Chapter 36
Diffraction
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Interference is the more general concept: it refers to the phenomenon of waves interacting. Waves will add constructively or destructively according to their phase difference. **Diffraction** usually refers to the spreading wave pattern from a finite-width aperture.

1. Diffraction by a single slit

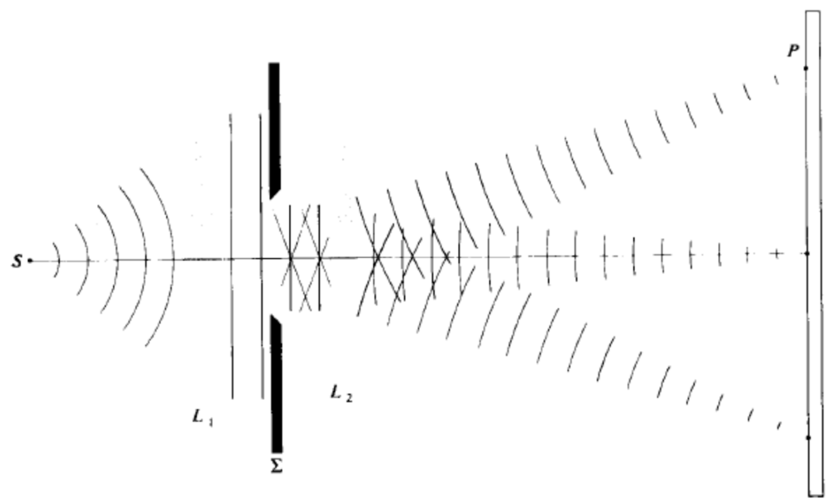
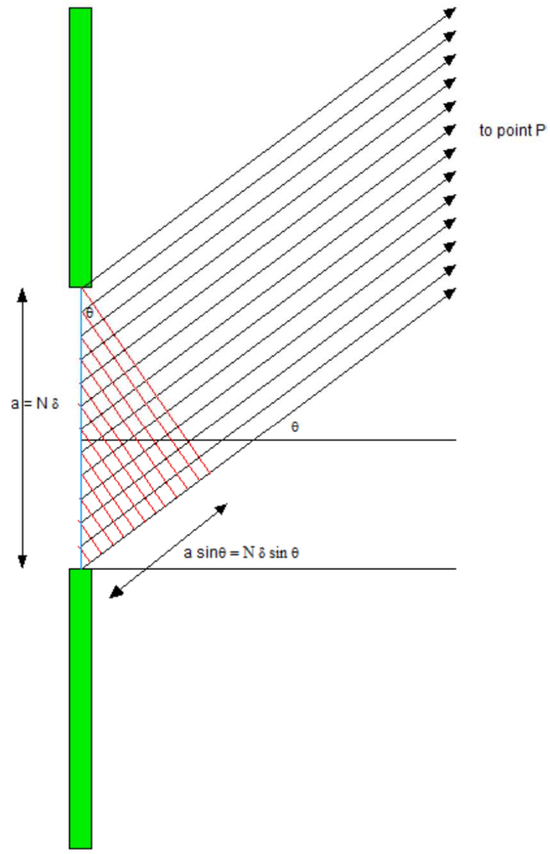


Fig. Single slit diffraction.

Imagine the slit divided into many narrow zones, width Δy (= $\delta = a/N$). Treat each as a secondary source of light contributing electric field amplitude $\Delta \boldsymbol{E}$ to the field at P.



We consider a linear array of N coherent point oscillators, which are each identical, even to their polarization. For the moment, we consider the oscillators to have no intrinsic phase difference. The rays shown are all almost parallel, meeting at some very distant point P. If the spatial extent of the array is comparatively small, the separate wave amplitudes arriving at P will be essentially equal, having traveled nearly equal distances, that is

$$E_0(r_1) = E_0(r_2) = ... = E_0(r_N) = E_0(r) = \frac{E_0}{N}$$

The sum of the interfering spherical wavelets yields an electric field at P, given by the real part of

$$\begin{aligned} E &= \mathrm{Re}[E_0(r)e^{i(kr_1-\omega t)} + E_0(r)e^{i(kr_2-\omega t)} + ... + E_0(r)e^{i(kr_N-\omega t)}] \\ &= \mathrm{Re}[E_0(r)e^{i(kr_1-\omega t)}[1 + e^{ik(r_2-r_1)} + e^{ik(r_3-r_1)} + ... + e^{ik(r_N-r_1))}]] \end{aligned}$$

((**Note**))

When the distances r_1 and r_2 from sources 1 and 2 to the field point P are large compared with the separation δ, then these two rays from the sources to the point P are nearly *parallel*. The path difference $r_2 - r_1$ is essentially equal to $\delta \sin\theta$.

Here we note that the phase difference between adjacent zone is

$$
\begin{aligned}
&k(r_2 - r_1) = \varphi = k\delta \sin\theta = k(\frac{a}{N}\sin\theta) \\
&k(r_3 - r_2) = \varphi \\
&k(r_4 - r_3) = \varphi \\
&------------------------ \\
&k(r_N - r_{N-1}) = \varphi
\end{aligned}
$$

where *k* is the wavenumber, $k = \dfrac{2\pi}{\lambda}$. It follows that

$$
\begin{aligned}
&k(r_2 - r_1) = \varphi \\
&k(r_3 - r_1) = 2\varphi \\
&k(r_4 - r_1) = 3\varphi \\
&------------------------ \\
&(r_N - r_1) = (N-1)\varphi
\end{aligned}
$$

Thus the field at the point P may be written as

$$E = \mathrm{Re}[E_0(r)e^{i(kr_1 - \omega t)}[1 + e^{i\varphi} + e^{i2\varphi} + \ldots + e^{i(N-1)\varphi}]]$$

We now calculate the complex number given by

$$
\begin{aligned}
Z &= 1 + e^{i\varphi} + e^{i2\varphi} + \ldots + e^{i(N-1)\varphi} \\
&= \frac{1 - e^{iN\varphi}}{1 - e^{i\varphi}} \\
&= \frac{e^{iN\varphi/2}(e^{iN\varphi/2} - e^{-iN\varphi/2})}{e^{i\varphi/2}(e^{i\varphi/2} - e^{-i\varphi/2})} \\
&= e^{i(N-1)\varphi/2}\frac{\sin(\frac{N\varphi}{2})}{\sin(\frac{\varphi}{2})}
\end{aligned}
$$

If we define *D* to be the distance from the center of the line of oscillators to the point P, that is

$$
\begin{aligned}
&kD = \frac{1}{2}(N-1)k\delta\sin\theta + kr_1 = \frac{1}{2}(N-1)\varphi + kr_1 \\
&k(D - r_1) = \frac{1}{2}(N-1)\varphi
\end{aligned}
$$

Then we have the form for E as

$$E = \mathrm{Re}[E_0(r)e^{i(kD-\omega t)}\frac{\sin(\frac{N\varphi}{2})}{\sin(\frac{\varphi}{2})}] = \mathrm{Re}[\tilde{E}e^{-i\omega t}]$$

The intensity distribution within the diffraction pattern due to N coherent, identical, distant point sources in a linear array is equal to

$$I = \langle S \rangle = \frac{c\varepsilon_0}{2}\left|\tilde{E}\right|^2$$

$$I = I_0\frac{\sin^2(\frac{N\varphi}{2})}{\sin^2(\frac{\varphi}{2})} = I_0\frac{\sin^2(\frac{\beta}{2})}{\sin^2(\frac{\beta}{2N})} = I_m\frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2}$$

in the limit of $N\to\infty$, where

$$\sin^2(\frac{\beta}{2N}) = \left(\frac{\beta}{2N}\right)^2$$

$$I_0 = \frac{c\varepsilon_0}{2}[E_0(r)]^2$$

$$I_m = I_0N^2 = \frac{c\varepsilon_0}{2}[NE_0(r)]^2 = \frac{c\varepsilon_0}{2}E_0{}^2$$

β is the phase difference

$$\beta = N\varphi = Nk\delta\sin\theta = ka\sin\theta$$

With

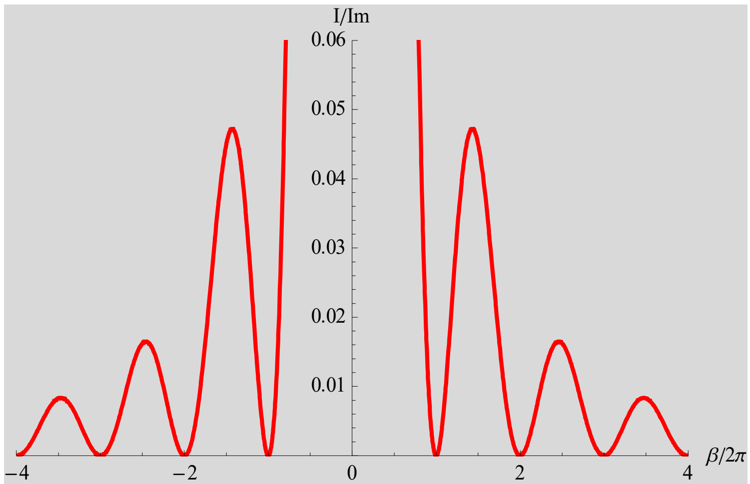
$$\varphi = k\delta\sin\theta$$

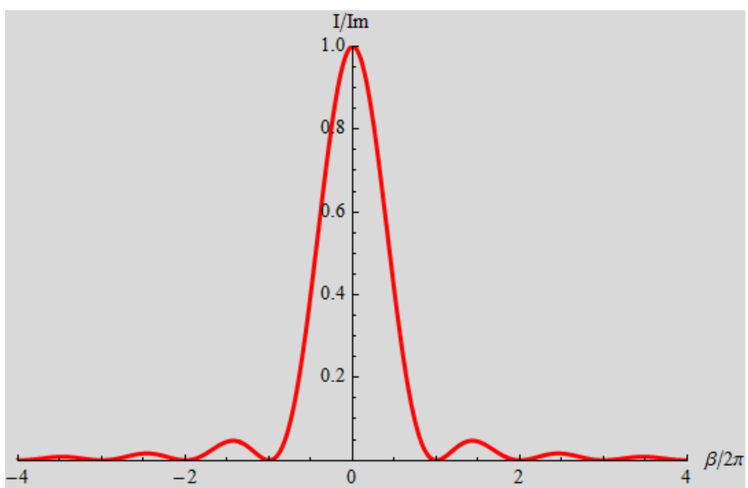
where $a = N\delta$. We make a plot of the relative intensity I/I_m as a function of β.

$$\frac{I}{I_m} = \frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2}$$

Note that

$$\int_{-\infty}^{\infty} \frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2} d\beta = 2\pi$$





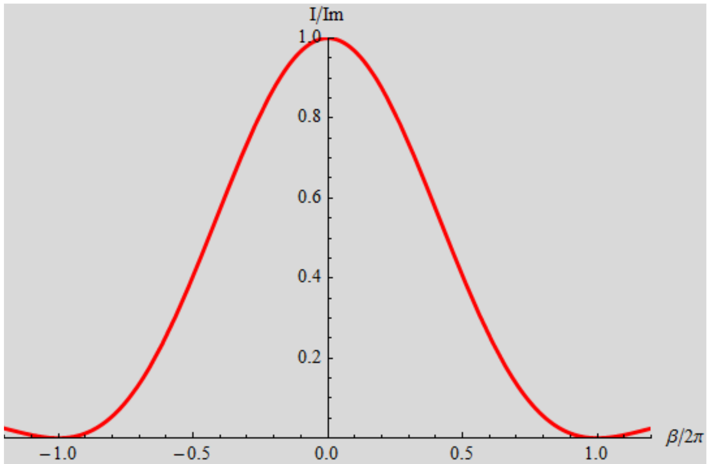
The numerator undergoes rapid fluctuations, while the denominator varies relatively slowly. The combined expression gives rise to a series of sharp principal peaks separated by small subsidiary maxima. The principal minimum occurs in directions in direction θ_{m} such that

$$\frac{\beta}{2} = \frac{ka}{2}\sin\theta = m\pi\ , \qquad a\sin\theta_m = \frac{1}{k}2m\pi = \frac{\lambda}{2\pi}2m\pi = m\lambda$$

or

$$\theta_m = m\frac{\lambda}{a}$$

2. Shape of the intensity



Here we examine the function form of the relative intensity

$$\frac{I}{I_0} = \frac{\sin^2(\frac{\beta}{2})}{(\frac{\beta}{2})^2},$$

where

$$\beta = \frac{2\pi}{\lambda}a\sin\theta \approx \frac{2\pi}{\lambda}a\theta .$$

in the small limit of θ. The function I/I_0 is equal to $4/\pi^2 = 0.405$ for $\beta = \pi$, and is ½ for $\beta = 2.78311 = 0.8859\ \pi$. The main feature of the intensity I/I_0 is that the intensity is large only in

$$-\pi < \beta < \pi , \qquad \text{or} \qquad -\frac{1}{2}\frac{\lambda}{a} < \sin\theta < \frac{1}{2}\frac{\lambda}{a}$$

or

$$\Delta(\sin\theta) = \frac{\lambda}{a}$$

$$\Delta\theta \approx \frac{\lambda}{a}$$

(diffraction limit)

For the diffraction pattern of a *circular aperture* of the diameter d, we have the condition of

$$\Delta\theta \approx 1.22\frac{\lambda}{d}$$

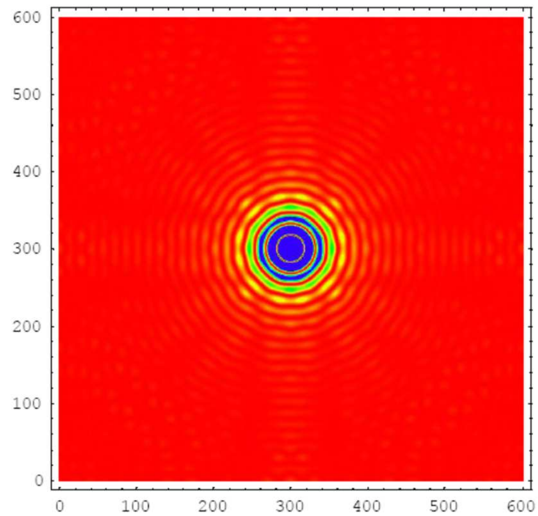


Fig. Fraunhofer diffraction pattern for a circular aperture (Mathematica). We use the FFT program of the Mathematica

3. Phasor diagram

In order to discuss the intensity I, we need to calculate the sum defined by

$$Z = E_0(r)[1 + e^{i\varphi} + e^{i2\varphi} + ... + e^{i(N-1)\varphi}]$$
$$= \frac{E_0}{N}[1 + e^{i\varphi} + e^{i2\varphi} + ... + e^{i(N-1)\varphi}]$$

in the complex plane, where $\varphi = \frac{\beta}{N} = k\delta\sin\theta$. For simplicity, here we solve this problem geometrically using the phasor diagram (in the real x-y plane). There are N isosceles triangular lattices (see the Figs. below). The first one is of length E_0/N and it has a phase equal to zero. The next one is of length E_0/N and it has a phase equal to φ. The next one is of length E_0/N and it has a phase equal to 2φ, and soon. So we get an equiangular polygon with N sides.

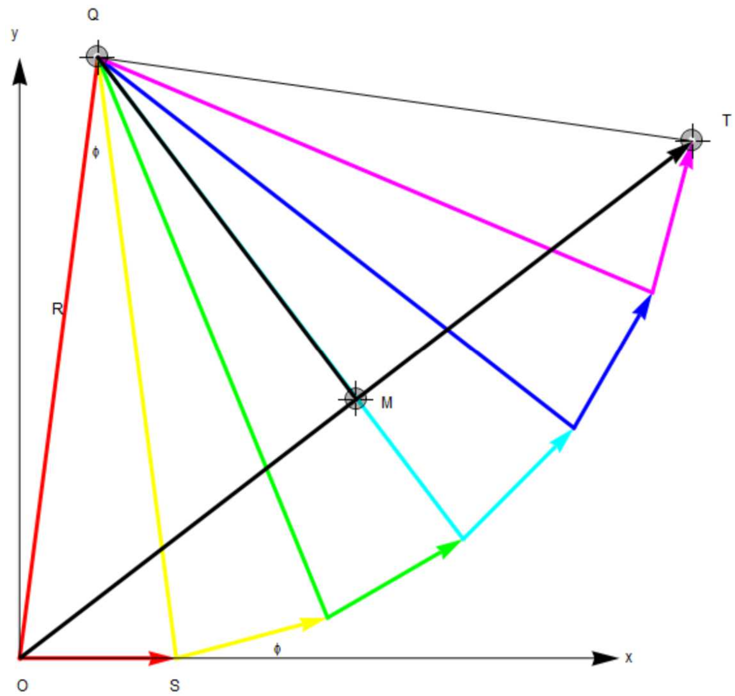


Fig. The resultant amplitude of $N = 6$ equally spaced sources with net successive phase difference φ. $\beta = N\,\varphi = 6\,\varphi$.

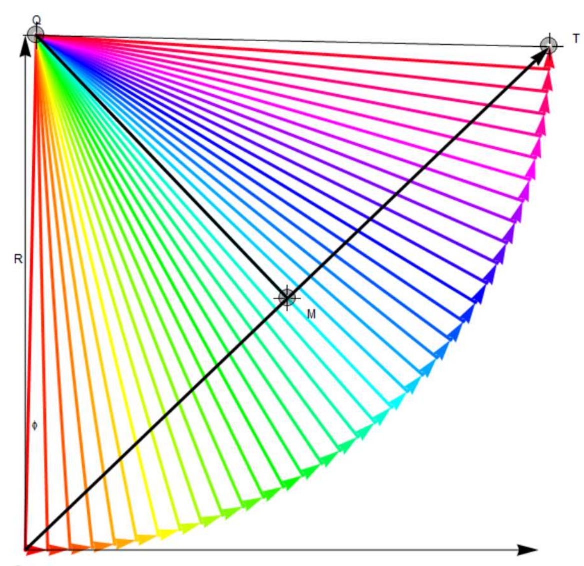
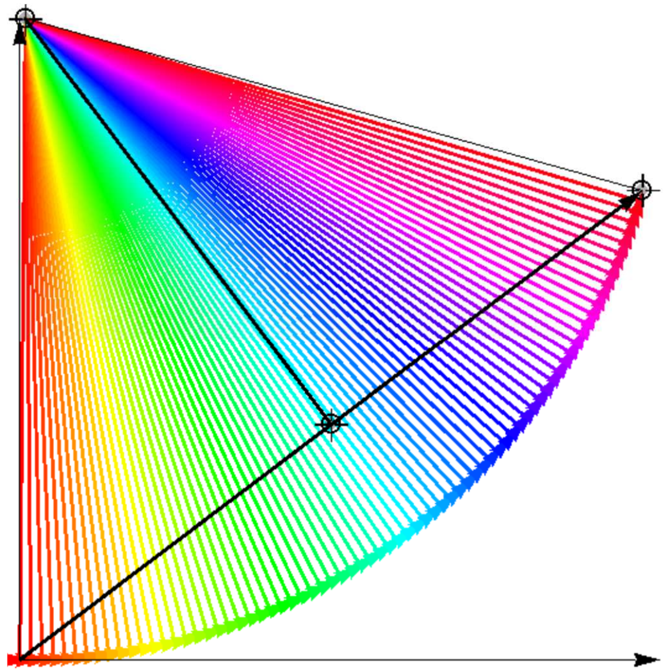


Fig. The resultant amplitude of $N = 36$ equally spaced sources with net successive phase difference φ.

We now consider the system with a very large N. We may imagine dividing the slit into N narrow strips. In the limit of large N, there is an infinite number of infinitesimally narrow strips. Then the curve trail of phasors become an arc of a circle, with arc length equal to the length E_0. The center C of this arc is found by constructing perpendiculars at O and T.



The radius of arc is given by

$$E_0 = R\beta = R(N\varphi), \quad \text{or} \qquad R\varphi = \frac{E_0}{N}$$

in the limit of large N, where R is the side of the isosceles triangular lattice with the vertex angle φ, and the phase difference β is given by

$$\beta = N\varphi = ka\sin\theta$$

with the value β being kept constant. Note that φ is the change of phase for two rays separated by $\delta = \dfrac{a}{N}$,

$$\varphi = k\delta\sin\theta, \qquad \text{or} \qquad \varphi = \frac{ka}{N}\sin\theta$$

Then the amplitude E_p of the resultant electric field at P is equal to the chord $\overline{OT}$, which is equal to

$$E_P = 2R\sin\frac{\beta}{2} = 2\frac{E_0}{\beta}\sin\frac{\beta}{2} = E_0\frac{\sin\frac{\beta}{2}}{\frac{\beta}{2}}.$$

Then the intensity I for the single slits with finite width a is given by

$$I = I_m\left(\frac{\sin\frac{\beta}{2}}{\frac{\beta}{2}}\right)^2.$$

where I_m is the intensity in the straight-ahead direction where $\beta = 0$.

The phase difference β is given by $\beta = ka\sin\theta = 2\pi\frac{a}{\lambda}\sin\theta = 2\pi p\sin\theta$. We make a plot of I/I_m as a function of θ, where $p = a/\lambda$ is changed as a parameter.

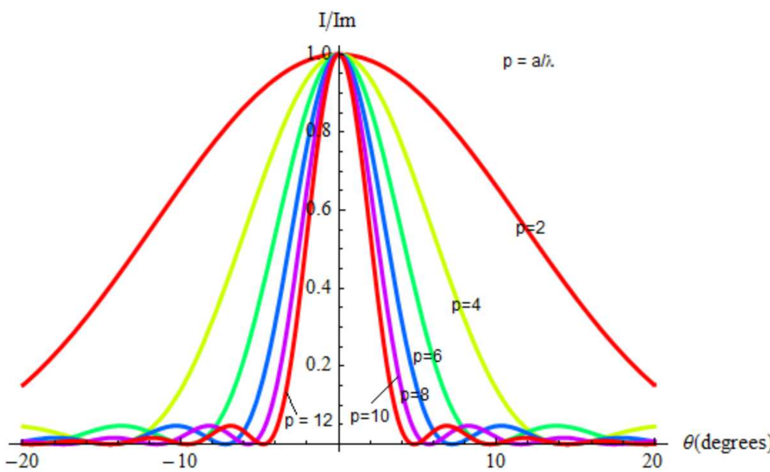


Fig. The relative intensity in single-slit diffraction for various values of the ratio $p = a/\lambda$. The wider the slit is the narrower is the central diffraction maximum.

4. Diffraction patterns

4.1 Young's double slit experiment (two slits with finite width)

We consider the Young's double slits (the slits are separated by d). Each slit has a finite width a.

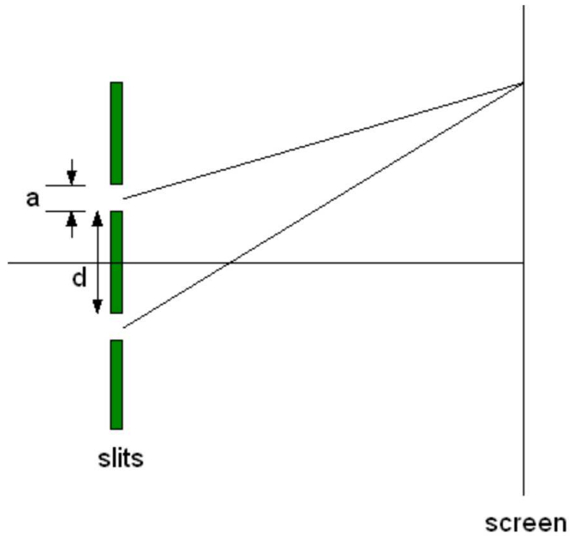


Fig. Geometric construction for describing the Young's double-slit experiment (not to scale).

The intensity is given by

$$I = I_0 \cos^2\left(\frac{\phi}{2}\right)\left(\frac{\sin\frac{\beta}{2}}{\frac{\beta}{2}}\right)^2,$$

where

$$\phi = kd\sin\theta = \frac{2\pi d}{\lambda}\sin\theta, \qquad \beta = ka\sin\theta = \frac{2\pi a}{\lambda}\sin\theta.$$

We note that the peak due to the double slit diffraction occurs at

$$\cos^2\left(\frac{\phi}{2}\right) = 1, \qquad \phi = 2m\pi \qquad \theta = \frac{\lambda}{d}m$$

The intensity becomes zero when

$$\sin^2\left(\frac{\beta}{2}\right) = 0, \qquad \beta = 2n\pi \qquad \theta = \frac{\lambda}{a}n$$

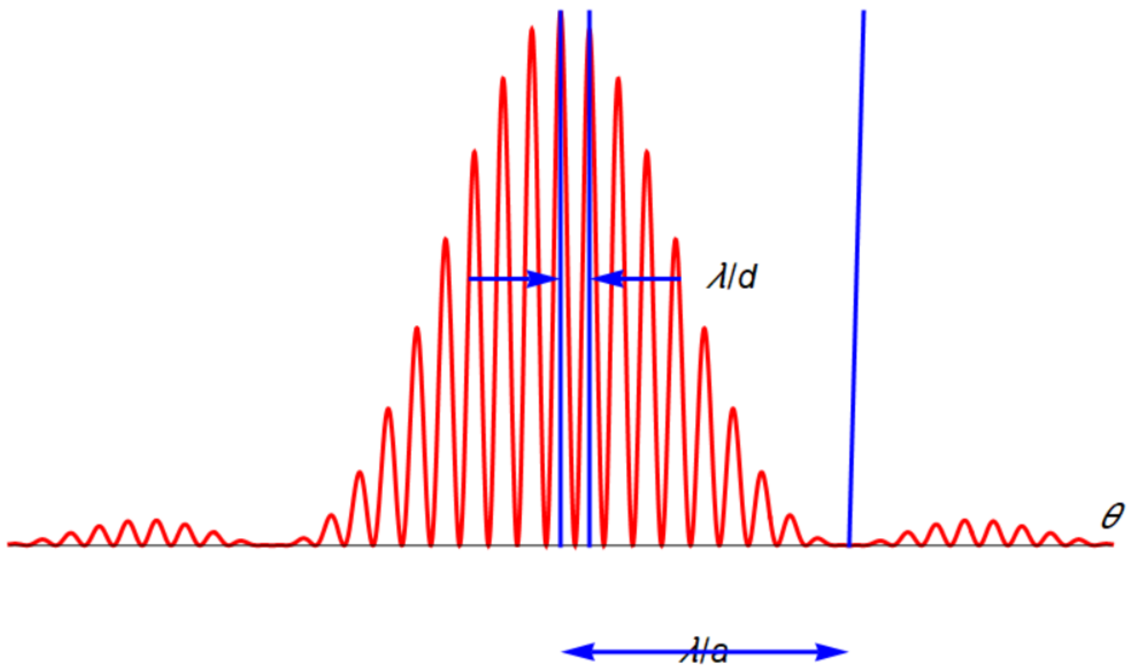
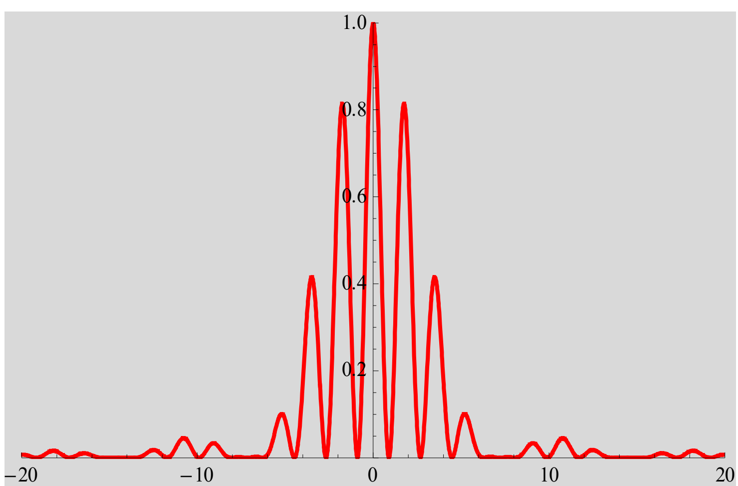


Fig. Diffraction pattern with the double slit with the distance d and the single slit with the distance a. $d >> a$.



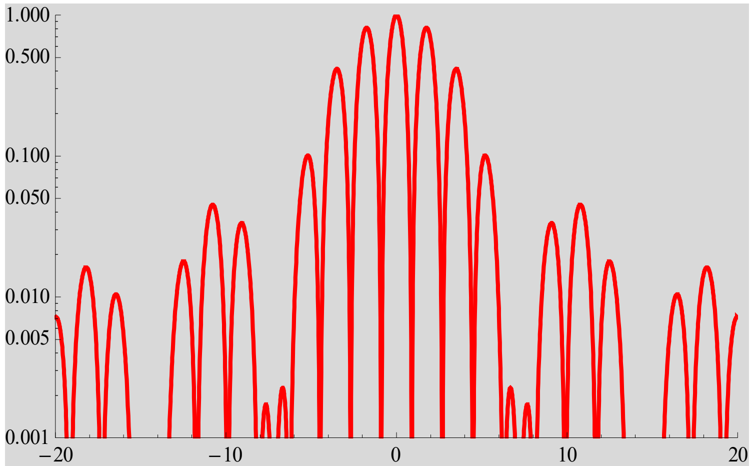


Fig. Intensity ratio I/I_0 vs angle θ (degrees) when $p = d/\lambda = 48$ and $q = a/\lambda = 4$.

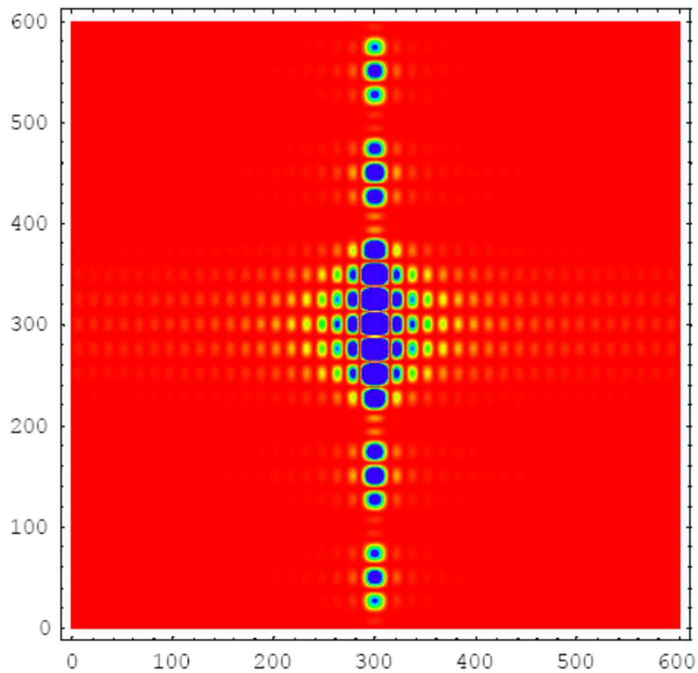


Fig. Fraunhofer diffraction pattern for the Young's double slits. See my article on the Fraunhofer diffraction in

http://physics.binghamton.edu/Sei_Suzuki/suzuki.html

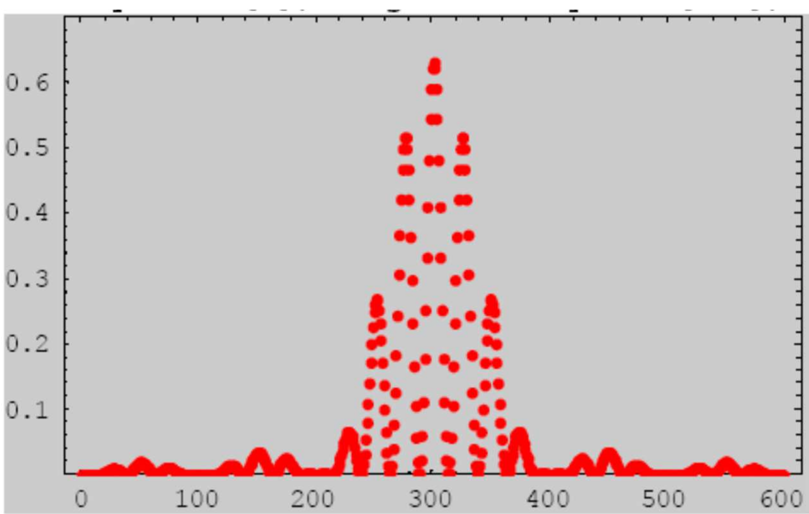


Fig. The intensity I as a function of y (x = 300) in the above Fraunhofer diffraction pattern.

4.2 DC SQUID

Analogy of the diffraction with double slits and single slit

See my article on the Josephson junction and DC SQUID for the detail;

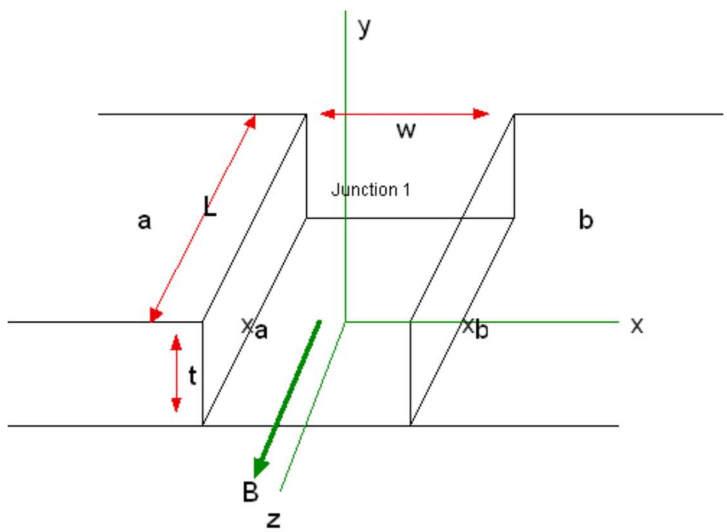


Fig. Diffraction effect of Josephson junction. A magnetic field $\boldsymbol{B}$ along the z direction, which is penetrated into the junction (in the normal phase).

We consider a junction (1) of rectangular cross section with magnetic field $\boldsymbol{B}$ applied in the plane of the junction, normal to an edge of width w.

$$J = J_0 \sin[\delta_1 + \frac{q}{\hbar c}\int_1^2 \boldsymbol{A}\cdot d\boldsymbol{l}],$$

with q = -2e. We use the vector potential $\boldsymbol{A}$ given by

$$\boldsymbol{A} = \frac{1}{2}(\boldsymbol{B}\times\boldsymbol{r}) = (-\frac{By}{2}, \frac{Bx}{2}, 0),$$

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi = (-By, 0, 0),$$

where

$$\chi = -\frac{Bxy}{2}.$$

Then we have

$$J = J_0 \sin[\delta_1 + \frac{q}{\hbar c}\int_{x_a}^{x_b}(-By)dx] = J_0 \sin[\delta_1 - \frac{qB}{\hbar c} yW],$$

$$dI_1 = JLdy = J_0 L \sin[\delta_1 - \frac{qB}{\hbar c} yW]dy,$$

Or

$$I_1 = J_0 L \int_{-t/2}^{t/2} \sin[\delta_1 - \frac{qB}{\hbar c} yW]dy.$$

Then we have

$$I_1 = J_0 L \frac{2\hbar c}{BWq}\sin(\delta_1)\sin(\frac{qB}{\hbar c}\frac{t}{2}W).$$

Here we introduce the total magnetic flux passing through the area Wt ($\Phi_W = BWt$), $I_c = J_0 Lt$, and

$$\frac{\Phi_W}{\Phi_0} = \frac{BWt}{\frac{2\pi\hbar c}{2e}} = \frac{eBWt}{\pi\hbar c}, \qquad \text{or} \qquad \pi\frac{\Phi_W}{\Phi_0} = \frac{eBWt}{\hbar c}.$$

Therefore, we have

$$I_1 = I_c \sin(\delta_1) \frac{\sin(\frac{\pi\Phi_W}{\Phi_0})}{\left(\frac{\pi\Phi_W}{\Phi_0}\right)}.$$

The total current is given by

$$I = I_1 + I_1 = I_c[\sin(\delta_1) + \sin(\delta_1)] \frac{\sin(\frac{\pi\Phi_W}{\Phi_0})}{\left(\frac{\pi\Phi_W}{\Phi_0}\right)},$$

Or

$$I = I_1 + I_1 = 2I_c \sin(\delta_0)\cos(\pi\frac{\Phi}{\Phi_0}) \frac{\sin(\frac{\pi\Phi_W}{\Phi_0})}{\left(\frac{\pi\Phi_W}{\Phi_0}\right)}.$$

The short period variation is produced by interference from the two Josephson junctions, while the long period variation is a diffraction effect and arises from the finite dimensions of each junction. The interference pattern of $|I|^2$ is very similar to the intensity of the Young's double slits experiment. If the slits have finite width, the intensity must be multiplied by the diffraction pattern of a single slit, and for large angles the oscillations die out.

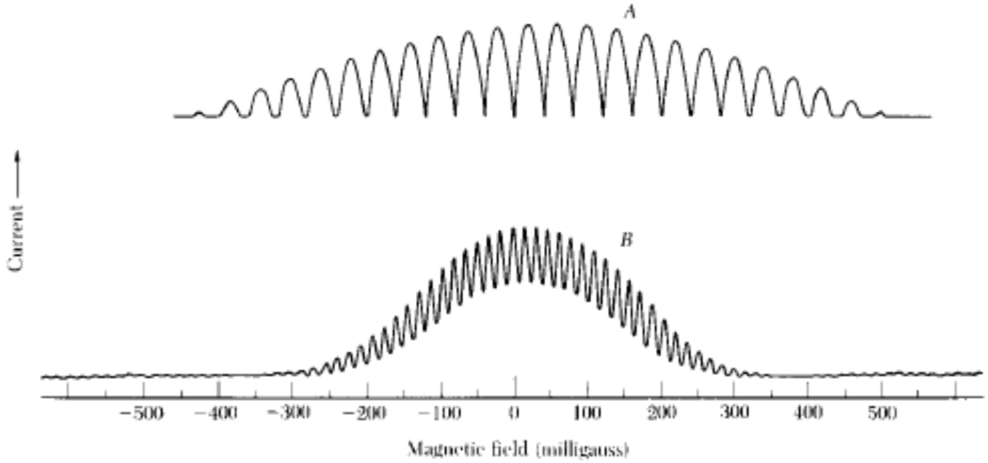
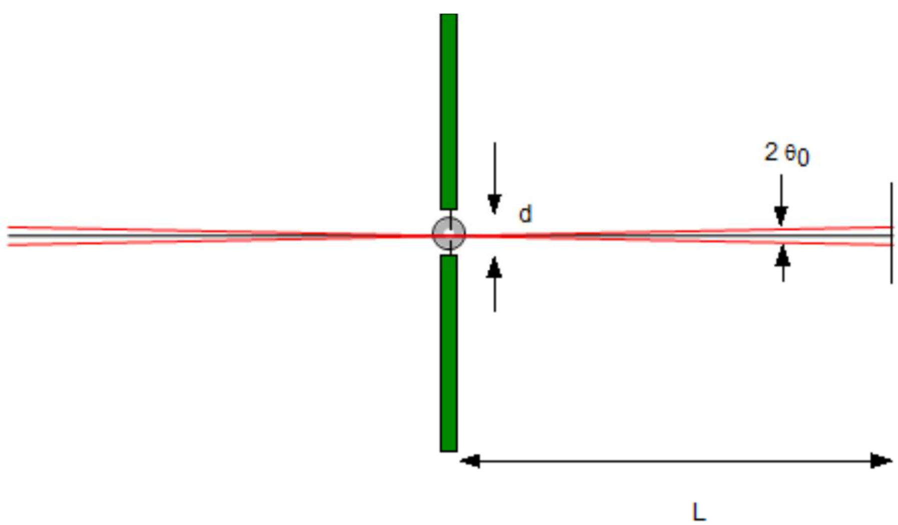


Figure 26 Experimental trace of J_{max} versus magnetic field showing interference and diffraction effects for two junctions A and B. The field periodicity is 39.5 and 16 mG for A and B, respectively. Approximate maximum currents are 1 mA (A) and 0.5 mA (B). The junction separation is 3 mm and junction width 0.5 mm for both cases. The zero offset of A is due to a background magnetic field. (After R. C. Jaklevic, J. Lambe, J. E. Mercereau and A. H. Silver.)

5. Diffraction by a circular aperture

5.1 Rayleigh's criterion



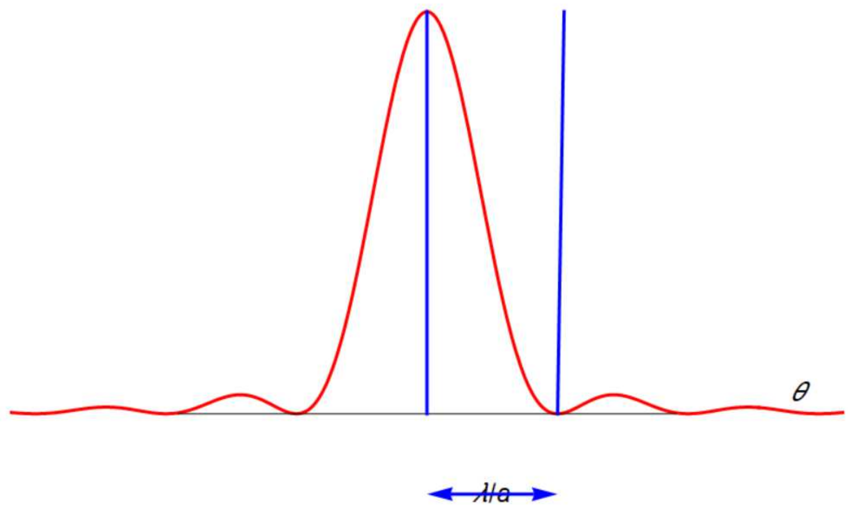
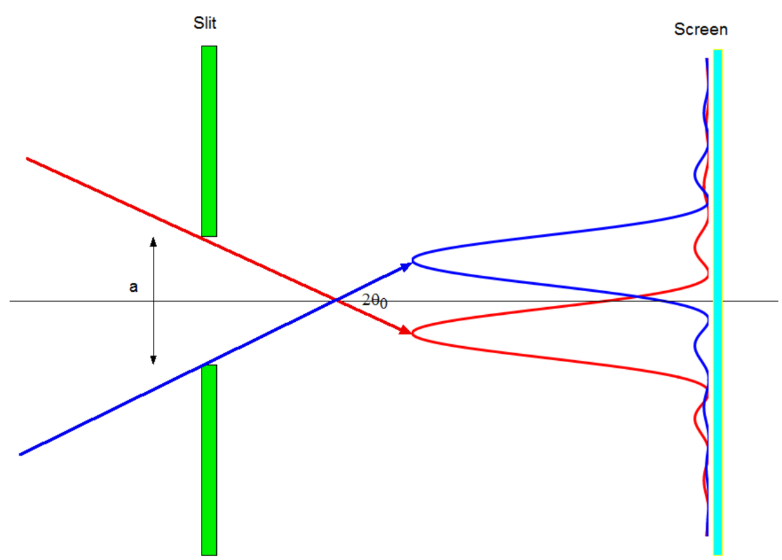


Fig. Diffraction patter of single-slit with a size a. The intensity becomes zero for $\Delta\theta = \dfrac{\lambda}{a}$.



We consider the angular separation of the two point-sources (centered at $\theta = \theta_0$ and $\theta = -\theta_0$) for the single slit with the width a. Noting that

$$\beta_+ = N\varphi_+ = \frac{2\pi a}{\lambda}\sin(\theta - \theta_0)\,, \qquad x_+ = \frac{\beta_+}{2\pi} = \frac{a}{\lambda}\sin(\theta - \theta_0)$$

$$\beta_- = N\varphi_- = \frac{2\pi a}{\lambda}\sin(\theta + \theta_0)\,, \qquad x_- = \frac{\beta_-}{2\pi} = \frac{a}{\lambda}\sin(\theta + \theta_0)$$

the intensity is given by

$$I \propto I(\beta_+) + I(\beta_-)$$

as a result of the superposition. The intensity $I(\beta_+)$ has a peak at $\theta = \theta_0$, while the intensity $I(\beta_-)$ has a peak at $\theta = -\theta_0$. We make a plot of the intensity as a function of

$$\beta = N\varphi = \frac{2\pi a}{\lambda}\sin\theta, \qquad \text{or} \qquad x = \frac{\beta}{2\pi} = \frac{a}{\lambda}\sin\theta \simeq \frac{a}{\lambda}\theta$$

where

$$x_0 = \frac{a}{\lambda}\sin\theta_0$$

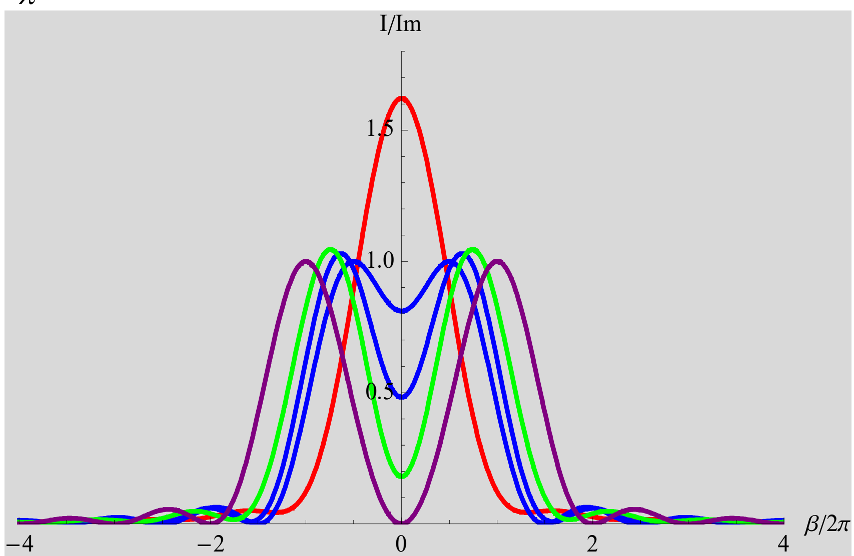


Fig. Superposition of the intensity $I/I_{\max}$ centered with $\theta = \theta_0$ and the intensity $I/I_{\max}$ centered with $\theta = -\theta_0$, as a function of $x = \beta/(2\pi)$, where $x_0 = \frac{a}{\lambda}\sin\theta_0$ is changed as a parameter. x_0 = 0.25 (red), 0.5 (blue), 0.60 (blue), 0.75 (green), and 1.00 (purple).

The Rayleigh's criterion is satisfied for $x_0 = 0.5$.

$$2x_0 = 1 = 2\frac{a}{\lambda}\theta_0 = \frac{a}{\lambda}(2\theta_0) = \frac{a}{\lambda}\theta_R \approx \frac{a}{\lambda}\sin\theta_R$$

or

$$\sin\theta_R = \frac{\lambda}{a}$$

where

$$\theta_R = 2\theta_0$$

For the circular aperture, we have

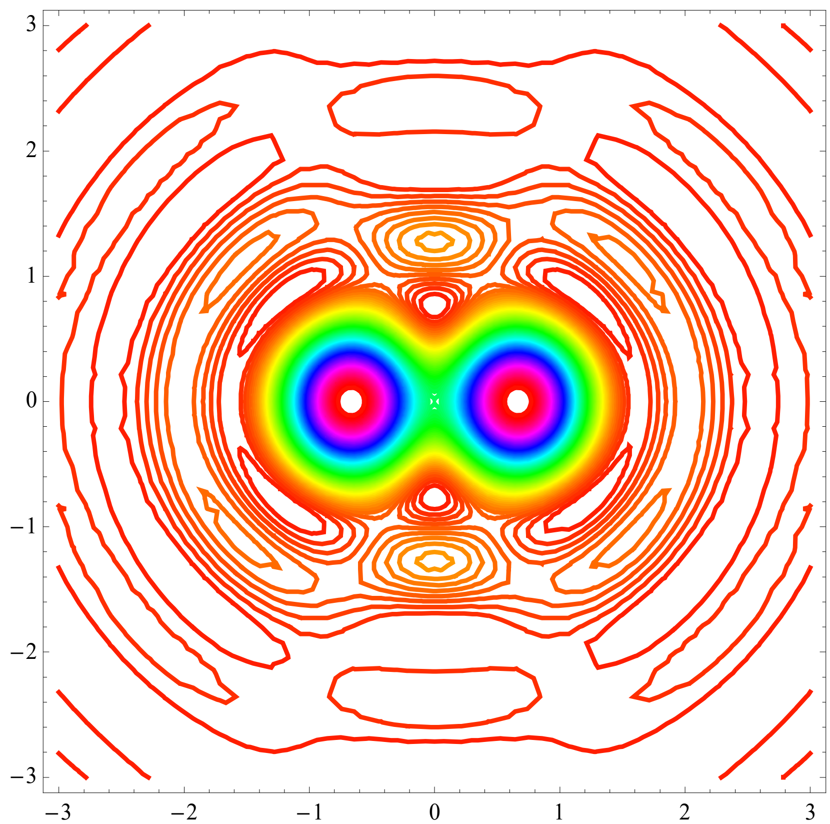
$$\sin\theta_R = 1.220\frac{\lambda}{d}$$

where d is the diameter of circular aperture.

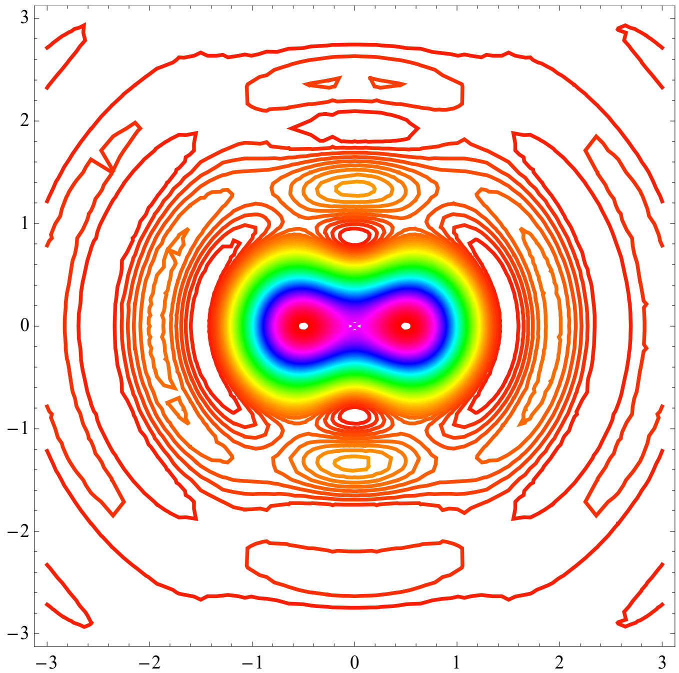
((**Mathematica**))

ContourPlot of the double peaks in the x-y plane.

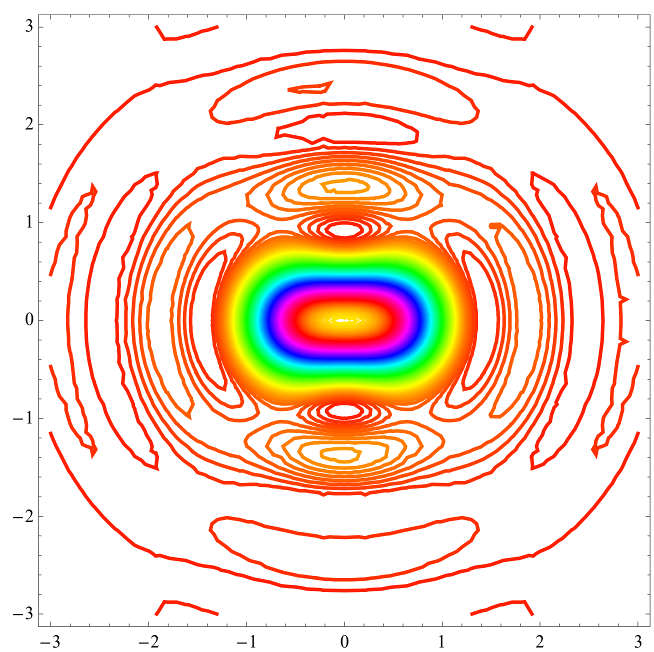
(a) $x_0 = 0.65$



(b) $x_0 = 0.50$



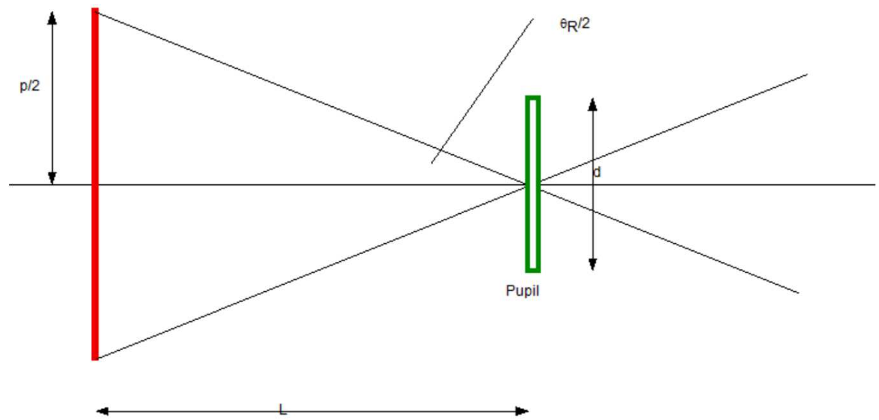
(c) $x_0 = 0.40$



5.2 Example
Problem 36-84

If you look at something 40 m from you, what is the smallest length (perpendicular to your line of sight) that you can resolve, according to Rayleigh's criterion? Assume the pupil of your eye has a diameter of 4.00 mm, and use 500 nm as the wavelength of the light reaching you.

((**Solution**))
d = 4.0 mm for the diameter of pupil
λ = 500 nm. L = 40 m.



We use the Rayleigh criterion,

$$\sin\theta_R = 1.22\frac{\lambda}{d} = 1.22\frac{500nm}{4.0mm} = 1.525\times10^{-4} \approx \theta_R$$

From the above figure, we have

$$\tan\frac{\theta_R}{2} = \frac{p/2}{L}$$
$$p = 2L\tan\frac{\theta_R}{2} \approx L\theta_R = 40m\times1.525\times10^{-4} = 6.1mm$$

5.3 Rayleigh criterion of iris diameter

We calculate the Rayleigh criterion of the iris diameter of human eyes a,

$$\theta_R = 1.22\frac{\lambda}{a}$$

Suppose that a = 5 mm = 5x10^{-3} m and the wavelength λ = 500 nm. Then we have

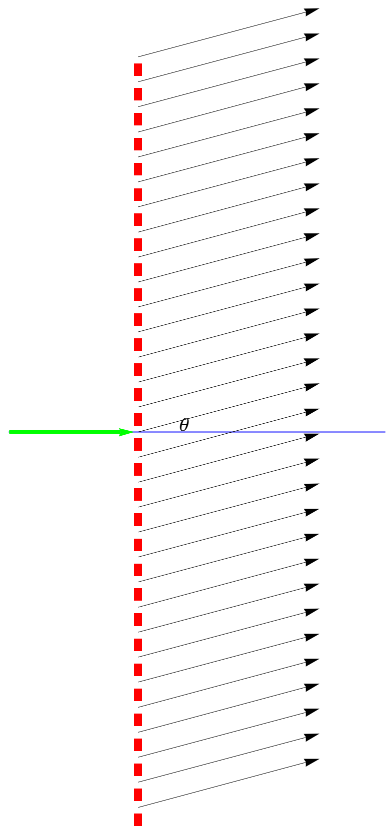
θ_R=1.22 x 10^{-4} rad.

Since 1 arcsec = $\frac{1}{3600}\times\frac{\pi}{180}$=4.84814 x 10^{-6} rad, we get

θ_R=25.16 arcsec.

6. Diffraction gratings

6.1 The definition

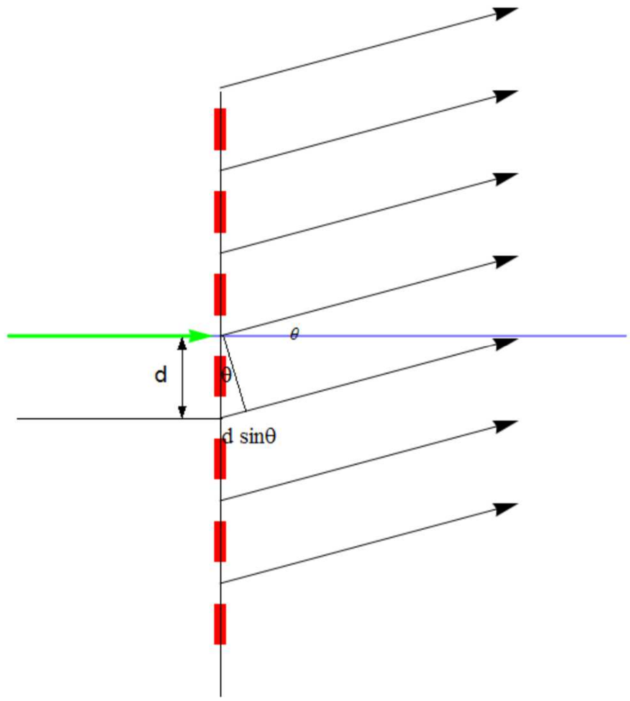


The diffracting grating consists of a large number of equally spaced parallel slits. A typical grating contains several thousand lines per centimeter. The intensity of the pattern on the screen is the result of the combined effects of interference and diffraction. Each slit produces diffraction, and the diffracted beams interfere with one another to form the final pattern.

6.2 Diffraction Grating, Types

A transmission grating can be made by cutting parallel grooves on a glass plate. The spaces between the grooves are transparent to the light and so act as separate slits. A reflection grating can be made by cutting parallel grooves on the surface of a reflective material.

6.3 Diffraction Grating



The condition for maxima is

$$d \sin \theta = m \lambda \text{ (bright)}$$

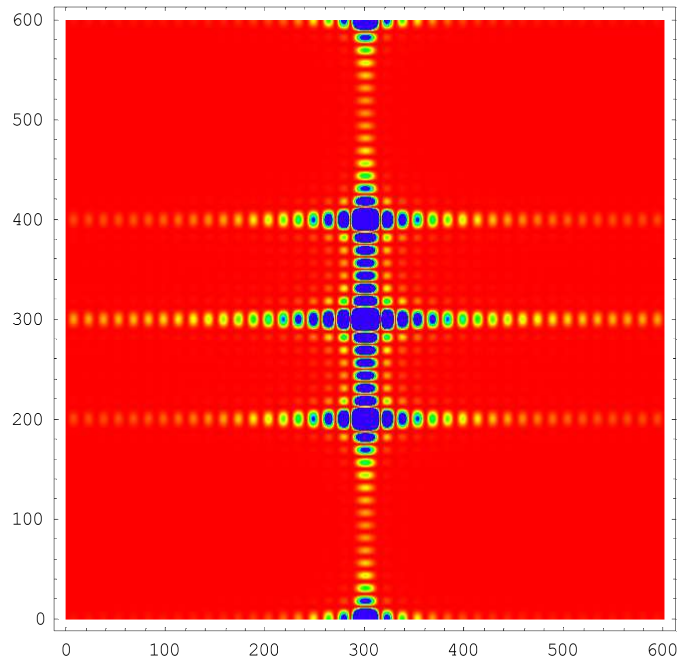
where $m = 0, 1, 2, \ldots$ The integer m is the order number of the diffraction pattern. If the incident radiation contains several wavelengths, each wavelength deviates through a specific angle.

6.4 Diffraction Grating, Intensity

All the wavelengths are seen at $m = 0$. This is called the zero-th order maximum. The first order maximum corresponds to $m = 1$. Note the sharpness of the principle maxima and the broad range of the dark areas

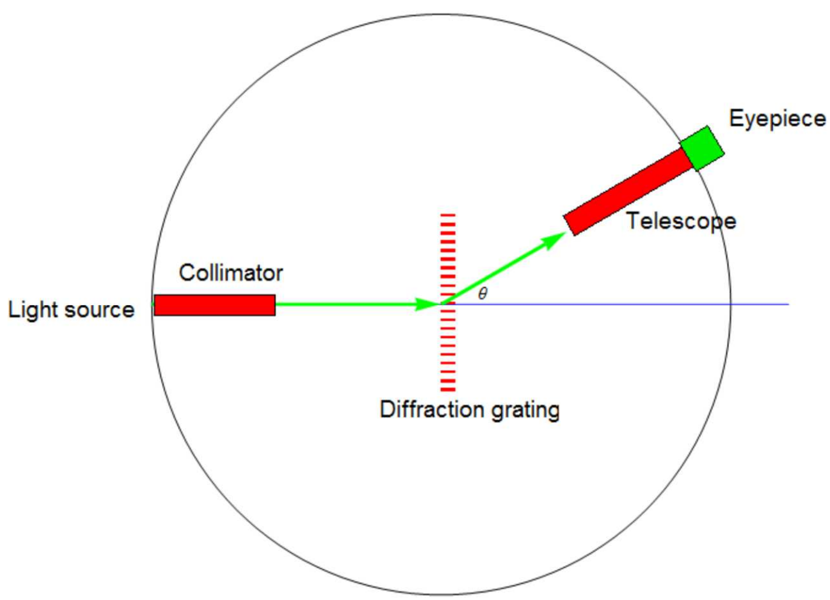
6.5 Characteristics of the intensity pattern

The sharp peaks are in contrast to the broad, bright fringes characteristic of the two-slit interference pattern. Because the principle maxima are so sharp, they are much brighter than two-slit interference patterns.



Fraunhofer diffraction pattern of diffraction grating (10 slits) (Mathematica)

6.6 Diffraction Grating Spectrometer



The diffraction grating spectroscopy consists of a slit, a collimator, a rotatable table, and a rotatable telescope. A transmission grating, consisting of a mask with a large number of evenly spaced slits, is positioned on the table with the slits vertical. Parallel light from the collimator is diffracted by the slits and the diffracted beams are combined to form an image of the collimator slit at the telescope focus. In the Sophomore laboratory we use the Hg (mercury) light source having the wavelengths listed below

Hg lamp

Color	Wavelength (nm)
Yellow	576.959
Yellow	579.065
Green	546.074 (intense)
Blue	435.835
Violet	404.656 (intense)

When the slit width of the diffraction grating is *d*, each spectrum of the mercury light is measured at the condition given by

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

The slit width *d* is typically denoted as the number of lines per inch (LPI); for eaxmaple, 15000 LPI. The slit width *d* is shorter than the wavelength λ.

1 inch = 25.40 mm = 25.40 x 10^6 nm

$$d = \frac{25.40\times 10^6\, nm}{1.50\times 10^4} = 1693 nm$$

6.7 Intensity with *N* slits

We now consider the intensity for the system with *N* slits. The electric field for each slit is given by

$$E_0 = \frac{E_0}{N}\sin(kr - \omega t)$$

$$E_1 = \frac{E_0}{N}\sin(kr - \omega t + \phi)$$

....

$$E_{N-1} = \frac{E_0}{N}\sin[kr - \omega t + (N-1)\phi]$$

where $\phi = kd\sin\theta$. In order to obtain the resultant electric field, we use the phasor diagram.

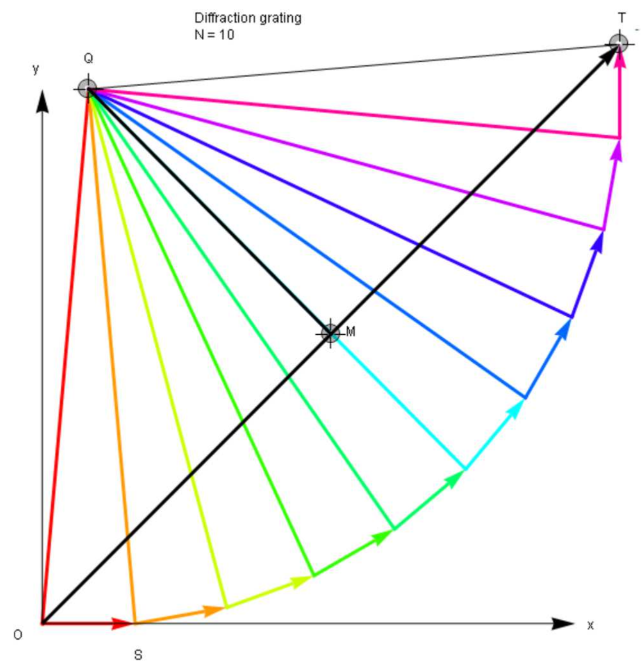


Fig. The phasor diagram of the diffraction grating ($N = 10$).

$$\angle OQS = \phi$$

$$\overline{OQ} = R$$

$$\overline{OS} = 2R\sin\left(\frac{\phi}{2}\right) = \frac{E_0}{N}$$

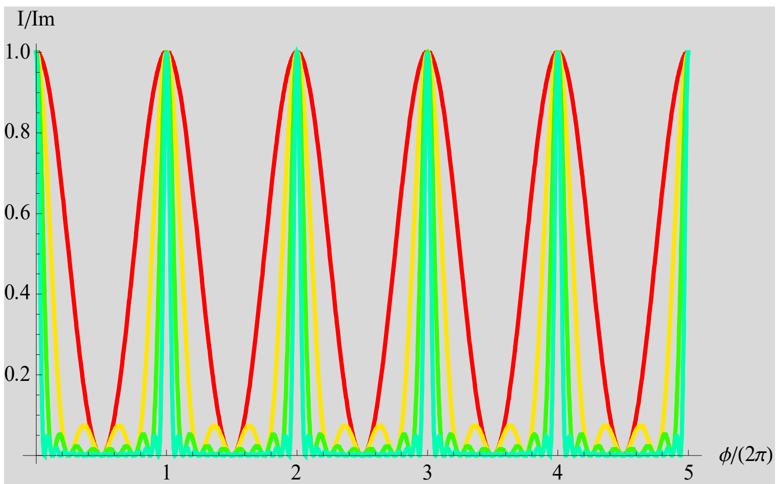
$$\overline{OT} = 2\overline{OM} = 2R\sin\left(\frac{N\phi}{2}\right) = \frac{E_0}{N}\frac{\sin\left(\frac{N\phi}{2}\right)}{\sin\left(\frac{\phi}{2}\right)}$$

where

$$\phi = \frac{2\pi}{\lambda} d\sin\theta$$

Then the intensity I is obtained as

$$I = \frac{I_0}{N^2}\frac{\sin^2\left(\frac{N\phi}{2}\right)}{\sin^2\left(\frac{\phi}{2}\right)} = I_0 \frac{\dfrac{\sin^2\left(\frac{N\phi}{2}\right)}{\left(\frac{N\phi}{2}\right)^2}}{\dfrac{\sin^2\left(\frac{\phi}{2}\right)}{\left(\frac{\phi}{2}\right)^2}}$$



The diffraction pattern ($N = 2$, 4, 8, and 16)

((**Another method for the derivation of the intensity**))

In the phasor diagram, the x and y components of the resultant electric field is given by

$$E_x = \frac{E_0}{N}\sum_{k=0}^{N-1}\cos(k\varphi)$$

$$E_y = \frac{E_0}{N}\sum_{k=0}^{N-1}\sin(k\varphi)$$

$$\boldsymbol{E}^2 = E_x^{\ 2} + E_y^{\ 2} = \frac{E_0^{\ 2}\sin^2(\frac{N\varphi}{2})}{N^2\sin^2(\frac{\varphi}{2})}$$

$$I_N = I_0\frac{\sin^2(\frac{N\varphi}{2})}{N^2\sin^2(\frac{\varphi}{2})}$$

For $N = 3$,

$$I_3 = \frac{1}{9}[1 + 2\cos\phi)^2$$

For $N = 4$

$$I_3 = \frac{1}{4}[\cos(\frac{\phi}{2}) + \cos(\frac{3\phi}{2})]^2$$

6.8 Resolution

$$I = \frac{I_0}{N^2}\frac{\sin^2\left(\frac{N\phi}{2}\right)}{\sin^2\left(\frac{\phi}{2}\right)}$$

where $\phi = \frac{2\pi}{\lambda}d\sin\theta$. What is of particular interest is that the pattern contains principal maximum when the denominator becomes zero, namely when

$$\sin\left(\frac{\phi}{2}\right) = 0$$

or

$$\phi = 2n\pi$$

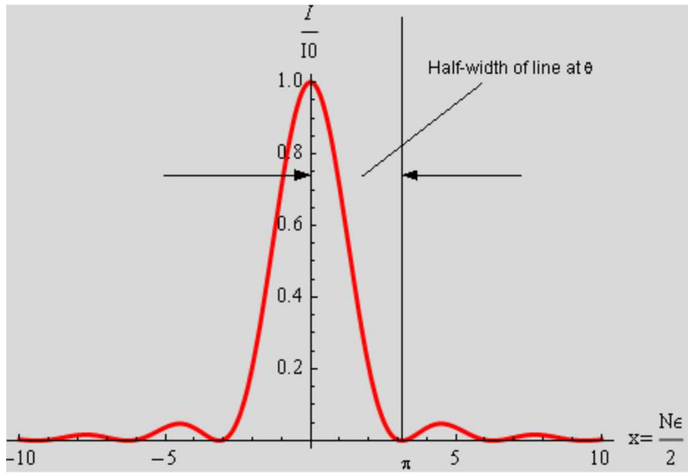
where n = 0, 1, 2, 3, 4, ….The intensity at the principal maximum can be found as follows. For $\phi = 2n\pi + \varepsilon$,

$$I = \frac{I_0}{N^2}\frac{\sin^2\left(\frac{N(2n\pi + \varepsilon)}{2}\right)}{\sin^2\left(\frac{2n\pi + \varepsilon}{2}\right)} = \frac{I_0}{N^2}\frac{\sin^2\left(\frac{N\varepsilon}{2}\right)}{\sin^2\left(\frac{\varepsilon}{2}\right)} \approx \frac{I_0}{N^2}\frac{\sin^2\left(\frac{N\varepsilon}{2}\right)}{\frac{\varepsilon^2}{4}} = I_0\frac{\sin^2\left(\frac{N\varepsilon}{2}\right)}{\left(\frac{N\varepsilon}{2}\right)^2}$$

When $x = \frac{N\varepsilon}{2}$, I is rewritten as

$$\frac{I}{I_0} = \frac{\sin^2 x}{x^2}$$

In the limit of $x \to 0$, I/I_0 tends to unity.



The width of the principal maximum is given by the first minimum of the function sin$x$/x, which occurs when $x = \pm\pi$. From the definition, we have

$$\Delta x = \Delta(\frac{N\varepsilon}{2}) = \pi$$

$$\Delta\phi = \Delta\varepsilon = \frac{2\pi}{N}$$

since $\phi = 2n\pi + \varepsilon$. The phase difference $\Delta\phi$ can be also written as

$$\Delta\phi = \frac{2\pi}{\lambda} d\Delta(\sin\theta) = \frac{2\pi}{\lambda} d\cos\theta\Delta\theta = \frac{2\pi}{N}$$

or

$$\Delta\theta_{hw} = \frac{\lambda}{Nd\cos\theta} \qquad \text{(half-width of line at } \theta\text{).}$$

The expression for $\Delta\theta$ is approximated by

$$\Delta\theta_{hw} \approx \frac{\lambda}{Nd}$$

This means that $\Delta\theta$ becomes very small in the limit of large N.

((**Analysis of resolution**))

$$\frac{I}{I_0} = \frac{1}{N^2}\frac{\sin^2\left(\frac{N\varphi}{2}\right)}{\sin^2\left(\frac{\varphi}{2}\right)} = \frac{1}{N^2}\frac{\sin^2(N\pi x)}{\sin^2(\pi x)}$$

where $\varphi = 2\pi\left(\frac{d}{\lambda}\right)\sin\theta \simeq 2\pi\left(\frac{d}{\lambda}\right)\theta = 2\pi x$, $\quad x = \left(\frac{d}{\lambda}\right)\theta$

The peak appears when $\sin(\pi x) = 0$; x = 0, 1, 2,….. The peak width can be estimated from $\sin(N\pi x) = 0$, as

$$N\pi x = \pm\pi\,, \quad |x| < \frac{1}{N}$$

Leading to the line-width as $2/N$. When N increases, the line-width becomes extremely narrow.

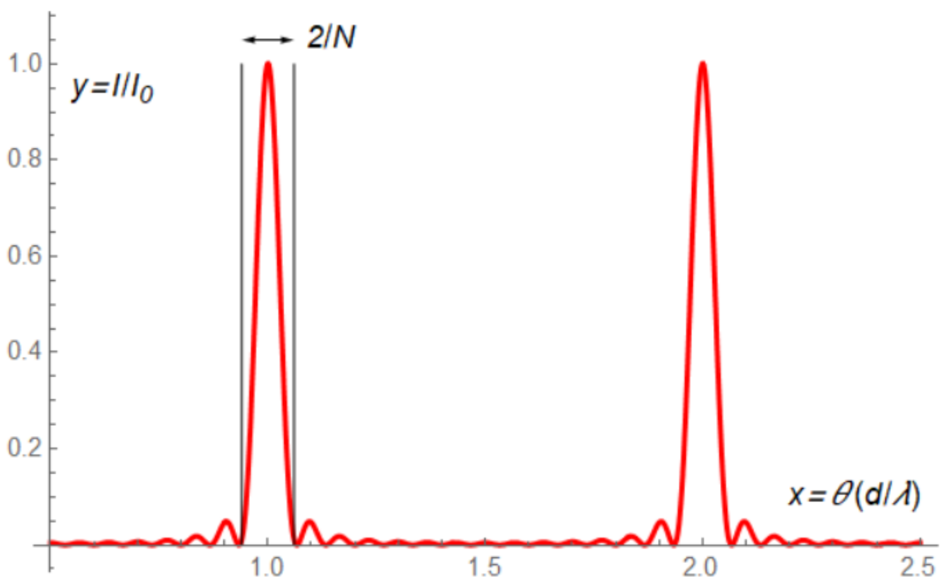


Fig. The diffraction pattern for the diffraction grating. The Intensity ratio I/I_0 as a function of $x = \frac{d}{\lambda}\theta$. N = 15. The peak appears at x = 0,1, 2, 3, . The line-width of the peak is $\Delta x = \frac{d}{\lambda}\Delta\theta = \frac{1}{N}$. The peak appears at $\theta = m\frac{\lambda}{d}$ with m = 0, 1, 2, 3,… The resolution is $\Delta\theta = \frac{\lambda}{Nd}$.

((**Example**)) **Diffraction grating**
2500 lines/inch. 1 inch = 2.54 cm. The separation distance d is

$d = 10.16$ μm.

We use the wavelength λ = 630 nm. We can observe the signal at

$$\theta_1 = \frac{\lambda}{d} = 3.55°.$$

6.9 Dispersion *D*

The dispersion D is defined by

$$D = \frac{\Delta\theta}{\Delta\lambda}$$

where $\Delta\theta$ is the angular separation of two lines whose wavelengths differ by $\Delta\lambda$. Using the relation

$$d \sin\theta = m\lambda$$
$$d \cos\theta \Delta\theta = m\Delta\lambda$$

we have

$$D = \frac{\Delta\theta}{\Delta\lambda} = \frac{m}{d\cos\theta}$$

6.10 Resolving power *R*

The resolving power R is defined by

$$R = \frac{\lambda_{avg}}{\Delta\lambda}$$ (resolving power defined).

where λ_{avg} is the mean wavelength of two emission lines that can barely be recognized as separate, and $\Delta\lambda$ is the wavelength difference between them.

Here we use the relations given by

$$d \sin\theta = m\lambda$$
$$d \cos\theta \Delta\theta = m\Delta\lambda$$

where

$$\Delta\theta \geq \Delta\theta_{hw} = \frac{\lambda}{Nd\cos\theta}$$

Then we have

$$m\Delta\lambda = d\cos\theta\Delta\theta \geq d\cos\theta\Delta\theta_{hw} = d\cos\theta\frac{\lambda}{Nd\cos\theta} = \frac{\lambda}{N}$$

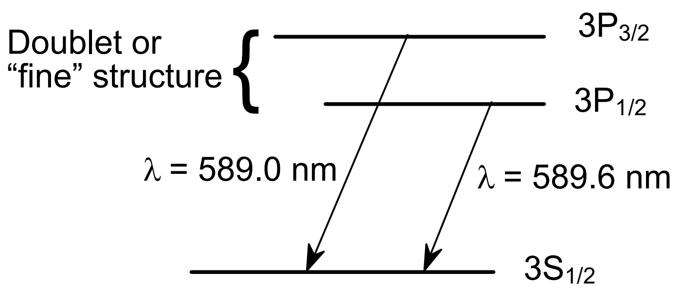
or

$$\boxed{R = \frac{\lambda}{\Delta\lambda} = Nm}$$ (resolving power of a grating).

The greater the number of slits N, the better the resolution. Also, the higher the order m of the diffraction-pattern maximum that we use, the better the resolution.

((**Example**))

For example, consider the case of Na D lines;



R is estimated as

$$R = \frac{\lambda_{avg}}{\Delta\lambda} = \frac{589.3}{0.6} = 982.2$$

6.11 Example
Problem 36-64

A diffraction grating illuminated by monochromatic light normal to the grating produces a certain line at angle θ. (a) What is the product of that line's half-width and the gratin's resolving power?.(b) Evaluate that product for the first order of a grating of slit separation 900 nm in light of wavelength 600 nm.

((**Solution**))

The phase ϕ is defined as

$$\phi = \frac{2\pi}{\lambda} d\sin\theta$$

for the diffraction grating with N slits. The constructive interference occurs when

$$\phi = 2\pi m \qquad \text{or} \qquad d\sin\theta = m\lambda$$

where m is interger. From the definition, we have

The line's half-width $\theta_{hw} = \dfrac{\lambda}{Nd\cos\theta}$

The grating's resolving power $R = \dfrac{\lambda_{avg}}{\Delta\lambda} = Nm$

(a)

$$R\theta_{hw} = Nm\frac{\lambda}{Nd\cos\theta} = \frac{m\lambda}{d\cos\theta} = \frac{d\sin\theta}{d\cos\theta} = \tan\theta$$

(b) d = 900 nm. λ = 600 nm.

For $m = 1$, $\sin\theta = \dfrac{\lambda}{d} = \dfrac{2}{3}$, or $\theta = 41.81°$

Then we have

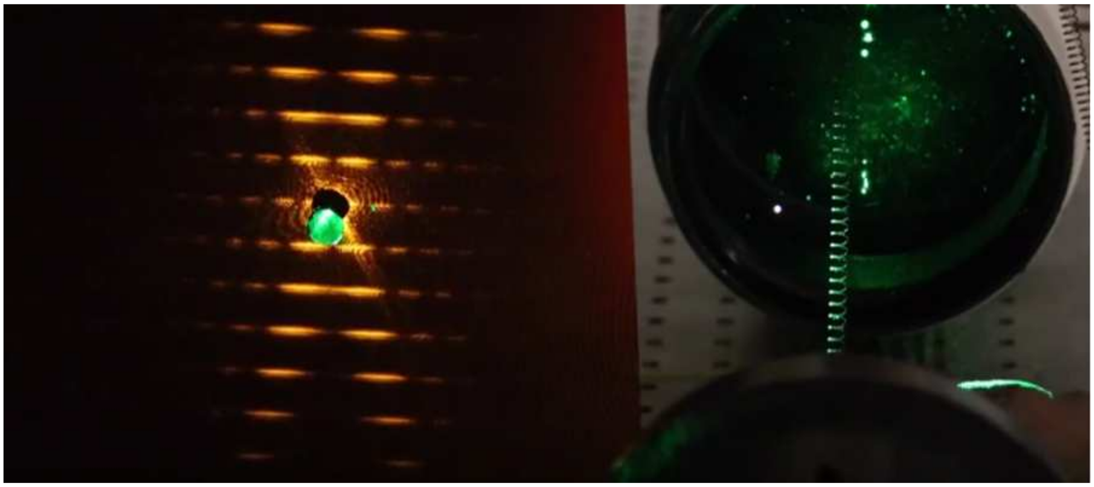
$$R\theta_{hw} = \tan\theta = \tan(41.81°) = 0.894$$

6.12 Compact disc

The tracks of a compact disc act as a diffraction grating, producing a separation of the colors of white light. The nominal track separation on a CD is 1.6 μm, coprresponding to about 625 tracks per mm,. This is in the range of ordinary laboratory diffraction gratings. For red light of wavelength 600 nm, this would give a first diffraction maximum at about 22°.

6.13 ((Example)) Diffraction grating of helical coil

A helical coil has a centerline shape of a helix. A helix (pl: helixes or helices) is a curve that forms a spiral or a coil in space. I found the pattern of the diffraction grating of the helical coil in the web site.

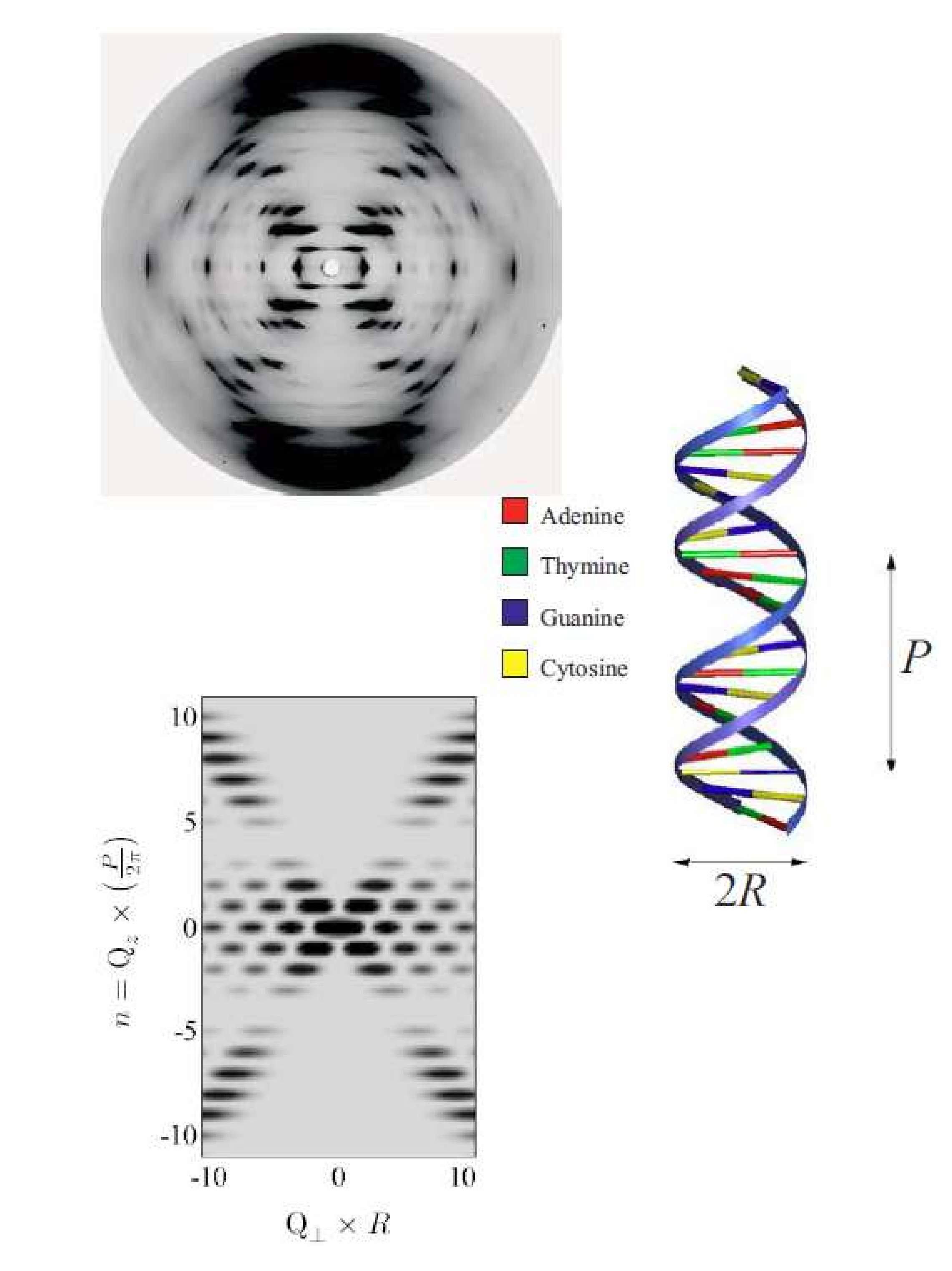


Experiment with Diffraction grating made from a helical coil. The diffraction pattern is very similar to that of DNA obtained by Rosalind Franklin.

https://www.youtube.com/watch?v=I9Ab8BLW3kA

((**Experimental results**))

Photo 51 was an X-ray diffraction image that gave them some crucial pieces of information. It was only after seeing this photo that Watson and Crick realized that DNA must have a double helical structure. The problem was that Photo 51 was actually made by Rosalind Franklin.



7. x-ray difraction

7.1 x-ray source

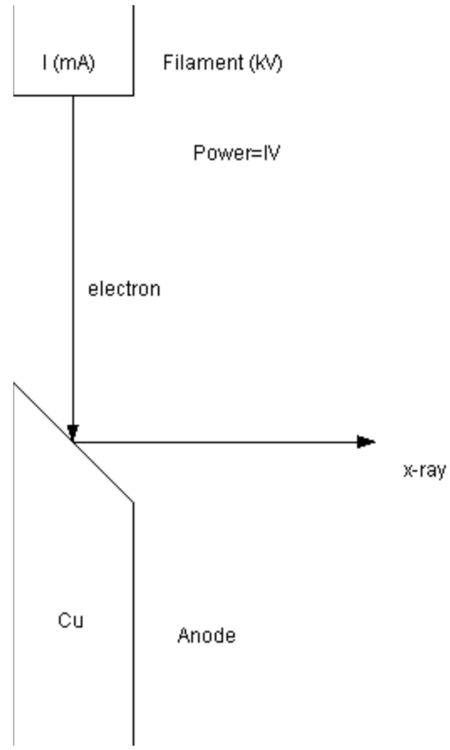


Fig. Schematic diagram for the generation of x-rays. Metal target (Cu or Mo) is bombarded by accelerating electrons. The power of the system is given by $P = I(\text{mA})\ V(\text{keV})$, where I is the current of cathode and V is the voltage between the anode and cathode. Typically, we have I = 30 mA and V = 50 kV: P = 1.5 kW.

We use two kinds of targets to generate x-rays: Cu and Mo.
The wavelength of $CuK_{\alpha 1}$, $CuK_{\alpha 2}$ and CuK_{β} lines are given by

$$\lambda_{K\alpha 1} = 1.540562\ \text{Å}. \quad \lambda_{K\alpha 2} = 1.544390\ \text{Å}, \ \lambda_{K\beta} = 1.392218\ \text{Å}.$$

The intensity ratio of $CuK_{\alpha 1}$ and $CuK_{\alpha 2}$ lines is 2:1.

The weighed average wavelength $\lambda_{K\alpha}$ is calculated as

$$\lambda_{K\alpha} = \frac{2\lambda_{K\alpha 1} + \lambda_{K\alpha 2}}{3} = 1.54184\ \text{Å}.$$

((**Note**)) The wavelength of MoKα is $\lambda_{K\alpha}$ = 0.71073 Å. Figure shows the intensity versus wavelength distribution for x rays from a Mo target. The penetration depth of MoK_{α} line is much longer than that of CuK_{α} l,ine.

$$\lambda_{K\alpha 1} = 0.709300\ \text{Å}. \quad \lambda_{K\alpha 2} = 0.713590\ \text{Å}, \qquad \lambda_{K\beta} = 0.632\ \text{Å}$$

$$\lambda_{K\alpha} = \frac{2\lambda_{K\alpha 1} + \lambda_{K\alpha 2}}{3} = 0.71073 \text{ Å}.$$

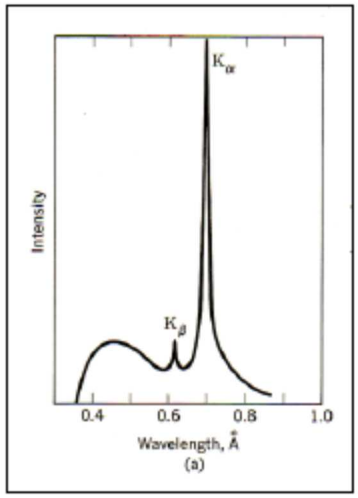


Fig. Intensitry vs wavelength distribution for x-rays from a Mo target bombarded by 30 keV electrons from C. Kittel, Introduction to Solid State Physics.

7.2 Principle of x-ray diffraction

x-ray (photon) behaves like both wave and particle. In a crystal, atoms are periodically located on the lattice. Each atom has a nucleus and electrons surrounding the nucleus. The electric field of the incident photon accelerates electrons. The electrons oscillate around a equilibrium position with the period of the incident photon. The nucleus does not oscillate because of the heavy mass.

Classical electrodynamics tells us that an accelerating charge radiates an electromagnetic field.

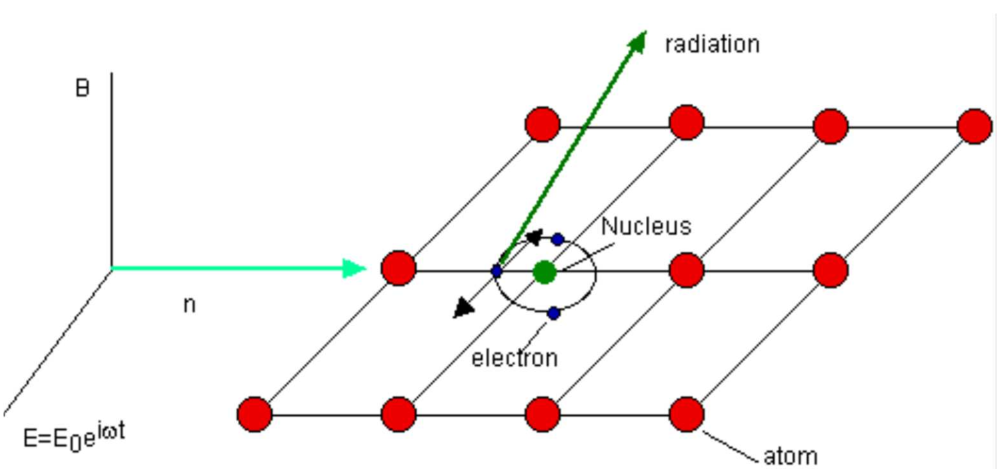


Fig. Schematic diagram for the interaction between an electromagnetic wave (x-ray) and electrons surrounding nucleus. The oscillatory electric field ($E = E_0 e^{i\omega t}$) of x-ray photon gives rise to the harmonic oscillation of the electrons along the electric field.

The instantaneous electromagnetic energy (radiation) flow is given by the pointing vector

$$\boldsymbol{S} \approx \frac{\dot{v}^2 \sin^2\theta}{R^2}\boldsymbol{n}$$

The direction of the velocity $\boldsymbol{v}$ (the direction of the oscillation) is along the x direction. The direction of the photon radiation is in the (x, y) plane.

7.3 Experimental configuration of x-ray scattering

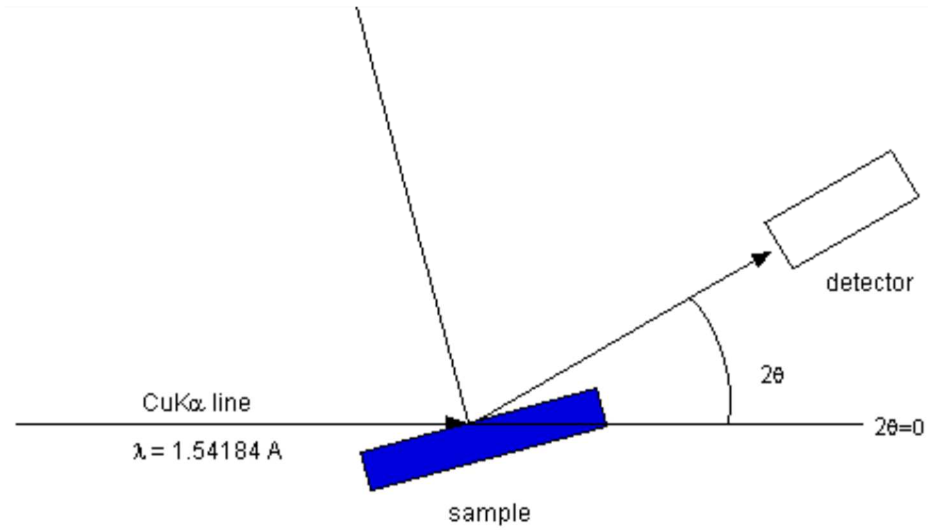


Fig. Example for the geometry of Ω (= θ) – 2θ scan for the (00L) x-ray diffraction. The Cu target is used. The direction of the incident x-ray is $2\theta = 0$. The angle between the detector and the direction of the incident x-ray is 2θ. W is the rotation angle of the sample.

((**Example**)) x-ray diffraction

We show two examples of the x-ray diffraction pattern whicha are obtained in my laboratory

(a) Stage- 3 $MoCl_5$ graphite intercalation compound (GIC). $MoCl_5$ are intercalated into empty graphite galleries. There are three graphene layers between adjacent $MoCl_5$ intercalate layers.

(b) Ni vemiculte. Vermiculite is a layered silicate (a kind of clays). In the interlamellar space, Ni layer are sandwiched between two water layers.

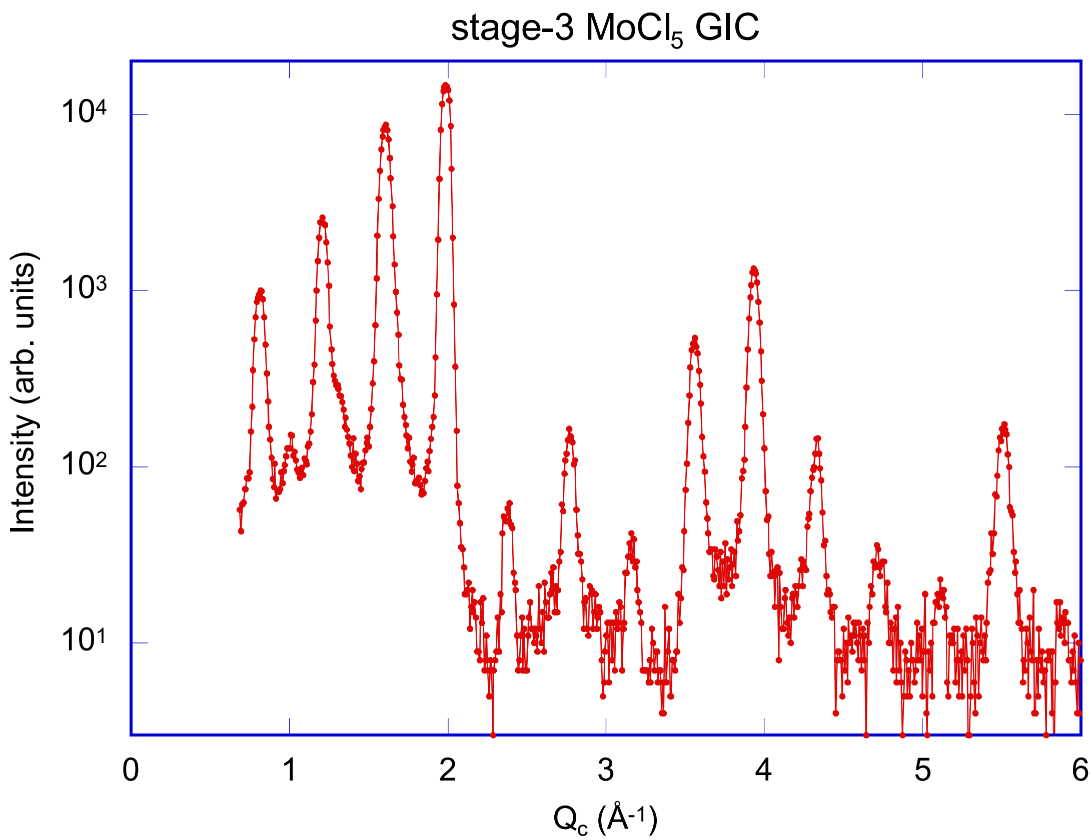


Fig. (00*L*) x-ray diffraction pattern of stage-3 $MoCl_5$ GIC.

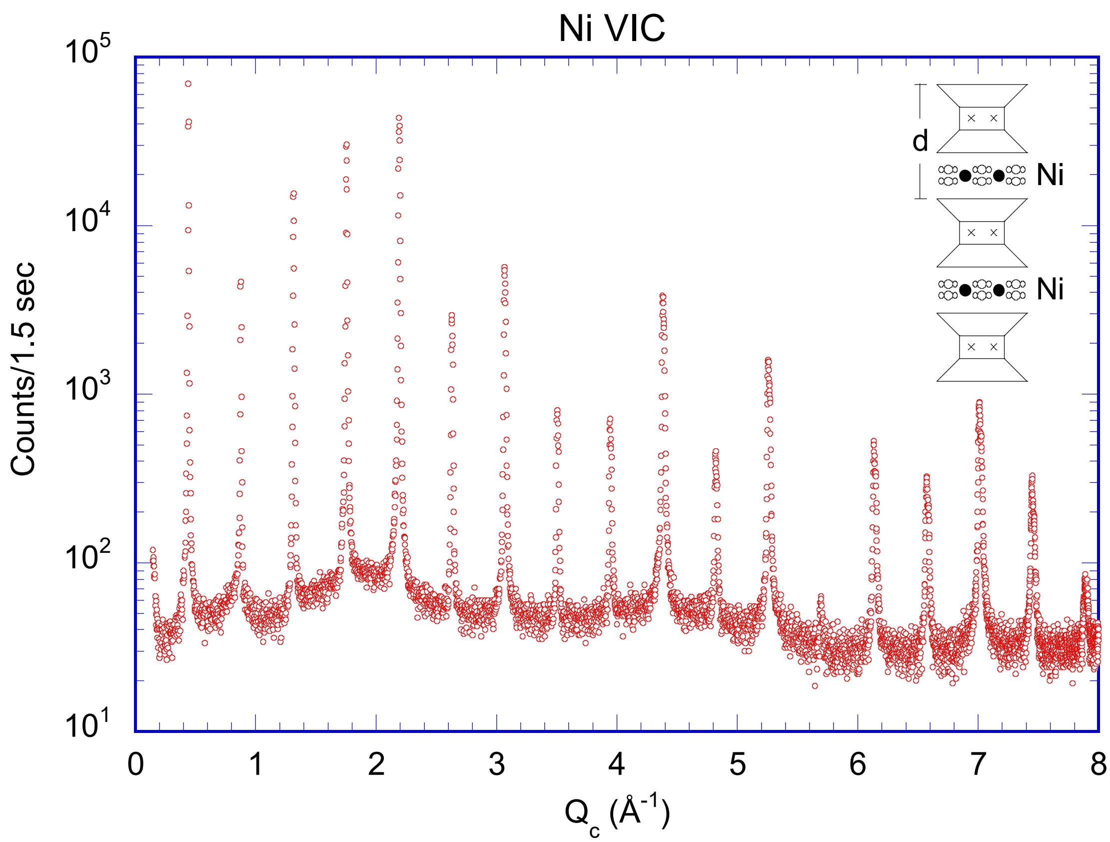


Fig. (00*L*) x-ray diffraction pattern of Ni-vermiculite with two water-layer hydration state.

8. Bragg condition

8.1. Bragg law

The incident x-rays are reflected specularly from parallel planes of atoms in the crystal.
(a) The angle of incoming x-rays is equal to the angle of outgoing x-rays.
(b) The energy of x-rays is conserved on reflection (elastic scattering).

The path difference for x-rays reflected from adjacent planes is equal to $\Delta d = 2d\sin\theta$. The corresponding phase difference is

$$\Delta\phi = k\Delta d = (2\pi/\lambda)2d\sin\theta.$$

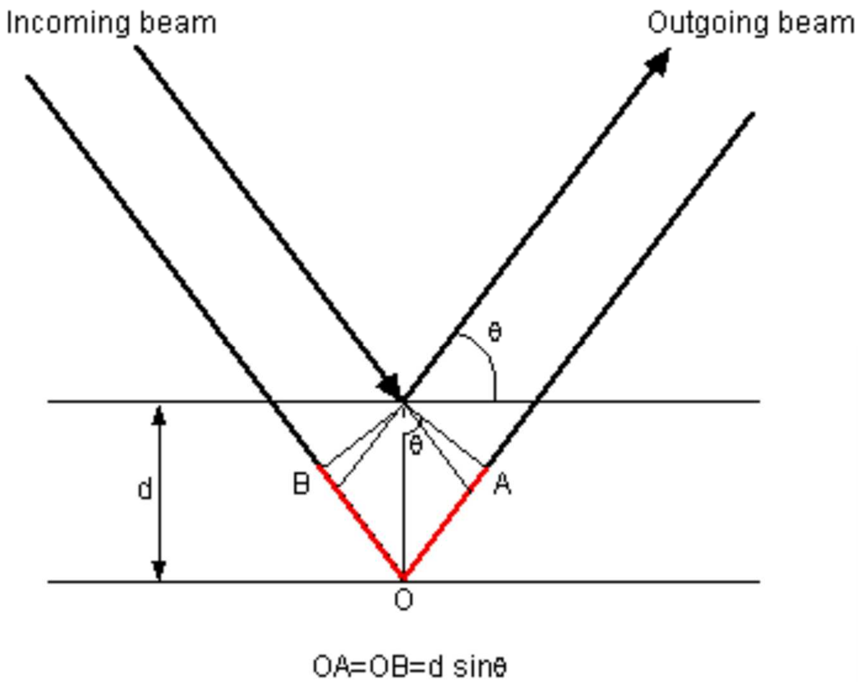
where k is the wave number ($k = 2\pi/\lambda$) and λ is the wave length.

Constructive interference of the radiation from successive planes occurs when $\Delta\phi = 2n\pi$, where n is an integer (Bragg's law).

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

The Bragg reflection can occur only for $\lambda \leq 2d$.

The Bragg law is a consequence of the periodicity of the lattice. The Bragg law does not refer to the composition of the basis of atoms associated with every lattice point. The composition of the bases determines the relative intensity of the various orders of diffraction.



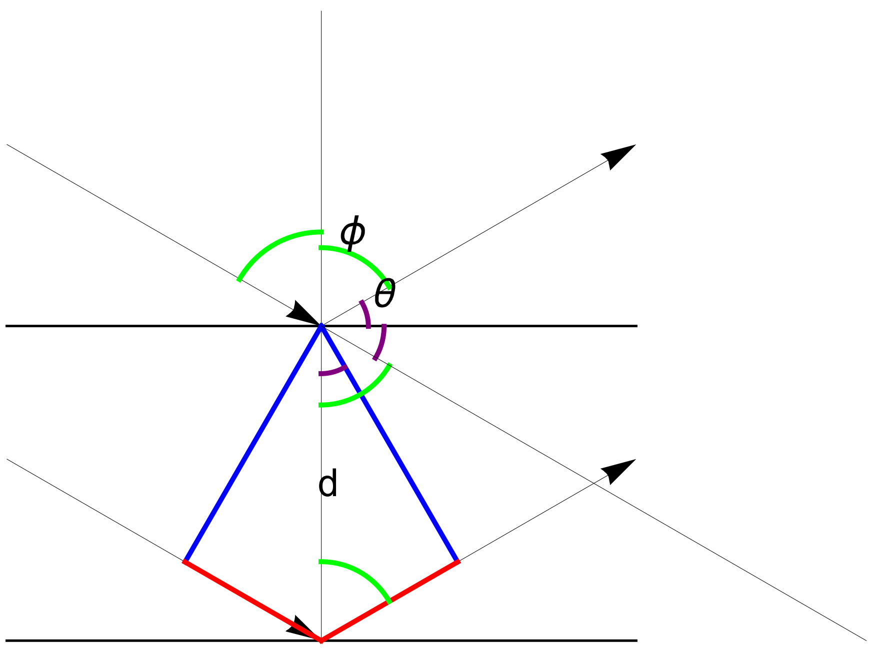


Fig. Geometry of the scattering of x-rays from planar arrays. The path difference between two rays reflected by planar arrays is $2d\sin\theta$.

8.2 Concept of Ewald sphere: introduction of reciprocal lattice

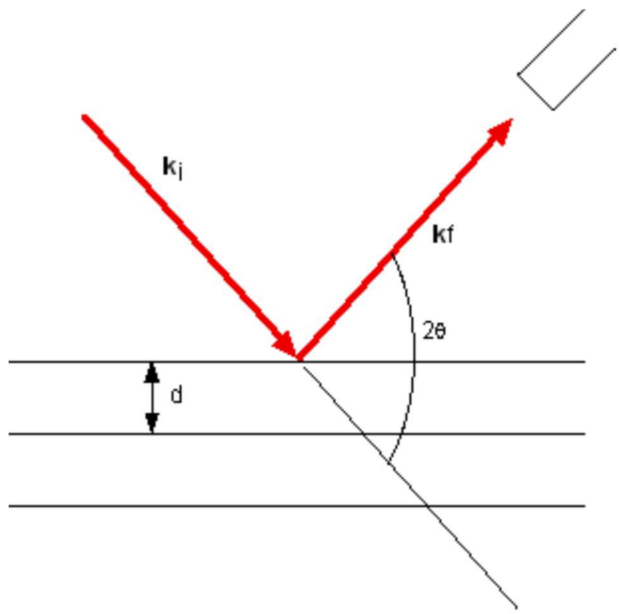


Fig. The geometry of the scattered x-ray beam. The incident x-ray has the wavevector k_i (= $\boldsymbol{k}$), while the outgoing x-ray has the wavevector $\boldsymbol{k}_f$ (= $\boldsymbol{k}'$). $|\mathbf{k}_i| = |\mathbf{k}_f| = 2\pi/\lambda$, where λ is the wavelength of x-ray.

Bragg law:

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

$\boldsymbol{k}_i$ is incident wavevector.
$\boldsymbol{k}_f$ is the outgoing wavevector.

$$|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$$

$\boldsymbol{Q}$ is the scattering vector:

$$\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f, \quad \text{or} \quad \boldsymbol{Q} = \boldsymbol{k}_f - \boldsymbol{k}_i$$

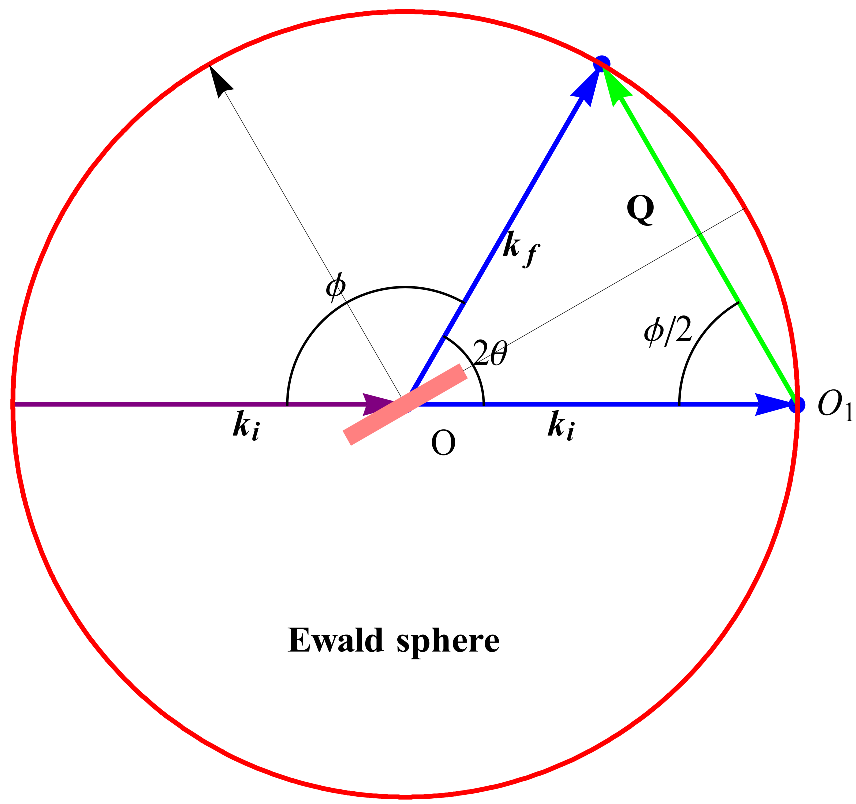


Fig. The geometry (Ewald sphere) using a circle with a radius k ($= 2\pi/\lambda$). The scattering vector $\boldsymbol{Q}$ is defined by $\boldsymbol{Q} = \boldsymbol{k}_f - \boldsymbol{k}_i$.

This is a part of the Ewald sphere. The detail of the Ewald sphere will be discussed later.

In the above configuration, $\boldsymbol{Q}$ is perpendicular to the surface of the system

$$|\boldsymbol{Q}| = 2|\boldsymbol{k}_i|\sin\theta = \frac{4\pi}{\lambda}\sin\theta = \frac{4\pi}{\lambda}\frac{n\lambda}{2d} = \frac{2\pi}{d}n \quad \text{(Bragg condition)}$$

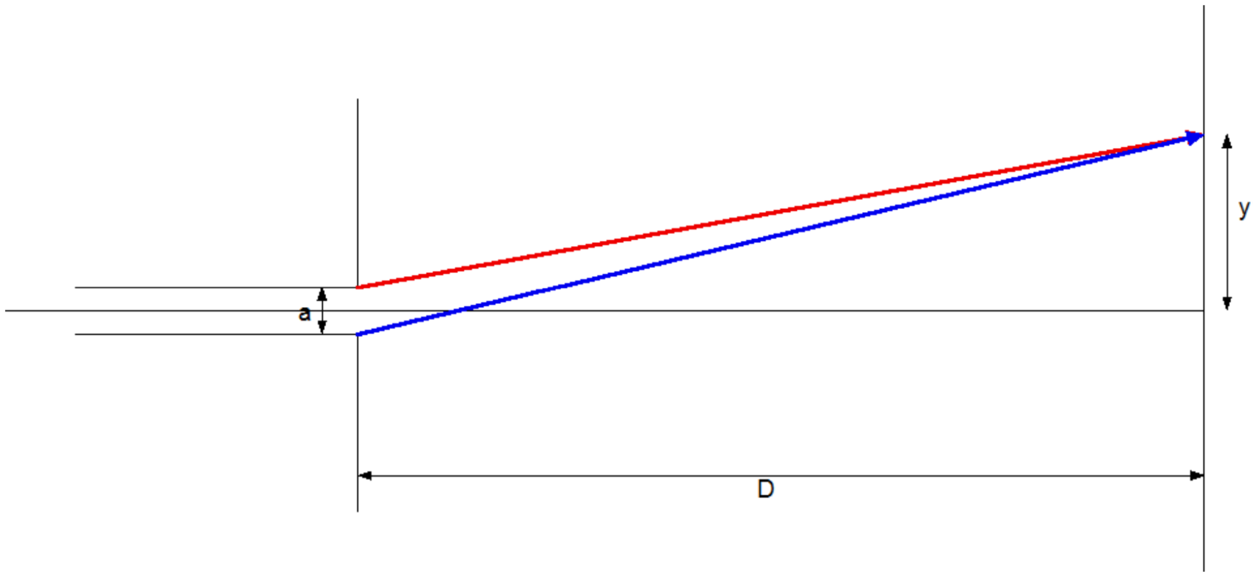
which coincides with the reciprocal lattice point. In other words, the Bragg reflections occur, when $\boldsymbol{Q}$ is equal to the reciprocal lattice vectors.

9. Typical examples

9.1 Problem 36-9 Single slit

A slit 1.00 mm wide is illustrated by light of wave length 589 nm. We see a diffraction pattern on a screen 3.00 m away. What is the distance between the first two diffraction minimum on the same side of the central diffraction maximum?

((**Solution**))



$a = 1.0$ mm
$D = 3.00$ m
$\lambda = 589$ nm

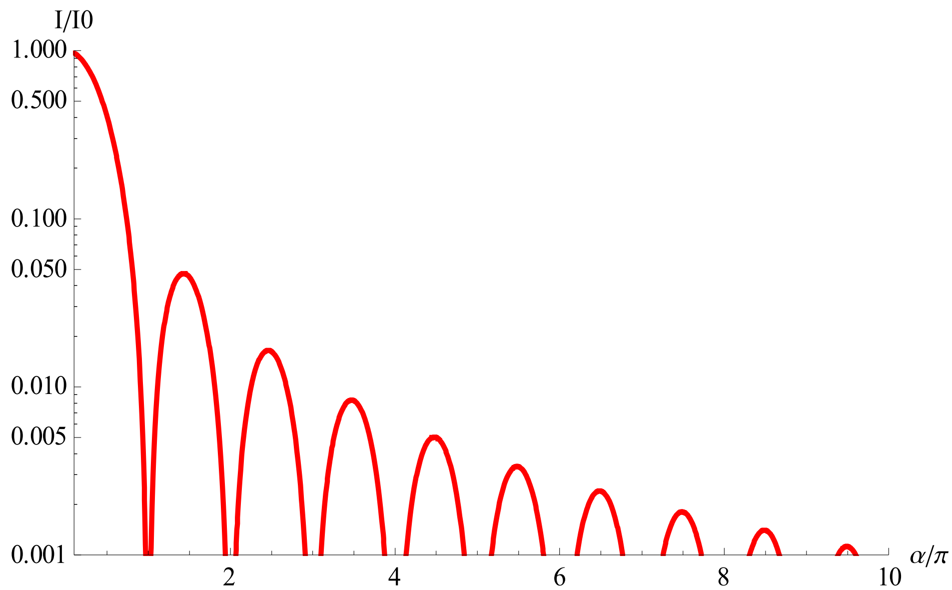
The intensity from the single slit is given by

$$\frac{I}{I_0} = \frac{\sin^2(\alpha)}{\alpha^2},$$

where

$$\alpha = \frac{\pi}{\lambda} a \sin\theta \approx \frac{\pi}{\lambda} a\theta .$$

When $\alpha = m\pi$, the intensity becomes zero.



The angle for the minimum intensity is

$$\alpha = \frac{\pi}{\lambda} a\theta = m\pi$$

$$\theta_n = \frac{m\lambda}{a}$$

Then we have

$$y_m = D\tan\theta_m \approx D\theta_m = D\frac{m\lambda}{a}$$

$$y_2 - y_1 = D\frac{\lambda}{a} = 1.767\,mm$$

9.2 Problem 36-56 (SP-36)

Derive this expression for the intensity pattern for a three-slit "grating":

$$I = \frac{1}{9} I_m (1 + 4\cos\phi + 4\cos^2\phi)$$

where

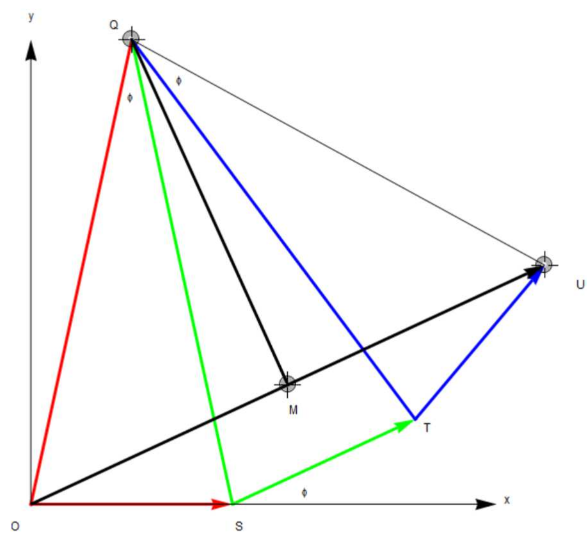
$\phi = (2\pi d \sin\theta)/\lambda$ and $a << \lambda$.

((**Solution**))

We consider the phasor diagram for the three-slit system

$$\overline{OS} = \overline{ST} = \overline{TU} = \frac{E_0}{3}$$

$$\angle QOS = \phi = \frac{2\pi}{\lambda} d \sin\theta$$



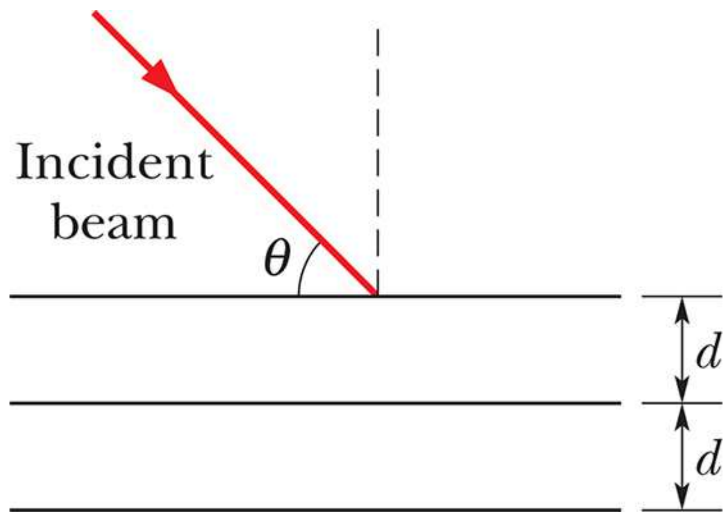
Noting that $\angle OQU = 3\phi$, $\overline{OQ} = R$, $\overline{OS} = 2R\sin\frac{\phi}{2}$, we have

$$\overline{OU} = 2\overline{OM} = 2R\sin\frac{3\phi}{2} = \frac{\sin\frac{3\phi}{2}}{\sin\frac{\phi}{2}}\overline{OS} = \frac{E_0}{3}\frac{\sin\frac{3\phi}{2}}{\sin\frac{\phi}{2}}$$

Then the intensity is obtained as

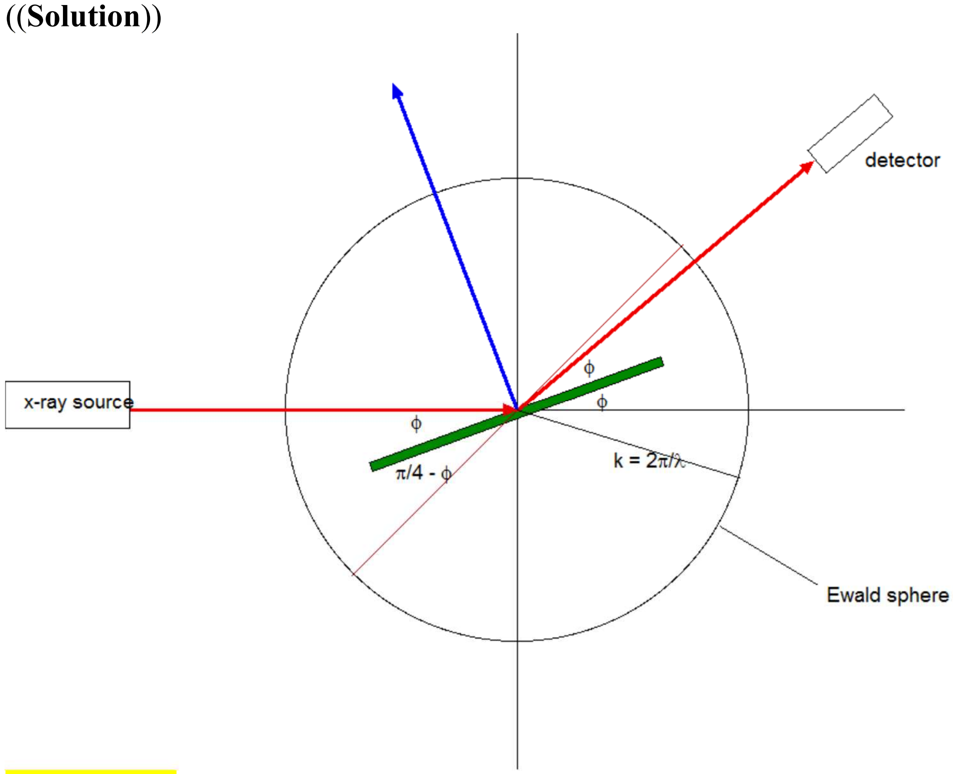
$$\begin{aligned}\frac{I}{I_0} &= \frac{1}{9}\frac{\sin^2\frac{3\phi}{2}}{\sin^2\frac{\phi}{2}} = \frac{1}{9}\frac{1-\cos(3\phi)}{1-\cos\phi} = \frac{1}{9}\frac{1-\cos(3\phi)}{1-\cos\phi} \\ &= \frac{1}{9}\frac{(1-\cos\phi)(1+2\cos\phi)^2}{1-\cos\phi} \\ &= \frac{1}{9}(1+2\cos\phi)^2 \\ &= \frac{1}{9}(1+4\cos\phi+4\cos^2\phi)\end{aligned}$$

9.3 Problem 36-73



In Fig., let a beam of x rays of wavelength 0.125 nm be incident on a NaCl crystal at angle θ = 45.0 to the top face of the crystal and a family of reflecting planes. Let the reflecting planes have separation d = 0.252 nm. The crystal is turned through angle φ around an axis perpendicular to the plane of the page until these reflecting planes give diffraction maxima. What are the (a) smaller and (b) larger value of φ if the crystal is turned clockwise and (c) smaller and (d) larger value of φ if it is turned counterclockwise?

((**Solution**))



d = 0.252 nm
λ = 0.125 nm

Bragg condition:

$2d\ \sin\phi = m\lambda$.

$m = 1$	$\phi_1 = 14.359°$	$45° - \phi_1 = 30.641°$
$m = 2$	$\phi_2 = 29.735°$	$45° - \phi_2 = 15.265°$
$m = 3$	$\phi_3 = 48.075°$	$-45° + \phi_3 = 3.075°$
$m = 4$	$\phi_4 = 82.747°$	$-45° + \phi_4 = 37.747°$

10. Rayleigh's criterion

Fraunhofer diffraction at a circular aperture is an effect of very great practical significance in the study of optical instrument. Here we derive the formula of Rayleigh criterion for the circular aperture. We consider the diffraction of radiation of wavelength λ (wave number $k = \dfrac{2\pi}{\lambda}$), incident normal to a circular aperture of radius a (at the point Q (x, y, 0)). Note that the incident wave is a plane wave with the wave vector $\boldsymbol{k}$.

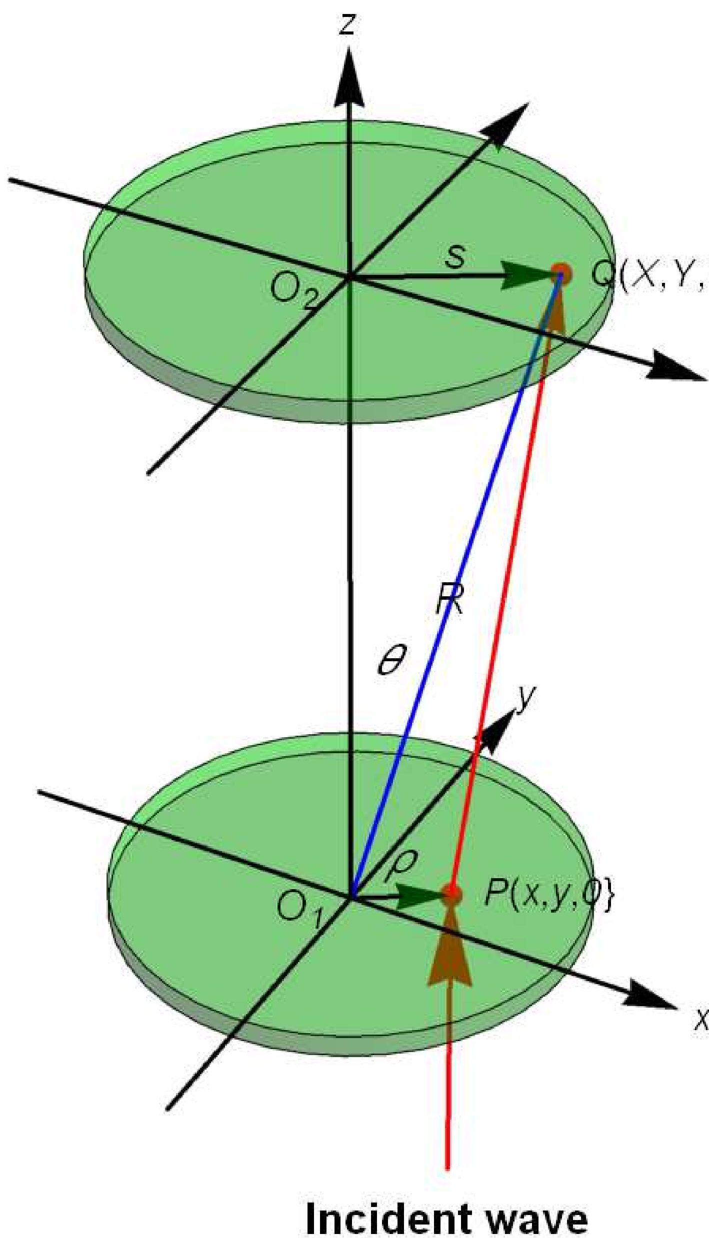


Fig. Geometry of Fraunhofer diffraction, circular aperture. $R\sin\theta = s$. $s = \left|\overrightarrow{O_2Q}\right|$

The electric field for the outgoing spherical wave emitted from the point P (x, y, 0) on circular aperture is given by

$$E_0 \frac{1}{r} e^{ikr},$$

at the detecting point B (X, Y, Z) with

$$
\begin{aligned}
r &= \left|\overrightarrow{PQ}\right| \\
&= \sqrt{(X-x)^2 + (Y-y)^2 + Z^2} \\
&\approx \sqrt{X^2 + Y^2 + Z^2 - 2xX - 2yY} \\
&= R[1 - \frac{2}{R^2}(xX + yY)]^{1/2} \\
&\approx R - \frac{1}{R}(xX + yY)
\end{aligned}
$$

where $R = \left|\overrightarrow{O_1Q}\right| = \sqrt{X^2 + Y^2 + Z^2}$. Thus, we have

$$
E_0 \frac{1}{r} e^{i(kr-\omega t)} = E_0 \frac{1}{R} e^{i(kR-\omega t)} e^{-ik(\frac{xX+yY}{R})}
$$

Suppose that $(x, y) = \rho(\cos\phi, \sin\phi)$ and $(X, Y) = s(\cos\Phi, \sin\Phi)$ in the 2D plane. Then we get

$$
\frac{xX + yY}{R} = \frac{s\rho}{R}\cos(\phi - \Phi).
$$

From the symmetry of the system, it is reasonable to assume that $\Phi = 0$ for the sake of simplicity.

$$
E_1 = E_0 \frac{1}{r} e^{i(kr-\omega t)} = E_0 \frac{1}{R} e^{i(kR-\omega t)} e^{-i\frac{ks\rho}{R}\cos\phi}.
$$

Using the principle of superposition, the resultant electric field is obtained as

$$
\begin{aligned}
E_1 &= \iint E_0 \frac{1}{r} e^{i(kr-\omega t)} da \\
&= E_0 \frac{1}{R} e^{i(kR-\omega t)} \iint e^{-i\frac{ks\rho}{R}\cos\phi} da \\
&= E_0 \frac{1}{R} e^{i(kR-\omega t)} \int_0^a \rho d\rho \int_0^{2\pi} d\phi e^{-i\frac{ks\rho}{R}\cos\phi}
\end{aligned}
$$

where da is the element of area for the circular aperture,

$$da = \rho d\rho d\phi .$$

Here we use the formula of the Bessel function,

$$J_0(u) = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{-iu\mathrm{os}\phi} ,$$

leading to

$$E_1 = 2\pi E_0 \frac{1}{R} e^{i(kR-\omega t)} \int_0^a \rho d\rho J_0(u_1 = \frac{ks\rho}{R}) .$$

Since $u_1 = \frac{ks\rho}{R}$, $du_1 = \frac{ks}{R} d\rho$, this integral can be written as

$$E_1 = 2\pi E_0 \frac{1}{R} e^{i(kR-\omega t)} \left(\frac{R}{ks}\right)^2 \int_0^{\frac{kas}{R}} u_1 du_1 J_0(u_1) .$$

Using the formula,

$$\int_0^u u_1 du_1 J_0(u_1) = uJ_1(u)$$
,

we get

$$E_1 = 2\pi E_0 \frac{1}{R} e^{i(kR-\omega t)} \left(\frac{R}{ks}\right)^2 \frac{kas}{R} J_1(\frac{kas}{R})$$
$$= [2\pi E_0 \frac{a^2}{R} e^{i(kR-\omega t)}] \frac{R}{ksa} J_1(\frac{kas}{R})$$

The intensity I is

$$I = \frac{|E_1|^2}{2\mu_0 c} = \frac{2\pi^2 E_0{}^2}{\mu_0 c R^2} \left[\frac{R}{ksa} J_1(\frac{kas}{R})\right]^2 .$$

We note that for $s = R\sin\theta$,

$$I(\theta) = \frac{|E_1|^2}{2\mu_0 c} = \frac{\pi^2 E_0{}^2}{2\mu_0 c R^2}\left[\frac{2J_1(ka\sin\theta)}{ka\sin\theta}\right]^2.$$

Since $\theta = 0$, we get

$$I(\theta = 0) = \frac{\pi^2 E_0{}^2}{2\mu_0 c R^2},$$

since $\dfrac{2J_1(u)}{u} = 1$ at $u = 0$. Finally, we get the intensity as

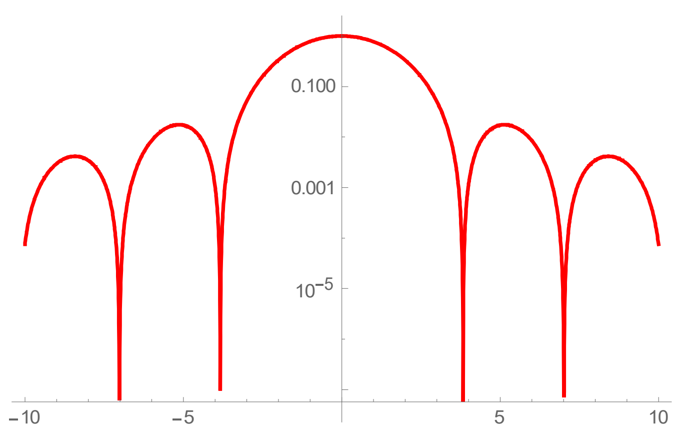
$$I(\theta) = I(\theta = 0)\left[\frac{2J_1(ka\sin\theta)}{ka\sin\theta}\right]^2.$$

We make a plot of $I(\theta)/I(\theta = 0)$ as a function of $x = ka\sin\theta = \dfrac{2\pi}{\lambda}a\sin\theta$. The intensity becomes zero when $x = 3.83171$.

$$\frac{2\pi}{\lambda}a\sin\theta = 3.83171.$$

When $D = 2a$ (diameter), we get the Rayleigh criterion

$$\boxed{D\sin\theta = \frac{3.83171}{\pi}\lambda = 1.21967\lambda}$$



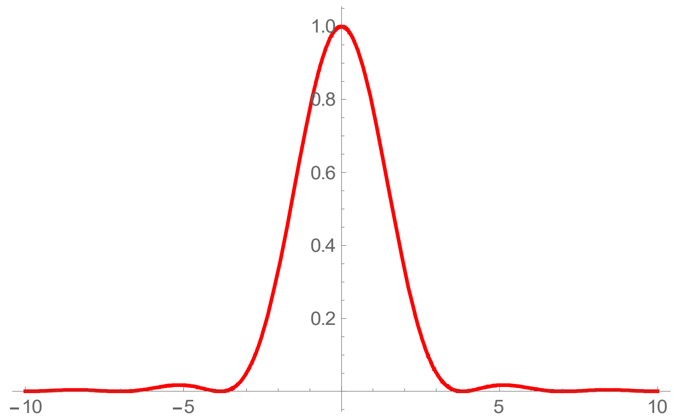


Fig. $I(\theta) = I(\theta = 0)\left[\dfrac{2J_1(x)}{x}\right]^2$ with $x = ka\sin\theta = \dfrac{2\pi a}{\lambda}\sin\theta$. $J_1(x)$ becomes zero at $x = 3.83171$, 7.0156, 10.1735. $\sin\theta = \dfrac{3.83171\lambda}{\pi(2a)} = \dfrac{\lambda}{D}1.2196$ with $D = 2a$.

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E. Hecht, Optics, Global Edition (Pearson, 2017).

G.B. Arfken, H.J. Weber, and F.E. Harris, Mathematical Methods for Physicists, seven-th edition (Elsevier, 2013).

11. Reflective diffraction grating

The diffraction grating is an optical device widely used for studying the spectrum and measuring the wavelength of light. Diffraction gratings are made by ruling fine grooves to produce a transmission grating or a reflecting grating. As illustrated in Fig. below, the rulings are parallel, and equally spaced. The best gratings are several inches in width and contain 5,000 to 30,000 grooves per inch. The spacing distance d is

$$d = \frac{2.54\ \text{cm}}{10^4} = 2540\ \text{nm},$$

for 10,000 lines per inch.

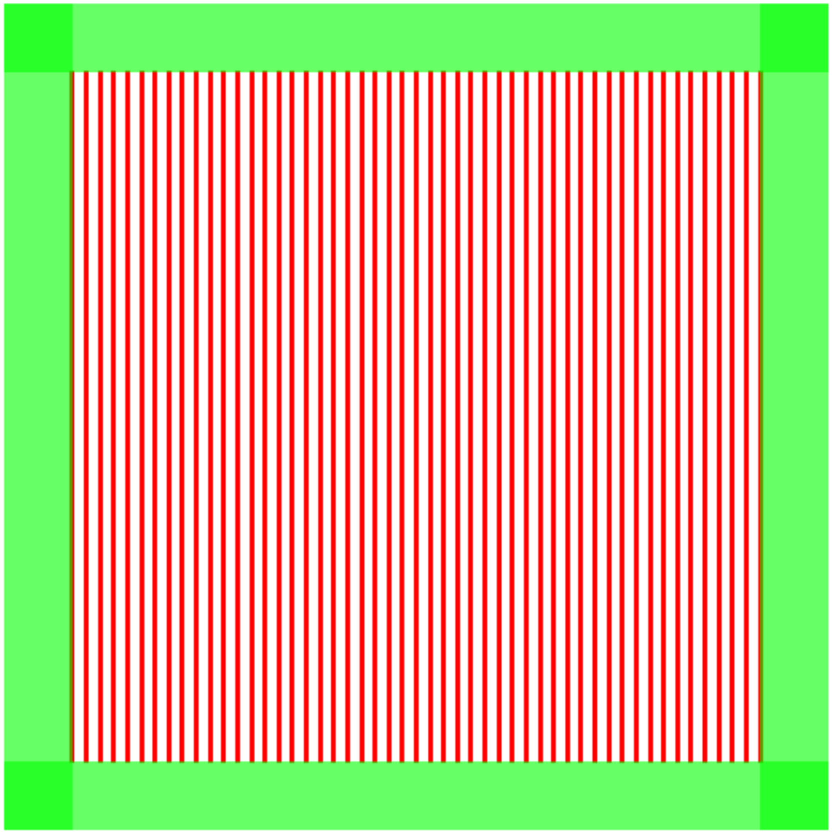


Fig. Schematic diagram of the grooves or rulings on a diffraction grating.

A diffraction grating is an optical device used to disperse light into a spectrum. It is ruled with closely-spaced, fine, parallel grooves, typically several thousand per centimeter, that produce interference patterns in a way that separates all the components of the incoming light. A diffraction grating can be used as the main dispersing element in a spectrograph. The diffraction pattern produced by the grating is described by the equation

$$d \sin\theta = m\lambda \,,$$

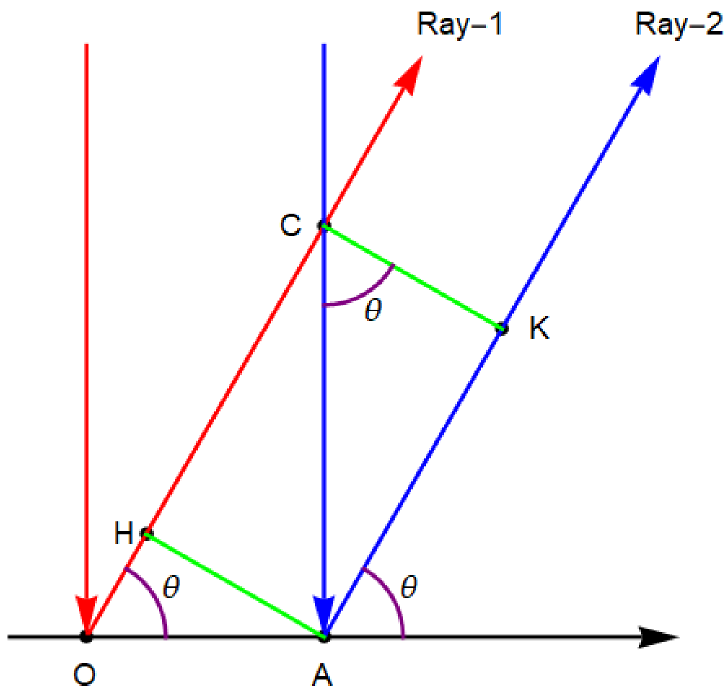
where m is the order number, λ is a selected wavelength, d is the spacing of the grooves, and θ is the angle of incidence of light.

11.2. Example-1: reflective diffraction grating

A **reflection grating** has grooves ruled onto a reflective coating on a surface that may be plane or concave, the latter being able to focus light. Its advantage over a transmission grating is that it produces a spectrum extending from ultraviolet to infrared, since the light doesn't pass through the grating material.

We consider the case when the ray-1 and ray-2 are normally incident on the surface of diffraction grating with a periodic structure. After the reflection on the surface grating, The diffracted ray-1 and ray-2 have a constructive interference when the angle is given by

$$d\sin\theta_m = m\lambda$$



The path difference between the ray-1 and ray-2 is

$$\overline{\mathrm{OH}} = d\sin\theta$$

where $\overline{OA} = d$

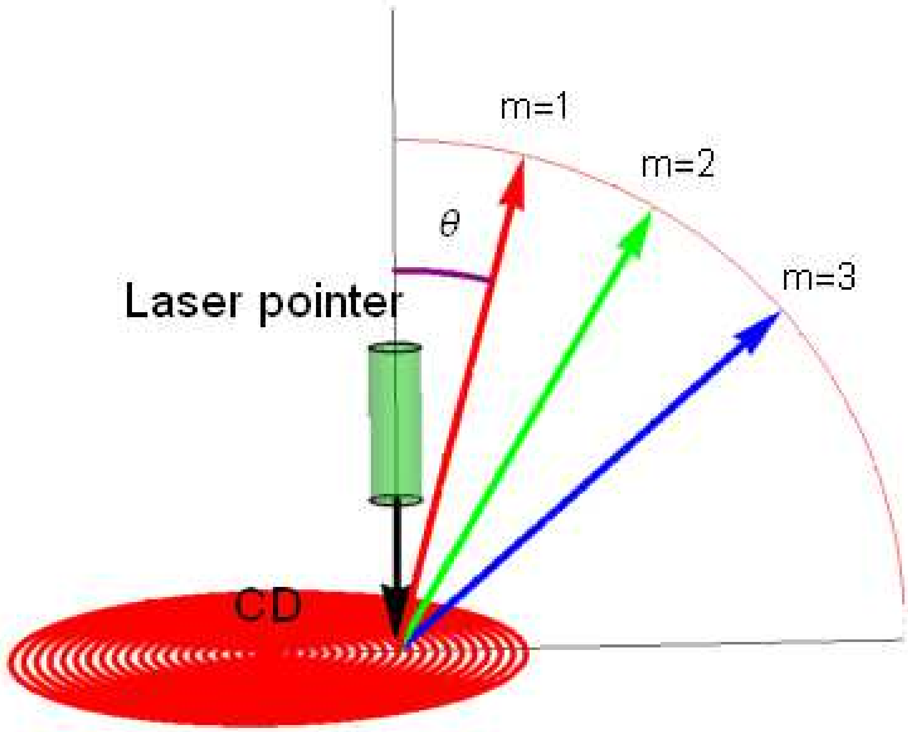
The phase difference is

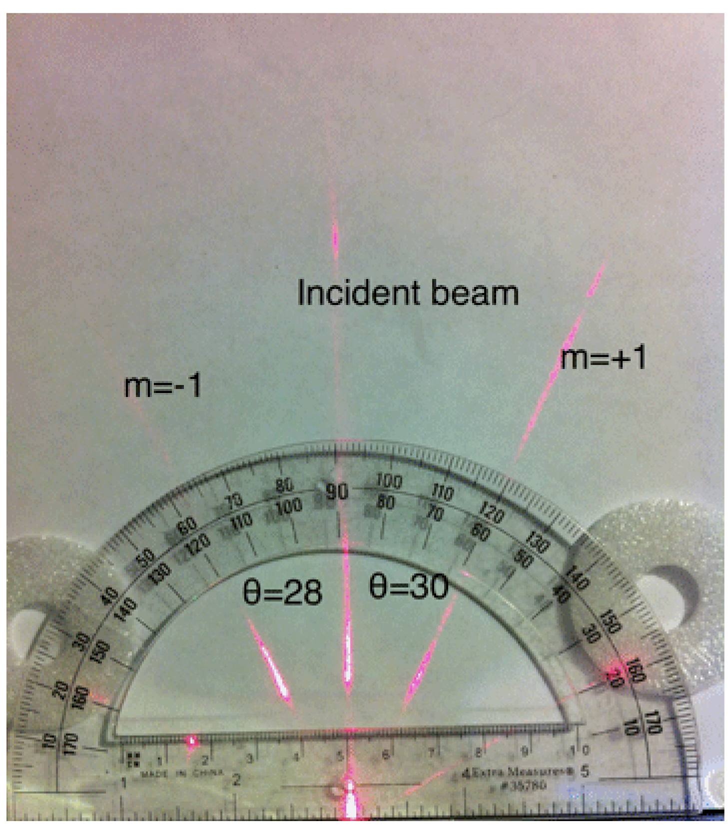
$$\Delta\phi = \frac{2\pi}{\lambda} d\sin\theta$$

The constructive interference occurs when

$$d\sin\theta_m = m\lambda$$

11.3 Experiment with CD and laser pointer


m=1
m=2
θ
m=3
Laser pointer
CD


Incident beam
m=-1
m=+1
θ=28
θ=30

From Engineering University of Colorado Boulder
https://www.teachengineering.org/content/uoh_/activities/uoh_diffraction/uoh_diffraction_activity1_figure2.gif

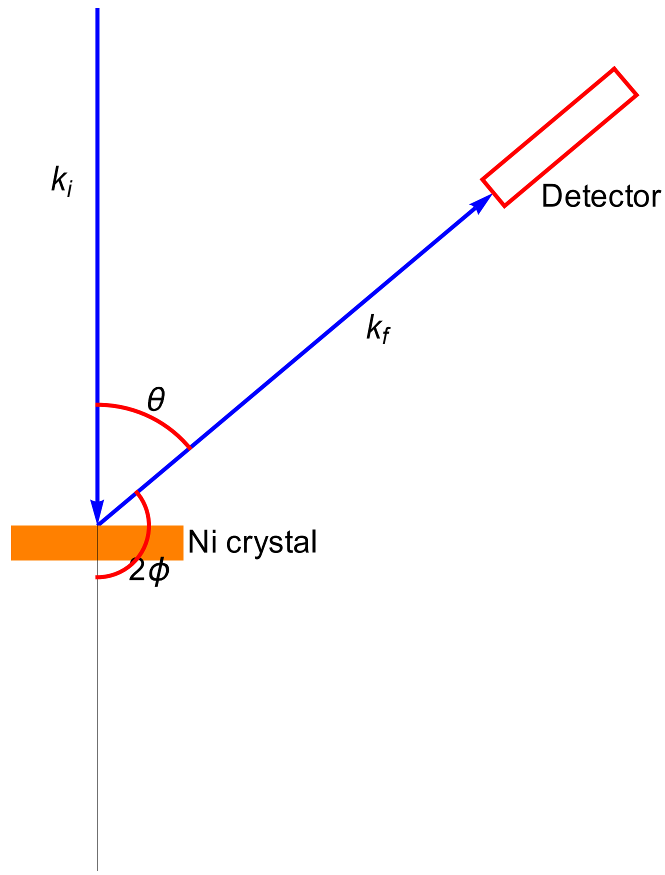
Fig. The laser beam is aligned with the normal of the CD surface (perpendicular to the CD). The incident and diffracted beams are clearly visible. The angles of the diffracted beams (the angle between the incident beam and diffracted beam) is measured.

11.4 Explanation of the formula using the Ewald sphere (Solid State Physics)

In order to understand the Bragg condition for the reflective diffraction grating, first we consider the Davisson-Germer experiment, where a two dimensional (2D) system [Ni <111> surface atomic separation *d*], plays the same role like the diffraction grating. In this experiment, the electron beam is incident at right angles to the Ni <111> surface. If it is regarded as the 2D lattice plane with the lattice constant *d*, it is predicted from the Bragg law (solid state physics) that a Bragg rod (ridge) is formed at the reciprocal lattice vector $\boldsymbol{G}_0$ in the reciprocal lattice space. ($|\boldsymbol{G}_0| = \frac{2\pi}{d}$). Thus, the Bragg condition occurs when

$$k_f \sin\theta = \frac{2\pi}{d} m, \qquad \text{or} \qquad \frac{2\pi}{\lambda}\sin\theta = \frac{2\pi m}{d}, \qquad \text{or} \qquad d\sin\theta = m\lambda,$$

using the Ewald sphere. In other words, the Bragg rod (ridge) with the reciprocal lattice vector $\boldsymbol{G}_0$ intersects with the Ewald sphere with radius $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$.



k_i
Detector
k_f
θ
Ni crystal
2ϕ

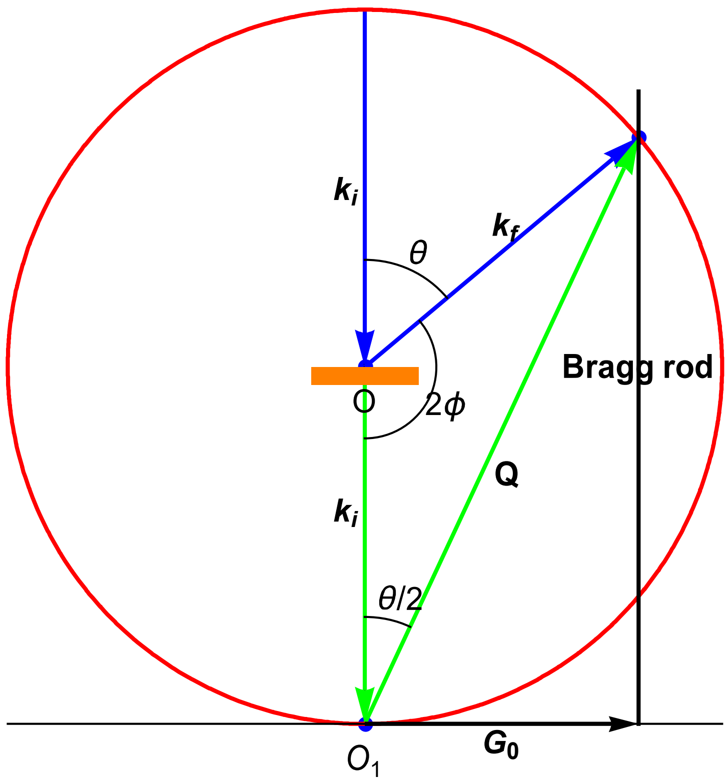


Fig. Ewald sphere (reciprocal lattice space) for the 2D structure system with a periodicity of distance *d*. The Bragg rod (ridge) is formed with $|\boldsymbol{G}_0| = \frac{2\pi}{d}$ in the reciprocal lattice space (see the textbook of Solid State Physics). According to the Bragg law, the Bragg reflection occurs when the condition $k_f \sin\theta = G_0$ is satisfied. In other words, the Bragg rod (ridge) for the 2D system intersects with the Ewald sphere with radius $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$. Since $k_f = \frac{2\pi}{\lambda}$ and $G_0 = \frac{2\pi}{d} m$, we get the Bragg condition, $d\sin\theta = m\lambda$.

Similar approach can be used for the reflective diffraction grating which forms a 1D structure. The light ray is incident at right angles to the diffraction grating. The Bragg condition occurs when the Bragg plane (for 1D system) denoted by the reciprocal lattice G_0 intersects with the Ewald sphere with radius $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$, where the Bragg plane is perpendicular to $\boldsymbol{G}_0$. In this case, we get the same Bragg condition as

$$k_f \sin\theta = G_0, \qquad \text{or} \qquad d\sin\theta = m\lambda .$$

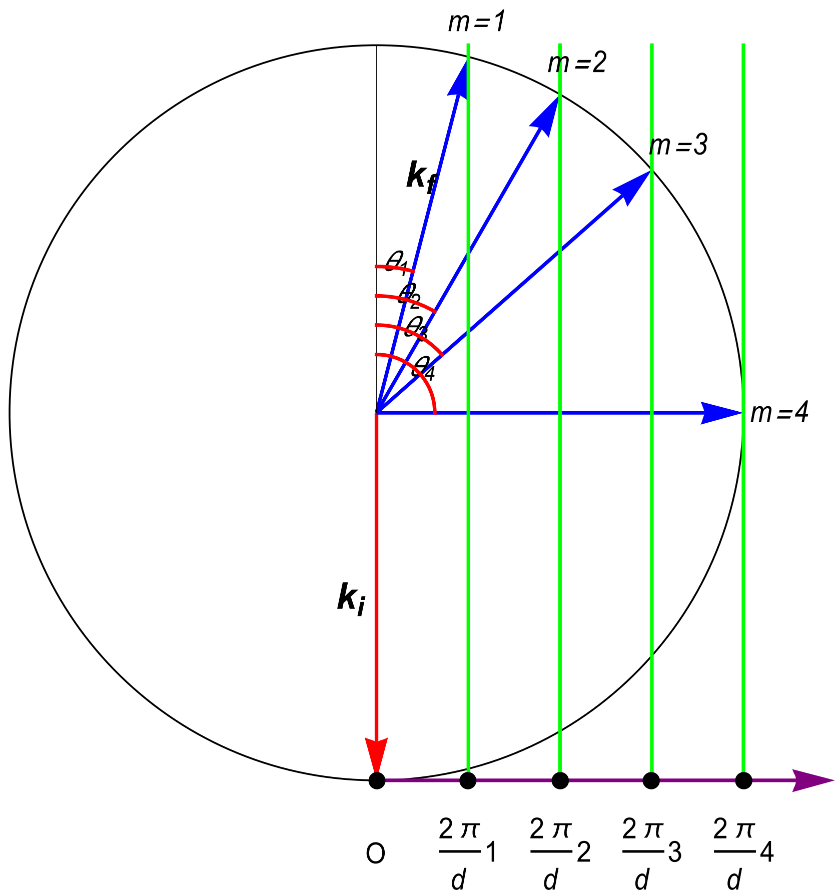


Fig. Ewald sphere for the reflective diffraction on the diffraction grating with the periodicity d.. The Bragg condition occurs when the Bragg rod (Bragg plane for the 1D system) intersects with the Ewald sphere with the radius $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \dfrac{2\pi}{\lambda}$, where λ is the wavelength of the light.

11.5 Example-2: reflective diffraction grating

We consider the case when the ray-1 and ray-2 are reflected on the surface of diffraction grating. The angle of the incident rays and the direction normal to the surface of grating is θ. After an ideal reflections on the grating, the reflected ray-1 and ray-2 lead to a constructive interference when the angle is satisfied by the condition

$$d \sin\theta_m = m\lambda.$$

where m =1, 2, 3,… The path difference between the ray-1 and ray-2 is

$$\overline{\mathrm{OH}} = d \sin\theta\,,$$

where $\overline{OA} = d$.

For simplicity, we assume that $d = 4\lambda$. We make a plot the constructive interference as follows.

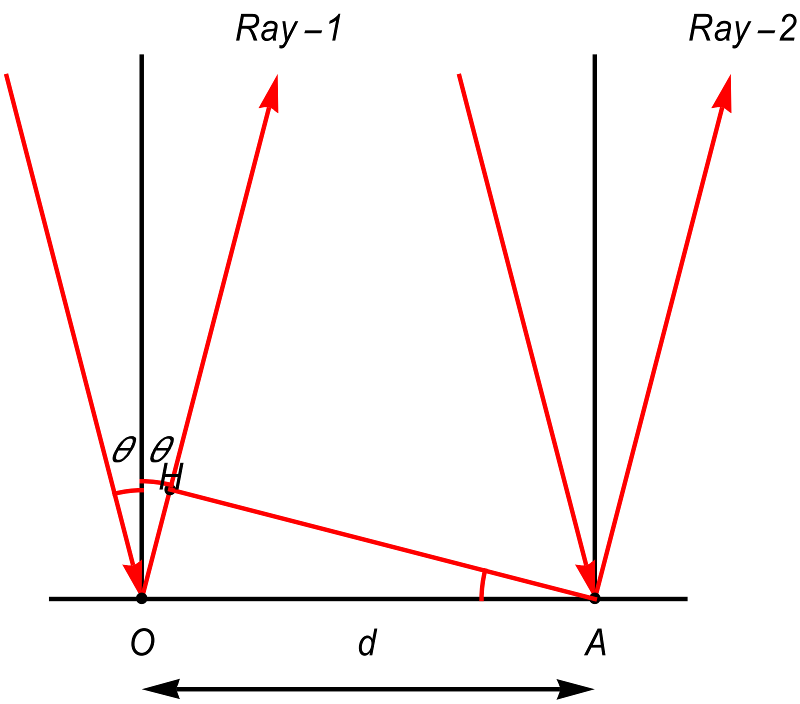


Fig. $d\sin\theta_m = m\lambda$ with m = 1. $d = 4\lambda$. $\angle \mathrm{OHA} = \frac{\pi}{2}$. $\overline{\mathrm{OH}} = d\sin\theta$ is the path difference between the ray 1 and ray-2.

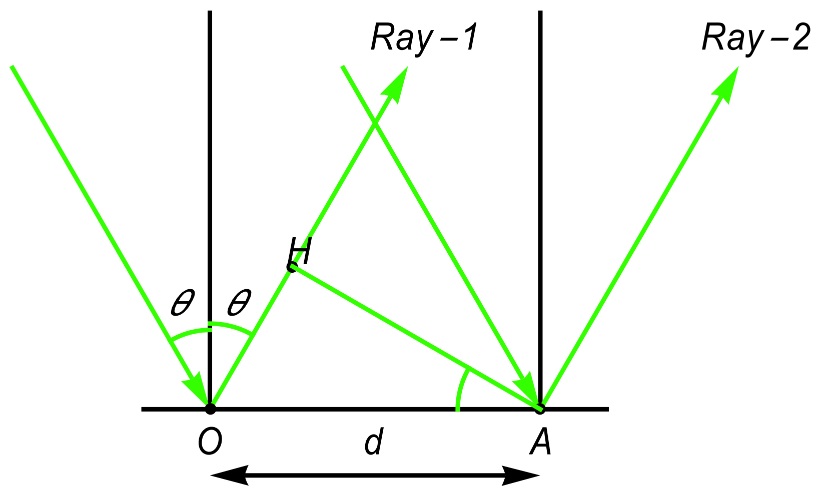


Fig. $d\sin\theta_m = m\lambda$ with $m = 2$. $d = 4\lambda$

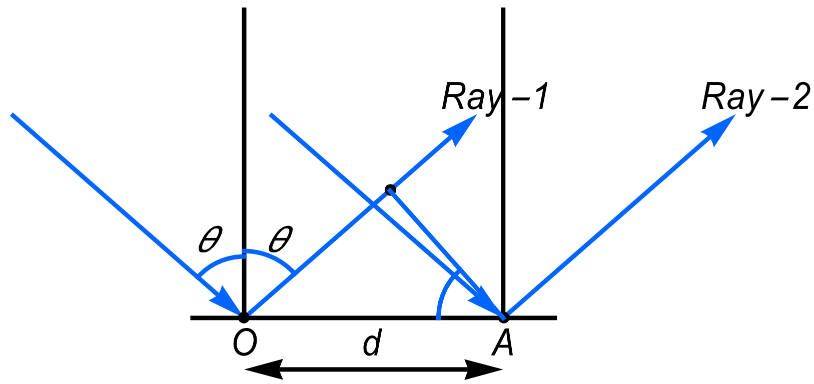


Fig. $d\sin\theta_m = m\lambda$ with $m = 3$. $d = 4\lambda$

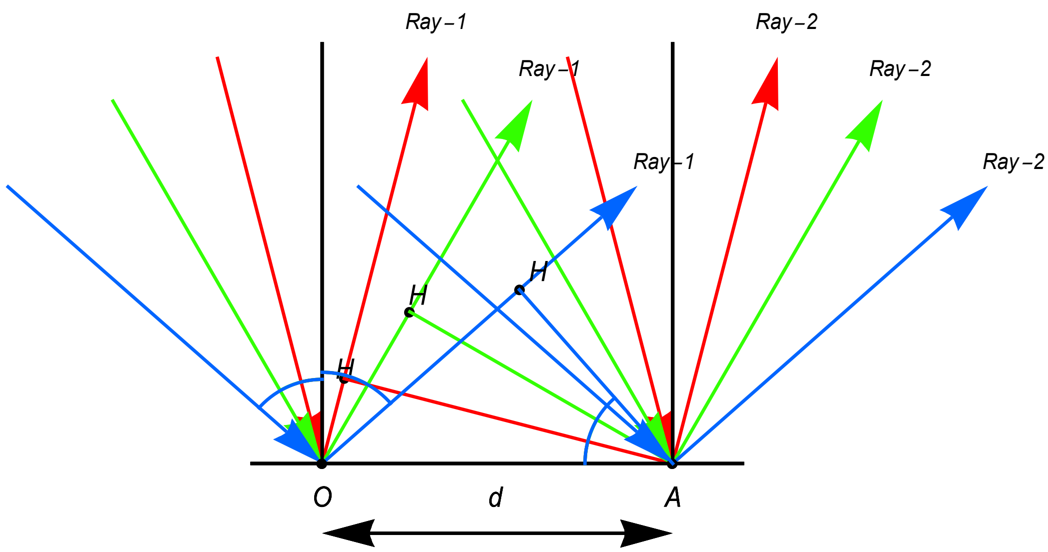


Fig. $d\sin\theta_m = m\lambda$ with $m = 1, 2, 3$. $d = 4\lambda$.

Ewald sphere for the 1D system (diffraction grating)

$$k_f \sin\theta = \frac{2\pi}{d},\ \frac{2\pi}{\lambda}\sin\theta = \frac{2\pi}{d},$$

Ewald sphere for the 1D system (diffraction grating)

$$k_f \sin\theta = \frac{2\pi}{d}, \qquad \frac{2\pi}{\lambda}\sin\theta = \frac{2\pi}{d}.$$

11.6 Bragg condition

Here we use the Ewald sphere to understand the Bragg condition. The wave vectors of the incident light and the reflected light are $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$. Note that $\theta_r = \theta_i = \theta$, where θ_i is the angle of incident between $\boldsymbol{k}_i$ and the direction normal to the surface of the diffraction and θ_r is the angle of reflection between $\boldsymbol{k}_f$ and the direction normal to the surface of the diffraction grating. Suppose that the diffraction grating has a 1D structure with periodicity *d*. Correspondingly, it forms a Bragg plane with $G_0 = \frac{2\pi}{d} m$ in the reciprocal latticespace, The Bragg refection occurs when the Bragg planes intersect with the Ewald sphere with the radius $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}$. The Bragg condition is obtained as

$$k_i \sin\theta = \frac{2\pi}{d} m , \qquad d \sin\theta = m\lambda$$

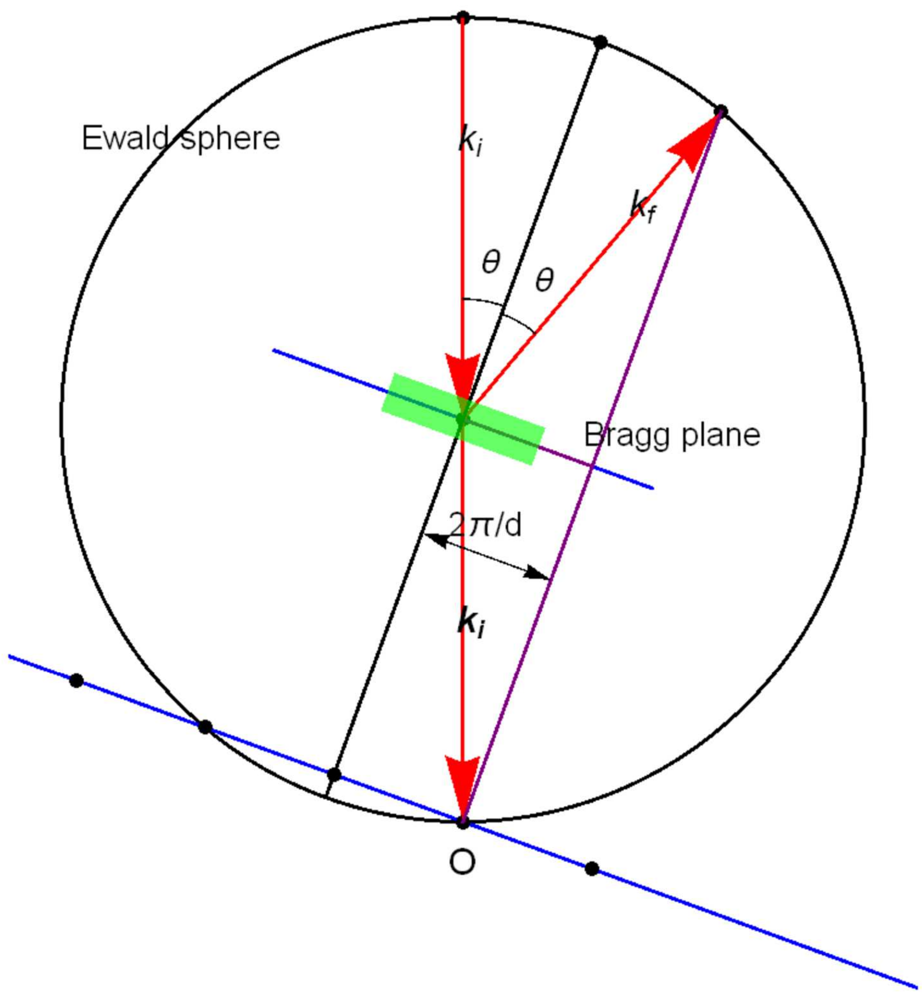
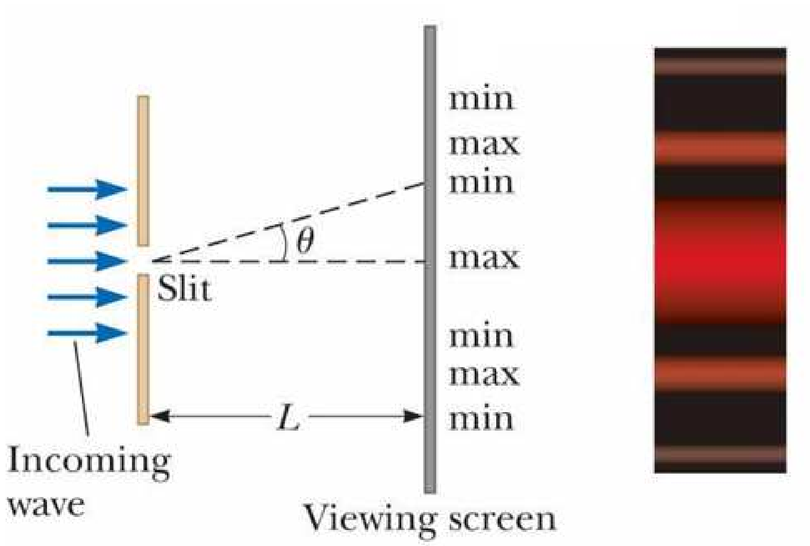


Fig. Ewald sphere for the diffraction grading with 1D periodicity. The 2D Bragg plane is formed with $G_0 = \frac{2\pi}{d} m$ in the reciprocal lattice space.

12. Heisenberg's principle of uncertainty with the use of diffraction with a single slit

12.1 Principle

Experimentally, the single slit in Fig. is made half as wide, the central fringe becomes wider. On the other hand, as the width of the single slit decreases, the central fringe becomes narrower.



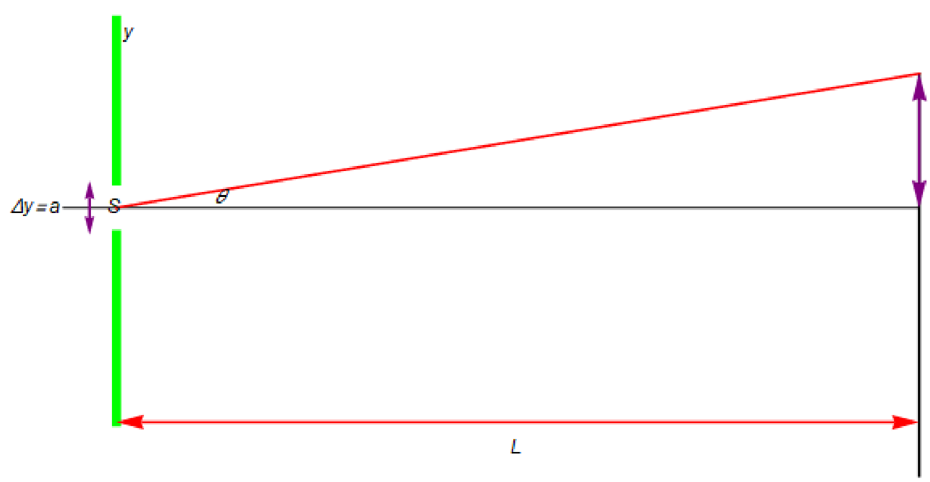


Fig. Single slit with the width a..

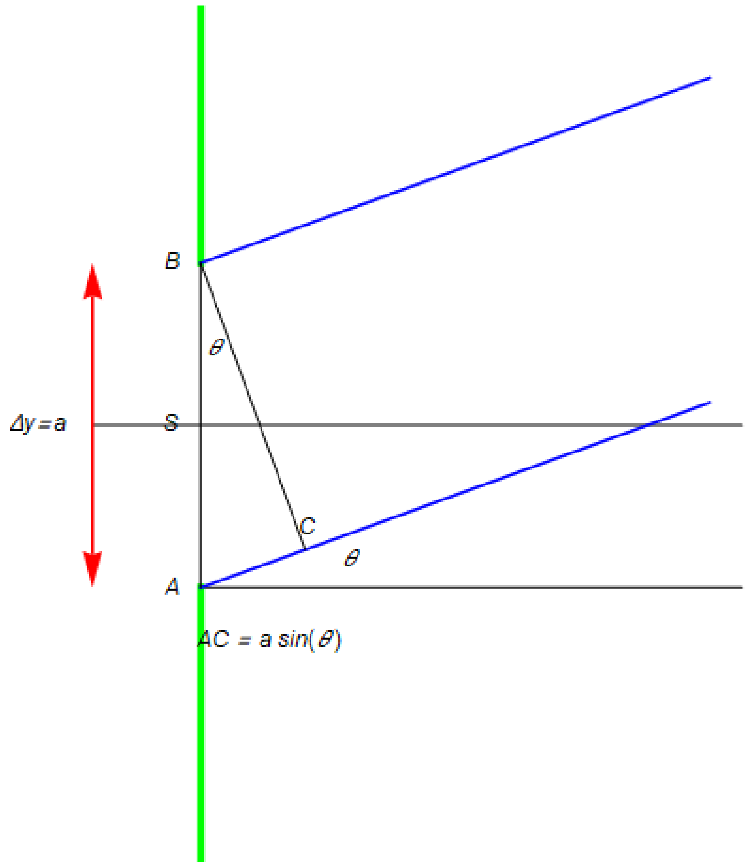


Fig. Path difference between two rays in the ingle slit with $\Delta y = a$, $AC = a\sin\theta$.

This result can be explained in terms of the Heisenberg's principle of uncertainty. The width of the slit is given by

$$\Delta y = a .$$

The change of the momentum along the y axis is

$$\Delta p_y = \frac{h}{\lambda}\sin\theta ,$$

where the momentum is h/λ using the de Broglie relation.

$$\Delta y \Delta p_y = \frac{h}{\lambda} a\sin\theta \approx \frac{h}{\lambda}\lambda = h ,$$

where $a\sin\theta = \lambda$. When the width Δy of the slit becomes smaller and smaller, the image of the screen becomes widely spread out. So such behavior can be explained by the Heisenberg's principle of uncertainty.

((**Heisenberg's discussion**))

I found an excellent article for the Heisenberg's principle of uncertainty, which Heisenberg himself discussed in his famous book [**W. Heisenberg, *The Physical Principles of the Quantum Theory* (Dover, 1949)**].

If electrons are made to pass through a slit of width *d*, then their co-ordinates in the direction of this width are known at the moment after having passed it with the accuracy $\Delta x = d$. If we assume the momentum in this direction to have been zero before passing through the slit (normal incidence), it would appear that the uncertainty relation is not fulfilled. But the electron may also be considered to be a plane de Broglie wave, and it is at once apparent that diffraction phenomena are necessarily produced by the slit. The emergent beam has a finite angle of divergence *d*, which is, by the simplest laws of optics,

$$\sin\alpha \approx \frac{\lambda}{d},$$

where λ is the wave-length of the de Broglie waves. Thus, the momentum of the electron parallel to the screen is uncertain, after passing through the slit, by an amount

$$\Delta p = \frac{h}{\lambda}\sin\alpha,$$

since h/λ is the momentum of the electron in the direction of the beam. Then, since $\Delta x = d$, we have

$$\Delta x \Delta p = \frac{h}{\lambda} d \sin\alpha \sim h. \qquad \text{(Heisenberg's principle of uncertainty)}$$

REFERENCES

W. Heisenberg, *The Physical Principles of the Quantum Theory* (Dover, 1949).

12.2 Fraunhofer diffraction power spectrum for the rectangle aperture

In optics, the Fraunhofer diffraction equation is used to model the diffraction of waves when the diffraction pattern is viewed at a long distance from the diffracting object, and also when it is viewed at the focal plane of an imaging lens. The *amplitude* in the diffraction pattern is simply the 2D Fourier transform of the aperture, besides scaling. We calculate the Fraunhofer diffraction power spectrum for the rectangle aperture with the sides Δx and Δy. We make a plot of power spectrum when Δx is changed as a parameter while Δy is kept constant. As the width Δx increases, the width of the spectrum decreases.

$$\Delta k_x \propto \frac{1}{\Delta x},$$

supporting the validity of the Heisenberg's principle of uncertainty, where $p_x = \hbar k_x$.

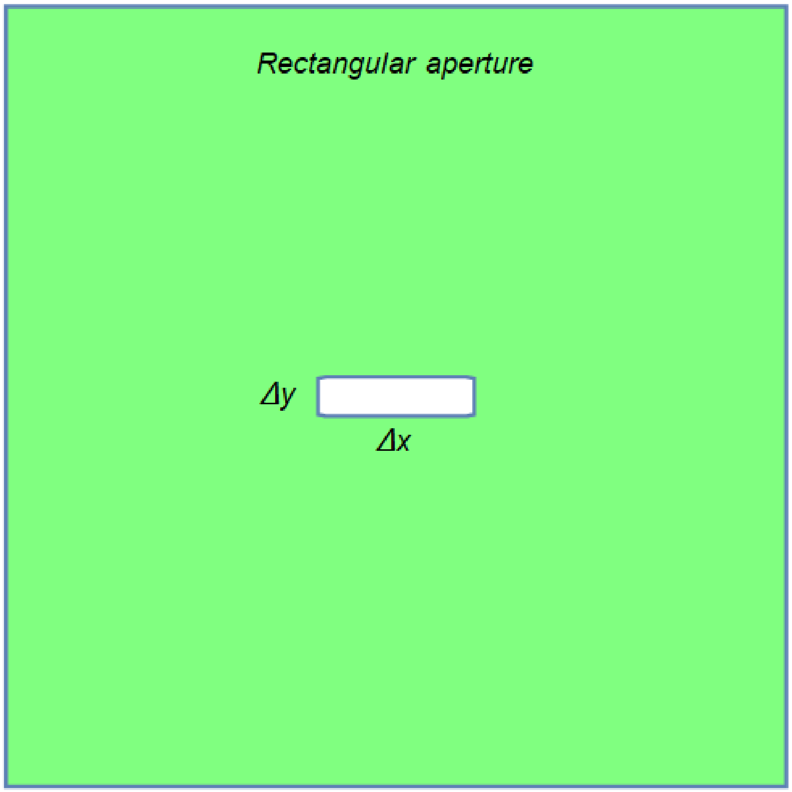


Fig. Rectangular aperture with sides of Δx and Δy.

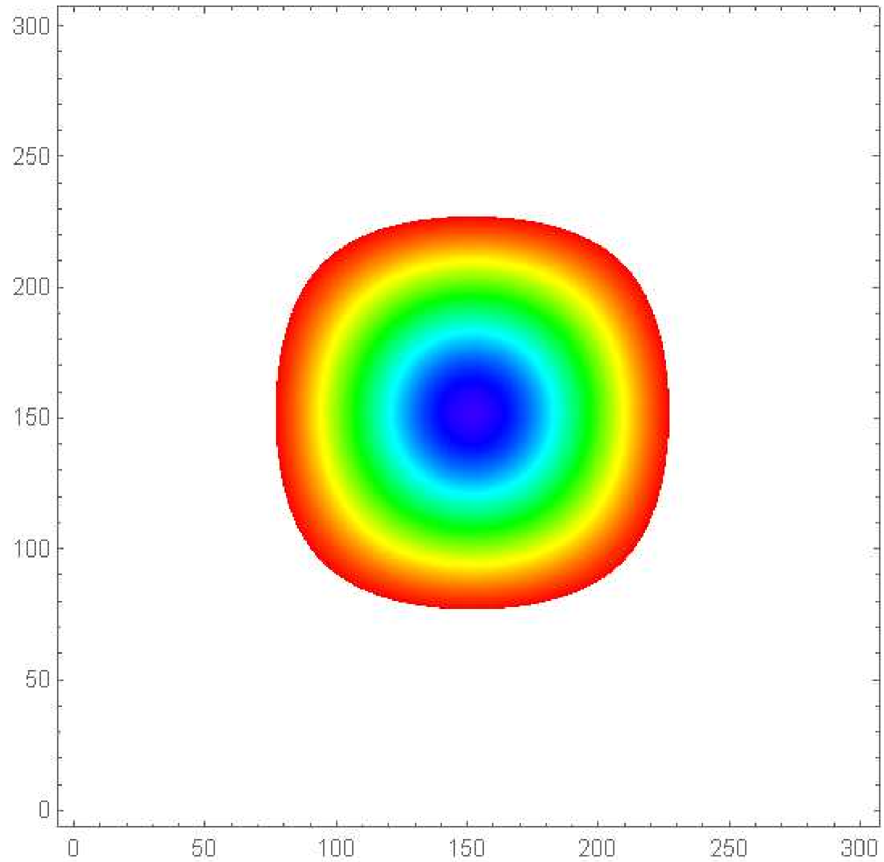


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 3$ and $\Delta y = 2$. Note that Δy is kept constant during this calculation here.

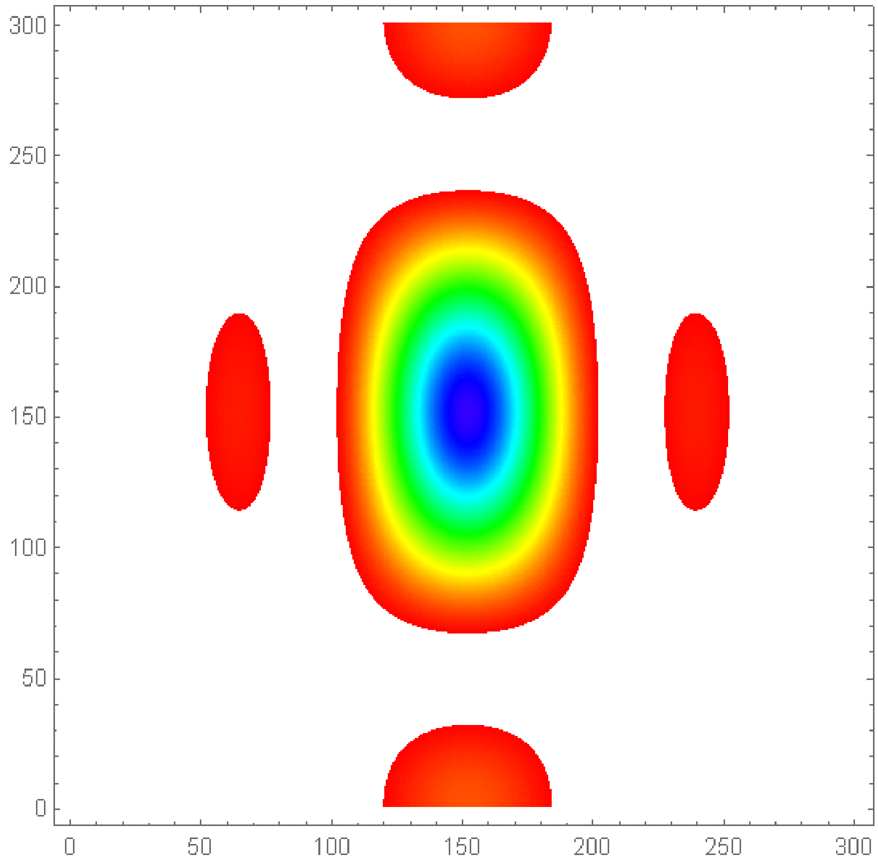


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 4$ and $\Delta y = 2$

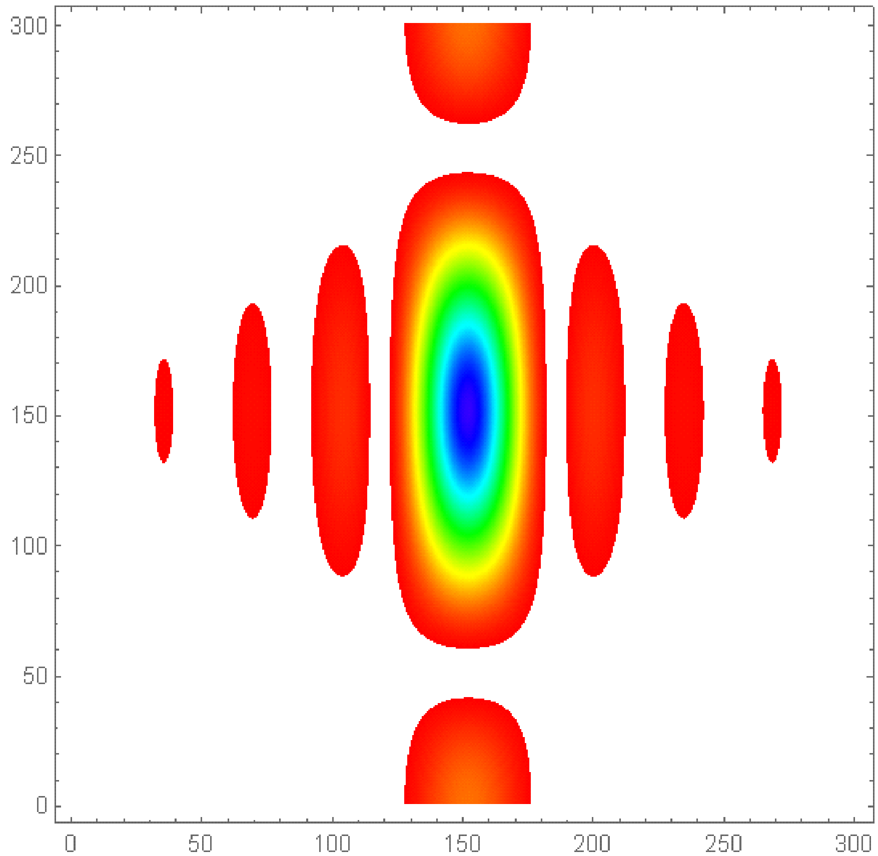


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 8$ and $\Delta y = 2$

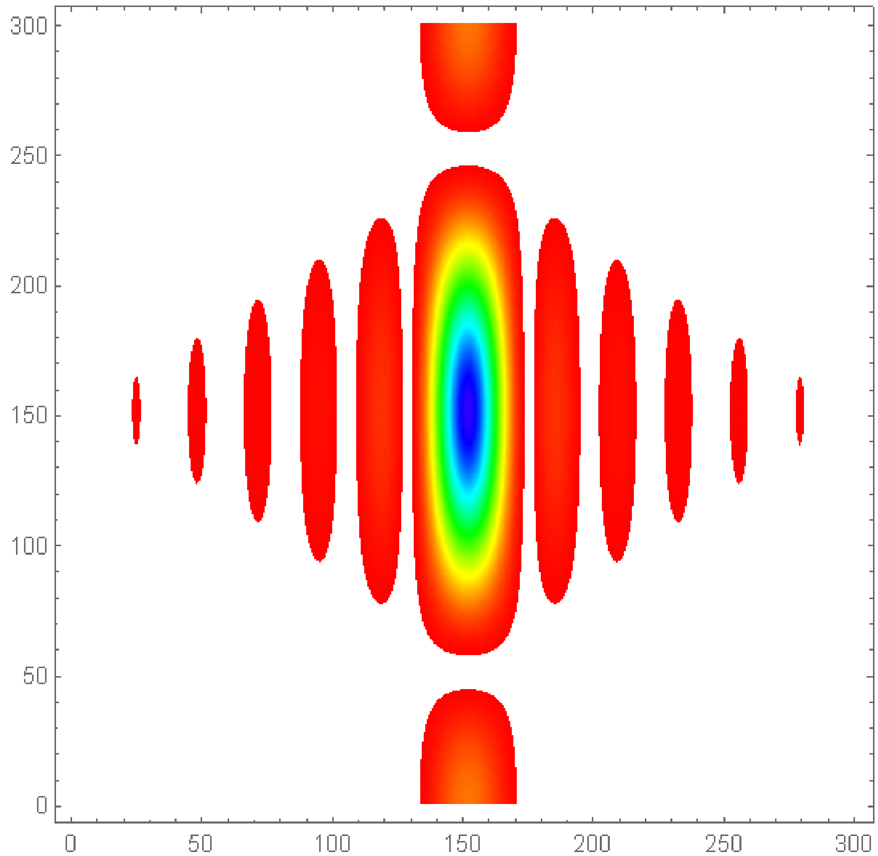


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 12$ and $\Delta y = 2$

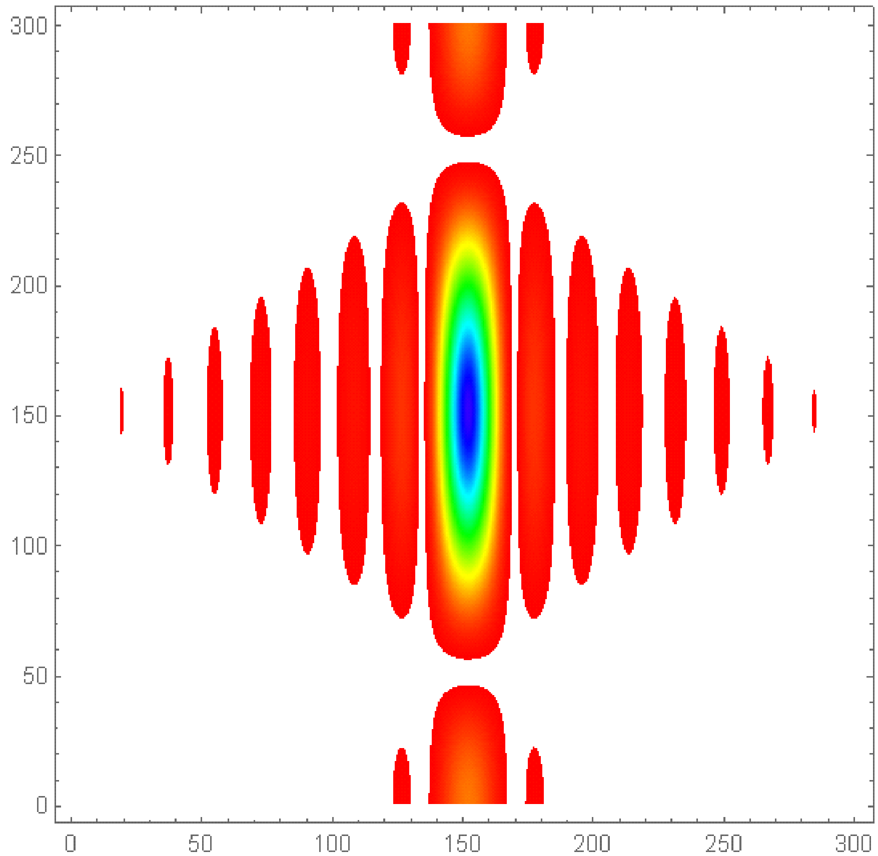


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 16$ and $\Delta y = 2$.

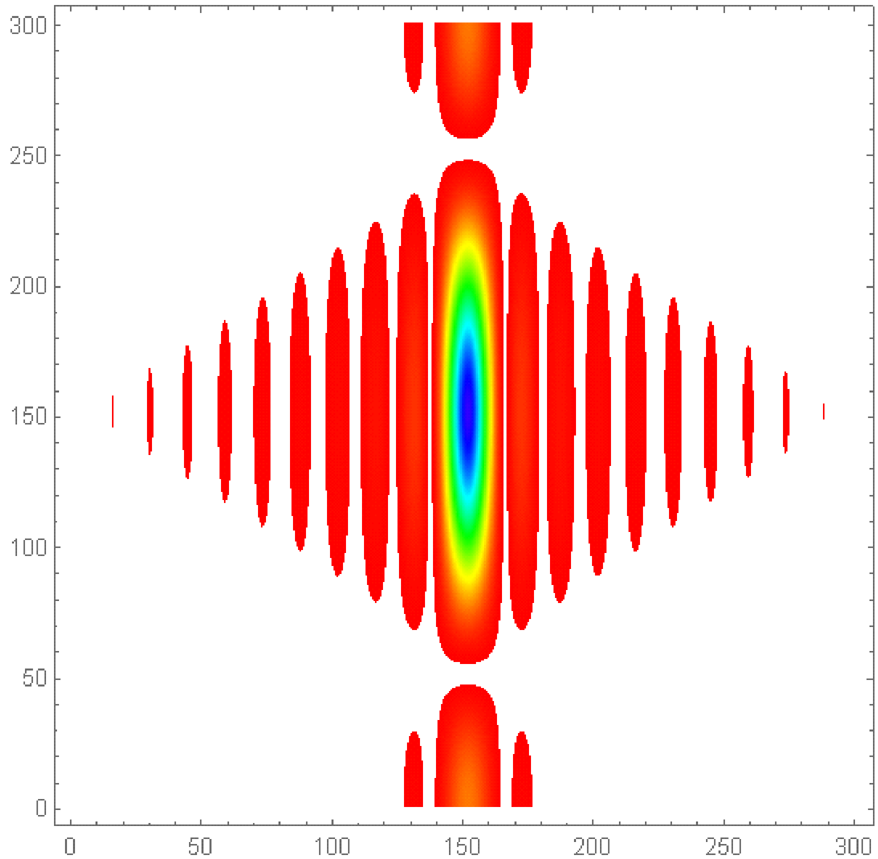


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 20$ and $\Delta y = 2$.

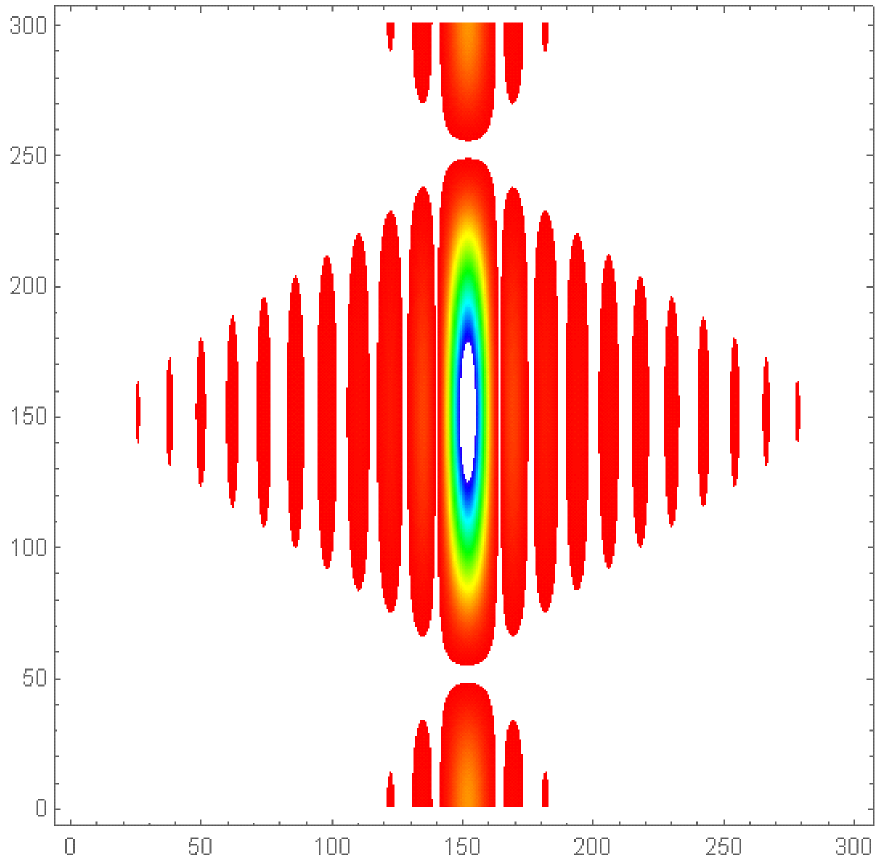


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 24$ and $\Delta y = 2$.

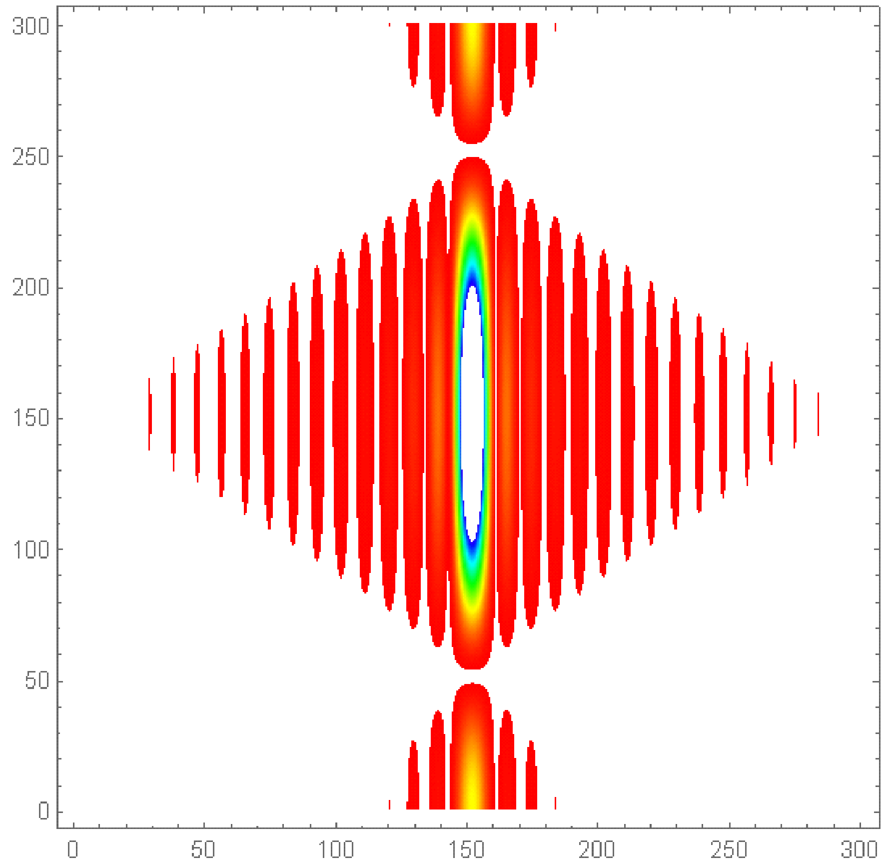


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 32$ and $\Delta y = 2$.

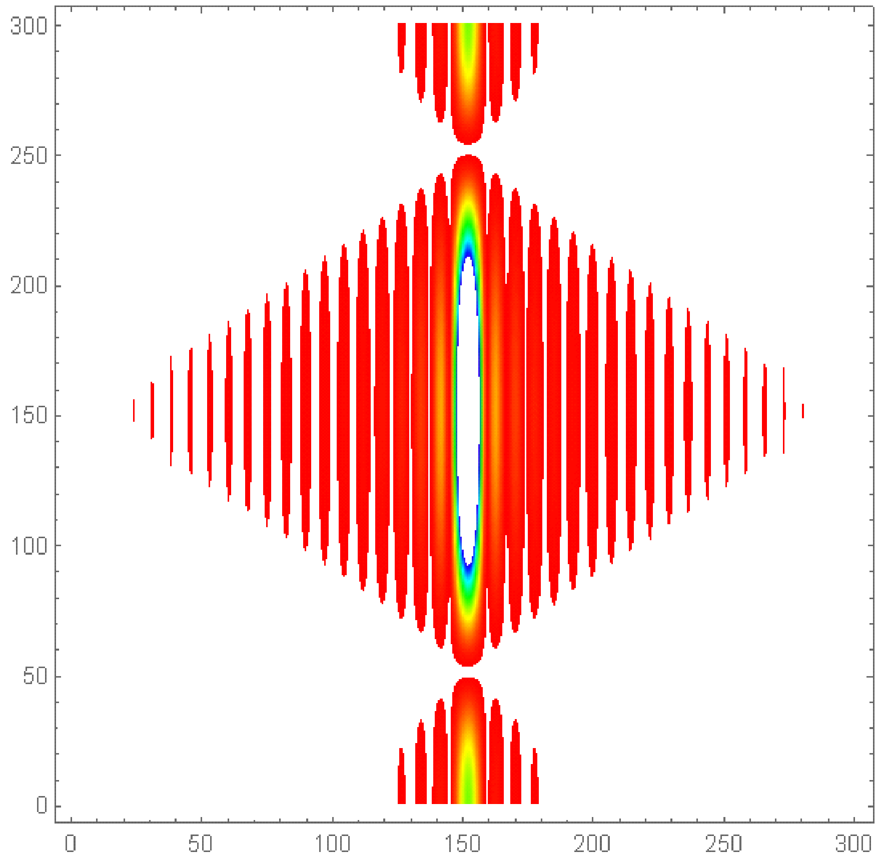


Fig. Fraunhofer diffraction power spectrum for the rectangle slit with widths $\Delta x = 40$ and $\Delta y = 2$.

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