to the XRF intensity[2]	Double scattering Rayleigh-Compton (this work)	Double scattering Compton-Rayleigh (this work)

Physical meaning of every chain of interactions (a,b) for the main processes affecting soft X-rays.

First order interaction

PHOTOELECTRIC

$$I_P^{(1)}(\vec{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{1+\operatorname{sgn}\gamma_0}{2}\,\frac{1-\operatorname{sgn}\gamma}{2}\sum_i \frac{|\gamma|}{\mu|\gamma_0| + \mu_0|\gamma|}$$

$$\delta(\lambda-\lambda_i)\; Q_{\lambda_i}(\lambda_0)\left[1-U(\lambda_0-\lambda_{ei})\right]$$

RAYLEIGH

$$I_R^{(1)}(\vec{\omega},\lambda) = I_0\,\frac{1+\operatorname{sgn}\gamma_0}{2}\,\frac{1-\operatorname{sgn}\gamma}{2}\,\frac{|\gamma|}{\mu|\gamma_0| + \mu_0|\gamma|}$$

$$\delta(\lambda-\lambda_0)\,\sigma\left[1+(\vec{\omega}\cdot\vec{\omega}_0)^2\right]\frac{F^2(\lambda_0, \vec{\omega}\cdot\vec{\omega}_0, Z)}{Z} \qquad \sigma = \frac{\rho N Z}{A}\frac{r_e^2}{2}$$

COMPTON

$$I_C^{(1)}(\hat{\omega},\lambda) = I_0\,\frac{1+\operatorname{sgn}\gamma_0}{2}\,\frac{1-\operatorname{sgn}\gamma}{2}\,\frac{|\gamma|}{\mu|\gamma_0| + \mu_0|\gamma|}$$

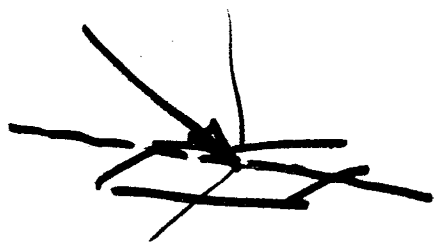
$$\sigma K_{KN}(\lambda,\lambda_0)\, S(\lambda_0, \vec{\omega}\cdot\vec{\omega}_0, Z)\, \delta\left((1-\hat{\omega}_0\cdot\hat{\omega})\lambda_c + \lambda_0 - \lambda\right)$$

SOME PROPERTIES OF THE FIRST ORDER INTERACTIONS

PHOTOELECTRIC

- Azimuthal symmetry
- Discrete at $\lambda = \lambda_i \quad (i=1,\dots,N)$
- Every line with different intensity given by $Q_{\lambda_i}(\lambda_0)$ and by the absorption

RAYLEIGH



- Plane of symmetry (not an axis)
- Discrete at $\lambda = \lambda_0$

COMPTON

- Plane of symmetry
- Discrete at $\lambda = \lambda_0 + \underbrace{\lambda_c \left(1 - \vec{\omega} \cdot \vec{\omega}_0\right)}_{\Delta\lambda}$

MANY ELEMENTS

- we assume isolated atoms

Mass absorption coefficient

$$\frac{\mu}{\rho} = \sum_j \underbrace{W_j}_{\text{weight fraction of element } j \text{ in the mixture}} \underbrace{\left(\frac{\mu}{\rho}\right)_j}_{\text{mass absorption coefficient of element } j}$$

$$\frac{\mu}{\rho}\left[\frac{cm^2}{g}\right] = \underbrace{\mu_0}_{\text{barn/electron}} \frac{NZ}{A} \qquad \mu\,[cm^{-1}] = \rho\left(\frac{\mu}{\rho}\right)$$

To get the composition dependence we must change from attenuation coefficients in $[cm^{-1}]$ to mass attenuation coeff in $[cm^2/g]$

$$I_p^{(1)}(\bar{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{|\gamma|}{\mu|\gamma_0| + \mu_0|\gamma|}\sum_i \delta(\lambda-\lambda_i)\,Q_{\lambda_i}(\lambda_0)$$

$$= \frac{I_0}{4\pi}\,\frac{|\gamma|}{\sum_j\left[\left(\frac{\mu_0}{\rho}\right)_j|\gamma_0| + \left(\frac{\mu}{\rho}\right)_j|\gamma|\right]W_j}\sum_i \delta(\lambda-\lambda_i)\,\underbrace{Q_{\lambda_i}}_{\text{has the factor } \left(\frac{\tau}{\rho}\right)_i W_i}(\lambda_0)$$

It is possible to write the following set of equations

$$\frac{4\pi}{|\gamma|} \frac{I_p^{(1)}(\vec{\omega}, \lambda_i)}{I_0} \sum_j W_j \left[\left(\frac{\mu_i}{\rho}\right)_j |\gamma_0| + \left(\frac{\mu_0}{\rho}\right)_j |\gamma| \right] = \underbrace{Q^*_{\lambda_i}(\lambda_0)}_{\text{for } W_i = 1} W_i$$

for as many lines as elements we get

$$\mathbb{I} \, \vec{W} = Q \, \vec{W}$$

and with the constraint

$$\sum_j W_j = 1$$

$$I^{(1)}(0,\vec{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{(1+\mathrm{sgn}\,\eta_0)}{2}\,\frac{(1-\mathrm{sgn}\,\eta)}{2}\,\frac{|\eta|}{\mu\,|\eta_0| + \mu_0|\eta|}\times$$

$$\sum_i \delta(\lambda-\lambda_i)\; Q_{\lambda_i}(\lambda_0)\left[1-\mathcal{U}(\lambda_0-\lambda_{e_i})\right]$$

$$I^{(2)}(0,\vec{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{(1+\mathrm{sgn}\,\eta_0)}{2}\,\frac{(1-\mathrm{sgn}\,\eta)}{2}\,\frac{|\eta|}{\mu\,|\eta_0| + \mu_0|\eta|}\times$$

$$\sum_i \delta(\lambda-\lambda_i)\sum_j \frac{Q_{\lambda_j}(\lambda_0)\,Q_{\lambda_i}(\lambda_j)}{2}\left[1-\mathcal{U}(\lambda_0-\lambda_{e_j})\right]\left[1-\mathcal{U}(\lambda_j-\lambda_{e_i})\right]\times$$

$$\left\{\frac{|\eta_0|}{\mu_0}\,\ln\left(1+\frac{\mu_0}{\mu_j|\eta_0|}\right)+\frac{|\eta|}{\mu}\,\ln\left(1+\frac{\mu}{\mu_j|\eta|}\right)\right\}$$

$$I^{(3)}(0,\vec{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{(1+\mathrm{sgn}\,\eta_0)}{2}\,\frac{(1-\mathrm{sgn}\,\eta)}{2}\,\frac{|\eta|}{\mu\,|\eta_0| + \mu_0|\eta|}\times$$

$$\sum_i \delta(\lambda-\lambda_i)\sum_j\sum_k \frac{Q_{\lambda_k}(\lambda_0)\,Q_{\lambda_j}(\lambda_k)\,Q_{\lambda_i}(\lambda_j)}{4}\times$$

$$\left[1-\mathcal{U}(\lambda_0-\lambda_{e_k})\right]\left[1-\mathcal{U}(\lambda_k-\lambda_{e_j})\right]\left[1-\mathcal{U}(\lambda_j-\lambda_{e_i})\right]\times$$

$$\left\{\frac{|\eta_0|}{\mu_0}\,\ln\left(1+\frac{\mu_0}{\mu_k|\eta_0|}\right)\left\{\frac{|\eta_0|}{\mu_0}\,\ln\left(1+\frac{\mu_0}{\mu_j|\eta_0|}\right)+\frac{|\eta|}{\mu}\,\ln\left(1+\frac{\mu}{\mu_j|\eta|}\right)\right\}+\right.$$

$$\frac{\eta^2}{\mu^2}\,\ln\left(1+\frac{\mu}{\mu_k|\eta|}\right)\ln\left(1+\frac{\mu}{\mu_j|\eta|}\right)+$$

$$\left.\frac{1}{\mu_k}\int_0^{\mu_k/\mu_j}\frac{ds}{\frac{\mu_k}{s}+\frac{\mu_0}{|\eta_0|}}\,\ln\left(\frac{1+s}{s}\right)+\frac{1}{\mu_j}\int_0^{\mu_j/\mu_k}\frac{ds}{\frac{\mu_j}{s}+\frac{\mu}{|\eta|}}\,\ln\left(\frac{1+s}{s}\right)\right\}$$

- gives a shorter tertiary expression but also the new **integrals** have a more stable numerical behavior for $\mu_0 < 1$ (as **may** occur with high excitation energies).
- the possibility of having line enhancement in a pure target is signaled (since photons are bosons they do not follow an exclusion principle).
  By example, the L lines of a pure element (of medium or high atomic number) suffer the enhancement of its own K lines.

HIGHER ORDER SCATTERING

$\lambda_0 \rightarrow Cr\ K\alpha_1$	primary
$\lambda_0 \rightarrow Fe\ K\alpha_1 \rightarrow Cr\ K\alpha_1$	secondary
$\lambda_0 \rightarrow Ni\ K\alpha_1 \rightarrow Fe\ K\alpha_1 \rightarrow Cr\ K\alpha_1$	tertiary
$\lambda_0 \rightarrow Zn\ K\alpha_1 \rightarrow Ni\ K\alpha_1 \rightarrow Fe\ K\alpha_1 \rightarrow Cr\ K\alpha_1$	fourth-order

FOURTH-ORDER XRF INTENSITY

$$I^{(4)}(\vec{\omega},\lambda) = \frac{I_0}{4\pi}\,\frac{(1+\operatorname{sgn}\eta_0)}{2}\,\frac{(1-\operatorname{sgn}\eta)}{2}\,\frac{|\eta|}{\mu_i|\eta_0| + \mu_0|\eta|}\times$$

$$\delta(\lambda-\lambda_i)\,\frac{Q_{\lambda_p}(\lambda_0)\,Q_{\lambda_k}(\lambda_p)\,Q_{\lambda_j}(\lambda_k)\,Q_{\lambda_i}(\lambda_j)}{8}\times$$

$$\left[1-\mathcal{U}(\lambda_0-\lambda_{e_p})\right]\left[1-\mathcal{U}(\lambda_p-\lambda_{e_k})\right]\left[1-\mathcal{U}(\lambda_k-\lambda_{e_j})\right]\left[1-\mathcal{U}(\lambda_j-\lambda_{e_i})\right]\times$$

$$\int_0^1\frac{d\eta'}{\eta'}\int_0^1\frac{d\eta''}{\eta''}\int_0^1\frac{ds}{s}\times$$

$$\frac{\mathcal{G}(a,a_0,a_1,a',a'')}{(a_1+a)(a_1+a_0)(a'+a)(a'+a_0)(a'+a_1)(a''+a)(a''+a_0)(a''+a_1)(a''+a')}$$

where

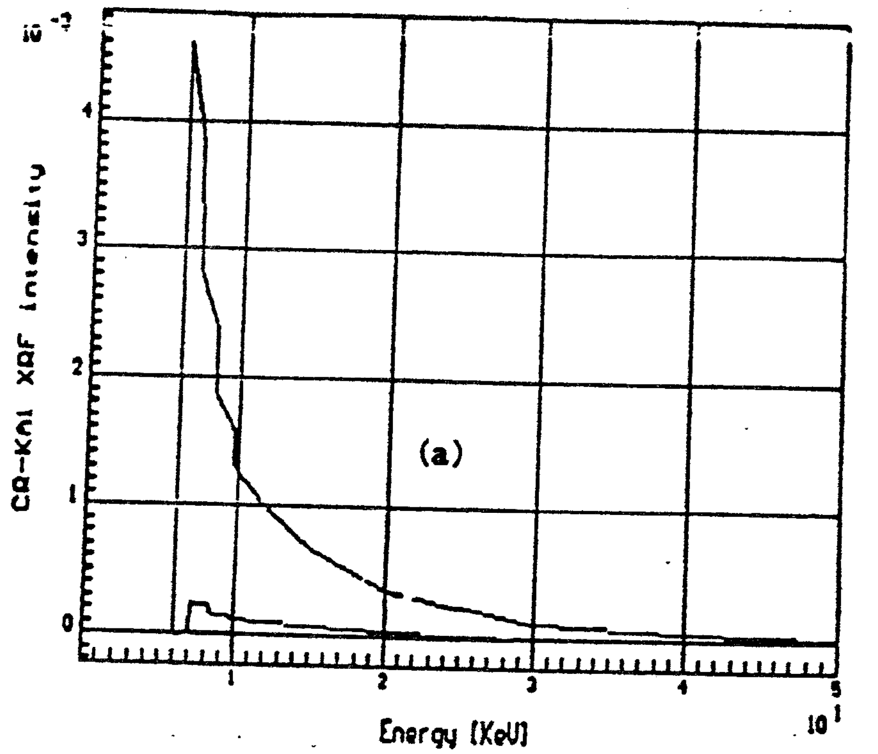
$$a = \frac{\mu_i}{|\eta|},\quad a_0 = \frac{\mu_0}{|\eta_0|},\quad a' = \frac{\mu_j}{\eta'},\quad a'' = \frac{\mu_k}{\eta''},\quad a_1 = \frac{\mu_p}{s},$$

and

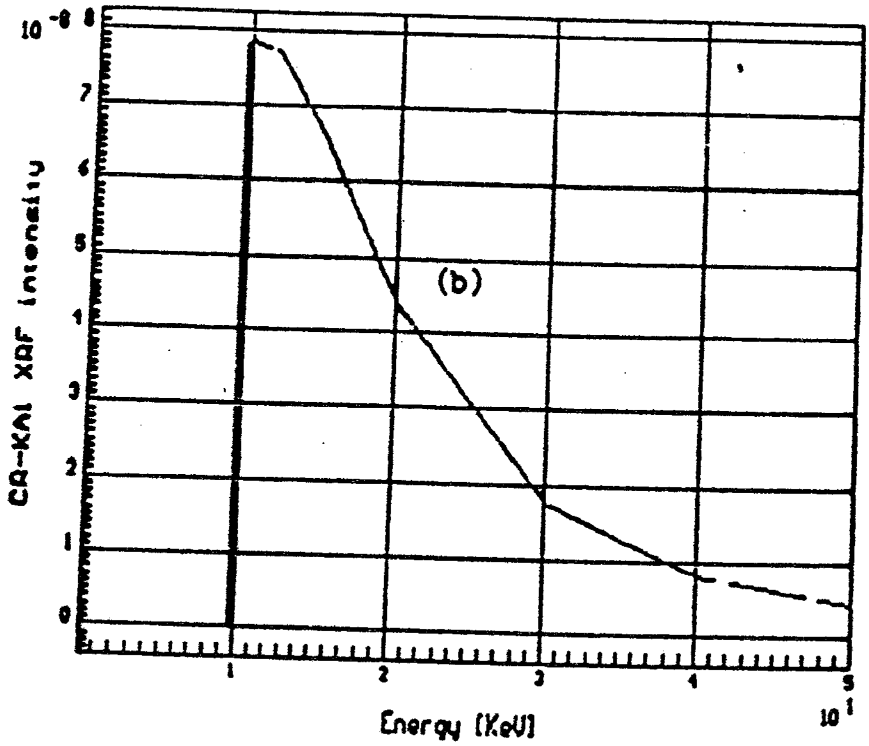
$$\mathcal{G}(a,a_0,a_1,a',a'')$$

a non reducible polynomial, positive definite, which does not admit any factorization in integer powers of its variables.

$$
\begin{aligned}
\mathcal{G}(a,a_0,a_1,a',a'') = {} & a'' \,(a'' \,((a' \,((8\, a_1 + 4\, a_0 + 4\, a)\, a' \\
& + a_1\, (8\, a_1 + 10\, a_0 + 10\, a) + a_0\, (4\, a_0 + 6\, a) + 2\, a^2) \\
& + a_1\, ((4\, a_0 + 4\, a)\, a_1 + a_0\, (2\, a_0 + 6\, a) + 4\, a^2) \\
& + a_0\, (2\, a\, a_0 + 2\, a^2))\, a'' + a' \\
& (a'\, ((8\, a_1 + 4\, a_0 + 4\, a)\, a' + a_1\, (16\, a_1 + 21\, a_0 + 21\, a) \\
& + a_0\, (8\, a_0 + 13\, a) + 5\, a^2) + a_1 \\
& (a_1\, (8\, a_1 + 21\, a_0 + 21\, a) + a_0\, (15\, a_0 + 30\, a) + 15\, a^2) \\
& + a_0\, (a_0\, (4\, a_0 + 11\, a) + 9\, a^2) + 2\, a^3) \\
& + a_1\, (a_1\, ((4\, a_0 + 4\, a)\, a_1 + a_0\, (5\, a_0 + 13\, a) + 8\, a^2) \\
& + a_0\, (a_0\, (2\, a_0 + 9\, a) + 11\, a^2) + 4\, a^2) \\
& + a_0\, (a_0\, (2\, a\, a_0 + 4\, a^2) + 2\, a^3)) \\
& + a'\, (a'\, ((a_1\, (8\, a_1 + 10\, a_0 + 10\, a) + a_0\, (4\, a_0 + 6\, a) \\
& + 2\, a^2)\, a' + a_1\, (a_1\, (8\, a_1 + 20\, a_0 + 20\, a) \\
& + a_0\, (15\, a_0 + 28\, a) + 13\, a^2) + a_0\, (a_0\, (4\, a_0 + 11\, a) + 8\, a^2) \\
& + a^3) + a_1\, (a_1\, ((10\, a_0 + 10\, a)\, a_1 + a_0\, (13\, a_0 + 28\, a) \\
& + 15\, a^2) + a_0\, (a_0\, (5\, a_0 + 21\, a) + 21\, a^2) + 5\, a^3) \\
& + a_0\, (a_0\, (5\, a\, a_0 + 8\, a^2) + 3\, a^3)) \\
& + a_1\, (a_1\, ((a_0\, (2\, a_0 + 6\, a) + 4\, a^2)\, a_1 \\
& + a_0\, (a_0\, (a_0 + 8\, a) + 11\, a^2) + 4\, a^3) \\
& + a_0\, (a_0\, (3\, a\, a_0 + 8\, a^2) + 5\, a^3)) + a_0^2\, (2\, a^2\, a_0 + 2\, a^3)) \\
& + a'\, (a'\, ((a_1\, ((4\, a_0 + 4\, a)\, a_1 + a_0\, (2\, a_0 + 6\, a) + 4\, a^2) \\
& + a_0\, (2\, a\, a_0 + 2\, a^2))\, a' + a_1 \\
& (a_1\, ((4\, a_0 + 4\, a)\, a_1 + a_0\, (6\, a_0 + 12\, a) + 6\, a^2) \\
& + a_0\, (a_0\, (2\, a_0 + 9\, a) + 9\, a^2) + 2\, a^3) \\
& + a_0\, (a_0\, (2\, a\, a_0 + 3\, a^2) + a^3)) \\
& + a_1\, (a_1\, ((a_0\, (4\, a_0 + 6\, a) + 2\, a^2)\, a_1 \\
& + a_0\, (a_0\, (2\, a_0 + 9\, a) + 9\, a^2) + 2\, a^3) \\
& + a_0\, (a_0\, (3\, a\, a_0 + 6\, a^2) + 3\, a^3)) + a_0^2\, (a^2\, a_0 + a^3)) \\
& + a_1\, (a_1\, (a_0\, (2\, a\, a_0 + 2\, a^2)\, a_1 \\
& + a_0\, (a_0\, (a\, a_0 + 3\, a^2) + 2\, a^3)) + a_0^2\, (a^2\, a_0 + a^3))
\end{aligned}
$$



CR(0.25) FE(0.25) NI(0.25) ZN(0.25) - INCIDENCE=15.0 TAKE-OFF=15.0

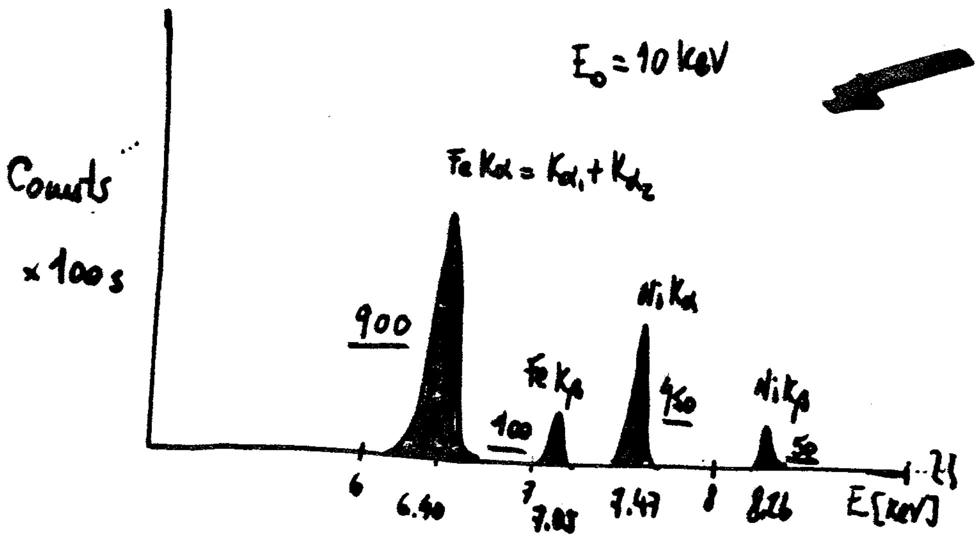


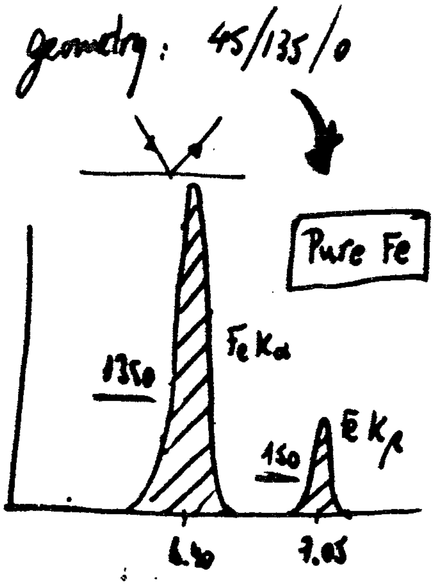
CR(0.25) FE(0.25) NI(0.25) ZN(0.25) - INCIDENCE=15.0 TAKE-OFF=15.0

A graphical comparison of the different orders of enhancement for a single chain of $K\alpha_1$ lines. The sample is Zn(25 %)-Ni(25 %)-Fe(25 %)-Cr(25 %) and the geometry is fixed. (a) All the orders are plotted in the same graphic to compare them. (b) The fourth order is plotted separately.

EXAMPLE

- Determine the composition of a binary steel Fe-Ni that has the following spectrum of emission





Data

Fe (Z=26)

$\boxed{\left(\frac{\mu}{\rho}\right)_{Fe}(10\text{ keV}) = 172.86}$

$\left(\frac{\tau}{\rho}\right)_{Fe}(10\text{ keV}) = 171.51$

$\boxed{\left(\frac{\mu}{\rho}\right)_{Fe}(6.40) = 70.46}$

$\left(\frac{\mu}{\rho}\right)_{Fe}(7.05) = 53.48$

$\left(\frac{\mu}{\rho}\right)_{Fe}(7.47) = 387.07$

$\left(\frac{\mu}{\rho}\right)_{Fe}(8.26) = 284.27$

$I_{K\alpha} : I_{K\beta} = 9:1$

$r_K = 8.33$

$\omega_K = 0.338$

Ni (Z=28)

$\boxed{\left(\frac{\mu}{\rho}\right)_{Ni}(10\text{ keV}) = 210.79}$

$\left(\frac{\tau}{\rho}\right)_{Ni}(10\text{ keV}) = 209.23$

$\boxed{\left(\frac{\mu}{\rho}\right)_{Ni}(6.40) = 91.89}$

$\left(\frac{\mu}{\rho}\right)_{Ni}(7.05) = 70.37$

$\left(\frac{\mu}{\rho}\right)_{Ni}(7.47) = 59.91$

$\left(\frac{\mu}{\rho}\right)_{Ni}(8.26) = 45.33$

$I_{K\alpha} : I_{K\beta} = 9:1$

$r_K = 7.85$

$\omega_K = 0.414$

We assume that $I(\vec{w},\lambda) = I^{(1)}(\vec{w},\lambda)$

and select Fe K_α that we have in both spectra (unknown sample and pure Fe)

We do the ratio $\dfrac{I_{Fe\text{-}unknown}}{I_{Fe\text{-}pure}}$ to factor out I_0 (that is unknown)

$$R = \frac{I_{Fe\text{-}u}}{I_{Fe\text{-}p}} = \frac{\cancel{Q^*_{Fe K_\alpha}(10\,\text{keV})}\; W_{Fe}}{\sum_j \left[\left(\frac{\mu}{\rho}\right)_j \left(\begin{smallmatrix}6.40\\ \text{keV}\end{smallmatrix}\right) + \left(\frac{\mu}{\rho}\right)_j \left(\begin{smallmatrix}10\\ \text{keV}\end{smallmatrix}\right)\right] W_j} \quad \frac{\left(\frac{\mu}{\rho}\right)_{Fe}\left(\begin{smallmatrix}6.40\\ \text{keV}\end{smallmatrix}\right) + \left(\frac{\mu}{\rho}\right)_{Fe}\left(\begin{smallmatrix}10\\ \text{keV}\end{smallmatrix}\right)}{\cancel{Q^*_{Fe K_\alpha}(10\,\text{keV})}}$$

$$\Rightarrow (R-1)\,W_{Fe} + R\left[\frac{\left(\frac{\mu}{\rho}\right)_{Ni}(6.40) + \left(\frac{\mu}{\rho}\right)_{Ni}(10)}{\left(\frac{\mu}{\rho}\right)_{Fe}(6.40) + \left(\frac{\mu}{\rho}\right)_{Fe}(10)}\right] W_{Ni} = 0 \qquad (E.1)$$

We have the additional equation

$$W_{Fe} + W_{Ni} = 1 \qquad (E.2)$$

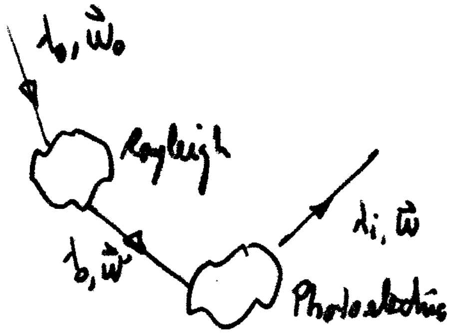
From (E.1) and (E.2) we get the composition.

$$\begin{aligned} -0.33\,W_{Fe} + 0.829\,W_{Ni} &= 0 \\ W_{Fe} + W_{Ni} &= 1 \end{aligned}$$

$$\begin{aligned} W_{Fe} - 2.51\,W_{Ni} &= 0 \\ -\quad W_{Fe} + W_{Ni} &= 1 \\ \hline -3.51\,W_{Ni} &= -1 \end{aligned}$$

$$\Rightarrow \boxed{\begin{aligned} W_{Ni} &= 0.285 \\ W_{Fe} &= 1 - W_{Ni} = 0.715 \end{aligned}}$$

Rayleigh - Photoelectric chain



$$I^{(2)}_{(R,P)}(\vec{\omega},\lambda) = \frac{1-\operatorname{sgn}\zeta}{2}\,\frac{1+\operatorname{sgn}\zeta_0}{2}\,\frac{I_0}{|\zeta_0|}\,\frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\zeta|}+\frac{\mu_0}{|\zeta_0|}}\,\frac{\sigma\, Q_i(\lambda_0)\left(1-U(\lambda_0-\lambda_{0i})\right)}{4\pi}$$

$$\left\{ \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\zeta'}{\zeta'}\, \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(+)})^2\right]}{\frac{\mu_i}{|\zeta|}+\frac{\mu_0}{\zeta'}}\, \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(+)}, Z)}{Z} + \right.$$

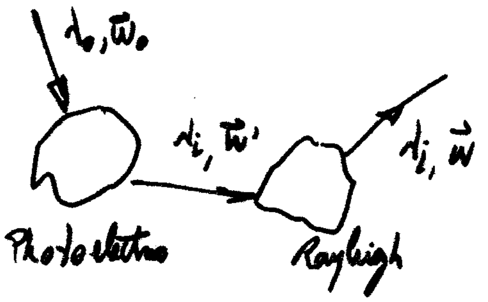
$$\left. + \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\zeta'}{\zeta'}\, \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(-)})^2\right]}{\frac{\mu_0}{|\zeta_0|}+\frac{\mu_0}{\zeta'}}\, \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(-)}, Z)}{Z} \right\}$$

where

$$\vec{\omega}'\cdot\vec{\omega}_0^{(\pm)} = \pm\zeta'\zeta_0 + \sqrt{1-\zeta'^2}\,\sqrt{1-\zeta_0^2}\,\cos(\varphi'-\varphi_0)$$

- Discrete $\lambda = \lambda_i$ $(i=1,\dots,N)$
- Azimuthal symmetry
- Modifies only the corresponding photoelectric line

Photoelectric-Rayleigh chain



$$I^{(2)}_{(P,R)}(\vec{\omega},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1+\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|}\,\frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\;\sigma\,\frac{Q_{\lambda_i}(\lambda_0)\left[1-u(\lambda_0-\lambda_{0i})\right]}{4\pi}$$

$$\left\{ \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'}\,\frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}^{(+)})^2\right]}{\frac{\mu_i}{|\eta|}+\frac{\mu_i}{\eta'}}\,\frac{F^2(\lambda_i,\vec{\omega}'\cdot\vec{\omega}^{(+)},Z)}{Z} + \right.$$

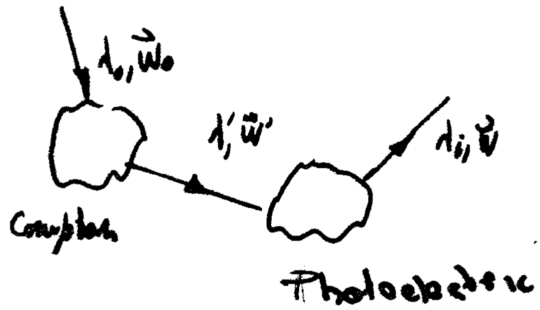
$$\left. + \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'}\,\frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}^{(-)})^2\right]}{\frac{\mu_0}{|\eta_0|}+\frac{\mu_i}{\eta'}}\,\frac{F^2(\lambda_i,\vec{\omega}'\cdot\vec{\omega}^{(-)},Z)}{Z} \right\}$$

where

$$\vec{\omega}'\cdot\vec{\omega}^{(\pm)} = \pm\eta'\eta + \sqrt{1-\eta'^2}\,\sqrt{1-\eta^2}\,\cos(\varphi'-\varphi)$$

- Discrete $\lambda=\lambda_i$ $(i=1,\dots,N)$
- Azimuthal symmetry
- Modifies only the corresponding photoelectric line

Compton - Photoelectric chain



$$I^{(2)}_{(C,P)}(\vec{w},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1+\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|}\,\frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\,\frac{\sigma}{2\pi}\int_{\lambda_0}^{\lambda_0+2\lambda_c}\frac{d\lambda'}{\lambda_c}\,S(\lambda_0,a',Z)\,K_{KN}(\lambda',\lambda_0)$$

$$Q_{\lambda_i}(\lambda')\left[1-U(\lambda'-\lambda_{ei})\right]\left\{\underset{(\alpha_2>\alpha_1)}{\int_{\alpha_1}^{\alpha_2}}\frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta|}+\frac{\mu'}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta_0^2)-(a'-\eta_0\eta')^2}}\right. +$$

$$\left. + \underset{(\beta_2>\beta_1)}{\int_{\beta_1}^{\beta_2}}\frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta_0|}+\frac{\mu'}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta_0^2)-(a'+\eta_0\eta')^2}}\right\}$$

where $a' = 1 + \dfrac{\lambda_0-\lambda'}{\lambda_c}$

$$\alpha_1 = \max\left(0,\ a'\eta_0 - \sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

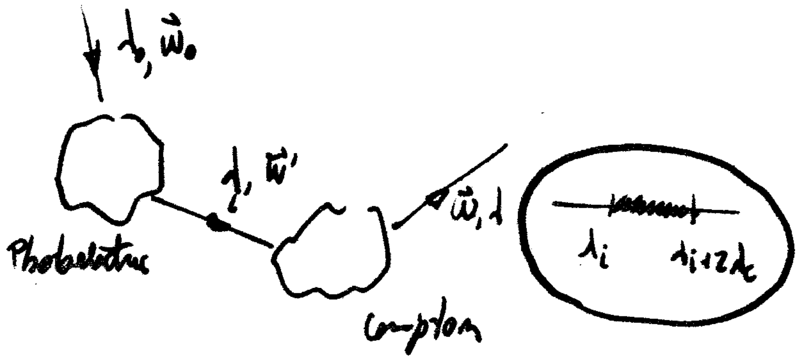
$$\alpha_2 = \min\left(1,\ a'\eta_0 + \sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

$$\beta_1 = -\min\left(0,\ a'\eta_0 + \sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

$$\beta_2 = -\max\left(-1,\ a'\eta_0 - \sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

- Discrete $\lambda = \lambda_i$ $(i=1,\dots,N)$
- Azimuthal symmetry
- Mode lines only the corresponding photoelectric line

Photoelectric - Compton chain



$$I^{(2)}_{(P,C)}(\vec{\omega},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1+\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|\lambda_c}\,\frac{K_{KN}(\lambda,\lambda_i)}{\frac{\mu}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\,\frac{\sigma\, Q_i(\lambda_0)\left[1-U(\lambda_0-\lambda_{e_i})\right] S(\lambda_i,a,Z)}{2\pi}$$

$$\Bigg\{ \underset{(\alpha_2>\alpha_1)}{\int_{\alpha_1}^{\alpha_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu}{|\eta|}+\frac{\mu_i}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a-\eta\eta')^2}} \;+$$

$$\underset{(\beta_2>\beta_1)}{\int_{\beta_1}^{\beta_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta|}+\frac{\mu_i}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a+\eta\eta')^2}} \Bigg\}$$

where $a = 1 + \frac{\lambda_i - \lambda}{\lambda_c}$

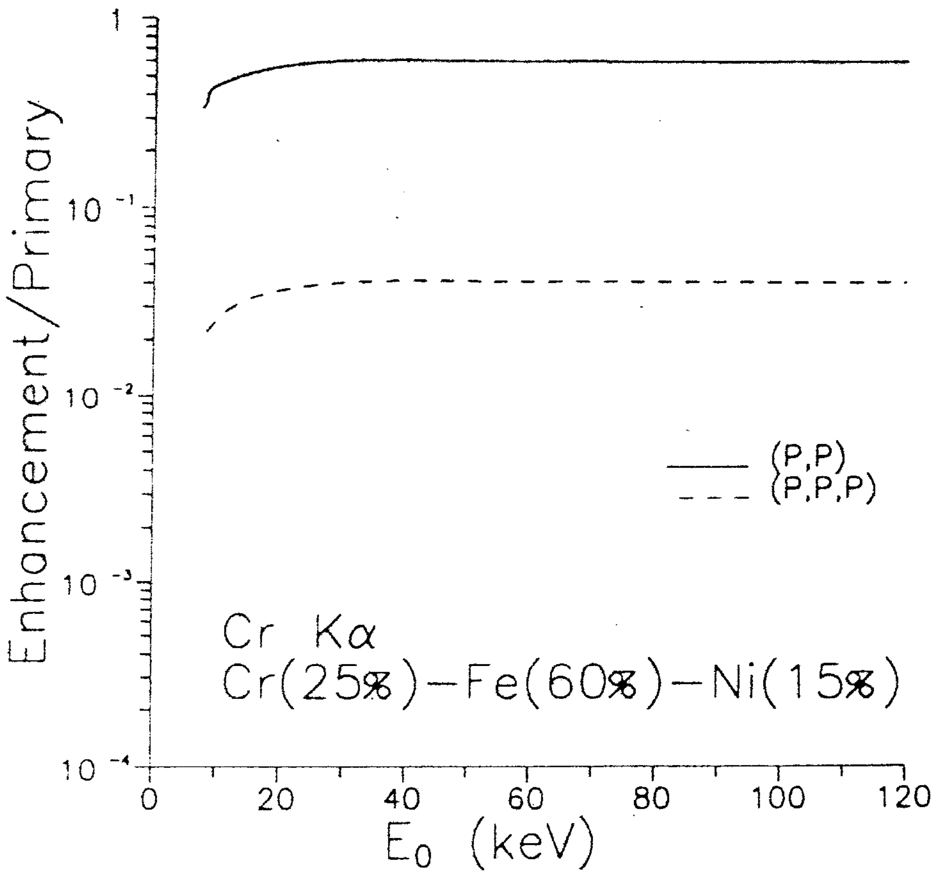
$$\alpha_1 = \max\left(0,\ a\eta - \sqrt{(1-\eta^2)(1-a^2)}\right)$$

$$\alpha_2 = \min\left(1,\ a\eta + \sqrt{(1-\eta^2)(1-a^2)}\right)$$

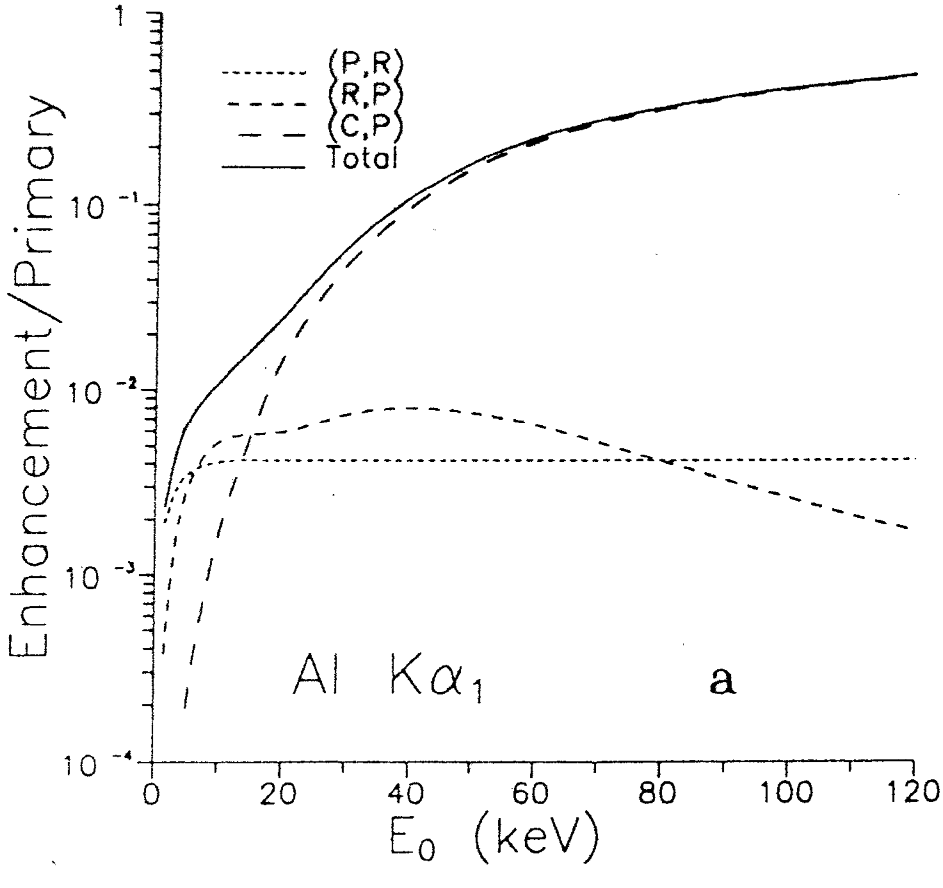
$$\beta_1 = -\min\left(0,\ a\eta + \sqrt{(1-a^2)(1-\eta^2)}\right)$$

$$\beta_2 = -\max\left(-1,\ a\eta - \sqrt{(1-\eta^2)(1-a^2)}\right)$$

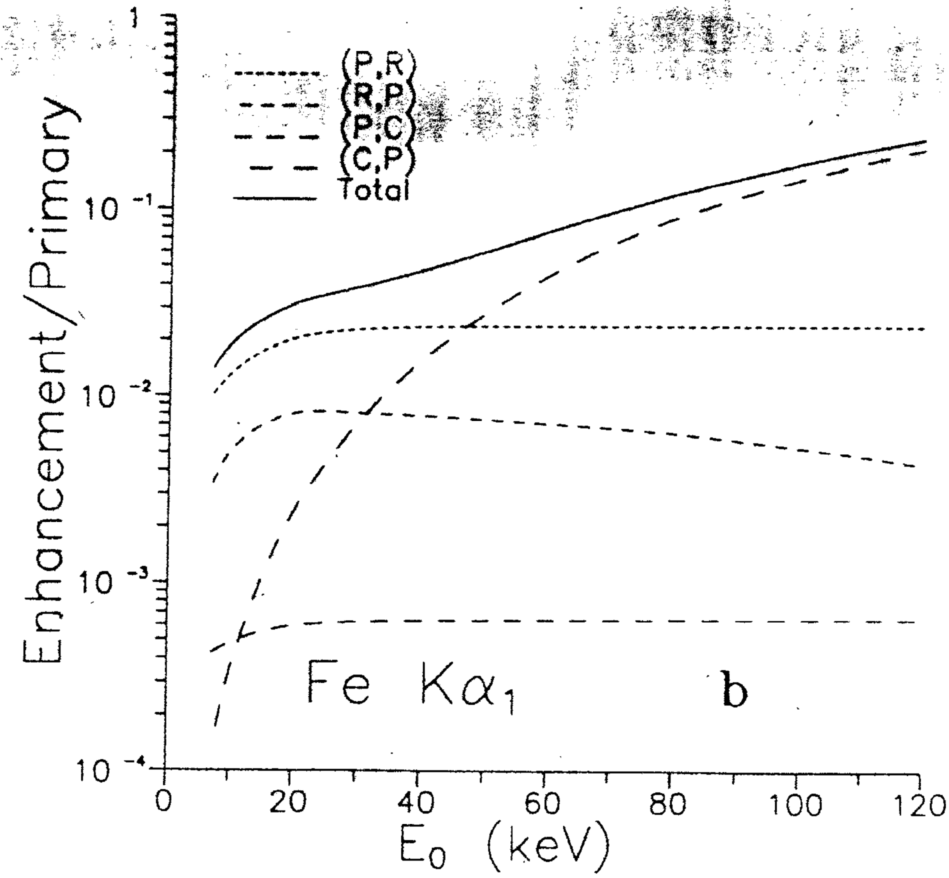
- Continuous $\lambda \in [\lambda_i, \lambda_i + 2\lambda_c]$
- Azimuthal symmetry (over the integrated intensity)
- Modifies the line shape (introduces a tail for lower energies than λ_i)
- May overlap to other lines



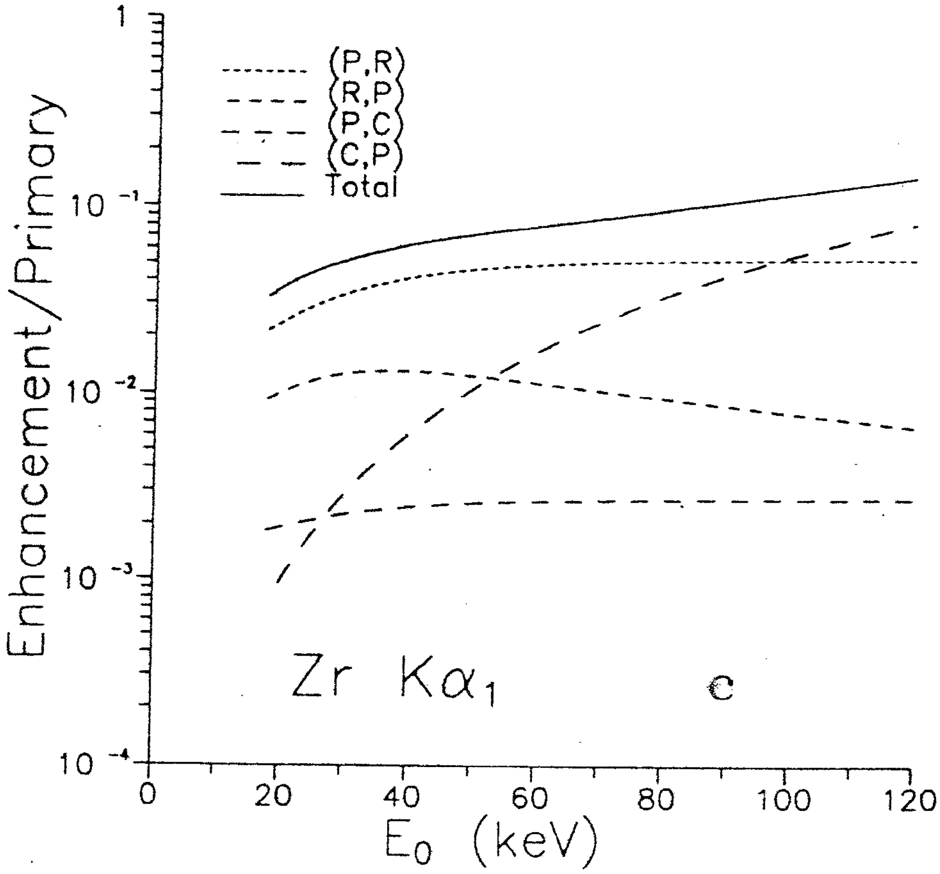
Enhancement/Primary
(P,P)
(P,P,P)
Cr Kα
Cr(25%)–Fe(60%)–Ni(15%)
E_0 (keV)



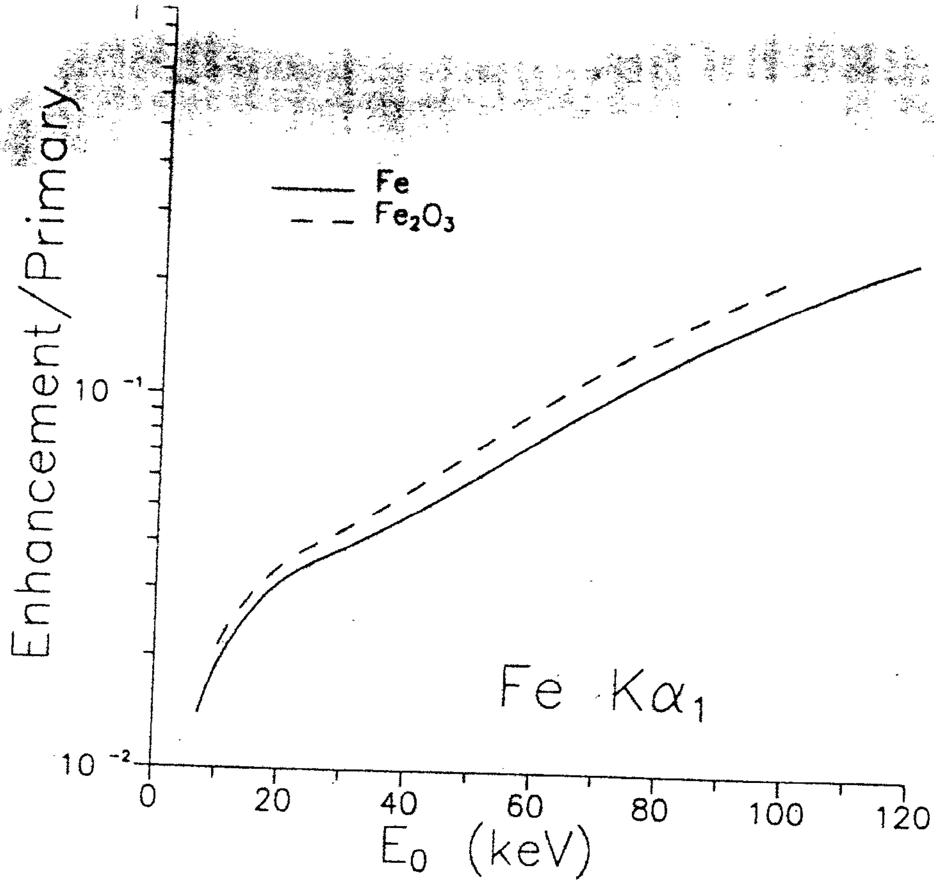
Enhancement/Primary
(P,R)
(R,P)
(C,P)
Total
Al $K\alpha_1$
a
E_0 (keV)

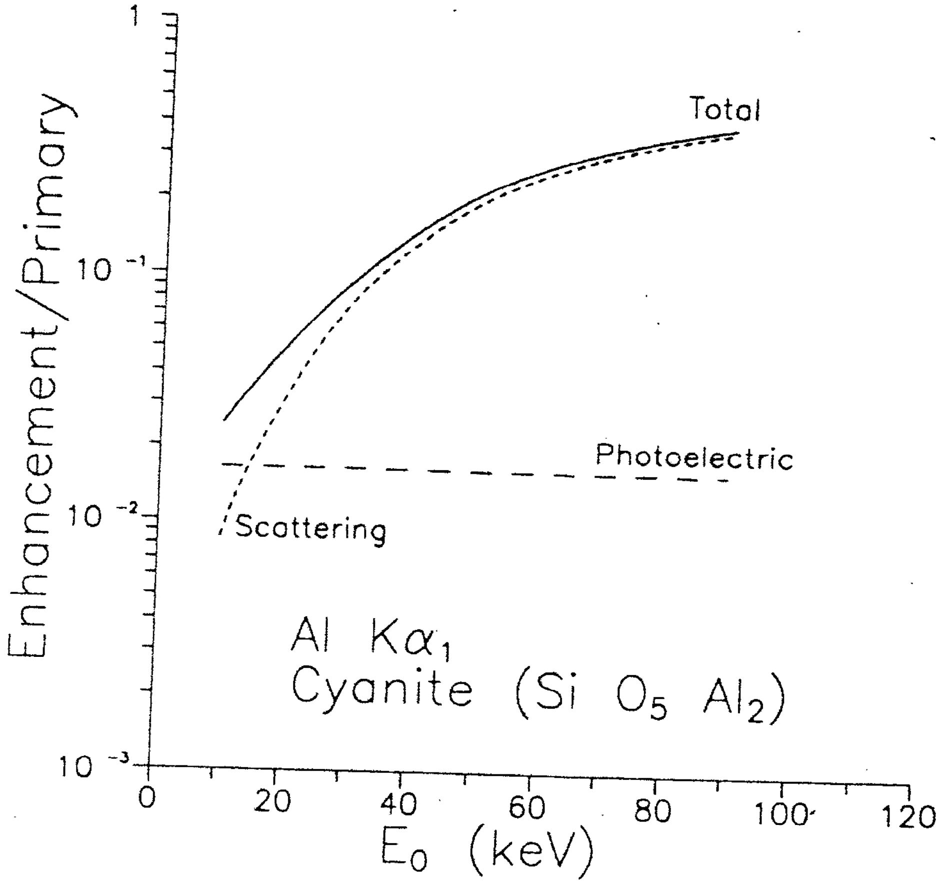


(P,R)
(R,P)
(P,C)
(C,P)
Total
Enhancement/Primary
Fe Kα1
b
E0 (keV)

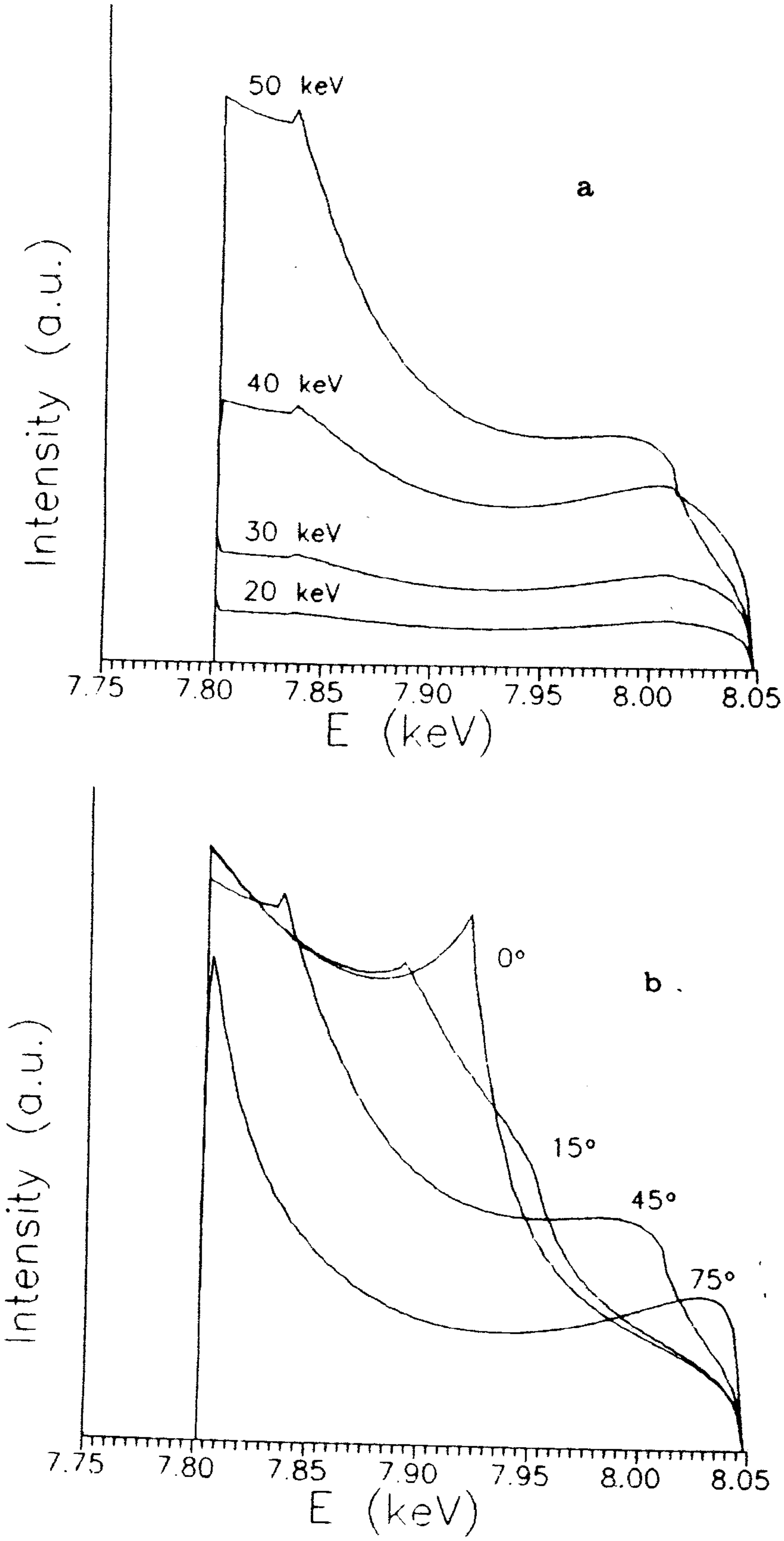


(P,R)
(R,P)
(P,C)
(C,P)
Total
Enhancement/Primary
Zr Kα1
c
E0 (keV)


Enhancement/Primary
Fe
Fe_2O_3
10^{-1}
10^{-2}
Fe $K\alpha_1$
0
20
40
60
80
100
120
E_0 (keV)

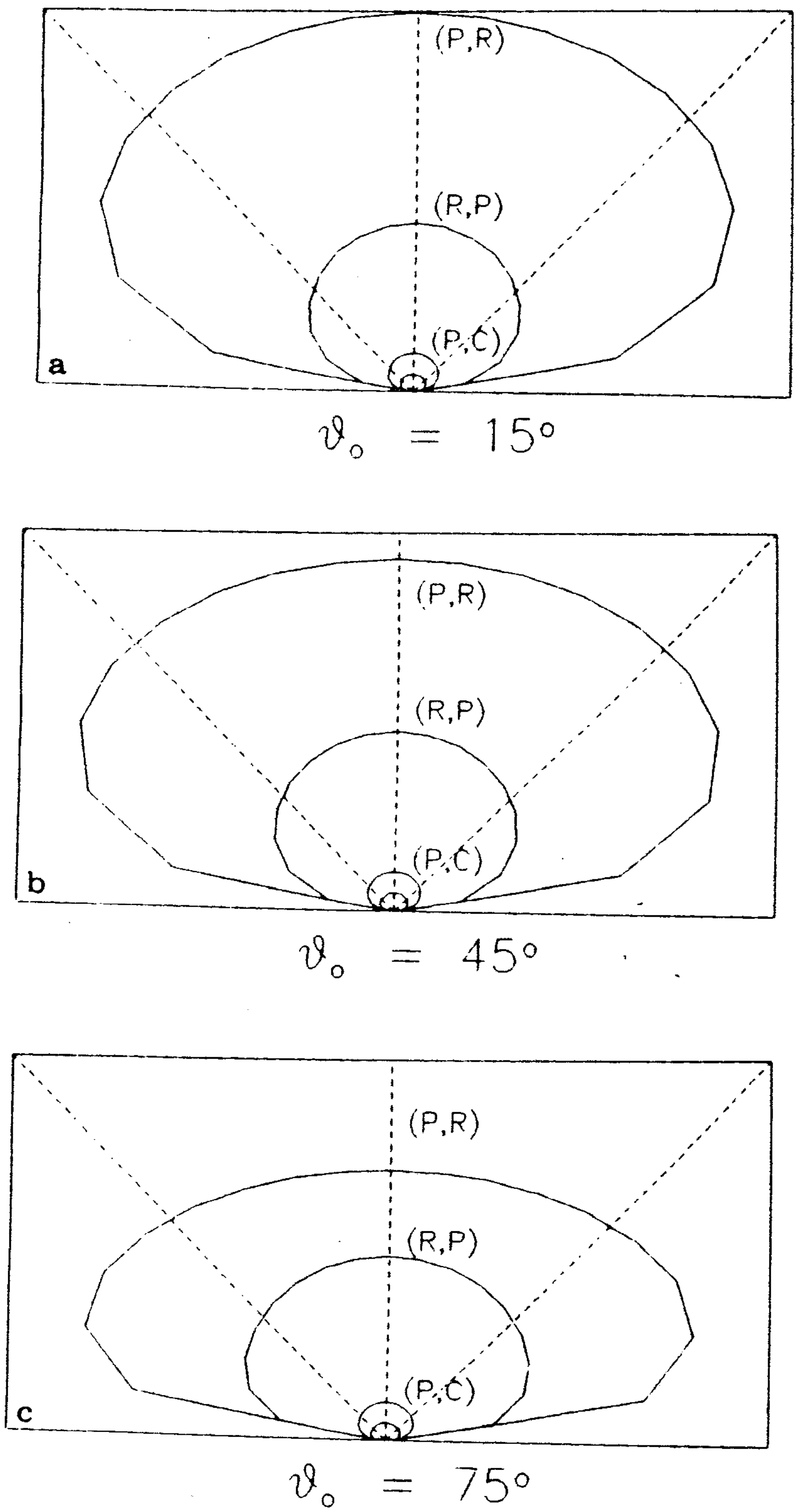

Enhancement/Primary
1
10^{-1}
10^{-2}
10^{-3}
Total
Photoelectric
Scattering
Al $K\alpha_1$
Cyanite (Si O_5 Al_2)
0
20
40
60
80
100
120
E_0 (keV)

THE CONTINUOUS SPECTRUM OF THE (P,C) CONTRIBUTION



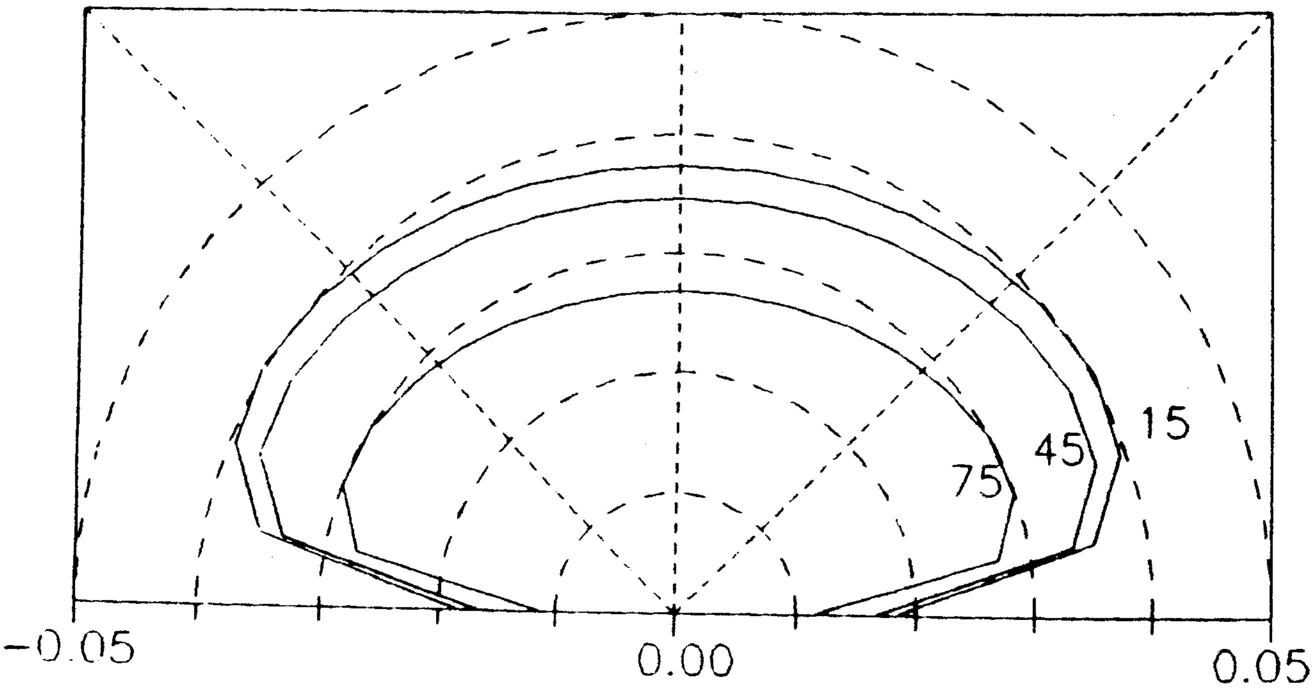
The (P,C) continuous contribution to the Cu $K\alpha_1$ line in a pure Cu sample for (a) variable excitation energy E_0 ($\vartheta_0 = 45^{\circ}$), and (b) variable angle of incidence ϑ_0 ($E_0 = 10$ keV).

POLAR INTENSITY AS A FUNCTION OF THE ANGLE OF INCIDENCE



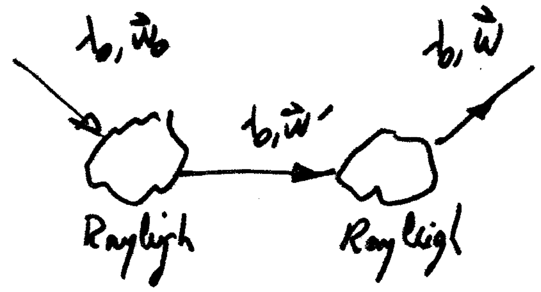
Polar graphs for the (R,P), (P,R), (C,P) and (P,C) contributions to the Zr $K\alpha_1$ in pure Zr excited with 20 keV x rays. The graphs correspond to polar angles of incidence ϑ_0 of (a) 15°, (b) 45° and (c) 75°.

POLAR INTENSITY (RELATIVE) AS A FUNCTION OF THE ANGLE OF INCIDENCE



This polar graph shows the total scattering contribution to the Zr $K\alpha_1$ line in a pure Zr sample excited with a 20 keV photon beam. The enhancement is plotted in units of the unmodified XRF line to show its importance. Since the XRF emission is isotropic, the polar plot should remain on a circular curve for an isotropic contribution. The shifts from the circular behavior signal an anisotropic behavior in that angular region.

Rayleigh-Rayleigh chain



$$I^{(2)}_{(R,R)}(\vec{\omega},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1+\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|}\,\frac{\delta(\lambda-\lambda_0)}{\frac{\mu_0}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\,\sigma^2$$

$$\Bigg\{ \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'} \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(+)})^2\right]\left[1+(\vec{\omega}'\cdot\vec{\omega}^{(+)})^2\right]}{\frac{\mu_0}{|\eta|}+\frac{\mu_0}{\eta'}} \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(+)}, z)}{z} \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}^{(+)}, z)}{z} +$$

$$\int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'} \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(-)})^2\right]\left[1+(\vec{\omega}'\cdot\vec{\omega}^{(-)})^2\right]}{\frac{\mu_0}{|\eta_0|}+\frac{\mu_0}{\eta'}} \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(-)}, z)}{z} \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}^{(-)}, z)}{z} \Bigg\}$$

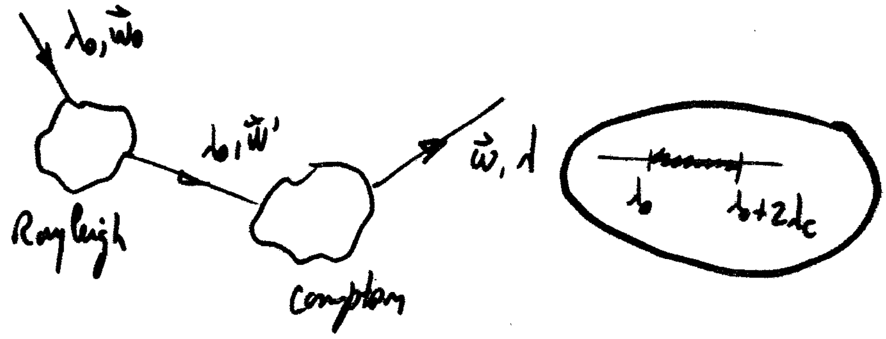
where

$$\vec{\omega}'\cdot\vec{\omega}_0^{(\pm)} = \pm\eta'\eta_0 + \sqrt{1-\eta'^2}\sqrt{1-\eta_0^2}\cos(\varphi'-\varphi_0)$$

$$\vec{\omega}'\cdot\vec{\omega}^{(\pm)} = \pm\eta'\eta + \sqrt{1-\eta'^2}\sqrt{1-\eta^2}\cos(\varphi'-\varphi)$$

- Discrete ($\lambda=\lambda_0$)
- Plane of symmetry
- Modifies also the coherent line

Rayleigh - Compton chain



$$I^{(2)}_{(R,C)}(\vec{w},\lambda) = \frac{1-\mathrm{sgn}\,\eta}{2}\,\frac{1+\mathrm{sgn}\,\eta_0}{2}\,\frac{I_0}{|\eta_0|\lambda_c}\,\frac{\sigma^2 K_{KN}(\lambda,\lambda_0)\,S(\lambda_0,a,Z)}{\frac{\mu}{|\eta|}+\frac{\mu_0}{|\eta_0|}}$$

$$\Bigg\{ \underset{(\alpha_2>\alpha_1)}{\int_{\alpha_1}^{\alpha_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{\eta'}+\frac{\mu}{|\eta|}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a-\eta'\eta)^2}}\sum_{i=1}^{2}\left(1+(\vec{w}_0\cdot\vec{w}_i'^{(+)})^2\right)\frac{F^2(\lambda_0,\vec{w}_0\cdot\vec{w}_i'^{(+)},Z)}{Z} +$$

$$\underset{(\beta_2>\beta_1)}{\int_{\beta_1}^{\beta_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta_0|}+\frac{\mu_0}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a+\eta'\eta)^2}}\sum_{i=1}^{2}\left[1+(\vec{w}_0\cdot\vec{w}_i'^{(-)})^2\right]\frac{F^2(\lambda_0,\vec{w}_0\cdot\vec{w}_i'^{(-)},Z)}{Z}\Bigg\}$$

where

$$a = 1+\frac{\lambda_0-\lambda}{\lambda_c}, \quad \varphi_1'^{(\pm)} = \varphi + \arccos\frac{a\mp\eta'\eta}{\sqrt{(1-\eta^2)(1-\eta'^2)}}, \quad \varphi_2'^{(\pm)} = \varphi + 2\pi - (\varphi_1'^{(\pm)}-\varphi)$$

$$\vec{w}_0\cdot\vec{w}_i'^{(\pm)} = \pm\eta_0\eta' + \sqrt{(1-\eta_0^2)(1-\eta'^2)}\,\cos(\varphi_i'^{(\pm)})$$

$$\alpha_1 = \max\left(0, a\eta - \sqrt{(1-\eta^2)(1-a^2)}\right)$$

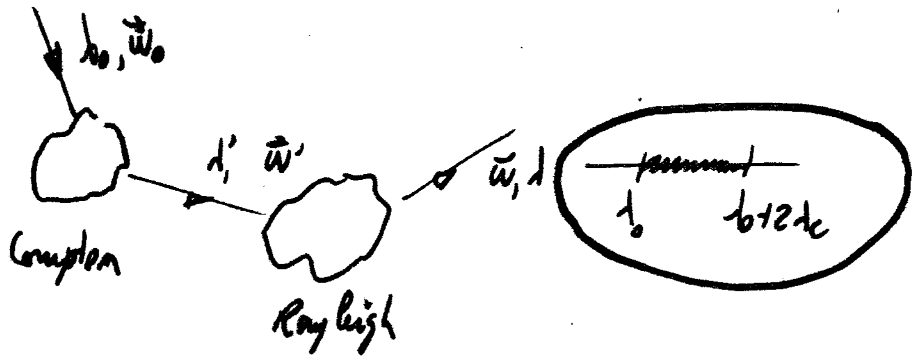
$$\alpha_2 = \min\left(1, a\eta + \sqrt{(1-\eta^2)(1-a^2)}\right)$$

$$\beta_1 = -\max\left(0, a\eta + \sqrt{(1-\eta^2)(1-a^2)}\right)$$

$$\beta_2 = -\min\left(-1, a\eta - \sqrt{(1-\eta^2)(1-a^2)}\right)$$

- Continuous $\lambda \in [\lambda_0, \lambda_0+2\lambda_c]$
- Modifies the Compton profile
- Overlaps the Compton-Rayleigh and Compton-Compton spectra
- May overlap other lines

Compton-Rayleigh chain



$$I^{(2)}_{(C,R)}(\vec{w},\lambda) = \frac{1-\operatorname{sgn}\gamma}{2}\,\frac{1+\operatorname{sgn}\gamma_0}{2}\,\frac{I_0}{|\gamma_0|\lambda_c}\,\frac{\sigma^c K_{KN}(\lambda,\lambda_0)\,S(\lambda_0,q,Z)}{\frac{\mu}{|\gamma|}+\frac{\mu_0}{|\gamma_0|}}$$

$$\Bigg\{ \int_{\substack{\alpha_1 \\ (\alpha_2>\alpha_1)}}^{\alpha_2} \frac{d\gamma'}{\gamma'}\,\frac{1}{\frac{\mu}{|\gamma|}+\frac{\mu}{\gamma'}}\,\frac{1}{\sqrt{(1-\gamma'^2)(1-\gamma_0^2)-(a-\gamma'\gamma_0)^2}}\sum_{i=1}^{2}\left(1+(\vec{w}\cdot\vec{w}_i'^{(+)})^2\right)\frac{F^2(\lambda,\vec{w}\cdot\vec{w}_i'^{(+)},Z)}{Z} +$$

$$\int_{\substack{\beta_1 \\ (\beta_2>\beta_1)}}^{\beta_2} \frac{d\gamma'}{\gamma'}\,\frac{1}{\frac{\mu_0}{|\gamma_0|}+\frac{\mu}{\gamma'}}\,\frac{1}{\sqrt{(1-\gamma'^2)(1-\gamma_0^2)-(a+\gamma'\gamma_0)^2}}\sum_{i=1}^{2}\left(1+(\vec{w}\cdot\vec{w}_i'^{(-)})^2\right)\frac{F^2(\lambda,\vec{w}\cdot\vec{w}_i'^{(-)},Z)}{Z}\Bigg\}$$

where $a = 1+\frac{\lambda_0-\lambda}{\lambda_c}$, $\varphi_1'^{(\pm)} = \arccos\frac{a\mp\gamma'\gamma_0}{\sqrt{(1-\gamma'^2)(1-\gamma_0^2)}}$, $\varphi_2'^{(\pm)} = 2\pi-\varphi_1'^{(\pm)}$

$$\vec{w}\cdot\vec{w}_i'^{(\pm)} = \pm\gamma\gamma' + \sqrt{(1-\gamma^2)(1-\gamma'^2)}\cos(\varphi_i'^{(\pm)}-\varphi)$$

$$\alpha_1 = \max\left(0, a\gamma_0-\sqrt{(1-\gamma_0^2)(1-a^2)}\right)$$

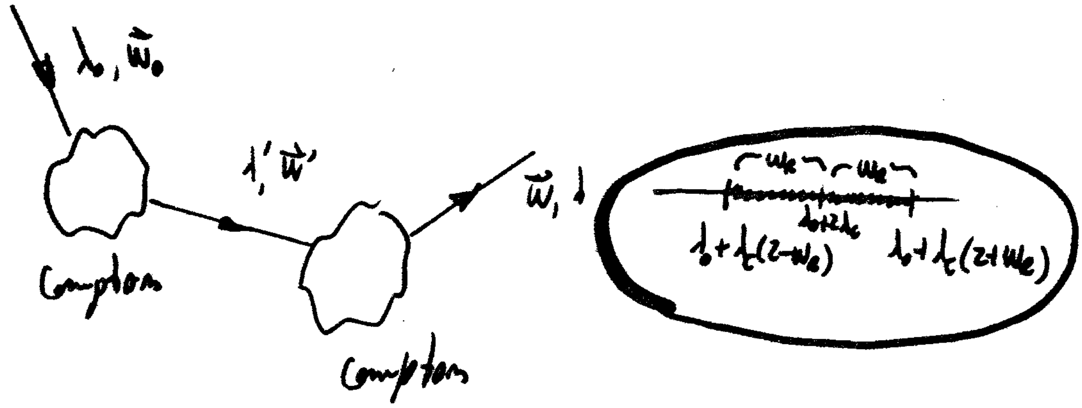
$$\alpha_2 = \min\left(1, a\gamma_0+\sqrt{(1-\gamma_0^2)(1-a^2)}\right)$$

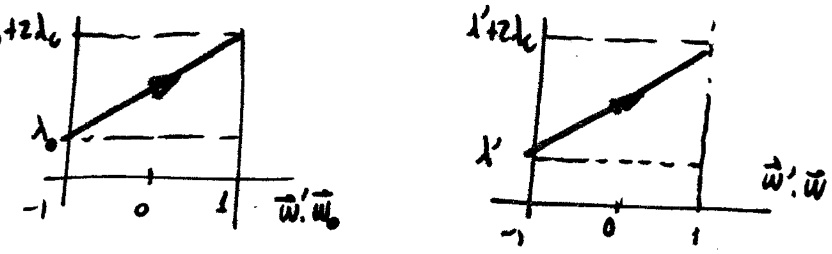
$$\beta_1 = -\min\left(0, a\gamma_0+\sqrt{(1-\gamma_0^2)(1-a^2)}\right)$$

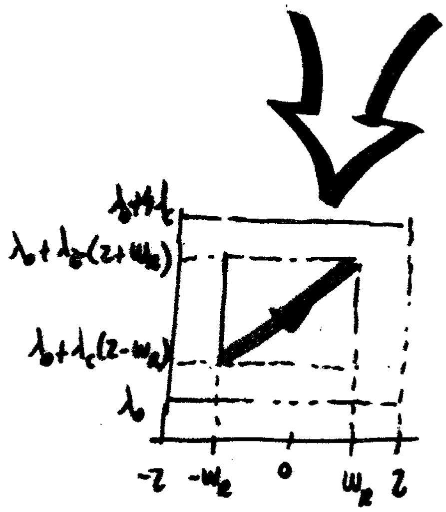
$$\beta_2 = -\max\left(-1, a\gamma_0-\sqrt{(1-\gamma_0^2)(1-a^2)}\right)$$

- Continuous $\lambda \in [\lambda_0, \lambda_0+2\lambda_c]$
- Modifies the Compton profile
- Overlaps the Rayleigh-Compton and Compton-Compton spectra
- May overlap other lines

Compton - Compton chain (detail)







$\vec{\omega}'.(\vec{\omega}+\vec{\omega}_0)$

$\vec{\omega}_R = \vec{\omega}+\vec{\omega}_0$

$\omega_R = \sqrt{2(1+\vec{\omega}.\vec{\omega}_0)}$

$$I^{(2)}_{(C,C)}(\vec{\omega},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1-\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|}\,\frac{\sigma^2}{\frac{\mu}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\int_0^\infty d\lambda' \int_{4\pi}\frac{d\vec{\omega}'}{|\eta'|}\,K_{KN}(\lambda,\lambda')\,K_{KN}(\lambda',\lambda_0)$$

$$S(\lambda', \vec{\omega}.\vec{\omega}', z)\,S(\lambda_0, \vec{\omega}'.\vec{\omega}_0, z)\,\delta\big(\lambda_c(1-\vec{\omega}'.\vec{\omega}_0)+\lambda_0-\lambda'\big)\,\delta\big(\lambda_c(1-\vec{\omega}'.\vec{\omega})+\lambda'-\lambda\big)$$

$$\left\{ \frac{1+\operatorname{sgn}\eta'}{2}\,\frac{1}{\frac{\mu}{|\eta|}+\frac{\mu'}{|\eta'|}} + \frac{1-\operatorname{sgn}\eta'}{2}\,\frac{1}{\frac{\mu_0}{|\eta_0|}+\frac{\mu'}{|\eta'|}} \right\}$$

Integration over λ' and Dirac-δ properties give

$$I^{(2)}_{(S,C)}(\vec{w},\lambda) = \frac{1-\mathrm{sgn}\,\eta}{2}\,\frac{1+\mathrm{sgn}\,\eta_0}{2}\,\frac{I_0}{|\eta_0|\lambda_c}\,\frac{\sigma^2}{\frac{\mu}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\int_{4\pi}\frac{d\vec{w}'}{|\eta'|}K_{kN}(\lambda,\tilde{\lambda})\,K_{kN}(\tilde{\lambda},\lambda_0)$$

$$S(\tilde{\lambda},\vec{w}\cdot\vec{w}';z)\,S(\lambda_0,\vec{w}'\cdot\vec{w}_0,z)\,\delta\left(2-\vec{w}'\cdot\vec{w}_R+\frac{\lambda_0-\lambda}{\lambda_c}\right)\left\{\frac{1+\mathrm{sgn}\,\eta'}{2}\,\frac{1}{\frac{\mu}{|\eta|}+\frac{\mu(\tilde{\lambda})}{|\eta'|}}+\frac{1-\mathrm{sgn}\,\eta'}{2}\,\frac{1}{\frac{\mu_0}{|\eta_0|}+\frac{\mu(\tilde{\lambda})}{|\eta'|}}\right\}$$

where $\tilde{\lambda} = \lambda_0 + \lambda_c(1-\vec{w}'\cdot\vec{w}_0)$

The δ-function can be written as

$$\delta\left(2-\vec{w}'\cdot\vec{w}_R+\frac{\lambda_0-\lambda}{\lambda_c}\right) =$$

$$= \delta\left(a - w_R\left(\eta'\eta_R + \sqrt{(1-\eta'^2)(1-\eta_R^2)}\,\cos(\varphi'-\varphi_R)\right)\right)$$

where

$$a = 2+\frac{\lambda_0-\lambda}{\lambda_c}\;,\quad \eta_R = \frac{\eta+\eta_0}{w_R}\;,\quad \varphi_R = \arccos\left(\frac{\sqrt{1-\eta_0^2}+\sqrt{1-\eta^2}\cos\varphi}{\sqrt{w_R^2-(\eta_0+\eta)^2}}\right)$$

for $\boxed{w_R \neq 0}$ we have

$$\delta\left(2-\vec{w}'\cdot\vec{w}_R+\frac{\lambda_0-\lambda}{\lambda_c}\right) =$$

$$= \frac{1}{w_R}\,\delta\left(\alpha-\eta'\eta_R-\sqrt{1-\eta'^2}\sqrt{1-\eta_R^2}\,\cos(\varphi'-\varphi_R)\right)$$

where $\alpha = \dfrac{a}{w_R}$.

The δ-function depends on η' <u>and</u> φ'. Is it possible to separate it into a part in φ' and a part in η'?

The condition into the δ satisfies for some values of $\cos(\varphi'-\varphi_R)$. Since the cosine function is defined in $[-1,1]$, that condition is equivalent to

$$\frac{(\alpha-\eta'\eta_R)^2}{(1-\eta'^2)(1-\eta_R^2)} \leq 1 \qquad ([illegible])$$

Condition (C.1) can be written as

$$(\alpha-\eta'\eta_R)^2 \le (1-\eta'^2)(1-\eta_R^2)$$

or

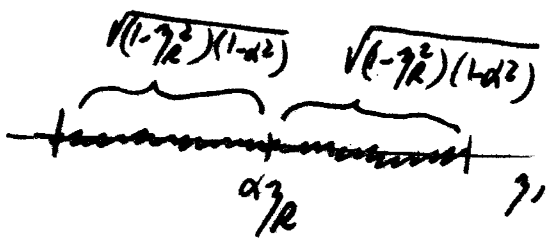
$$(\alpha^2+\eta_R-1) - 2\alpha\eta_R\eta' + \eta'^2 \le 0 \qquad \text{(C.2)}$$

which can be expressed as

$$(\eta'-\eta_1')(\eta'-\eta_2') \le 0 \qquad (\eta_1' \text{ and } \eta_2' \text{ are the roots of (C.2)})$$

$$\eta_{1,2}' = \alpha\eta_R \pm \sqrt{(1-\eta_R^2)(1-\alpha^2)}$$

Then we have that η' satisfies



We will use also the δ-function property $\delta[g(x)] = \sum_n \frac{\delta(x-x_n)}{|g'(x_n)|}$, $g(x_n)=0, g'(x_n)\neq 0$ to extract the φ' dependence of the δ

$$\delta\left(\alpha-\eta'\eta_R-\sqrt{1-\eta'^2}\sqrt{1-\eta_R^2}\cos(\varphi'-\varphi_R)\right) = \sum_{i=1}^{2}\frac{\delta(\varphi'-\varphi_i')}{|g'(\varphi_i')|}$$

$$= \sum_{i=1}^{2}\frac{\delta(\varphi'-\varphi_i')}{\sqrt{(1-\eta'^2)(1-\eta_R^2)-(\alpha-\eta'\eta_R)^2}}$$

where $\varphi_1 = \varphi_R + \arccos\left(\frac{\alpha-\eta'\eta_R}{\sqrt{(1-\eta'^2)(1-\eta_R^2)}}\right)$

$$\varphi_2 = 2\pi + \varphi_R - (\varphi_1-\varphi_R)$$

Finally

$$\delta\left(z - \vec{w}' \cdot \vec{w}_R + \frac{\lambda_0 - \lambda}{\lambda_c}\right) = \frac{1}{w_R} \frac{\delta(\varphi' - \varphi_1') + \delta(\varphi' - \varphi_2')}{\sqrt{(1-\gamma'^2)(1-\gamma_R^2) - (\alpha - \gamma'\gamma_R)^2}}$$

$$\left\{ \mathcal{U}\left(\gamma' - (\alpha\gamma_R - \sqrt{(1-\gamma_R^2)(1-\alpha^2)}\right) - \mathcal{U}\left(\gamma' - (\alpha\gamma_R + \sqrt{(1-\gamma_R^2)(1-\alpha^2)})\right) \right\}$$

By substituting in the last expression of $I^{(2)}_{(C,C)}$ we obtain after some algebra

$$I^{(2)}_{(C,C)}(\vec{w},\lambda) = \frac{1 - \operatorname{sgn}\gamma}{2} \; \frac{1 + \operatorname{sgn}\gamma_0}{2} \; \frac{I_0}{|\gamma_0| \lambda_c w_R} \; \frac{\sigma^2}{\frac{\mu}{|\gamma|} + \frac{\mu_0}{|\gamma_0|}}$$

$$\left\{ \int_{\substack{\alpha_1 \\ (\alpha_2 > \alpha_1)}}^{\alpha_2} \frac{d\gamma'}{\gamma'} \frac{1}{\sqrt{(1-\gamma'^2)(1-\gamma_R^2) - (\alpha - \gamma'\gamma_R)^2}} \sum_{i=1}^{2} \frac{K_{KN}(\lambda, \tilde{\lambda}_i^{(+)}) K_{KN}(\tilde{\lambda}_i^{(+)}, \lambda_0)\, S(\tilde{\lambda}_i^{(+)}, \vec{w} \cdot \vec{w}_i'^{(+)}, z)\, S(\lambda_0, \vec{w}_0 \cdot \vec{w}_i'^{(+)}, z)}{\frac{\mu}{|\gamma|} + \frac{\mu(\tilde{\lambda}_i^{(+)})}{\gamma'}} + \right.$$

$$\left. + \int_{\substack{\beta_1 \\ (\beta_2 > \beta_1)}}^{\beta_2} \frac{d\gamma'}{\gamma'} \frac{1}{\sqrt{(1-\gamma'^2)(1-\gamma_R^2) - (\alpha + \gamma'\gamma_R)^2}} \sum_{i=1}^{2} \frac{K_{KN}(\lambda, \tilde{\lambda}_i^{(-)}) K_{KN}(\tilde{\lambda}_i^{(-)}, \lambda_0)\, S(\tilde{\lambda}_i^{(-)}, \vec{w} \cdot \vec{w}_i'^{(-)}, z)\, S(\lambda_0, \vec{w}_0 \cdot \vec{w}_i'^{(-)}, z)}{\frac{\mu_0}{|\gamma_0|} + \frac{\mu(\tilde{\lambda}_i^{(-)})}{|\gamma'|}} \right\}$$

where $\tilde{\lambda}_i^{(\pm)} = \lambda_0 + \lambda_c (1 - \vec{w}' \cdot \vec{w}_{0i}^{(\pm)})$

$$\vec{w}' \cdot \vec{w}_{0i}^{(\pm)} = \pm \gamma'\gamma_0 + \sqrt{1-\gamma'^2}\sqrt{1-\gamma_0^2} \cos(\varphi_i'^{(\pm)})$$

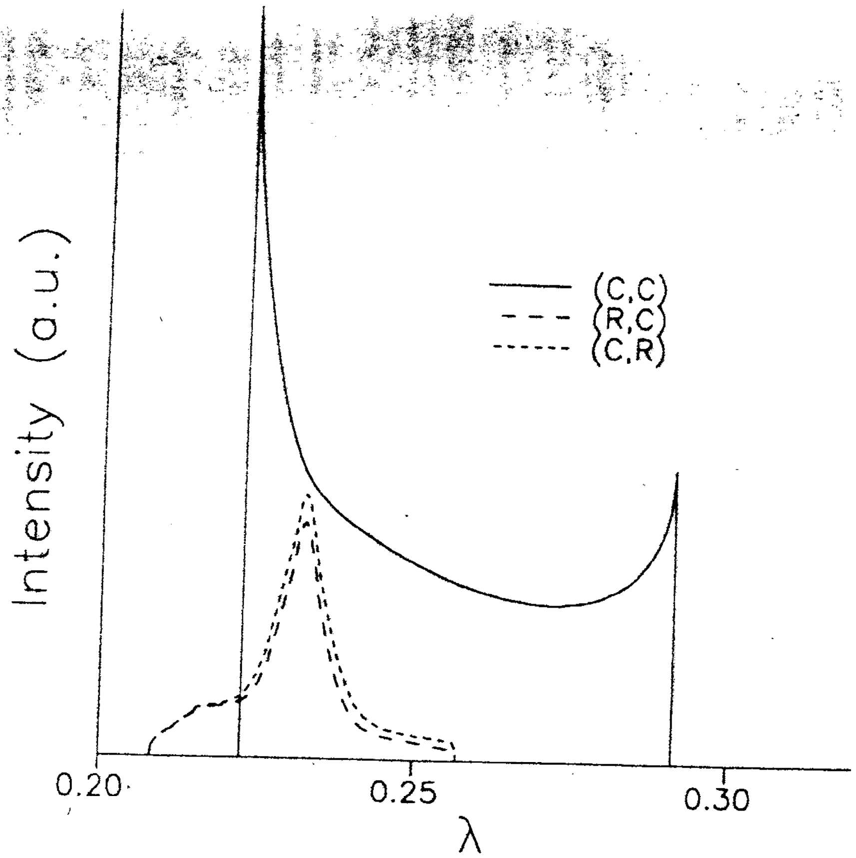
$$\alpha_1 = \max\left(0, \alpha\gamma_R - \sqrt{(1-\alpha^2)(1-\gamma_R^2)}\right)$$

$$\alpha_2 = \min\left(1, \alpha\gamma_R + \sqrt{(1-\alpha^2)(1-\gamma_R^2)}\right)$$

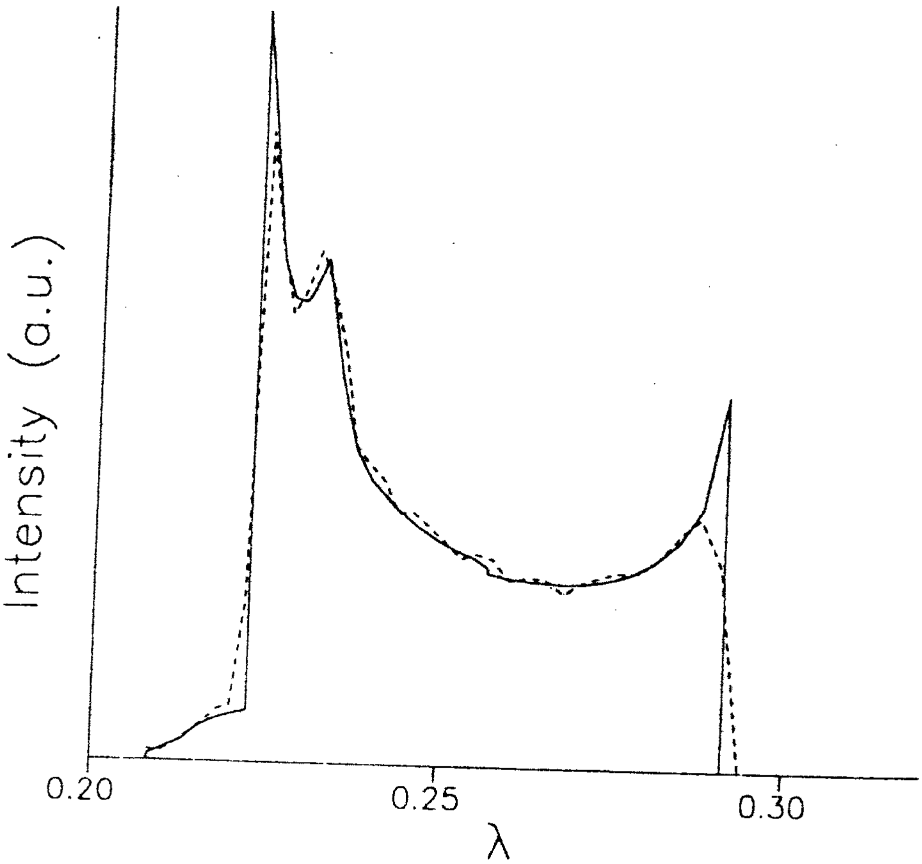
$$\beta_1 = -\min\left(0, \alpha\gamma_R + \sqrt{(1-\alpha^2)(1-\gamma_R^2)}\right)$$

$$\beta_2 = -\max\left(-1, \alpha\gamma_R - \sqrt{(1-\alpha^2)(1-\gamma_R^2)}\right)$$

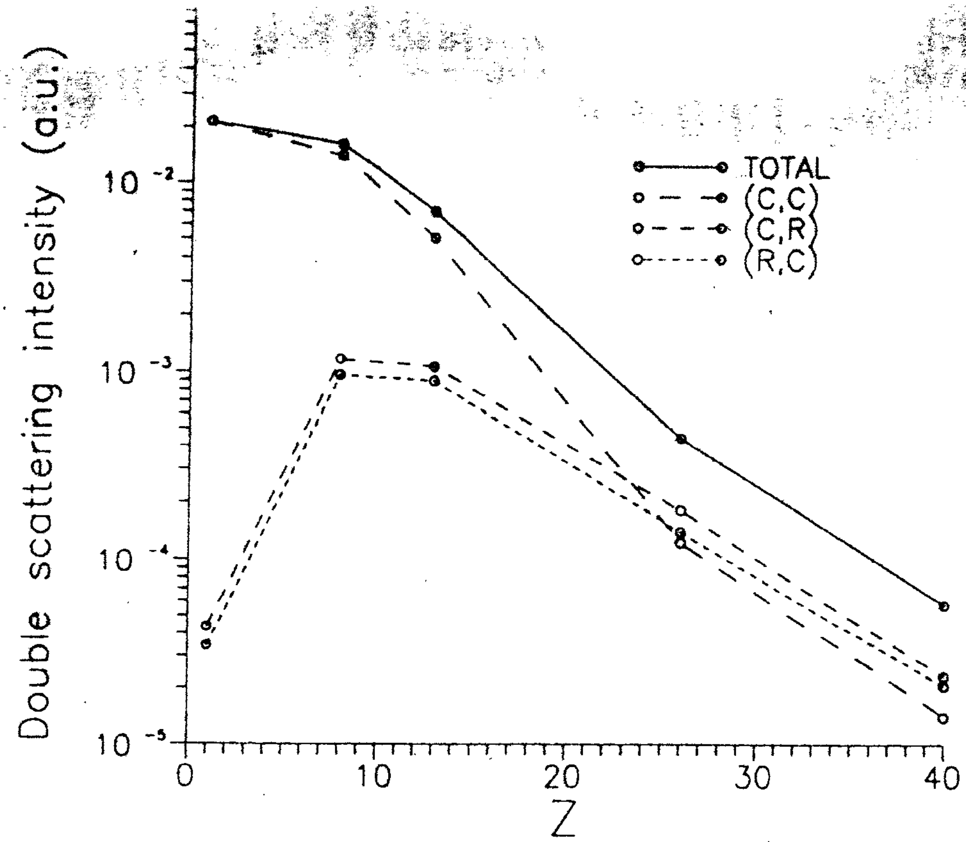
- Continuous $\lambda \in [\lambda_0 + \lambda_c(z - w_R), \lambda_0 + \lambda_c(z + w_R)]$
- Overlaps the Compton-Rayleigh and the Rayleigh-Compton chains
- Modifies the Compton profile

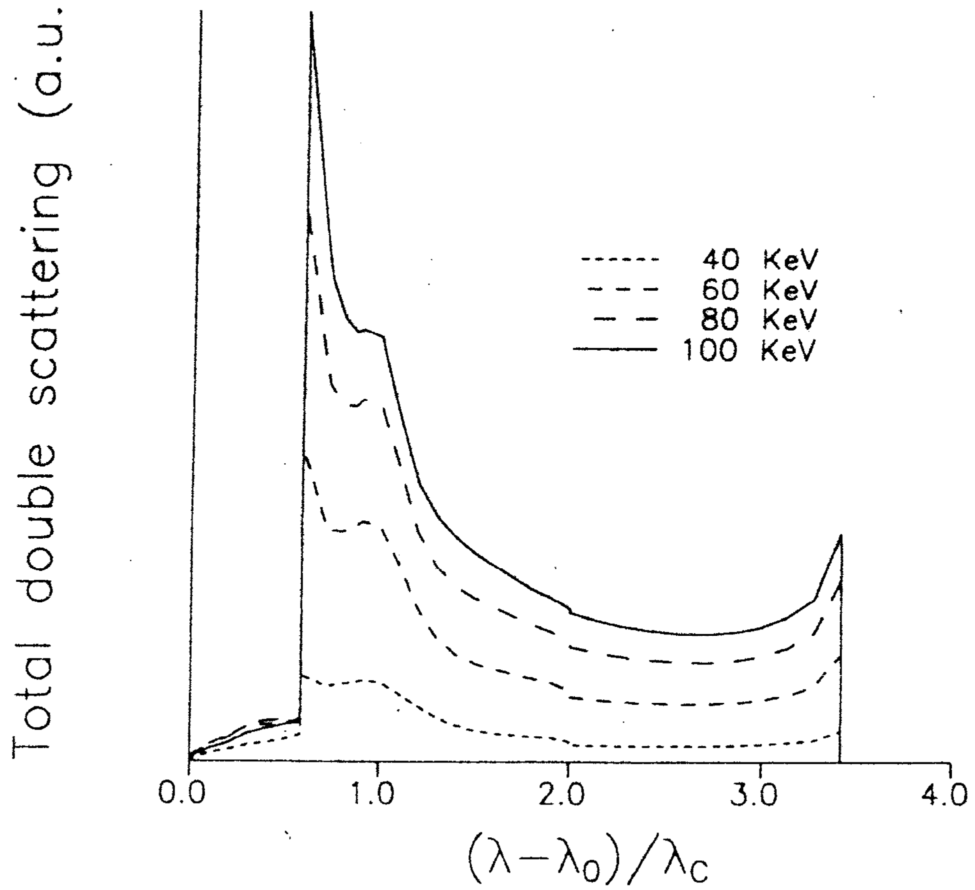


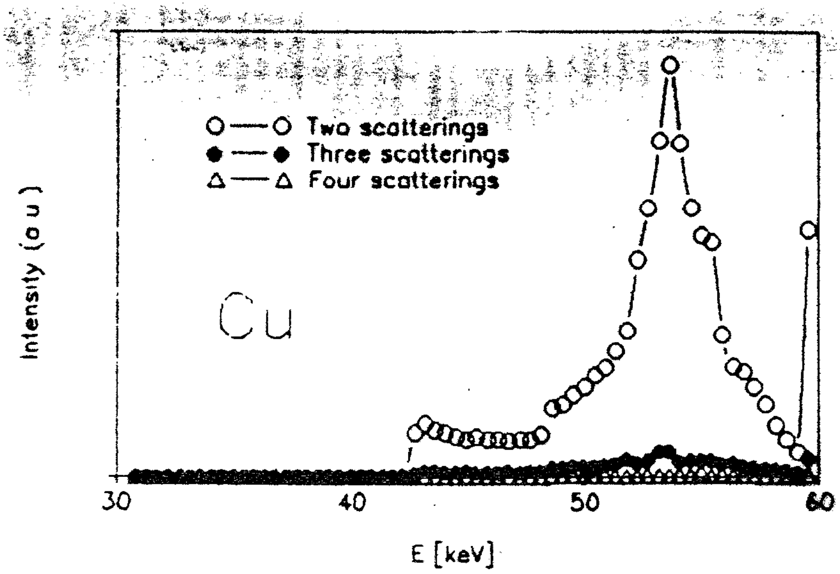
Intensity (a.u.)
(C,C)
(R,C)
(C,R)
0.20
0.25
0.30
λ

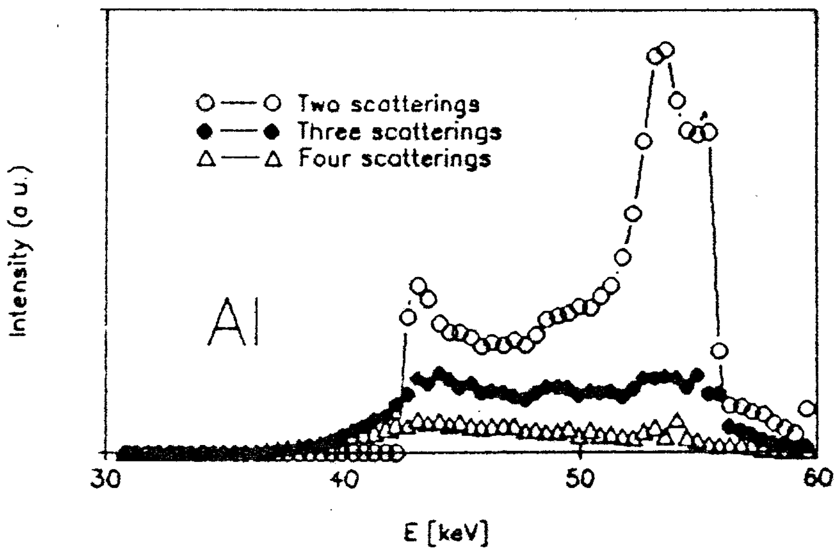


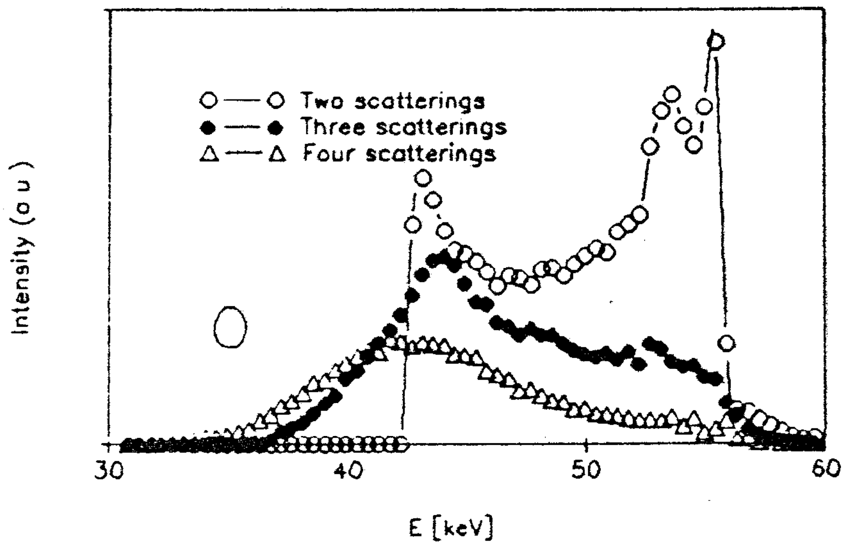
Intensity (a.u.)
0.20
0.25
0.30
λ


Double scattering intensity (a.u.)
TOTAL
(C,C)
(C,R)
(R,C)
10^{-2}
10^{-3}
10^{-4}
10^{-5}
0
10
20
30
40
Z


Total double scattering (a.u.)
40 KeV
60 KeV
80 KeV
100 KeV
0.0
1.0
2.0
3.0
4.0
$(\lambda-\lambda_0)/\lambda_C$


Two scatterings
Three scatterings
Four scatterings
Intensity (a u)
Cu
30
40
50
60
E [keV]

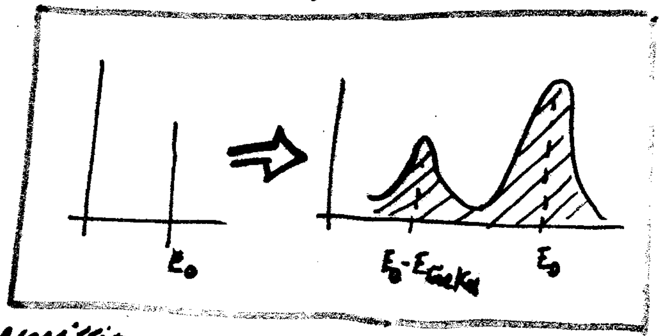

Two scatterings
Three scatterings
Four scatterings
Intensity (a u.)
Al
30
40
50
60
E [keV]


Two scatterings
Three scatterings
Four scatterings
Intensity (a u)
O
30
40
50
60
E [keV]

Detector response

$$R(E_0,E) = \left(1-\chi(E_0)\right)\frac{0.9395}{FWHM(E_0)}\, e^{-2.773\frac{(E-E_0)^2}{FWHM^2(E_0)}} +$$

$$\chi(E_0)\,\frac{0.9395}{FWHM(E_0-E_{K_\alpha Ge})}\, e^{-2.773\frac{(E_0-E_{K_\alpha Ge}-E)^2}{FWHM^2(E_0-E_{K_\alpha Ge})}}$$



where

$\phi(E_0)$ = efficiency at energy E_0

$\chi(E_0)$ = probability of escape peak emission

$$\chi(E_0) = 0.5\, \omega_{K_{Ge}}\left(1-\frac{1}{r_{K_{Ge}}}\right)\left[1-\frac{\mu_{Ge}(Ge\,k_\alpha)}{\mu_{Ge}(E_0)}\ln\left(1+\frac{\mu_{Ge}(E_0)}{\mu_{Ge}(Ge\,k_\alpha)}\right)\right]U(E_0-E_{GeK})$$

$FWHM(E)$ = full width at half maximum

$$FWHM(E) = 2.355\sqrt{(\Delta E_0)^2+\varepsilon E_0}$$

effective Fano factor

Some properties

$$\int R(E_0,E)\,dE = 1$$

NORMALIZATION

$$\tilde{I}(E) = \int R(E',E)\, I(E')\, \phi(E')\, dE'$$

efficiency

Comparison with experimental data

- If data are in energy we must transform our theoretical spectrum to energy (originally in wavelength)

- We have a part of the spectrum composed of discrete lines and a part with continuum. How do the discrete lines add to the continuum?
  We know the intensity of every line, not the distribution.
  We should assign a distribution (gaussian) to each line whose FWHM is given by the natural line width. After that we have a full continuous spectrum.

- Experimental data are in MCA format so we must divide the energy range as in a MCA, and digitalize the spectrum.

- Experimental data are of detected photons so we simulate a response function of a state-of-the-art radiation detector having
  - line broadening as a function of energy
  - efficiency as a function of energy
  - escape peak creation

Computation of X-Ray spectra

CODE: $\boxed{\text{SHAPE}}$

Reference: SHAPE: a computer simulation of energy dispersive X-ray spectra.

Author(s): J.E. Fernández and M. Sumini

Description: X-ray spectrum theoretical computation taking into account multiple scattering (photon-photon) processes of photoelectric, Rayleigh and Compton effects, for any element or mixture. Results allow the identification of different chain contributions of multiple scattering, and include detector response modification.
Geometry of excitation-detection and energy of the monochromatic source are interactively defined, as much as sample composition and detector characteristics.

THE CODE

NAME	SHAPE
MODULES	SHAPE1, SHAPE2
LANGUAGE	Pascal
COMPUTER	IBM PC
REQUIREMENTS	400 KB RAM
	Numerical coprocessor (recommended)
	Parameters data base
USAGE	Interactive

SHAPE1

Evaluates the first and second order contributions of the photoelectric effect and the Rayleigh and Compton scattering.

Computes the theoretical spectrum (in wavelength) on the surface of the target.

SHAPE2

Converts the wavelength spectrum to energy.

Converts monochromatic contributions into continuous ones.

Produces an MCA discretized spectrum simulating 1024 channels.

Filters the response through a Ge solid-state detector characteristic function.

PARAMETERS DATA BASE

PARAM containing the atomic number, the chemical symbol, the atomic weight, the density and the conversion constant from barns/atom to cm^2/g.

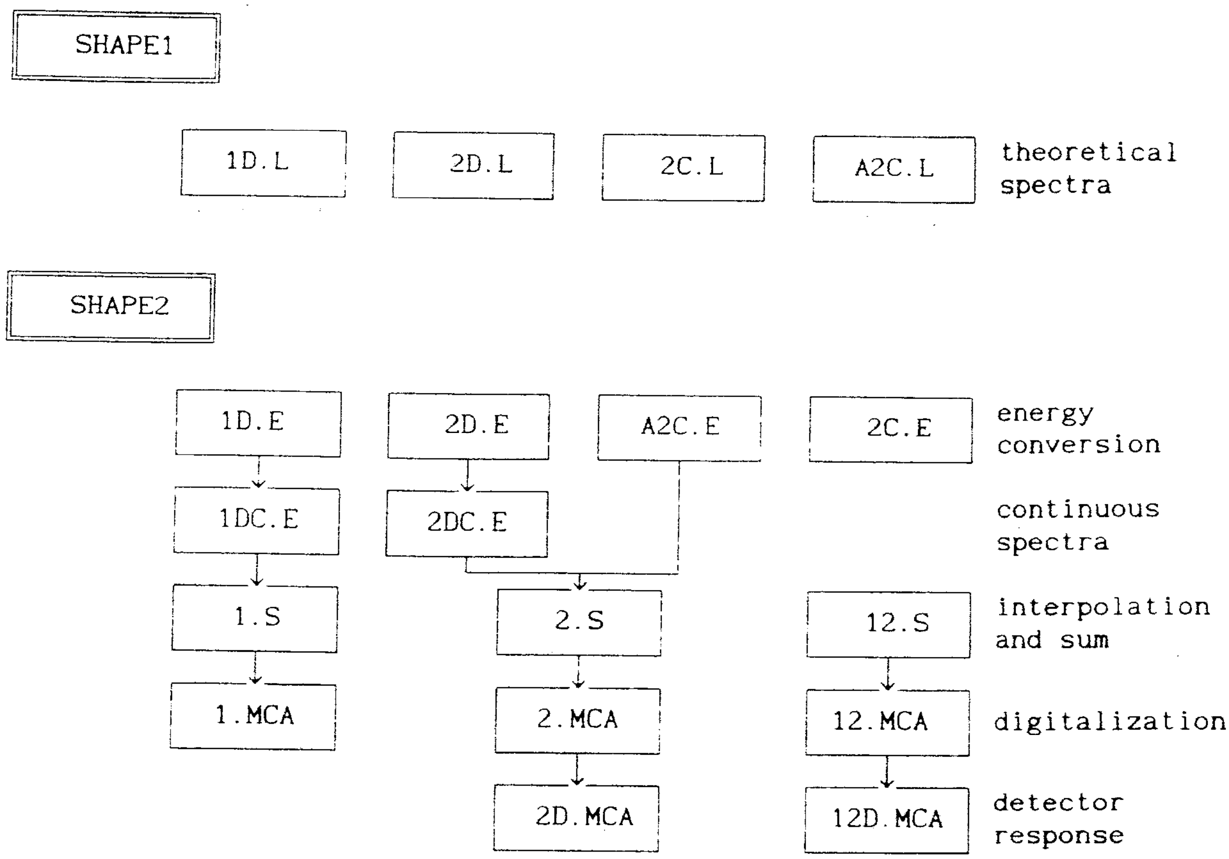
MCMASTER containing the McMaster coefficients for the photoelectric series K, L and M, and for integrated coherent and incoherent scattering.

EDGES containing the data related to the spectral series as spectral symbol, absorption edge energy, absorption edge jump, and fluorescence yield

LINES containing the data on every single line as the spectral series to which it belongs, its spectroscopic symbol, its energy, and its line fraction.

CROMER containing the parameters for computing the coherent and the incoherent scattering functions.

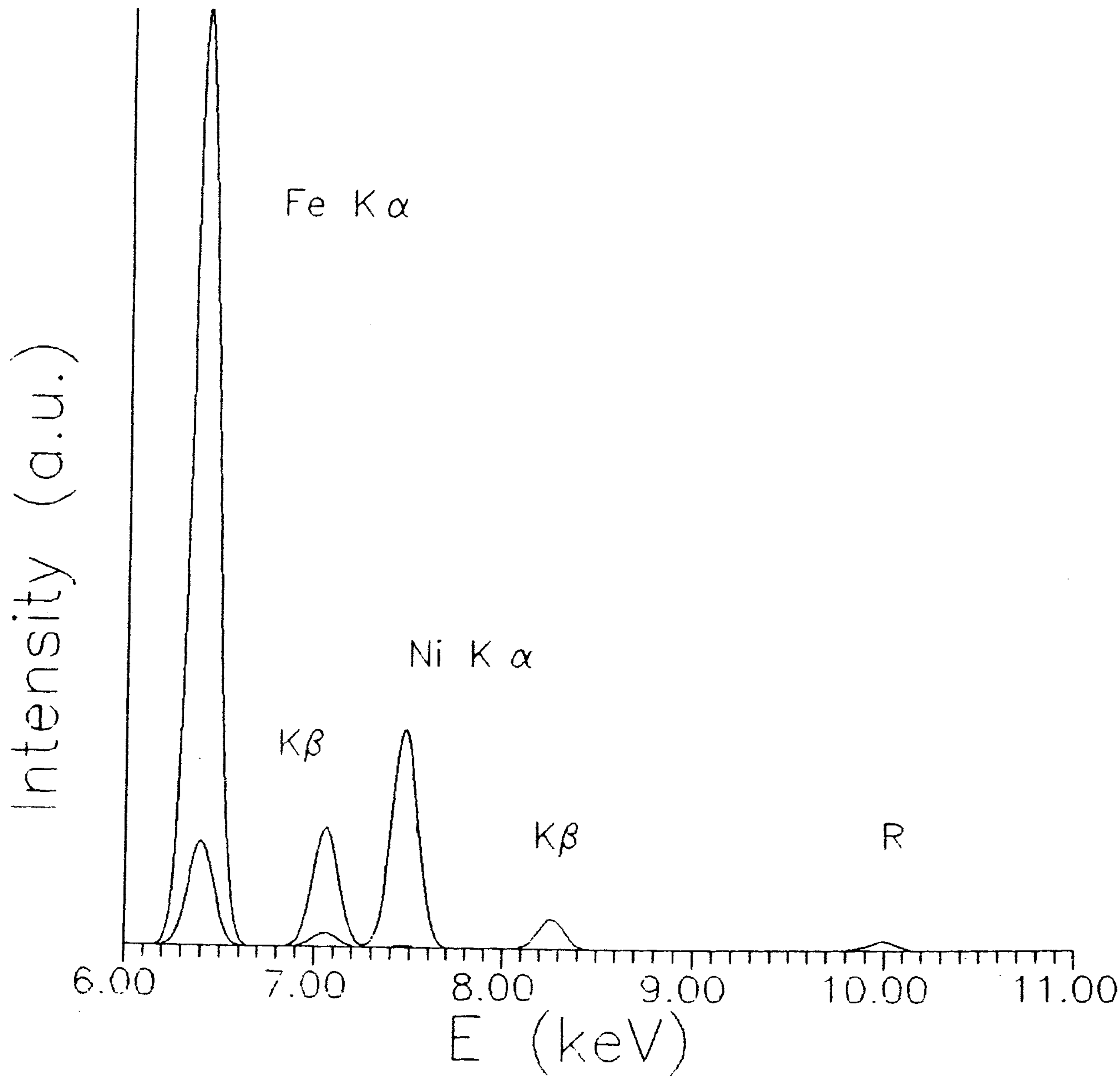
SHAPE'S FILE OUTPUT



File output of the two steps of SHAPE for the different stages of computation.

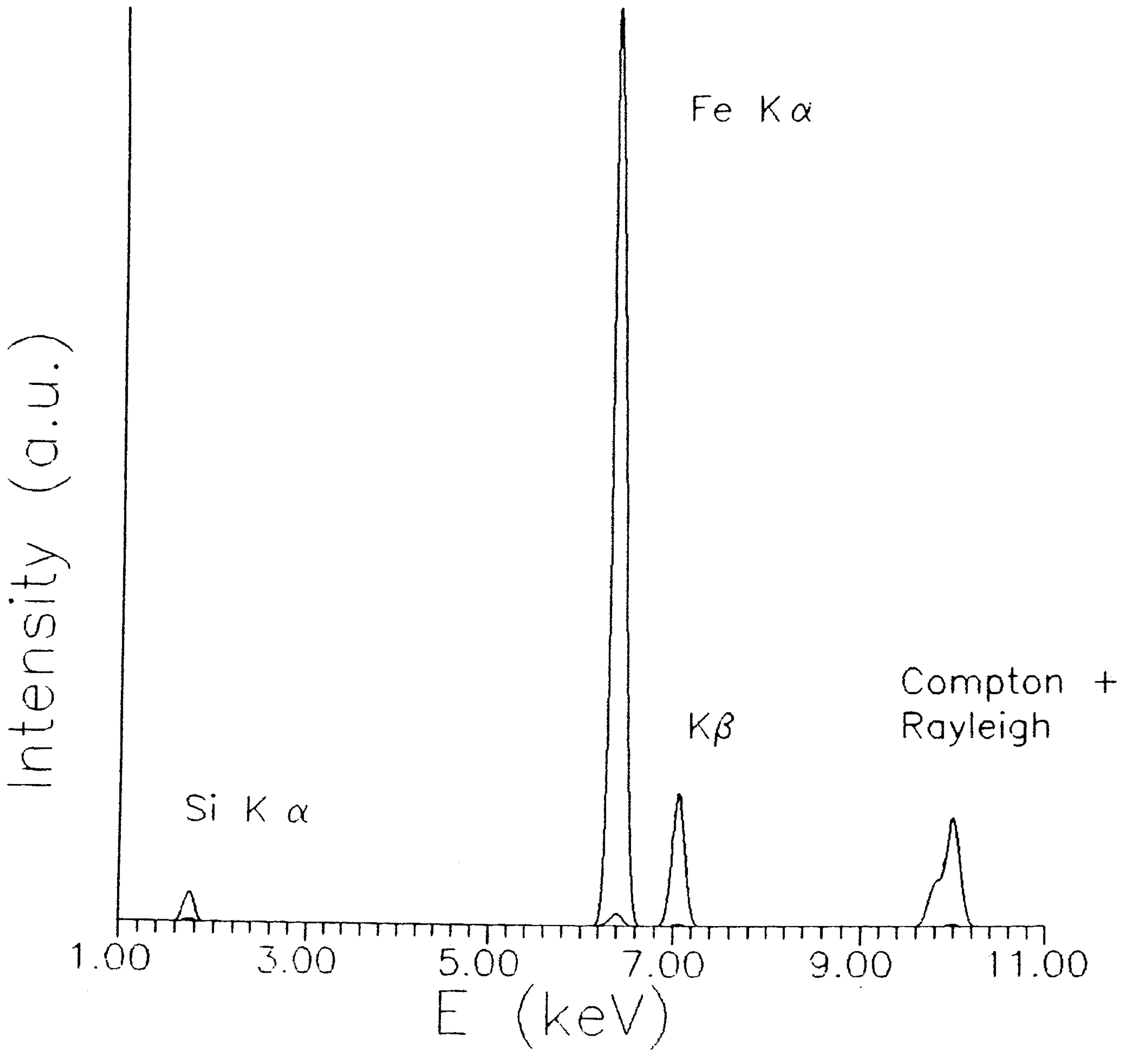
TEST PROBLEM

SAMPLE	Fe (75%) - Ni (25%)
EXCITATION ENERGY	10 keV
GEOMETRY (45/135/0)	Polar incidence 45°
	Polar take-off 45°
	Azimuthal angle 0°
COMMENTS	XRF characteristic lines showing the total and second order contributions.



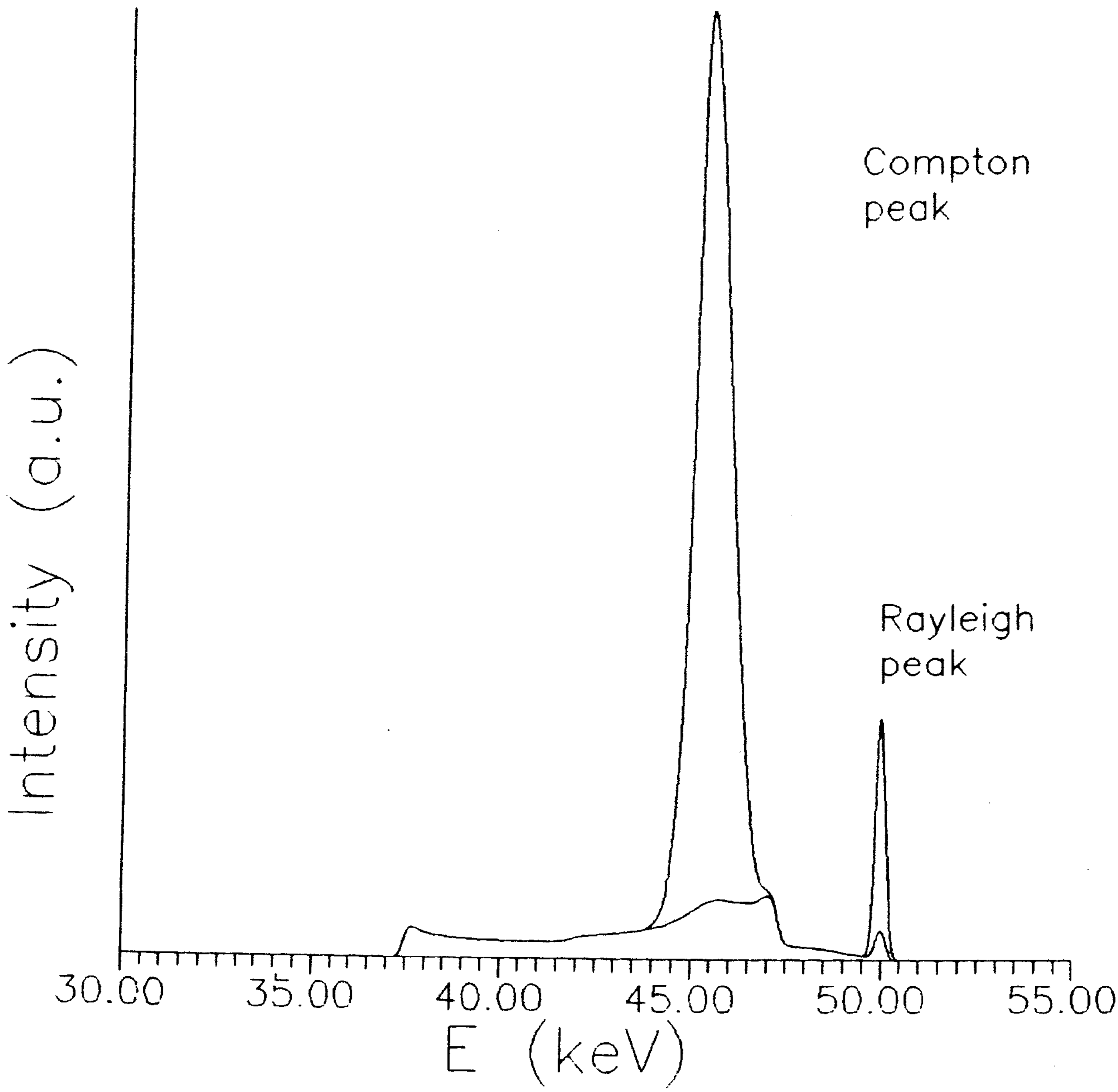
TEST PROBLEM

SAMPLE	SiO_2 (90%) - Fe_2O_3 (10%)
EXCITATION ENERGY	10 keV
GEOMETRY (45/135/0)	Polar incidence 45°
	Polar take-off 45°
	Azimuthal angle 0°
COMMENTS	Fe XRF characteristic lines
	showing the enhancement due to
	scattering



TEST PROBLEM

SAMPLE	SiO_2 (90%) - Fe_2O_3 (10%)
EXCITATION ENERGY	50 keV
GEOMETRY (45/135/0)	Polar incidence 45°
	Polar take-off 45°
	Azimuthal angle 0°
COMMENTS	Scattering spectrum showing the importance of the second order contribution.



TEST PROBLEM

SAMPLE	H_2O
EXCITATION ENERGY	59.54 keV (^{241}Am)
GEOMETRY (45/135/0)	Polar incidence 45°
	Polar take-off 45°
	Azimuthal angle 0°
COMMENTS	Comparison with experimental data obtained with a 5mm thick pure Ge detector (same as simulated by SHAPE).