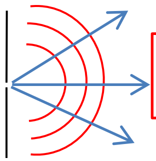
Diffraction

Wavenumber $k = \frac{2\pi}{\lambda}$ $\quad \omega = 2\pi f$ Frequency $\quad$ Wave speed $c = f\lambda$ $\quad \omega = ck$ $\quad$ Wave power input $P = \frac{1}{2}ZA^2\omega^2$ $\quad$ Z = Wave impedance

The *Huygens-Fresnel Principle* states: *"Every unobstructed point of a wavefront, at a given instant, serves as a source of spherical secondary wavelets (with the same frequency as that of the primary wave). The amplitude of the optical field at any point beyond is the superposition of all these wavelets (considering their amplitudes and relative phases)."*

Hence to determine the *wavefield* beyond an illuminated edge of slit, we need to add up the effect of spherical wave sources in the vicinity of the slit or *aperture*.

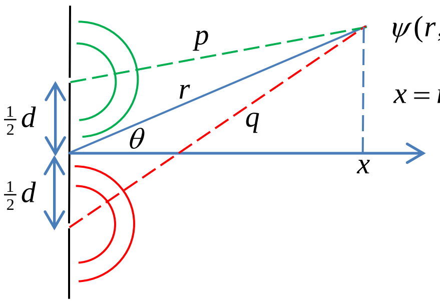
An infinitesimally thin slit



$$\psi(r,t) = \frac{Ae^{i(kr-\omega t)}}{r}$$

Two infinitesimally thin slits

'Young's double slits'



$$\psi(r,t) = \frac{Ae^{i(kp-\omega t)}}{p} + \frac{Ae^{i(kq-\omega t)}}{q}$$

$$x = r\cos\theta$$

Cosine Rule:

$$p^2 = r^2 + \tfrac{1}{4}d^2 - rd\cos\left(90^\circ - \theta\right)$$

$$p^2 = r^2 + \tfrac{1}{4}d^2 - rd\sin\theta$$

$$q^2 = r^2 + \tfrac{1}{4}d^2 - rd\cos\left(90^\circ + \theta\right)$$

$$p^2 = r^2 + \tfrac{1}{4}d^2 + rd\sin\theta$$

$$p = r\sqrt{1 + \tfrac{1}{4}\frac{d^2}{r^2} - \frac{d\sin\theta}{r}}$$

$$q = r\sqrt{1 + \tfrac{1}{4}\frac{d^2}{r^2} + \frac{d\sin\theta}{r}}$$

Assume $r \gg d$

$$\therefore \psi(r,t) \approx \frac{Ae^{-i\omega t}}{r}\left(e^{ikp} + e^{ikq}\right)$$

Only the phase term will vary significantly when $r \gg d$

Binomial expansion:

$$p \approx r + \tfrac{1}{8}\frac{d^2}{r} - \tfrac{1}{2}d\sin\theta$$

$$q \approx r + \tfrac{1}{8}\frac{d^2}{r} + \tfrac{1}{2}d\sin\theta$$

$$\therefore \psi(r,t) \approx \frac{Ae^{-i\omega t}}{r}e^{ik\left(r+\frac{1}{8}\frac{d^2}{r}\right)}\left(e^{-i\frac{1}{2}kd\sin\theta} + e^{i\frac{1}{2}kd\sin\theta}\right)$$

$$\psi(r,t) \approx \frac{2Ae^{-i\omega t}}{r}e^{ik\left(r+\frac{1}{8}\frac{d^2}{r}\right)}\cos\left(\tfrac{1}{2}kd\sin\theta\right)$$

$$|\psi|^2 \approx \frac{A^2}{r^2}\cos^2\left(\tfrac{1}{2}kd\sin\theta\right)$$ wave **power**

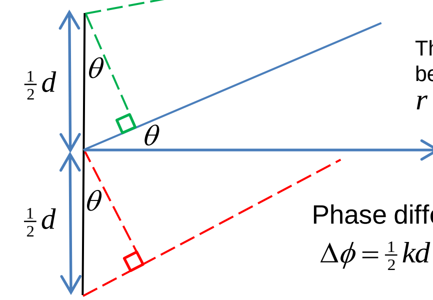
Hence *maxima* when

$\frac{1}{2}kd\sin\theta = n\pi$ $\quad$ n is an integer

$$\theta = \sin^{-1}\left(\frac{2n\pi}{kd}\right) = \sin^{-1}\left(\frac{n\lambda}{d}\right) \qquad |n| < \frac{d}{\lambda}$$

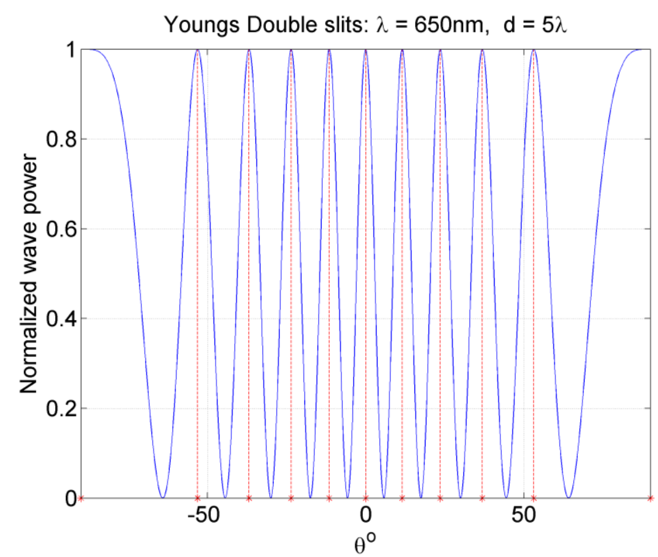
Equivalent geometry is wavelet sources are at the same angle (i.e. plane waves) but separated by $d\sin\theta$

Phase difference $\Delta\phi = -\frac{1}{2}kd\sin\theta$



This only works because $r \gg d$

Phase difference $\Delta\phi = \frac{1}{2}kd\sin\theta$

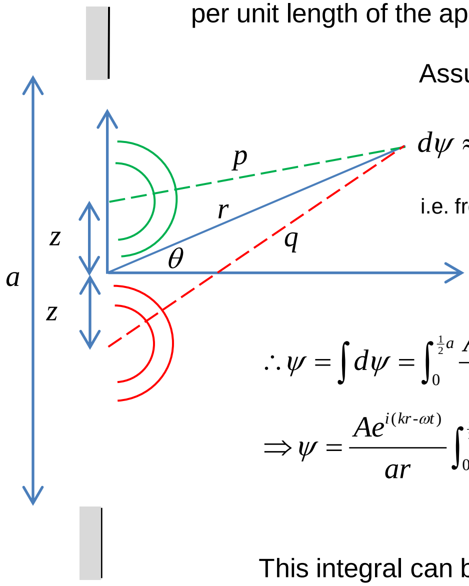


$$\sin\theta = \cos\left(90^\circ - \theta\right) \qquad -\sin\theta = \cos\left(90^\circ + \theta\right) \qquad \cos x = \tfrac{1}{2}\left(e^{ix} + e^{-ix}\right)$$

The diffraction pattern of a finite width slit

The analysis of the double slit can be extended to include pairs of infinitesimal slits which cover the whole aperture width *a*

Define *A/a* in this case to be the illumination amplitude per unit length of the aperture



Assuming $r \gg a$

$$d\psi \approx \frac{A}{a}dz\frac{e^{-i\omega t}}{r}e^{ik\left(r+\frac{1}{2}\frac{z^2}{r}\right)}\left(e^{-ikz\sin\theta}+e^{ikz\sin\theta}\right)$$

i.e. from Double slit analysis, but use $\frac{1}{2}d \to z$

$$\therefore \psi = \int d\psi = \int_0^{\frac{1}{2}a}\frac{Ae^{-i\omega t}}{ar}e^{ik\left(r+\frac{1}{2}\frac{z^2}{r}\right)}\left(e^{-ikz\sin\theta}+e^{ikz\sin\theta}\right)dz$$

$$\Rightarrow \psi = \frac{Ae^{i(kr-\omega t)}}{ar}\int_0^{\frac{1}{2}a}e^{\frac{ikz^2}{2r}}\left(e^{-ikz\sin\theta}+e^{ikz\sin\theta}\right)dz$$

This integral can be simplified into two regimes:

Fraunhofer – or 'linear phase' with *z* $\quad e^{\frac{ikz^2}{2r}} \approx \text{constant}$

$$\frac{k\left(\frac{1}{2}a\right)^2}{2r} \ll 1$$

$$\frac{2\pi a^2}{8\lambda r} \ll 1$$

$$r \gg \frac{\pi a^2}{4\lambda}$$

$$\boxed{r \gg \frac{a^2}{\lambda}}$$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{ar}\int_0^{\frac{1}{2}a}\left(e^{-ikz\sin\theta}+e^{ikz\sin\theta}\right)dz$$

$$\psi = \frac{2Ae^{i(kr-\omega t)}}{ar}\int_0^{\frac{1}{2}a}\cos(kz\sin\theta)\,dz$$

$$\psi = \frac{2Ae^{i(kr-\omega t)}}{ar}\left[\frac{\sin(kz\sin\theta)}{k\sin\theta}\right]_0^{\frac{1}{2}a}$$

$$|\psi|^2 = \frac{A^2}{r^2}\left(\frac{\sin\left(\frac{1}{2}ka\sin\theta\right)}{\frac{1}{2}ka\sin\theta}\right)^2$$

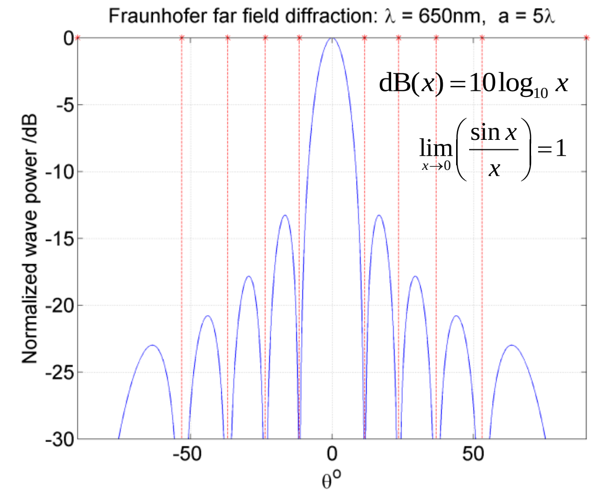
$$\theta = 0;\quad |\psi|^2 = |\psi_0|^2 = \frac{A^2}{r^2}$$

$$\boxed{\therefore \left|\frac{\psi}{\psi_0}\right|^2 = \left(\frac{\sin\left(\frac{1}{2}ka\sin\theta\right)}{\frac{1}{2}ka\sin\theta}\right)^2}$$

Hence *zeros* when:

$\frac{1}{2}kd\sin\theta = n\pi \quad$ *n* is a non-zero integer

$$\boxed{\theta = \sin^{-1}\left(\frac{2n\pi}{kd}\right) \quad |n| < \frac{kd}{2\pi}}$$



Fresnel – or 'quadratic phase' with *z*

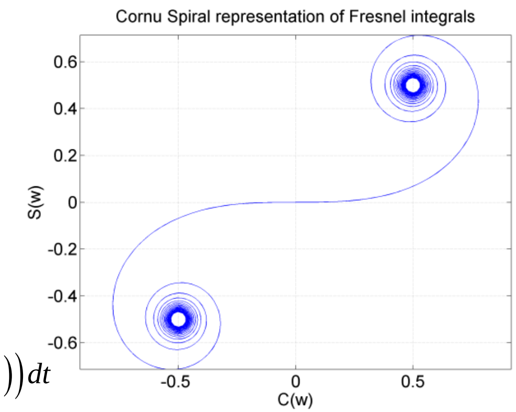
$\theta = 0°$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{ar}\int_0^{\frac{1}{2}a}e^{\frac{ikz^2}{2r}}dz$$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{ar}\int_0^{\frac{1}{2}a}e^{\frac{i\pi z^2}{\lambda r}}dz \quad \leftarrow k = \frac{2\pi}{\lambda}$$

$$\frac{1}{2}\pi t^2 = \frac{\pi z^2}{\lambda r} \Rightarrow t = z\sqrt{\frac{2}{\lambda r}}$$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{ar}\sqrt{\tfrac{1}{2}\lambda r}\int_0^{\frac{1}{2}a\sqrt{\frac{2}{\lambda r}}}\left(\cos\left(\tfrac{1}{2}\pi t^2\right)+i\sin\left(\tfrac{1}{2}\pi t^2\right)\right)dt$$



$$\boxed{\begin{aligned}|\psi|^2 &= \frac{A^2\lambda}{2a^2r}\left|C(w)+iS(w)\right|^2\\ w &= \tfrac{1}{2}a\sqrt{\frac{2}{\lambda r}}\\ C(w) &= \int_0^w\cos\left(\tfrac{1}{2}\pi t^2\right)dt\\ S(w) &= \int_0^w\sin\left(\tfrac{1}{2}\pi t^2\right)dt\end{aligned}}$$

Fresnel Integrals
These can't be evaluated exactly, but *can* be evaluated numerically

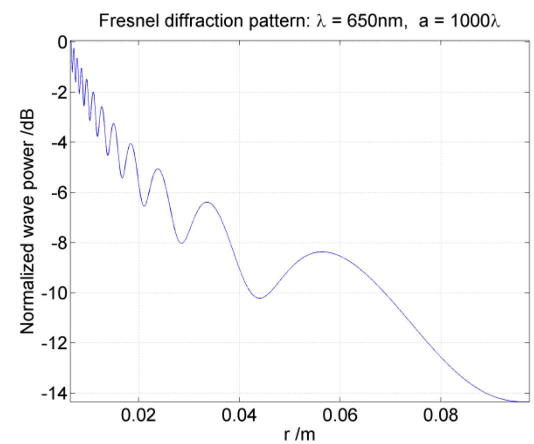
$$w^2 = \tfrac{1}{4}a^2\frac{2}{\lambda r}$$

$$r = \frac{a^2}{2\lambda w^2}$$

$$r \gg a$$

$$\therefore \frac{a^2}{2\lambda w^2} \gg a$$

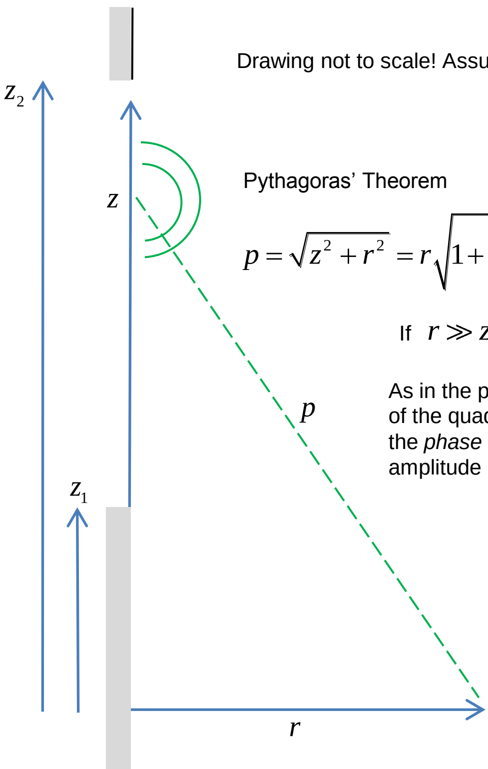
$$\boxed{\lambda \ll \frac{a}{2w^2}}$$



Generalized Fresnel wavefield

We can derive the Fresnel regime wavefield for more general geometries, and apply this to determine the diffraction pattern of a 'knife edge.'

Consider the uniformly illuminated aperture to extend from z_1 to z_2.



Drawing not to scale! Assume $r \gg z_2 - z_1$

Pythagoras' Theorem

$$p = \sqrt{z^2 + r^2} = r\sqrt{1 + \frac{z^2}{r^2}} \approx r\left(1 + \tfrac{1}{2}\frac{z^2}{r^2}\right) = r + \tfrac{1}{2}\frac{z^2}{r}$$

If $r \gg z$ as well as $r \gg z_2 - z_1$

As in the previous examples, the effect of the quadratic term in z will only effect the *phase* significantly and not the amplitude

$$\psi(r,t) = \int_{z_1}^{z_2} \frac{A}{a}\frac{e^{i(kp-\omega t)}}{p}dz$$

$$r \gg z, \quad p \approx r + \tfrac{1}{2}\frac{z^2}{r}$$

$$\therefore \psi(r,t) \approx \frac{Ae^{i(kr-\omega t)}}{r}\int_{z_1}^{z_2} e^{\frac{ikz^2}{2r}}dz$$

In this case, absorb a into constant A which could be calculated by direct wave intensity measurement.

$$k = \frac{2\pi}{\lambda}$$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{r}\int_{z_1}^{z_2} e^{\frac{i\pi z^2}{\lambda r}}dz$$

Consider substitution $\tfrac{1}{2}\pi t^2 = \frac{\pi z^2}{\lambda r} \Rightarrow t = z\sqrt{\frac{2}{\lambda r}} \Rightarrow dz = dt\sqrt{\tfrac{1}{2}\lambda r}$

$$\psi = \frac{Ae^{i(kr-\omega t)}}{r}\sqrt{\tfrac{1}{2}\lambda r}\int_{z_1\sqrt{\frac{2}{\lambda r}}}^{z_2\sqrt{\frac{2}{\lambda r}}}\left(\cos\left(\tfrac{1}{2}\pi t^2\right) + i\sin\left(\tfrac{1}{2}\pi t^2\right)\right)dt$$

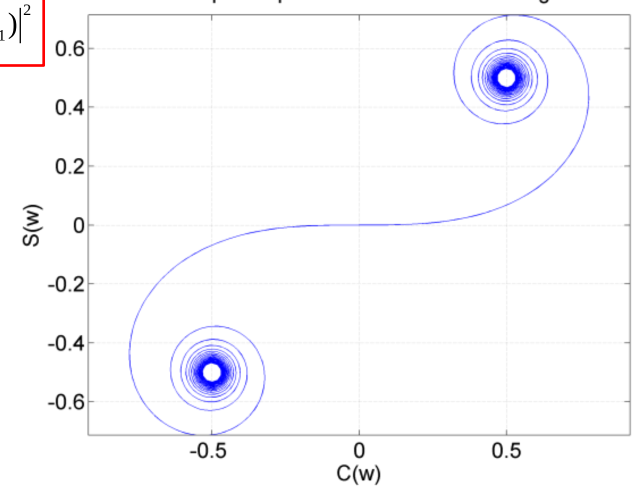
$$|\psi|^2 = \frac{A^2\lambda}{2r}\left|C(w_2) - C(w_1) + iS(w_2) - iS(w_1)\right|^2$$

$$w_{1,2} = z_{1,2}\sqrt{\frac{2}{\lambda r}}$$

$$C(w) = \int_0^w \cos\left(\tfrac{1}{2}\pi t^2\right)dt$$

$$S(w) = \int_0^w \sin\left(\tfrac{1}{2}\pi t^2\right)dt$$

Cornu Spiral representation of Fresnel integrals



Now for a **'knife edge'**

$$z_1 = z, \quad z_2 = \infty$$

$$|\psi|^2 = \frac{A^2\lambda}{2r}\left|C(\infty) - C(w) + iS(\infty) - iS(w)\right|^2$$

$$w = z\sqrt{\frac{2}{\lambda r}}$$

From the Cornu Spiral one can see that

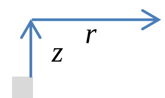
$$S(\infty) = C(\infty) = \tfrac{1}{2}$$

$$\therefore |\psi|^2 = \frac{A^2\lambda}{2r}\left|\tfrac{1}{2}(1+i) - C(w) - iS(w)\right|^2$$

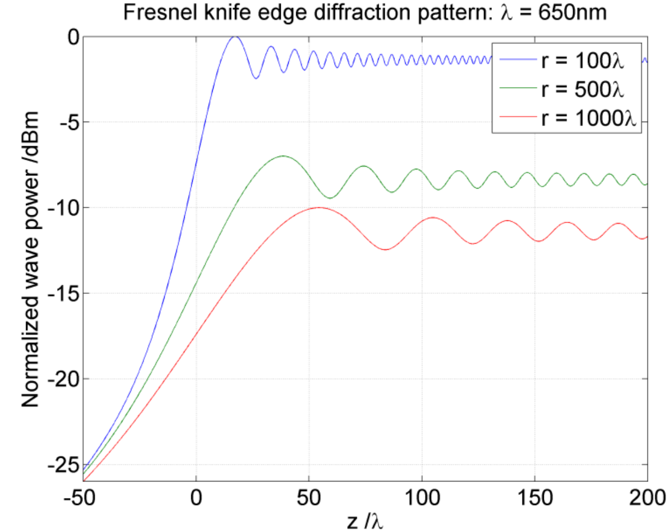
Now if we are *above* the knife edge by z (rather than below) we must exchange its *sign*. Since w is proportional to z :

$$|\psi|^2 = \frac{A^2\lambda}{2r}\left|\tfrac{1}{2}(1+i) + C(w) + iS(w)\right|^2$$

$$w = z\sqrt{\frac{2}{\lambda r}}$$

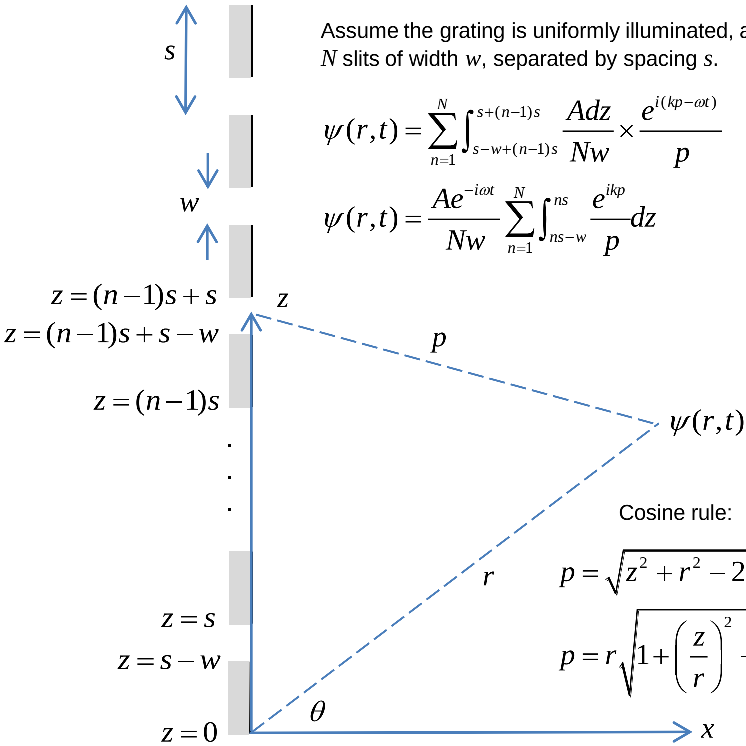


Fresnel knife edge diffraction pattern: λ = 650nm



$$S(\pm w) = \pm S(w) \qquad C(\pm w) = \pm C(w)$$

Far-field (Fraunhofer) diffraction pattern of a grating



Assume the grating is uniformly illuminated, and consists of N slits of width w, separated by spacing s.

$$\psi(r,t)=\sum_{n=1}^{N}\int_{s-w+(n-1)s}^{s+(n-1)s}\frac{A\,dz}{Nw}\times\frac{e^{i(kp-\omega t)}}{p}$$

$$\psi(r,t)=\frac{Ae^{-i\omega t}}{Nw}\sum_{n=1}^{N}\int_{ns-w}^{ns}\frac{e^{ikp}}{p}dz$$

Cosine rule:

$$p=\sqrt{z^2+r^2-2zr\cos\left(\tfrac{1}{2}\pi-\theta\right)}$$

$$p=r\sqrt{1+\left(\frac{z}{r}\right)^2-\frac{2z}{r}\sin\theta}$$

Assume 'far-field' (Fraunhofer) scenario – i.e. $r \gg z$

$$\therefore\ p\approx r\left(1-\frac{z}{r}\sin\theta\right)=r-z\sin\theta$$

i.e. *plane waves* arriving at r,θ

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nwr}\sum_{n=1}^{N}\int_{ns-w}^{ns}e^{-ikz\sin\theta}dz$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nwr}\sum_{n=1}^{N}\left[\frac{e^{-ikz\sin\theta}}{-ik\sin\theta}\right]_{ns-w}^{ns}$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nwr}\sum_{n=1}^{N}\frac{1}{-ik\sin\theta}\left(e^{-ikns\sin\theta}-e^{-ik(ns-w)\sin\theta}\right)$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nwr}\sum_{n=1}^{N}\frac{1}{-ik\sin\theta}e^{-ik(ns-\frac{1}{2}w)\sin\theta}\left(e^{-ik\frac{1}{2}w\sin\theta}-e^{ik\frac{1}{2}w\sin\theta}\right)$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{1}{\frac{1}{2}kw\sin\theta}\frac{1}{2i}\left(e^{ik\frac{1}{2}w\sin\theta}-e^{-ik\frac{1}{2}w\sin\theta}\right)\sum_{n=1}^{N}e^{-ik(ns-\frac{1}{2}w)\sin\theta}$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}e^{-ik\frac{1}{2}w\sin\theta}\sum_{n=1}^{N}\left(e^{-iks\sin\theta}\right)^n$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}e^{-ik\frac{1}{2}w\sin\theta}\frac{e^{-iks\sin\theta}-e^{-ik(N+1)s\sin\theta}}{1-e^{-iks\sin\theta}}$$

The last step uses the formula for the sum of a *geometric series*

$$\sum_{n=1}^{N}ar^{n-1}=a+ar+...+ar^{N-1}=a\frac{1-r^N}{1-r}\quad\therefore\ a\frac{1-r^N}{1-r}=\frac{a}{r}\sum_{n=1}^{N}r^n\ \Rightarrow\ \boxed{\sum_{n=1}^{N}r^n=\frac{r-r^{N+1}}{1-r}}$$

$$\therefore\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}e^{-ik\frac{1}{2}w\sin\theta}\frac{e^{-iks\sin\theta}e^{-i\frac{1}{2}kNs\sin\theta}\left(e^{i\frac{1}{2}kNs\sin\theta}-e^{-i\frac{1}{2}kNs\sin\theta}\right)}{e^{-i\frac{1}{2}ks\sin\theta}\left(e^{i\frac{1}{2}ks\sin\theta}-e^{-i\frac{1}{2}ks\sin\theta}\right)}$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}e^{-ik\frac{1}{2}w\sin\theta}\frac{e^{-i\frac{1}{2}ks\sin\theta}e^{-i\frac{1}{2}kNs\sin\theta}\times2i\sin\left(\frac{1}{2}kNs\sin\theta\right)}{2i\sin\left(\frac{1}{2}ks\sin\theta\right)}$$

$$\psi(r,t)\approx\frac{Ae^{i(kr-\omega t)}}{Nr}\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}e^{-ik\frac{1}{2}(w+s+Ns)\sin\theta}\frac{\sin\left(\frac{1}{2}kNs\sin\theta\right)}{\sin\left(\frac{1}{2}ks\sin\theta\right)}$$

$$|\psi|^2\approx\frac{A^2}{N^2r^2}\left(\frac{\sin\left(\frac{1}{2}kw\sin\theta\right)}{\frac{1}{2}kw\sin\theta}\times\frac{\sin\left(\frac{1}{2}kNs\sin\theta\right)}{\sin\left(\frac{1}{2}ks\sin\theta\right)}\right)^2$$

$$\boxed{|\psi|^2\approx\frac{A^2}{N^2r^2}\left(\frac{\sin\left(\frac{\pi}{\lambda}w\sin\theta\right)}{\frac{\pi}{\lambda}w\sin\theta}\times\frac{\sin\left(\frac{\pi}{\lambda}Ns\sin\theta\right)}{\sin\left(\frac{\pi}{\lambda}s\sin\theta\right)}\right)^2}\quad\longleftarrow\quad k=\frac{2\pi}{\lambda}$$

wavenumber

Zeros at: $\frac{\pi}{\lambda}w\sin\theta=n\pi$

$$\boxed{\theta=\sin^{-1}\left(\frac{n\lambda}{w}\right)\quad n\in\mathbb{Z},n\neq0}$$

$\frac{\pi}{\lambda}Ns\sin\theta=m\pi$

$$\boxed{\theta=\sin^{-1}\left(\frac{m\lambda}{Ns}\right)\quad m\in\mathbb{Z}}$$

Maxima ('grating lobes') at: $\frac{\pi}{\lambda}s\sin\theta=q\pi$

$$\boxed{\theta=\sin^{-1}\left(\frac{q\lambda}{s}\right)\quad q\in\mathbb{Z}}$$

Far-Field diffraction summary

$$|\psi|^2 = \frac{A^2}{N^2 r^2}\left(\frac{\sin\left(\frac{\pi}{\lambda} w \sin\theta\right)}{\frac{\pi}{\lambda} w \sin\theta} \times \frac{\sin\left(\frac{\pi}{\lambda} N s \sin\theta\right)}{\sin\left(\frac{\pi}{\lambda} s \sin\theta\right)}\right)^2$$

This is the actual formula for the **diffraction pattern wave power**. It incorporates all the maxima and minima effects described above.

n, m, p are integers

Envelope due to finite slit width

Zeros at: $\theta = \sin^{-1}\left(\frac{n\lambda}{w}\right); \; n \neq 0$

Maxima due to slit spacing

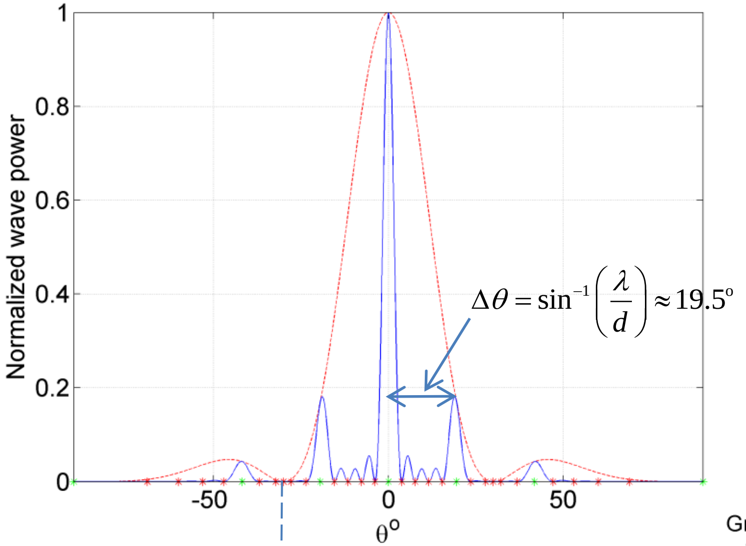
Maxima at: $\theta = \sin^{-1}\left(\frac{m\lambda}{s}\right)$

Fine structure due to number of slits
(i.e. overall size of aperture)

Zeros at: $\theta = \sin^{-1}\left(\frac{p\lambda}{Ns}\right)$

But *maxima* when $\frac{p}{N}$ integer m

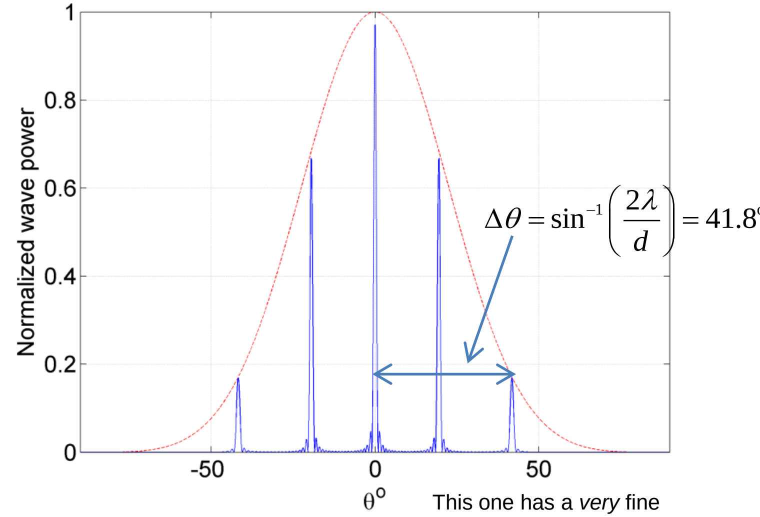
Grating Fraunhofer far field diffraction
λ = 650nm, s = 3λ, w = 2λ, N = 5



$$\Delta\theta = \sin^{-1}\left(\frac{\lambda}{d}\right) \approx 19.5^\circ$$

$$\Delta\theta = \sin^{-1}\left(\frac{\lambda}{w}\right) = 30^\circ$$

Grating Fraunhofer far field diffraction
λ = 650nm, s = 3λ, w = 1λ, N = 20



$$\Delta\theta = \sin^{-1}\left(\frac{2\lambda}{d}\right) = 41.8^\circ$$

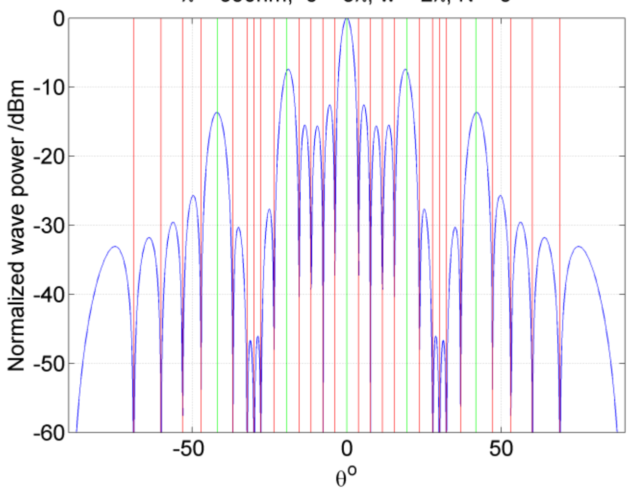
This one has a *very* fine structure since N is large

Almost all of these diffraction effects result in a *main lobe* of angular width (in radians)

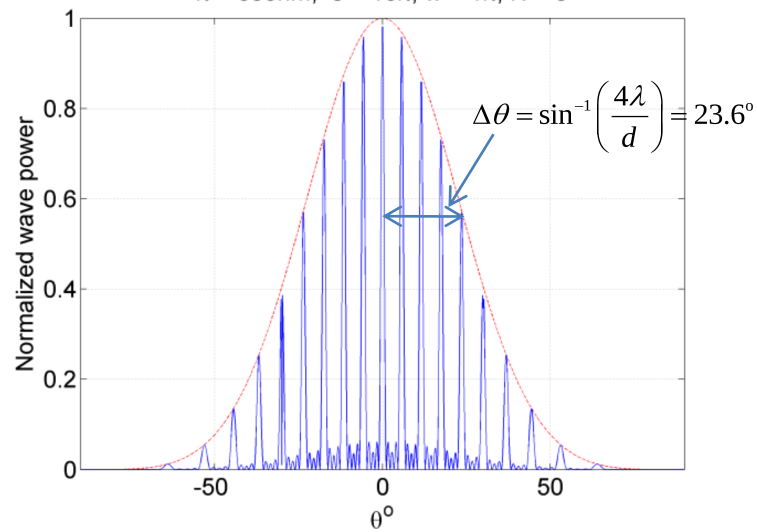
$$\Delta\theta \approx \frac{\lambda}{d}$$

where d is a characteristic length of the grating, slit etc. For any optical instrument, the 'resolving power' is likely to be diffraction limited. So this ratio gives *the minimum angular deviation* that two objects could be **resolved** via an optical system.

Grating Fraunhofer far field diffraction
λ = 650nm, s = 3λ, w = 2λ, N = 5



Grating Fraunhofer far field diffraction
λ = 650nm, s = 10λ, w = 1λ, N = 5

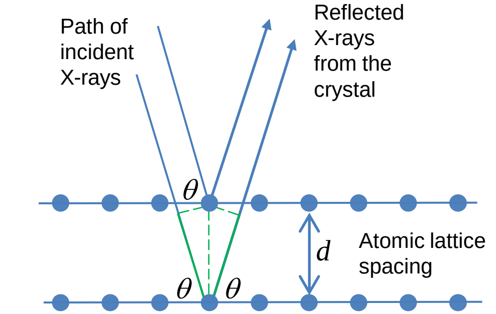


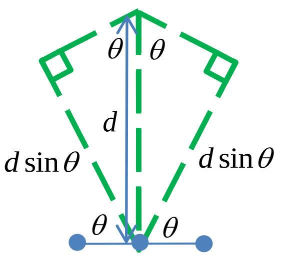
$$\Delta\theta = \sin^{-1}\left(\frac{4\lambda}{d}\right) = 23.6^\circ$$

*1 arc-second is 1/3600 of a degree

e.g. for the James Web space telescope, d = 6.5m. So for Infra-Red light of wavelength 3.15μm, $\Delta\theta$ is about 0.1 arc-seconds*.

Bragg's law of X-ray diffraction from atoms in a crystal lattice

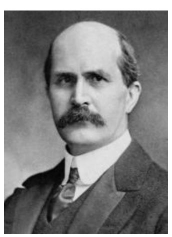




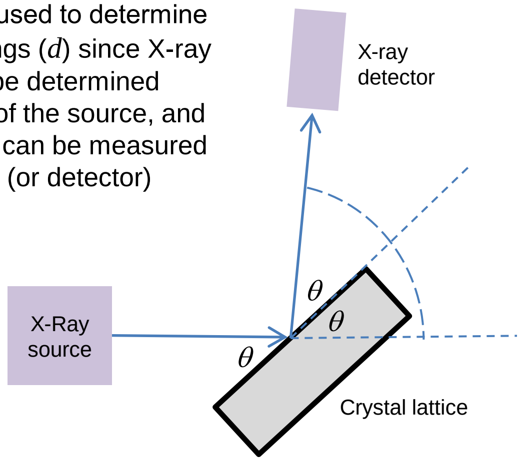
Reflected rays will constructively interfere when the *path difference* between the rays reflecting off nearby atomic layers is an integer multiple of the wavelength of the X-rays

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

Bragg's law can be used to determine atomic lattice spacings (d) since X-ray wavelengths λ can be determined from the properties of the source, and the diffraction angle can be measured via rotating a crystal (or detector) as shown



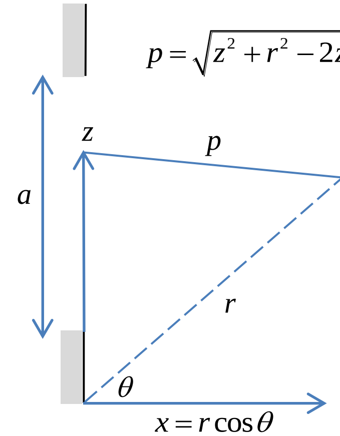
Sir William Henry Bragg 1862-1942



Modelling general diffraction effects from a finite width slit

We can use a computer to evaluate the wavefield in the vicinity of a finite width slit which is uniformly illuminated. We are therefore not restricted to the limitations of the Fraunhofer and Fresnel regimes

$$p = \sqrt{z^2 + r^2 - 2zr\cos\left(\tfrac{1}{2}\pi - \theta\right)} = \sqrt{z^2 + r^2 - 2zr\sin\theta}$$

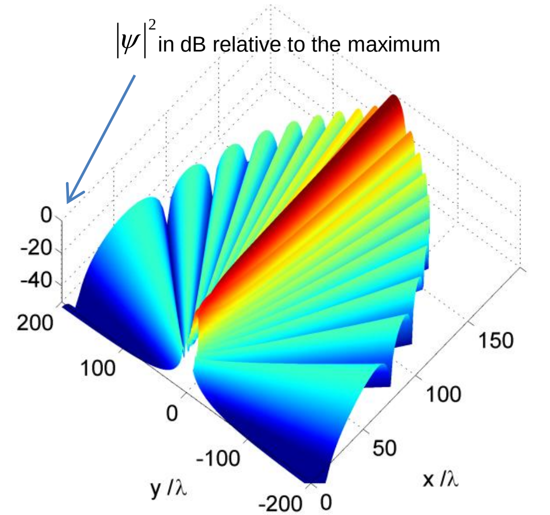


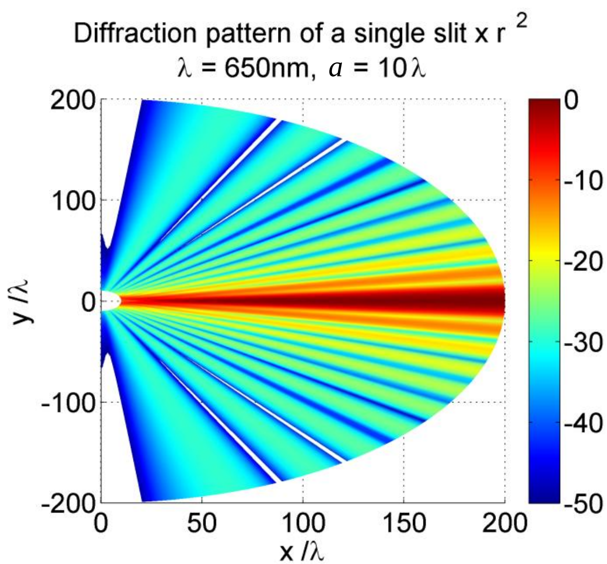
$$\psi(r,t) = \frac{A}{a} e^{-i\omega t} \int \frac{e^{ikp}}{p} dz$$

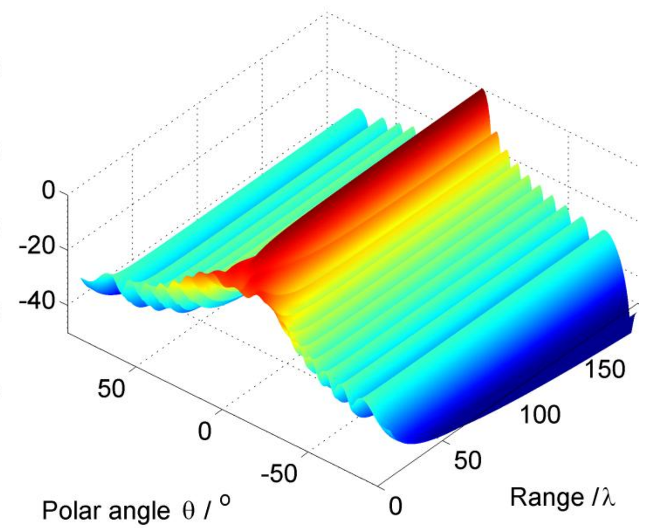
The idea is to evaluate the wavefield power at various r and θ values. The integral is approximated by a *sum* based on a large number of finite dz values

In the examples below :

$$dz = \tfrac{1}{500} a$$







All three plots are visualizations of the same wavefield power in **normalized decibels**.

Decibels are a useful measure of power over a large range of values $\mathrm{dB}(x) = \log_{10} x$