Particle-wave duality

The X-ray spectrum, Compton-effect,
The theory of de Broglie
The uncertainty relation by Heisenberg
The Scroedinger equation

Chapter 7 of the textbook
Elementary Physics 3

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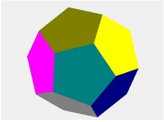


Ole Witt-Hansen 1980 (2017)

Informative remark: The present chapter is a translation from a Danish textbook of Elementary Physics. However, the texts in the figures are not translated. On the other hand the figures and the supplementing text should speak for themselves.

Contents

1. The particle nature of the photon

In chapter 6, on the photoelectric effect, we realized that light, when observed at the atomic level behave as particles having the energy $E_{photon} = h\nu$, where h is Planck's constant and ν is the frequency of the light.
In this section we shall first, based on the special theory of relativity, draw some conclusions concerning the momentum and the "mass" and of the photon.
Since the photons move with the speed of light they must have rest mass zero. This follows from the relativistic formula for the mass:

$$(1.1) \qquad m = \frac{m_0}{\sqrt{1 - v^2/c^2}} \quad \Rightarrow \quad m_0 = m\sqrt{1 - v^2/c^2}$$

Since $1 - v^2/c^2 = 0$ for the photon, it follows that the rest mass m_0 is zero.
To obtain a formula for the momentum of the photon, we shall use the relativistic formula:

$$(1.2) \qquad E^2 - p^2c^2 = m_0c^4 \quad \wedge \quad m_0 = 0 \quad \Rightarrow \quad p = \frac{E}{c}$$

The energy of the photon can hereafter be written in various ways.

$$(1.3) \qquad p = \frac{E}{c} \quad \Leftrightarrow \quad p = \frac{h\nu}{c} \quad \Leftrightarrow \quad p = \frac{h}{\lambda}$$

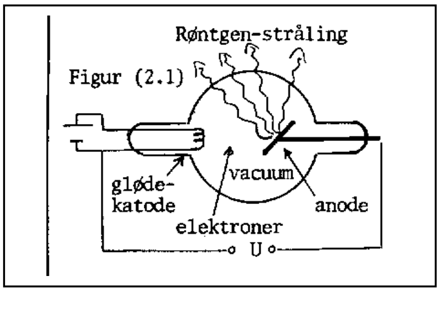
In obtaining the last expression, we have used that: $c = \lambda\nu$. Even if the rest mass of the photon is zero, one can assign an equivalent mass to the photon when using Einstein's equivalence between energy and mass: $E = mc^2$.

$$(1.4) \qquad h\nu = mc^2 \quad \Rightarrow \quad m = \frac{h\nu}{c^2} = \frac{p}{c}$$

We notice that (1.4) comply with the classical formula for the momentum: $p = mv$.

2. X-rays

In 1895 the physicist Roentgen observed that from the anode in a discharge tube was emitted a very penetrating radiation. The observation demanded however, that the tube was connected to high voltage more than 10 *kV.*
What Roentgen actually discovered was that a fluorescent screen placed in the vicinity of the tube lit up. The conclusion of Roentgen was that from the anode was emitted a radiation, which was able to penetrate the thin glass tube and also paper and other more easy materials, but that the radiation was stopped by metals and other hard materials, like thick glass. The radiation is called Roentgen-radiation, or X-rays, (since the radiation was considered mysterious at that time)



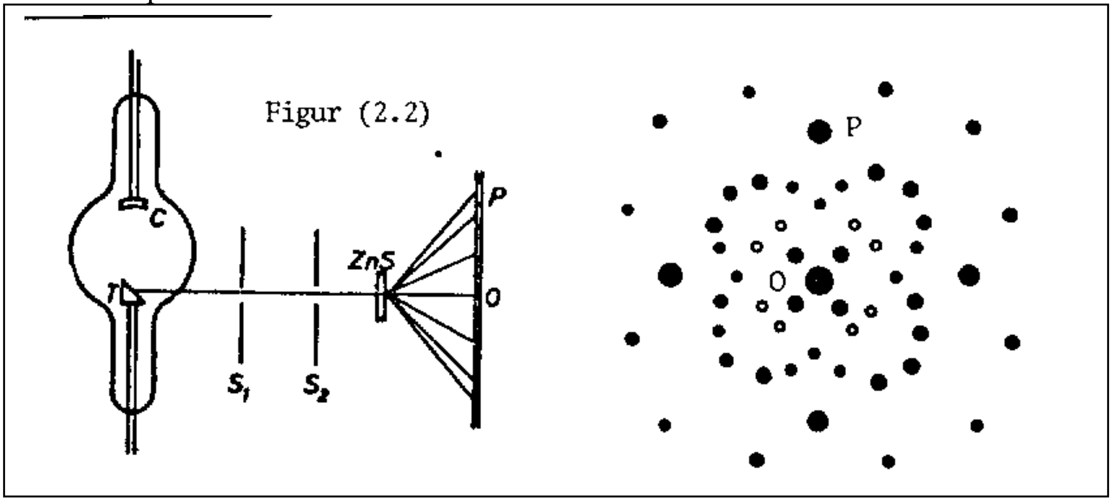
In the figure (2.1) is schematically shown the basic device of the Roentgen tube. In the tube there is high vacuum. The electrons are emitted spontaneously from the glow-cathode, because of its high temperature.
Following they are accelerated towards the anode.
Using an acceleration voltage of 50 *kV,* the electrons will have a kinetic energy of 50 *keV*, when they hit the anode.

In a collision, the electrons will loose most of their kinetic energies at a very short distance (and time), which means a violent deceleration.
Most of the energy of the electrons will be converted to heat in the anode, and some energy will end as electromagnetic radiation, according to the Maxwell equations.

Right from the discovery of the X-rays, it was therefore the general opinion that the X-rays were in fact electromagnetic radiation.
The first attempts to determine the wavelength using diffraction in prisms or optical grids showed, however, no deflection whatsoever. The conclusion was then that if the Roentgen-radiation was in fact electromagnetic radiation, it must have a wavelength less than 1 *nm* (10^{-9}).
It is, however, not possible to manufacture optical grids intended for that tiny wavelength, and the German physicist Von Laue therefore suggested that instead of optical grids, one could use the crystal grids of certain atoms to conduct the interference experiments with X-rays.

An experiment equipped to determine the wavelength in this manner was performed by Friedrich and Knipping in 1913. The schematic setup is shown below.

To the left is the X-ray tube. There were used two screens S_1 and S_2 made of lead to obtain a single narrow beam, which was then sent through a thin crystal of *ZnS*. After the passage of the beam the result of the scattering was registered on a photographic record.
When the photographic record was developed it showed a black spot were the beam had passed the crystal without deflection, but moreover and around the central spot there was a regular pattern of much weaker spots, which showed that a minor part of the beam had been scattered and by interference reinforced in various directions.
This phenomenon is well known from optical grids. To the left in the figure (2.2) is shown the diffraction pattern.



Figur (2.2)

Doing a complicated analysis of the interference pattern, Von Laue could establish that the X-ray radiation had wavelengths in the interval 0.01 – 0.1 *nm*.

3. The X-ray spectrum. The Bragg-condition

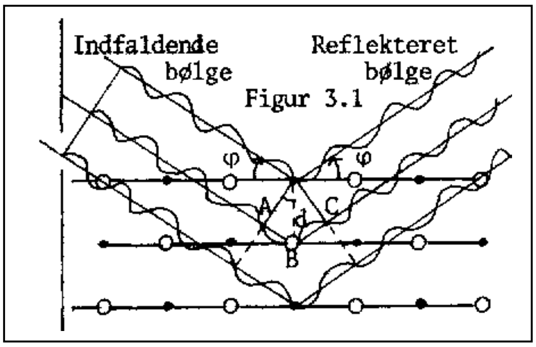
The interference pattern that is observed when the X-ray beam passes through a crystal is fairly complex to analyze, and shortly after Von Laue's discoveries, the Englishman W. Bragg, suggested that the reflected radiation from the surface of the crystal might be easier to analyze than that of the transmitted beam

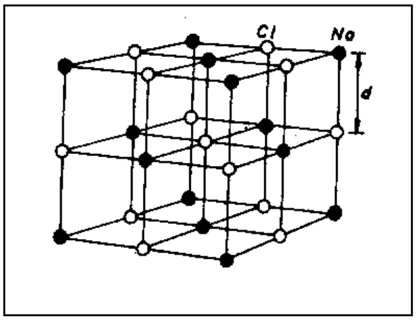
When the X-rays fall into the surface of a crystal they will be scattered by single atoms in the same manner as it is the case for an optical reflection grid. The reflected waves will interfere according to Huygens principle and by superposition be reinforced in certain directions, dependent of the wavelength and the geometry of the crystal. By measuring of the angle of deflection, and with knowledge of the structure of the crystal, it is possible to determine the wavelength in somewhat the same manner as it is done with the optical grid, but with one significant difference, since the crystal consists not only of one, but of multiple layers of "grids".

For a crystal like *NaCl* the geometry is particular simple, since it has a cubic crystal structure.
The crystal consists of a series of parallel planes, where each plane has aligned atoms.
Such a set of parallel planes are called Bragg planes. The distance between the planes is called the grid-separation *d*.

The incoming wave will be scattered on each of the Bragg planes, and by interference it will result in a transmitted wave and a reflected wave. The angle of reflection will comply with that of the law of reflection from optics.

The point is, however, that the reflected wave from the different Bragg planes will in general not be in phase, and they will therefore quench each other by interference.
The reflected waves from the Bragg planes will be in phase only at certain specific angles of the incoming X-rays, and only at these angles a reflected wave will be observed.
We shall now derive the condition for having a reflected wave, using the so called Bragg-condition that a reflected wave must fulfil.





The figure shows a plane X-ray beam, which falls into a cubic crystal. It appears from the figure that the condition that two waves from different Bragg-planes are in phase is that their difference in path length *ABC* is an integral number of wavelengths. If the glancing angle is φ, we find the Bragg-condition.

$$(3.2) \qquad |AB|+|BC| = n\lambda \qquad 2d\sin\varphi = n\lambda\,, \quad n = 1,2,3...$$

For a cubic grid, (as for example *NaCl*), it is relatively simple to find an expression for the grid separation *d*. In the figure above is shown how we perceive how the cubic grid is built.
The volume *V* that each molecule occupies can be found from:

$$V = \frac{M}{\rho N_A}$$

Where *M* is the mole mass, ρ is the density and N_A is Avogadro's number.

Since both the Na^+ ions and the Cl^- ions scatter the waves, the volume per scattering atom must be half the size of the volume of the molecule.

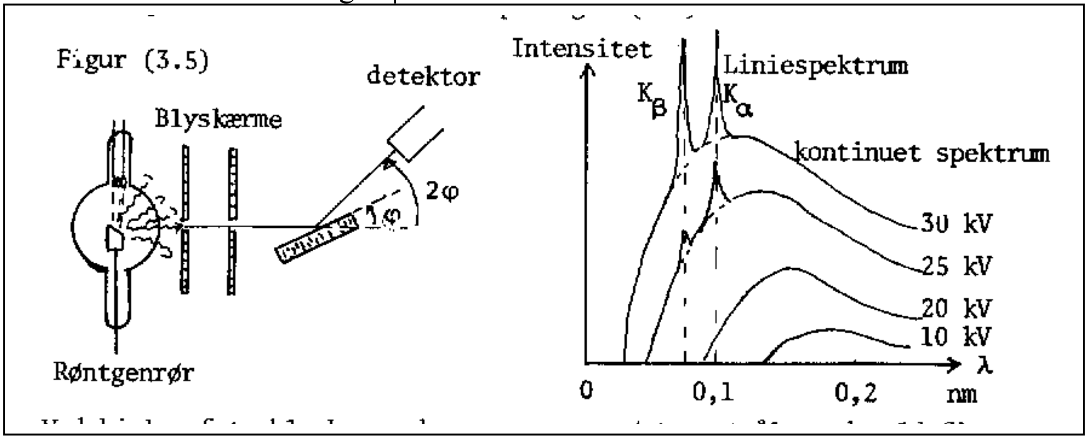
If the volume of a molecule is put to d^3, which is the volume of a cube having the side d, then we find the expression for the Bragg separation distance d:

$$(3.4)\qquad d^3 = \frac{M}{2\rho N_A} \quad \Rightarrow \quad d = \sqrt[3]{\frac{M}{2\rho N_A}} \quad \textit{which gives} \quad d_{NaCl} = 2.8\,10^{-10}\,m$$

The Bragg condition (3.2) has been central for the spectroscopy of X-rays, where also the intensity distribution as a function of the wavelength has been determined.

One may apply a setup, schematically shown to the left in figure (3.5) together with some characteristic X-ray spectra shown to the right.
By using two lead screens each with a narrow slit, then a X-ray beam with a well defined direction is formed. The beam is then reflected on a swivel crystal.
The wavelength of the X-rays having a reflection angle φ can then be evaluated using the Bragg-condition.
Finally a detector belongs to the X-ray spectroscope that can measure the intensity of the radiation which is reflected at an angle φ.

Figur (3.5)



If you map the intensity as a function of wavelength λ then we may find curves that are shown in the figure to the right
The distribution of the intensity is strongly dependent on the voltage U over the X-ray tube.
The spectrum is continuous, but for higher anode voltage superimposed by a line spectrum.

In any case the continuous spectrum is sharply confined by a least wavelength λ_{min} .
If we calculate the corresponding frequency: $\nu_{\max} = c / \lambda_{\min}$, we will find that there is a direct proportionality between $\nu_{\max}$ and the acceleration voltage U.

This proportionality can, however, easily be explained from the quantum hypothesis.
The decelerating electrons will, with their collision with the anode material, emit electromagnetic radiation as photons.
The maximum energy that a photon can obtain, must be equal to the kinetic energy of the incoming electron, which corresponds to that the electron looses all its energy in just one collision, which gives the condition:

$$(3.7) \qquad \tfrac{1}{2}mv^2 = Ue \quad and \quad Ue = h\nu_{\max} \quad and \quad \lambda_{\min} = \frac{c}{\nu_{\max}} \quad \Rightarrow \quad \lambda_{\min} = \frac{hc}{Ue}$$

The minimum wavelength calculated in (3.7), appears to be in perfect agreement with the results from experiments.
It should be noticed that from a classical calculation, you will find no minimum for the wavelength. The continuous spectrum is produced because the electrons loose their energy in several collisions with the atoms in the anode. In each collision a photon is emitted (brake radiation), and the emitted photons comprise the continuous spectrum.

The main part of the electrons energy goes to heating the anode, which means that an X-ray tube can only be active for a short period, unless the anode is cooled.

The overlapping line spectra in the continuous spectrum can be understood from the atom model of Bohr, since it may happen that one on the incoming electrons shoots out one of the hard bound electron in the *K*-shell of one of the atoms in the anode material, leaving a vacant hole.
In a very short time the vacant stationary state in the *K*-shell will be filled by one of the outer electrons, and at the same time the atom will emit a photon with frequency υ, the energy of which comply with the frequency condition: $h\nu = E_{K-shell} - E_{outer}$.
For heavier metals this jump in energy is so large that the emitted photon is in the X-ray region. This characteristic radiation with a definite frequency is seen as the line spectra in the mapping of the intensity in figure (3.5).

Notice that only if the acceleration voltage is above 25 *kV*, the line spectra appear which comply with the binding energies of the electrons in the *K*-shell in the heavier metals.
Experimentally one also finds that the different anode materials have their own characteristic line spectra, representing the energy levels in the particular atom.

X-rays are often characterized by their hardness, since a large acceleration voltage gives “hard” X-rays, while a lower acceleration voltage gives “soft” X-rays.

X-ray scanning and making X-ray photos are based on the different softness of various materials, (bones, flesh, wood, metal). X-ray photos are not ordinary photos, (a real image depicted on some photographic screen through a lens), but a shadow image of the parts of the objects that most effectively stop the X-rays. Taking two or more X-ray photos from different angles, one is able to reconstruct a fracture in a bone, or perhaps identifying the presence of cancer cells.

It is amazing that it was only in the 1960s that one has been aware of the health danger for living creatures of X-rays in larger doses. X-rays are dangerous, because they damage or kill living cells, that on sight can cause cancer..

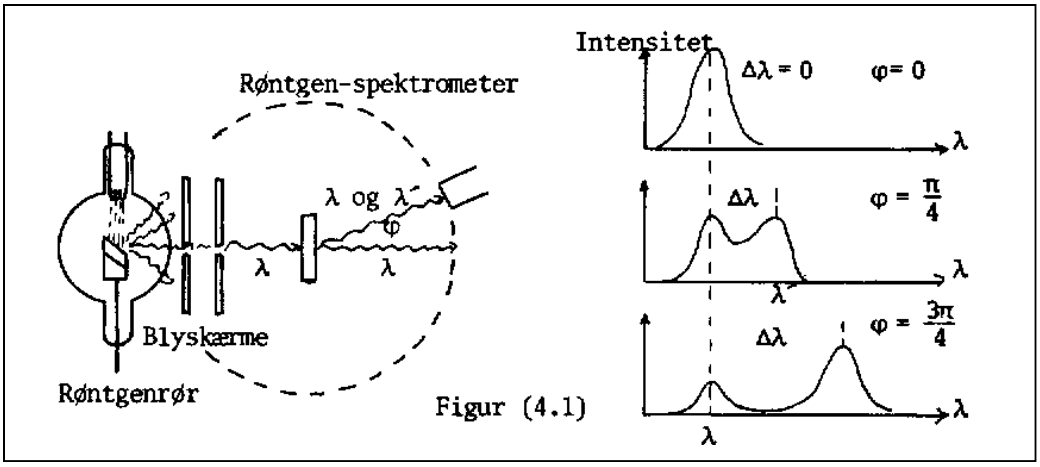
But the damaging effect on the human tissue has also had a positive application, since the X-rays are used to destroy cancer tissue.
When fighting the cancer cells with X-rays, it is impossible totally to avoid damaging the healthy tissue, so one either rotates the person along an axis with the malign cells placed in the centre of the axix, or one rotates the X-ray apparatus around an axis with the malign cells in centre.

When I was a boy in the fifties, then in the larger stores selling shoes, there were installed X-ray apparatus (believe it or not), so from above you could look down and see how your toes fitted in the shoes. That was of course great fun, and boys could look in the apparatus for several minutes. They disappeared, however abruptly in the mid fifties, and I have never heard anything about this fatal mistake concerning public health, and it has never been mentioned since, and I believe one has chosen to "forget" this betrayal from the medical authorities.

4. The Compton effect

When passing a non crystalline material an X-ray beam will be scattered on its atoms, and because of the random distribution of the atoms, the beam will be scattered in all directions.
A.H. Compton made in 1932 an experiment, which showed that an initially monochromatic (only one wavelength) beam after being scattered an angle φ had two components, where the wavelength of the one component was unaltered while the other showed an extension of the wavelength.

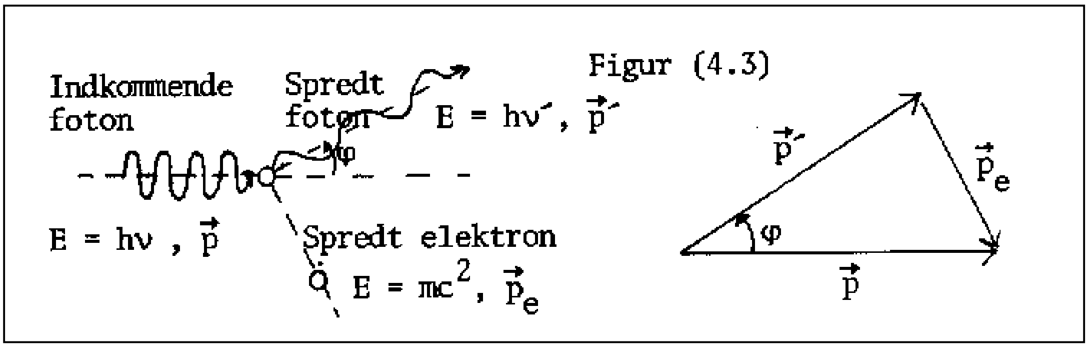
This split in wavelength of the scattered beam is called the Compton-effect.
The spilt of the wavelength Δλ, was furthermore observed to grow systematically with the scattering angle φ.
Below is shown schematically the setup for the experiment to measure the Compton effect along with some graphs of the X-ray spectrum at different scattering angles.



Figur (4.1)

The Compton effect can not be explained from classical electromagnetism.
That electromagnetic radiation will be scattered when it passes a transparent material is what could be expected, but the observed change in wavelength is inexplicable.

Compton showed, however, that the effect can be explained from the quantum hypothesis.
Namely if the incoming beam is perceived as consisting of photons, he showed that the extension of the wavelength corresponded to the energy that a photon looses with an elastic collision with an electron.
We shall then show how the extension of the wavelength may be determined by such a collision, using energy and momentum conservation in a relativistic mechanical derivation.



In figure (4.3) is schematically shown a collision where a photon having energy $h\nu$ and momentum $p = \frac{h}{\lambda}$ hits a resting electron with energy $m_0 c^2$.

After the collision, the photon has the energy $h\nu'$, the momentum $p' = \frac{h}{\lambda}$, while the electron has the energy mc^2 and momentum p_e.

For the photon, the relation between energy and momentum is $E = pc$.

For the electron we have the relativistic formula for the relation between momentum and energy:

$$E^2 - p_e{}^2 c^2 = m_0{}^2 c^4 \quad \Leftrightarrow \quad m^2 c^4 - p_e{}^2 c^2 = m_0{}^2 c^4 \quad \Leftrightarrow \quad p_e{}^2 = m^2 c^2 - m_0{}^2 c^2$$

The relativistic conservation of energy may be expressed by the equation.

$$h\nu + m_0 c^2 = h\nu' + mc^2$$

By dividing this equation with c and using: $\frac{\nu}{c} = \frac{1}{\lambda}$ it gives:

$$(4.4) \qquad \frac{h}{\lambda} + m_0 c = \frac{h}{\lambda'} + mc \quad \Rightarrow \quad mc = m_0 c + \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\right)$$

For the collision applies conservation of momentum. This can be illustrated by the triangle composed by the vectors $\vec{p}, \vec{p}\,'$ *and* $\vec{p}_e$, as shown in figure (4.3) above, expressing: $\vec{p} = \vec{p}\,' + \vec{p}_e$. The deflection angle φ is the angle between $\vec{p}$ *and* $\vec{p}\,'$.

We now take the square of the relation: $\vec{p}_e = \vec{p} - \vec{p}\,'$, from which we get:

$$p_e{}^2 = p^2 + p'^2 - 2pp'\cos\varphi \quad \Rightarrow \quad p_e{}^2 = \left(\frac{h}{\lambda}\right)^2 + \left(\frac{h}{\lambda'}\right)^2 - 2\frac{h^2}{\lambda\lambda'}\cos\varphi$$

Inserting in this equation: $p_e{}^2 = mc^2 - m_0{}^2 c^2$, we find

$$(4.5) \qquad m^2 c^2 = m_0{}^2 c^2 + \left(\frac{h}{\lambda}\right)^2 + \left(\frac{h}{\lambda'}\right)^2 - 2\frac{h^2}{\lambda\lambda'}\cos\varphi$$

To eliminate m^2c^2 we take the square of (4.4). This gives:

$$(4.6) \qquad m^2c^2 = m_0{}^2c^2 + (\frac{h}{\lambda})^2 + (\frac{h}{\lambda'})^2 - 2\frac{h^2}{\lambda\lambda'}\cos\varphi + 2m_0c(\frac{h}{\lambda} - \frac{h}{\lambda'})$$

By subtracting (4.5) from (4.6), we get the equation:

$$(4.7) \qquad 2m_0c(\frac{h}{\lambda} - \frac{h}{\lambda'}) = 2\frac{h^2}{\lambda\lambda'}(1-\cos\varphi) \quad \Leftrightarrow \quad \Delta\lambda = \lambda' - \lambda = \frac{h}{m_0c}(1-\cos\varphi)$$

Inserting the mass of the electron, we find: $\frac{h}{m_0c}$ =2.4 *pm.*

This is referred to as the Compton wavelength for the electron. As you can see from (4.7) then $\Delta\lambda$ grows with the deflection angle φ , and it has its maximum when $\varphi = \pi$.

According to (4.7) one should expect that all photons would have an extension of wavelength. When this is not the case, however, it can be explained because the photon in such cases has had a collision with one of the heavily bounded electrons, which act as a collision with the atom as a whole, and in the calculation (4.7), we should therefore replace the electron mass by the mass of the atom. In that case the Compton wavelength becomes several thousand times less, and the Compton effect disappears.

5. Particle waves. The assumption of de Broglie

The particle properties of light had already been discovered around 1900 and later experimentally established with the photoelectric effect. About 20 years later in 1924 the French physicist de Broglie put forward the hypothesis that not only the photons, but all atomic particles exhibited particle properties as well as wave properties.

According to this hypothesis should e.g. electrons have particle properties, which in principle could be demonstrated by interference experiments.

For a photon, we have the relation for the momentum: $p = \frac{h}{\lambda}$.

de Broglie then assumed that a similar relation was valid for all atomic particles, such that for a particle with momentum p, one could assign a wavelength λ, according to the formula:

$$(5.1) \qquad p = \frac{h}{\lambda} \quad \Leftrightarrow \quad \lambda = \frac{h}{p} \quad \Leftrightarrow \quad \lambda = \frac{h}{mv}$$

The wavelength calculated from (5.1) is called the de Broglie wavelength.

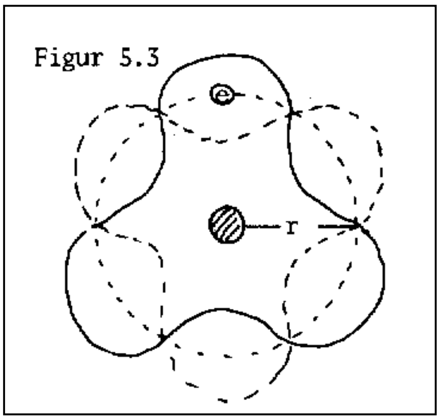
5.2 Example

For an electron, we find the momentum p, and thus the de Broglie wavelength:

$$\tfrac{1}{2}mv^2 = E \quad \Leftrightarrow \quad \frac{p^2}{2m} = E \quad \Rightarrow \quad p = \sqrt{2mE} \quad \Rightarrow \quad \lambda = \frac{h}{\sqrt{2mE}}$$

If we insert $h = 6.63\ 10^{-34}$ *Js*, $m = 9.11\ 10^{-31}$ *kg* and $E = 100$ *eV* = $1.6\ 10^{-17}$ *J.* we will find a de Broglie wavelength λ = $1.23\ 10^{-10}$ *m*. This length corresponds approximately to the double of the Bohr radius, and it is in the same region as

X-rays are. It should therefore in principle be possible to determine the de Broglie wavelength for the electrons in the same manner as the determination of the wavelengths for X-rays.
There was also a profund idea behind de Broglie's introduction of wavelengths for particles. Since according to de Broglie should the stationary states (as introduced by Bohr) correspond to standing waves for the electrons.
In this manner could de Broglie namely in a simple fashion explain Bohr's quantization condition for the angular momentum, according to which: $L = n\hbar,\ n = 1,2,3...$



Figur 5.3

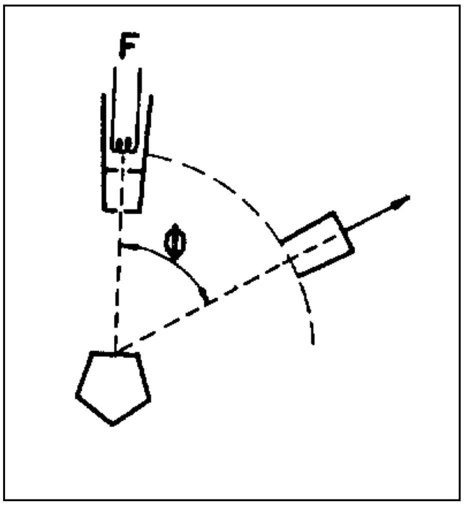
In figure (5.3) is illustrated how de Broglie perceived the circular movement of the electron around the nucleus as a standing circular wave. The possible stationary states should then correspond to that the standing wave should fulfil a "border condition".
As it is seen from the figure, this border condition must be that the circumference of the circular path is an integral number of de Broglie wavelengths.
If the radius in the circular orbit is r, it results in the condition.

$$2\pi r = n\lambda \ \wedge \ \lambda = \frac{h}{mv} \ \Rightarrow \ 2\pi r = n\frac{h}{mv} \ \Leftrightarrow$$

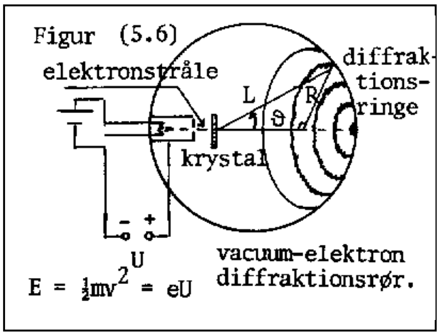
(5.4) $$mvr = n\frac{h}{2\pi}, \quad n = 1,2,3... \quad \Rightarrow \quad L = n\hbar \ , \ n = 1,2,3,...$$

We see that the hypothesis of the de Broglie wavelength leads the quantization condition of the angular momentum initially introduced by Bohr, and for the hydrogen atom it gives the correct energy level, when (5.4) is inserted in the classical expression for the energy of the electron. (Elementary Physics 3: Chapter 6, section 10)

In spite of this (and other results), there were in the beginning only little confidence in the proposition of the particle waves. It was simply too far fetched from the classical conceptions. The theory was however confirmed directly, by a famous electron interference experiment performed by Davidson and Germer in 1927.



The experimental arrangement is shown in figure (5.5) to the left.
The electrons are emitted from the glow thread F, and are accelerated through a voltage of about 100 V.
The electron beam falls perpendicular in on a Nickel crystal, where the electrons are spread in all directions. Using a Faraday cup, (able to register the accumulated charge), it is possible to measure the intensity of the scattered beam in all directions.
The experiment showed that there were some maxima in certain directions. Furthermore Davidson and Germer showed that the position of the observed maxima could be predicted from the Bragg-condition. $2d\sin\varphi = n\lambda$, after inserting the de Broglie wavelength for the electron.



The de Broglie wavelength for the electron can, however, also be determined experimentally by letting the electron beam pass through a thin crystal as illustrated in figure (5.6).
If you place a photographic plate or a fluorescent screen on the other side of the crystal, you will observe a series of concentric rings. If we think of the crystal as a two dimensional optical grid, then the radius in the circles can be calculated from the deflecting angle in the same manner as for an ordinary optical grid with grid constant *d*. With the designations in the figure, We then find from the optical grid-equation:

(5.7)
$$d\sin\varphi = n\lambda \quad \wedge \quad \sin\varphi = \frac{R}{L} \quad \Rightarrow \quad \lambda = \frac{dR}{nL}$$

In (5.7) λ is the wavelength for the electrons determined experimentally from an interference experiment.
The wavelength for the electrons can, however, also be determined from the de Broglie formula, when the energy of the electron is known.

$$\lambda = \frac{h}{\sqrt{2mE}}$$

With a comparison with (5.7) an excellent agreement is found, which confirms de Broglie’s theory.

The experimental fact that atomic particles have wave properties, and that electromagnetic waves show particle properties has been named the *particle–wave* duality.

Atomic phenomena have apparently both particle and wave properties. That it is so, was indeed a very surprising, (not to say shocking), experience emerging from the many experiments performed in the late 1800s.
In physics, however, it is not the degree of comprehensibility that is decisive for a theory, but rather the agreement of theory with data from experiments and the capability of the theory to predict the results of new experiments.

Bohr’s theory as well as that of de Broglie had certainly fundamental elements necessary for understanding the atomic world, but both theories were incomplete in several areas, and until the end of 1920 one lacked a theory that tied together the wave description and the particle description in one unified description of the atomic world.

6. The Heisenberg uncertainty relations

Her we shall discuss some simple examples of particle waves and derive some essential consequences of the particle-wave duality. We initiate by the remark that if we apply the wave description of the electrons circular motion around the nucleus, we completely loose any conception of its position in the orbit. On the other hand the angular momentum, and thereby the momentum of the electron is precisely determined.

It turns out to be a fundamental consequence of the particle–wave duality that if you seek to determine the momentum of an atomic particle precisely, then you are referred to the wave description, but at the same time you loose completely the significance of the position of the particle.
On the other hand, if we try to determine the position precisely, then we loose completely information of its momentum.
Momentum and position are, using an expression of Bohr, *complementary*. They can not be determined simultaneously with an arbitrary precision.

We shall then discuss this phenomenon a little more closely.

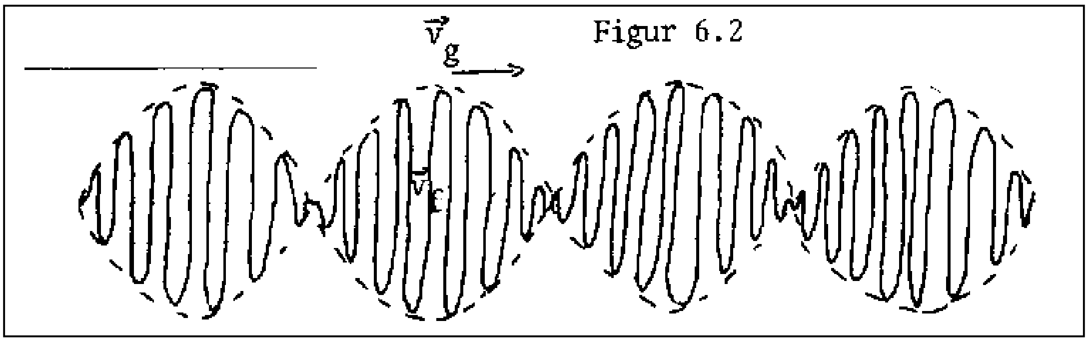
First we consider a superposition of two harmonic (particle) waves having the same amplitude, but with slightly different angular frequencies and wave numbers.

$$\begin{aligned} u(x,t) &= A\cos(\omega_1 t - k_1 x) + A\cos(\omega_2 t - k_2 x) \\ &= 2A\cos(\frac{\omega_2-\omega_1}{2}t - \frac{k_2-k_1}{2}x)\cos(\frac{\omega_2+\omega_1}{2}t - \frac{k_2+k_1}{2}x) \\ &= 2A\cos(\tfrac{1}{2}\Delta\omega t - \tfrac{1}{2}\Delta k x)\cos(\omega t - kx) \end{aligned} \tag{6.1}$$

In the rewriting of (6.1), we have applied the inverse logarithmic formulas for the addition of two cosine functions, and furthermore we have put:

$$\Delta\omega = \omega_2 - \omega_1,\ \Delta k = k_2 - k_1 \text{ and } \omega = \tfrac{1}{2}(\omega_2+\omega_1)\ ,\ k = \tfrac{1}{2}(k_2+k_1).$$

What we see is, that we may perceive the superposition of the two harmonic waves as one wave propagating with the phase velocity $v_p = \frac{\omega}{k}$.
(This expression comes about if we follow a point of constant phase in the second cosine function).
For instance $\omega t - kx = 0 \ \Rightarrow\ v_p = \frac{x}{t} = \frac{\omega}{k}$. At the same time the wave has a time an position dependent amplitude: $A(x,t) = 2A\cos(\tfrac{1}{2}\Delta\omega t - \tfrac{1}{2}\Delta k x)$.
If we follow a point, where the phase in the amplitude has maximum, that is: $\tfrac{1}{2}\Delta\omega t - \tfrac{1}{2}\Delta k x = 0$, we find the so called group velocity: $v_g = \frac{x}{t} = \frac{\Delta\omega}{\Delta k}$.
If ω is given as a function of k: $\omega = \omega(k)$, then we may for small changes identify the group velocity with the derivative $\frac{d\omega}{dk}$.
Below is sketched what the wave function (6.1) may look like. We have earlier in Elementary physics 2, in the section on waves encountered such a wave function in the paragraph on shock waves.


Figur 6.2

The dashed line marks the variation of the amplitude. It is this form that propagates with the group velocity v_g, while the phase in the oscillations propagates with the phase velocity v_p.

We see that the propagation of a superposition of two waves is characterized both by a phase-velocity and a group velocity. The observed velocity, however, is the group velocity, since this means that we follow a point with constant amplitude. If $\omega = \omega(k)$, we have thus:

(6.3) $\quad v_p = \dfrac{\omega}{k}$ (Phase velocity) $\qquad v_g = \dfrac{d\omega}{dk}$ (Group velocity)

If the speed of propagation (as it also is the case for sound waves) does not depend on the frequency, then $\omega = v k$, where the frequency v is constant, then the phase velocity and group velocity are the same.

For a particle we have according to de Broglie: $E = \hbar\omega \ and \ p = \hbar k$.
The phase and group velocities can therefore be evaluated as:

$$v_p = \frac{E}{p} \quad and \quad v_g = \frac{dE}{dp}.$$

For a non relativistic particle: $E = \dfrac{p^2}{2m}$, and we therefore find:

$$v_f = \frac{E}{p} = \frac{p}{2m} = \tfrac{1}{2}v, \quad \text{while} \quad v_g = \frac{dE}{dp} = v \text{ (the speed of the particle).}$$

Clearly, when you describe an atomic particle or a beam of such particles by a harmonic wave, then the positions of the particles are completely indefinite. On the other hand, the momentums of the particles are completely determined. This follows, if we evaluate the momentum from the de Broglie relation:

$$p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k \text{ , where } k = \frac{2\pi}{\lambda} \text{ is the wave number.}$$

The wave number is completely determined for a plane harmonic wave and so is the momentum according to the de Broglie relation.

If we want information on the position of a particle, we must describe it by a “pulse”, a so called *wave packet*, which has a confined extent in space. The position of the wave packet is then to be identified with the position of the particle.

We shall then try, using a superposition of harmonic waves which have wave numbers between k_1 and k_2 . If we want a superposition having all wave numbers between k_1 and k_2 it can be done by evaluating the integral.

$$u(x,t) = \int_{k_1}^{k_2} A\cos(\omega t - kx)dk \tag{6.4}$$

We then assume that $\omega = \omega(k)$, and if the interval [k_1 , k_2] is small, then it is a fair approximation to assume that ω is a linear function of k in the interval, such that $v_g = \frac{d\omega}{dk}$ is a constant.

In that case we may evaluate the integral.

$$\begin{aligned} u(x,t) &= \frac{A}{\frac{d\omega}{dk}t - x}\left[\sin(\omega t - kx)\right]_{k_1}^{k_2} \\ &= \frac{A}{\frac{d\omega}{dk}t - x}(\sin(\omega_2 t - k_2 x) - \sin(\omega_1 t - k_1 x)) \\ &= \frac{2A}{\frac{d\omega}{dk}t - x}\sin(\tfrac{1}{2}\Delta\omega t - \tfrac{1}{2}\Delta kx)\cos(\frac{\omega_1 + \omega_2}{2}t - \frac{k_1 + k_2}{2}x) \\ &= 2A\frac{\sin(\frac{1}{2}\Delta k(\frac{\Delta\omega}{\Delta k}t - x))}{\frac{d\omega}{dk}t - x}\cos(\omega t - kx) \end{aligned} \tag{6.5}$$

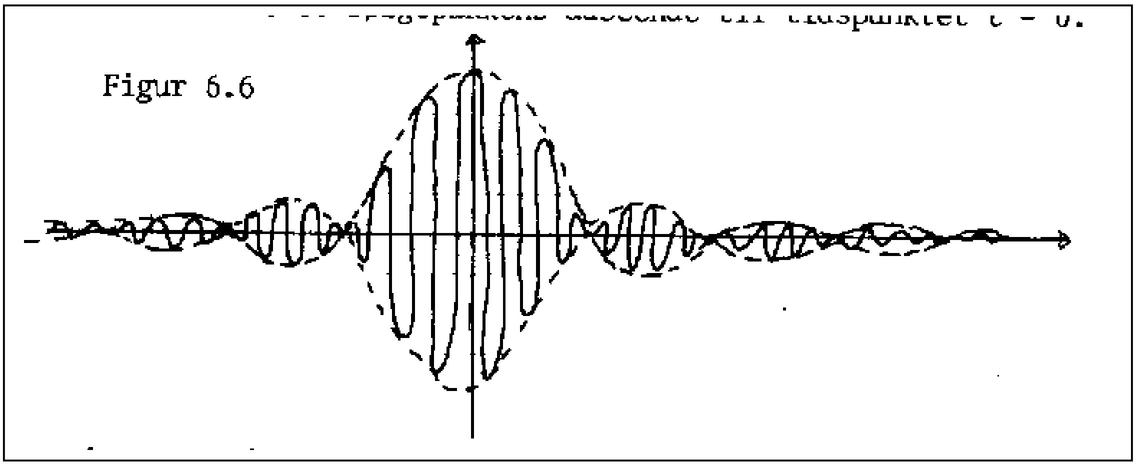
As it was the case for the superposition of the two harmonic waves, we perceive (6.5) as a harmonic wave with a time dependent amplitude. To understand the variation of the amplitude, we notice that the function: $\frac{\sin kx}{x} \rightarrow 1 \quad for \quad x \rightarrow 0$ and that the function essentially is different from zero only in the interval $-\pi \le kx \le \pi$.

About the superposition (6.5) we remark that, if ω is a linear function of k, we may identify $\frac{\Delta\omega}{\Delta k}$ with the group velocity $v_g = \frac{d\omega}{dk}$, and $-\pi \le \frac{1}{2}\Delta k(\frac{\Delta\omega}{\Delta k}t - x) \le \pi$.

The maximum of the amplitude moves with the group velocity, determined by the denominator.

$$\frac{d\omega}{dk}t - x = 0 \quad \Rightarrow \quad v_g = \frac{x}{t} = \frac{d\omega}{dk} \ .$$

Below is sketched the form of the wave packet at $t = 0$.



Figur 6.6

To estimate the spatial extend of the wave packet, we shall consider it at the time $t = 0$.
At that time the wave packet is essentially only different from zero in the interval $-\frac{2\pi}{\Delta k} \le x \le \frac{2\pi}{\Delta k}$.
Should we therefore estimate the uncertainty Δx in the position of a particle described by the wave packet above, we must have: $\Delta x \ge \frac{2\pi}{\Delta k} \quad \Rightarrow \quad \Delta x \Delta k \ge 2\pi$.
Δk may, however, also be perceived as the uncertainty on the wave number of the particle, and causes a uncertainty on the momentum of the particle. If we use the de Broglie's relation:

$$p = \frac{h}{\lambda} = \hbar k \quad \Rightarrow \quad \Delta p = \hbar \Delta k .$$

Thus we find:

(6.7) $$\Delta x \Delta k \ge 2\pi \quad \Rightarrow \quad \hbar \Delta k \Delta x \ge 2\pi \quad \Rightarrow \quad \Delta x \Delta p \ge h$$

The last inequality is Heisenberg's famous *uncertainty relation*.

The relation expresses that in the particle–wave duality description of an atomic particle it is impossible simultaneously to determine the momentum and the position of a particle with unlimited accuracy.
The position and the momentum can only be determined such that the product of the uncertainties on the position and momentum do not exceed *h,* Planck's constant,(which indeed is a very small number, even in an atomic scale).

One might argue that the derivation of this result is based on a very specific wave function, but it turns out that (6.7) is quite general, and that it is a fundamental consequence of the particle wave duality.

Clearly the description of the motion of a particle using a wave function has some peculiar consequences. The question is whether we must completely abandon the conception of a particle located at a certain point?
This paradox, however, has been circumvented by the so called *probability interpretation*, of quantum physical predictions, according to which the absolute square of the (complex) wave

function should be interpreted as the *probability* of finding the atomic particle in a certain volume element.

The probability interpretation of the wave mechanics has, however, (also from a more philosophical point of view), some conspicuous consequences.

From mechanics we are used to the deterministic point of view, that is, if we know the momentum and the position of a particle, and we know the forces that act on the particle, then we can calculate the position of the particle at any later time. And this is (in principle) possible with unlimited accuracy. But with the probability interpretation this is no longer the case.

In the wave mechanics the position of a particle is given by a (complex) wave function $\psi(x,t)$, where $|\psi(x,t)|^2$ is the *probability* of finding the particle in the volume element *dV.*

In a similar manner, which we shall not substantiate, one may calculate the probability that a particle has a momentum in the interval: $d^3\vec{p} = dp_x dp_y dp_z$.

In the wave mechanics one is compelled to (at least partly) to abandon the *determinism* of the classical physics, according to which, one may (in principle) with unlimited accuracy predict the state of a system once the initial conditions and the acting forces are known.

In the wave mechanics one may at most establish that the system has a certain probability to be found at a certain position and having a certain momentum at a given time.
And what is more intriguing. Two different systems, having the same initial conditions may later be "found" in two different states.

This has been named *the indeterminism in quantum physics*.

This *indeterminism* has (especially among non-physicists) been the subject of exaggerated interpretation and even crude misconception, since they have extrapolated the concept of indeterminism to other phenomenon in the macroscopic material world and even to the human conscience.
Some of these philosophical speakers have taken the indeterminism in quantum physiucs as a proof that, (even with the sufficient amount of information), one is not able to predict the future, and even the development of human life.
In the extreme they have challenged the concept of a free will. Pursuing this line of thinking into the absurd, the conclusion may be that over life on earth is still in the hands of " The Lord".

Firstly, we should emphasize that indeterminism is a phenomenon that is bound to atomic particles. In quantum statistics one may prove that the positions and the momentums of larger systems, can be established with a probability, proportional to the inverse of Avogadro's number: (6.0 10^{23}).

And for two hundred years we have known that determinism prevails in classical mechanics. Miracles do not exist (outside the human mind).

The rational facts are, however, that quantum mechanics is nothing but a precise mathematical formalism, by which one may calculate the probabilities of the development of an atomic system in time, and these precise mathematical probabilities excludes exactly the conception of a "higher determination".

"If the Lord determines our future, at least he does it by throwing dices", as it polemically has been stated. Some physicist (including Einstein) has had difficulties in abandoning the principle of determinism, which otherwise has rule for over 200 years.

On the other hand no physicist can discard a theory if it gives a correct description of nature, and can make correct prediction of nature, no matter how odd it may look like and how far it is from everyday experience in the macroscopic world.

Anyway, there is nothing whatsoever in quantum physics which can substantiate a metaphysic or religious view of the material world.

We shall end this section by stating the differential equation, which (non relativistic) determine the development of a quantum mechanical wave function.
From this rather complex differential equation one may in principle calculate the wave function for an arbitrary atomic system at any later time, once the dynamic potentials are known.

The equation is, (as mentioned earlier), the famous Schroedinger equation.
It was first published in 1928 by the Austrian physicist K. E. Schroedinger, following the theoretical work of Bohr, de Broglie, Heisenberg among others.

The mathematical formalism on which the Schroedinger equation is founded goes far beyond a textbook on "Elementary Physics", so we have no real opportunity to explain, interpret or apply the equation, but it is only stated for the sake of completeness.

One flagrant difference to classical physics is that physical quantities: momentum, energy and so on are replaced by differential operators, acting on the wave function.
This formalism has been imported from the Hamiltonian analytical mechanics, (as it is also the case with statistical mechanics).

A particle moving in a potential $V(x,t)$ is described by a wave function: $\psi(x,t)$.
The probability that a particle is situated in the volume element $dV = dxdydz$ at the time t is calculated as $|\psi(x,t)|^2 dV$.

The momentum of the particle at time t can be calculated from the operator $i\hbar\frac{\partial}{\partial x}$ applied on the wave function. (i is the complex unit $i^2=-1$).

The wave function is the solution to the Scroedinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{6.8}$$

Where ∇^2 is the Laplace operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

The Scroedinger equation may be perceived as the fundamental equation in the non relativistic quantum mechanics, analogous to the role of Newton's 2. law in classical mechanics.

In the relativistic quantum mechanics, on the other hand, applies the Dirac equations, but they are considerably more mathematically complex.