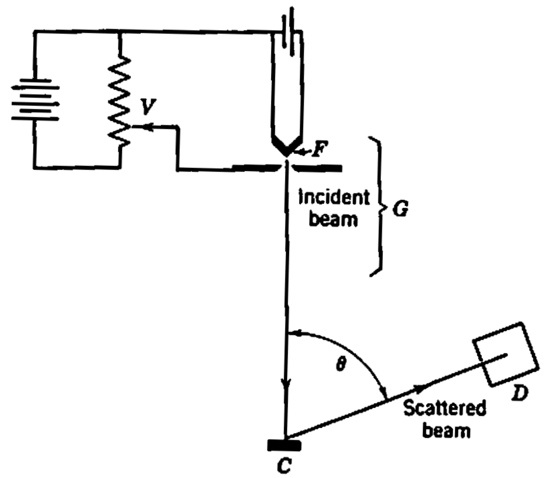


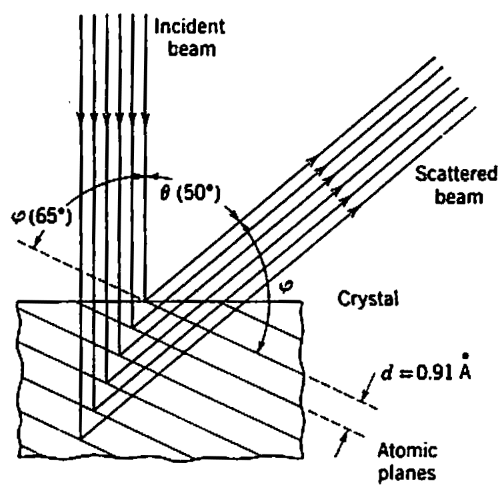
Since light waves behave like particles under certain circumstances, it is not unreasonable to assume that particles sometime behave like waves (matter waves). Louis de Broglie proposed that the wavelength of the matter waves is related to the linear momentum of the particle:

$$\lambda = \frac{h}{p}$$

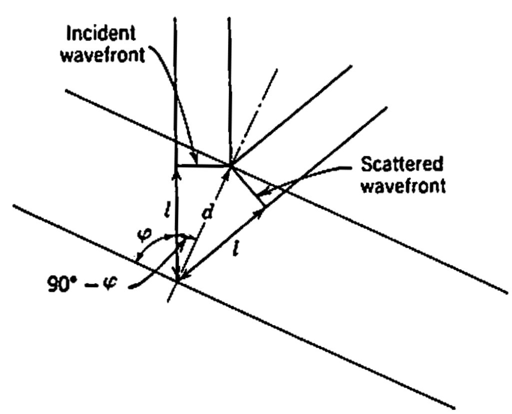
This relation is known as the **de Broglie relation**.

The predictions by de Broglie were confirmed by an experiment carried out by Davisson and Germer with electrons. De Broglie received the 1929 Nobel Prize in Physics for his work on matter waves.

The apparatus used by Davisson and Germer is shown in the Figure on the top of this page. The electrons are accelerated by a variable potential difference V, and the electrons scattered from a crystal are detected as function of the scattering angle θ in a detector D. The energy and angular distributions observed by looking at the scattering yields as function of angle and energy indicate that the observed distributions require constructive interference to be explained.



Consider a model where the atoms in the crystal are located in planes that are separated by a distance d, as shown in the Figure on the right. Assuming that the angle of incidence is equal to the angle of reflection, we can determine the path-length difference of the two rays shown in the bottom right part of the Figure. This difference is equal to



$$\Delta path = 2l = 2d\cos\left(\frac{1}{2}\pi - \varphi\right) = 2d\sin(\varphi)$$

Constructive interference occurs when the path length difference is equal to an integer number of wavelengths:

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

This relation is known as the **Bragg relation**.
The experiments with electrons show that the diffraction patterns observed have the same characteristics as the diffraction patterns observed with light. The electrons indeed behave like waves!

Note: Since h is small, the wavelength of macroscopic objects is small (since p is large). The wave nature of particles only appears when we look at microscopic scales.

The fact that particles sometimes behave like waves and waves sometimes behave like particles is known as **the wave-particle duality**. For any given situation, only one model applies (either the wave model or the particle model). This is known as **the principle of complementarity**.

If a particle behaves like a wave, we expect that the properties of the wave are similar to the properties of EM waves:

$$\varepsilon(x,t) = A\sin\left\{2\pi\left(\frac{x}{\lambda} - \nu t\right)\right\}$$

The intensity of the EM wave is proportional to the average of ε^2 over one cycle:

$$I = \frac{1}{\mu_0 c}\overline{\varepsilon^2}$$

which should be proportional to the average number of photons per unit volume.
The corresponding matter wave, also called the **de Broglie wave**, is given by

$$\Psi(x,t) = A\sin\left\{2\pi\left(\frac{x}{\lambda} - \nu t\right)\right\}$$

The square of the wave function, averaged over one period, is a measure of the probability of finding a particle in a unit volume around position x at time t. The EM wave is a solution of the wave equation; the wavefunction Ψ is the solution of the Schrödinger equation, as will be discussed in Chapter 5. The use of wavefunctions emphasizes the role of probability in predicting the time-evolution of a system.
In classical mechanics, the assumption was made that if we know the position and the linear momentum of a particle at time $t = 0$, the equations of motion can be used to determine the position and linear momentum at any later time. We say that classical mechanics is

deterministic. We will see that quantum mechanics is not deterministic and there are limits to how accurately we can measure the position and the linear momentum of an object. The precission of our measurements is limited by the **Heisenberg uncertainty principle:**

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

where $\hbar = h/2\pi$. Due to the smallness of h, the effects of Heisenberg's uncertainty principle are not observable in the macroscopic world. The Heisenberg uncertainty principle limits the accuracy of our measurements; it is consistent with the fact that the act of making a measurement disturbs the system and changes its state.

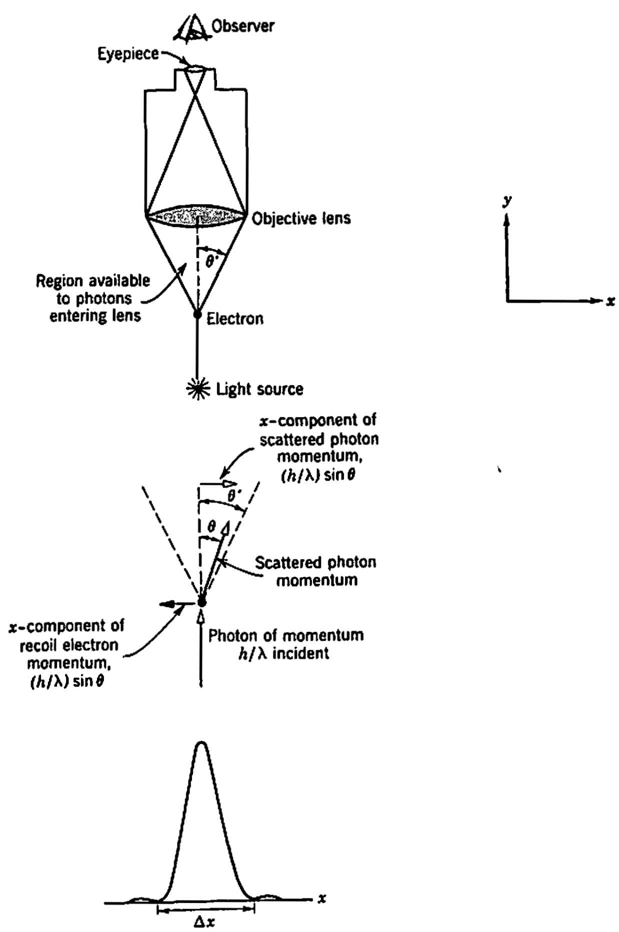
Consider the following **thought experiment** of making a measurement of the position of an electron using an optical microscope, as shown in the Figure at the bottom right. We want to determine the position of the electron by using a beam of photons and measuring the diffraction pattern generated by the scattered photons. Initially the photon is travelling in the y direction. After the interaction with the electron, the photon is moving at an angle θ. Assuming that the scattering angle is small, the change in its wavelength is small. The x component of the linear momentum of the scattered photon is equal to

$$p_{\gamma,x} = \frac{h}{\lambda}\sin\theta$$

Since linear momentum is conserved, the linear momentum of the electron after the interaction is equal to

$$p_{e,x} = -\frac{h}{\lambda}\sin\theta$$

We thus see that as a result of the scattering process, the linear momentum of the electron changes.



The scattered photons will produce a diffraction pattern on the screen. The resolving power of the microscope, and thus the accuracy with which we can determine the position of the electron, is limited by the width of the central peak of this diffraction pattern:

$$\Delta x = \frac{\lambda}{\sin\theta'}$$

where θ' is the maximum scattering angle of the photons. The corresponding uncertainty in the x component of the linear momentum of the electron is

$$\Delta p_x = 2p_{e,x} = 2\frac{h}{\lambda}\sin\theta'$$

The product of the uncertainties of the x position and linear momentum is this equal to

$$\Delta x \Delta p_x = \left(\frac{\lambda}{\sin\theta'}\right)\left(2\frac{h}{\lambda}\sin\theta'\right) = 2h > \frac{\hbar}{2}$$

We see that we can improve the spatial resolution of the microscope by reducing the wavelength. But shorter wavelengths correspond to larger momenta and thus a larger uncertainty in the linear momentum of the electron after the interaction with the photons.

Heisenberg's uncertainty relation can also be rewritten in terms of the uncertainty in energy E and time t. Consider a non-relativistic particle of mass m moving with a linear momentum p in the x direction. If its linear momentum is uncertain, its total energy will also be uncertain:

$$E = \frac{p_x^2}{2m} \quad \Rightarrow \quad \Delta E = \frac{2p_x \Delta p_x}{2m} = \frac{p_x \Delta p_x}{m} = v_x \Delta p_x$$

If the time required to make the measurement is Δt, the position of the particle is uncertain by $v_x\,\Delta t$. The uncertainty relation can now be rewritten as

$$\Delta x \Delta p_x = \left(v_x \Delta t\right)\left(\frac{\Delta E}{v_x}\right) = \boxed{\Delta E \Delta t \geq \frac{\hbar}{2}}$$

Example Problem 3.29

The lifetime of an excited state of a nucleus is usually 10^{-12} seconds. What is the uncertainty in the energy of the γ-ray emitted?

The uncertainty principle limits the accuracy of the energy of the excited state:

$$\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{0.6582 \times 10^{-15}}{2 \times 10^{-12}} = 3.3 \times 10^{-4} \text{ eV}$$

Assuming the ground state is stable, its lifetime is infinite and its energy is known with high accuracy. The uncertainty in the energy of the γ-ray is thus equal to 3.3×10^{-4} eV.
Note: the best γ-ray detectors have an energy resolution of about 1 keV, and the resolution of the energy of γ-rays is thus limited by the detector resolution.

Example Problem 3.28
(a) Consider an electron whose position is somewhere in an atom of diameter 1 Å. What is the uncertainty in the electron's linear momentum? Is this consistent with the binding energy of electrons in atoms? (b) Imagine an electron is somewhere in a nucleus of diameter 10^{-12} cm. What is the uncertainty in the electron's linear momentum? Is this consistent with the binding energy of nuclear constituents? (c) Consider now a neutron, or a proton, in such a nucleus. What is the uncertainty in the neutron's, or proton's, linear momentum? Is this consistent with the binding energy of nuclear constituents?

(a) The uncertainty of the position of the electron is 0.5 Å. The uncertainty of its linear momentum can be determined using the uncertainty principle:

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{0.6582 \times 10^{-15}}{2\left(0.5 \times 10^{-10}\right)} = 6.6 \times 10^{-6} \text{ eV s/m}$$

Assuming that the uncertainty in p is similar to the value of p, we can now estimate the energy of the electron:

$$E = \frac{p^2}{2m} = \frac{p^2c^2}{2mc^2} \geq \frac{\left(6.6 \times 10^{-6}\right)^2 \left(2.998 \times 10^8\right)^2}{2\left(0.511 \times 10^6\right)} = 3.8 \text{ eV}$$

Compare this to the potential energy of an electron at a distance of 0.5 Å from a proton:

$$U = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{\left(0.5 \times 10^{-10}\right)} = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \frac{\hbar c}{\left(0.5 \times 10^{-10}\right)} = \frac{1}{137} \frac{\left(0.6582 \times 10^{-15}\right)\left(2.998 \times 10^8\right)}{\left(0.5 \times 10^{-10}\right)} = 29 \text{ eV}$$

The kinetic energy of the electron, assuming it is in a circular orbit, is half the potential energy, and the total energy of the electron is thus 45 eV, consistent with the minimum value of 4 eV obtained from the uncertainty principle.

(b) The uncertainty of the position of the electron is 0.5×10^{-14} m. The uncertainty of its linear momentum can be determined using the uncertainty principle:

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{0.6582 \times 10^{-15}}{2\left(0.5 \times 10^{-14}\right)} = 0.066 \text{ eV s/m}$$

Assuming that the uncertainty in p is similar to the value of p, we can now estimate the energy of the electron:

$$E = \frac{p^2}{2m} = \frac{p^2c^2}{2mc^2} \geq \frac{\left(3.3 \times 10^{-2}\right)^2 \left(2.998 \times 10^8\right)^2}{2\left(0.511 \times 10^6\right)} = 381 \text{ MeV}$$

This binding energy is very large, much larger than the typical binding energy of nuclear constituents that are typically between 2 MeV and 9 MeV.

(c) The uncertainty of the position of the neutron is 0.5×10^{-14} m. The uncertainty of its linear momentum can be determined using the uncertainty principle:

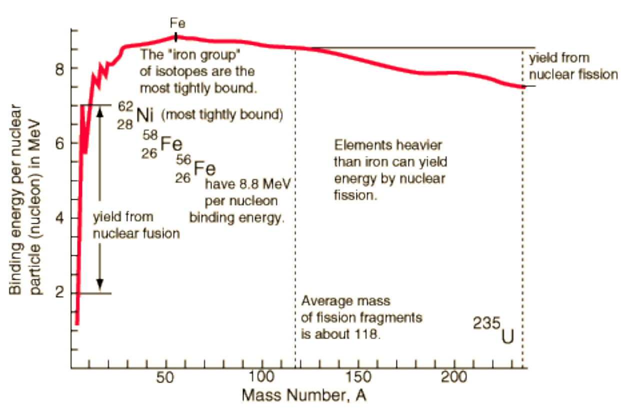
$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{0.6582 \times 10^{-15}}{2\left(0.5 \times 10^{-14}\right)} = 0.066 \text{ eV s/m}$$

Assuming that the uncertainty in p is similar to the value of p, we can now estimate the energy of the neutron:

$$E = \frac{p^2}{2m} = \frac{p^2c^2}{2mc^2} \geq$$

$$\frac{\left(6.6 \times 10^{-2}\right)^2 \left(2.998 \times 10^8\right)^2}{2\left(939.6 \times 10^6\right)} = 0.21 \text{ MeV}$$

The known binding energy of nucleons is consistent with this lower limit. Typical values are between 2 MeV and 9 MeV, as shown in the Figure on the right.



Now consider some important properties of matter waves. Assume we are considering a free particle of mass m, moving along the x axis with velocity v. Its wavelength is equal to

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

The de Broglie wavefunction of this particle is given by

$$\Psi(x,t) = A\sin\left\{2\pi\left(\frac{x}{\lambda} - \nu t\right)\right\}$$

At time t, this wavefunction has a maximum at position x. A short time dt later, the maximum has moved a distance dx. The following equation related dx and dt:

$$\frac{x}{\lambda} - \nu t = \frac{x+dx}{\lambda} - \nu(t+dt) \quad \Rightarrow \quad 0 = \frac{dx}{\lambda} - \nu dt \quad \Rightarrow \quad \text{velocity of propagation} = \frac{dx}{dt} = \lambda\nu$$

Using the expression of the de Broglie wavelength we can rewrite the velocity of propagation as

$$\text{velocity of propagation} = \lambda\nu = \frac{h}{p}\frac{E}{h} = \frac{\frac{p^2}{2m}}{p} = \frac{p}{2m} = \frac{1}{2}v$$

The velocity of propagation of the matter wave is thus half the velocity of propagation of the particle. **Note:** please note the difference between frequency ν and velocity v in these equations.

Is this a problem? Answer: No! Why not?

- The wave function considered above cannot represent a particle since it is not localized in space.
- In order to describe a particle in terms of a wavefunction we need to create a combination of waves. A combination of waves has two characteristic velocities (or node velocities): the velocity of propagation of the high-frequency component and the velocity of propagation of the envelope, also called the **group velocity**. As we will see, the group velocity is the velocity of the particle.

It is common to use κ instead of $1/\lambda$ in the wavefunction. The wave function is then written as

$$\Psi(x,t) = A\sin\left\{2\pi(\kappa x - \nu t)\right\}$$

Consider sum of two matter waves with slightly different wavelengths and frequencies:

$$\begin{aligned}\Psi_{1+2}(x,t) &= \left(\sin\{2\pi(\kappa x - \nu t)\} + \sin\{2\pi((\kappa + d\kappa)x - (\nu + d\nu)t)\}\right) \\ &= 2\cos\left\{2\pi\left(\frac{d\kappa}{2}x - \frac{d\nu}{2}t\right)\right\}\sin\{2\pi(\kappa x - \nu t)\}\end{aligned}$$

In this derivation we have assumed that $d\nu$ and $d\kappa$ are much smaller than ν and κ. The cosine term represents the low-frequency component of the sum; the sine term represents the high-frequency component. We can associated a velocity with each of these two components:

High-frequency component:

Consider the nodes in the high-frequency component:

$$2\pi(\kappa x - \nu t) = \pi n \quad \text{where } n = 0, \pm 1, \pm 2, ...$$

This equation can be rewritten as

$$x = \frac{n}{2\kappa} + \frac{\nu}{\kappa}t$$

The node velocity is thus equal to

$$\text{node velocity} = \frac{dx}{dt} = \frac{\nu}{\kappa} = \omega$$

Low-frequency component:

Consider the nodes in the low-frequency component:

$$2\pi\left(\frac{d\kappa}{2}x - \frac{d\nu}{2}t\right) = \pi\left(n + \frac{1}{2}\right) \quad \text{where } n = 0, \pm 1, \pm 2, ...$$

This equation can be rewritten as

$$x = \frac{\left(n + \frac{1}{2}\right)}{d\kappa} + \frac{d\nu}{d\kappa}t$$

The node velocity, or **group velocity**, is equal to

$$\text{node velocity} = \frac{dx}{dt} = \frac{d\nu}{d\kappa}$$

For particle waves we know that

$$\nu = \frac{E}{h} \quad \Rightarrow \quad d\nu = \frac{dE}{h}$$
$$\kappa = \frac{1}{\lambda} = \frac{p}{h} \quad \Rightarrow \quad d\kappa = \frac{dp}{h}$$

Assuming that the particle is moving at non-relativistic speeds, the energy E is approximately equal to $p^2/2m$. Substituting this in the previous expression we obtain for the group velocity

$$\text{group velocity} = \frac{d\nu}{d\kappa} = \frac{\frac{dE}{h}}{\frac{dp}{h}} = \frac{dE}{dp} = \frac{p}{m} = v$$

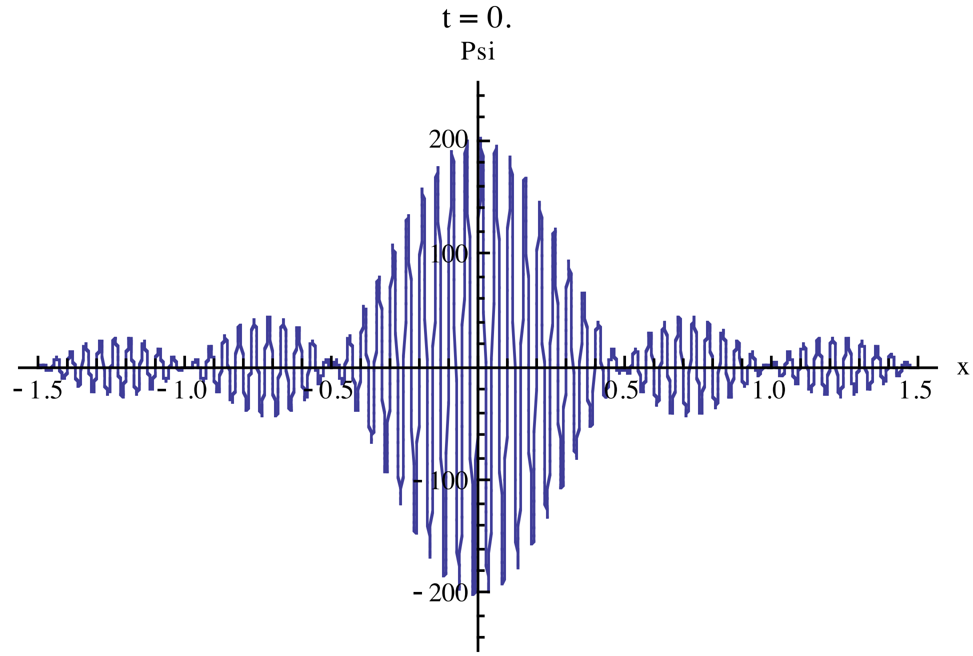
We thus conclude that **the group velocity is equal to the particle velocity**.

In general, we find that we need to add many different matter waves to describe a particle. Consider for example the sum of 201 matter waves of the same amplitude but with values of κ between 19 and 21 with a step size of 0.01 (the units of κ are 1/units of x). The result of this sum is the wavefunction shown in the Figure on top of the next page. The particle is most likely located in the region around $x = 0$. Defining the uncertainty in x to be equal to half width at half maximum, we conclude from the Figure that $\Delta x = 0.3$. Since κ varies between 19 and 21, the uncertainty in κ is equal to 1. The product of these two uncertainties is thus equal to

$$\Delta x \Delta \kappa = 0.3$$

In this particular case, the product of these uncertainties is large since we have given each individual wavefunction the same weight in our summation. If the amplitude of the individual waves would have been described by a Gaussian distribution, the product of the uncertainties in k and x would have been smaller. The limiting value of this product is $1/4\pi$:

$$\Delta x \Delta \kappa \geq \frac{1}{4\pi}$$



The uncertainty in κ can be rewritten as

$$\Delta\kappa = \Delta\left(\frac{1}{\lambda}\right) = \Delta\left(\frac{p}{h}\right) = \frac{1}{h}\Delta p$$

The product of the uncertainties can thus be rewritten as

$$\Delta x \Delta\kappa = \frac{1}{h}\Delta x \Delta p \geq \frac{1}{4\pi} \quad \text{or} \quad \Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

which is the Heisenberg uncertainty principle.