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SCHOOL ON THE USE OF SYNCHROTRON RADIATION IN SCIENCE AND TECHNOLOGY:
"John Fuggle Memorial"

3 November - 5 December 1997

Miramare - Trieste, Italy

Evaluation of a scattered radiation field relevant for multiple energy X-ray holography

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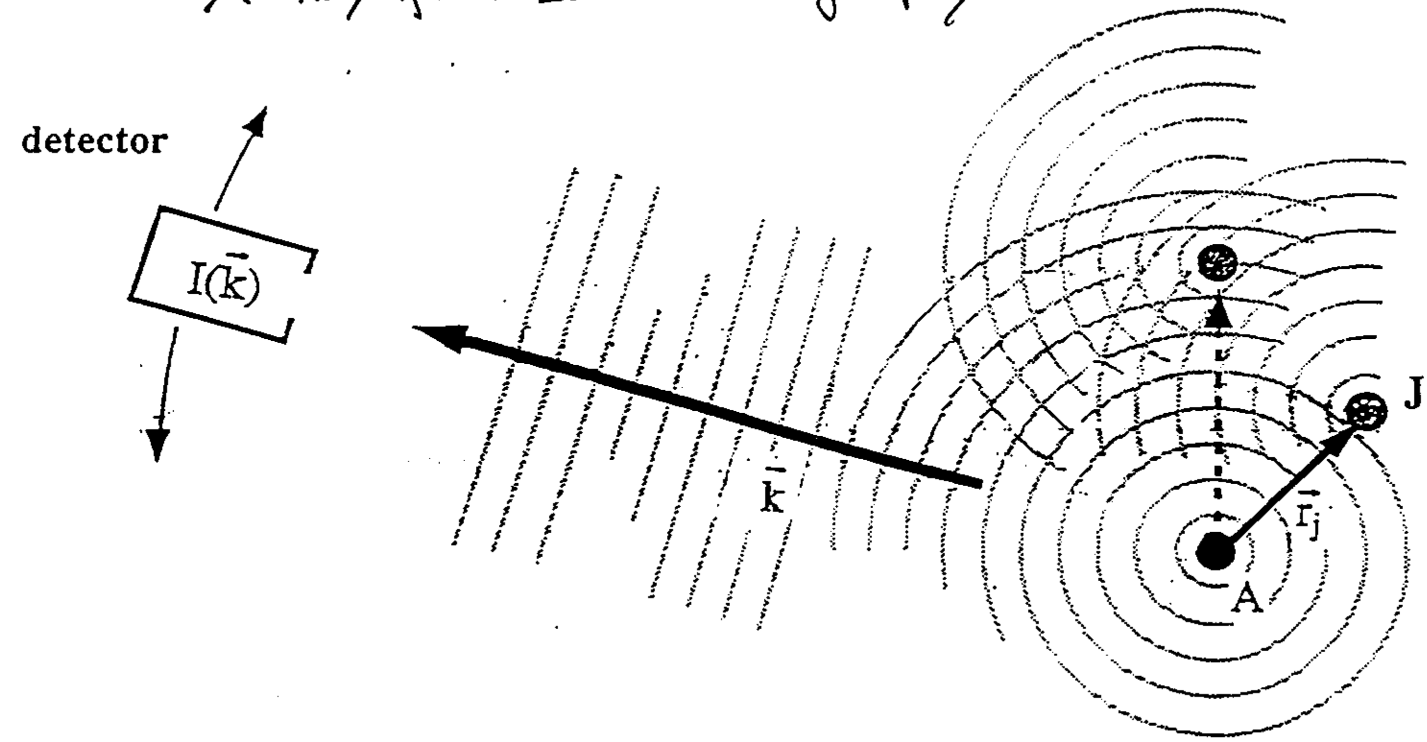
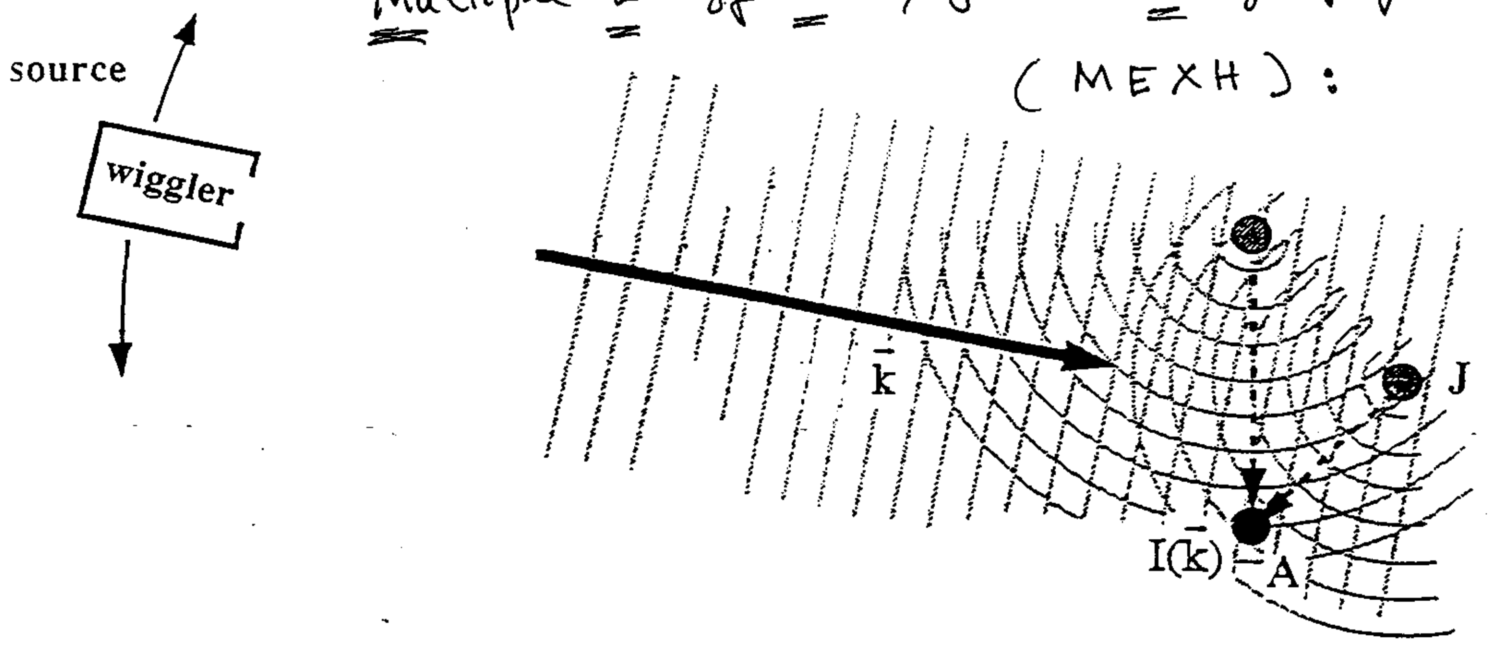
X-ray fluorescence holography:



Multiple Energy X-ray fluoresc. Holography

(MEXH):



References: Fadley, Materlik et al. Phys. Rev. Lett. 76, 3132 (1996)
" " " Synch. Rad. News 9, N.3, 30 (1996)

Electro-magnetic field:

$$A_\mu = A_\mu^{rad} + A_\mu^{ext}$$

Dirac:

$$\left[\gamma^\mu (i\partial_\mu - e A_\mu^{ext}) - m\right]\psi = e\gamma^\mu A_\mu^{rad}\psi$$

Maxwell:

$$\Box A_\mu^{rad} = e\bar{\psi}\gamma_\mu\psi$$

$$\bar{\psi} = \psi^\dagger\gamma^0$$

Must solve the Maxwell equation!

Write Dirac eq. in compact form:

$$\left[S^{ext}\right]^{-1}\psi = e\,\gamma^{\mu}A_{\mu}$$

its formal solution is:

$$\psi = \psi^{ext} + S^{ext}\,e\,\gamma^{\mu}A_{\mu}$$

$$\left\{\begin{array}{l} \text{where} \quad \left[S^{ext}\right]^{-1}\psi^{ext} = 0 \\ \text{i.e. } \underline{\text{electron only in the field } A_{\mu}^{ext} \text{ of the atom!}} \end{array}\right.$$

New Maxwell equation:

$$\Box A_{\mu}^{rad} = e\,\bar{\psi}^{ext}\gamma_{\mu}\psi^{ext} +$$

$$+ e^{2}\Big[\bar{\psi}^{ext}\gamma_{\mu}S^{ext}\gamma^{\nu}A_{\nu}^{rad}\psi +$$

$$+ \bar{\psi}\gamma^{\nu}A_{\nu}^{rad}S^{ext}\gamma_{\mu}\psi^{ext}\Big] +$$

$$+ O(e^{3})$$

Since I drop $O(e^3)$, then in the r.h.s. I can substitute $\psi \to \psi^{ext}$!

Let's go to numbers!

Take the following projection:

$$\underbrace{\langle 0|}_{\text{photon vacuum}} \langle \Psi_n | \text{Maxwell equation} \; |\Psi_n\rangle \underbrace{|1_i\rangle}_{\text{1 initial photon}}$$

$|\Psi_n\rangle \equiv$ core electron state of <u>atom n</u>

One gets:

$$\Box \langle A_\mu^{rad}(x)\rangle = e^2 \int d^4x' \, K_{\mu\nu}^{(n)}(x|x') \langle A_\nu^{rad}(x')\rangle$$

$$\langle A_\mu^{rad} \rangle = \langle 0 | A_\mu^{rad} | 1_i \rangle$$

$$K_{\mu\nu}^{(n)}(x|x') = \langle \Psi_n | \bar{\Psi}^{ext}(x) \gamma_\mu S^{ext}(x,x') \gamma^\nu \Psi^{ext}(x') | \Psi_n \rangle +$$

$$+ \left\langle \begin{matrix} x \leftrightarrow x' \\ \mu \leftrightarrow \nu \end{matrix} \right\rangle$$

I want only radiation: Take $A_0^{rad} = 0$.
Solve for $\mu \equiv j = 1, 2, 3$:

$$\langle A_j^{rad}(x) \rangle = A_j^{ref}(x) + e^2 \int d^4x' D_{ret}(x-x') \int d^4x'' K_{jl}^{(n)}(x'|x'') \langle A_l^{rad}(x'') \rangle$$

Dropping again terms $O(e^3)$:

$$\langle A_j^{rad}(x) \rangle = A_j^{ref}(x) + e^2 \int d^4x' D_{ret}(x-x') \int d^4x'' K_{jl}^{(n)}(x'|x'') A_l^{ref}(x'')$$

$$A_j^{ref}(x) = \vec{\varepsilon}_j \, e^{i(\vec{k}\cdot\vec{x} - \omega t)} \qquad j = 1,2,3 \qquad \omega \equiv |\vec{k}|$$

$\vec{\nabla}\cdot\vec{A}^{ref} = 0$, $\vec{\varepsilon}\cdot\vec{k} = 0$, radiation condition

$$D_{ret}(x-x') = \frac{1}{8\pi^2}\int_{-\infty}^{+\infty} dk\, e^{ik(t-t')}\, \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$$

$$= \frac{1}{4\pi|\vec{x}-\vec{x}'|}\,\delta\Big(|\vec{x}-\vec{x}'|-(t-t')\Big)$$

Taking the fourier transform of $K^{(m)}$ on time:

$$K_{j\ell}^{(m)}(x'|x'') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\, e^{ik(t''-t')}\, K_{j\ell}^{(m)}(k;\vec{x}'|\vec{x}'')$$

(static field A^{ext} !)

one finally obtains (let's sum on the atoms m):

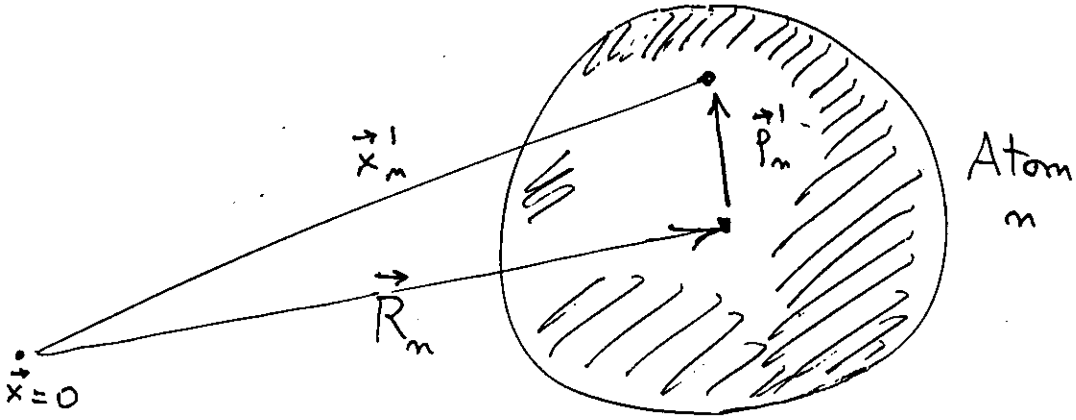
$$\left(A_j^{rad}(\vec{k};\vec{x}) \equiv e^{ikt}\langle A_j^{rad}(x)\rangle\right)$$

$$A_j^{rad}(\vec{k};\vec{x}) = \varepsilon_j\, e^{i\vec{k}\cdot\vec{x}} +$$

$$+ \frac{e^2}{4\pi}\sum_{m=1}^{N}\iint d^3x'_m\, d^3x''_m\, \frac{e^{ik|\vec{x}-\vec{x}'_m|}}{|\vec{x}-\vec{x}'_m|}\, K_{j\ell}^{(m)}(k;\vec{x}'_m,\vec{x}''_m)\,\varepsilon_\ell\, e^{i\vec{k}\cdot\vec{x}''_m}$$

$$A_j^{rad}(\vec{k};\vec{x}) \equiv A_j^{ref} + A_j^{obj} \ldots$$

Take $\vec{x}=0$ for simplicity.



then
$$\frac{e^{ik|\vec{x}-\vec{x}'_n|}}{|\vec{x}-\vec{x}'_n|} \underset{R_n \text{ large}}{\cong} \frac{e^{ikR_n}}{R_n} \cdot e^{-i\vec{k}_n\cdot\vec{\rho}'_n}$$

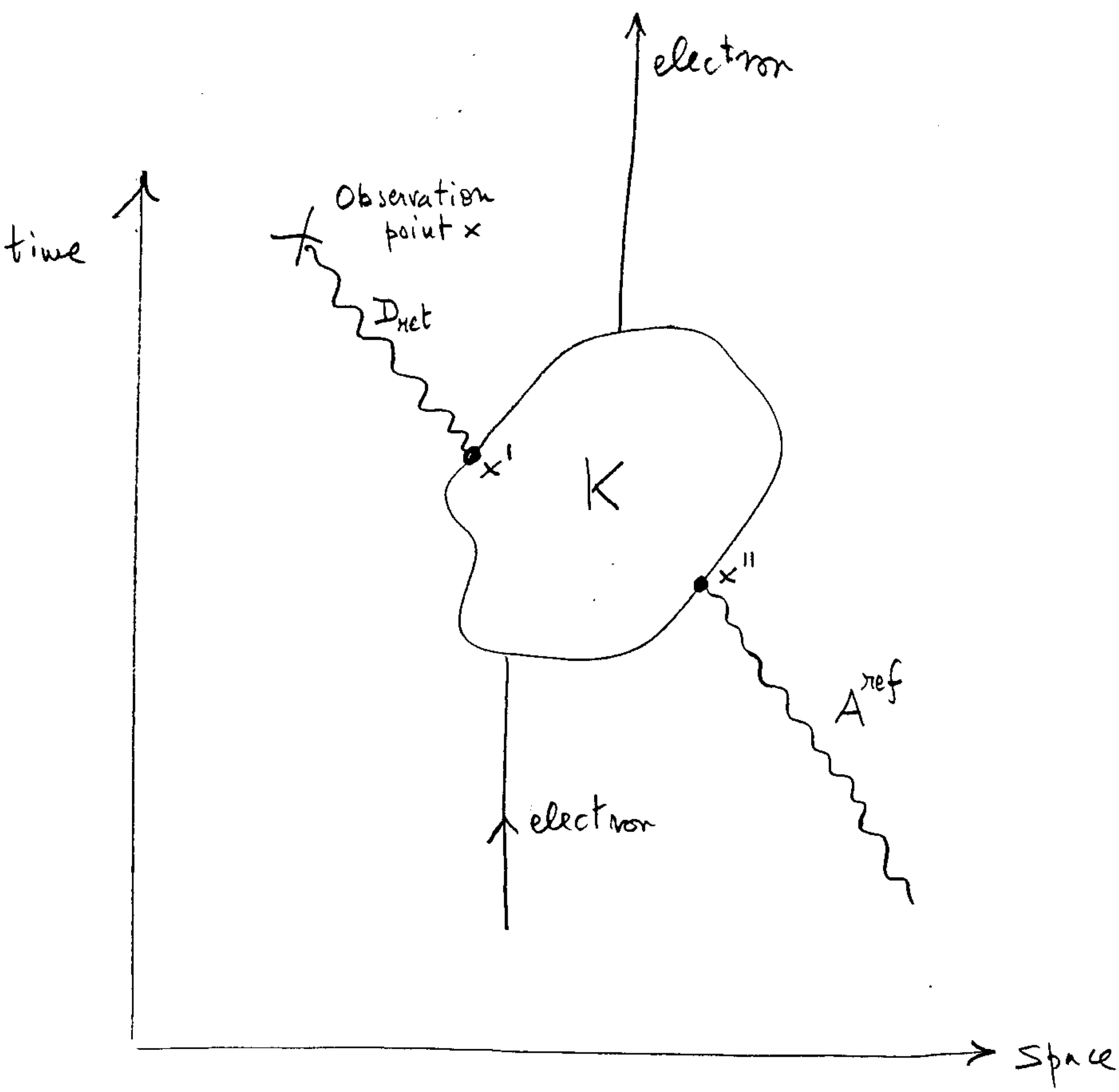
This is called <u>P</u>lane <u>W</u>ave <u>A</u>pproximation (PWA)

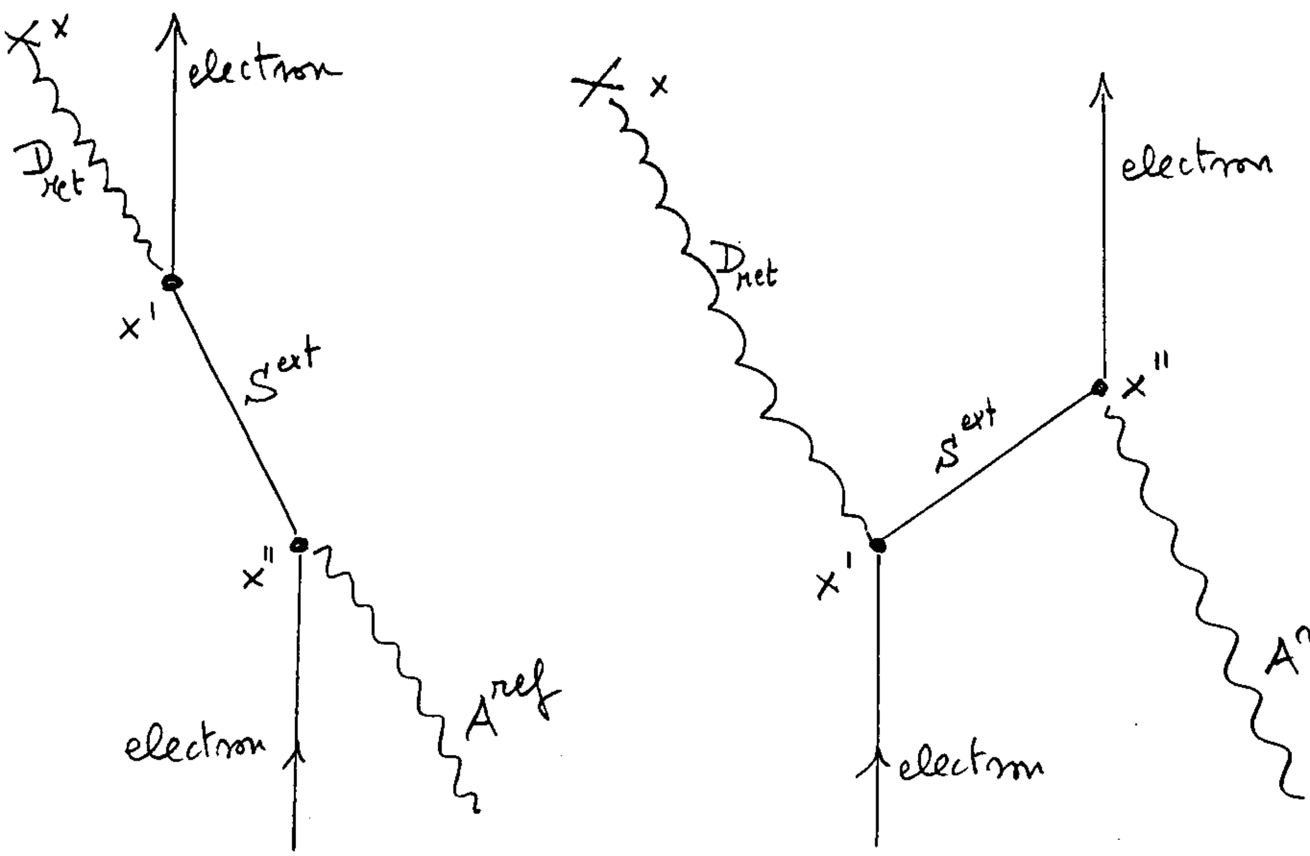
Finally obtain in the PWA:

$$A_j^{obj}(\vec{k};\vec{x}=0) = \sum_{n=1}^{N} \frac{e^{i(kR_n+\vec{k}\cdot\vec{R}_n)}}{R_n} f_{jl}^{(n)} \varepsilon_l$$

where $f^{(n)}$ is the scattering amplitude of the photon from the n^{th}-Atom:

$$f_{jl}^{(n)} = \iint d^3\rho'_n\, d^3\rho''_n\, e^{-i\vec{k}_n\cdot\rho'_n} \frac{e^2}{4\pi} K_{jl}^{(n)}(\vec{x}'_n|\vec{x}''_n)\, e^{i\vec{k}\cdot\rho''_n}$$


electron
time
Observation point x
D_{ret}
x'
K
x''
A^{ref}
electron
space


x
electron
D_{ret}
x'
S^{ext}
x''
electron
A^{ref}
x
electron
D_{ret}
S^{ext}
x''
x'
A^{ref}
electron