Quantum dynamics with x-rays

$9^{30} - 12^{30}$
break $11^{00} - 11^{15}$

DAY 1 – MONDAY

→ intro slides:

- historical perspective on lasers
- atomic physics and quantum optics
- novel coherent light sources
- x-ray incentives in quantum
- x-rays for imaging
- further nuclear incentives
- incentive on quant. optics with x-rays
- the trinity: x-ray physics
  quantum optics/phys
  nuclear transitions
  (few atoms)

→ we start with a part on x-rays:

(1) How do we generate x-rays?

Photos!

First x-ray shots by Röntgen in Würzburg 1895
with x-ray tube "Crookes tube"
→ cathode rays

How does this work?

→ Bremsstrahlung
→ $K\alpha$

(?) Bohr model
why not bound $\bar{e}$ in atom?

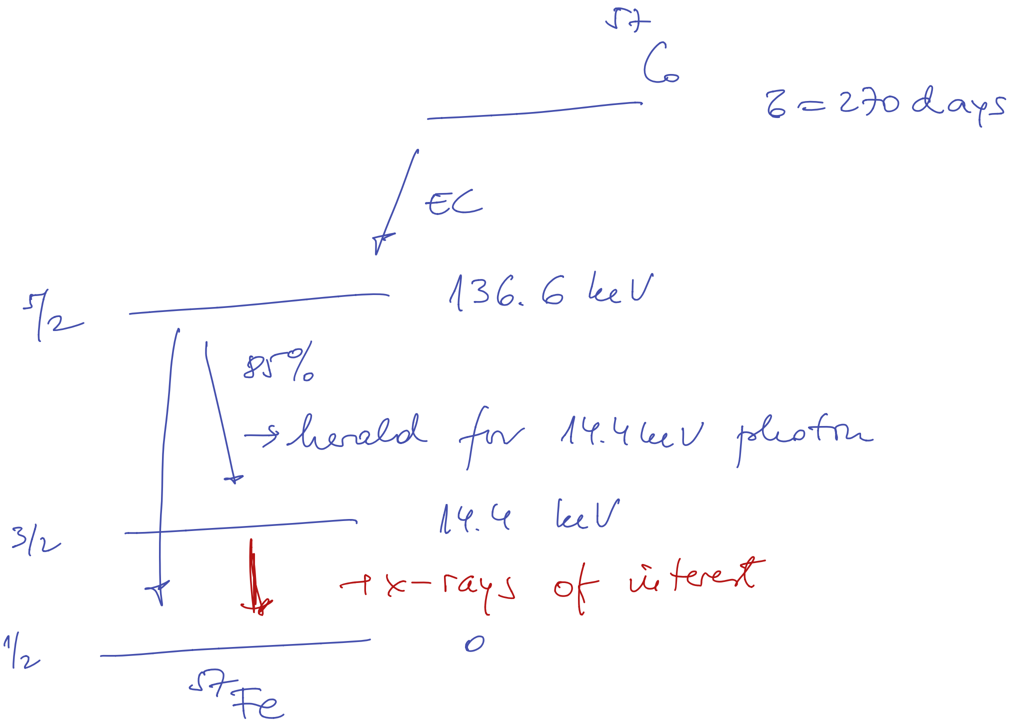
→ What about radioactive sources?

For instance decay of $^{57}_{27}Co$ to $^{57}_{26}Fe$ by EC

$p + e^- \to n + \nu_e$ called "electron capture"

in our case

$$^{57}_{27}Co + e^- \to {}^{57}_{26}Fe + \nu_e$$



But

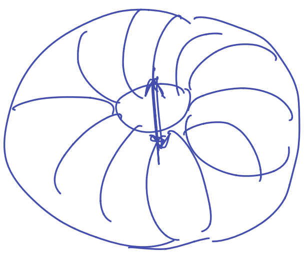
→ not tunable

→ not very strong

→ is all the time "ON" → not really controlable!

Generation of electromagnetic radiation:

Hertz tested Maxwell's theory on electromagnetism.
Use a dipole oscillator that emits radiation.



→ no rad. in the direction of oscillation

→ max. rad. power is observed $\perp$ to the oscillation direction.

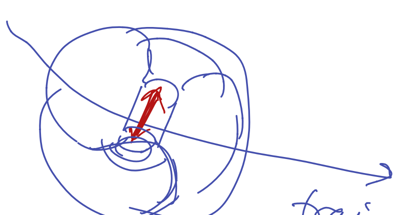
Larmor formula for radiated power:

$$P = \frac{e^2}{6\pi\varepsilon_0 m^2 c^3}\left(\frac{d\vec{p}}{dt}\right)^2$$

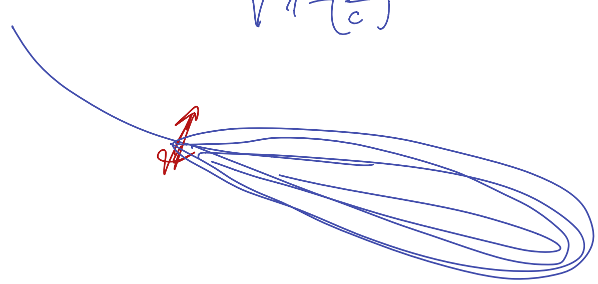
Now let us assume that our oscil. dipole is moving at high speed → transform from rest frame to laboratory frame

Lorentz transformation

$$\gamma = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \frac{E}{m_0 c^2}$$



→



$$\beta = \frac{v}{c}$$

graphs

few examples for different values of β.

Let us apply this transf for circular acceleration → Larmor formula

$$P = \frac{e^2 c}{6\pi\varepsilon_0} \frac{1}{(m_0 c^2)^4} \cdot \frac{E^4}{R^2}$$

→ $\sim \frac{E^4}{m_0^4}$ need large γ

→ $\sim \frac{1}{R^2}$ rad. loss needs large R

→ small m_0.

check about mass:

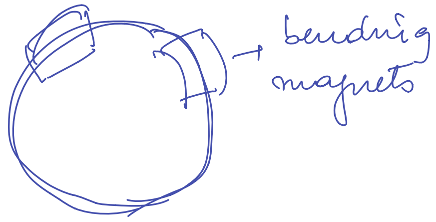
electron vs. proton $m_p / m_e = 1836 \simeq 2 \cdot 10^3$

$$\frac{P(e)}{P(p)} = \left(\frac{m_p}{m_e}\right)^4 \simeq 10^{13} \quad !!!$$

huge difference ⇒ bremsstrahlung is emitted mainly by electrons (positrons) ⇒ all x-ray sources rely on that!!!

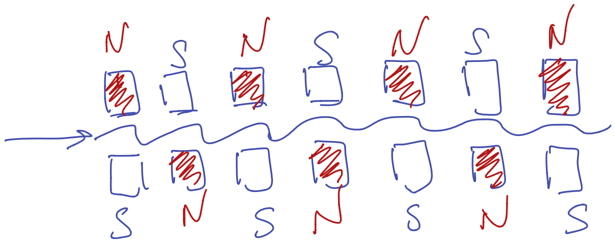
⇒ many powerful sources use CIRCULAR ACCEL. of HIGHLY RELATIVISTIC EL.!

Actually nowadays we do not use

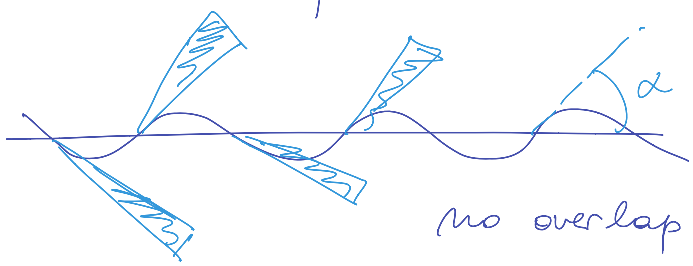


use undulators

periodic magnetic structures



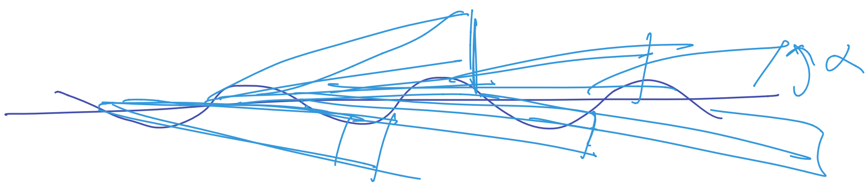
Some classification:



$\alpha > \frac{1}{\gamma}$

WIGGLER

no overlap of light cones!



$\alpha < \frac{1}{\gamma}$

UNDULATOR

radiation cones overlap, wave trains can interfere constructively!

Similar principle also for Free Electron Laser!

→ <u>wiggler</u> : $I \sim N_e N_p$

$N_e \to \bar{e}/\text{bunch}$

$N_p \to$ magnet poles.

→ emission of single $\bar{e}$ in diff. periods indep.

→ em. of diff. $\bar{e}$ indep.

→ undulator

$I \sim N_e N_p^2$

→ em. of single $\bar{e}$ in different periods coherent

→ em. of diff. $\bar{e}$ independent

→ free electron laser

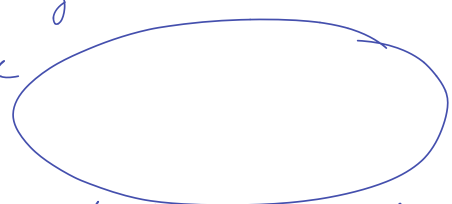
$I \sim N_e^2 N_p^2$

Self Amplified Spont. Emission

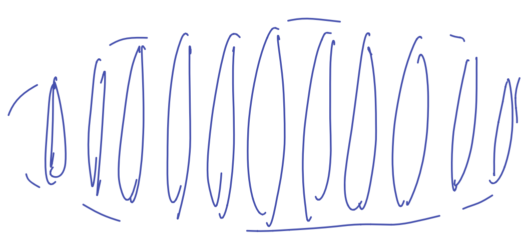
→ movie LCLS + photos DESY, etc.

microbunching

electron pulse



interacts with the light emitted by itself and individual $\bar{e}$ are accel/decel. so that they bunch in "slices"



each slice creates an x-ray pulse.
light of $\bar{e}$ in one microbunch (slice) adds up coherently!

② Characterization of light

one typically speaks of BRILLIANCE

$$\frac{\#\ \text{photons}}{\text{second} \cdot (0.1\%\ \text{BW}) \cdot \text{mrad}^2 \cdot \text{mm}^2}$$

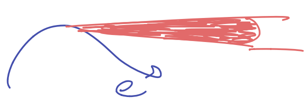
See it as a way to quantify the flux:

- normalized to bandwidth (BW)

  $0.1\%\ \text{BW} = 10^{-3} \cdot \dfrac{\text{width of freq. spectrum}}{\text{characteristic freq.}}$

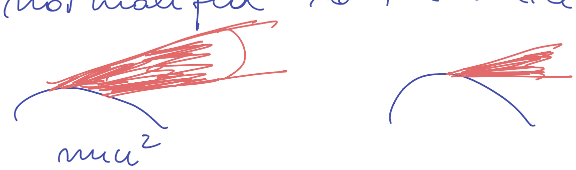
  (how monochromatic!)

- normalized to the emission opening angle

  $\sim \text{mrad}^2$ (how well collimated?)

- normalized to the source size

  how large is the effective source?

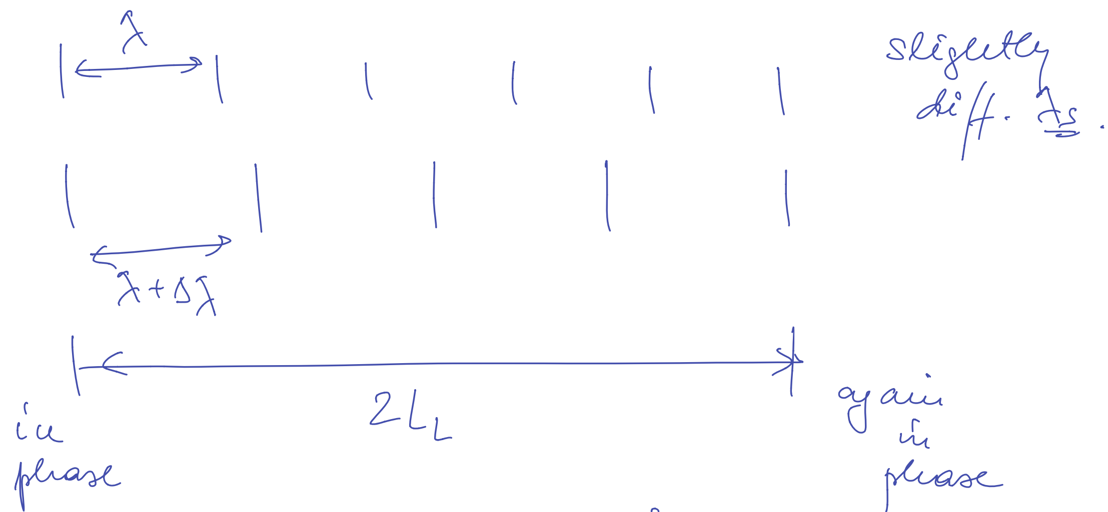
Graph on brilliances of sources!

+ slide on coherence / temporal / spatial

COHERENCE → very important concept

→ temporal

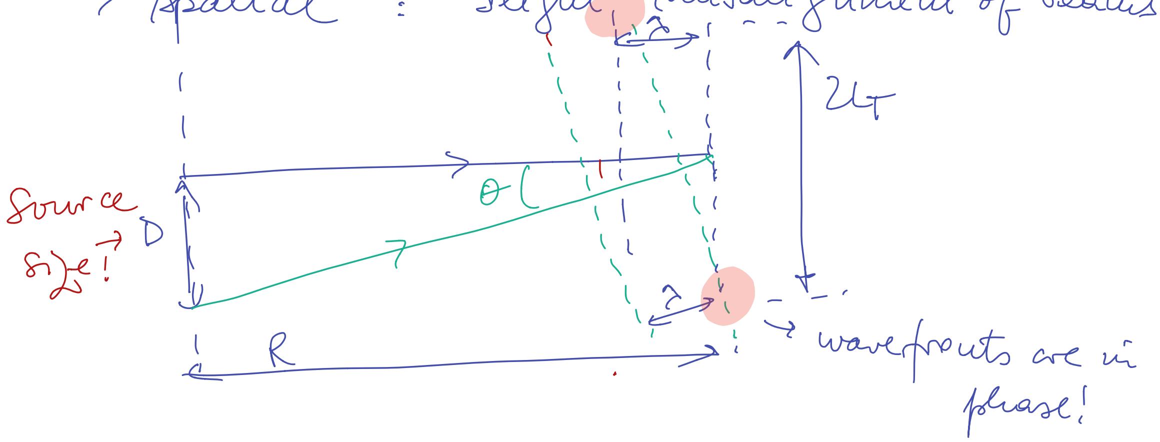
perfectly monochromatic light is fully coherent!



"coherence length" → $L_L = \frac{\lambda^2}{2\Delta\lambda}$

- interference is possible over this distance!
- use monochromator "wavelength filter"
- not good for SR, XFEL

→ spatial : slight misalignment of beams



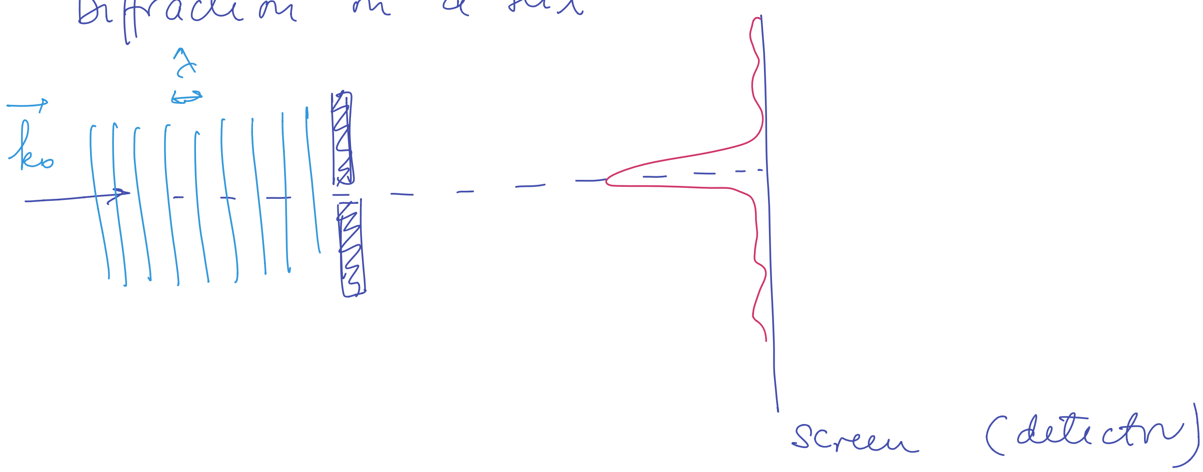
$$\theta = \frac{\lambda}{2L_T} = \frac{D}{R} \Rightarrow \text{coherence length}$$

$$L_T = \frac{\lambda}{2}\frac{R}{D}$$

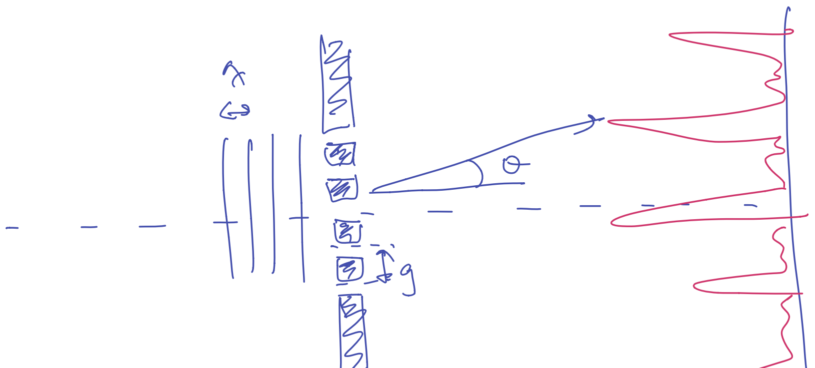
- interference is possible over this distance!
- reduce source size $\underline{\underline{D}}$ via aperture
- very good for XFEL!

③ On diffraction using x-rays

Diffraction on a slit



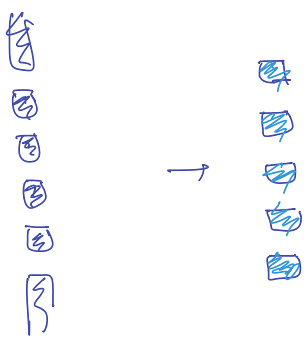
Now let us consider a grating



$\lambda = g \sin\theta$

diffraction on grating

Theorem of Babinet: complementary object yield the same diff. pattern!



now let us imagine

$\lambda = 0{,}63\,\mu m$ (visible)

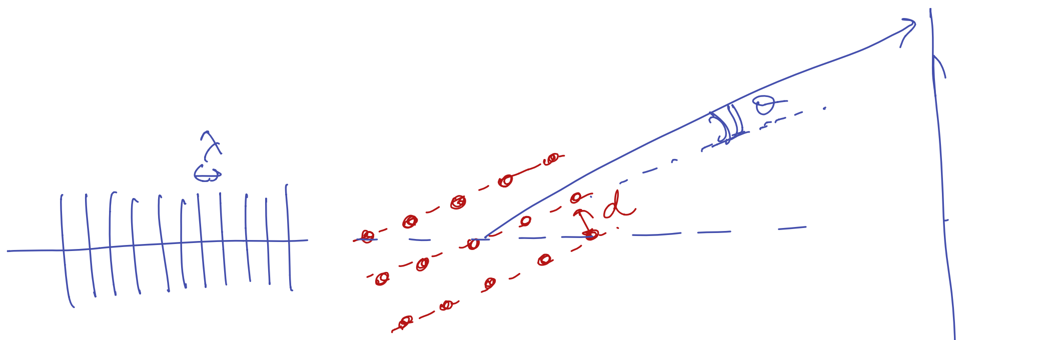
$\theta = 10°$

$g = 3{,}6\,\mu m$

and scale up to x-rays

$$\left.\begin{array}{l} \lambda = 0.1\,nm \\ \theta = 10° \\ g = 0.6\,nm \end{array}\right\} \to \text{interatomic distances.}$$

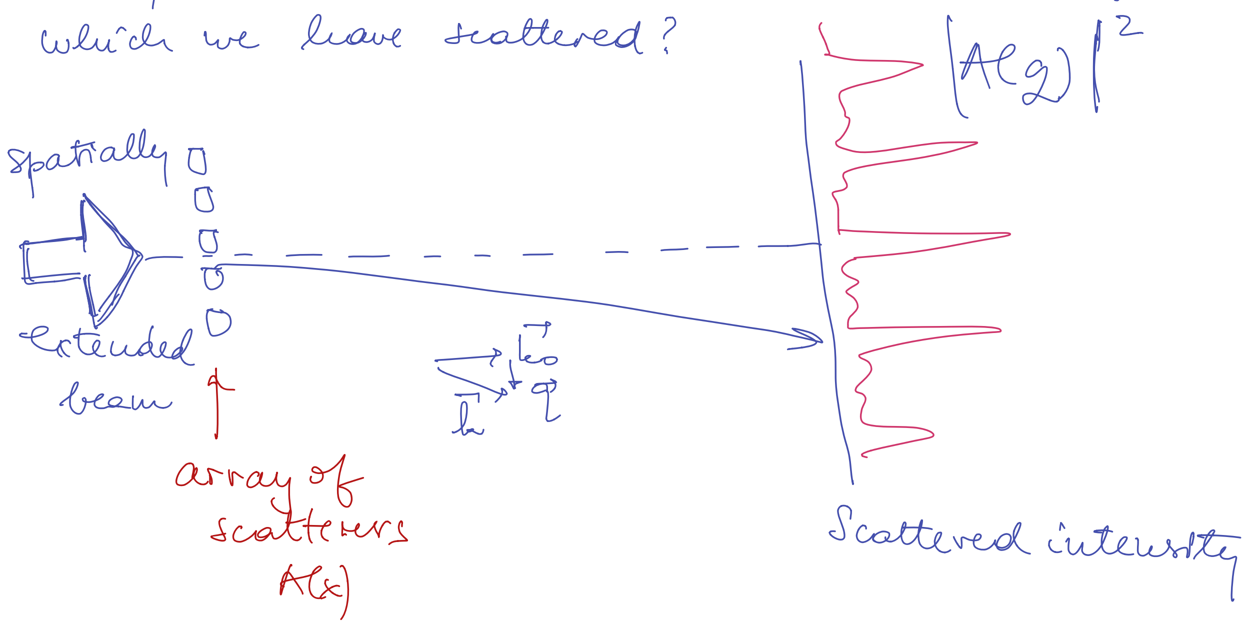
our complementary grating is a crystal lattice with atoms!



$(n)\lambda = 2d\sin\theta$

Bragg equation

Now, how can we determine the structure off which we have scattered?



$\vec{q} = \vec{k} - \vec{k}_0$ momentum transfer

$$A(q) = \int A(x)\, e^{iqx}\, dx \rightarrow \text{Fourier transform.}$$

we determine $|A(q)|^2$

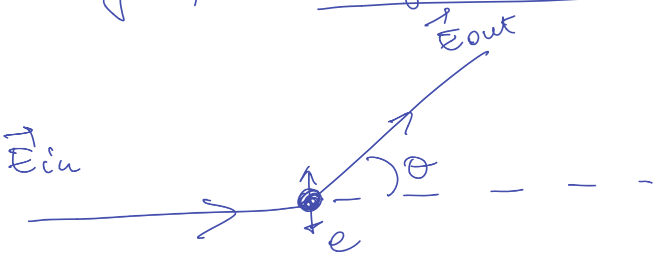
we want to extract $A(x)$.

PHASE PROBLEM

"Form factor"

Let us check this in more detail:

→ Scattering from single electron:



$$\underbrace{\vec{E}_{out}(\vec{r},t) = -\frac{r_e}{r}\vec{E}_{in}(t')\cos\theta}$$

r_e → Thomson scat. length.

↳ in vector form works for $\vec{r} >> \lambda$!!!

$$r_e = \frac{e^2}{4\pi\varepsilon_0 c^2 m}$$

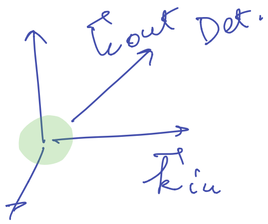
$$t' = t - \frac{r}{c}$$ (take retardation effects into account!)

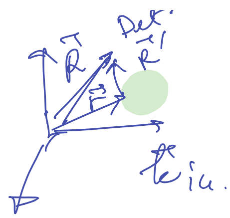
→ surface $\int$ over all directions is independent of $\frac{r_e}{r}$!

→ emission ⊥ to electron motion induced by incident field (same story as for x-ray production!!!)

→ Scattering from charge distribution

charge @ origin and at $\vec{r}$





relative phase before scattering $e^{-i\vec{k}_{in}\cdot\vec{r}}$

after scattering $e^{+i\vec{k}_{out}\cdot\vec{r}}$

$$\vec{K} = \vec{k}_{out} - \vec{k}_{in}$$

$$\underbrace{E_{out}(\vec{R}', t)}_{\text{from charge @ } \vec{r}} = E_{origin}\, e^{i\vec{K}\cdot\vec{r}}$$

phase

from charge @ origin

Now remember we aim to consider a charge density:

$$\vec{E}_{out}(\vec{R}, t) = E_{origin} \cdot \iint \rho(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, d^3r$$

this is the form factor.

so basically our $A(q)$ is called a form factor!

SINGLE ATOM $\quad f^0(\vec{K}) = \int \rho(r)\, e^{i\vec{K}\cdot\vec{r}}\, d^3r$

MOLECULE $\quad f^{mol}(\vec{K}) = \sum_{\vec{r}_j} f_j(\vec{K}) \cdot e^{i\vec{K}\cdot\vec{r}_j}$

$\boxed{\text{CRYSTAL}}$

$$f^{cryst}(\vec{k}) = \underbrace{\sum_{\vec{r}_j} f_j(\vec{k}) \cdot e^{i\vec{k}\cdot\vec{r}_j}}_{\to \text{unit cell}} \times \underbrace{\sum_{\vec{R}_n} e^{i\vec{k}\cdot\vec{R}_n}}_{\text{lattice}}$$

Photo

the phase is actually very important!
So we try to use whatever else we know to impose constraints

- know part of the molecule already
- exploit mathematical properties (symmetries, non-negative density, etc.)
- object support, aperture, some area of zero signal
- oversampling

Algorithm starting from a guess!
Use for biological samples → crystallization of ribosomes, other proteins.
Problem: need crystals of certain size, some molecules do not allow that!
→ XFEL can image single molecules!