Chapter 11 Diffraction

Reading Assignment:

1. D. Sherwood, Crystals, X-rays, and Proteins-chapter 5 and 7

Contents

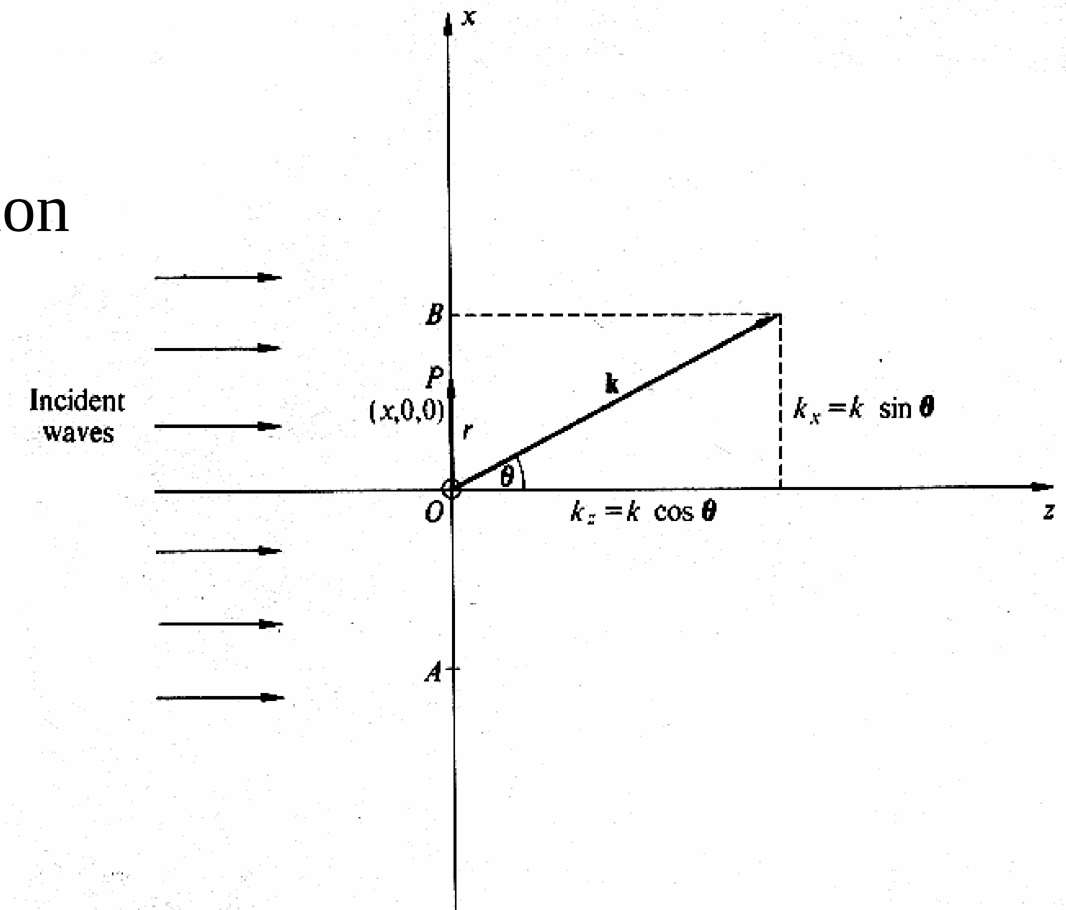
Diffraction by 1-D Obstacles

- geometric arrangement

diffraction pattern amplitude $F(\vec{k})$

$$F(\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\bullet\vec{r}} d\vec{r}$$

$f(\vec{r})$: amplitude function



xz plane

obstacle- along x-axis

$$\vec{r} = (x, 0, 0)$$

$$f(\vec{r}) \to f(x)$$

$$\vec{k} = (k_x, 0, k_z)$$

$$\vec{k}\bullet\vec{r} = k_x x = kx\sin\theta \qquad \theta : \text{scattering angle}$$

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Diffraction by 1-D Obstacles

- geometric arrangement

$$F(\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\cdot\vec{r}} d\vec{r} = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$$

$$\rightarrow F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx \ (\because k\text{: constant})$$

- in general, $F(\sin\theta)$ is complex

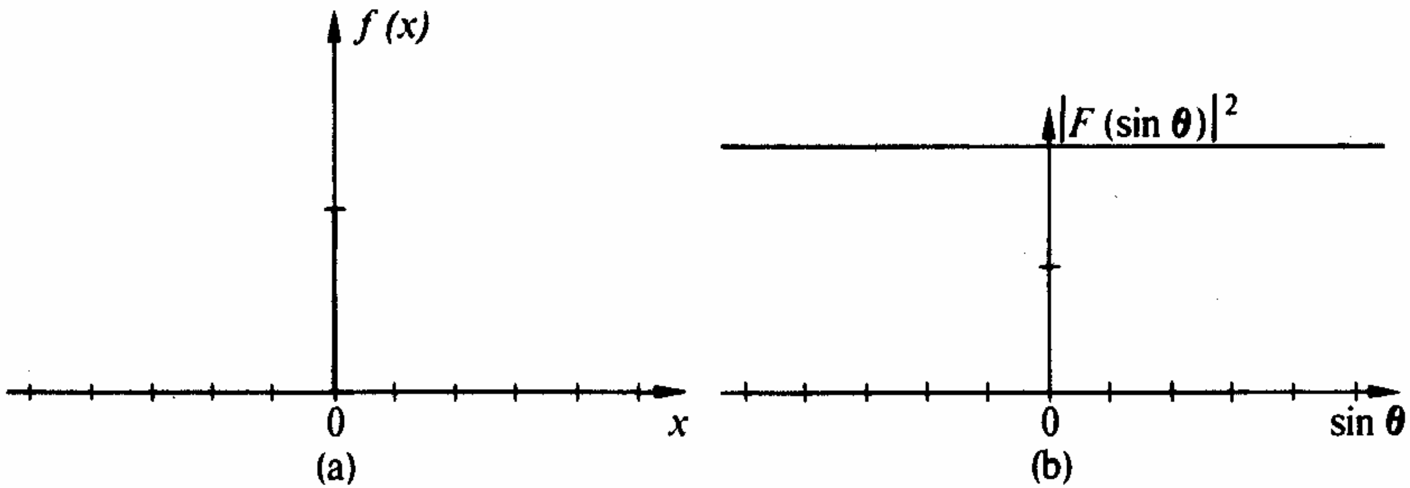
intensity of diffraction pattern $\left|F(\sin\theta)\right|^2$

Diffraction by 1-D Obstacles

- one narrow slit

  an infinite opaque sheet along the *x*-axis containing narrow slit at the origin

- narrowness- compared to the wavelength
- amplitude function- δ function



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Diffraction by 1-D Obstacles

- $f(x) = \delta(x)$

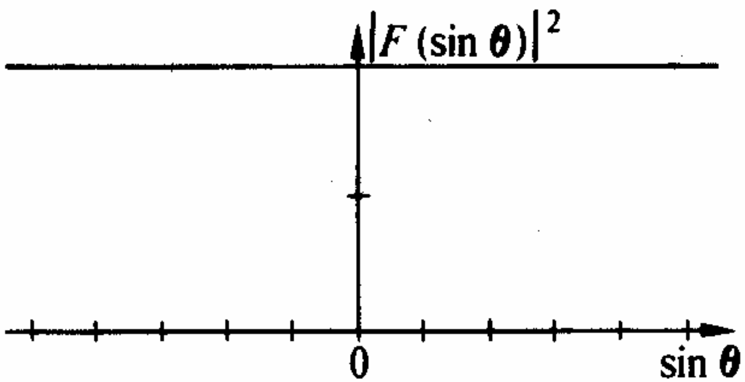
- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx = \int_{-\infty}^{\infty} \delta(x) e^{ikx\sin\theta} dx$

$$= \left[e^{ikx\sin\theta} \right]_{x=0} = 1$$

- intensity $\sim |F(\sin\theta)|^2 = 1$

- intensity is uniform at all angles

- a single narrow slit $\equiv$ an active point source



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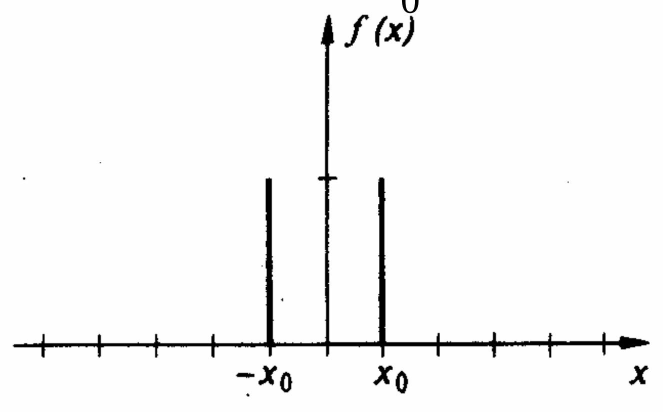
Diffraction by 1-D Obstacles

- two narrow slit

  a pair of δ functions, one at $+x_0$, and the other at $-x_0$



- $f(x) = \delta(x+x_0) + \delta(x-x_0)$

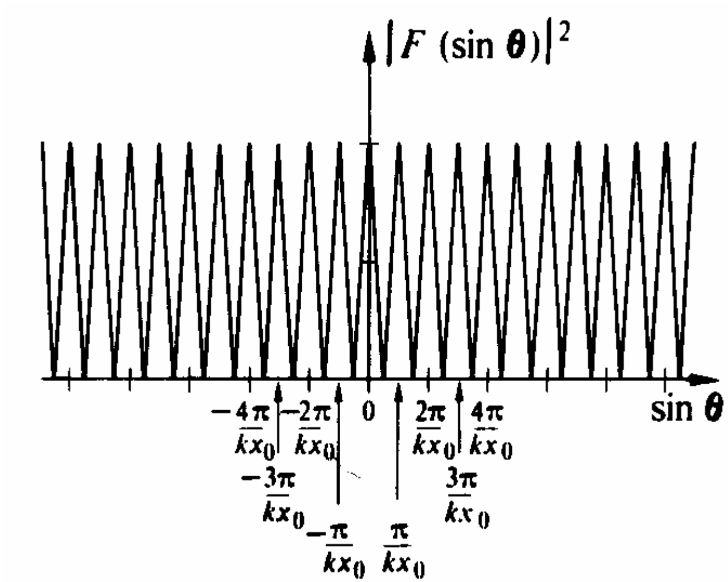
- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$

$$= \int_{-\infty}^{\infty} \delta(x+x_0) e^{ikx\sin\theta} dx + \int_{-\infty}^{\infty} \delta(x-x_0) e^{ikx\sin\theta} dx$$

$$= e^{-ikx_0\sin\theta} + e^{ikx_0\sin\theta} = 2\cos(kx_0\sin\theta)$$

$$(\because \int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx = f(x_0))$$

- $|F(\sin\theta)|^2 = 4\cos^2(kx_0\sin\theta)$



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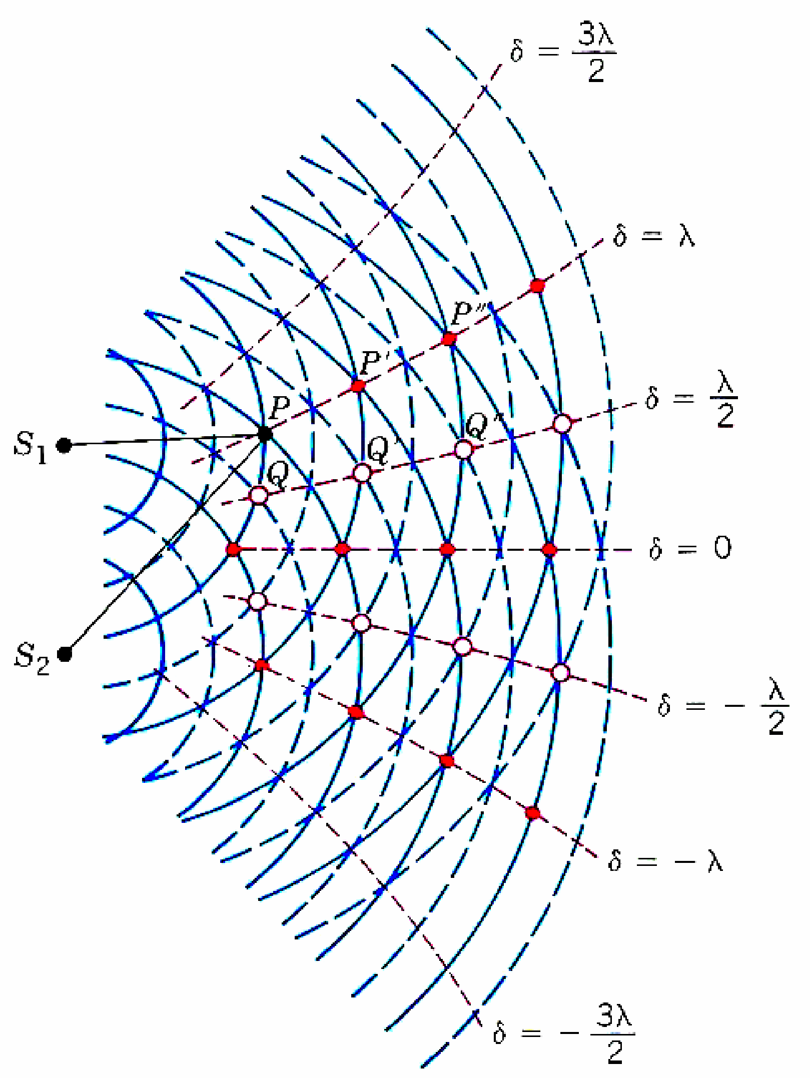
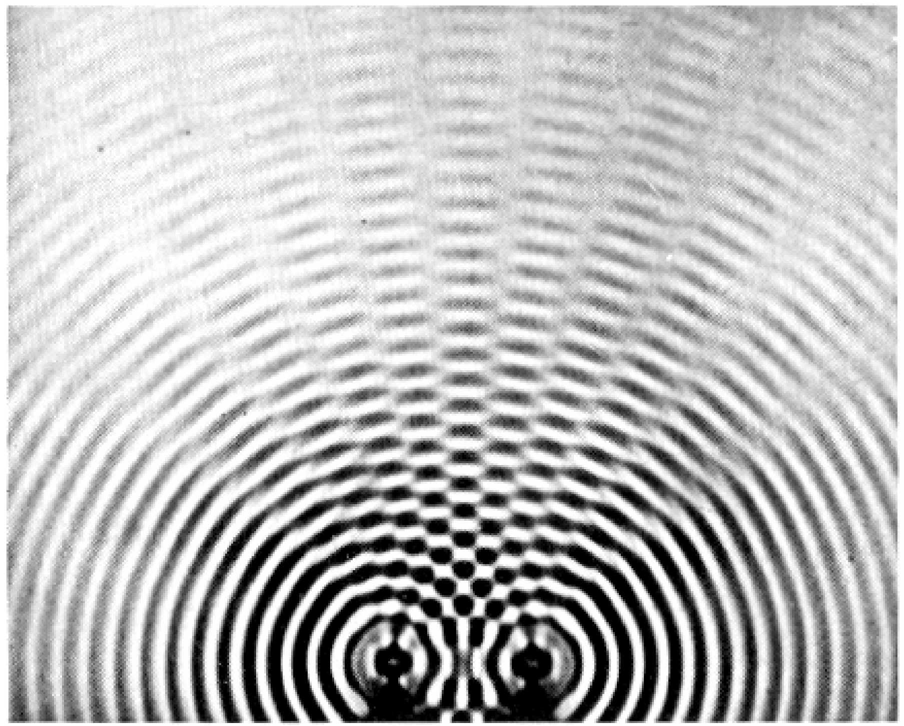
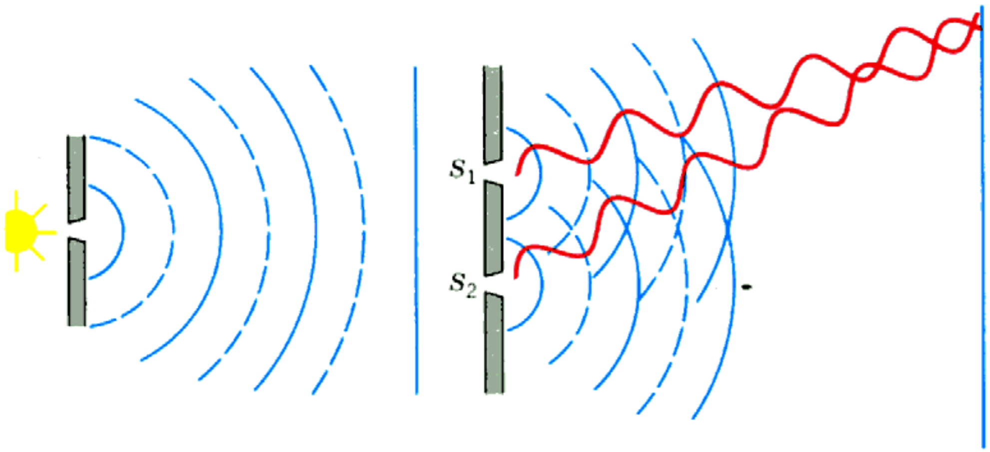
Interference



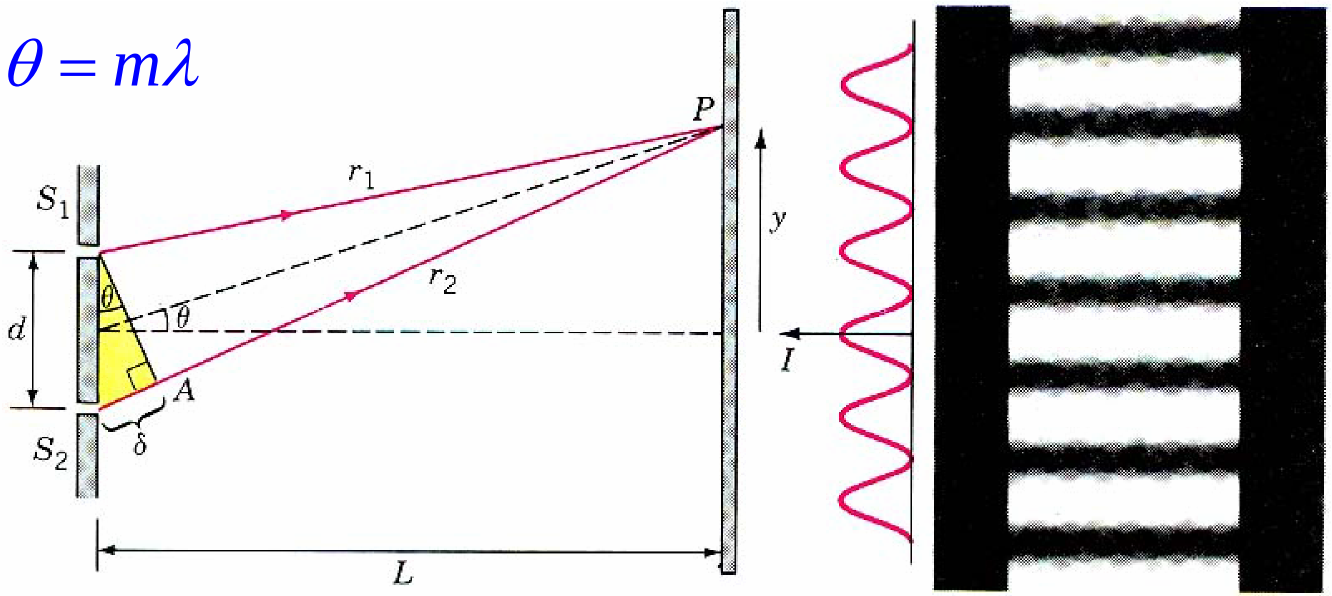


Young's Experiment



maxima

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



Diffraction by 1-D Obstacles

- three narrow slits

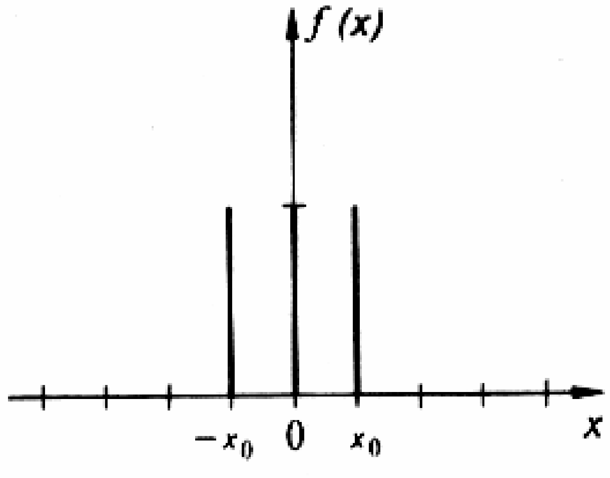
$$f(x) = \delta(x + x_0) + \delta(x) + \delta(x - x_0)$$

- $$F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$$

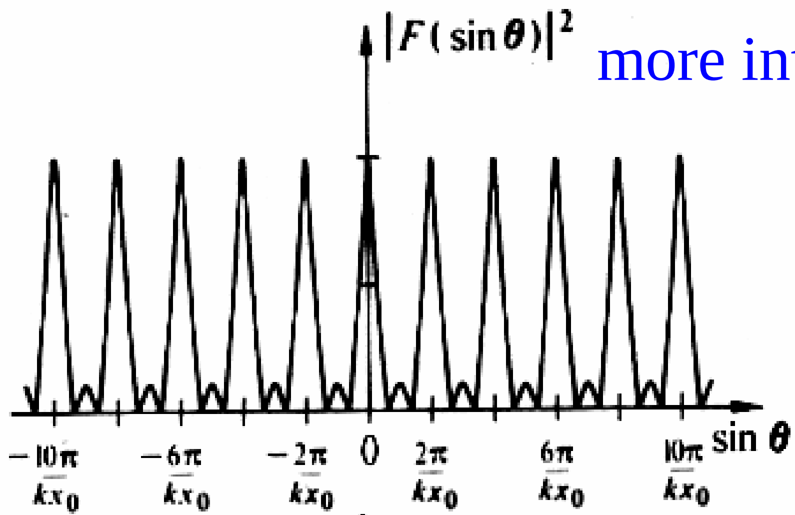
$$= 1 + 2\cos(kx_0 \sin\theta)$$

- $$\left|F(\sin\theta)\right|^2 = [1 + 2\cos(kx_0 \sin\theta)]^2$$

nine times more intense



(a)



(b)

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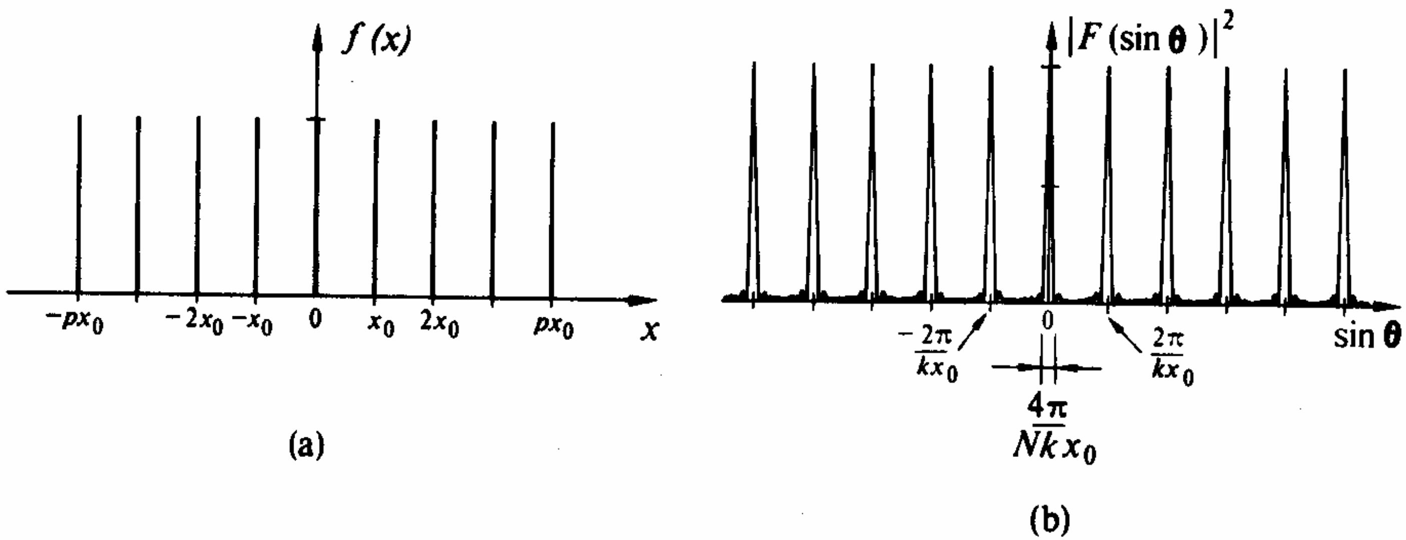
Diffraction by 1-D Obstacles

- N narrow slits

  equally spaced by a distance $x_0 \rightarrow N\ \delta$ function

  $N = 2p + 1$ (odd number)

- $f(x) = \sum_{n=-p}^{n=p} \delta(x - nx_0)$



Diffraction by 1-D Obstacles

- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$

$$= e^{-ikpx_0\sin\theta} + e^{-ik(p-1)x_0\sin\theta} + \cdots + 1 + \cdots + e^{ikpx_0\sin\theta}$$

$$= e^{-ikpx_0\sin\theta}(1 + e^{ikx_0\sin\theta} + \cdots + e^{ik2px_0\sin\theta})$$

$$= e^{-ikpx_0\sin\theta}\left(\frac{1-e^{ik(2p+1)x_0\sin\theta}}{1-e^{ikx_0\sin\theta}}\right) = e^{-ikpx_0\sin\theta}\left(\frac{1-e^{ikNx_0\sin\theta}}{1-e^{ikx_0\sin\theta}}\right)$$

$$= \frac{\sin\dfrac{Nkx_0\sin\theta}{2}}{\sin\dfrac{kx_0\sin\theta}{2}}$$

- $|F(\sin\theta)|^2 = \dfrac{\sin^2\dfrac{Nkx_0\sin\theta}{2}}{\sin^2\dfrac{kx_0\sin\theta}{2}}$

*main peak

angular width- $4\pi / Nkx_0$

separated by- $2\pi / kx_0$

N - 2 subsidiary peaks

Diffraction by 1-D Obstacles

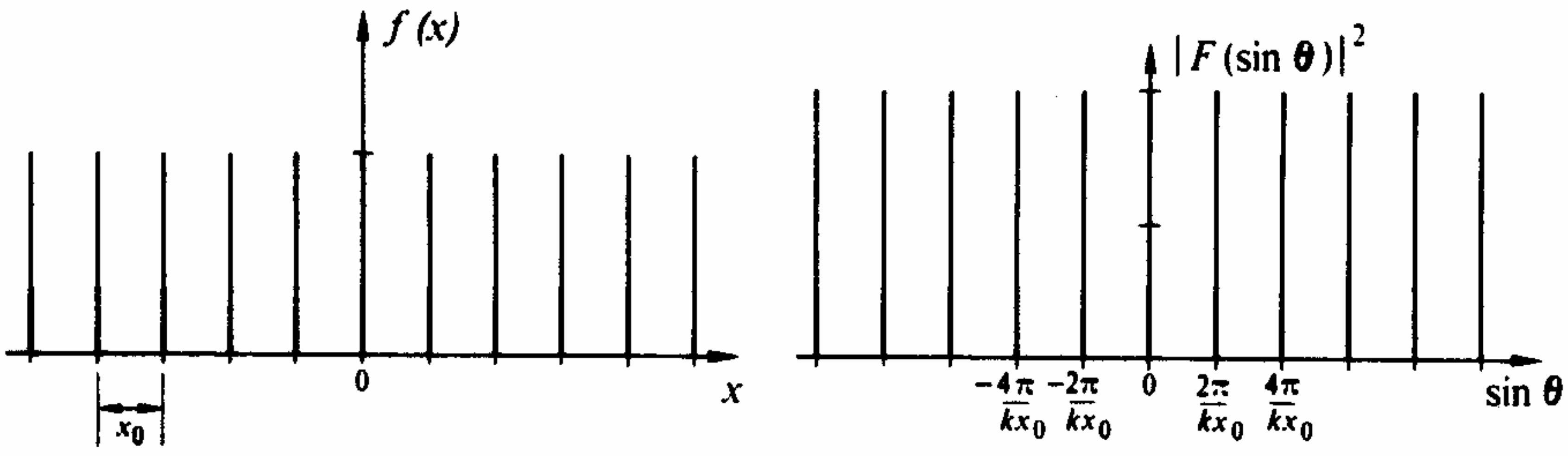
- infinite number of narrow slits
  separated by a distance x_0 $\rightarrow$ infinite array of δ function

- $f(x) = \sum_{n=-\infty}^{n=\infty} \delta(x - nx_0)$

- $F(\sin\theta) = \sum_{n=-\infty}^{n=\infty} \delta(\sin\theta - \frac{2n\pi}{kx_0})$

*infinitely sharp peak

$$\Delta(\sin\theta) = \frac{2\pi}{kx_0}$$



(a) (b)

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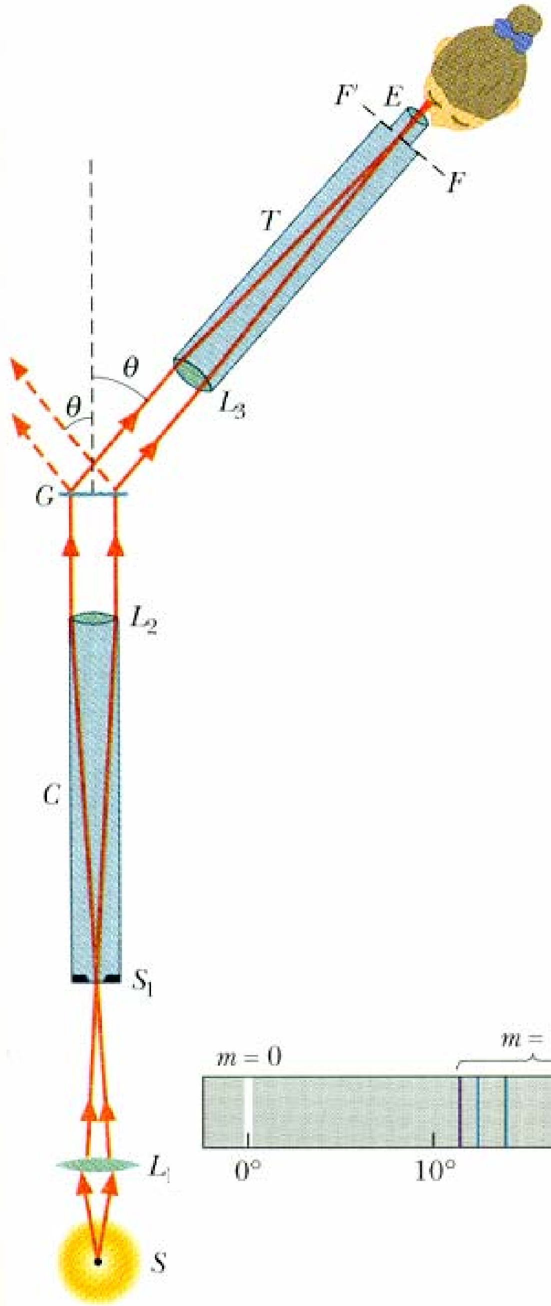
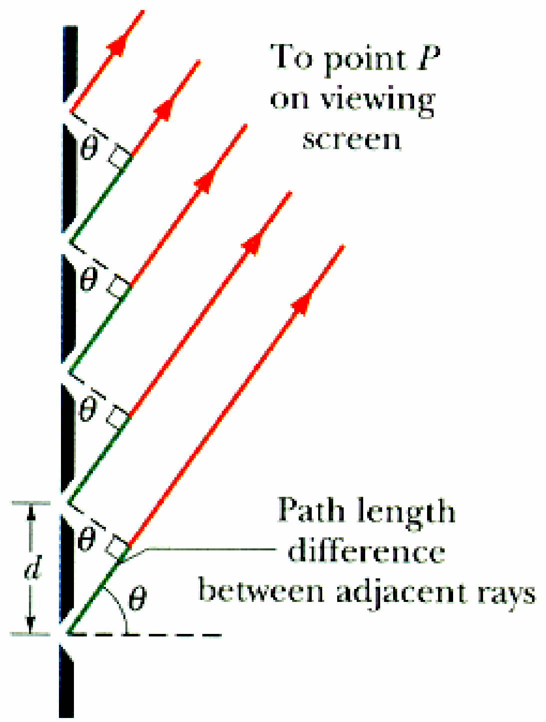
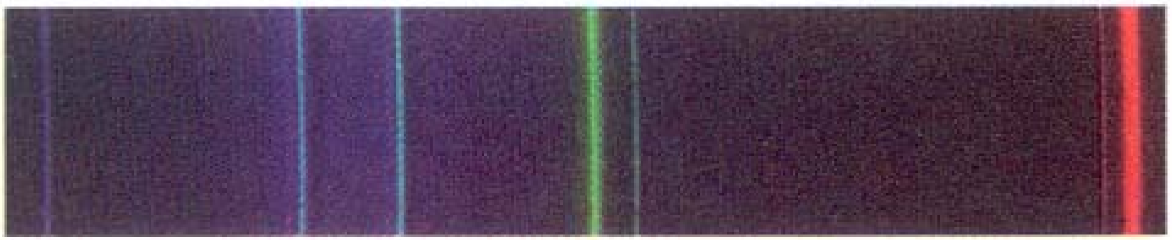
Grating Spectroscope

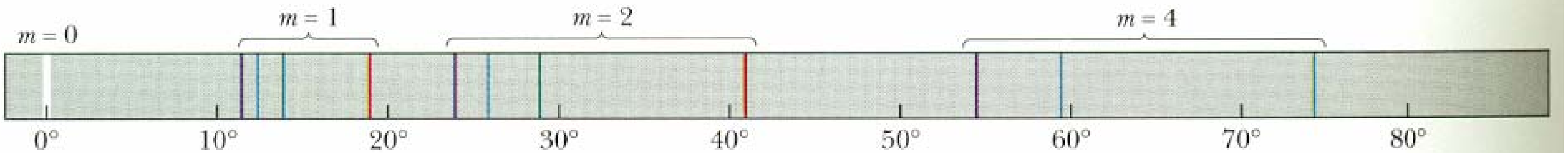




$$d\sin\theta = m\lambda$$



visible emission line of cadmium



visible emission line from hydrogen

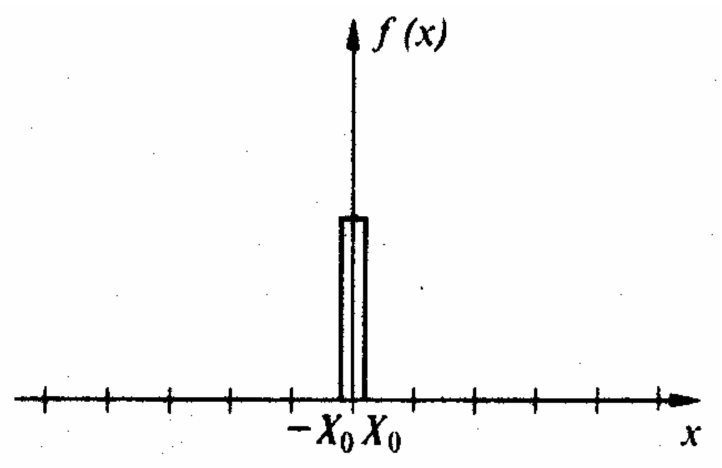
D. Halliday, Fundamentals of Physics

Diffraction by 1-D Obstacles

- one wide slit

  an opaque screen containing a slit which is wide

  $\sim 100\lambda$



$$- f(x) = 0 \quad if \quad -\infty < x < -X_0$$
$$1 \quad if \quad -X_0 < x < +X_0$$
$$0 \quad if \quad +X_0 < x < \infty$$

$$- \mathrm{F}(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$$

$$= \int_{-X_0}^{X_0} f(x) e^{ikx\sin\theta} dx = \left[\frac{e^{ikx\sin\theta}}{ik\sin\theta} \right]_{-X_0}^{X_0}$$

Diffraction by 1-D Obstacles

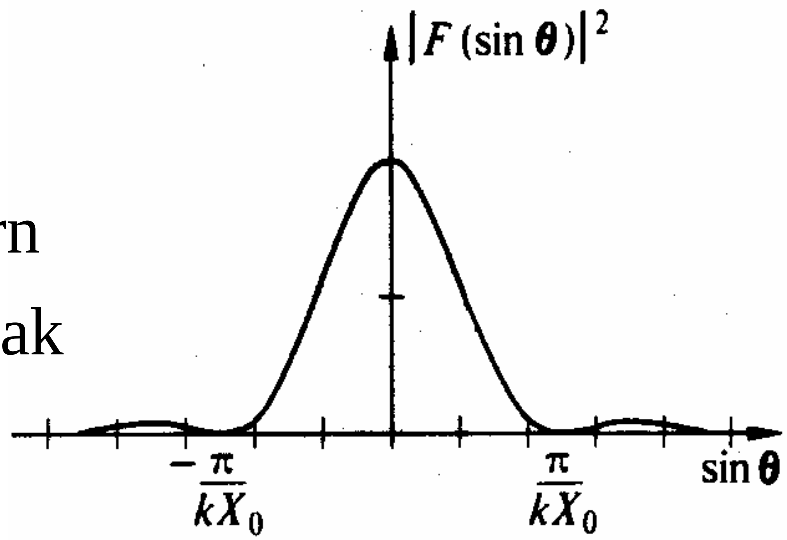
- $F(\sin\theta) = \left[\dfrac{e^{ikx\sin\theta}}{ik\sin\theta}\right]_{-X_0}^{X_0} = \dfrac{e^{ikX_0\sin\theta} - e^{-ikX_0\sin\theta}}{ik\sin\theta}$

$$= 2X_0 \frac{\sin(kX_0\sin\theta)}{kX_0\sin\theta}$$

- intensity~$\left|F(\sin\theta)\right|^2 = 4X_0^2 \dfrac{\sin^2(kX_0\sin\theta)}{(kX_0\sin\theta)^2}$

- $2X_0 \rightarrow \Delta(\sin\theta) = 2\pi / kX_0$
- the wider slit,

  the narrow the diffraction pattern
- secondary peak-very rapidly weak



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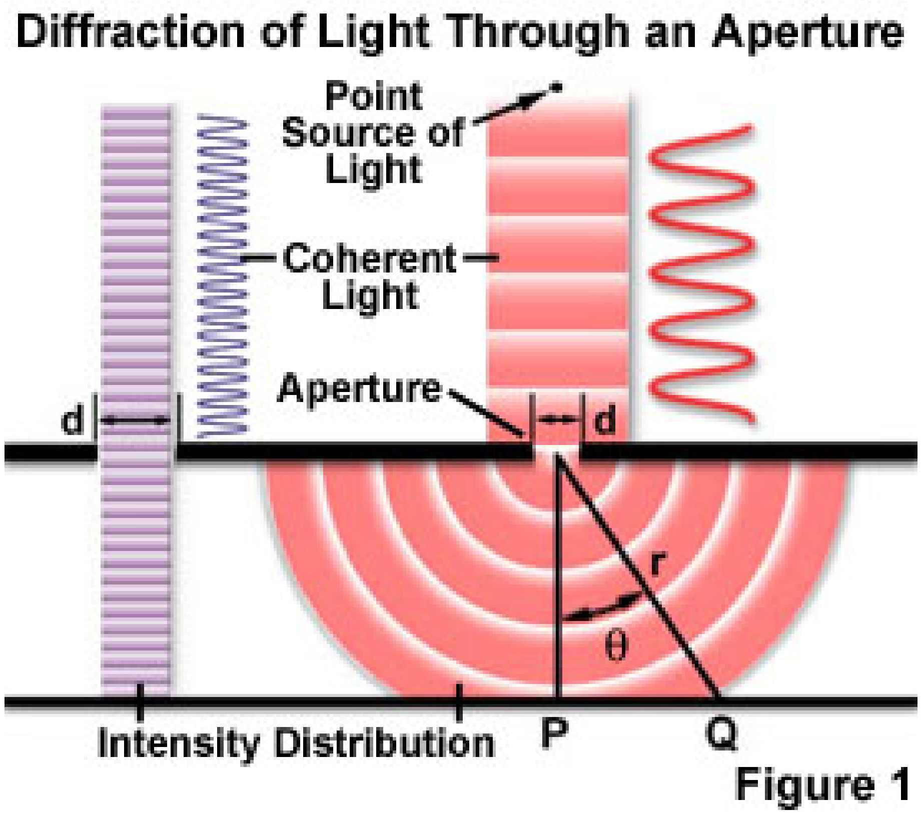
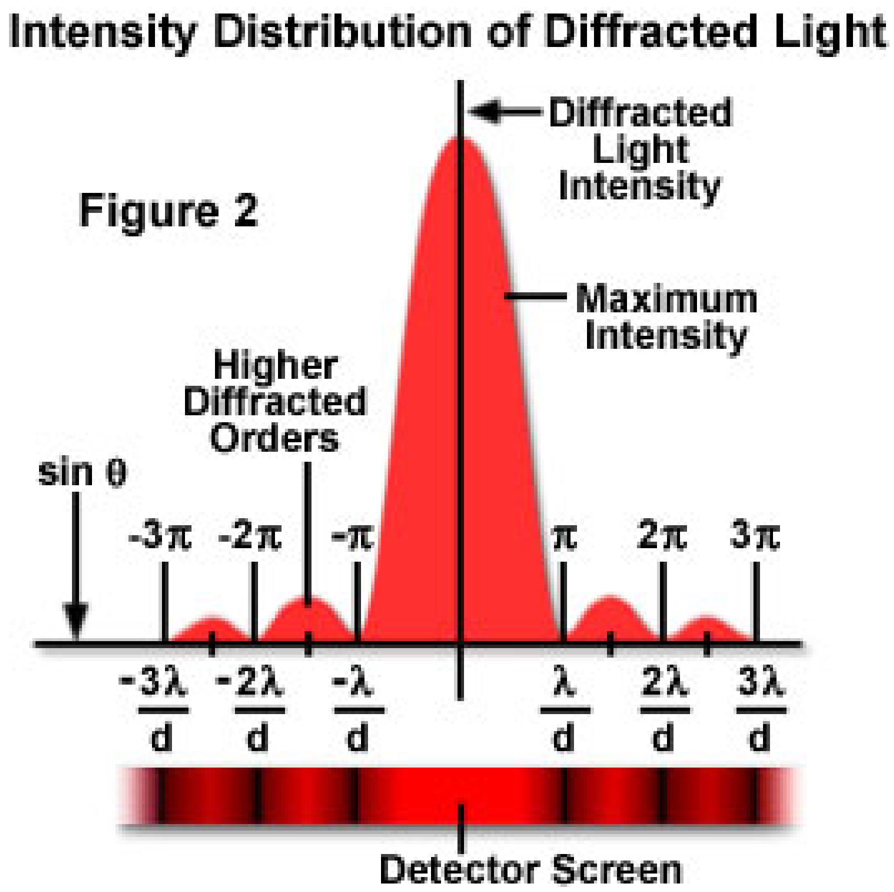
Single-Slit Diffraction





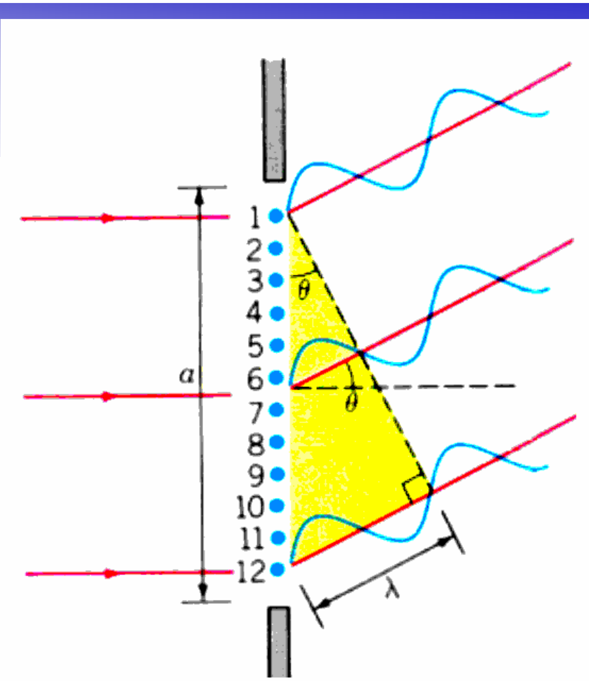
$$\delta \approx d \sin\theta, \text{ for minima } \sin\theta = m\frac{\lambda}{d}$$

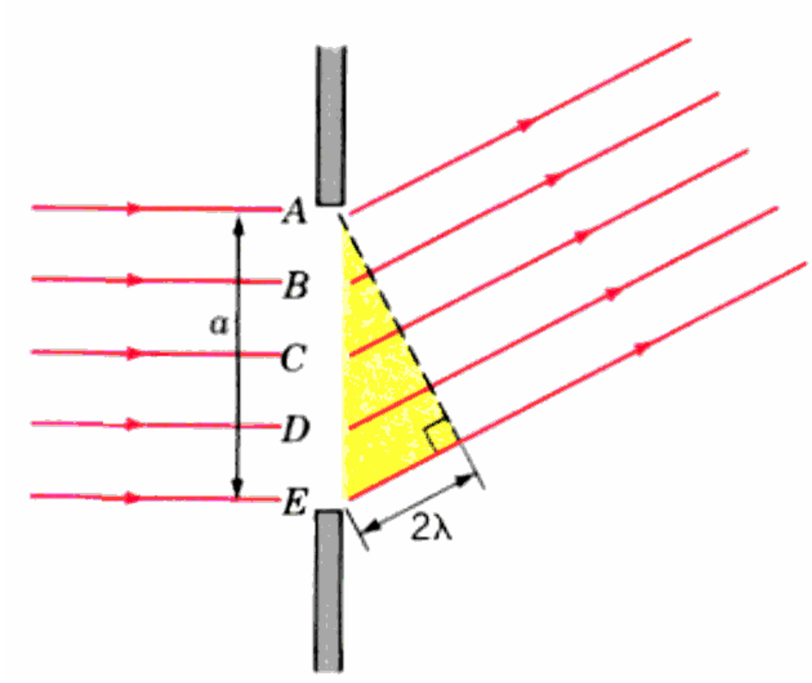
http://micro.magnet.fsu.edu/primer/java/diffraction/basicdiffraction/

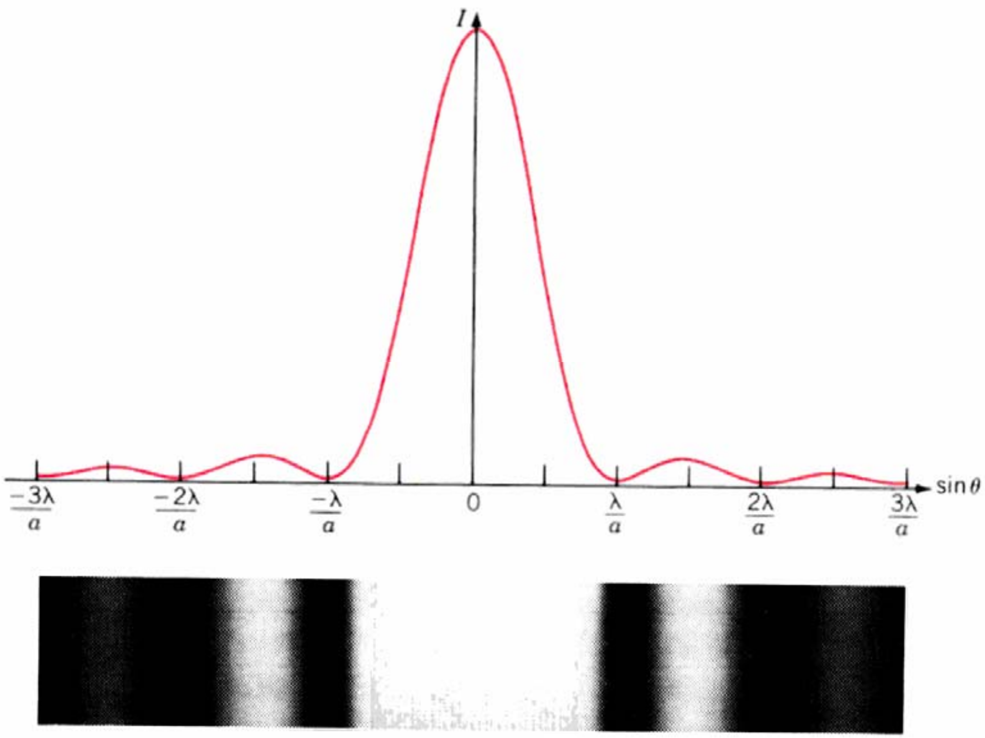
Single-Slit Diffraction

- $\delta \approx d \sin \theta$

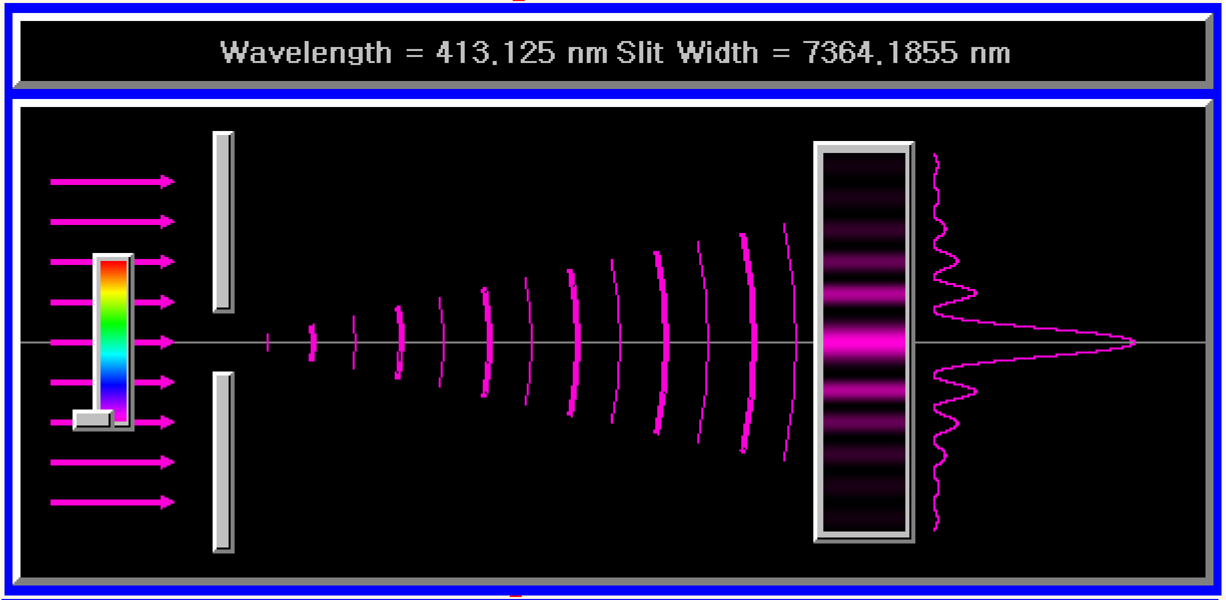
for minima $\sin \theta = m \dfrac{\lambda}{d}$, m=1,2,3,$\cdots$

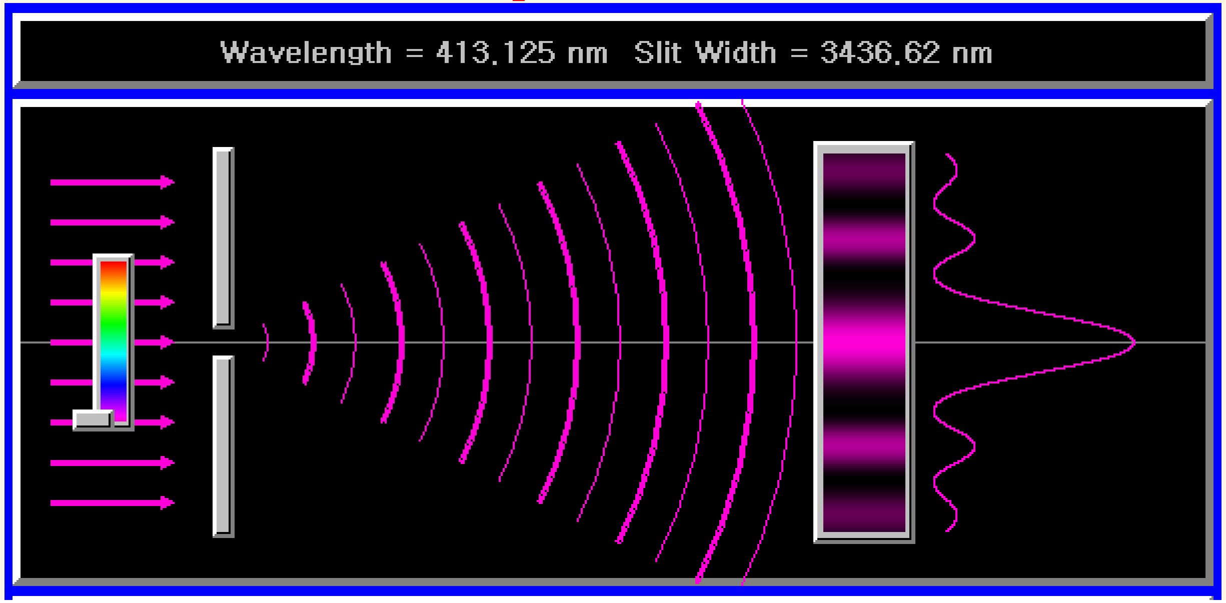




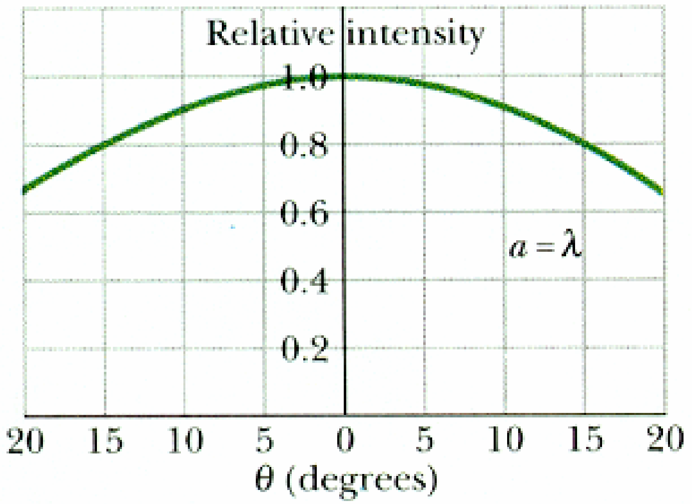


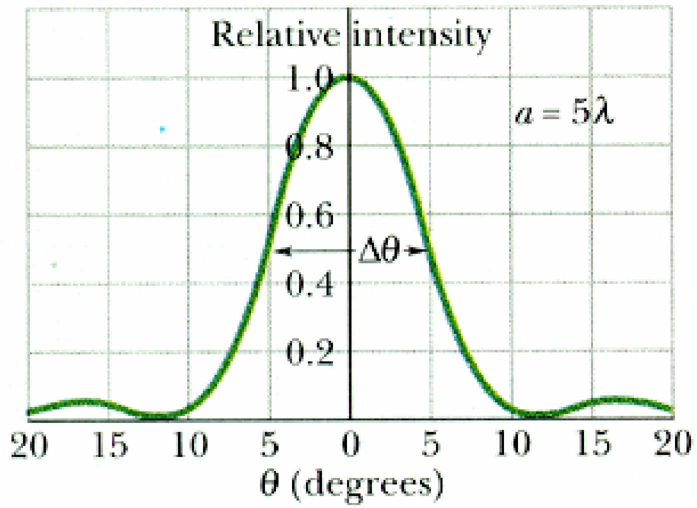
Single-Slit Diffraction

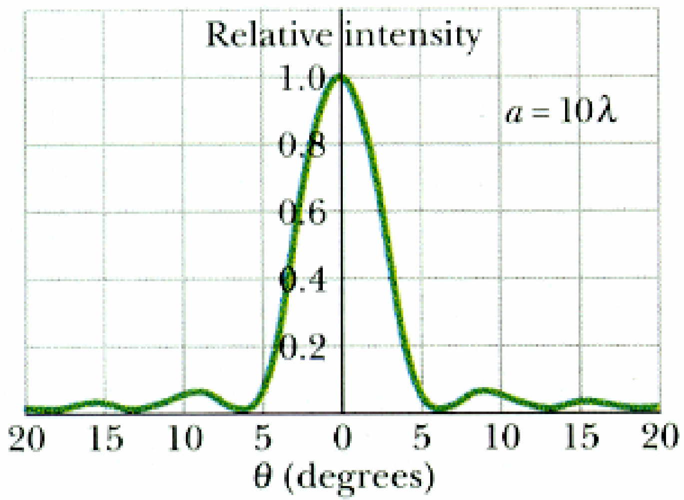




http://www.phys.hawaii.edu/~teb/optics/java/slitdiffr/







D. Halliday, Fundamentals of Physics

Convolution

- $c(\vec{u}) = f(\vec{r}) * g(\vec{r}) = \int_{all\ \vec{r}} f(\vec{r}) g(\vec{u}-\vec{r}) d\vec{r} = \int_{all\ \vec{r}} f(\vec{u}-\vec{r}) g(\vec{r}) d\vec{r}$

- integrand is a function of $\vec{u}$ and $\vec{r}$

  integration is taken over $\vec{r} \rightarrow$ function of $\vec{u}$

- $g(\vec{r})$ vs. $g(\vec{u}-\vec{r})$ or $g(x)$ vs. $g(u-x)$ for 1-D

  reflection+displacement

- example

  $f(x)$: δ function, $g(x)$: arbitrary function

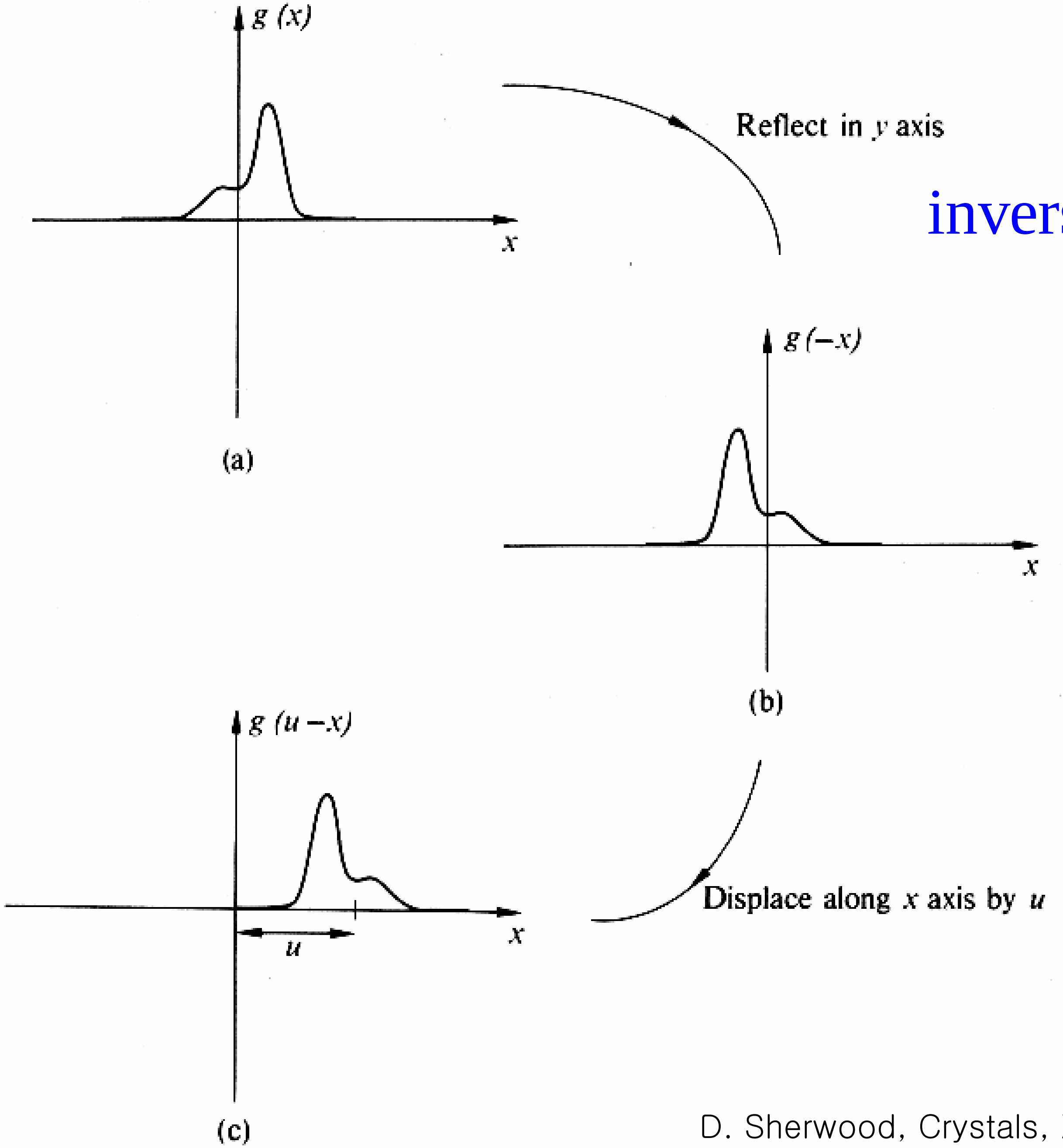
  $$c(u) = \int_{-\infty}^{\infty} f(x) g(u-x) dx = \int_{-\infty}^{\infty} \delta(x+x_o) g(u-x) dx$$

  $$+ \int_{-\infty}^{\infty} \delta(x-x_0) g(u-x) dx$$

  $$= g(u+x_0) + g(u-x_0)$$

http://www.jhu.edu/~signals/convolve/index.html

inversion in 3-D



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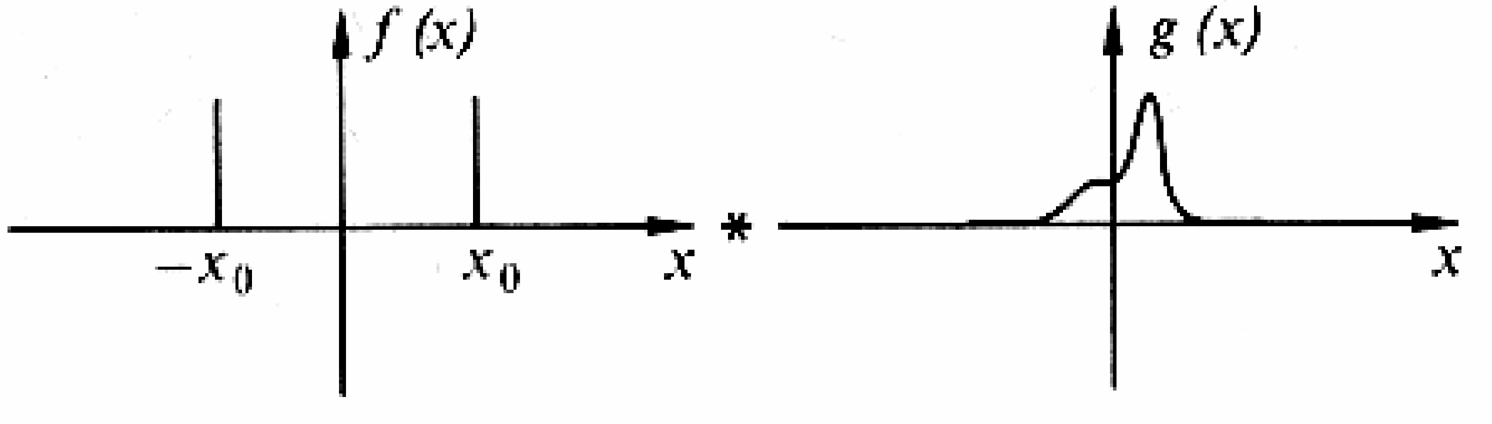
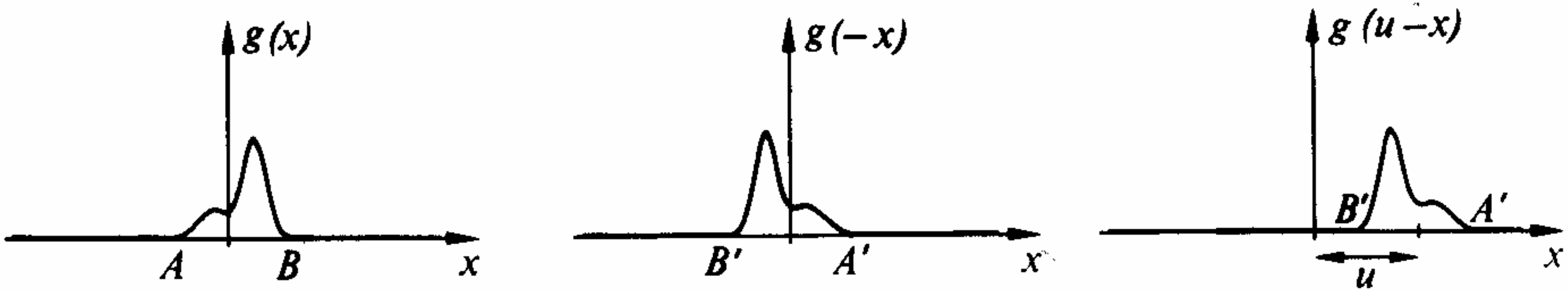
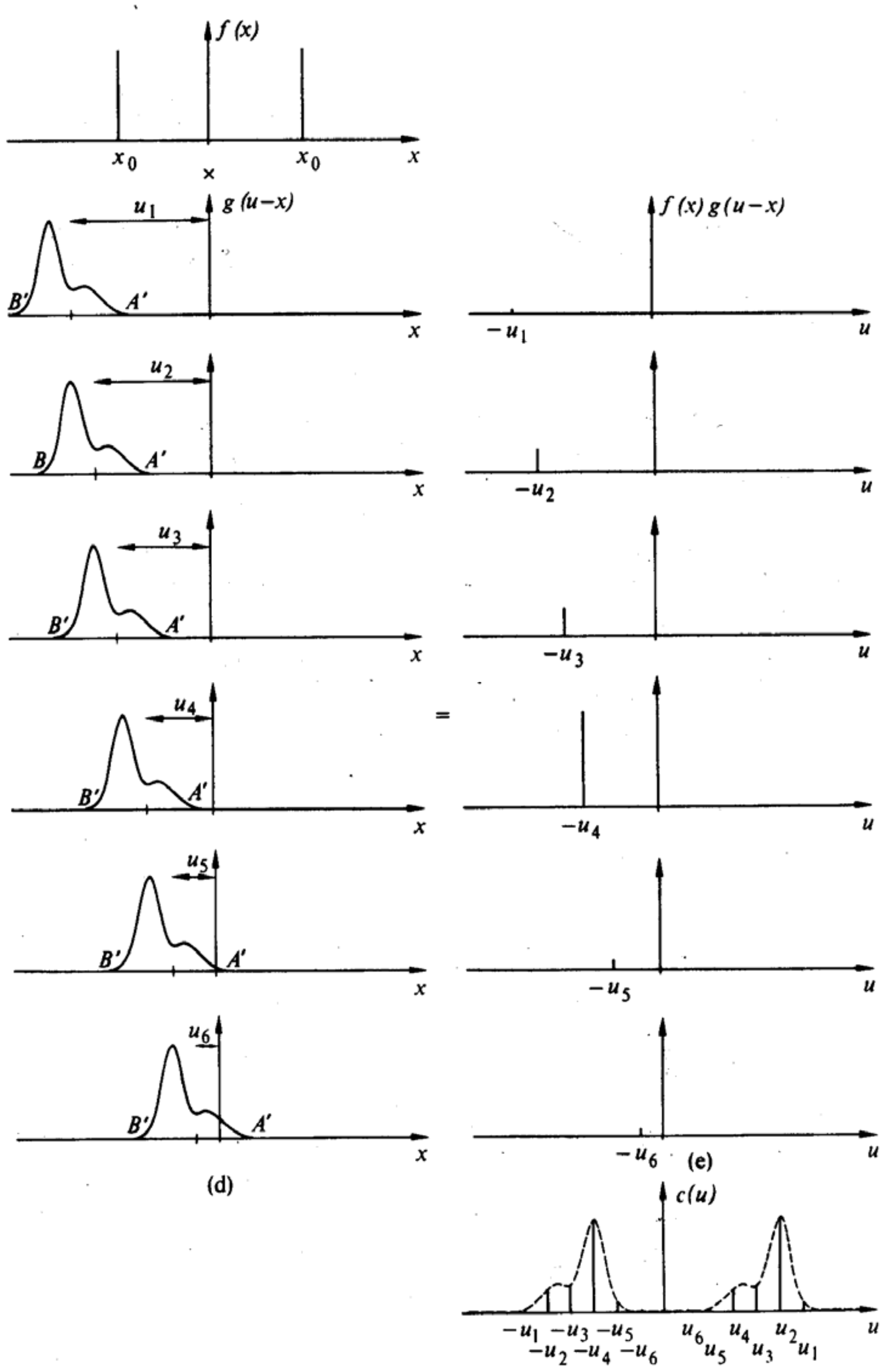


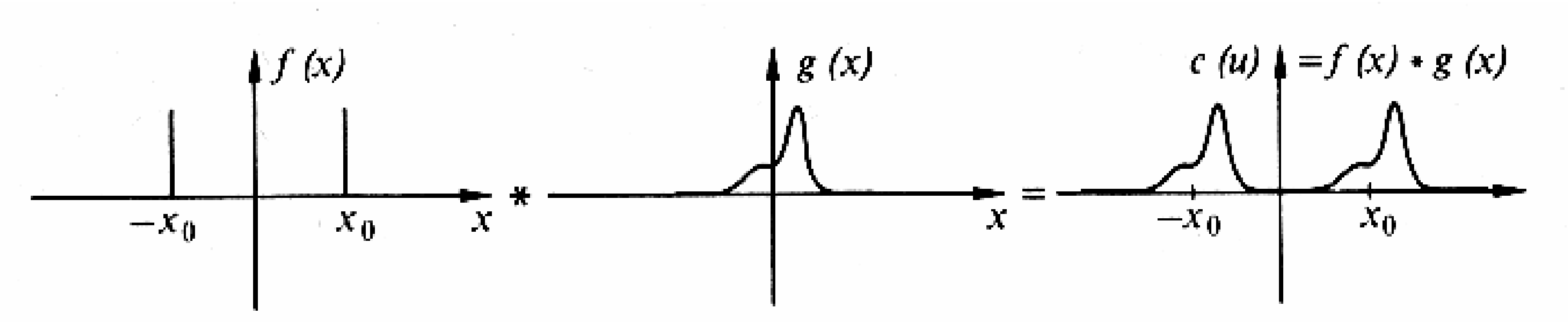
f (x)
g (x)
−x0
x0
x
*
x

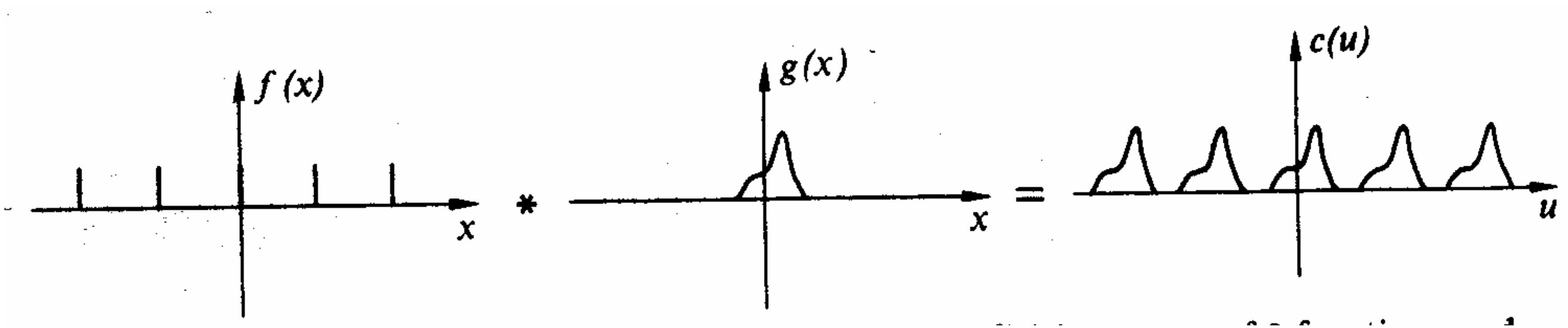


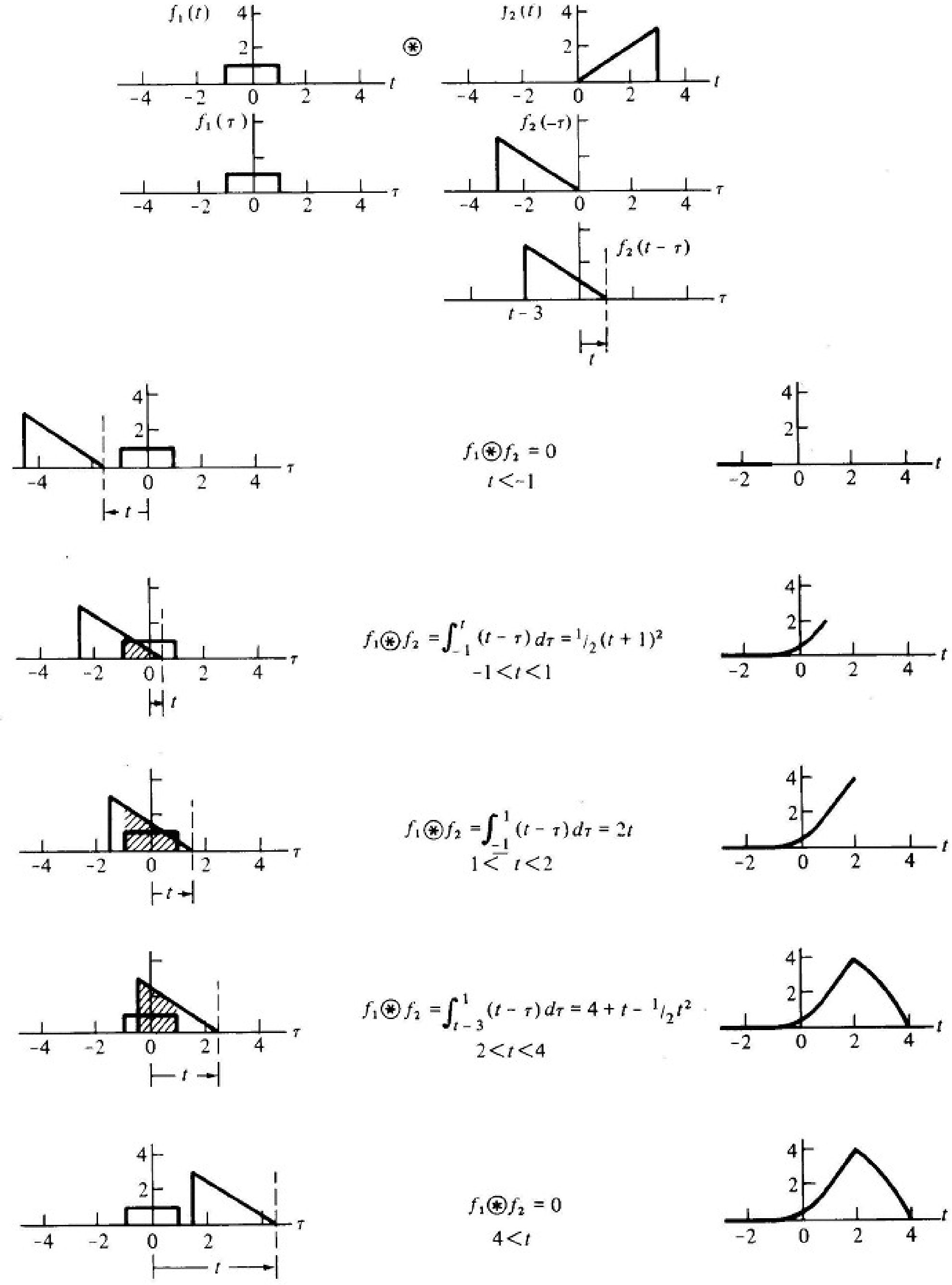
g (x)
A
B
x
g (−x)
B′
A′
x
g (u −x)
B′
A′
u
x



f (x)
x0
x0
x
×
g (u−x)
f (x) g (u−x)
u1
u2
u3
u4
u5
u6
B′
A′
−u1
−u2
−u3
−u4
−u5
−u6
u
=
(d)
(e)
c(u)
−u1 −u3 −u5 u6 u4 u2
−u2 −u4 −u6 u5 u3 u1


f (x)
−x0
x0
x
*
g (x)
x
=
c (u)
= f (x) * g (x)
−x0
x0


f (x)
x
*
g(x)
x
=
c(u)
u



The convolution of a rectangular and a triangular pulse.

Diffraction by 1-D Obstacles

- two wide slit

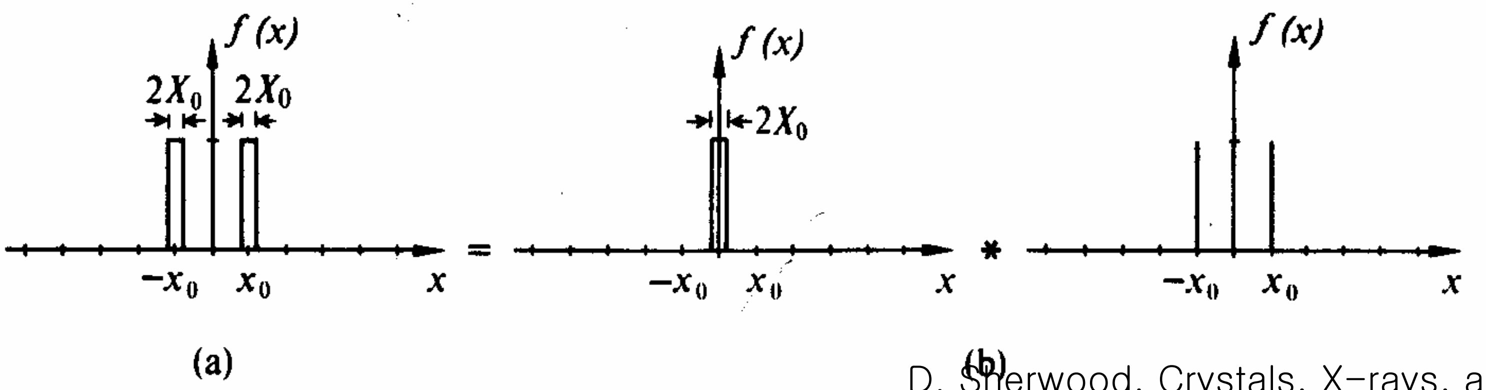
slits , each of width $2X_0$, centered at $x = -x_0$ and $x = x_0$

- $f(x) = 0 \;\; if \;\; -\infty < x < -(x_0 + X_0)$

$$
\begin{aligned}
&1 \;\; if \;\; -(x_0 + X_0) < x < -(x_0 - X_0) \\
&0 \;\; if \;\; -(x_0 - X_0) < x < (x_0 - X_0) \\
&1 \;\; if \;\; (x_0 - X_0) < x < (x_0 + X_0) \\
&0 \;\; if \;\; (x_0 + X_0) < x < \infty
\end{aligned}
$$

- $f(x)$ is convolution of one wide slit and two narrow slit

$f(two\ wide\ slit) = f(one\ wide\ slit) * f(two\ narrow\ slit)$



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Diffraction by 1-D Obstacles

- Fourier transform

$$Tf(two\ wide\ slit) = T[f(one\ wide\ slit) * f(two\ narrow\ slit)]$$

- Fourier transform of a convolution is the product of the individual Fourier transforms

$$Tf(two\ wide\ slit) = Tf(one\ wide\ slit) \cdot Tf(two\ narrow\ slit)]$$

- one wide slit

$$F(\sin\theta) = 2X_0 \frac{\sin(kX_0 \sin\theta)}{kX_0 \sin\theta}$$

- two narrow slit

$$F(\sin\theta) = 2\cos(kx_0 \sin\theta)$$

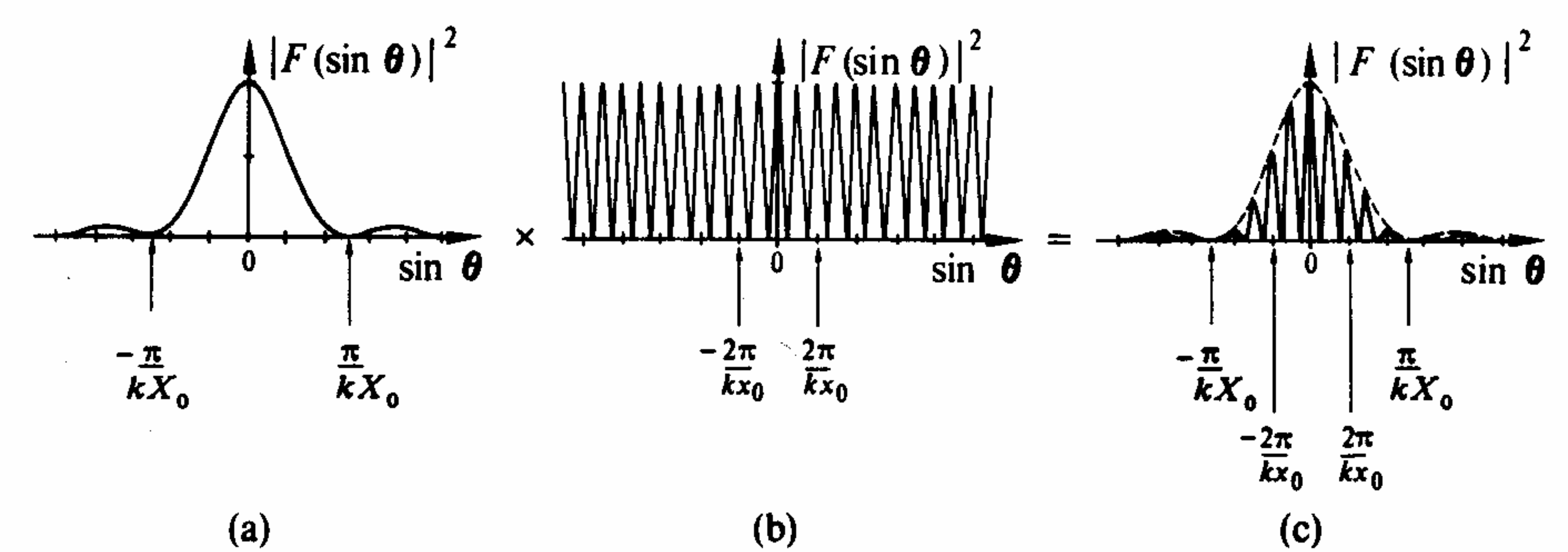
Diffraction by 1-D Obstacles

- two wide slit

$$F(\sin\theta) = 4X_0 \frac{\sin(kX_0 \sin\theta)}{kX_0 \sin\theta} \cos(kx_0 \sin\theta)$$

-intensity

$$\left|F(\sin\theta)\right|^2 = 16X_0^2 \frac{\sin^2(kX_0 \sin\theta)}{(kX_0 \sin\theta)^2} \cos^2(kx_0 \sin\theta)$$



Diffraction by 1-D Obstacles

- two wide slit

  form of diffraction pattern is a series of $\cos^2$ fringes

  modulated by $(\sin\alpha/\alpha)^2$

- $\cos^2$ function- first zero $kx_0 \sin\theta_1 = \pi/2$

  $\sin\theta_1 = \pi/(2kx_0)$

- $(\sin\alpha/\alpha)^2$ function- first zero $kX_0 \sin\theta_2 = \pi$

  $\sin\theta_2 = \pi/(kX_0)$

- $x_0 \gg X_0 \rightarrow \theta_2 > \theta_1$

Diffraction by 1-D Obstacles

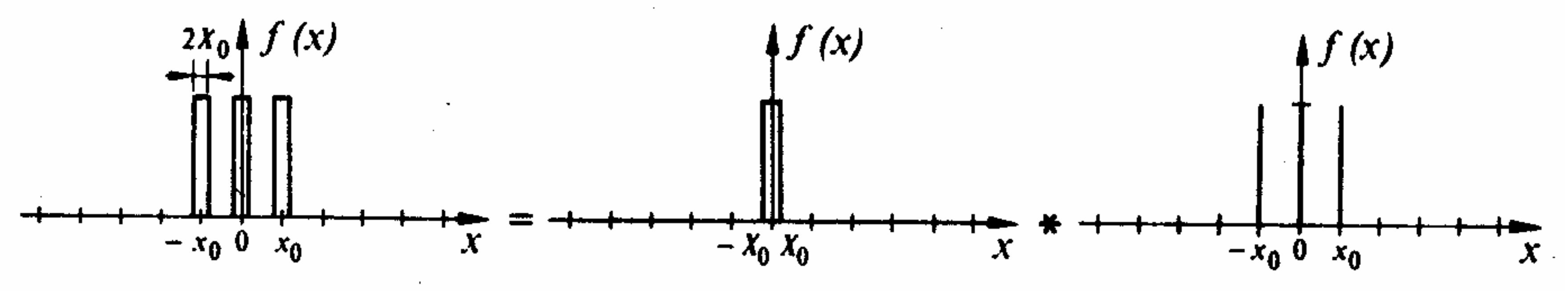
- three wide slit
- amplitude function

$$f(three\ wide\ slit) = f(one\ wide\ slit) * f(three\ narrow\ slits)$$

$$Tf(threeo\ wide\ slit) = T[f(one\ wide\ slit) * f(three\ narrow\ slits)]$$

$$Tf(threeo\ wide\ slit) = Tf(one\ wide\ slit) * Tf(three\ narrow\ slits)$$

- $F(\sin\theta) = 2X_0 \dfrac{\sin(kX_0 \sin\theta)}{kX_0 \sin\theta}[1 + 2\cos(kx_0 \sin\theta)]$

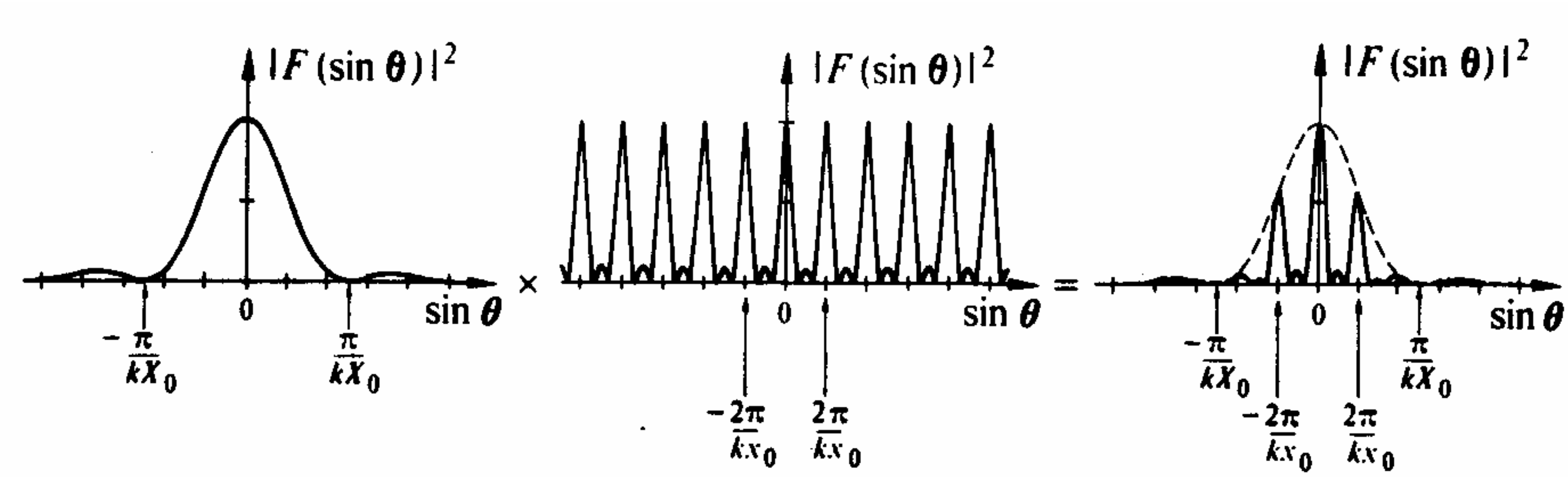


Diffraction by 1-D Obstacles

- three wide slits

- intensity

$$\left|F(\sin\theta)\right|^2 = 4X_0^2 \frac{\sin^2(kX_0\sin\theta)}{(kX_0\sin\theta)^2}[1+2\cos(kx_0\sin\theta)]^2$$



Diffraction by 1-D Obstacles

- N wide slits

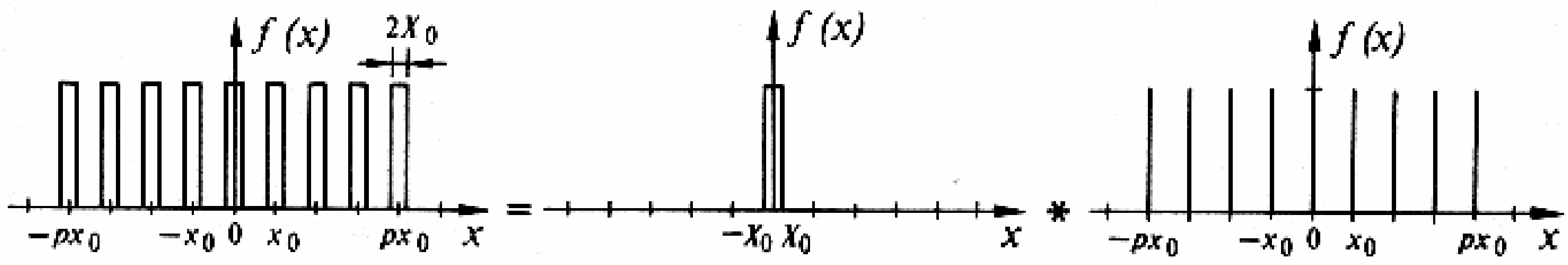
  width of $2X_0$, centered on a δ function

- amplitude function

$$f(N\ wide\ slit) = f(one\ wide\ slit) * f(N\ narrow\ slits)$$

$$Tf(N\ wide\ slit) = T[f(one\ wide\ slit) * f(N\ narrow\ slits)]$$

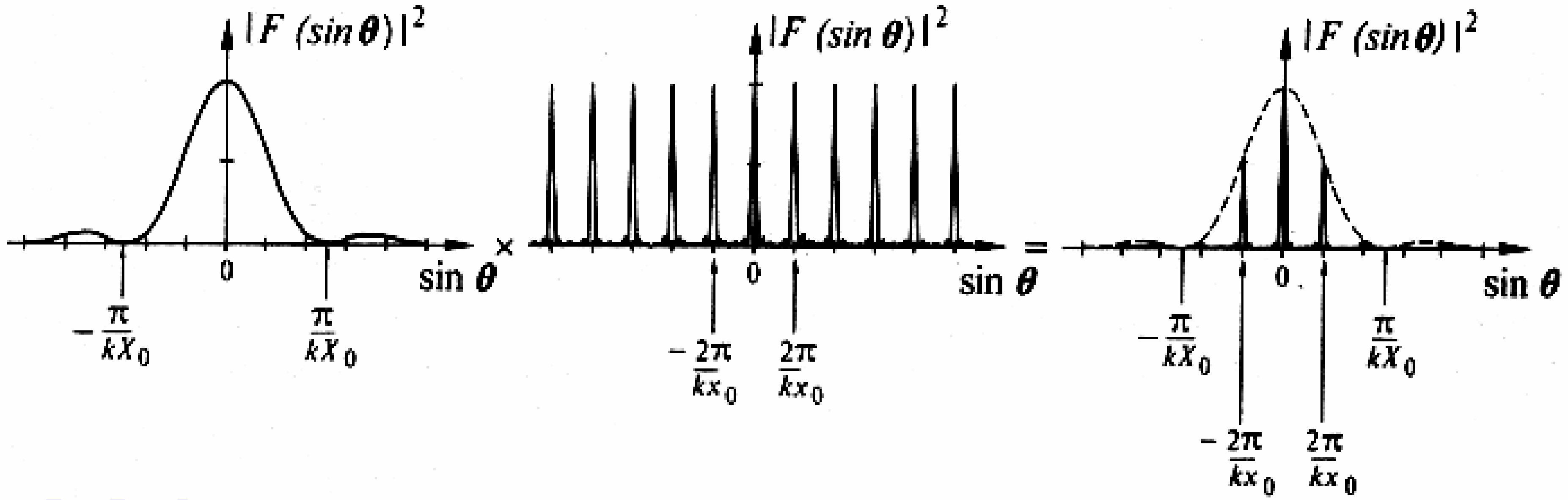
$$Tf(N\ wide\ slit) = Tf(one\ wide\ slit) * Tf(N\ narrow\ slits)$$



Diffraction by 1-D Obstacles

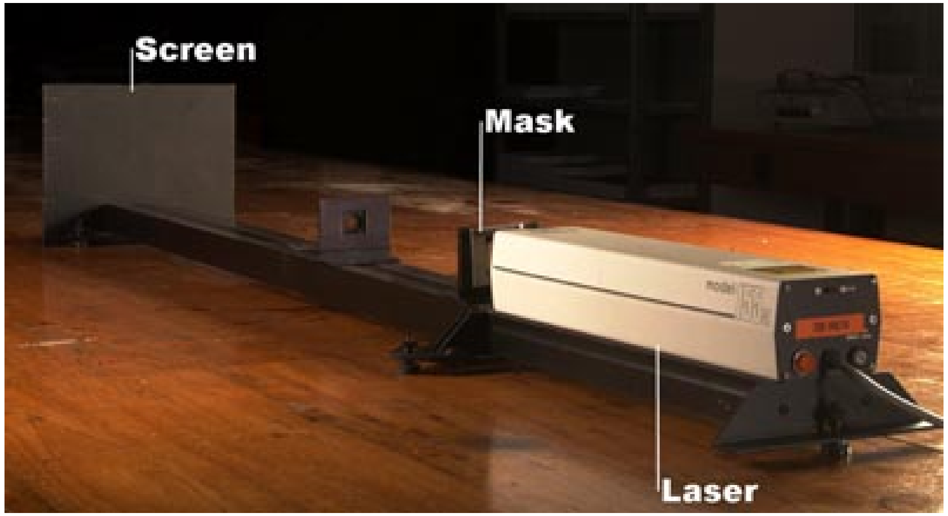
- N wide slits
- intensity

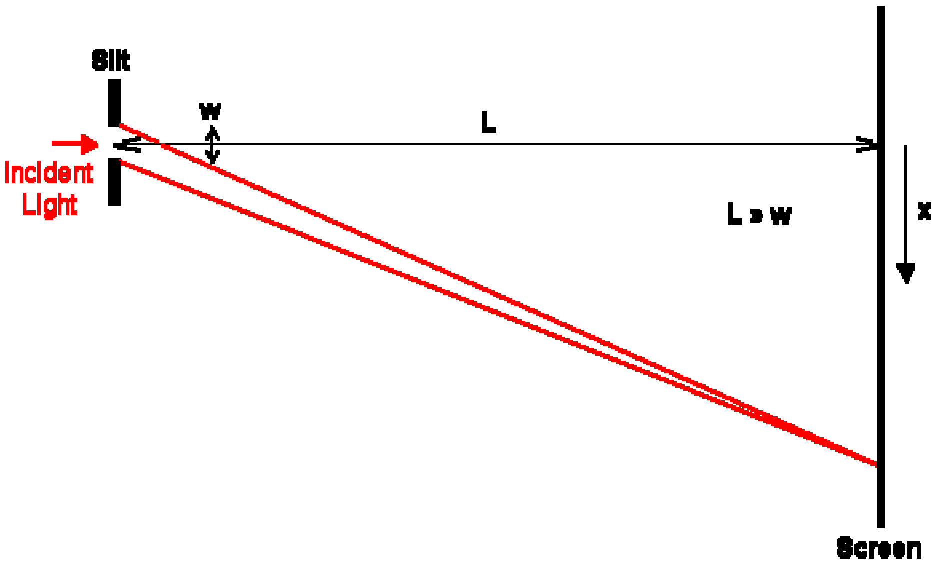
$$|F(\sin\theta)|^2 = 4X_0^2 \frac{\sin^2(kX_0\sin\theta)}{(kX_0\sin\theta)^2} \frac{\sin^2 \dfrac{Nkx_0\sin\theta}{2}}{\sin^2 \dfrac{kx_0\sin\theta}{2}}$$

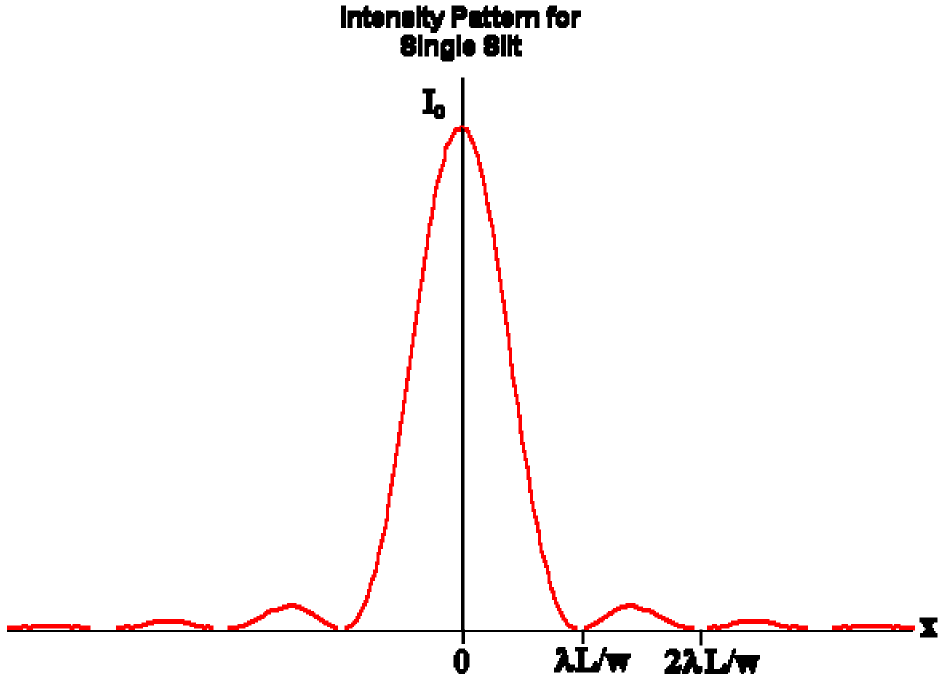


D. Sherwood, Crystals, X-rays, and Proteins

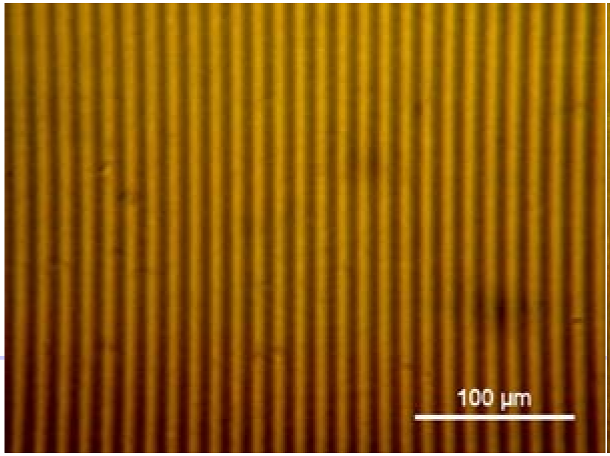
Experiments

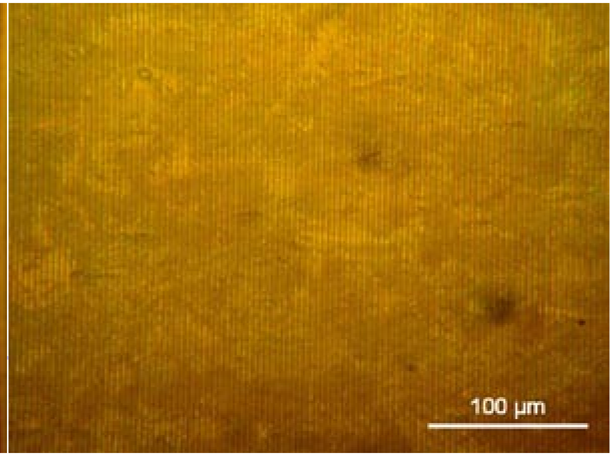






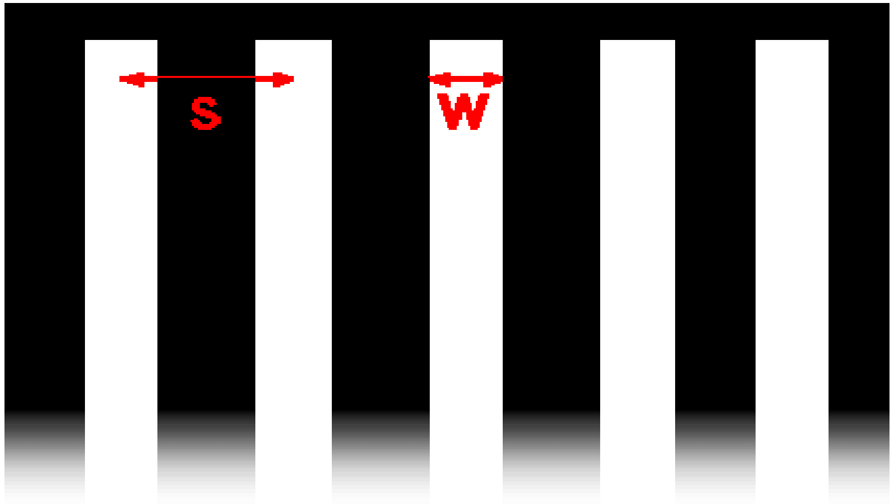
http://www.msm.cam.ac.uk/doitpoms/tlplib/diffraction/index.php





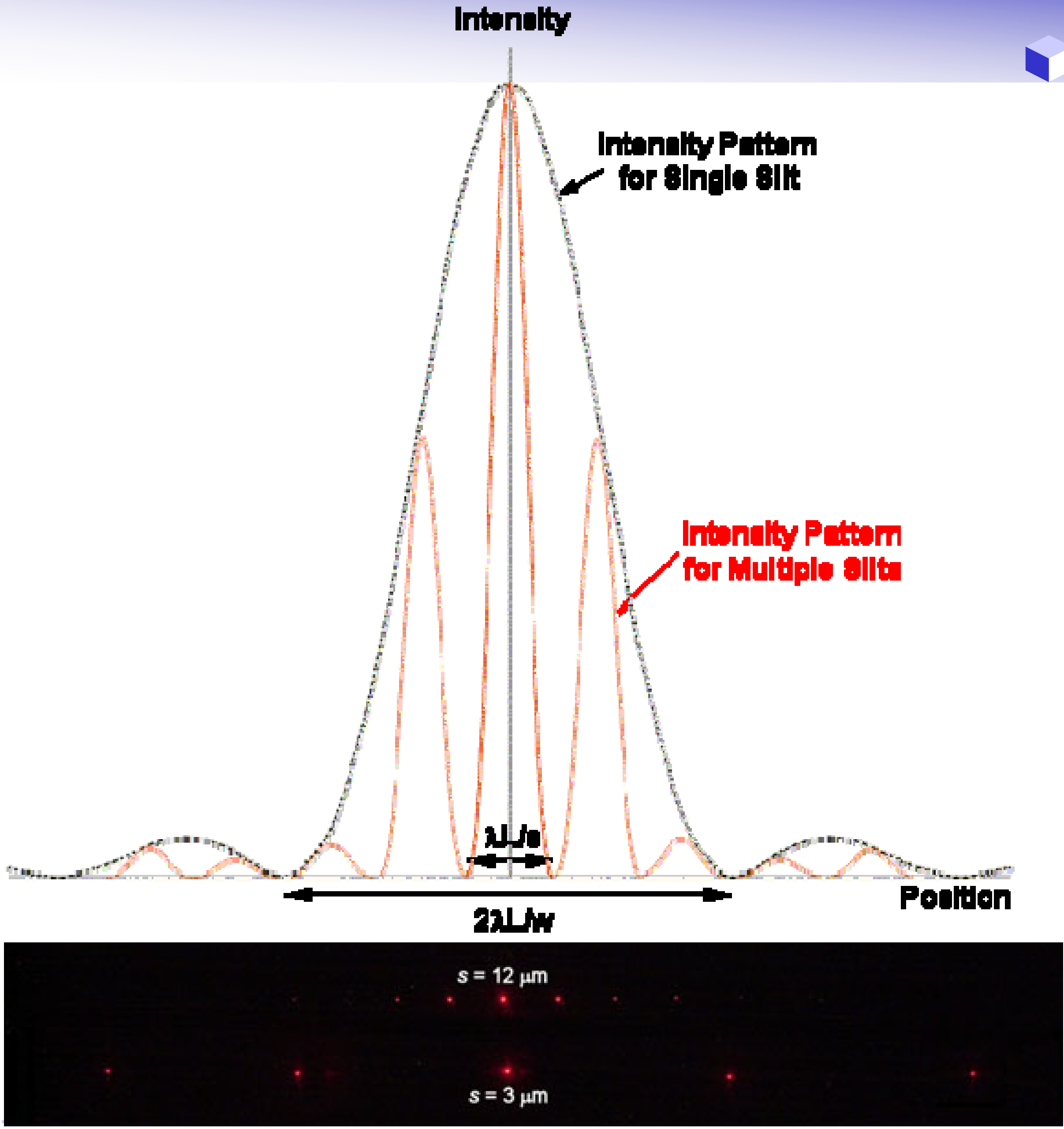
(a) s = 12 μm

(b) s = 3 μm



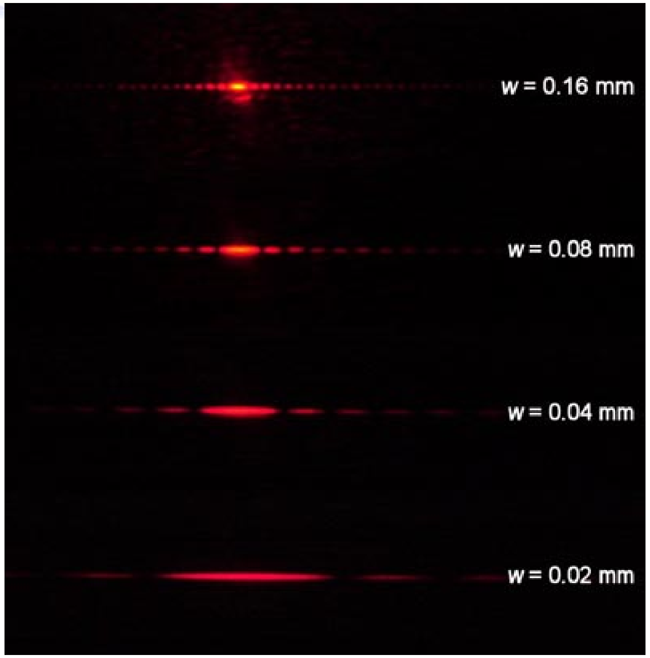
Slit spacing s and slit width w

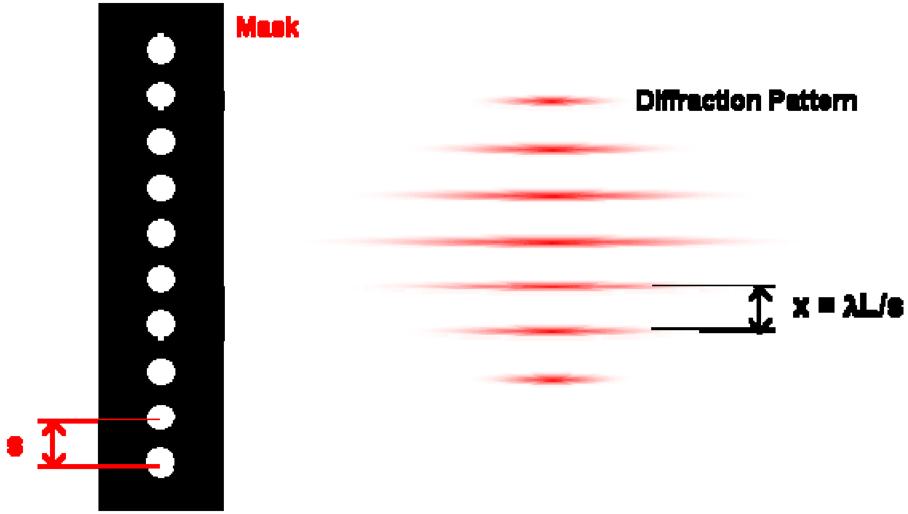
http://www.msm.cam.ac.uk/doitpoms/tlplib/diffraction/index.php

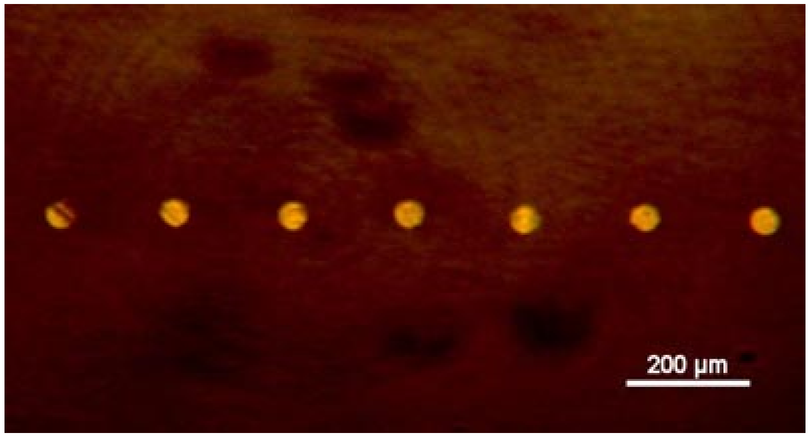


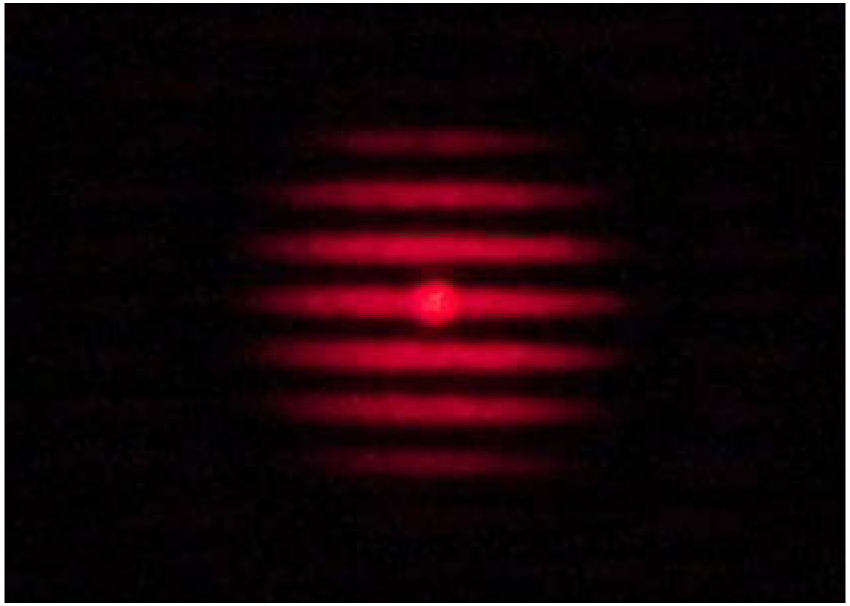
Diffraction patterns from gratings (a) and (b).

http://www.msm.cam.ac.uk/doitpoms/tlplib/diffraction/index.php









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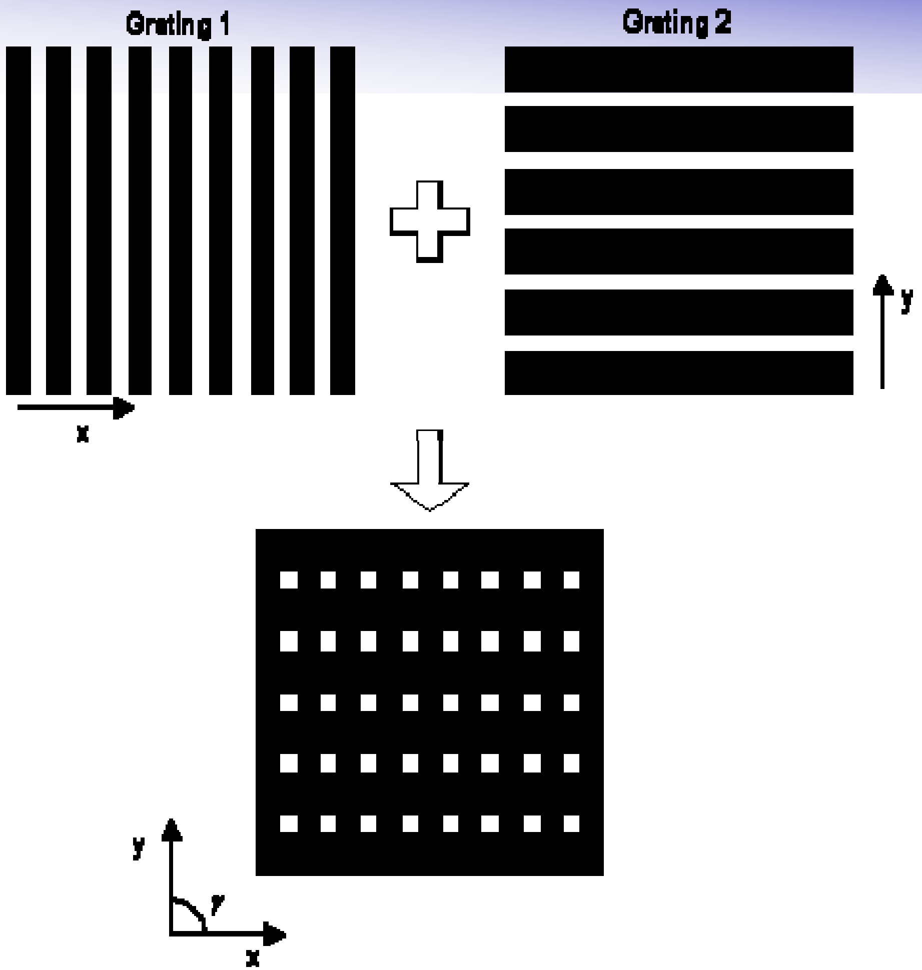

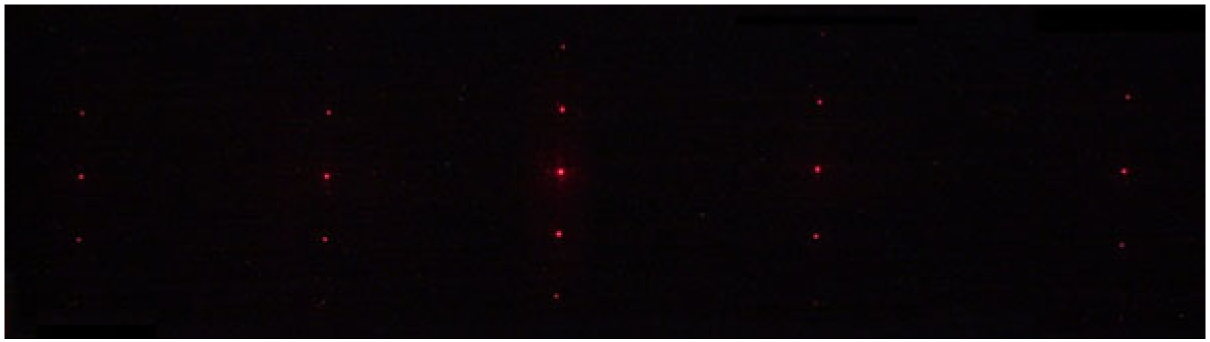

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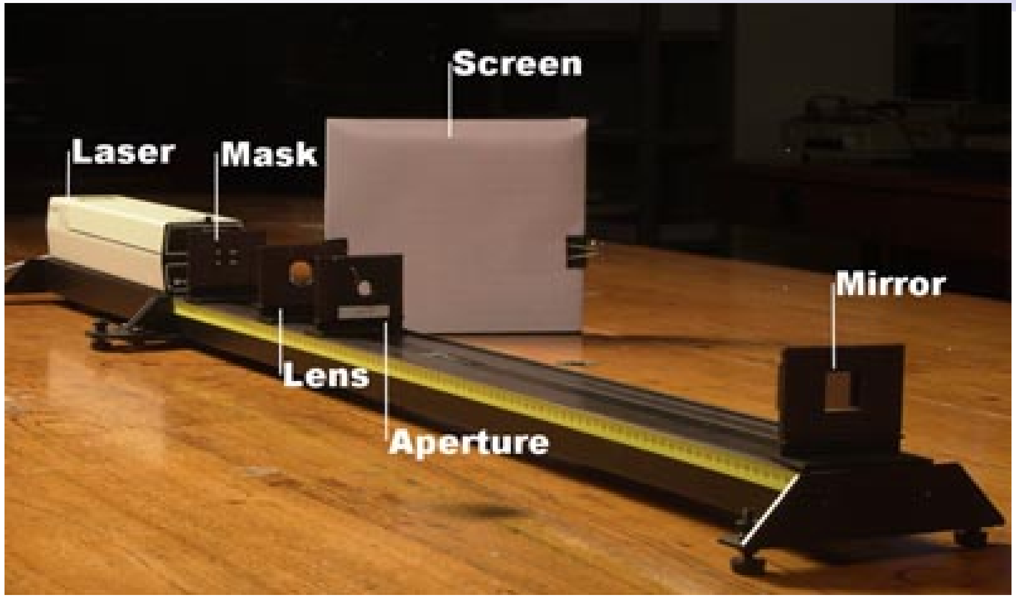
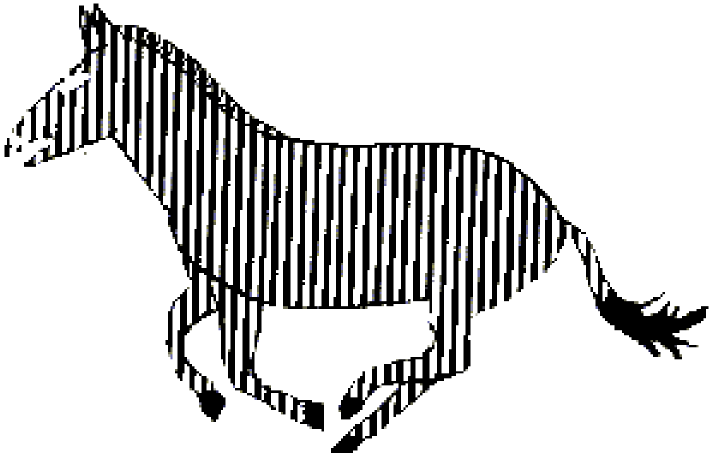
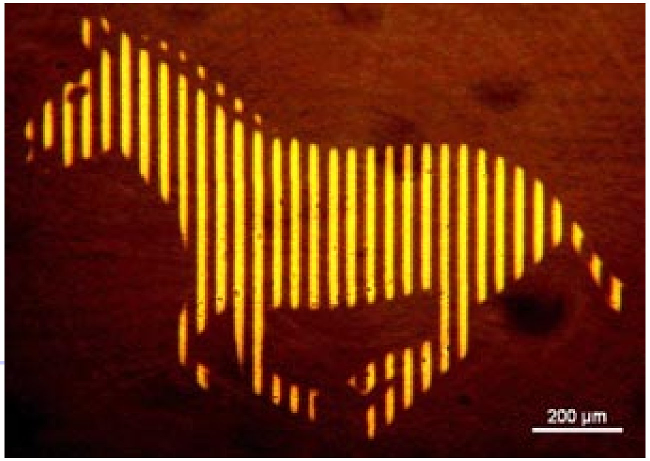






The zebra

http://www.msm.cam.ac.uk/doitpoms/tlplib/diffraction/index.php

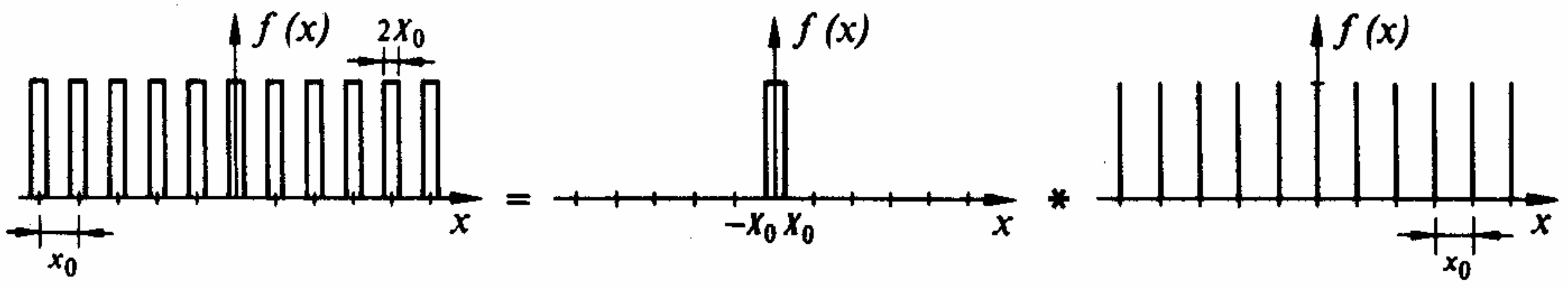
Diffraction by 1-D Obstacles

- infinite wide slits
- amplitude function

$$f(\infty\ wide\ slit) = f(one\ wide\ slit) * f(\infty\ narrow\ slits)$$

$$Tf(\infty\ wide\ slit) = T[f(one\ wide\ slit) * f(\infty\ narrow\ slits)]$$

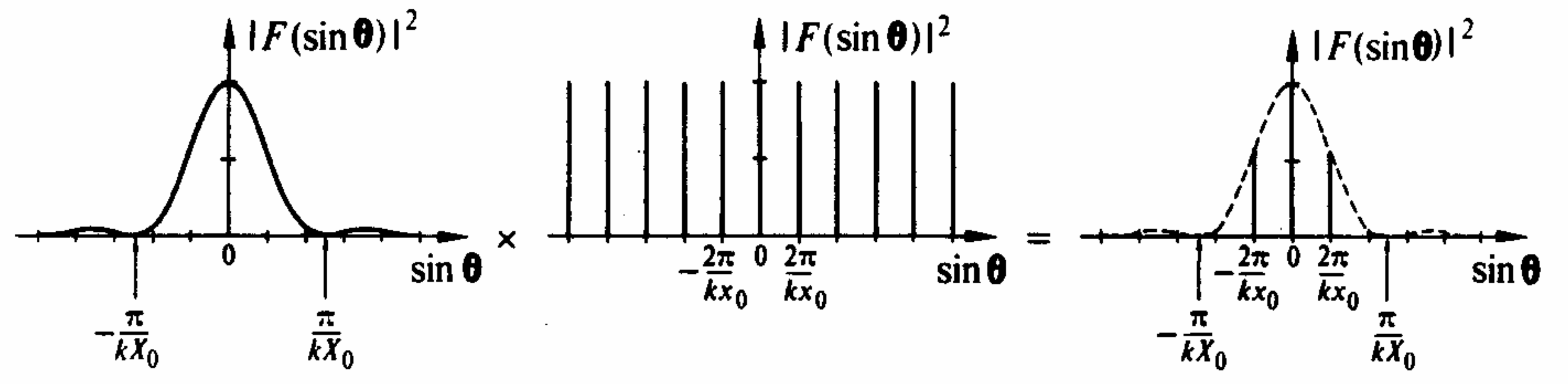
$$Tf(\infty\ wide\ slit) = Tf(one\ wide\ slit) * Tf(\infty\ narrow\ slits)$$



Diffraction by 1-D Obstacles

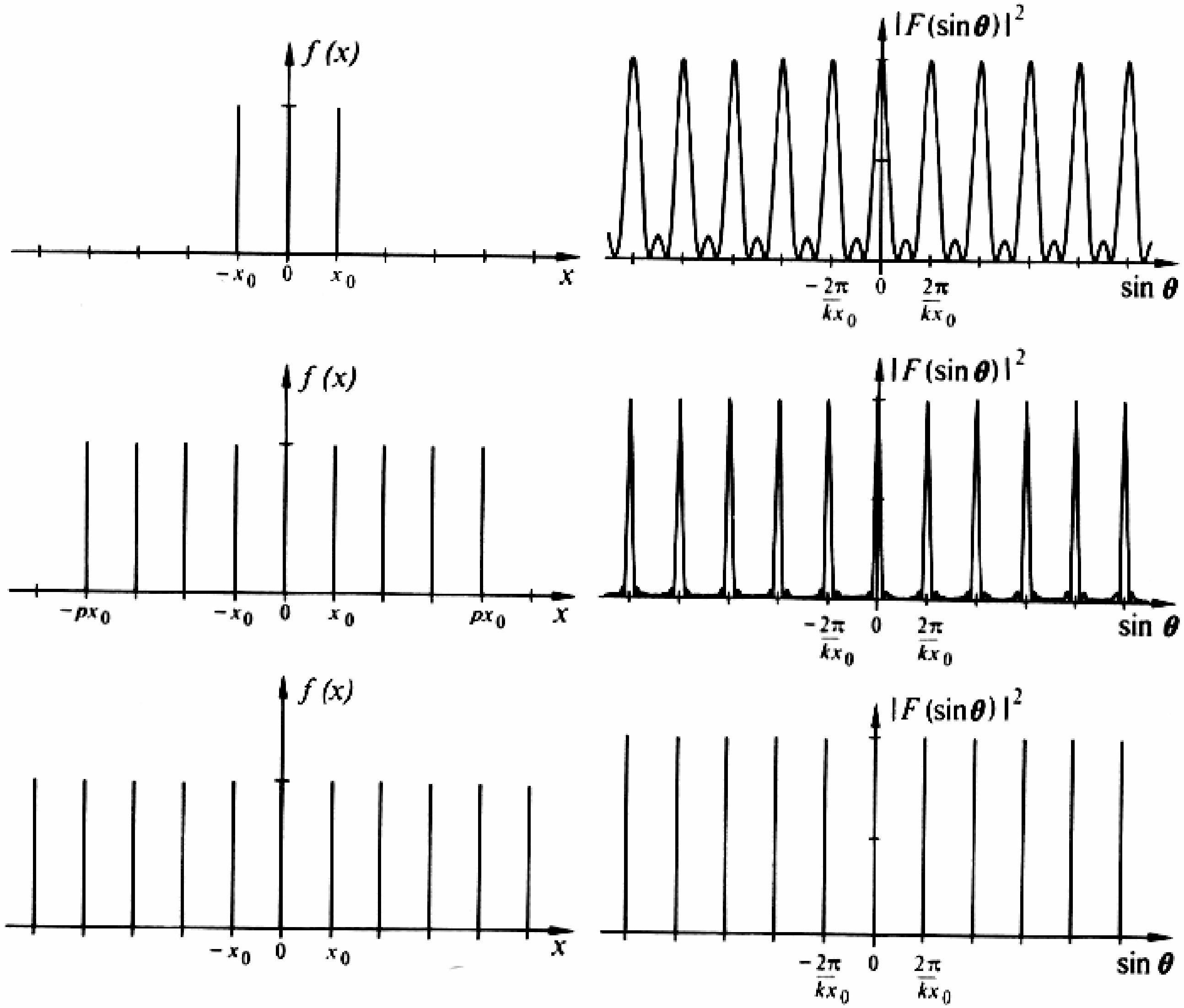
- infinite number of wide slits
- intensity

$$\left|F(\sin\theta)\right|^2 = 4X_0^2 \frac{\sin^2(kX_0\sin\theta)}{(kX_0\sin\theta)^2}\left|\sum_{n=-\infty}^{n=\infty}\delta(\sin\theta-\frac{2n\pi}{kx_0})\right|^2$$



Diffraction by 1-D Obstacles

- significance of the diffraction pattern



D. Sherwood, Crystals, X-rays, and Proteins

Diffraction by 1-D Obstacles

- narrow slits

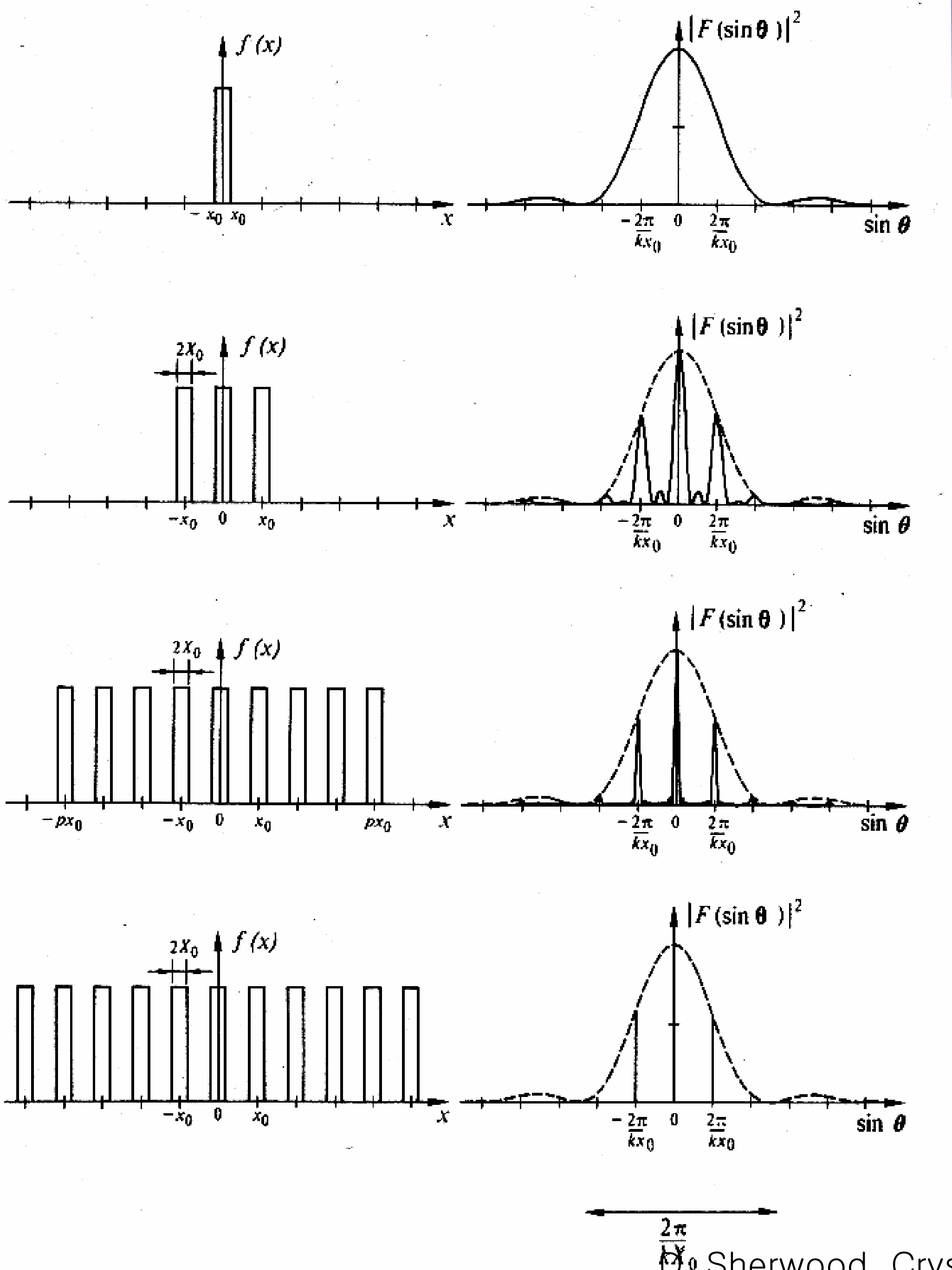
1. As the number of slits increases, the main peaks become sharper and narrower, whilst the subsidiary peaks become rapidly less intense
2. The position and separation of the main peaks is constant independent of the number of peaks. The man peaks are separated by an angular deflection given by

$$\Delta(\sin\theta) = \frac{2\pi}{kx_0}$$

The distance is determined soly by λ and separation x_0 of any two neighboring narrow slits.

Diffraction by 1-D Obstacles

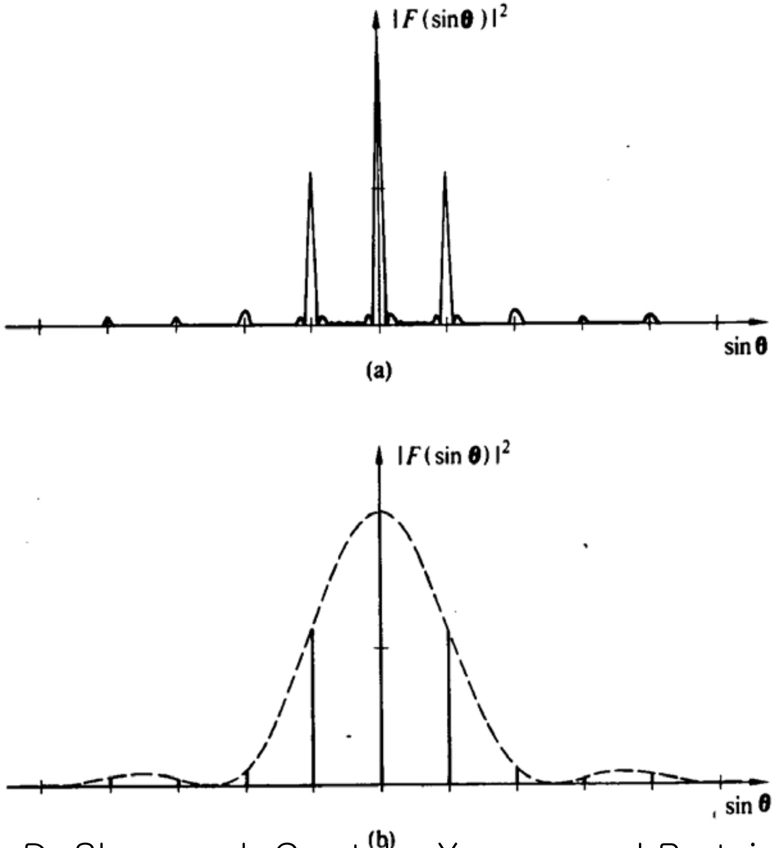
- narrow slits
- The position of the main peak in a diffraction pattern is determined solely by the lattice spacing in an obstacle.
- The shape of the main peak is determined by the overall shape of the obstacle.



D. Sherwood, Crystals, X-rays, and Proteins

Diffraction by 1-D Obstacles

- wide slits
- The effect of the motif (one wide slit) is to alter the intensity of each main peak, but the position of the main peaks are unchanged
- intensity envolope
  $\rightarrow$ structure of motif



D. Sherwood, Crystals, X-rays, and Proteins

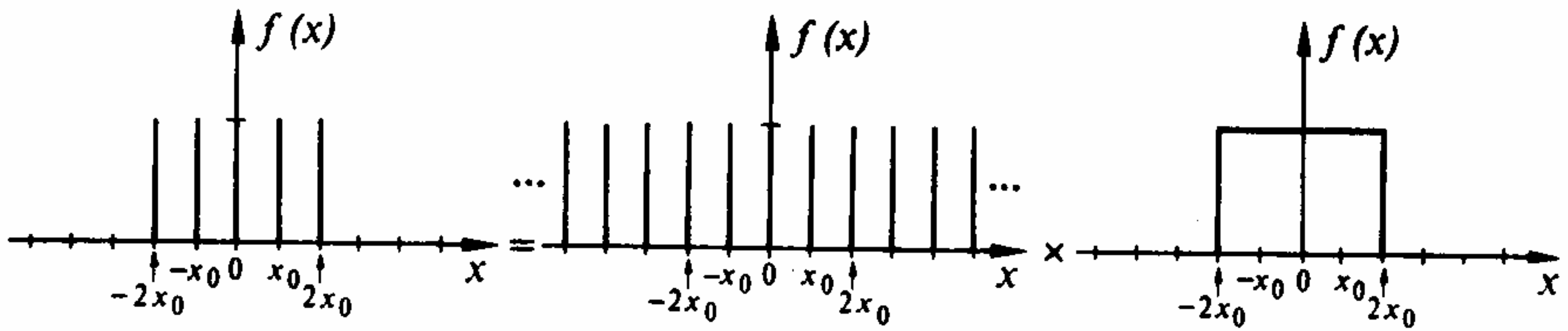
Diffraction by 1-D Obstacles

- another way of looking at N wide slits
- shape function

  is zero everywhere outside an obstacle

  corresponds to the macroscopic shape of the obstacle

  within the obstacle



Diffraction by 1-D Obstacles

- finite lattice

$$f(\textit{finite lattice}) = f(\textit{infinite lattice}) \bullet f(\textit{shape function})$$

$$f(\textit{obstacle}) = f(\textit{motif}) * f(\textit{finite lattice})$$

$$f(\textit{obstacle}) = f(\textit{motif}) * [f(\textit{infinite lattice}) \bullet f(\textit{shape function})]$$

- diffraction pattern

$$F(\sin\theta) = Tf(\textit{obstacle})$$

$$= T\{f(\textit{motif}) * [f(\textit{infinite lattice}) \bullet f(\textit{shape function})]\}$$

$$= Tf(\textit{motif}) \bullet T[f(\textit{infinite lattice}) \bullet f(\textit{shape function})]$$

$$= Tf(\textit{motif}) \bullet [Tf(\textit{infinite lattice}) * Tf(\textit{shape function})]$$

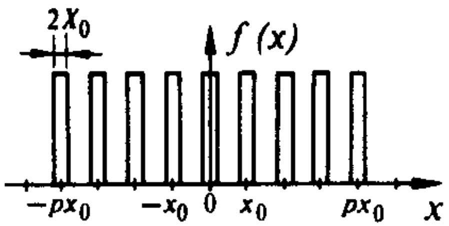
Diffraction by 1-D Obstacles

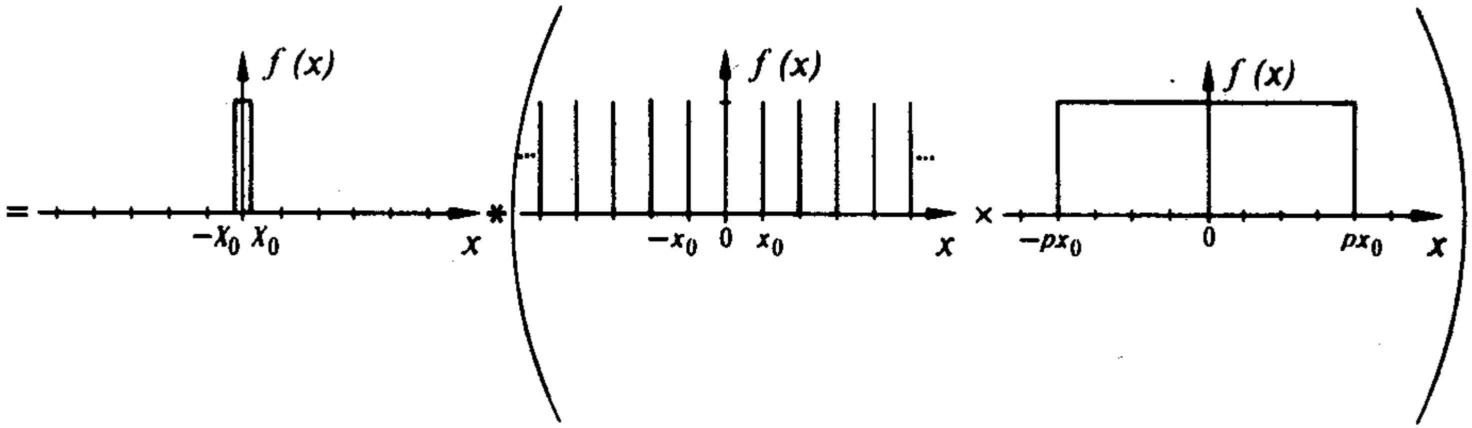
- N wide slits

$$f(N\ \ wide\ slits) = f(one\ wide\ slit) * f(N\ \ narrow\ slits)$$

$$f(N\ \ wide\ slits) = f(one\ wide\ slit) *$$

$$[f(\infty\ narrow\ slits) \bullet f(shape\ function)]$$





Diffraction by 1-D Obstacles

- diffraction pattern

$$Tf(N\ \ wide\ slits) = T\{f(one\ wide\ slit) *$$
$$[f(\infty\ narrow\ slits) \bullet f(shape\ function)]\}$$
$$= Tf(one\ wide\ slit) \bullet T[f(\infty\ narrow\ slits) \bullet f(shape\ function)]$$
$$= Tf(one\ wide\ slit) \bullet Tf(\infty\ narrow\ slits) * Tf(shape\ function)$$

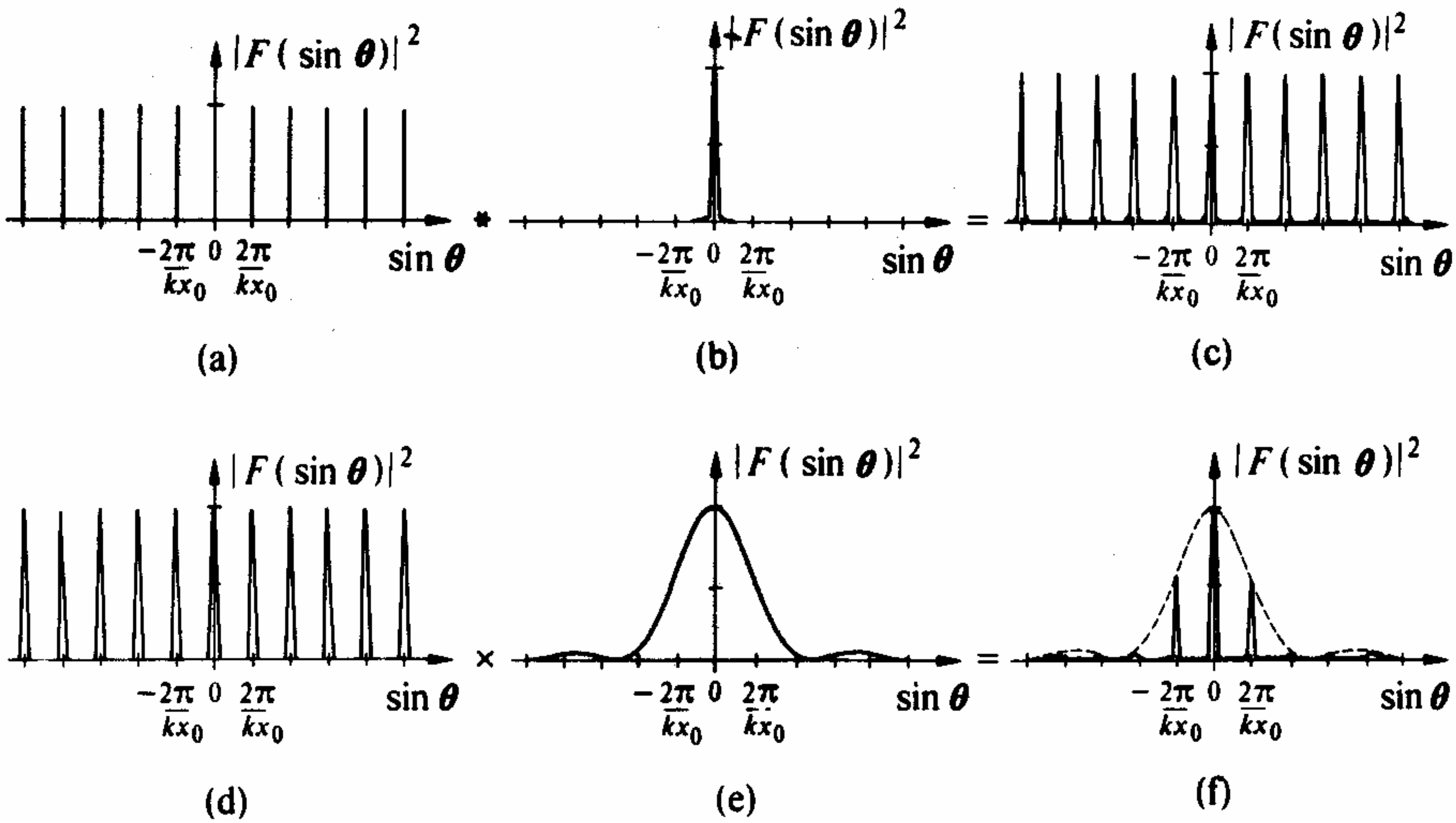
- three types of structural information

that concerning the lattice

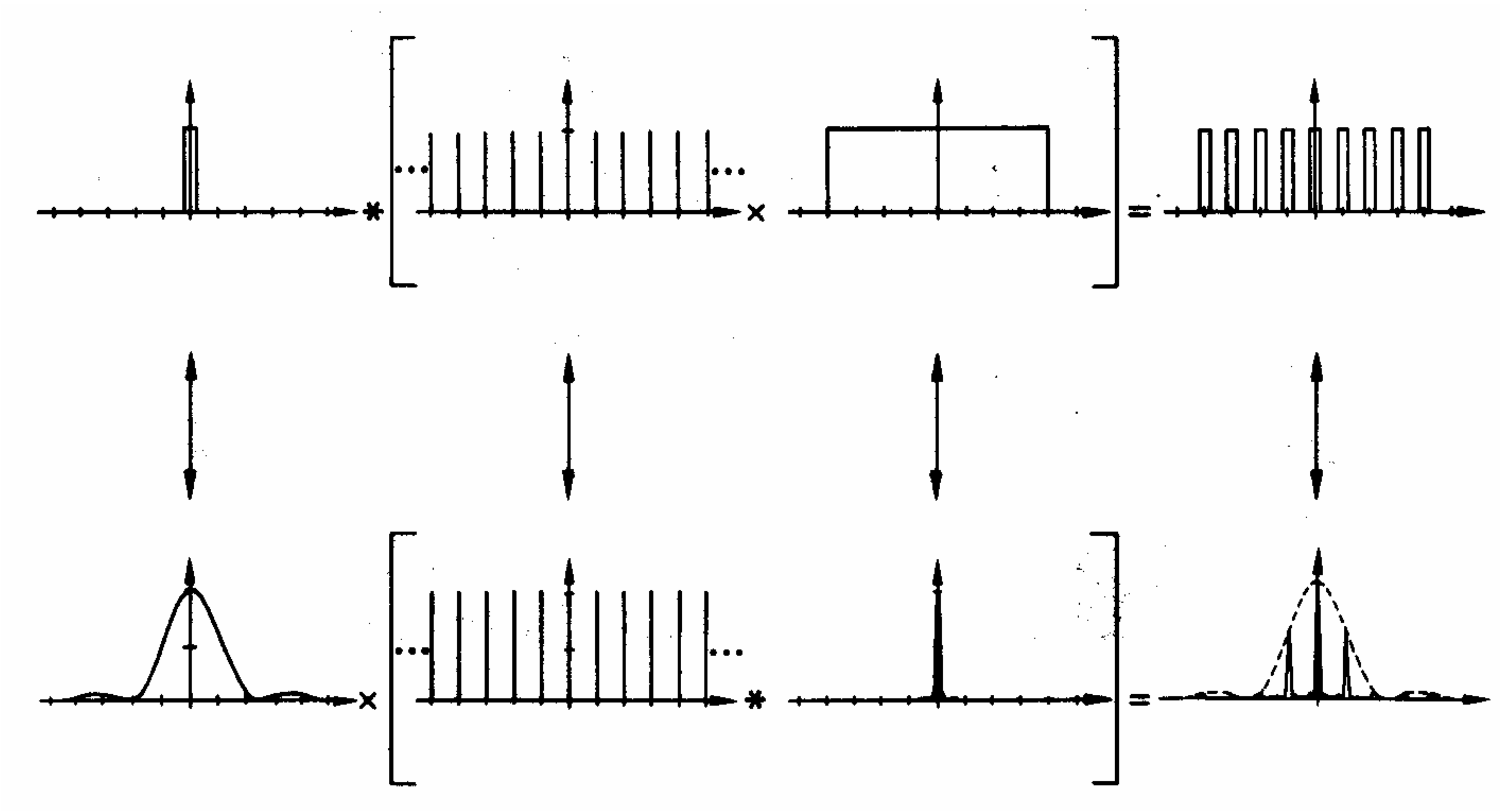
that concerning the motif

that concerning the shape of the entire crystal

Diffraction by 1-D Obstacles



Diffraction by 1-D Obstacles



D. Sherwood, Crystals, X-rays, and Proteins

Summary

- the position of the main peaks gives information
  on the lattice

- the shape of each main peak gives information
  on the overall object shape

- the set of intensities of all the main peaks gives information
  on the structure of the motif