Interference

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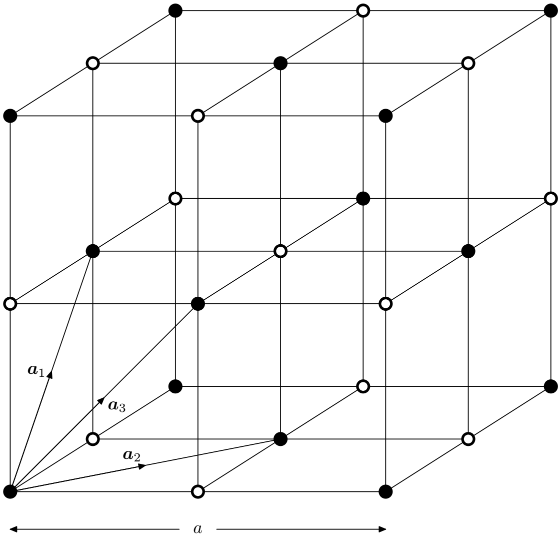
Crystal

- a crystal is a regular array of identical unit cells
- location $\boldsymbol{x}_l = l_1 \boldsymbol{a}_1 + l_2 \boldsymbol{a}_2 + l_3 \boldsymbol{a}_3$
- $l_1 = -M_1, -M_1 + 1, \dots, M_1 - 1, M_1$
- l_2 and l_3 likewise
- each unit cell serves as an antenna
- it is excited by a primary electromagnetic wave
- and emits a secondary wave
- response is described by a complex number f
- which describes the responsiveness and the retardation



Unit cell and primitive cell of NaCl like crystal

Source, crystal and detector

- the X-ray source is at $\boldsymbol{x}_{\rm s} = -R_{\rm s}\boldsymbol{n}_{\rm in}$
- the detector is at $\boldsymbol{x}_{\rm d} = +R_{\rm d}\boldsymbol{n}_{\rm out}$
- what is the distance between source and a unit cell?
- $r_{{\rm s}l} = |\boldsymbol{x}_{\rm s} - \boldsymbol{x}_l| = |R_{\rm s}\boldsymbol{n}_{\rm in} + \boldsymbol{x}_l|$
- $= R_{\rm s}|\boldsymbol{n}_{\rm in} + R_{\rm s}^{-1}\boldsymbol{x}_l|$
- $= R_{\rm s}\sqrt{1 + 2R_{\rm s}^{-1}\boldsymbol{x}_l \cdot \boldsymbol{n}_{\rm in} + \dots}$
- $= R_{\rm s} + \boldsymbol{x}_l \cdot \boldsymbol{n}_{\rm in} + \dots$
- distance between detector and unit cell likewise
- $r_{{\rm d}l} = R_{\rm d} - \boldsymbol{x}_l \cdot \boldsymbol{n}_{\rm out} + \dots$

Spherical wave

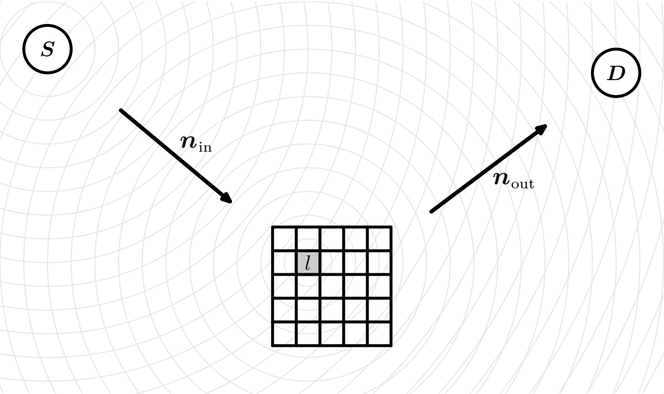
- for simplicity, we work with a scalar electric field E
- wave equation $\Delta E + k^2 E = 0$
- vacuum wave number $k = \omega / c = 2\pi / \lambda$
- spherical solution for primary field

$$E_{\rm pr} = A \frac{{\rm e}^{{\rm i}kr}}{r}$$

- field strength at distance r from source
- secondary field emitted by unit cell

$$E_{\rm sd} = f E_{\rm pr}(r_{{\rm s}l}) \frac{{\rm e}^{{\rm i}kr}}{r}$$

- field strength at distance r from unit cell



X-ray scattering.Primary field emitted at source $\boldsymbol{S}$. A secondary field is emitted by the unit cell labeled l. It is detected at $\boldsymbol{D}$.

Detected intensity

- field strength of secondary wave at detector

$$E_l = Af\,\frac{\mathrm{e}^{\,\mathrm{i}kR_\mathrm{s}}}{R_\mathrm{s}}\,\frac{\mathrm{e}^{\,\mathrm{i}kR_\mathrm{d}}}{R_\mathrm{d}}\,\mathrm{e}^{\,\mathrm{i}k\boldsymbol{n}_\mathrm{in}\cdot\boldsymbol{x}_l}\,\mathrm{e}^{\,-\mathrm{i}k\boldsymbol{n}_\mathrm{out}\cdot\boldsymbol{x}_l}$$

- this is the contribution from unit cell l
- the entire field strength is the superposition

$$E = \sum_l E_l = Af\,\frac{\mathrm{e}^{\,\mathrm{i}kR_\mathrm{s}}}{R_\mathrm{s}}\,\frac{\mathrm{e}^{\,\mathrm{i}kR_\mathrm{d}}}{R_\mathrm{d}}\sum_l \mathrm{e}^{\,-\mathrm{i}\boldsymbol{\Delta}\cdot\boldsymbol{x}_l}$$

- wave vector transfer

$$\boldsymbol{\Delta} = k(\boldsymbol{n}_\mathrm{out} - \boldsymbol{n}_\mathrm{in})$$

- detected intensity of secondary waves

$$|E|^2 = \frac{|A|^2|f|^2}{R_\mathrm{s}^2R_\mathrm{d}^2}\left|\sum_l \mathrm{e}^{\,-\mathrm{i}\boldsymbol{\Delta}\cdot\boldsymbol{x}_l}\right|^2$$

- the sum has three factors, $\Sigma = F_1 F_2 F_3$
- each of the form

$$F = \sum_{l=-M}^{M} \mathrm{e}^{-\mathrm{i}\, l\, \boldsymbol{\Delta} \cdot \boldsymbol{a}}$$

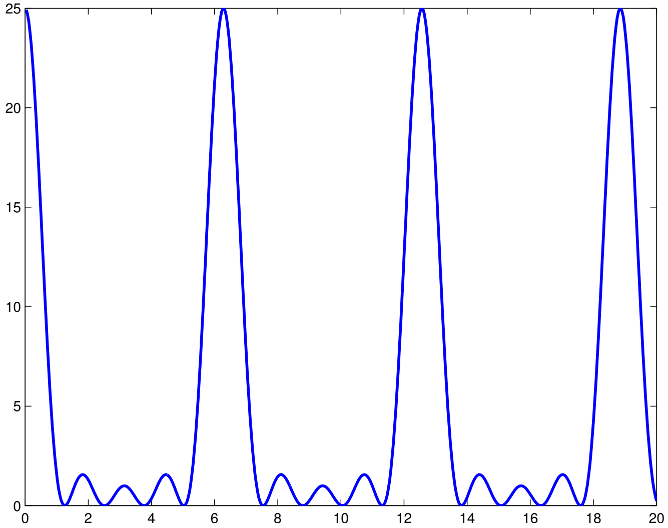
- with

$$z = \mathrm{e}^{-\mathrm{i} \boldsymbol{\Delta} \cdot \boldsymbol{a}}$$

- the factor is

$$F = \sum_{l=-M}^{M} z^l = \frac{\sin(N \boldsymbol{\Delta} \cdot \boldsymbol{a}/2)}{\sin(\boldsymbol{\Delta} \cdot \boldsymbol{a}/2)}$$

- where $N = 2M + 1$ (number of unit cells in this dimension)
- intensity at detector is proportional to $|\Sigma|^2 = |F_1|^2 |F_2|^2 |F_3|^2$

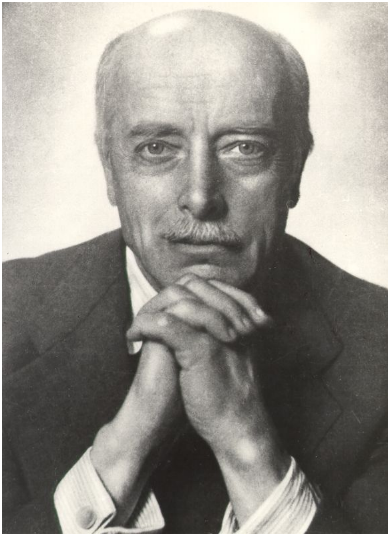


$|F|^2$ versus $\boldsymbol{\Delta}\cdot\boldsymbol{a}$ for $N=5$

Laue conditions

- Each factor is tiny unless $\boldsymbol{\Delta}\cdot\boldsymbol{a}_i$ is an integer multiple of 2π
- this must be fulfilled for $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$
- Laue conditions

  $$\boldsymbol{\Delta}\cdot\boldsymbol{a}_i=\nu_i\,2\pi$$
- sharp refraction peak if Laue conditions are fulfilled
- recall that $\boldsymbol{\Delta}=k(\boldsymbol{n}_{\text{out}}-\boldsymbol{n}_{\text{in}})$ depends on angles and wave number
- different kinds of X-ray diffraction experiments
- Max von Laue 1912, Nobel prize 1914
- William Henry and William Lawrence Bragg, father and son, 1914, Nobel prize 1915
- proof that X-rays were not particles, but electromagnetic waves



Max von der Laue, German physicist

Massive particle diffraction

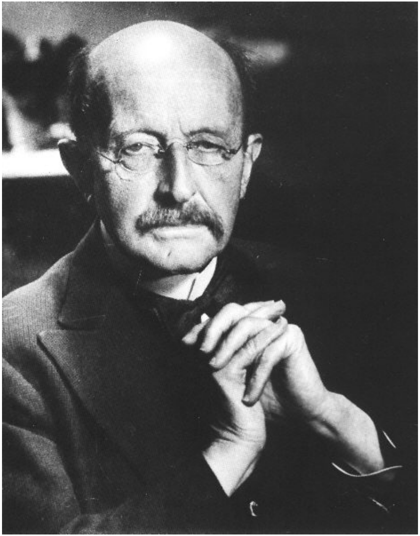
- In 1937, George P. Thomson discovered that electrons produced the same refraction pattern as X-rays
- provided the momentum p was identified with $\hbar k$
- predicted before by Louis de Broglie
- in 1946 the same was discovered for neutrons
- today preferred because only nucleons are visible
- dedicated nuclear reactors and spallation sources

George P.Thomson, British physicist

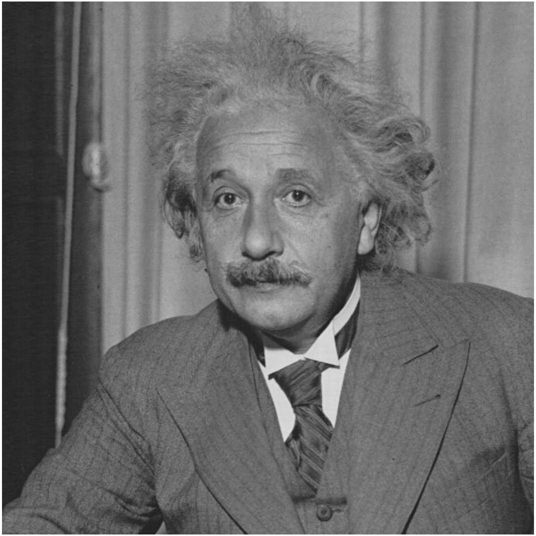
Louis de Broglie, French physicist

Quantum physics

- normally: *equal equations have equal solutions* (Feynman)
- now: same solutions must come from same equations
- guess the mathematical framework of quantum physic
- probability
- complex probability amplitudes
- interference
- Hilbert space, linear operators, observables, states, expectation values

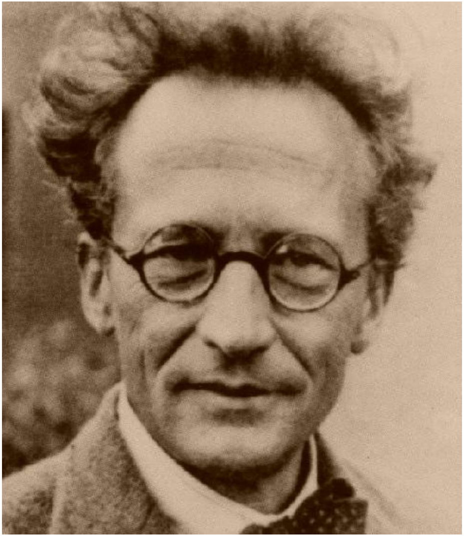


Max Planck, German physicist

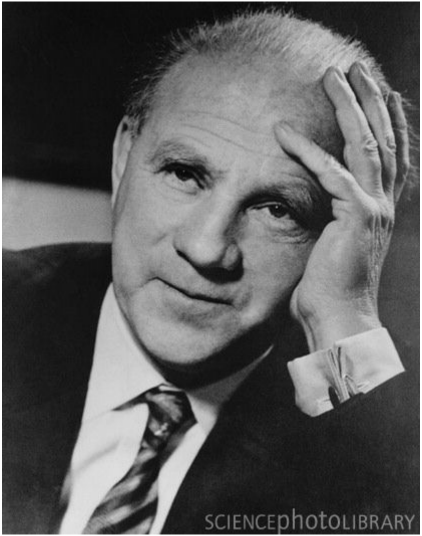


Albert Einstein, German physicist

David Hilbert, German mathematician



Erwin Schrödinger, Austrian physicist



Werner Heisenberg, German physicist

Differential cross section

- the target has n scatterer per unit volume
- beam intensity $I = I(x)$
- the beam is weakened by scattering

  $$\mathrm{d}I(x) = -I(x)\,\sigma\,n\,\mathrm{d}x$$
- therefore

  $$I(x) = I(0)\,\mathrm{e}^{-\sigma n x}$$
- cross section is solid angle integral

  $$\sigma = \int \mathrm{d}\Omega\,\sigma_{\mathrm{d}}(\vartheta)$$
- differential cross section depends on scattering angle ϑ
- but normally not on azimuth ϕ

Neutron-O_2 scattering

- oxygen nuclei at $\pm a\boldsymbol{n}/2$
- O_2 molecule held together by common electron cloud
- ignored by neutrons
- differential cross section is

$$\sigma_{\mathrm{d}} = \left| f\,\mathrm{e}^{-\mathrm{i}a\boldsymbol{\Delta}\cdot\boldsymbol{n}/2} + f\,\mathrm{e}^{+\mathrm{i}a\boldsymbol{\Delta}\cdot\boldsymbol{n}/2} \right|^2$$

- i.e.

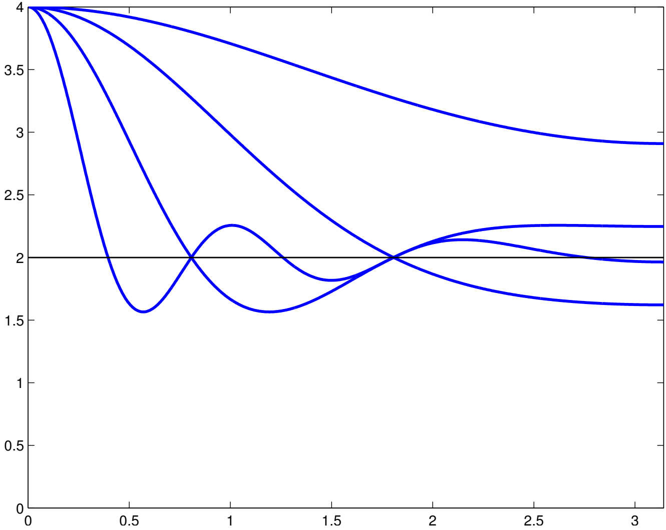
$$\sigma_{\mathrm{d}} = 4|f|^2 \cos^2 \frac{a\boldsymbol{\Delta}\cdot\boldsymbol{n}}{2}$$

- average over direction $\boldsymbol{n}$ (randomly oriented molecules)

$$\overline{\sigma_{\mathrm{d}}} = 2|f|^2 \left\{ 1 + \frac{\sin(\Delta a)}{\Delta a} \right\}$$

Constructive, destructive and no interference

- M refers to the randomly oriented molecule, A to the atom
- differential cross section
  $$\sigma_{\rm d}^{\rm M} = 2\left\{1 + \frac{\sin(\Delta a)}{\Delta a}\right\}\sigma_{\rm d}^{\rm A}$$
- scattering on an atom is isotropic
- cross section for scattering on a randomly oriented molecule depends on scattering angle
- via
  $$\Delta = k|\boldsymbol{n}_{\rm out} - \boldsymbol{n}_{\rm in}| = 2k\sin\frac{\vartheta}{2}$$
- for $\Delta a \to 0$ (slow or forward): amplitudes add, cross section for scattering on molecule is four times as large as for atom, full interference
- fast neutrons: cross section for molecule is twice that for atom - no interference
- intermediate: constructive or destructive interference



The ratio of molecular to atomic differential cross section is plotted vs. scattering angle ϑ. The curves are for $ka = 1$, 2, 4, and 8, according to decrease at forward direction. Values below 2 mean destructive interference.