### Diffraction

#### 1. Introduction

The deviation of a wave from rectilinear propagation, which occurs when a region of the wave front is obstructed, is called diffraction.

Is there any other situation when the wave departs from rectilinear propagation? Yes, we've already studied reflection and refraction. There is also the bend of light beams in inhomogeneous materials (responsible of the mirages, see Wikipedia). When do we have diffraction? Not when the obstacle has dimensions of the order of the wavelength, because diffraction shows up even at the edge of a semi-infinite screen. The important point is that for diffraction to appear the curvature radii of the obstacles must have dimensions of the order of the wavelength (Sommerfeld).

There is an approximate explanation of diffraction, based on the Huygens principle and on Fresnel's work and a rigorous theory initiated by Kirchhoff, much too difficult to treat.

There is "little" difference between interference and diffraction: *interference* appears when the number of sources is finite, diffraction when it is infinite.

**2.** Spherical waves (Mircea S. Rogalschi, Stuart B. Palmer Advanced university physics, 2006)

In spherical coordinates the Laplace operator is:

$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left( \frac{\partial^2}{\partial \varphi^2} \right)$$
(D1)

If the problem has a spherical symmetry, as e.g. for a point-like source, physical quantities depend only on *r* and *t*. The derivatives along  $\theta$  and  $\varphi$  are zero. The wave eq. in vacuum writes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi(r,t)}{\partial r}\right) - \frac{1}{c^2}\frac{\partial^2\psi(r,t)}{\partial t^2} = 0$$

This may also be written as

$$\frac{\partial^2}{\partial r^2} (r\psi(r,t)) - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} (r\psi(r,t)) = 0$$
 (D2)

# From Wikipedia (slightly changed) till end

Diffraction arises because of the way in which waves propagate; this is described by the <u>Huygens–Fresnel principle</u>. *The propagation of a wave can be visualized by considering every point on a wavefront as a point source for a secondary spherical wave*. The subsequent propagation and addition of all these spherical waves form the new wavefront. When waves are added together, their sum is determined by the relative phases as well as the amplitudes of the individual waves, an effect which is often known as wave <u>interference</u>. The summed amplitude of the waves can have any value between zero and the sum of the individual amplitudes. Hence, diffraction patterns usually have a series of maxima and minima.



Diffraction through a hole in a screen, photo in a ripple tank; water waves move from upper left to lower right, bump into the obstacle with a hole in the middle of the figure. Spherical (cylindrical) waves result. For the ripple tank see fine simulations at <u>http://www.falstad.com/ripple/</u>

See esp. the Fourier applet http://www.falstad.com/fourier/

The form of a diffraction pattern can be determined from the sum of the phases and amplitudes of the Huygens wavelets at each point in space. There are various analytical models which can be used to do this including the <u>Fraunhofer diffraction</u> equation for the <u>far field</u> and the <u>Fresnel diffraction</u> equation for the <u>near field</u> end

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This is a differential eq. for the function  $r\psi(r,t)$  having the same form as the wave eq. In 1D for the function  $\psi(x,t)$ . The solution (d'Alembert) is

$$r\psi(r,t) = f(r-ct) + g(r+ct)$$
(D3)

For any component of the electric or magnetic field this gives:

$$\psi(r,t) = \frac{1}{r}f(r-ct) + \frac{1}{r}g(r+ct)$$
(D4)

The first term is an outgoing perturbation with amplitude falling off as 1/r, known as the direct wave. The second term is an incoming spherical disturbance toward a point detector. For a harmonic spherical wave we find

$$\psi(r,t) = \frac{A}{r} \exp[i(\omega t - kr)]$$
(D5)

*Remark*: the intensity diminishes with a factor  $1/r^2$ . Therefore the total energy flux through a sphere of radius *r* remains the same, but this energy is spread over a surface larger and larger.

#### 3. The Huygens-Fresnel diffraction

Eq. (D5) will be used to give a mathematical expression to the Huygens-Fresnel principle. In the following figure S is the point-like source of monochromatic light,  $\Delta S_1$  and  $\Delta S_2$  are two small areas belonging to the wave front, P is the observation point, R is the distance between S and the wave front, r is the distance between  $\Delta S_1$ (or  $\Delta S_2$ ) and P.  $Q_1$  and  $Q_2$  are the points around which we sketch the secondary waves prescribed by the Huygens-Fresnel principle.  $R_1 = R_2 = R$ ,  $r_1 = r_2 = r$ .

*Remark*: if the points  $Q_1$  and  $Q_2$  are not on the spherical wave front, or if P is not so symmetrically disposed the distances  $SQ_1$  and  $SQ_2$  wouldn't be equal, nor would be equal  $Q_1P$  and  $Q_2P$ .



The spherical wave from S arrives in  $Q_1$  or  $Q_2$  as

$$\psi_1(Q_1,t) = \frac{A}{R_1} \exp[i(\omega t - kR_1)] \quad \text{and} \quad \psi_2(Q_2,t) = \frac{A}{R_2} \exp[i(\omega t - kR_2)]$$

The same relations apply in the propagation from  $Q_1$  and  $Q_2$  toward P. The amplitudes are different, because we assume the secondary waves from  $Q_i$  to be proportional to  $\Delta S_i$  and the propagation from  $Q_i$  to P introduces a factor  $\frac{\exp[ikr_i]}{r_i}$ . The resultant wave at P is:

$$\psi(P,t) = C \left[ \frac{A \exp[i(\omega t - kR_1 - kr_1)]}{R_1 r_1} \Delta S_1 + \frac{A \exp[i(\omega t - kR_2 - kr_2)]}{R_2 r_2} \Delta S_2 \right]$$

Dividing the wave front in small areas d*S* and transforming sum in integral we find:

$$\psi(P,t) = CAe^{i\omega t} \int_{\Sigma} \frac{A \exp[i(-kR - kr)]}{Rr} dS$$
(D6)

The constant *C* is not known from this deduction based on interference only. It turns out (from Kirchhoff formulation) that it depends on:

- a phase shift of secondary waves
- the angles between the initial propagation, the surface normal and the propagation direction of secondary waves.

#### 4. The results of Kirchhoff

We give without proof the results of Kirchhoff for the case  $R, r >> \lambda$ . The angles are defined in the following figure:



The result is:

$$\psi(P) = -\frac{i}{\lambda} A e^{i\omega t} \int_{\Sigma} \frac{e^{-ik(R+r)}}{Rr} [\cos(\vec{u}_n, \vec{u}_r) - \cos(\vec{u}_n, \vec{u}_R)] dS$$
(D7)

The two additional effects included in the Kirchhoff relation are:

- a phase shift by  $\pi/2$
- an angular dependence on both directions of propagations, defined by the *obliquity factor*  $K(\vec{u}_r, \vec{u}_R) = \frac{1}{2} [\cos(\vec{u}_n, \vec{u}_r) - \cos(\vec{u}_n, \vec{u}_R)]$

## 5. The Fraunhoffer diffraction

Assume R, r >> dimensions of the aperture. Then the obliquity factor could be considered constant and the variations of R and r over the aperture are small and 1/Rr could be considered constant too. The changes in R+r affects, however, the phase contribution of different elements from the aperture, due to the large value of the wave vector k. (D7) reduces to:

$$\psi(P) = A(\Sigma)e^{i\omega t} \int_{\Sigma} e^{-ik(R+r)} dS$$
(D8)

When the distances of both the source and the point of observation from the aperture  $\Sigma$  are large, the wave front may be considered plane. The approximation is known as the *far field* or the *Fraunhoffer diffraction*. Denote by (*X*, *Y*) the coordinates in the plane of the aperture and by  $\alpha, \beta$  the direction cosines of  $\vec{u}_r$ . Put  $p = \frac{\alpha}{\lambda}$ ,  $q = \frac{\beta}{\lambda}$ . The Fraunhoffer diffraction formula is given by:

$$\Psi(p,q) = \Psi_0 \int_{\Sigma} A(X,Y) \exp[-2\pi i (pX+qY)] dX dY$$
(D9)

Quantities p and q are known as *spatial frequencies* and (D9) is a 2D Fourier transform.

Example 1. Far field diffraction by a slit



The slit has width *b* in the *Y*-direction and is illuminated by a hpw. The problem is 1D.

$$\Psi(\theta) = \Psi_0 \int_{-b/2}^{b/2} \exp[-2\pi i Y \sin \theta / \lambda] dY = \Psi_0 b \frac{\sin(\pi b \sin \theta / \lambda)}{\pi b \sin \theta / \lambda} = \Psi_0 b \frac{\sin \delta}{\delta}$$
(D10)

The corresponding intensity is:

$$I(\theta) = I_0 \left(\frac{\sin \delta}{\delta}\right)^2$$
(D11)

Example 2. Diffraction grating.

The intensity diffracted by *N* slits is a composition of relations (I10) and (D11):

$$I = I_0 \left( \frac{\sin \frac{kb \sin \theta}{2}}{\frac{kb \sin \theta}{2}} \right)^2 \left( \frac{\sin \frac{Nkd \sin \theta}{2}}{\sin \frac{kd \sin \theta}{2}} \right)^2$$
(D12)

Remember: *b* is the width of each slit, *d* is the distance between two slits. The figure is drawn for N=5.



In 2D (*Wikipedia*):



In 3D: used to investigate crystal structures and molecular structures.

### 6. Fresnel diffraction

If the source and the observation point are close to the obstacle we deal with near field or Fresnel diffraction. The explanation of the diffraction pattern is made using the construction made first by Fresnel. In the following figure *S* is a point-like source, *P* is the observation point and  $r_0$  is the distance between *P* and the wave front reaching the aperture. The Fresnel method is applied if *S* and *P* are close to the axis and if  $\lambda \ll r_0$ , *R*, dimensions of the aperture.



Fresnel's construction



front view

#### Fresnel zones

With the center in the observation point *P* draw the sphere of radius  $r_0$  and then successive spheres with radii  $r_0 + \lambda/2$ ,  $r_0 + 2\lambda/2$ ,  $r_0 + 3\lambda/2$ , ...,  $r_0 + m\lambda/2$ , until all the surface of the aperture is covered. These spheres produce on the wave front surface a family pf spherical zones called *Fresnel zones*.

*Remark*: Spherical zones are actually bordered by planes, not by spheres, but if  $\lambda \ll r_0$ , *R*, dimensions of the aperture the constructed spheres may be approximated with planes.

The reason for this construction is that the path difference between beams originating from adjacent Fresnel zones differs by  $\lambda/2$  and then contributions from adjacent zones have opposed phases. As we shall demonstrate, Fresnel zones have almost equal areas. Therefore their contributions in *P* are almost equal, except for the obliquity factor, diminishing from the center toward the border. But the contribution from the *p*'th zone equals half the sum of contributions from its neighbors:

 $E_p = -\frac{E_{p-1} + E_{p+1}}{2}$ . The minus appears from the  $\lambda/2$  path difference.

*Problem*: Show that areas of different Fresnel zones are almost equal. *Hint*: the area of a spherical zone is given by the following argument (from *Mathematica*): the solution until the end



The <u>surface area</u> of a <u>spherical segment</u>. Call the <u>radius</u> of the <u>sphere</u> R, the upper and lower <u>radii</u> h and a, respectively, and the height of the <u>spherical segment</u> h. The zone is a <u>surface of revolution</u> about the <u>z-axis</u>, so the <u>surface area</u> is given by

$$S = 2\pi \int x \sqrt{1 + {x'}^2} \, dz. \tag{1}$$

In the *xz*-plane, the equation of the zone is simply that of a <u>circle</u>,

$$x = \sqrt{R^2 - z^2} \,, \tag{2}$$

so

$$x' = -z \left(\frac{R^2}{2} - z^2\right)^{-1/2}$$
(3)

$$x'^2 = \frac{z^2}{R^2 - z^2},$$
 (4)

and

$$S = 2\pi \int_{\sqrt{R^2 - a^2}}^{\sqrt{R^2 - b^2}} \sqrt{R^2 - z^2} \sqrt{1 + \frac{z^2}{R^2 - z^2}} dz$$
(5)

$$= 2\pi R \int_{\sqrt{R^2 - a^2}}^{\sqrt{R^2 - b^2}} dz$$
(6)

$$= 2\pi R \left( \sqrt{R^2 - b^2} - \sqrt{R^2 - a^2} \right)$$
(7)

$$= 2\pi R h. \tag{8}$$

This result is somewhat surprising since it depends only on the *height* of the zone, not its vertical position with respect to the sphere.

The result is:  $S = 2\pi Rh$ , where *R* is the radius of the wave-front sphere and *h* is the height of the zone. Let's compute the area of the spherical cap with height h=OAand radius  $\rho_j = AQ$  containing *j* zones (actually *j*-1 zones and the cap) (see e.g. http://mathworld.wolfram.com/SphericalCap.html)



The area is  $S_j = 2\pi Rh$ . From triangles *SAQ* and *PAQ* we find:  $h = \frac{r_j^2 - r_0^2}{2(R + r_0)}$ .

But  $r_j = r_0 + j\frac{\lambda}{2}$ . Hence  $r_j^2 - r_0^2 = jr_0\lambda + j^2\left(\frac{\lambda}{2}\right)^2 \approx jr_0\lambda$ . The height becomes

 $h = j \frac{r_0}{R + r_0} \frac{\lambda}{2}$  and the area  $S_j = j \frac{2\pi R r_0}{R + r_0} \frac{\lambda}{2}$ . The area of the j'th Fresnel zone is

 $\Delta S_j = S_j - S_{j-1} = \frac{\pi R r_0}{R + r_0} \lambda$ . It does not depend on *j*, so it is the same for all Fresnel

zones. the end

The amplitudes of the fields arriving in P are different only concerning  $r_j$  and the obliquity factor; the radius R is the same for all and their areas are equal. As the order j increases, so do the distance  $r_j$  and the angle, so we expect the electric field contribution to decrease steadily. Assume

$$E_j = \frac{E_{j-1} + E_{j+1}}{2} \tag{D13}$$

Compute the total field in *P*:

$$E(P) = \frac{E_1}{2} + \left(\frac{E_1}{2} - E_2 + \frac{E_3}{2}\right) + \left(\frac{E_3}{2} - E_4 + \frac{E_5}{2}\right) + \left(\frac{E_5}{2} - E_6 + \frac{E_7}{2}\right) + \dots (-1)^{m-1} \frac{E_m}{2}$$

Or, because the brackets are almost zero:

$$E(P) = \frac{E_1}{2} + (-1)^{m-1} \frac{E_m}{2}$$
(D14)

Applications: see the lectures.

# X-ray diffraction

See Wikipedia

http://en.wikipedia.org/wiki/File:X-ray\_diffraction\_pattern\_3clpro.jpg



