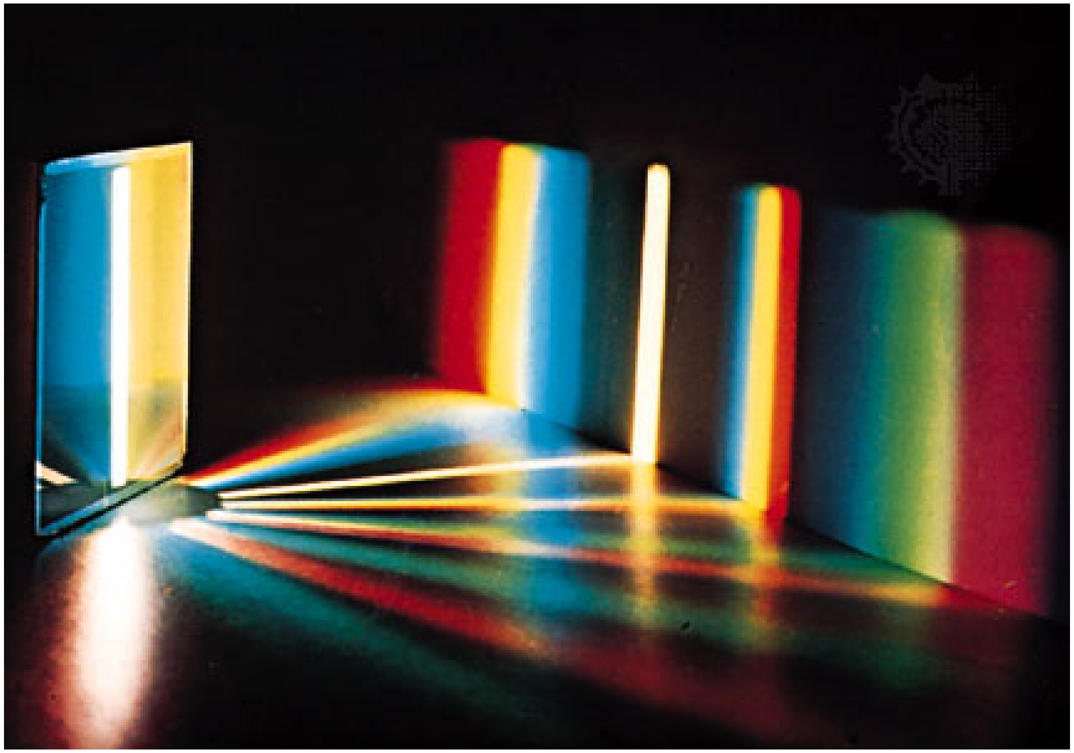
33. Diffraction: a few important illustrations

Babinet's Principle

Diffraction gratings

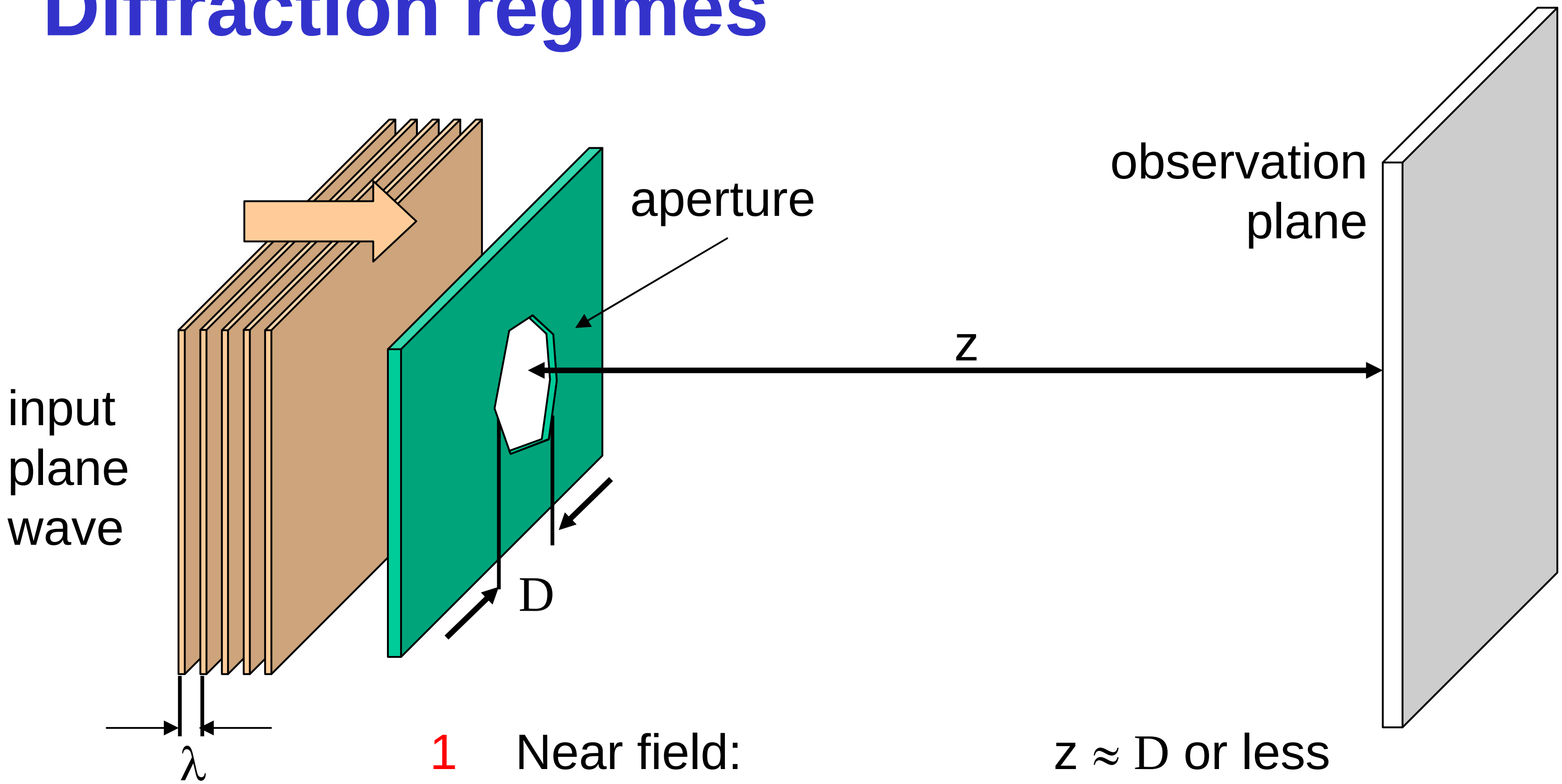
X-ray diffraction:
Bragg scattering
and crystal structures



A lens transforms a Fresnel diffraction problem into a Fraunhofer diffraction problem

Diffraction and image resolution: the Rayleigh criterion

Diffraction regimes



Note: this is the typical ordering of the regimes; if the aperture is smaller than the wavelength, then regimes **2** and **3** could be swapped.

1 Near field: $z \approx D$ or less

2 Fresnel diffraction: $z >> D$ (paraxial)

3 Fraunhofer diffraction: $z >> \pi D^2/\lambda$ and $z >> D$

In the Fraunhofer regime, the diffraction pattern is a Fourier transform.

Babinet's Principle

Jacques Babinet
1794-1872

Fraunhofer diffraction is a Fourier transform:

$$E_A(x_0, y_0) \propto \iint \exp\left\{-\frac{jk}{z}(x_0 x_1 + y_0 y_1)\right\} Aperture(x_1, y_1)\, dx_1 dy_1$$

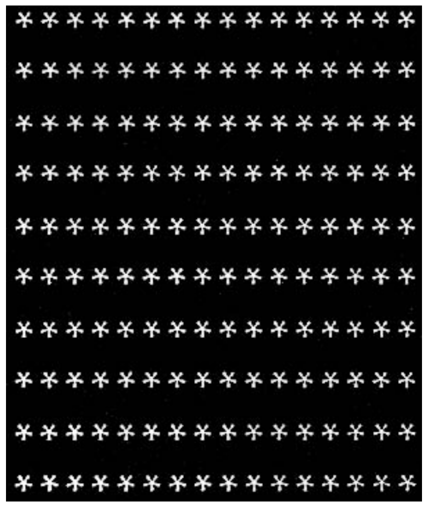
A complementary aperture (one which is the inverse of the original one) must give a related diffraction pattern:

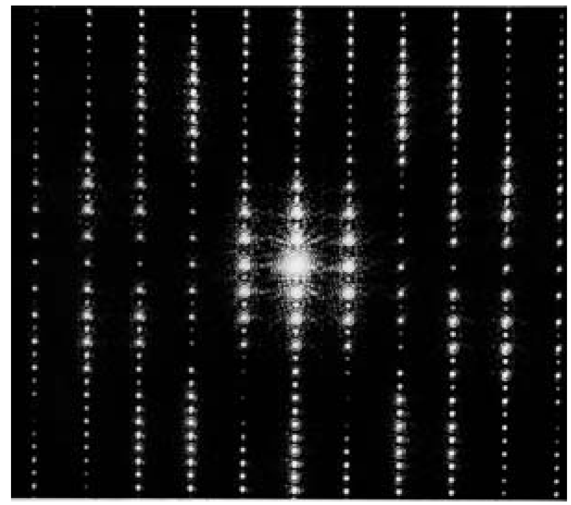
$$E_C(x_0, y_0) \propto \iint \exp\left\{-\frac{jk}{z}(x_0 x_1 + y_0 y_1)\right\} \left[1 - Aperture(x_1, y_1)\right] dx_1 dy_1$$

Thus: $E_C(x_0, y_0) = -E_A(x_0, y_0)$ at all points except $x_0 = y_0 = 0$

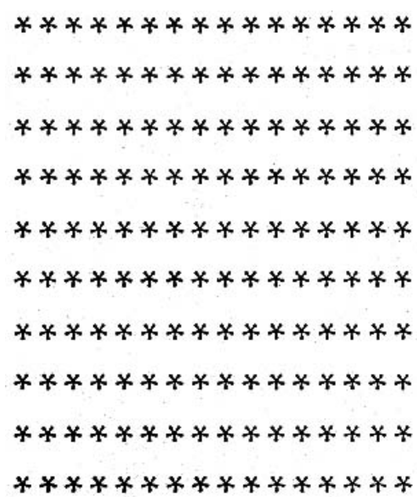
Babinet's Principle in action

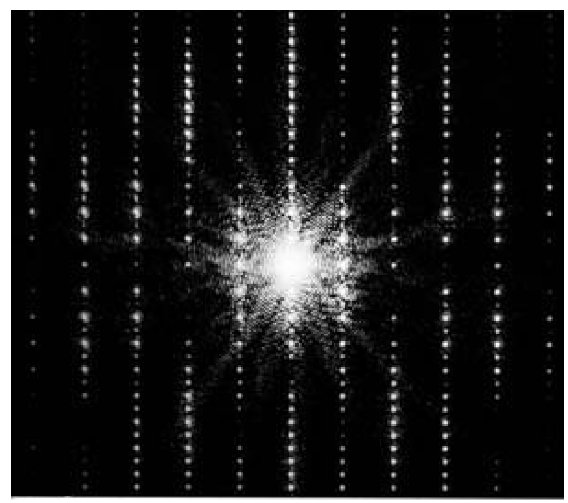
an array
of holes





an array of
anti-holes





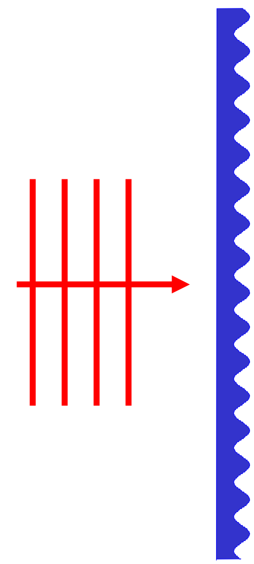
The Diffraction Grating

A diffraction grating is a slab
with a periodic modulation
of any sort on one of its surfaces.

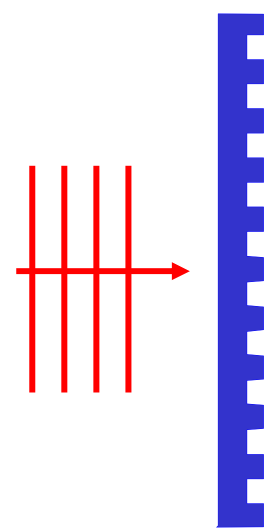
The modulation can be in
transmission, reflection, or
the phase delay of a beam.

The grating is then said to be
a transmission grating,
reflection grating, or
phase grating, respectively.

What happens when a
plane wave illuminates
an object of this sort?

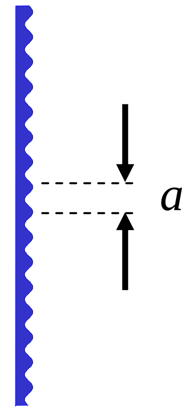


A sinusoidal
modulation



A square
modulation

Diffraction Grating Mathematics



As an example, consider a sinusoidal modulation of the transmission:

$$Aperture(x_1, y_1) = A + B\cos(2\pi x_1 / a)$$

where a is the "grating spacing." The Fraunhofer diffracted field is:

$$E\left(x_0, y_0\right) \propto \iint Aperture(x_1, y_1)\, \exp\left\{-\frac{jk}{z}(x_0 x_1 + y_0 y_1)\right\}\, dx_1 dy_1$$

Ignoring the y_1 integration, the x_1 integral is just the Fourier transform of a constant (A) plus $B\cos(2\pi x_1/a)$:

$$E(x_0) \propto \int \left[A + B\cos(2\pi x_1 / a)\right]\exp\left\{-\frac{jk}{z}(x_0 x_1)\right\} dx_1$$

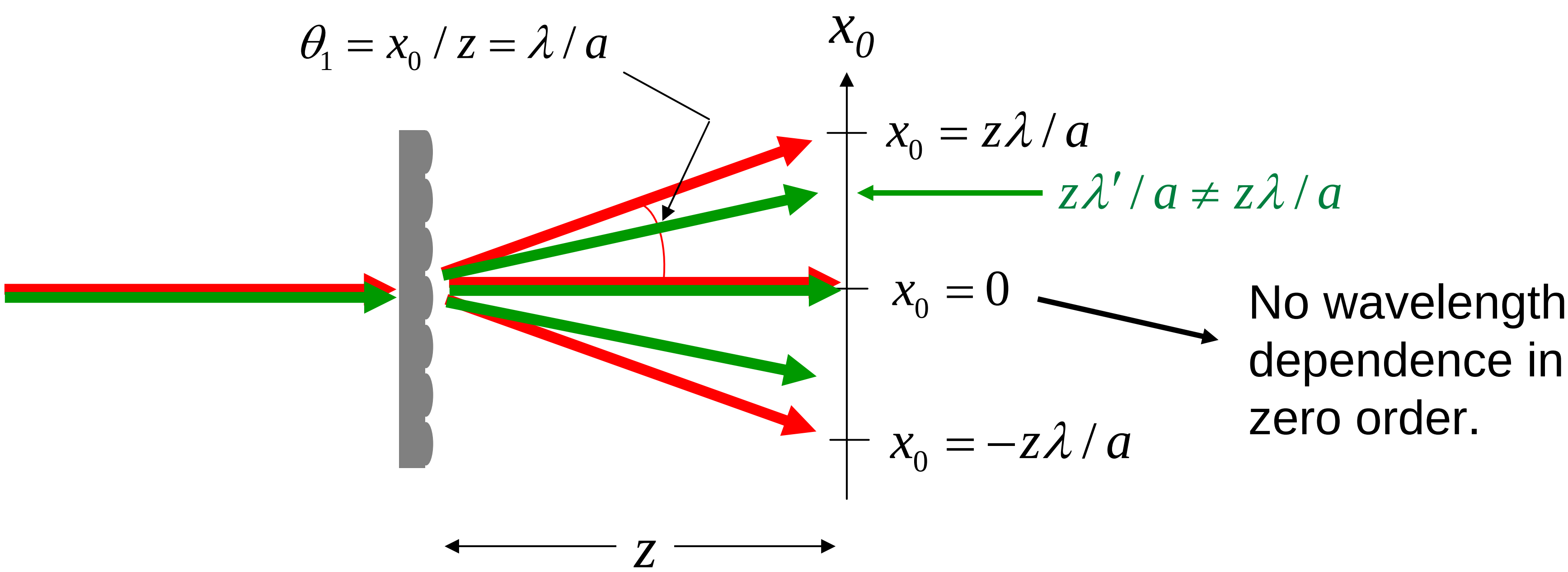
$$\propto \pi B\delta([kx_0 / z] - 2\pi / a) + 2\pi A\delta([kx_0 / z]) + \pi B\delta([kx_0 / z] + 2\pi / a)$$

$x_0 = z\lambda / a$ — first order

$x_0 = 0$ — zeroth order

$x_0 = -z\lambda / a$ — negative first order

Diffraction orders



Because x_0 depends on λ for the +1 and –1 orders, different wavelengths are separated.

The longer the wavelength, the larger its diffraction angle.
(except for zeroth order)

Diffraction Grating Mathematics: Higher Orders

What if the periodic modulation of the transmission is not sinusoidal?

Since it's periodic, we can use a Fourier Series for it:

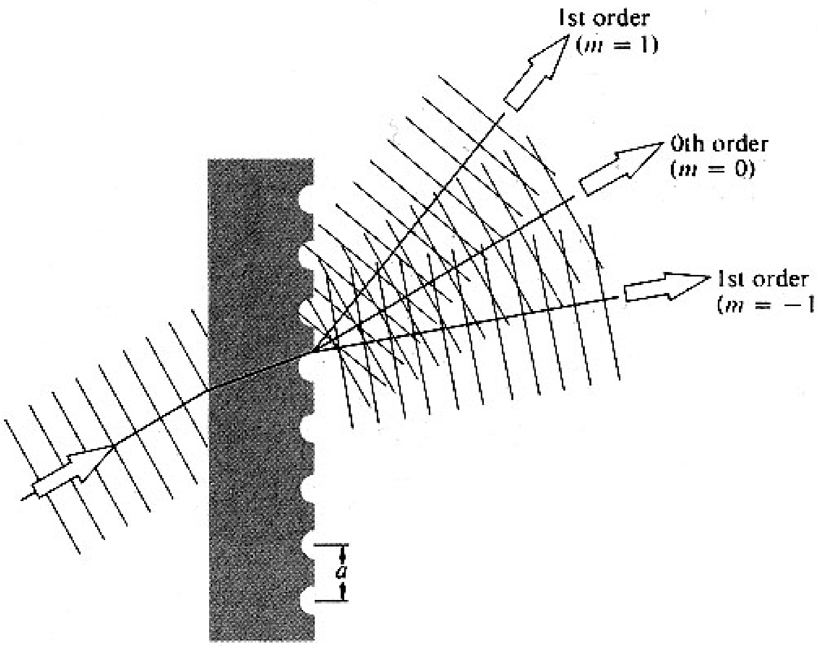
$$Aperture(x_1, y_1) = A_0 + A_1 \cos(2\pi x_1 / a) + A_2 \cos(4\pi x_1 / a) + A_3 \cos(6\pi x_1 / a) + \ldots$$

Keeping up to third order, the resulting Fourier Transform is:

$$\begin{array}{llll}
\propto \pi A_3 \delta([kx_0 / z] - 6\pi / a) & \rightarrow & x_0 = 6\pi z / ka = 3 z\lambda / a & \text{3rd order} \\
+\pi A_2 \delta([kx_0 / z] - 4\pi / a) & \rightarrow & x_0 = 4\pi z / ka = 2 z\lambda / a & \text{2nd order} \\
+\pi A_1 \delta([kx_0 / z] - 2\pi / a) & \rightarrow & x_0 = 2\pi z / ka = 1 z\lambda / a & \text{1st order} \\
+2\pi A_0 \delta([kx_0 / z]) & \rightarrow & x_0 = 0 & \text{0th order} \\
+\pi A_1 \delta([kx_0 / z] + 2\pi / a) & \rightarrow & x_0 = -2\pi z / ka = -1 z\lambda / a & \text{-1st order} \\
+\pi A_2 \delta([kx_0 / z] + 4\pi / a) & \rightarrow & x_0 = -4\pi z / ka = -2 z\lambda / a & \text{-2nd order} \\
+\pi A_3 \delta([kx_0 / z] + 6\pi / a) & \rightarrow & x_0 = -6\pi z / ka = -3 z\lambda / a & \text{-3rd order}
\end{array}$$

A square modulation is commonly used. It has many orders.

The Grating Equation



An order of a diffraction grating occurs if:

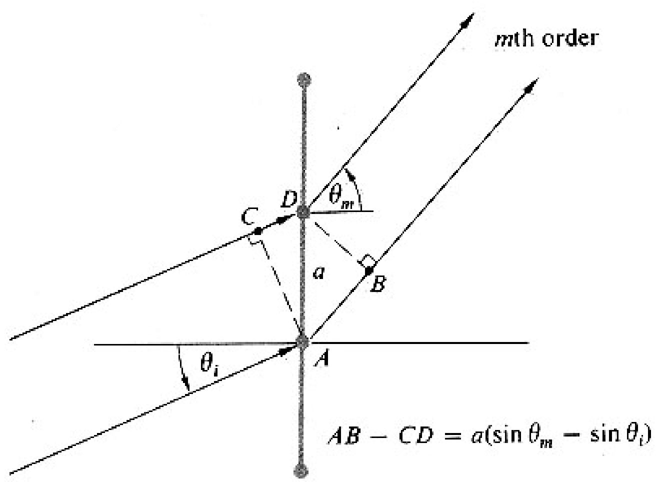
$$a\,[x_0 / z] = m\lambda \quad \text{or}$$

$$a \sin(\theta_m) = m\lambda$$

where m is an integer.

This equation assumed normal incidence and a small diffraction angle, however. One can derive a more general result, the "grating equation," using a tilted input beam:

$$\boxed{a\left[\sin(\theta_m) - \sin(\theta_i)\right] = m\lambda}$$

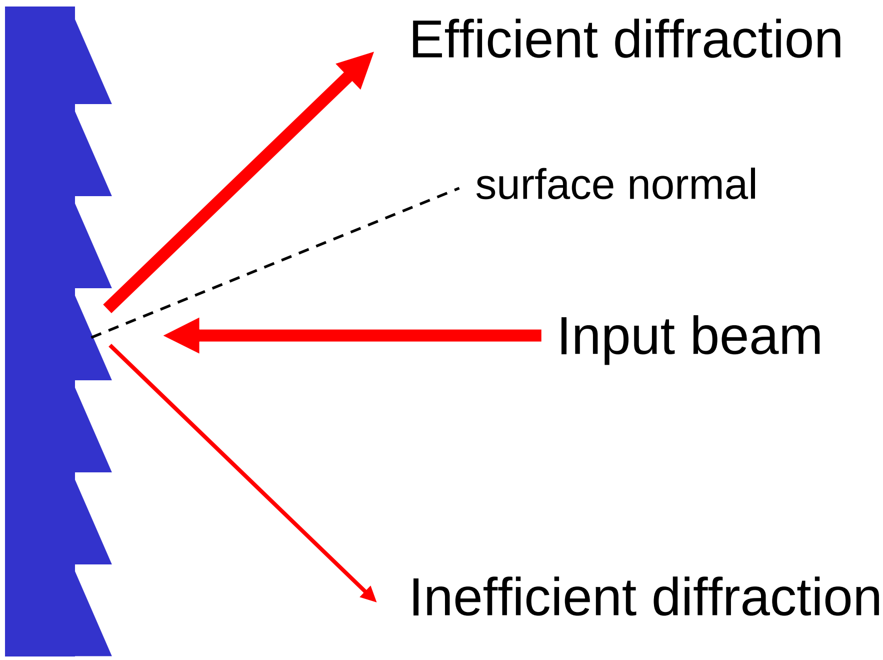


Remember that the diffracted angle can be negative, too. But it cannot be larger than ±90°.

Blazed Diffraction Grating

By tilting the facets of the grating so the desired diffraction order coincides with the specular reflection from the facets, the grating efficiency can be increased.

"Specular" means angle of incidence equals angle of reflection.

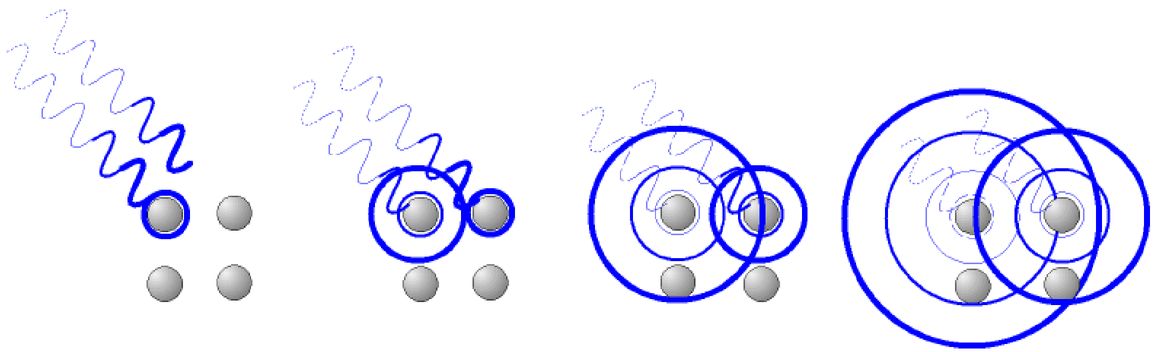


Even though both diffracted beams satisfy the grating equation, one is vastly more intense than the other.

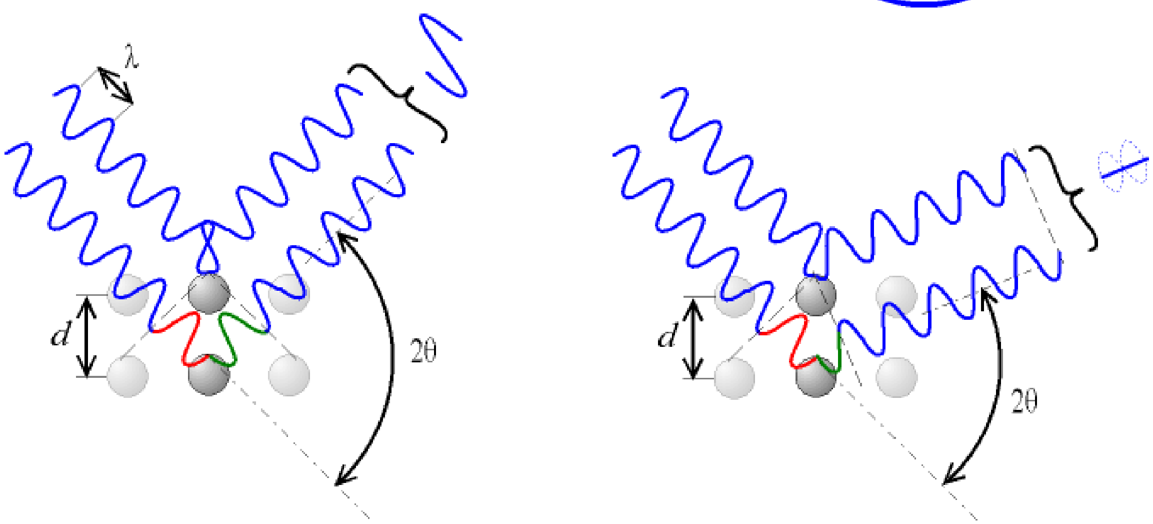
Diffraction from a periodic array: Bragg's Law

We can also derive the grating condition by looking at the path length difference between waves scattered from adjacent sites in a periodic array.

This leads us to Bragg's Law, for scattering of x-rays from crystalline materials. This is really equivalent to the grating diffraction problem.

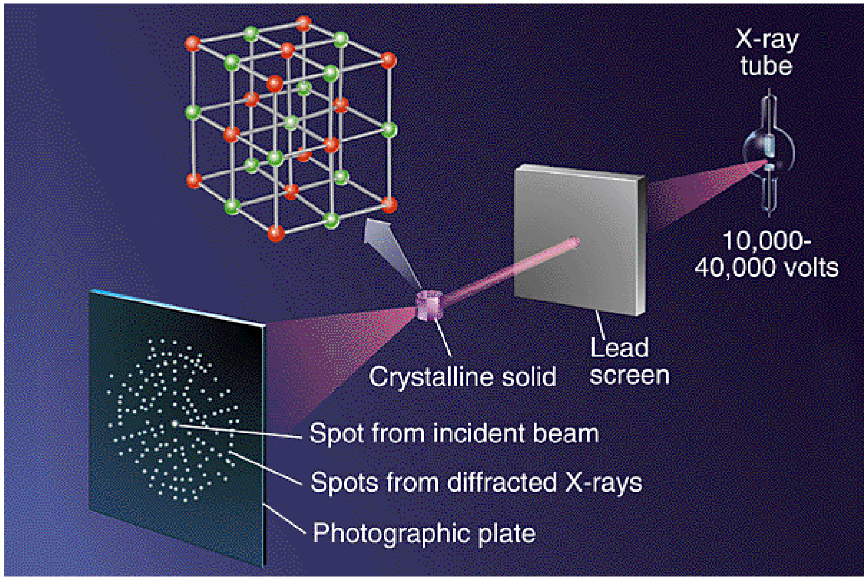


A periodic array of atoms in a lattice is illuminated by a plane wave. Each atom produces a scattered spherical wave.



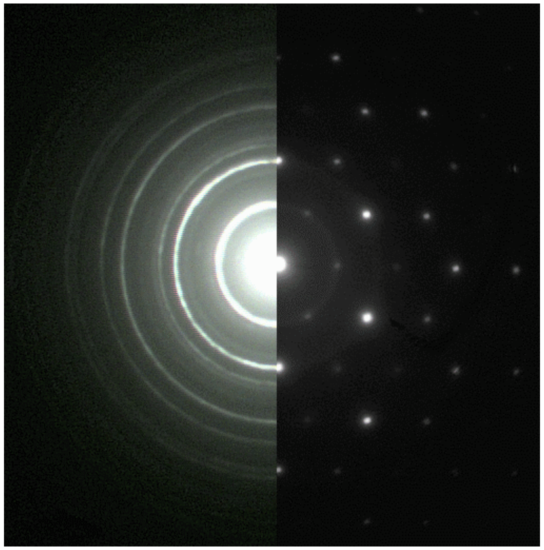
At a certain specific angle, the scattered waves interfere constructively, just as in the case of waves scattered from a grating.

X-ray Crystallography

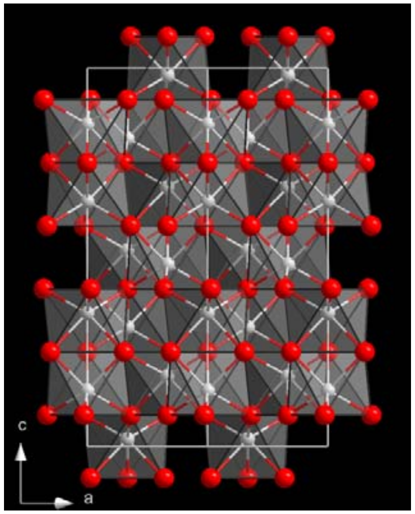


The tendency of diffraction to expand the smallest structure into the largest pattern is the key to the technique of x-ray crystallography, in which x-rays diffract off the nuclei of crystals, and the diffraction pattern reveals the crystal molecular structure.

This is the standard method for determining the crystal structure of any solid.

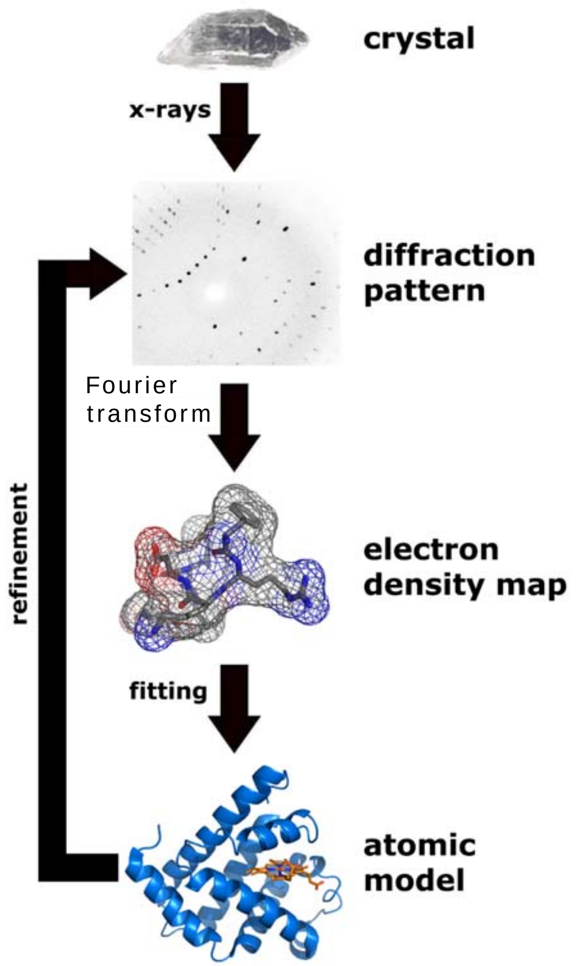


X-ray diffraction pattern from polycrystalline (left) and single-crystal (right) Cr_2O_3



crystal structure of Cr_2O_3

Application: Finding the structures of biomolecules

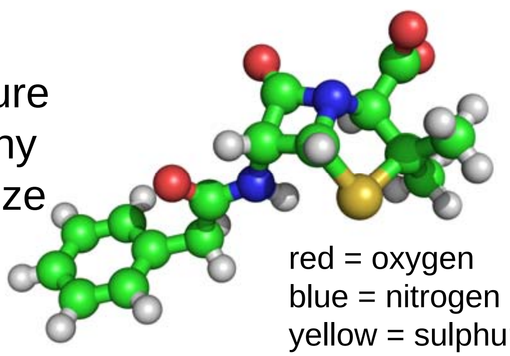


Knowing where all the atoms are in a large molecule is difficult. But it is crucial for understanding how molecules interact and function.

If you can persuade the molecules to form a crystal, that is, to arrange themselves regularly in space, then you can use x-ray diffraction to find the location of every atom.

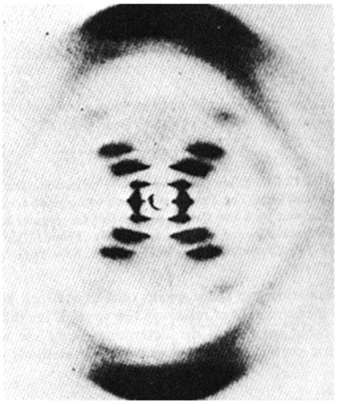
This idea is most important in biology.
A classic example:

the three-dimensional structure of penicillin, solved by Dorothy Crowfoot Hodgkin (Nobel Prize in Chemistry, 1964)



red = oxygen
blue = nitrogen
yellow = sulphur
green = carbon
white = hydrogen

The most important x-ray diffraction pattern in history

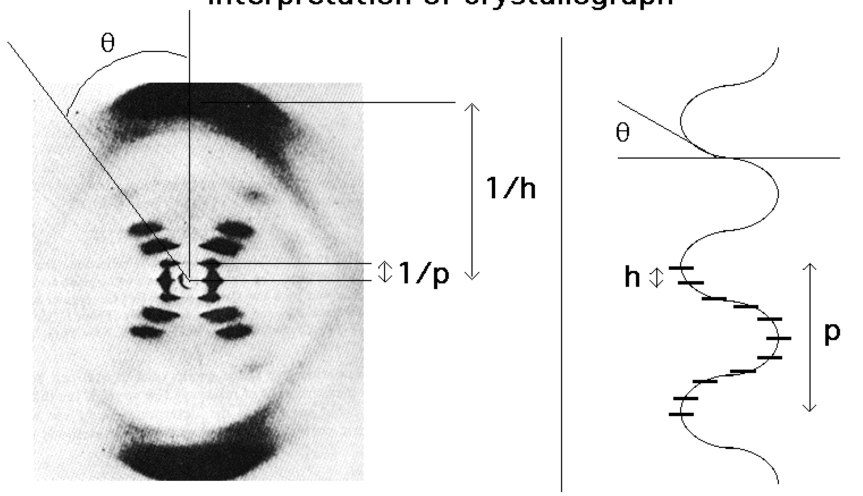


X-ray diffraction pattern from B form of DNA

Data obtained by Rosalind Franklin, 1952.

Nobel prize obtained by Crick and Watson, 1962

Interpretation of crystallograph



θ - tilt of helix (angle from perpendicular to long axis)

h = 3.4 Å (Distance between bases)

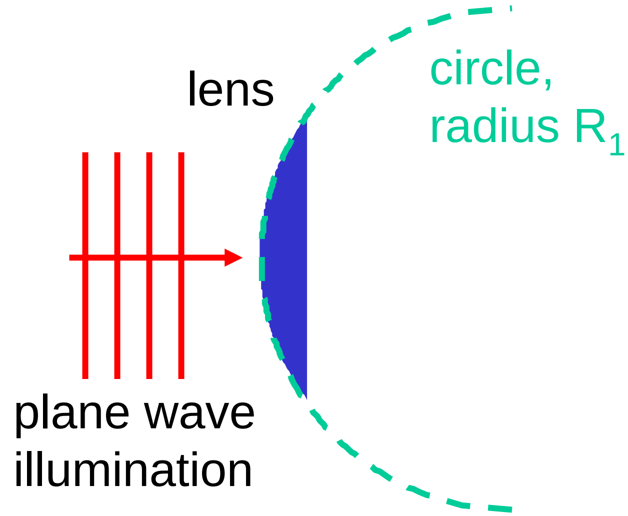
p = 34 Å (Distance for one complete turn of helix; Repeat unit of the helix)

Diffraction treatment of a spherical lens

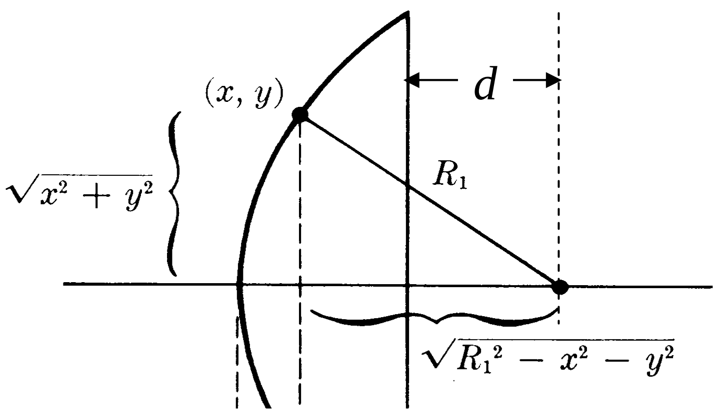
An ideal lens has unity transmission, but it introduces a phase delay proportional to its thickness at a given point (x_1,y_1):

$$lens(x_1, y_1) = \exp[\,j(n-1)k \cdot \Delta(x_1, y_1)]$$

where $\Delta(x_1,y_1)$ is the thickness at the point (x_1,y_1).



Compute $\Delta(x_1,y_1)$:



$$\Delta(x, y) = \sqrt{R_1^2 - x^2 - y^2} - d$$

$$lens(x_1, y_1) = \exp\left[\, j(n-1)k\left\{\sqrt{R_1^2 - (x_1^2 + y_1^2)} - d\right\}\right]$$

$$\sqrt{R_1^2 - x_1^2 - y_1^2} = R_1\sqrt{1-(x_1^2 + y_1^2)/R_1^2} \approx R_1 - \frac{x_1^2 + y_1^2}{2R_1}$$

$$lens(x_1, y_1) \approx \exp[-jk(n-1)\left(x_1^2 + y_1^2\right)\big/2R_1]$$

where we have neglected constant (independent of x_1, y_1) phase delays.

In the focal plane, the diffraction problem is Fraunhofer

A lens has a phase delay proportional to its thickness at a given point (x_1,y_1):

$$lens(x_1, y_1) = \exp\left[-j\frac{(n-1)k}{2R_1}\left(x_1^2 + y_1^2\right)\right]$$

If we substitute this result into the <u>Fresnel</u> (not Fraunhofer) integral:

$$E(x_0, y_0) \propto \iint\limits_{Aperture} \exp\left\{ jk\left[\frac{(-2x_0x_1 - 2y_0y_1}{2z} + \frac{(x_1^2 + y_1^2)}{2z}\right]\right\} lens(x_1, y_1)\, dx_1 dy_1$$

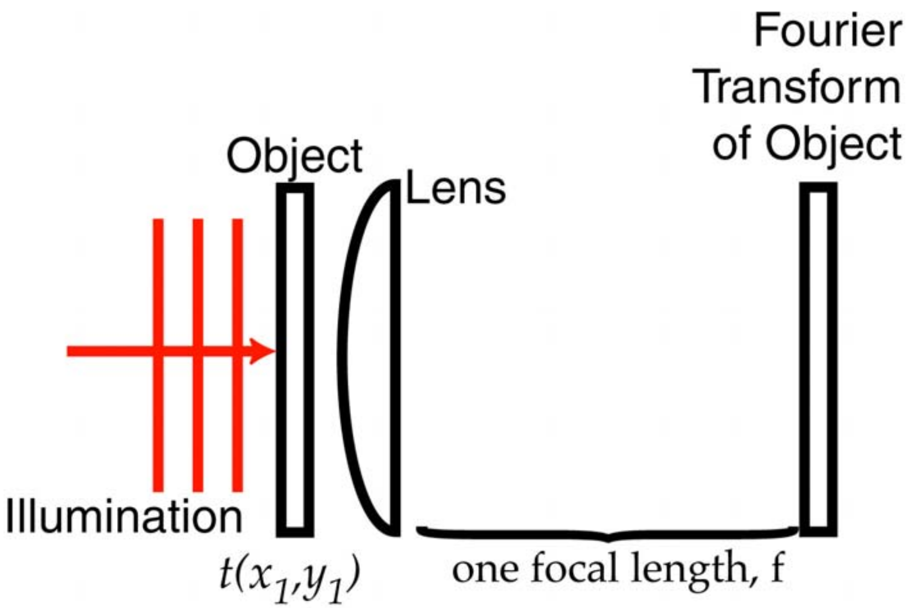
the quadratic terms x_1^2 and y_1^2 will cancel provided that:

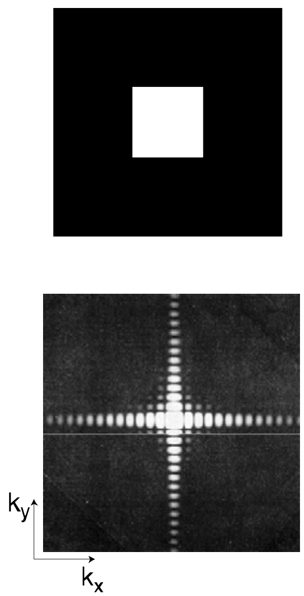
$$(n-1)(k/2R_1) = (k/2z) \qquad \text{or} \qquad 1/z = (n-1)(1/R_1)$$

But this is the Lensmaker's Formula! The distance z which satisfies this condition is the focal length of the lens!

A lens brings the far field in to its focal plane

If we look in a plane one focal length beyond a lens, we are in the Fraunhofer regime, even if it isn't far away! So we see the Fourier Transform of any object that is in front of the lens.





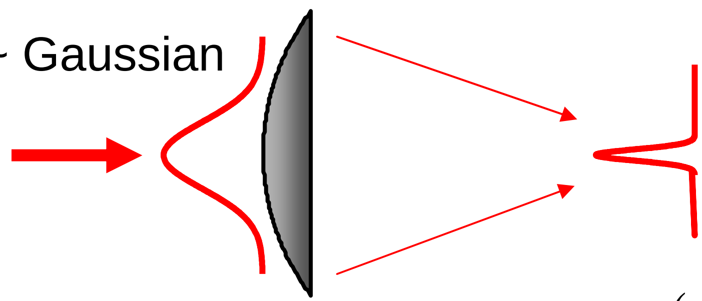
Object: an opaque screen with a square hole

Focal plane: sinc(x) * sinc(y)

A lens in this configuration is said to be a "Fourier-Transforming lens."

A focused Gaussian beam produces a Gaussian spot at the focus. But a focused plane wave produces an Airy pattern.

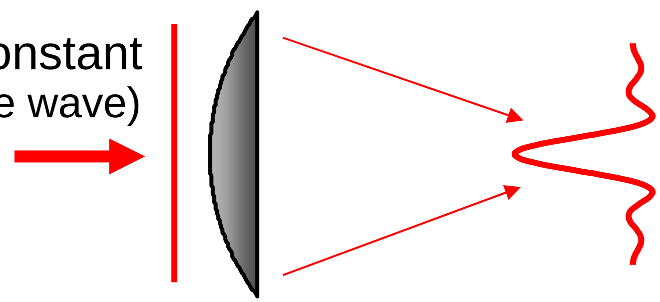
input: $I(x_1,y_1)$ ~ Gaussian



in the Fourier plane: still Gaussian, but narrower: ρ_{spot} depends on w_{input}

$$Gaussian(x_0, y_0) \propto FT\{Gaussian(x_1, y_1)\}$$

input: $I(x_1,y_1)$ ~ constant
(plane wave)



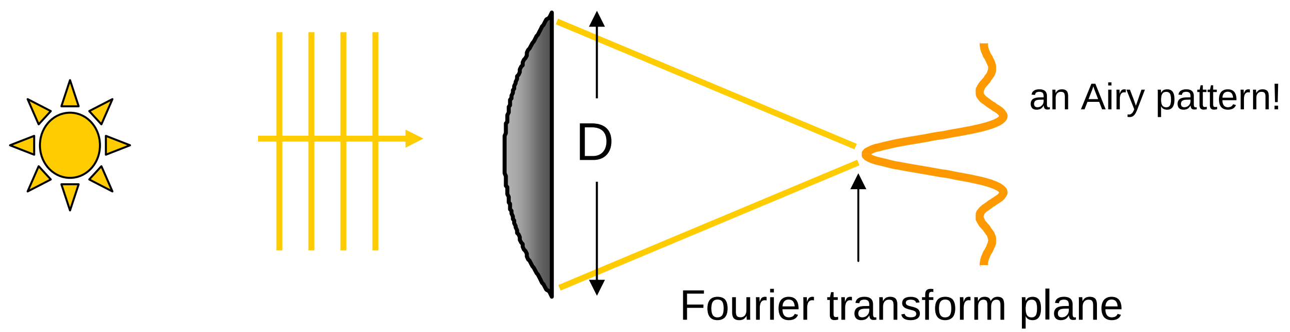
in the Fourier plane: an Airy pattern $[J_1(\rho)/\rho]^2$

$$Airy(x_0, y_0) \propto FT\{const(x_1, y_1),\ \text{for } r < R_{lens}\}$$

The size of the Airy pattern is determined by the size of the lens.

Application: resolution limit of a telescope

Consider a telescope looking at a distant star…



In this case, the telescope pupil (the size of the lens) is the limiting aperture. A plane wave illuminating this circular aperture produces an Airy pattern in the image plane. The size of this image is determined by the size of the lens, D, and the focal length, f, according to:

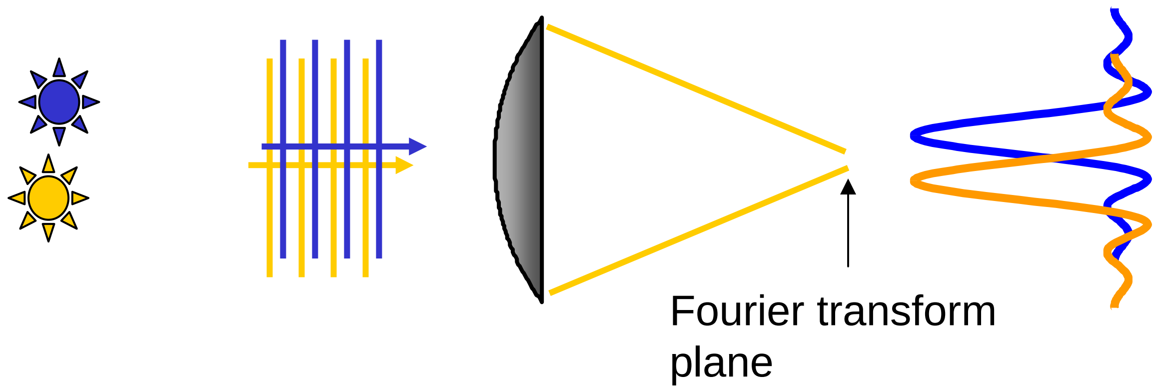
$$\rho_{spot} = 1.22 \frac{\lambda f}{D} = 1.22\lambda \left(f /\# \right)$$

The angular spread $\Delta\theta$ is given by ρ_{spot}/f, and therefore:

$$\Delta\theta = 1.22\,\lambda / D$$

Application: resolution limit of a telescope

Now consider a telescope looking at two distant stars…



<u>Rayleigh criterion:</u> it is possible to resolve the two stars when the peak of the Airy pattern of one coincides with the first minimum of the Airy pattern of the other one.

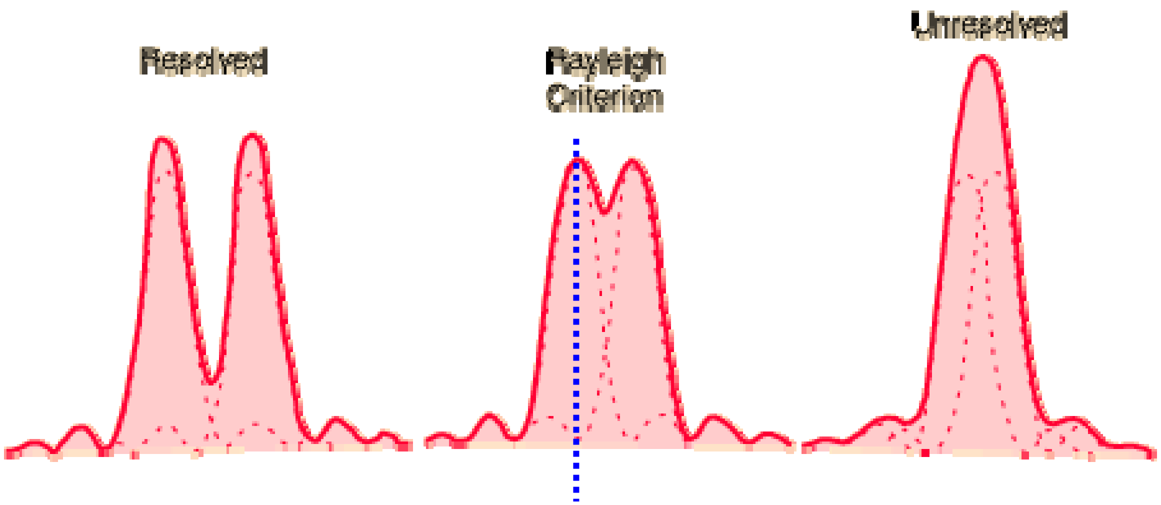
Thus, the telescope is able to resolve two stars if they are separated in the sky by at least an angle of:

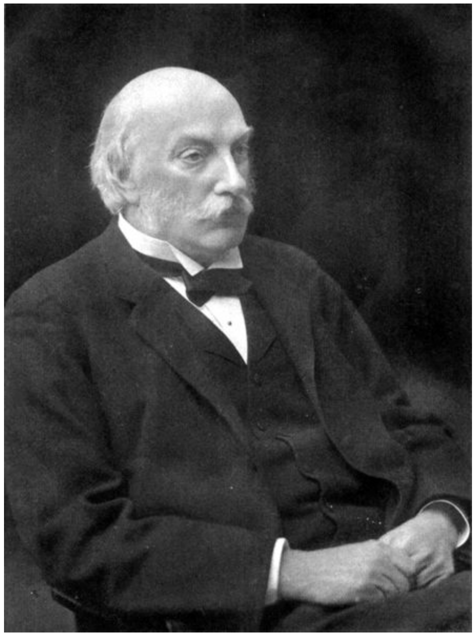
$$\Delta\theta_{\min} = 1.22\,\lambda/D$$

Resolution can be improved by (a) decreasing λ, or (b) increasing D.

The Rayleigh criterion

Once again, Rayleigh is The Man…



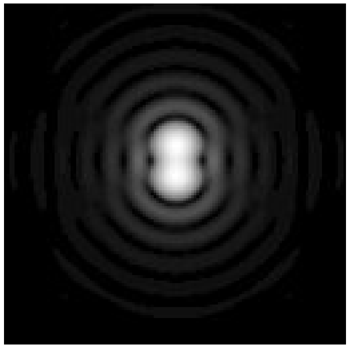


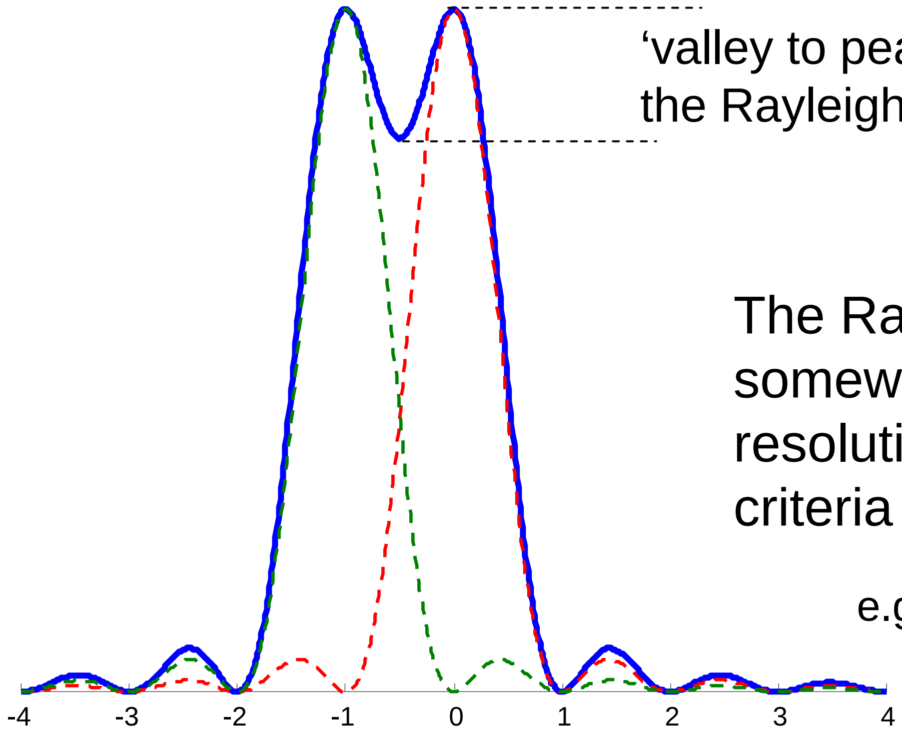
John William Strutt,
3rd Baron Rayleigh
1842 - 1919

“This rule is convenient on account of its simplicity and it is sufficiently accurate in view of the necessary uncertainty as to what exactly is meant by resolution.”

The Rayleigh criterion

These two Airy patterns are just barely resolved, according to Rayleigh's criterion.





'valley to peak ratio' = 73% when the Rayleigh criterion is satisfied.

The Rayleigh criterion is a somewhat arbitrary definition of resolution. There are other criteria that are also often used.

e.g., see Sparrow Criterion

Application: resolution limit of a telescope

Hubble space telescope

The size of the reflecting mirror in Hubble is:

$$D = 2.4 \text{ meters}$$

So, for green light,

$$\lambda = 500 \text{ nanometers}$$

the resolving power of Hubble is:

$$\Delta\theta_{\min} \approx 2.5\times10^{-7} \text{ radians}$$
$$= 0.05 \text{ arc-seconds}$$

In fact, Hubble usually achieves a resolution of about 0.1 arc-sec, which is about two times the diffraction limit. This is limited by spherical abberation of the focusing mirror.