Quantum Physics 2005

Notes-1

Course Information, Overview,

The Need for Quantum Mechanics

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Topic Overview

1. Why and when do we use quantum mechanics?
2. Probability waves and the Quantum Mechanical State function; Wave packets and particles
3. Observables and Operators
4. The Schrodinger Equation and some special problems (square well, step barrier, harmonic oscillator, tunneling)
5. More formal use of operators
6. The single electron atom/ angular momentum

Intellectual overview

- The study of quantum physics includes several key parts:
  - Learning about experimental observations of quantum phenomena.
  - Understanding the meaning and consequences of a probabilistic description of physical systems
  - Understanding the consequences of uncertainty
  - Learning about the behavior of waves and applying these ideas to state functions
  - Solving the Schrodinger equation and/or carrying out the appropriate mathematical manipulations to solve a problem.

The course

- 2 lecture/studios per week T/F 12-2
- Reading quiz and exercises every class = 15% of grade
- Homework=35%
- 2 regular exams = 30%
- Final = 20%

Textbook

- Required: Understanding Quantum Physics by Michael Morrison
- Recommended:
  Fundamentals of Physics by Halliday, Resnick…
  Handbook of Mathematical Formulas by Spiegel (Schaums Outline Series)
- References:
  Introduction to the Structure of Matter, Brehm and Mullen
  Quantum Physics, Eisberg and Resnick

Academic Integrity

- Collaboration on homework and in-class exercises is encouraged. Copying is discouraged.
- Collaboration on quizzes and examinations is forbidden and will result in zero for that test and a letter to the Dean of Students.
- Formula sheets will be supplied for exams. Use of any other materials results in zero for the exam and a letter to the DoS.

The class really starts now.

Classical Mechanics

- A **particle** is an indivisible point of mass.
- A **system** is a collection of particles with defined forces acting on them.
- A **trajectory** is the position and momentum (**r**(t), **p**(t))of a particle as a function of time.
- If we know the trajectory and forces on a particle at a given time, we can calculate the trajectory at a later time. By integrating through time, we can determine the trajectory of a particle at all times.

$$m\frac{d^2\vec{r}}{dt^2} = -\nabla V(\vec{r},t); \quad \vec{p}(t) = m\frac{d\vec{r}}{dt}$$

Some compelling experiments: The particlelike behavior of electromagnetic radiation

- Simple experiments that tell us that light has both wavelike and particle-like behavior
  - The photoelectric effect (particle)
  - Double slit interference (wave)
  - X-ray diffraction (wave)
  - The Compton effect (particle)
  - Photon counting experiments (particle)

The photoelectric effect

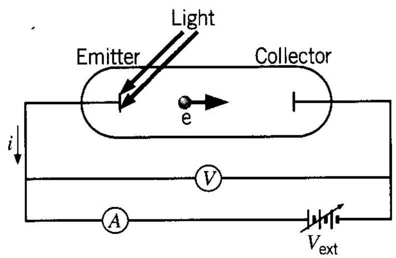


FIGURE 3.10 Apparatus for observing the photoelectric effect. The flow of electrons from the emitter to the collector is measured by the ammeter A as a current i in the external circuit. A variable voltage source V_{ext} establishes a potential difference between the emitter and collector, which is measured by the voltmeter V.

Krane

Krane

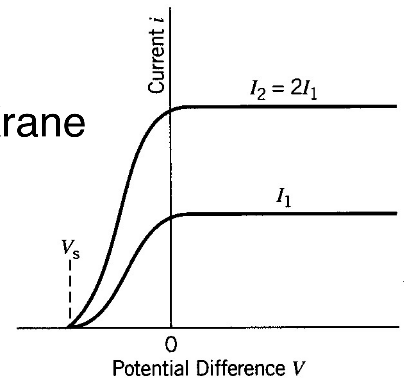


FIGURE 3.11 The photoelectric current i as a function of the potential difference V for two different values of the intensity of the light. When the intensity is doubled, the current is doubled (twice as many photoelectrons are emitted), but the stopping potential V_s remains the same.

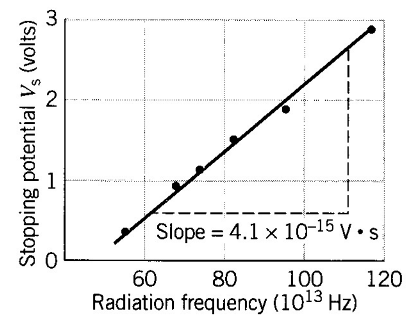


FIGURE 3.12 Millikan's results for the photoelectric effect in sodium. The slope of the line is h/e; the experimental determination of the slope gives a way of determining Planck's constant. The intercept should give the cutoff frequency; however, in Mil-

Krane

- In a photoelectric experiment, we measure the voltage necessary to stop an electron ejected from a surface by incident light of known wavelength.

Interpretation of the photoelectric effect experiment

Einstein introduced the idea that light carries energy in quantized bundles - photons.

The energy in a quantum of light is related to the frequency of the electromagnetic wave that characterizes the light.

The scaling constant can be found from the slope of eV_{stop} vs wave frequency, ν. It is found that:

$$eV_{stop} = h\nu - \Phi_{material} = E_{photon} - \Phi$$

where $h = 6.626x10^{-34}$ joule-sec

For light waves in vacuum, $c = \lambda\nu = 3x10^{8}$ m/s,

so we can also write:

$$eV_{stop} = \frac{hc}{\lambda} - \Phi_{material}$$

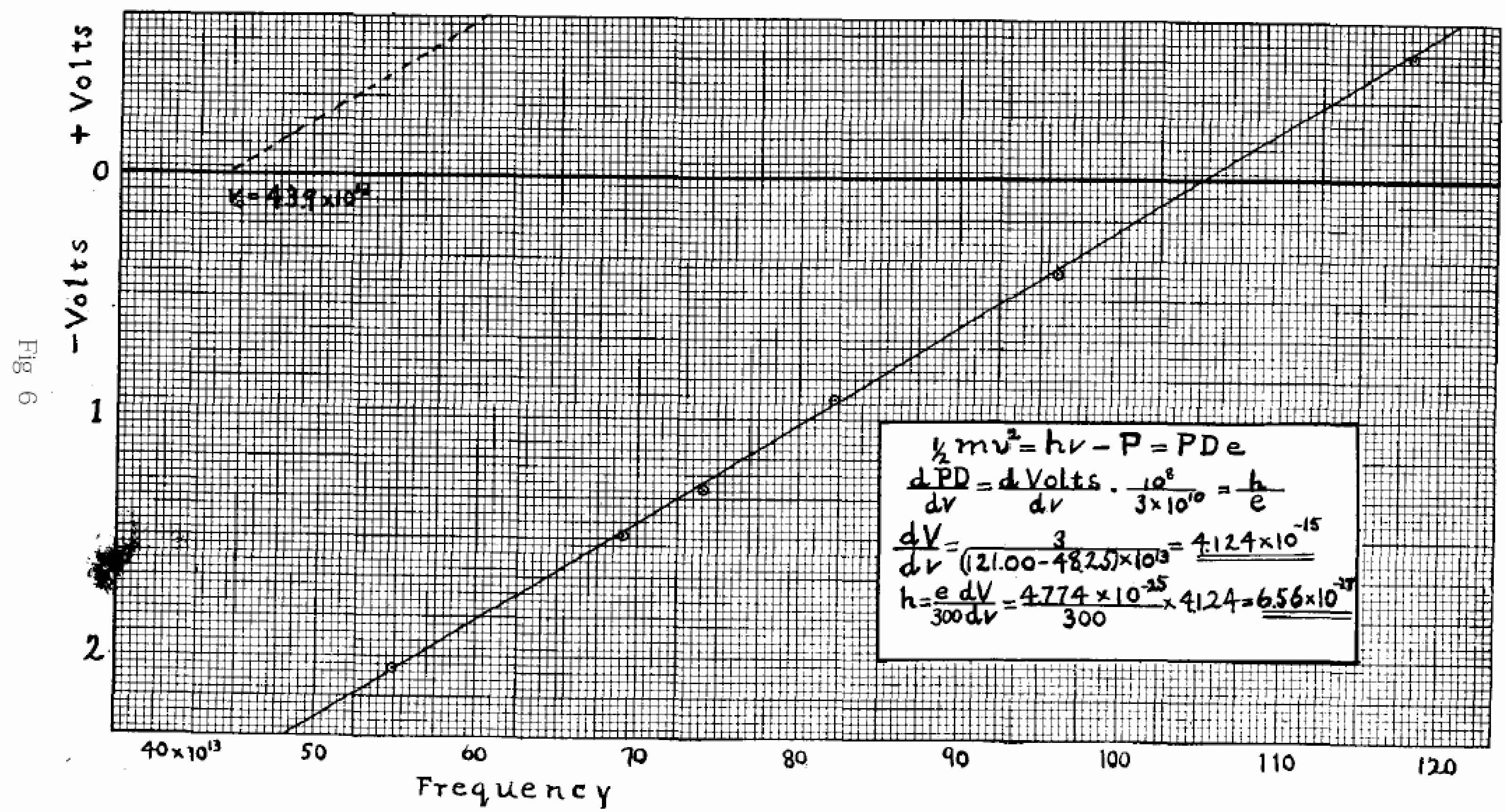
A convenient (non-SI) substitution is $hc = 1240$ eV-nm.

from Millikan's 1916 paper

1. *That there exists for each exciting frequency* v, *above* a certain *critical value, a definitely determinable maximum velocity of emission of corpuscles.*
2. *That there is a linear relation between V and v.*
3. *That* $\frac{dV}{d\nu}$ *or the slope of the V v line is numerically equal to* h/e.
4. *That at the critical* frequency ν_0 *at which* v = o, $p = h\nu_0$, *i. e., that the intercept* of *the Vv* line on *the* v axis is *the lowest* frequency *at which the metal* in *question can be photoelectrically active.*
5. *That the contact* $E.M.F.$ *between* any *two* conductors is given *by the equation*

$$\text{Contact E.M.F.} = h/e(\nu_0 - \nu_0') - (V_0 - V_0').$$

R. A. Millikan, Phys Rev 7, 355, (1916)



Compton scattering

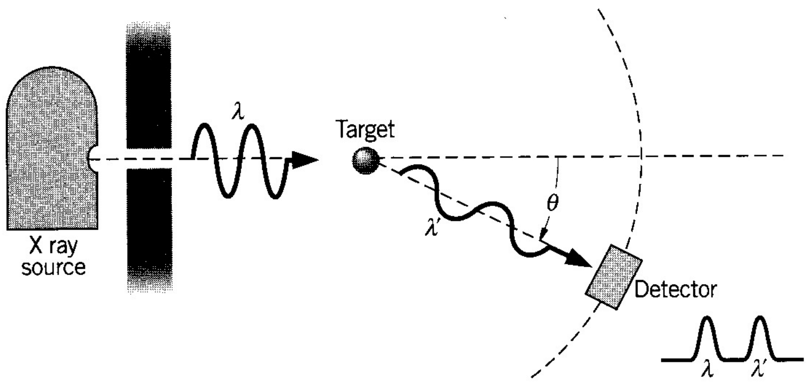


FIGURE 3.19 Schematic diagram of Compton scattering apparatus. The wavelength λ' of the scattered X rays is measured by the detector, which can be moved to different positions θ. The wavelength difference $\lambda' - \lambda$ varies with θ.

(from Krane)

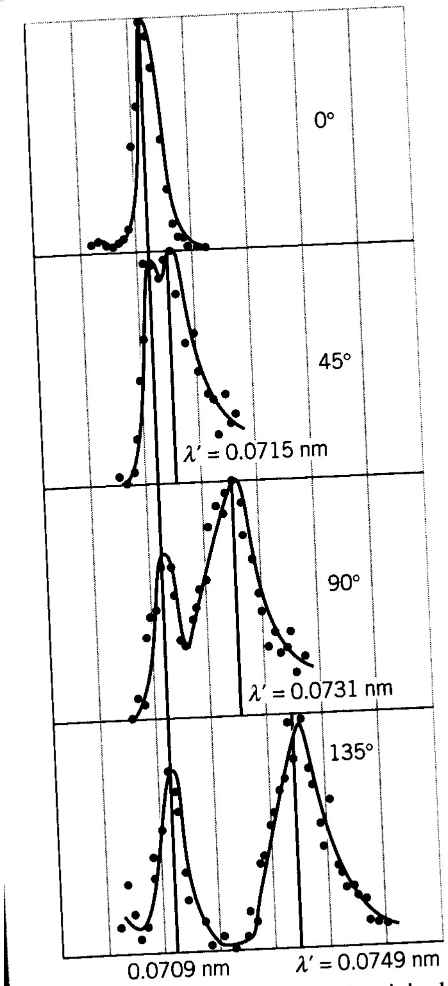


FIGURE 3.20 Compton's original results for X-ray scattering.

- The Compton effect involves scattering of electromagnetic radiation from electrons.
- The scattered x-ray has a shifted wavelength (energy) that depends on scattered direction

Compton effect

We use energy and momentum conservation laws:

Energy

$hv' = h\nu - K_{electron}$: K = kinetic energy

Momentum

x component: $\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma mv\cos\theta$

y component: $0 = \frac{h}{\lambda'}\sin\phi + \gamma mv\sin\theta$

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{mc}\left(1-\cos\phi\right)$$

m = mass of electron;

γ=relativistic correction to electron momentum mv

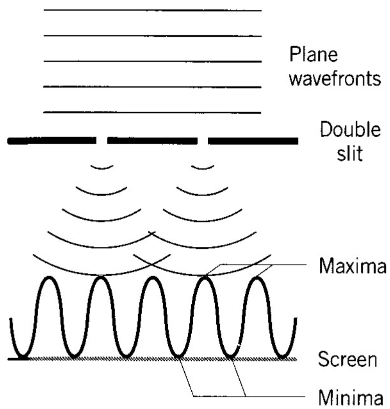
Conclusions from the Compton Effect

X-ray quanta of wavelength λ have:

Kinetic energy: $K = \dfrac{hc}{\lambda}$

Momentum: $p = \dfrac{h}{\lambda}$

Double slit interference



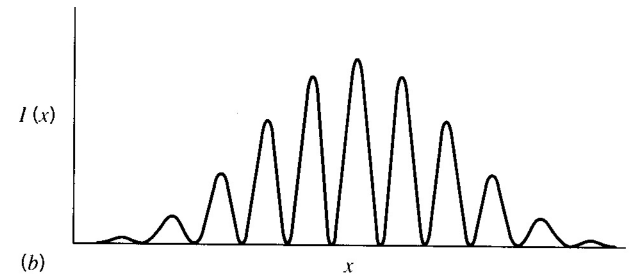


FIGURE 5-10 Results from the two-slit experiment using photons. (*a*) Measured photon intensity as a function of position. From M. Cagnet, *Atlas of Optical Phenomena*, Springer-Verlag (1962). (*b*) Calculated photon intensity.

The intensity maxima in a double slit wave interference experiment occur at:

$$d \sin\theta = n\lambda$$

where d is the distance between the slits.

(The width of the overall pattern depends on the width of the slits.)

X-ray diffraction

- In x-ray diffraction, x-ray waves diffracted from electrons on one atom interfere with waves diffracted from nearby atoms.
- Such interference is most pronounced when atoms are arranged in a crystalline lattice.

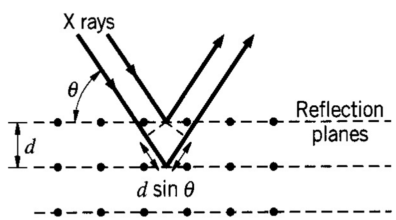


FIGURE 3.5 A beam of X rays reflected from a set of crystal planes of spacing d. The beam reflected from the second plane travels a distance $2d \sin \theta$ greater than the beam reflected from the first plane.

Bragg diffraction maxima are observed when:

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

$d =$ the distance between adjacent planes of atoms in the crystal.

Laue X-ray Diffraction Pattern

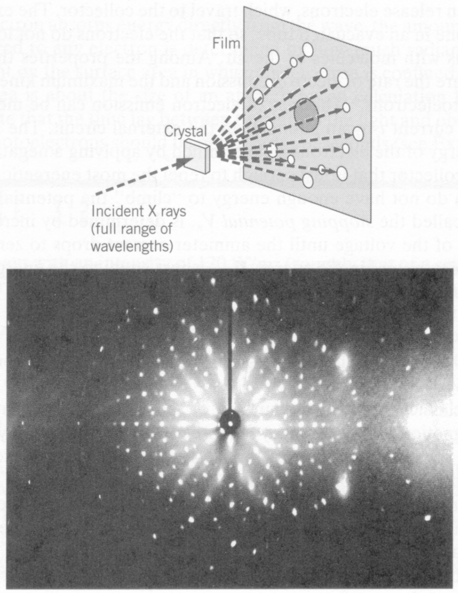


FIGURE 3.7 (Top) Apparatus for observing X-ray scattering by a crystal. An interference maximum (dot) appears on the film whenever a set of crystal planes happens to satisfy the Bragg condition for a particular wavelength. (Bottom) Laue pattern of NaCl crystal.

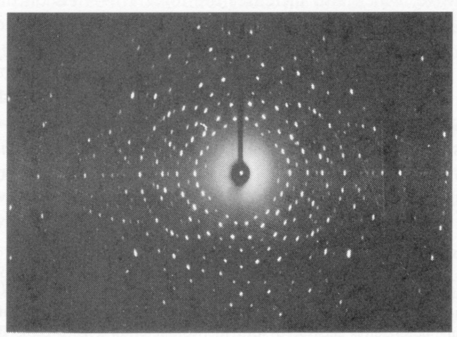


FIGURE 3.8 Laue pattern of a quartz crystal. The difference in crystal structure and spacing between quartz and NaCl makes this pattern look different from Figure 3.7.

- A Laue diffraction pattern is observed when x-rays of many wavelengths are incident on a crystal and diffraction can therefore occur from many planes simultaneously.

…pretty

from Krane

The bottom line on light

- In many experiments, light behaves like a wave (c=phase velocity, ν=frequency, λ=wavelength).
- In many other experiments, light behaves like a quantum particle (photon) with properties:

energy: $E_{photon} = h\nu = \dfrac{hc}{\lambda}$

momentum: $p = \dfrac{h}{\lambda}$

and thus: $E = pc$

Some compelling experiments: The wavelike behavior of particles

- Experiments that tell us that electrons have wave-like properties
  - electron diffraction from crystals (waves)
- Other particles
  - proton diffraction from nuclei
  - neutron diffraction from crystals

Electron diffraction from crystals

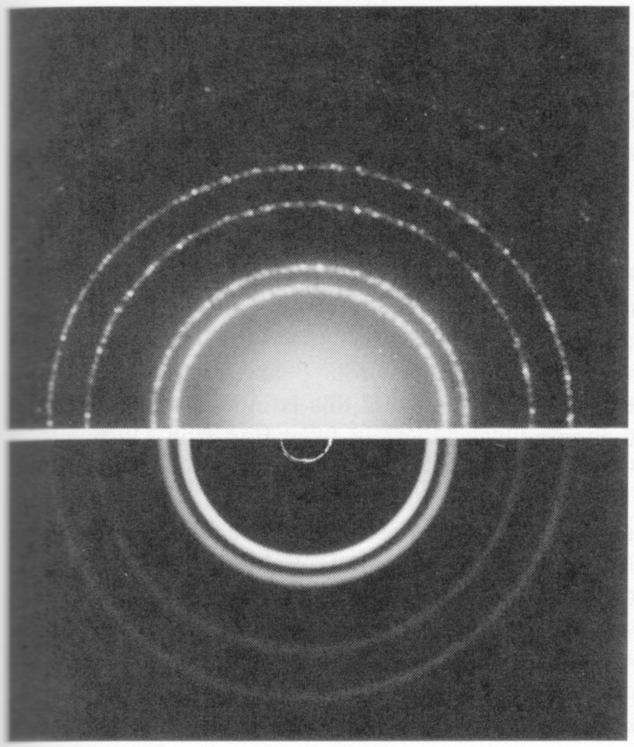
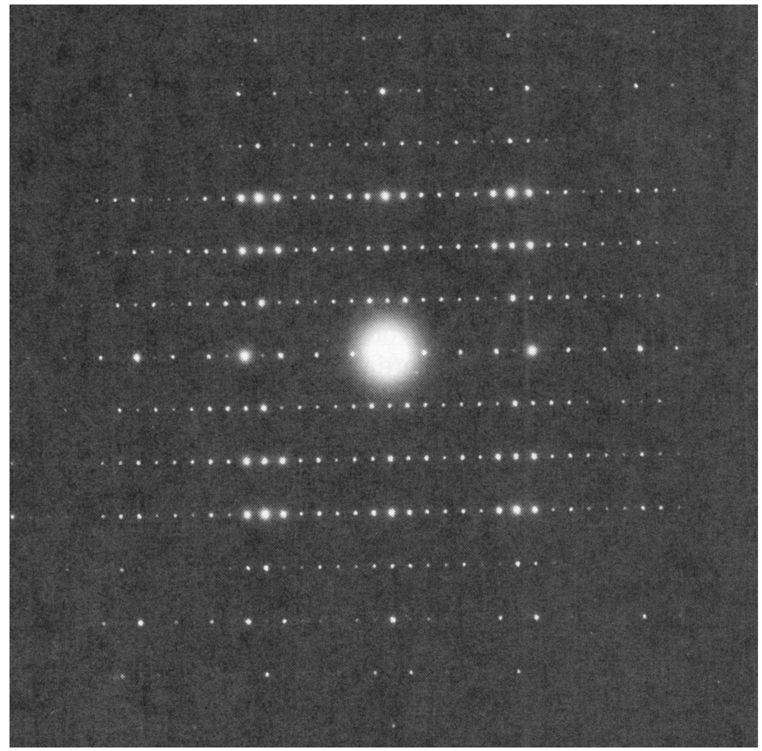


FIGURE 4.3 Comparison of X-ray diffraction and electron diffraction. The upper half of the figure shows the result of scattering of 0.071 nm X rays by an aluminum foil, and the lower half shows the result of scattering of 600 eV electrons by aluminum. (The wavelengths are different so the scales of the two halves have been adjusted.)



- electron diffraction patterns from single crystal (above) and polycrystals (left) [from Krane]

Proton diffraction from nuclei

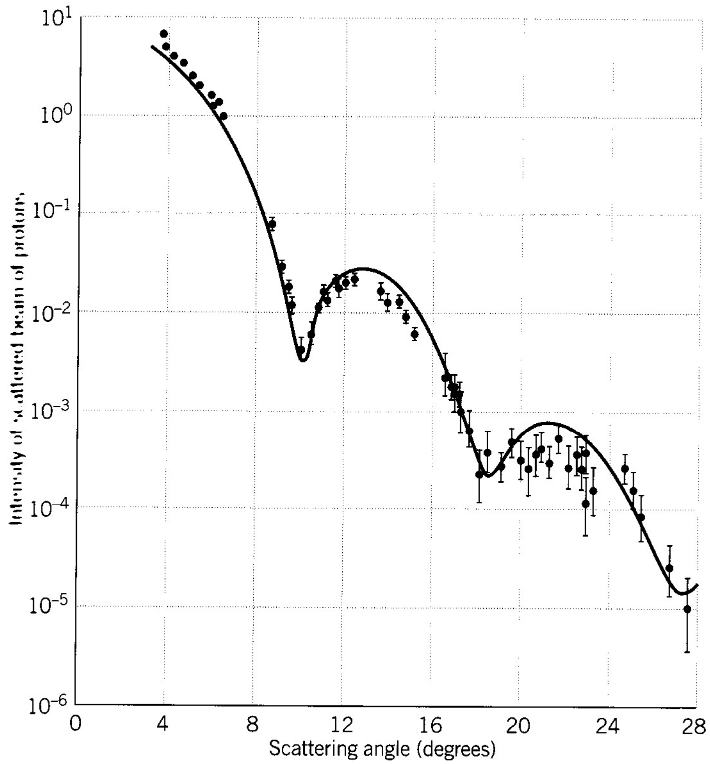


FIGURE 4.8 Diffraction of 1 GeV protons by oxygen nuclei. The pattern of maxima and minima is similar to that of single-slit diffraction of light waves.

from Krane

Neutron diffraction

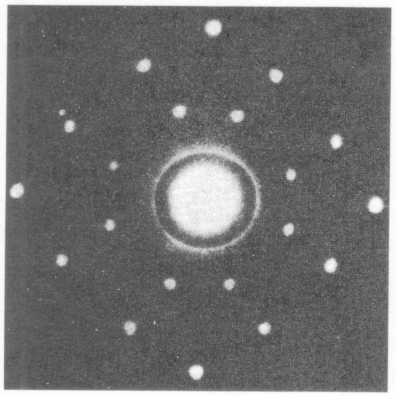
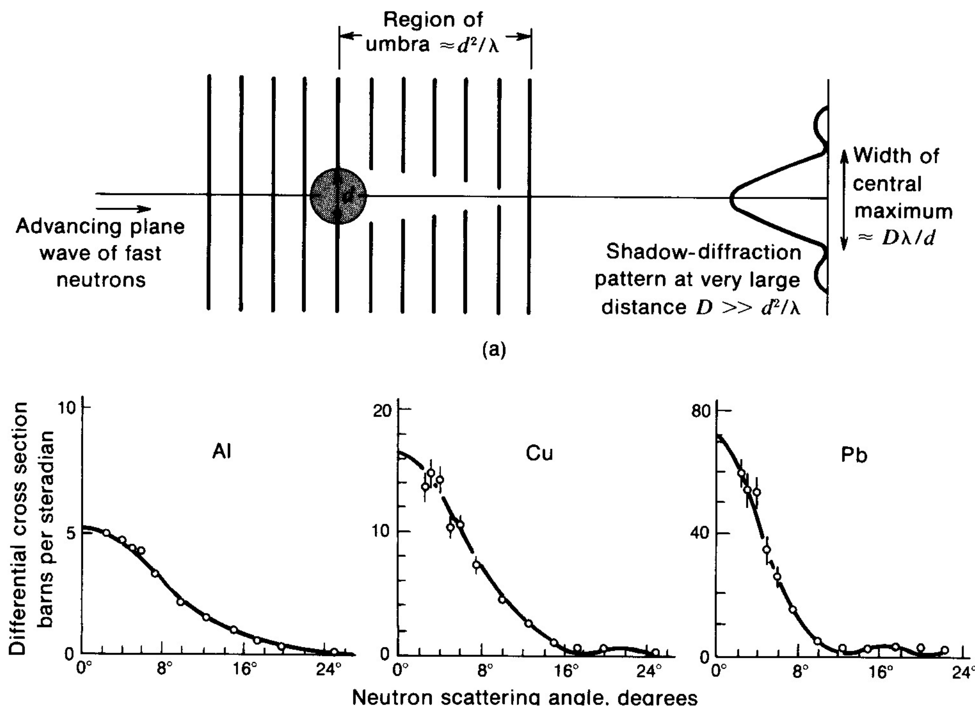


FIGURE 4.7 Diffraction of neutrons by a sodium chloride crystal.

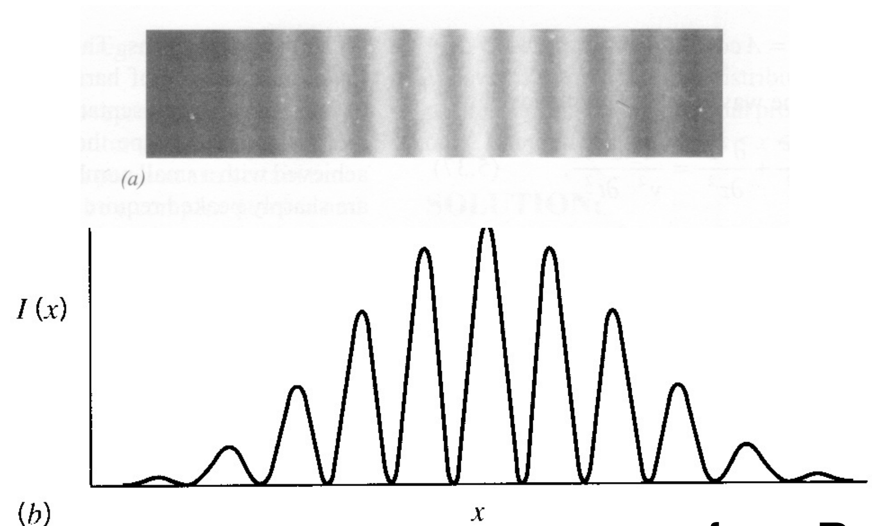
from Krane



Diffraction of fast neutrons from Al, Cu, and Pb nuclei. [from French, after A Bratenahl, Phys Rev 77, 597 (1950)]

Electron double slit interference

- Electron interference from passing through a double slit



from Rohlf

FIGURE 5-11 Results from the two-slit experiment using electrons.
(*a*) Measured electron intensity as a function of position. From C. Jönsson, Zeit. Phys. **161**, 454 (1961). (*b*) Calculated electron intensity.

Helium diffraction from LiF crystal

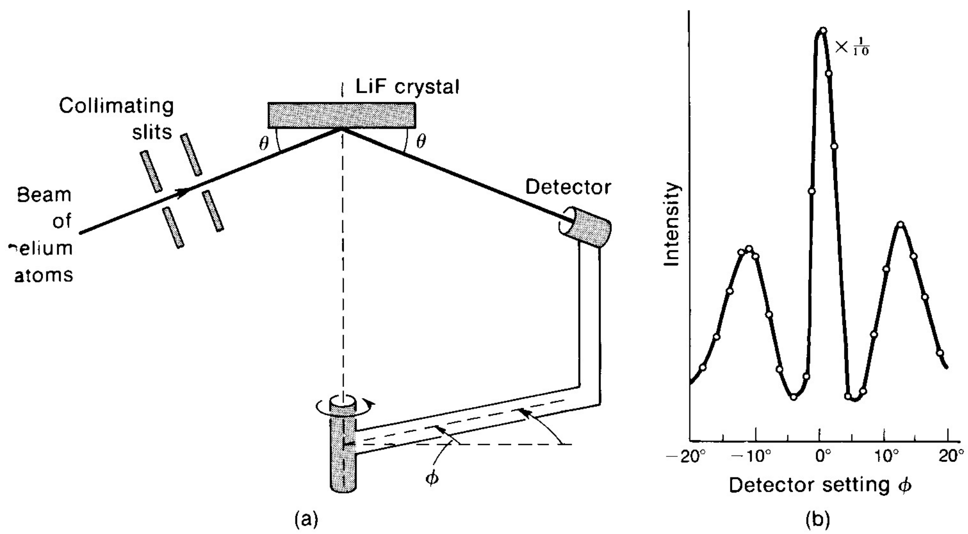
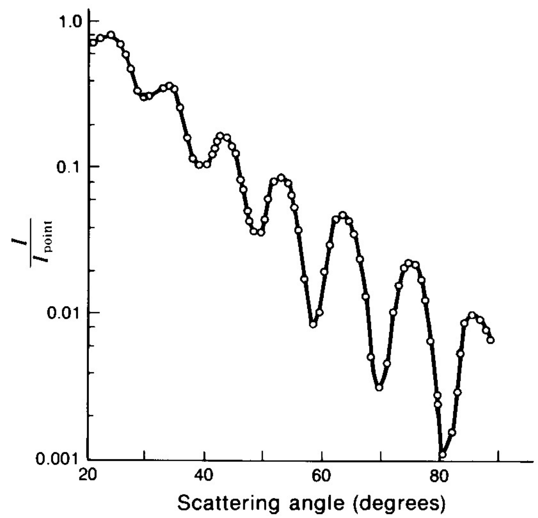


Fig. 2-16 (a) Experimental arrangement used by Stern et al. *to investigate crystal diffraction of neutral helium atoms. (b) Experimental results showing central reflection peak* ($\phi = 0°$), *plus first-order diffraction peaks* ($\phi = 11°$). *In the experiment,* $\theta = 18.5°$.

from French after Estermann and Stern, Z Phys 61, 95 (1930)

Alpha scattering from niobium nuclei



Angular distribution of 40 MeV alpha particles scattered from niobium nuclei.
[from French after G. Igo et al., Phys Rev 101, 1508 (1956)]

The bottom line on particles

- In many experiments, electrons, protons, neutrons, and heavier things act like particles with mass, kinetic energy, and momentum:

$p = mv$ and $K = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ for non-relativistic particles

- In many other experiments, electrons, protons, neutrons, and heavier things act like waves with :

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}$$

The De Broglie hypothesis

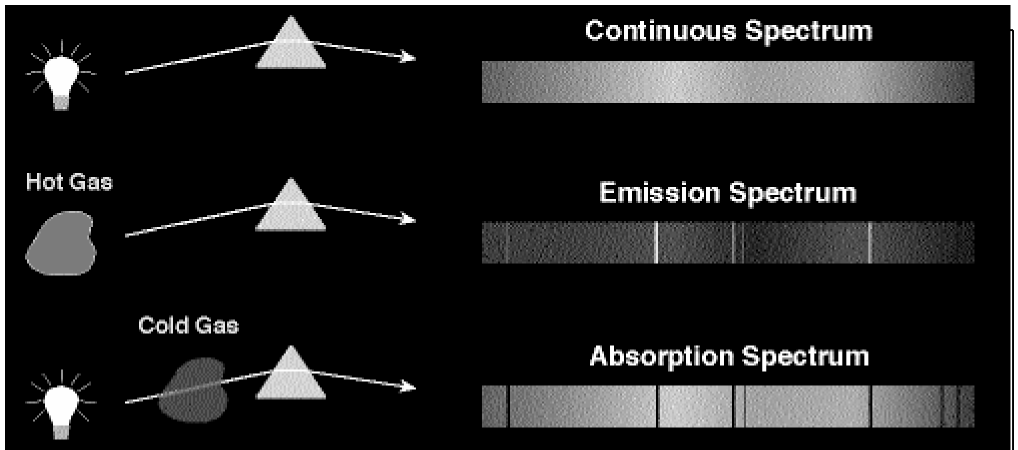
$$p = \frac{h}{\lambda}$$

for everything

Some other well-known experiments and observations

- optical emission spectra of atoms are quantized
- the emission spectrum of a hot object (blackbody radiation) cannot be explained with classical theories

Emission spectrum of atoms



from a random astronomy website

For hydrogen:

$$h\nu = -13.6eV\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Blackbody radiation

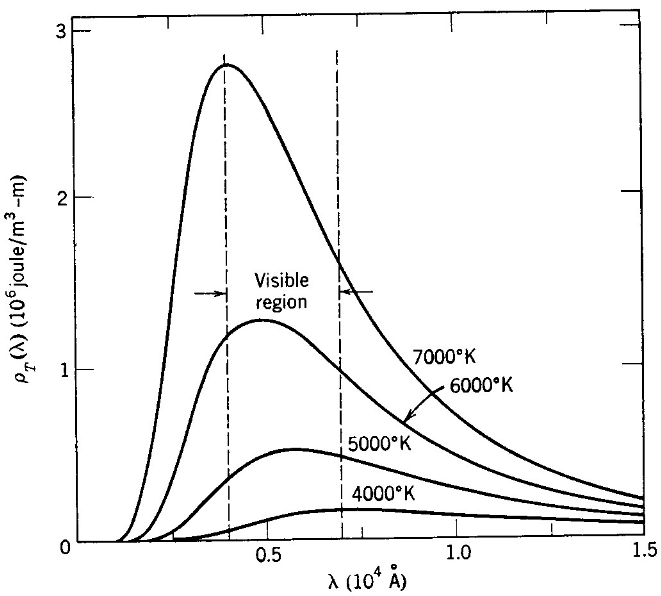


Figure 1-12 Planck's energy density of blackbody radiation at various temperatures as a function of wavelength. Note that the wavelength at which the curve is a maximum decreases as the temperature increases.

$$\rho_T(\lambda)\, d\lambda = \frac{8\pi hc}{\lambda^5} \frac{d\lambda}{e^{hc/\lambda kT} - 1}$$

from Eisberg and Resnick

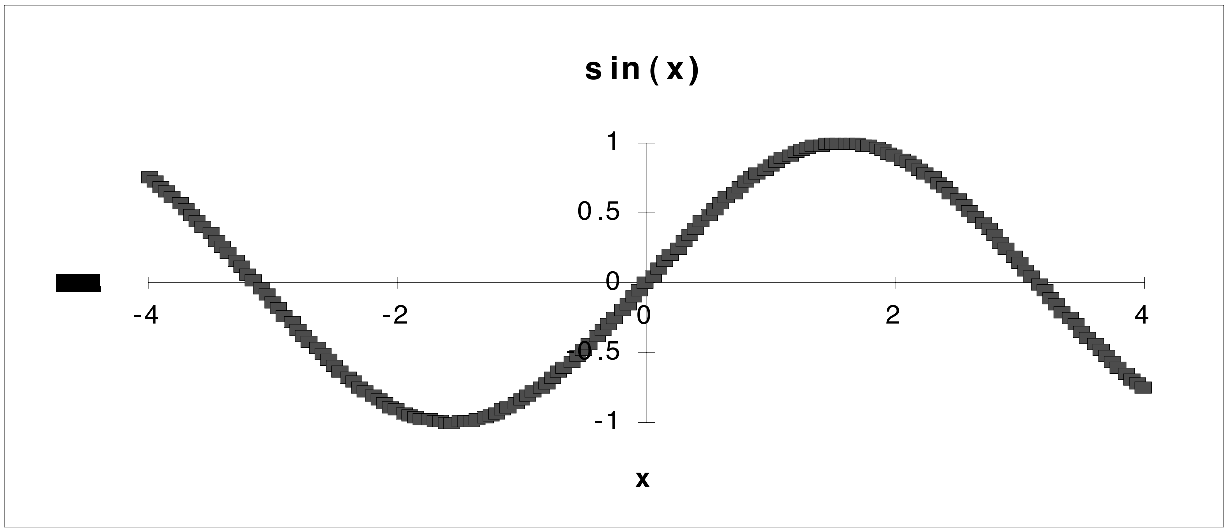
A review of wave superposition and interference

Many of the neat observations of quantum physics can be understood in terms of the addition (superposition) of harmonic waves of different frequency and phase.

In the next several pages I review some of the basic relations and phenomena that are useful in understanding wave phenomena.

Harmonic waves

y=A sin($k(x \pm vt)+\varphi$) or y=Asin($kx \pm \omega t+\varphi$)



$$\lambda = wavelength; \quad k = \frac{2\pi}{\lambda}$$

$$T = period; \quad \omega = \frac{2\pi}{T} = 2\pi\nu$$

Phase and phase velocity

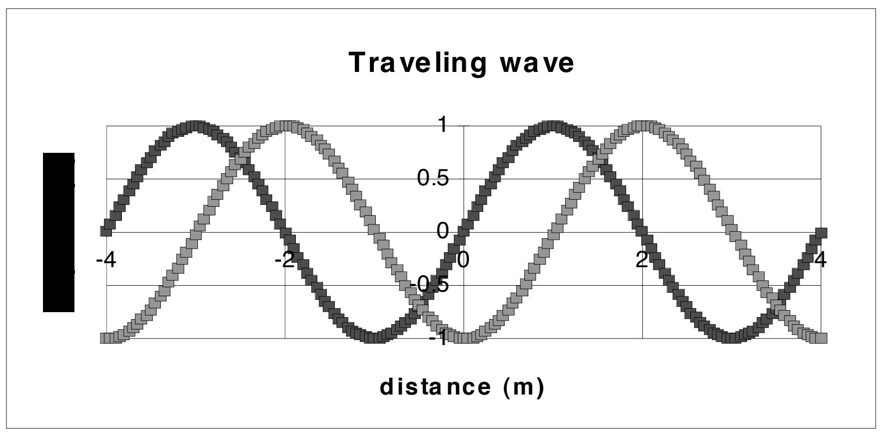
$y = A\sin(kx \pm \omega t)$

$(kx \pm \omega t)$ = phase

when change in phase=2π = repeat

<u>Phase velocity</u> = speed with which point of constant phase moves in space.

$v_p = \omega / k = \lambda \nu$



Complex Representation of Travelling Waves

Doing arithmetic for waves is frequently easier using the complex representation using:

$$e^{i\theta} = \cos\theta + i\sin\theta$$

So that a harmonic wave is represented as

$$\psi(x,t) = A\cos(kx - \omega t + \varepsilon)$$

$$\psi(x,t) = \mathrm{Re}\left[Ae^{i(kx-\omega t+\varepsilon)}\right]$$

Adding waves: same wavelength and direction, different phase

$$\psi_1 = \psi_{01} \sin(kx + \omega t + \phi_1)$$

$$\psi_2 = \psi_{02} \sin(kx + \omega t + \phi_2)$$

taking the form:

$$\psi_R = \psi_1 + \psi_2 = \psi_0 \sin(kx + \omega t + \alpha)$$

we find:

$$\left|\psi_0^2\right| = \psi_{01}^2 + \psi_{02}^2 + 2\psi_{01}\psi_{02} \cos(\phi_1 - \phi_2)$$

and:

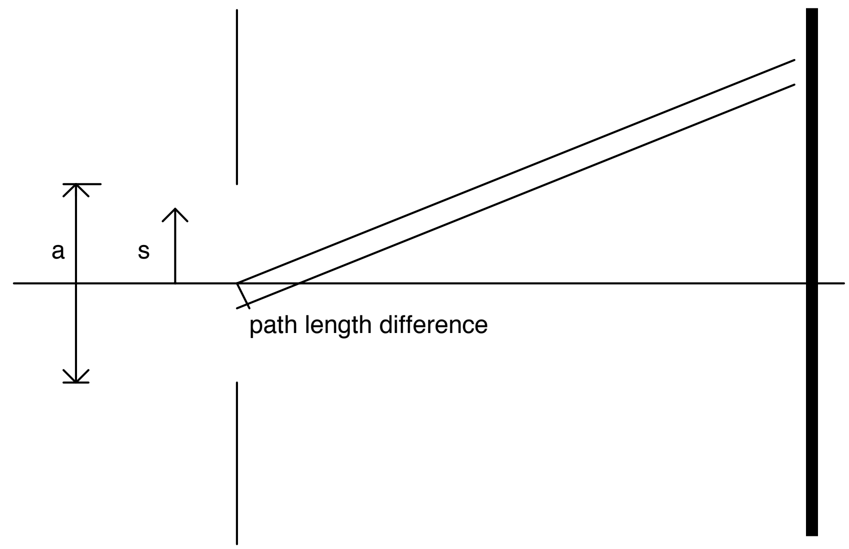
$$\tan\alpha = \frac{\psi_{01} \sin\phi_1 + \psi_{02} \sin\phi_2}{\psi_{01} \cos\phi_1 + \psi_{02} \cos\phi_2}$$

Adding like-waves, in words

- Amplitude
  - When two waves are in phase, the resultant amplitude is just the sum of the amplitudes.
  - When two waves are 180^0 out of phase, the resultant is the difference between the two.
- Phase
  - The resultant phase is always between the two component phases. (Halfway when they are equal; closer to the larger wave when they are not.)

(see adding_waves.mws)

Another useful example of added waves: diffraction from a slit



Let's take the field at the view screen from an element of length on the slit *ds* as $E_s ds$

Ignore effects of distance except in the path length.

Single slit diffraction

$$d\omega = \mathrm{Re}(\psi_s e^{i(kz(s)-\omega t)} ds)$$

$$z(s) = z_0 + s\sin\theta$$

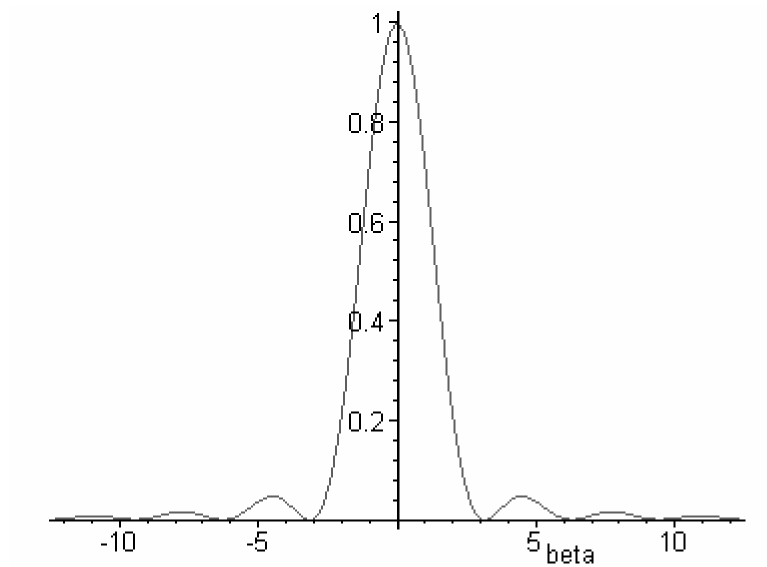
$$\psi(\theta) = \psi_s e^{i(kz_0-\omega t)} \int_{-a/2}^{a/2} e^{iks\sin\theta} ds$$

$$= \psi_s e^{i(kz_0-\omega t)} a \frac{\sin\beta}{\beta}$$

where

$$\beta = \frac{ak}{2}\sin\theta$$

$$\psi^2 = (\psi_s a)^2 \frac{\sin^2\beta}{\beta^2}$$



First zero at $\beta=\pi$, so $\sin\theta = \frac{2\pi}{ak} = \frac{\lambda}{a}$

Adding waves: traveling in opposite directions

Equal amplitudes:

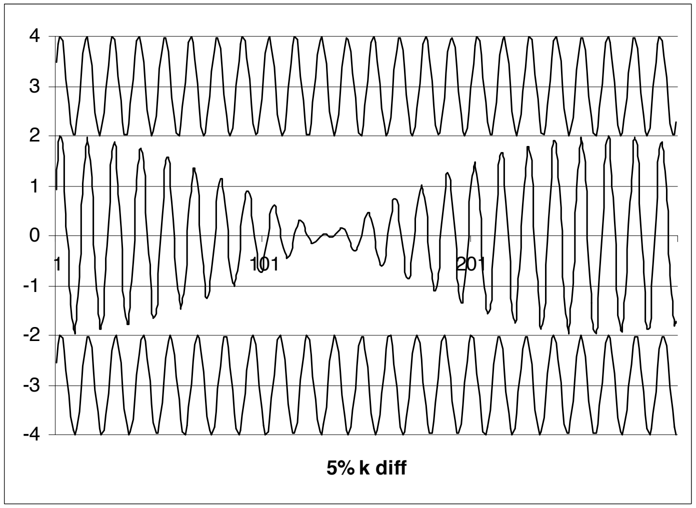
$$\psi_R = \psi_0 (\sin(kx - \omega t + \varepsilon_1) + \sin(kx + \omega t + \varepsilon_2))$$

$$\psi_R = 2\psi_0 \sin(kx + \frac{\varepsilon_1 + \varepsilon_2}{2}) \cos \omega t$$

- The resultant wave does not appear to travel – it oscillates in place on a harmonic pattern both in time and space separately

=Standing wave

Adding waves: different wavelengths



BEATS

$$\psi_1 = \psi_{01}\cos(k_1 x - \omega_1 t)$$

$$\psi_2 = \psi_{01}\cos(k_2 x - \omega_2 t)$$

$$\psi = 2\psi_{01}\cos\frac{1}{2}\left[\left(k_1 + k_2\right)x - (\omega_1 + \omega_2)t\right]$$

$$\times\cos\frac{1}{2}\left[\left(k_1 - k_2\right)x - \left(\omega_1 - \omega_2\right)t\right]$$

$$= \psi_{01}\cos\left[\bar{k}x - \bar{\omega}t\right]\cos\left[\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right]$$

- The resultant wave has a quickly varying part that waves at the average wavelength of the two components.
- It also has an envelope part that varies at the difference between the component wavelengths.

Adding waves: group velocity

- Note that when we add two waves of differing ω and *k* to one another, the envelope travels with a different speed:

monochromatic wave 1: $v_{phase_1} = \frac{\omega_1}{k_1}$

monochromatic wave 2: $v_{phase_2} = \frac{\omega_2}{k_2}$

beat envelope: $v_{group} = \frac{\Delta\omega}{\Delta k}$

see group_velocity.mws

Adding many waves to make a pulse

- In order to make a wave pulse of finite width, we have to add many waves of differing wavelengths in different amounts.
- The mathematical approach to finding out how much of each wavelength we need is the Fourier transform:

$$f(x) = \frac{1}{\pi}\left[\int_0^\infty A(k)\cos kx\,dk + \int_0^\infty B(k)\sin kx\,dk\right]$$

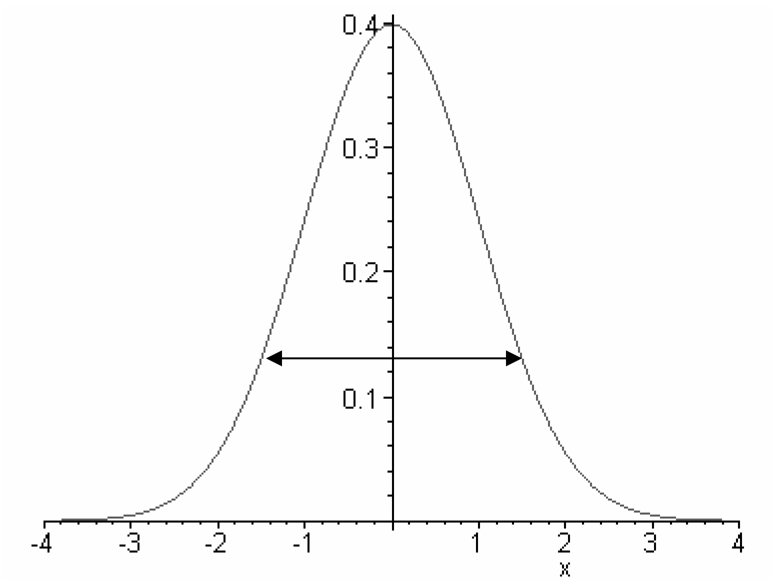
where:

$$A(k) = \int_{-\infty}^{\infty} f(x)\cos kx\,dx$$

$$B(k) = \int_{-\infty}^{\infty} f(x)\sin kx\,dx$$

The Fourier transform of a Gaussian pulse

- We can think of a Gaussian pulse as a localized pulse, whose position we know to a certain accuracy $\Delta x = 2\sigma_x$.



$$f(x) = \frac{1}{\sigma_x \sqrt{2\pi}} e^{-x^2/2\sigma_x^2}$$

Finding the transform

I will drop overall multiplicative constants

because I am interested in the shape of A(k)

$$A(k) \propto \int_{-\infty}^{\infty} e^{-x^2/2\sigma_x^2} e^{-ikx} dx = \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx$$

$$where \quad a = 1/2\sigma_x^2$$

(solving by completing the square:)

$$A(k) \propto \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx = \int_{-\infty}^{\infty} e^{-\left(x\sqrt{a} - \frac{ik}{2\sqrt{a}}\right)^2 - k^2/4a} dx$$

letting $\beta = x\sqrt{a} - \dfrac{ik}{2\sqrt{a}}$

$$A(k) \propto \frac{1}{\sqrt{a}} e^{-k^2/4a} \int_{-\infty}^{\infty} e^{-\beta^2} d\beta = \sqrt{\frac{\pi}{a}} e^{-k^2/4a} = \sqrt{\frac{\pi}{a}} e^{-k^2\sigma_x^2/2}$$

Transform of a Gaussian pulse: The Heisenberg Uncertainty Principle

We can rewrite this in the standard form of a Gaussian in k:

$$A(k) \propto e^{-k^2/2\sigma_k^2} \quad \text{where} \quad \sigma_k^2 = 1/\sigma_x^2$$

The result then is that $\sigma_x\sigma_k=1$ for a Gaussian pulse. You will find that the product of spatial and wavenumber widths is always equal to or greater than one. Since the deBroglie hypothesis relates wavelength to momentum, $p=h/\lambda$ we thus conclude that $\sigma_x\sigma_p>=h/2\pi$. This is a statement of the **Heisenberg Uncertainty Principle**.

The Heisenberg Uncertainty Principle

- This principle states that you cannot know both the position and momentum of a particle simultaneously to arbitrary accuracy.
  - There are many approaches to this idea. Here are two.
    - The act of measuring position requires that the particle intact with a probe, which imparts momentum to the particle.
    - Representing the position of localized wave requires that many wavelengths (momenta) be added together.
    - The act of measuring position by forcing a particle to pass through an aperture causes the particle wave to diffract.

The Heisenberg Uncertainty Principle

- Position and momentum are called conjugate variables and specify the trajectory of a classical particle. We have found that if one wants to specify the position of a Gaussian wave packet, then:

$$\Delta x \Delta p = \hbar$$

- Similarly, angular frequency and time are conjugate variables in wave analysis. (They appear with one another in the phase of a harmonic wave.)

$$\Delta \omega \Delta t = 1$$

- Since energy and frequency are related Planck constant we have, for a Gaussian packet:

$$\Delta E \Delta t = \hbar$$

The next stages

- We have seen through experiment that particles behave like waves with wavelength relationship: $p=h/\lambda$.
- The next stage is to figure out the relationship between whatever waves and observable quantities like position, momentum, energy, mass…
- The stage after that is to come up with a differential equation that describes the wavy thing and predicts its behavior.
- There is still a lot more we can do before actually addressing the wave equation.

References

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Addendum – Energy and momentum

The notation for energy, momentum, and wavelength
in Morrison is somewhat confusing because he does not always clearly
distinguish between total relativistic energy (which includes mass energy),
and kinetic energy (which does not.)
Here goes my version:

1) Classical kinetic energy-momentum relation: $T = \frac{1}{2} m_0 v^2 = \frac{p^2}{2m_0}$

2) Relativistic total energy-momentum relationship: $E^2 = p^2c^2 + m_0^2c^4$
with $E = T + m_0c^2$.

When you want to find the wavelength from classical kinetic energy, use 1 and $p = \frac{h}{\lambda}$:

$$T = \frac{p^2}{2m_0} = \frac{h^2}{2m_0\lambda^2} \quad \Rightarrow \quad \lambda = \frac{h}{\sqrt{2m_0T}} = \frac{hc}{\sqrt{2m_0c^2T}}$$

When you want to find the wavelength for a relativistic particle use 2 and $p = \frac{h}{\lambda}$:

$$\lambda = \frac{hc/E}{\sqrt{1+\left(\frac{m_0c^2}{E}\right)^2}} = \frac{hc/\left(T + m_0c^2\right)}{\sqrt{1+\left(\frac{m_0c^2}{\left(T+m_0c^2\right)}\right)^2}}$$

Addendum – comparing classical and relativistic formulas for wavelength

1) Classical: $\lambda = \frac{h}{\sqrt{2m_0T}} = \frac{hc}{\sqrt{2m_0c^2T}}$

2) Relativistic: $\lambda = \frac{hc/\left(T + m_0c^2\right)}{\sqrt{1-\left(\frac{m_0c^2}{\left(T + m_0c^2\right)}\right)^2}} = \frac{hc}{\sqrt{\left(T + m_0c^2\right)^2 - \left(m_0c^2\right)^2}} = \frac{hc}{m_0c^2\sqrt{\left(\frac{T}{m_0c^2}+1\right)^2 - 1}}$

To compare the two expressions, let's Taylor expand eq. 2 in $\frac{T}{m_0c^2}$:

$$\lambda = \frac{hc}{m_0c^2\sqrt{\left(\frac{T}{m_0c^2}+1\right)^2 - 1}} \cong \frac{hc}{m_0c^2\sqrt{2\frac{T}{m_0c^2}}} = \frac{hc}{\sqrt{2m_0c^2T}}$$

They become the same at small T!

Addendum – comparing classical and relativistic formulas for wavelength

1) Classical: $\lambda = \dfrac{h}{\sqrt{2m_0 T}} = \dfrac{hc}{\sqrt{2m_0 c^2 T}}$

2) Relativistic: $\lambda = \dfrac{hc}{m_0 c^2 \sqrt{\left(\dfrac{T}{m_0 c^2} + 1\right)^2 - 1}}$

To find the difference between the two forms, let's keep all the terms in $\dfrac{T}{m_0 c^2}$:

$$\lambda = \frac{hc}{m_0 c^2 \sqrt{\left(\dfrac{T}{m_0 c^2} + 1\right)^2 - 1}} \cong \frac{hc}{m_0 c^2 \sqrt{\left(\left(\dfrac{T}{m_0 c^2}\right)^2 + 2\dfrac{T}{m_0 c^2} + 1\right) - 1}} = \frac{hc}{\sqrt{2Tm_0 c^2}\sqrt{\left(\left(\dfrac{T}{2m_0 c^2}\right) + 1\right)}}$$

$$\lambda_{\mathrm{Re}lativistic} \cong \lambda_{Classical} \frac{1}{\sqrt{\left(\left(\dfrac{T}{2m_0 c^2}\right) + 1\right)}} \cong \lambda_{Classical}\left(1 - \left(\frac{T}{4m_0 c^2}\right)\right)$$