Diffraction by 1-D Obstacles

- geometric arrangement

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

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

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

xz plane

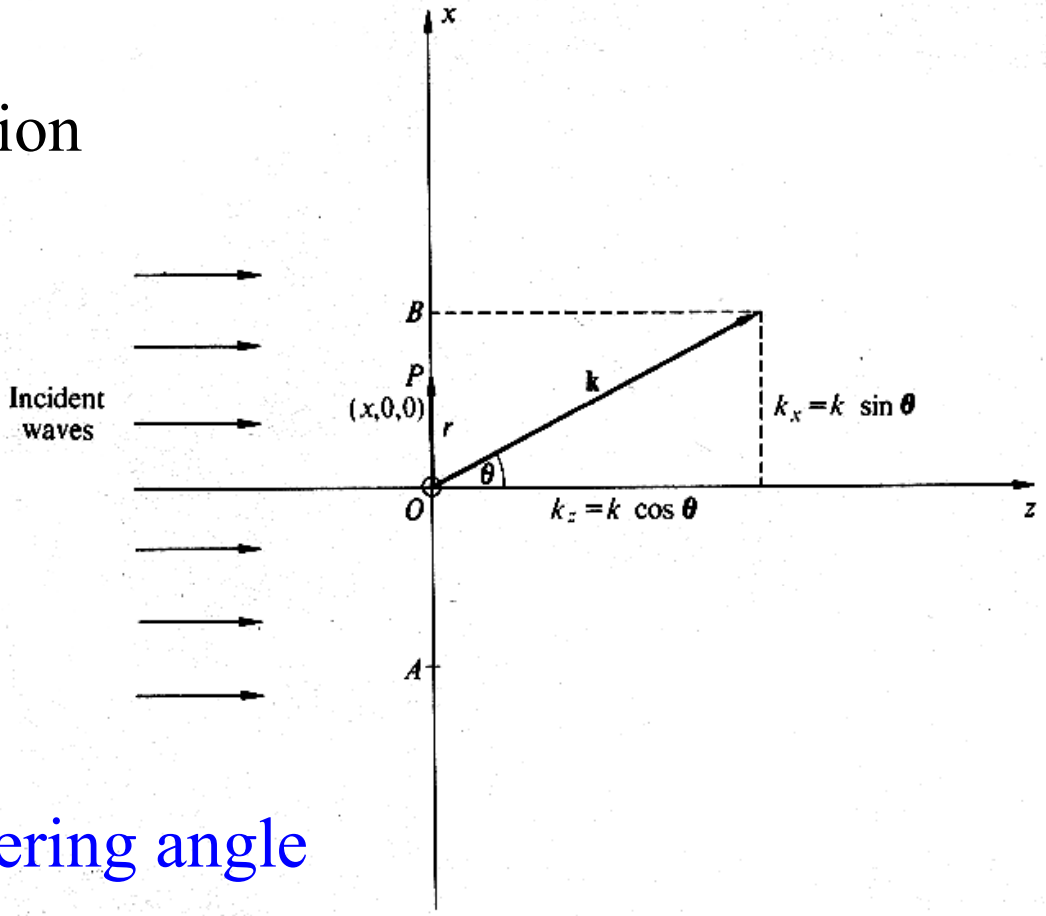
obstacle- along x-axis

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

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

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

$\vec{k}\cdot\vec{r} = k_x x = kx\sin\theta$ scattering angle



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 $\left|F(\sin\theta)\right|^2$

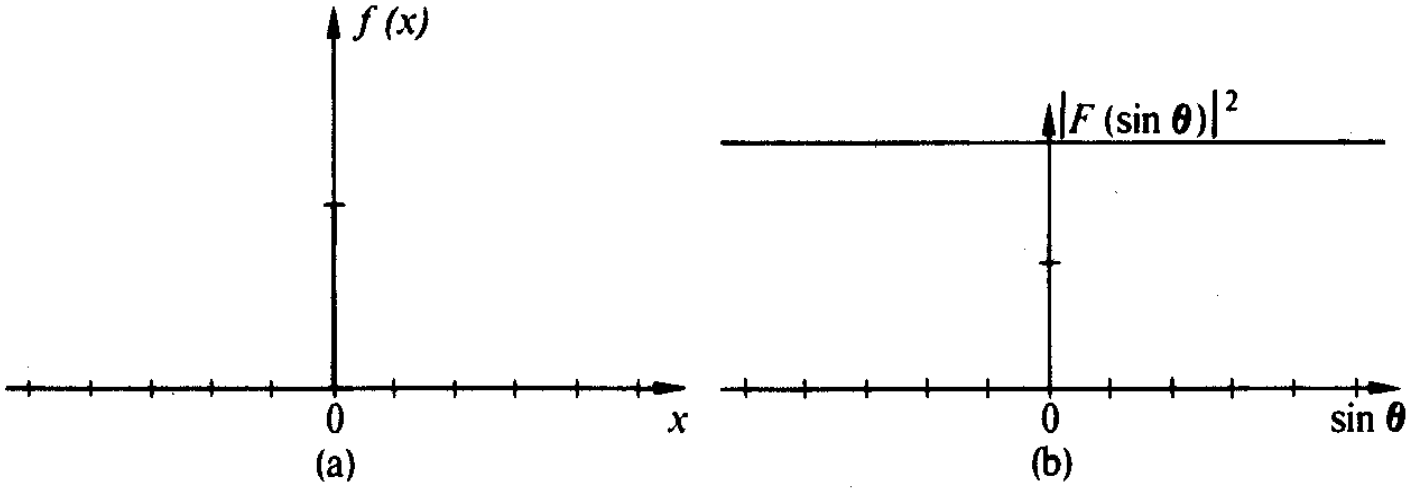
Diffraction by 1-D Obstacles

- 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



Diffraction by 1-D Obstacles

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

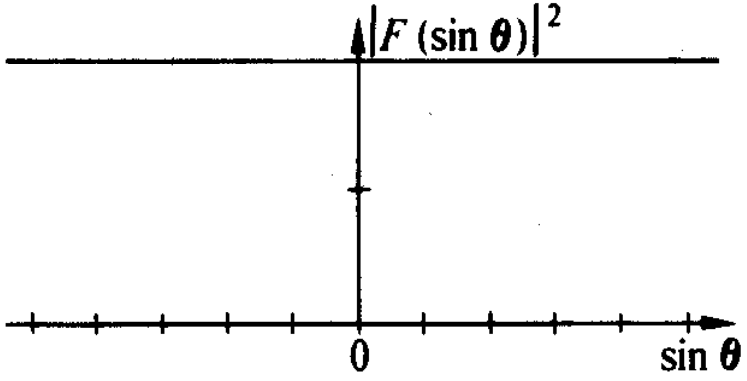
- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx = \int_{-\infty}^{\infty} \delta(x) e^{ikx\sin\theta} dx$

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

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

- intensity is uniform at all angles

- a single narrow slit ≡ an active point source

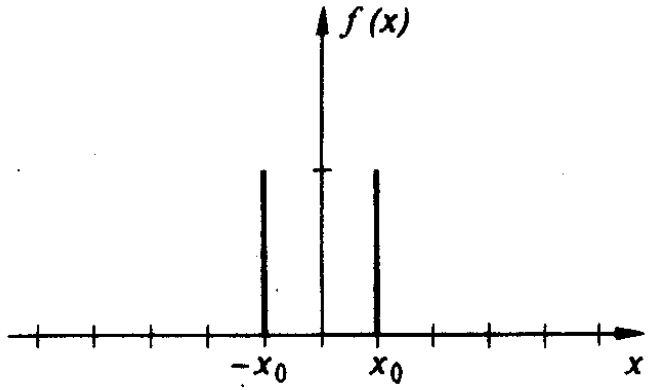


Diffraction by 1-D Obstacles

- two narrow slit

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

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



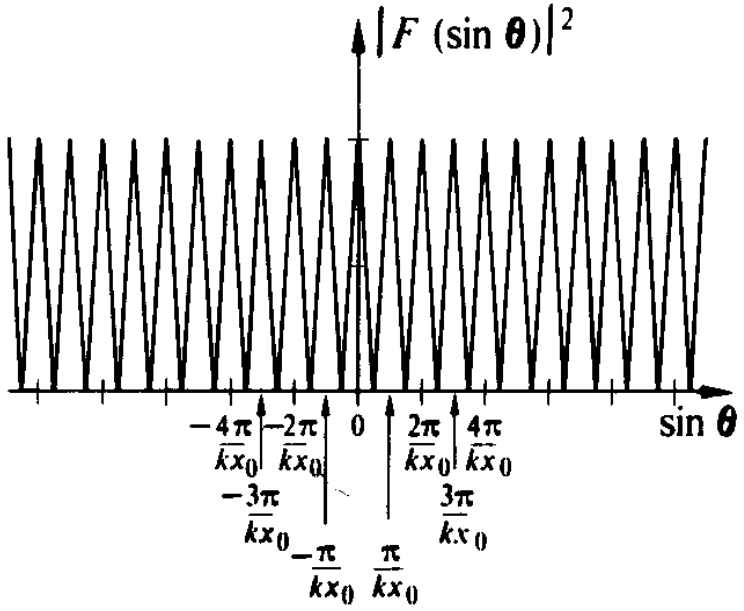
- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$

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

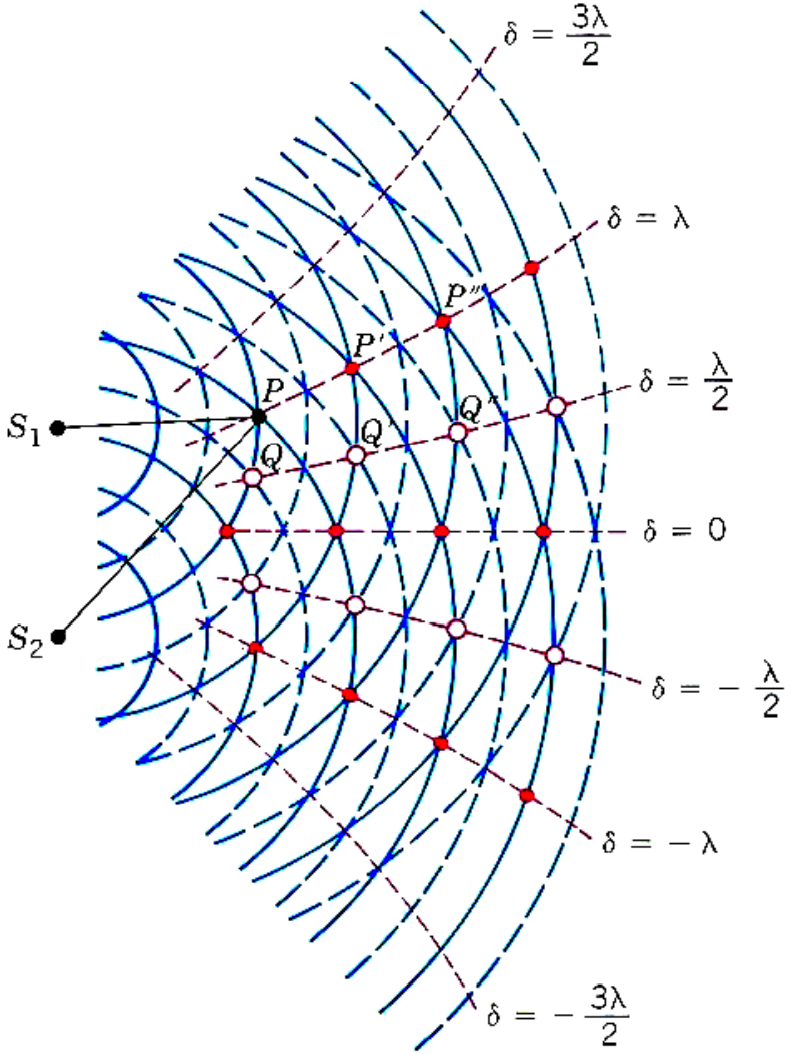
$$= e^{-ikx_0\sin\theta} + e^{ikx_0\sin\theta} = 2\cos(kx_0\sin\theta)$$

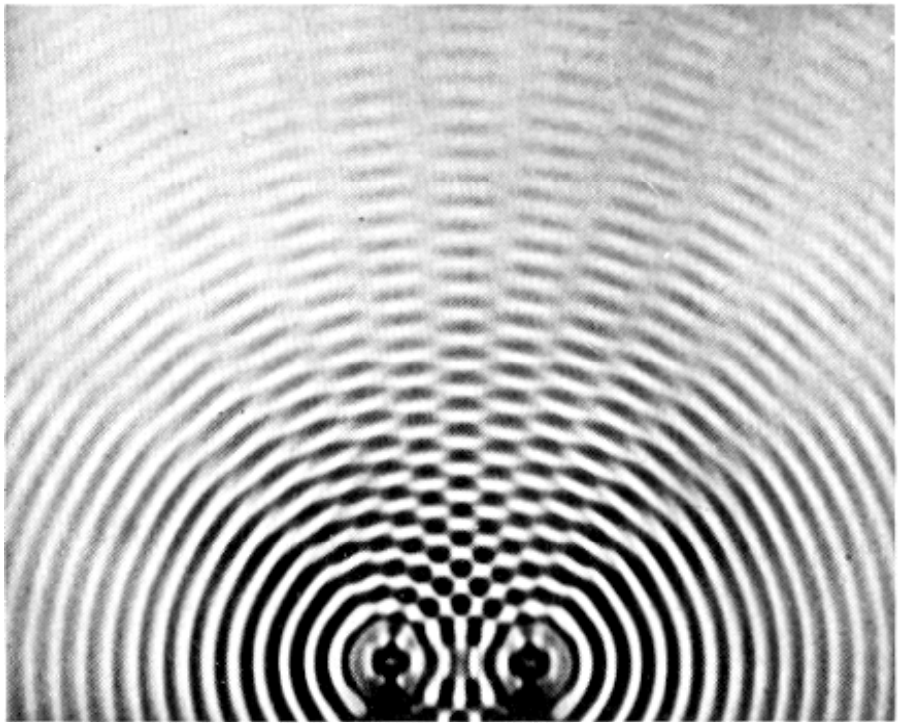
$$\left(\because \int_{-\infty}^{\infty} f(x)\delta(x - x_0)dx = f(x_0)\right)$$

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

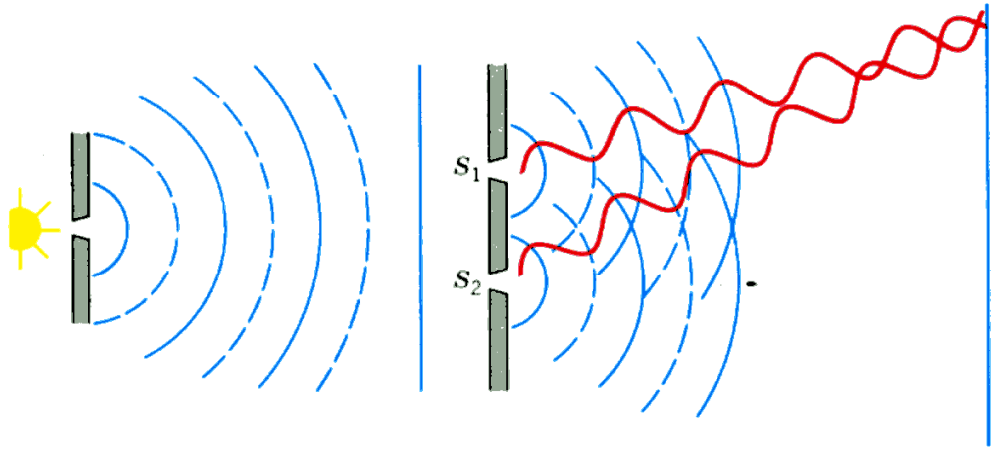


Interference



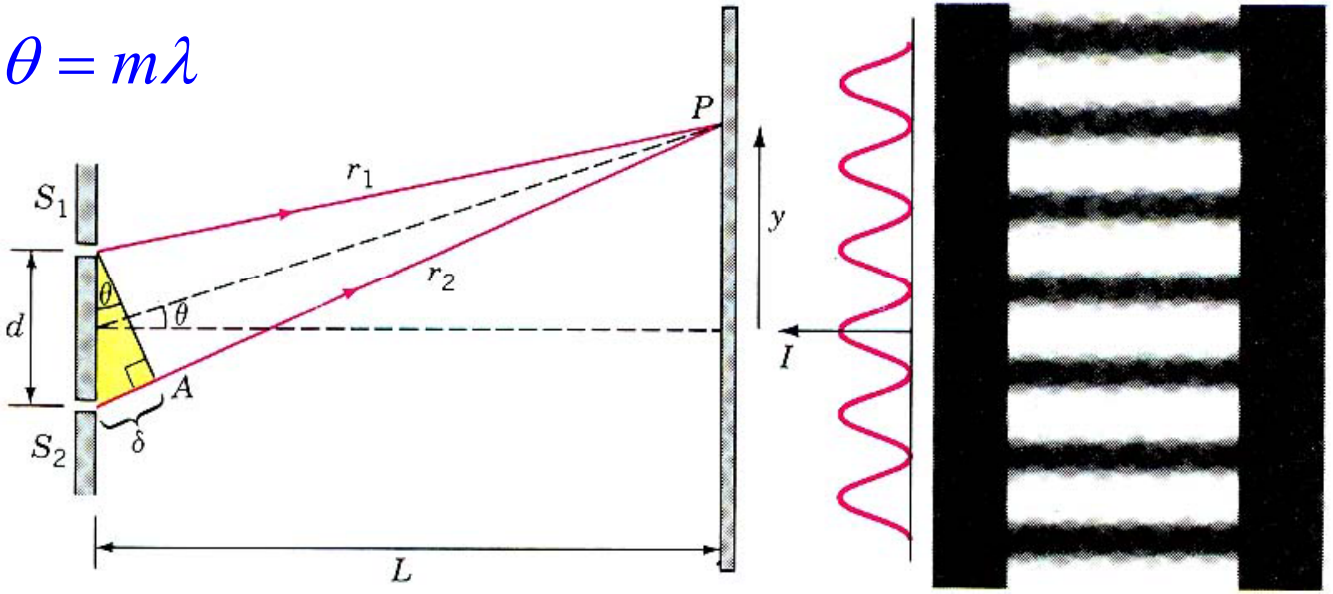


Young's Experiment



maxima

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



Diffraction by 1-D Obstacles

- three narrow slits

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

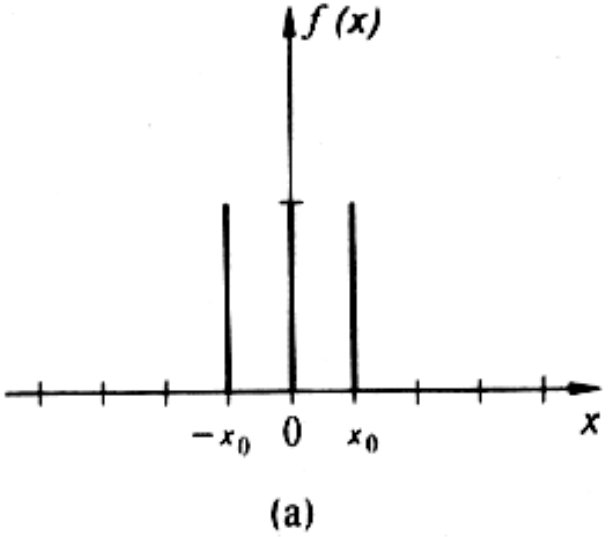
- $F(\sin\theta) = \int_{-\infty}^{\infty} f(x) e^{ikx\sin\theta} dx$

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

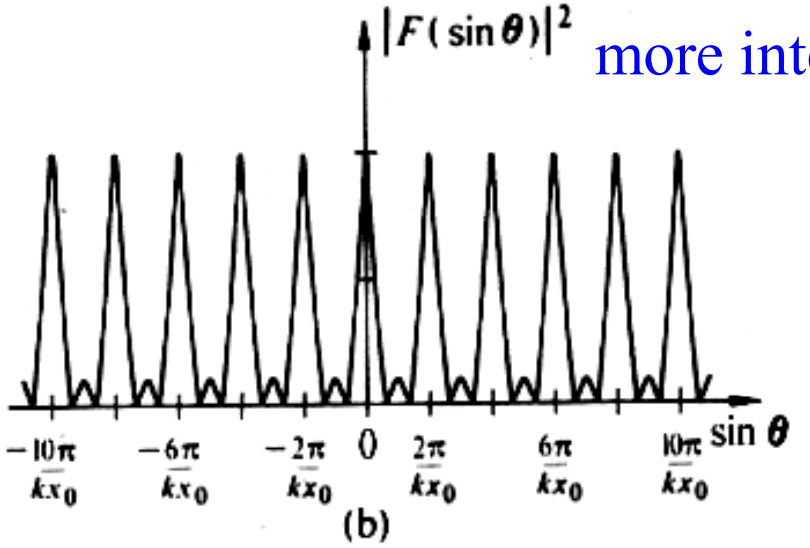
- $\left|F(\sin\theta)\right|^2 = [1 + 2\cos(kx_0 \sin\theta)]^2$

nine times

more intense



(a)



(b)

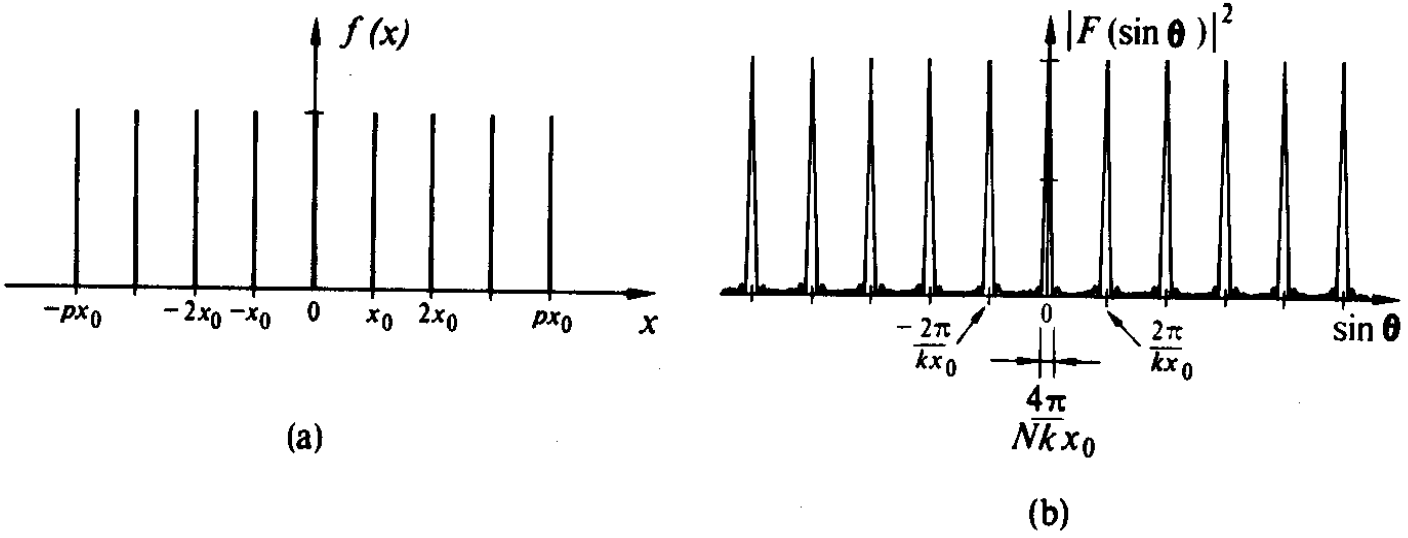
Diffraction by 1-D Obstacles

- N narrow slits

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

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

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



Diffraction by 1-D Obstacles

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

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

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

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

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

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

*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

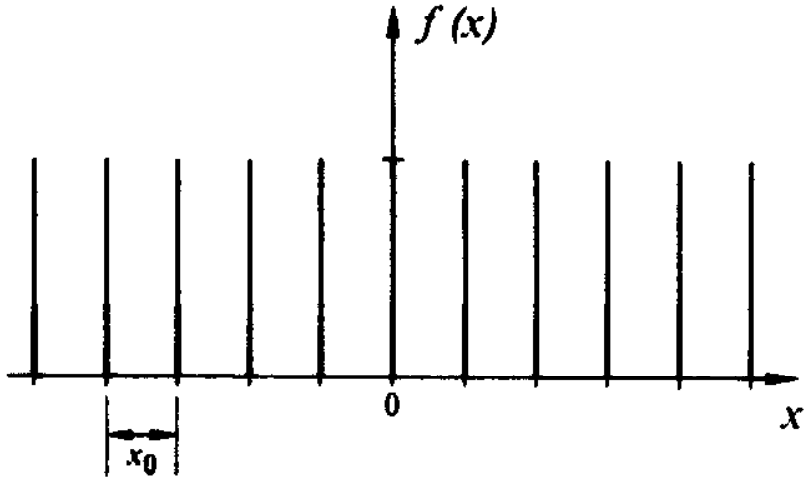
  separated by a distance $x_0 \rightarrow$ infinite array of δ function

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

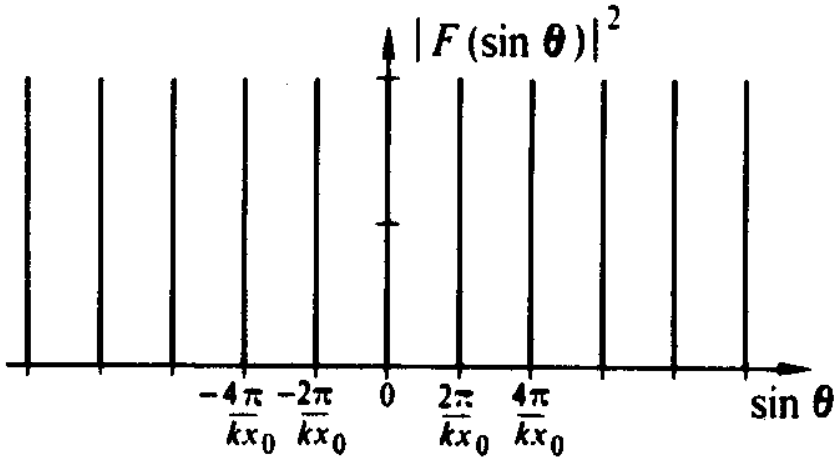
- $F(\sin\theta) = \sum_{n=-\infty}^{n=\infty} \delta(\sin\theta - \frac{2n\pi}{kx_0})$

*infinitely sharp peak

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

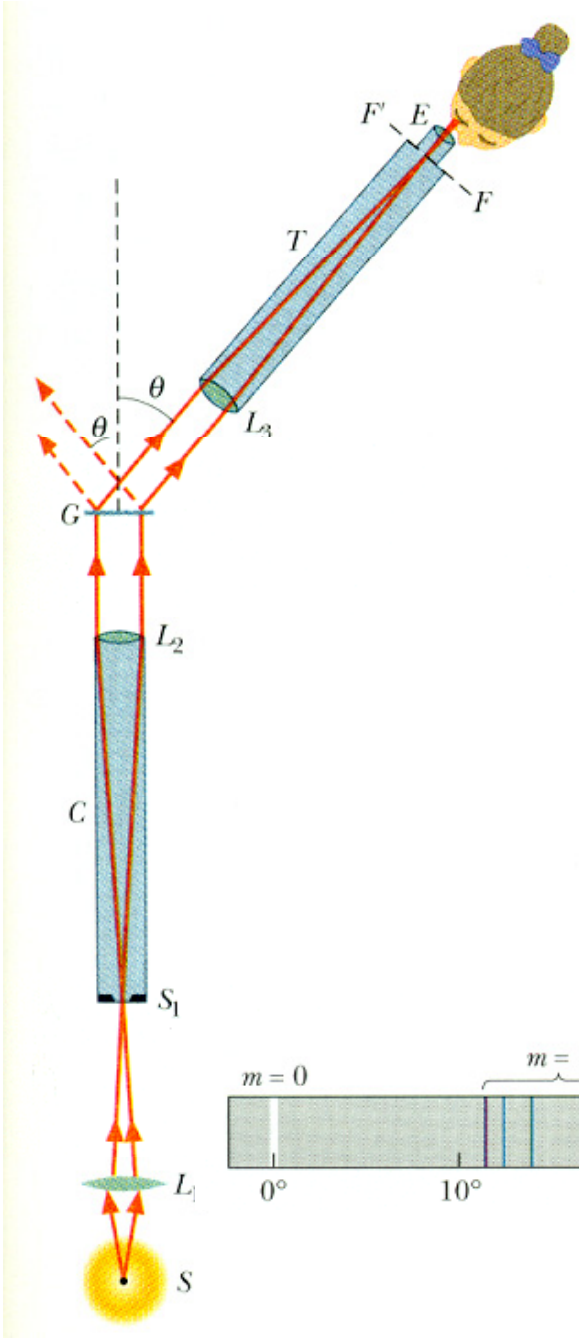


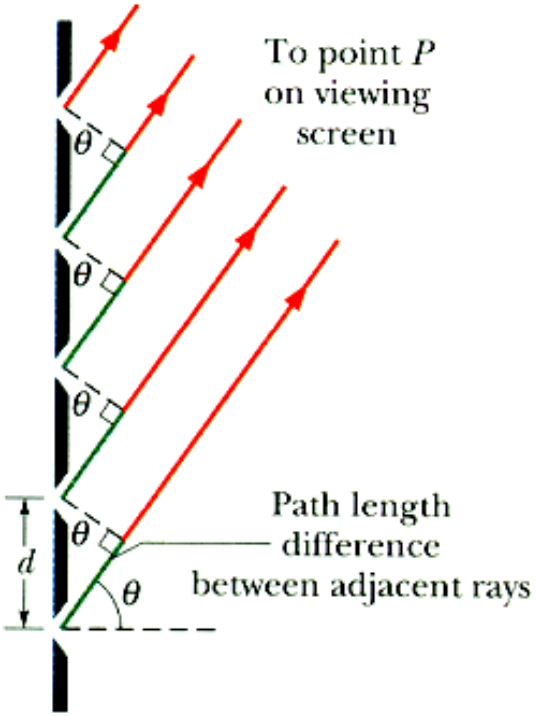
(a)



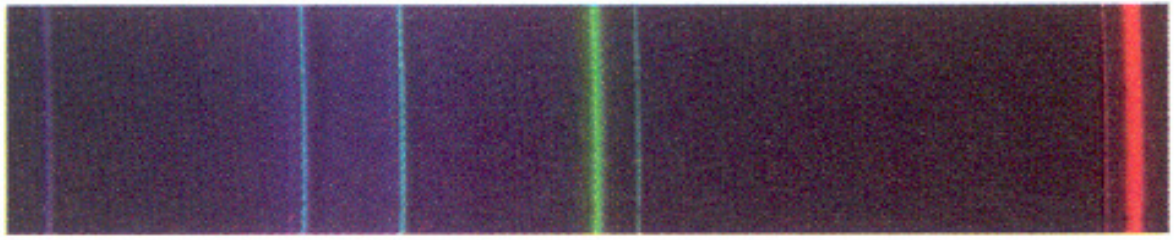
(b)

Grating Spectroscope

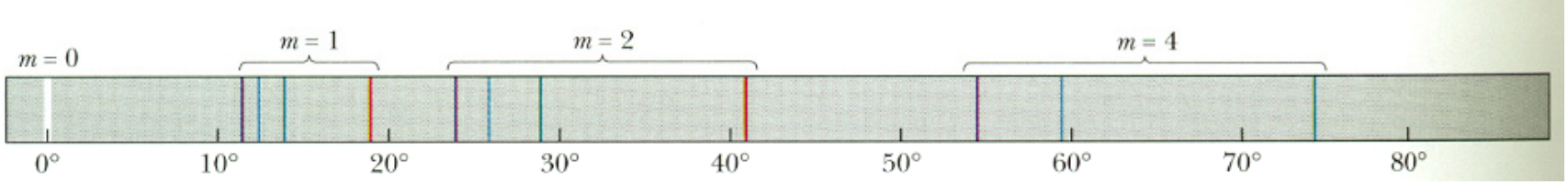




$$d \sin\theta = m\lambda$$



visible emission line of cadmium



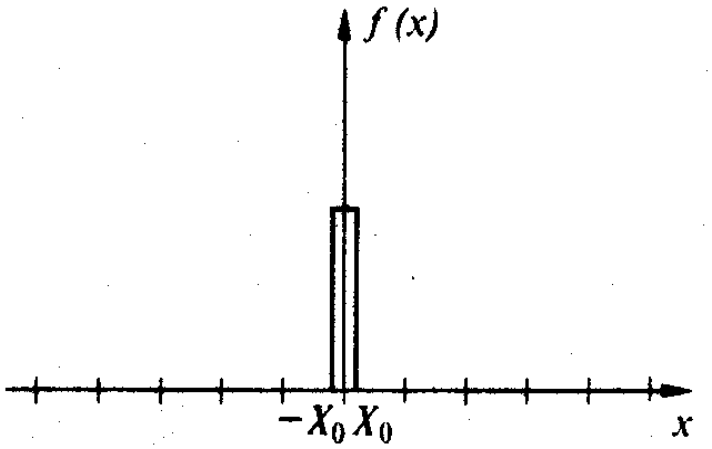
visible emission line from hydrogen

Diffraction by 1-D Obstacles

- one wide slit

  an opaque screen containing a slit which is wide

  $\sim 100\lambda$



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

  $1 \quad if \quad -X_0 < x < +X_0$

  $0 \quad if \quad +X_0 < x < \infty$

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

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

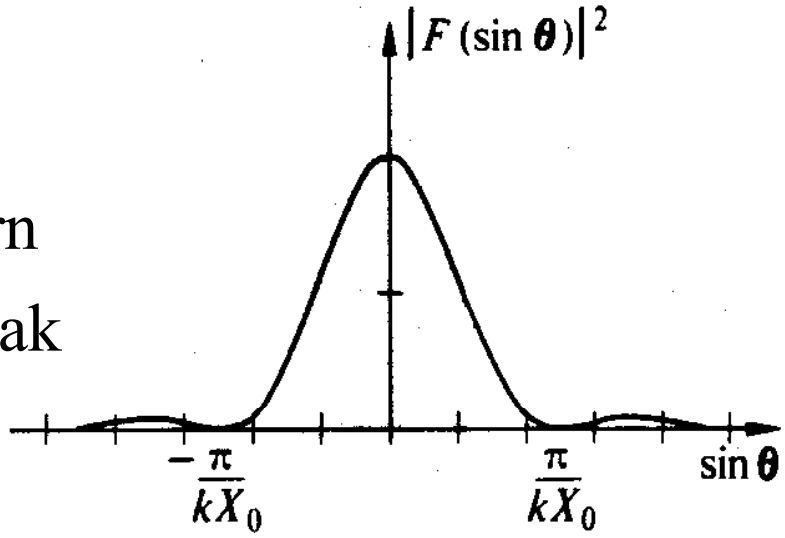
Diffraction by 1-D Obstacles

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

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

$$- \text{intensity} \sim \left|\mathrm{F}(\sin\theta)\right|^2 = 4X_0^2 \frac{\sin^2(kX_0\sin\theta)}{(kX_0\sin\theta)^2}$$

- $2\mathrm{X}_0 \rightarrow \Delta(\sin\theta) = 2\pi / kX_0$
- the wider slit,
  the narrow the diffraction pattern
- secondary peak-very rapidly weak



Single-Slit Diffraction

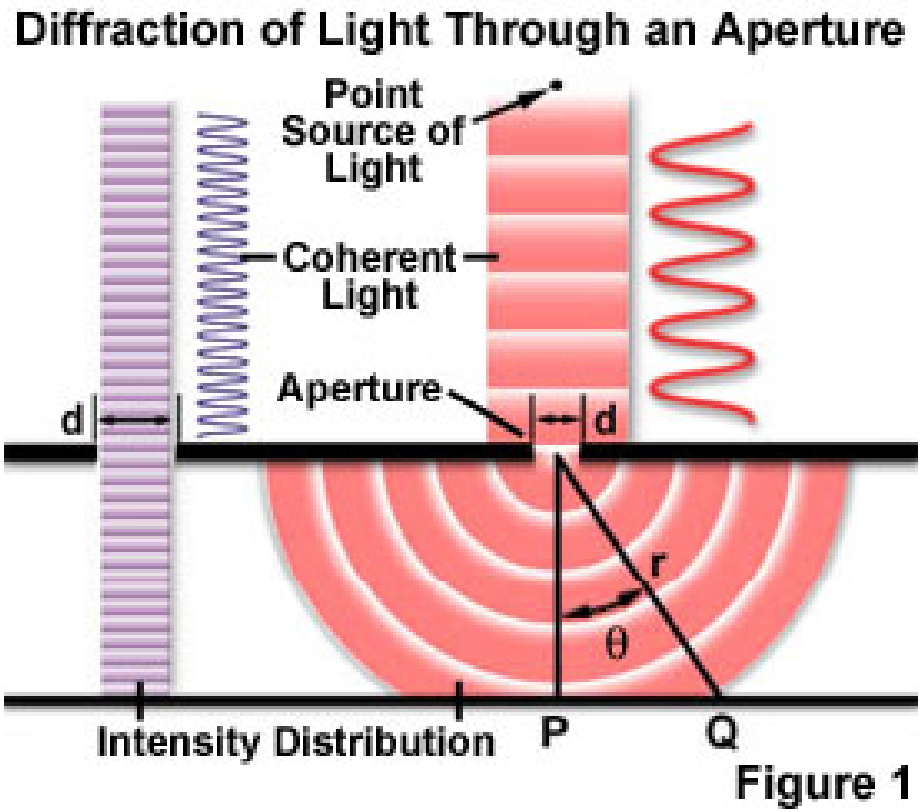


Figure 1

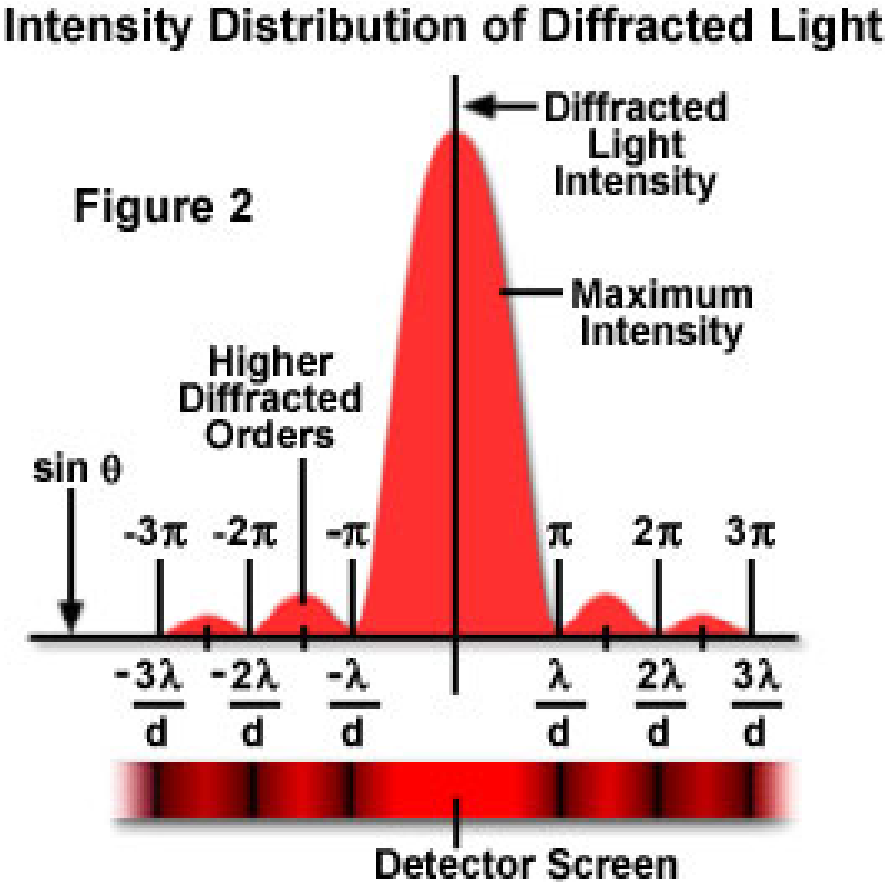


Figure 2

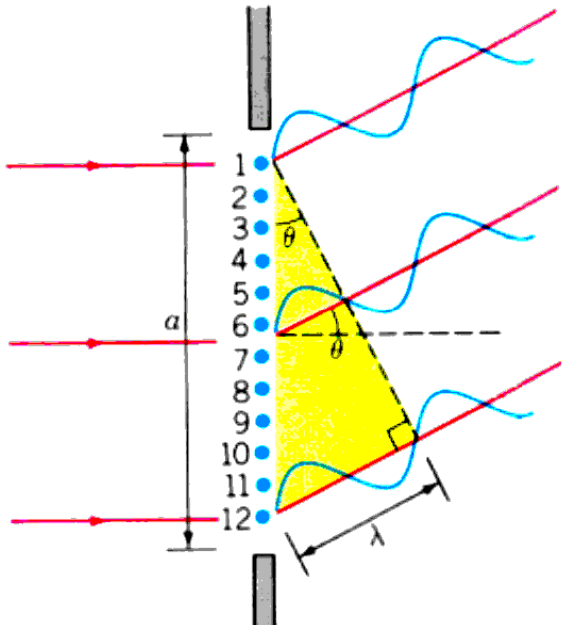
$$\delta \approx d \sin\theta, \text{ for minima } \sin\theta = m\frac{\lambda}{d}$$

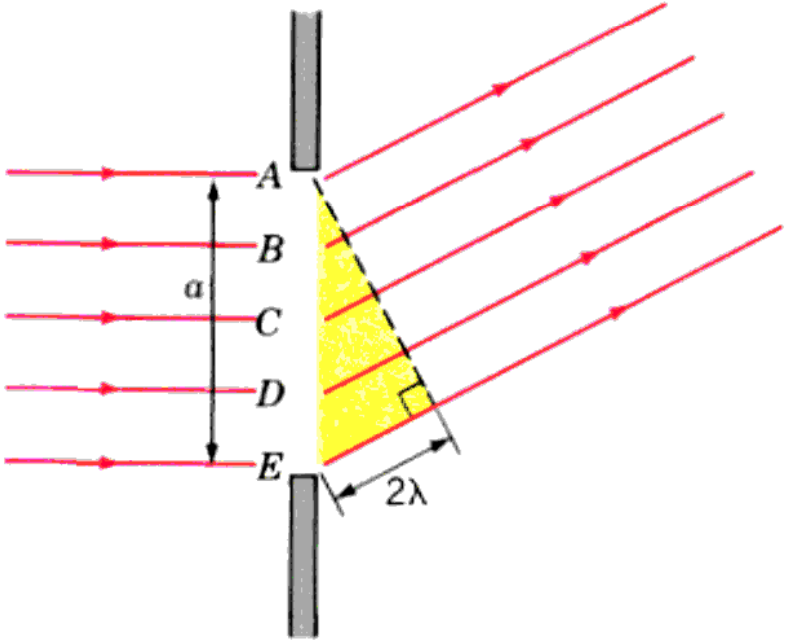
http://micro.magnet.fsu.edu/primer/java/diffraction/basicdiffraction/

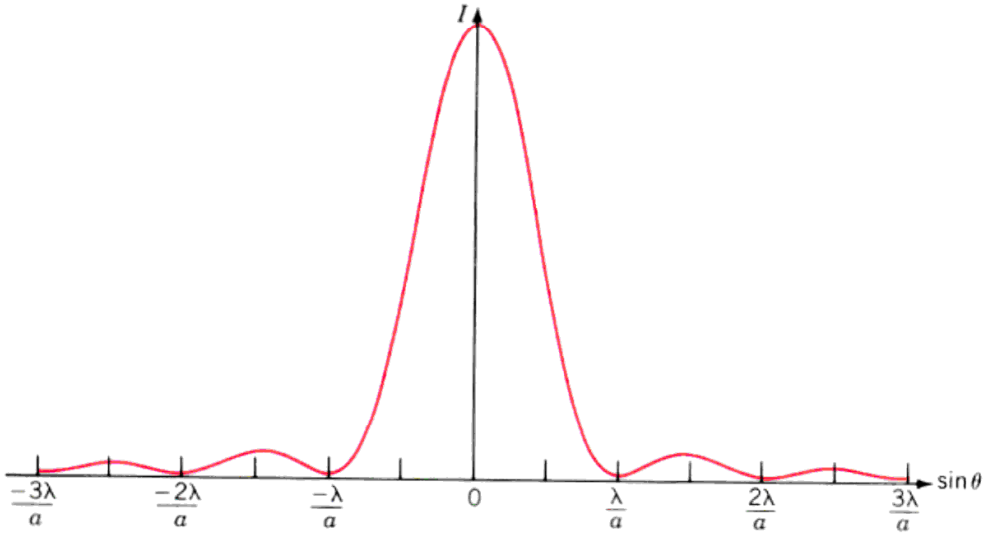
Single-Slit Diffractio

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

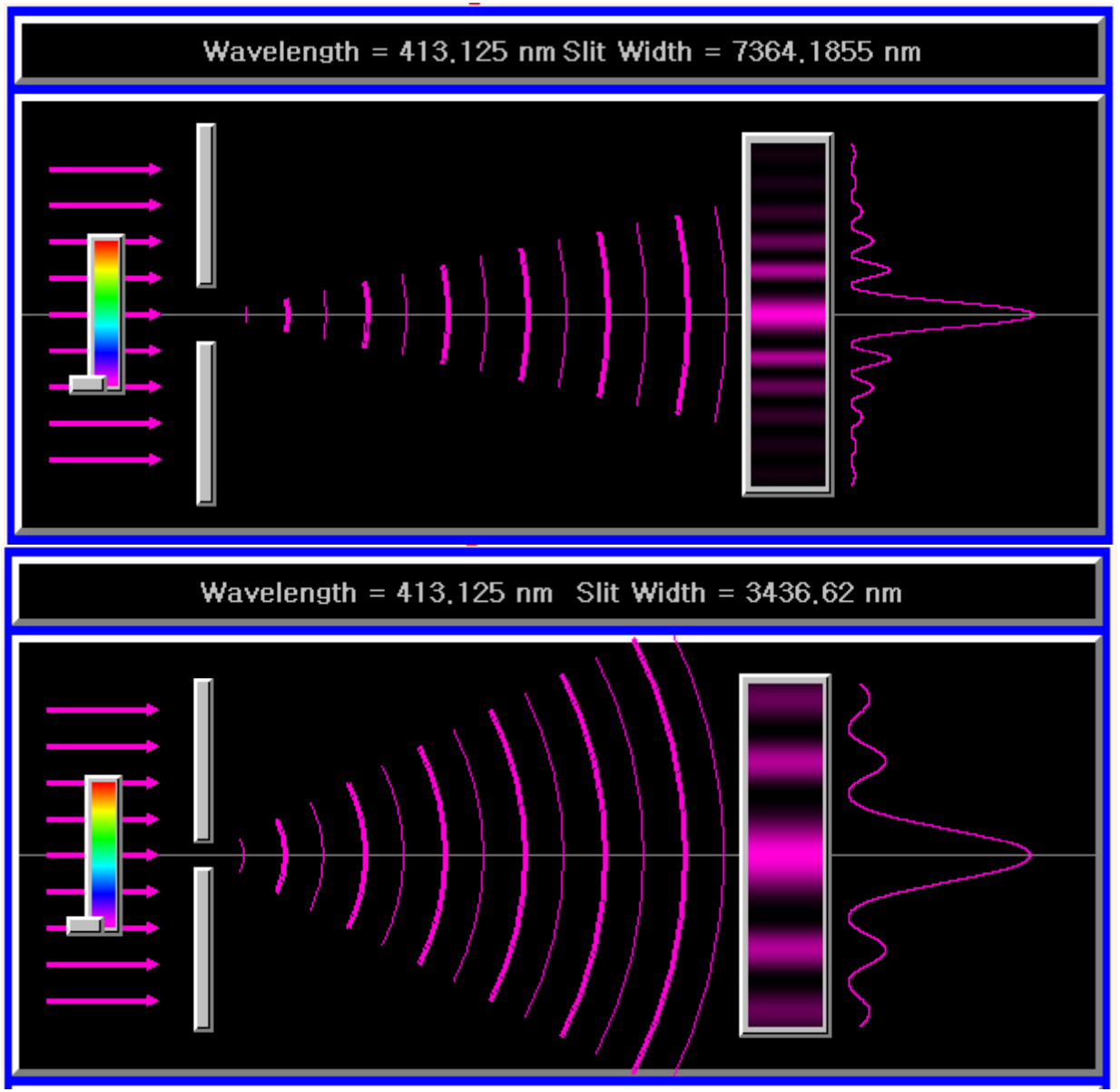
for minima $\sin\theta = m\dfrac{\lambda}{d}$, m=1,2,3,$\cdots$



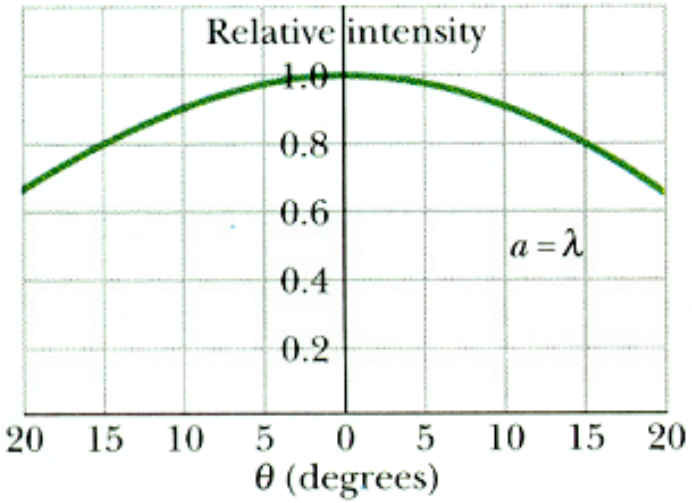


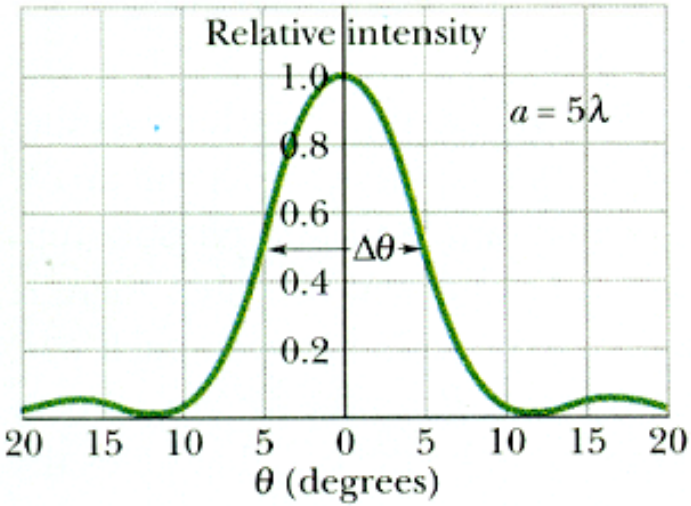


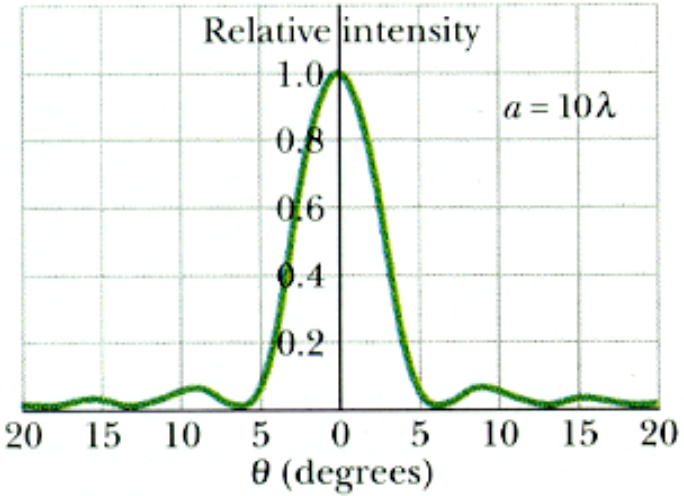
Single-Slit Diffraction



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


Relative intensity
1.0
0.8
0.6
0.4
0.2
$a = \lambda$
20 15 10 5 0 5 10 15 20
θ (degrees)


Relative intensity
1.0
0.8
0.6
0.4
0.2
$a = 5\lambda$
$\Delta\theta$
20 15 10 5 0 5 10 15 20
θ (degrees)


Relative intensity
1.0
0.8
0.6
0.4
0.2
$a = 10\lambda$
20 15 10 5 0 5 10 15 20
θ (degrees)

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

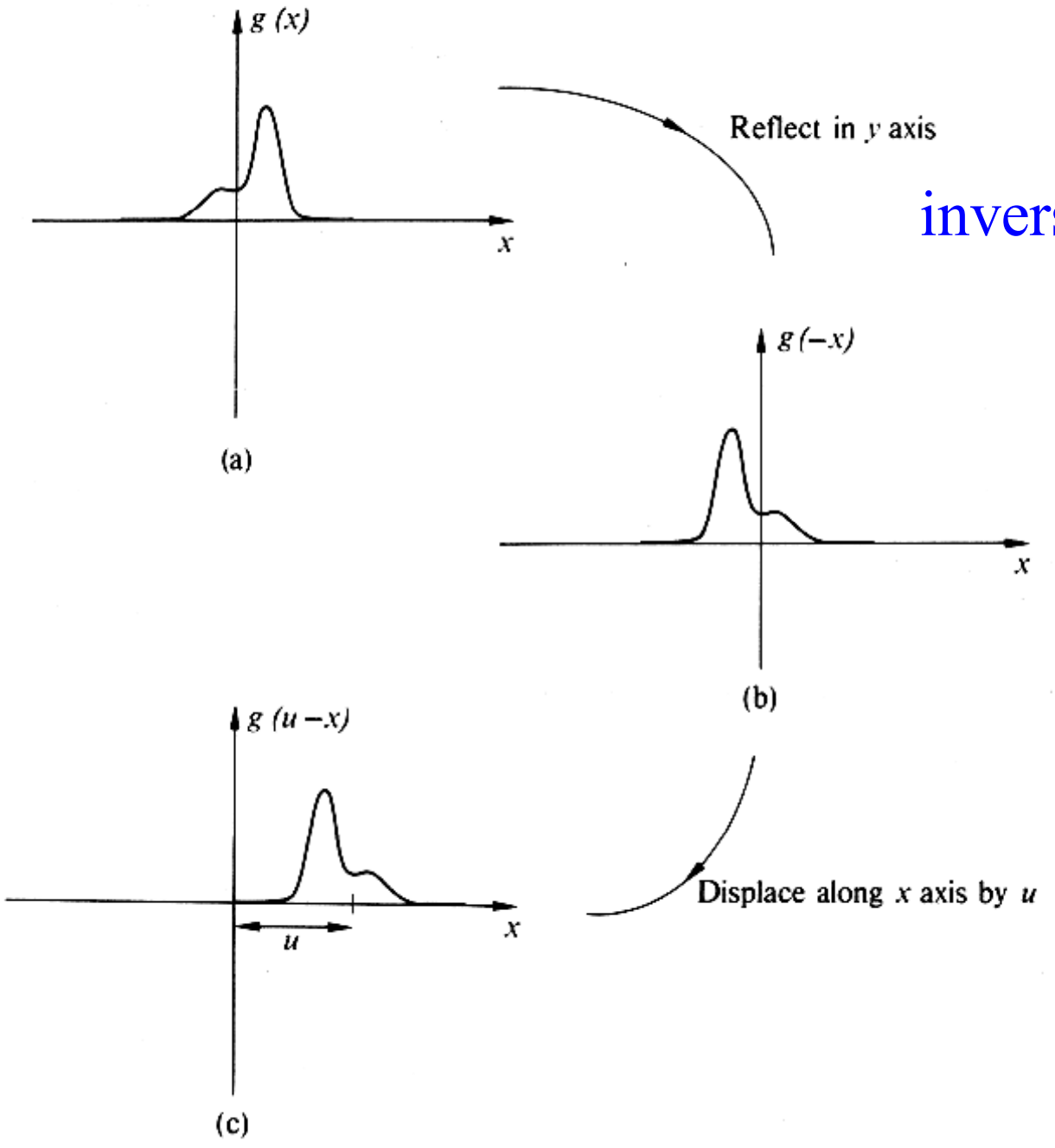
- example

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

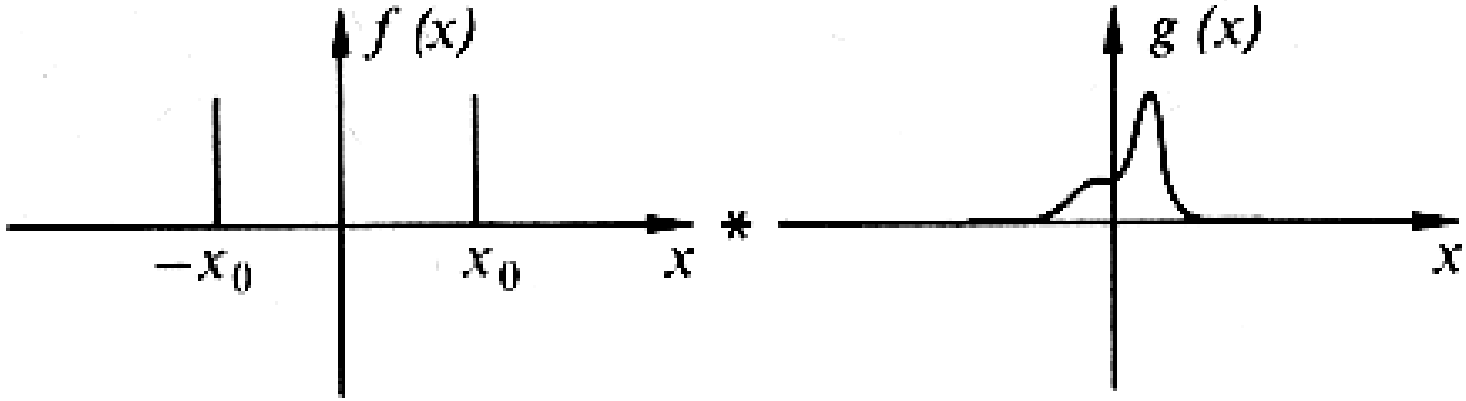
  $$\text{c(u)} = \int_{-\infty}^{\infty} f(x) g(u - x) dx = \int_{-\infty}^{\infty} \delta(x + x_o) g(u - x) dx$$

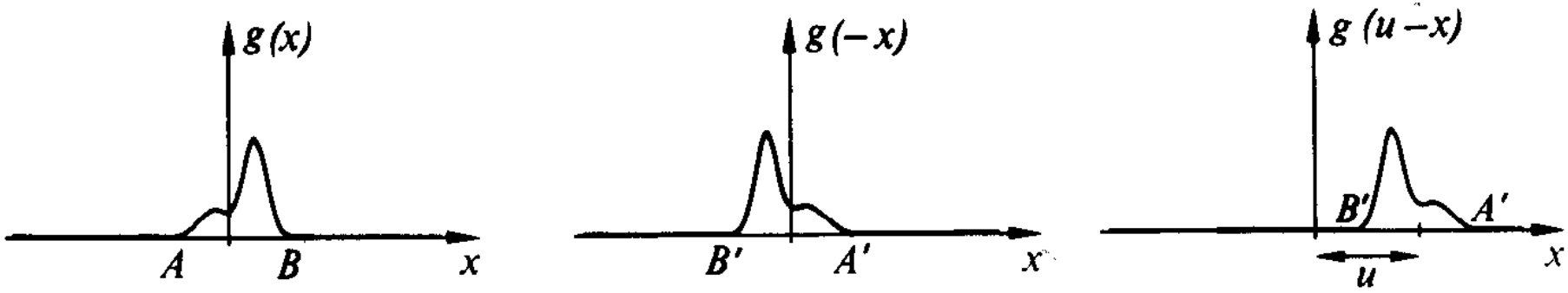
  $$+ \int_{-\infty}^{\infty} \delta(x - x_0) g(u - x) dx$$

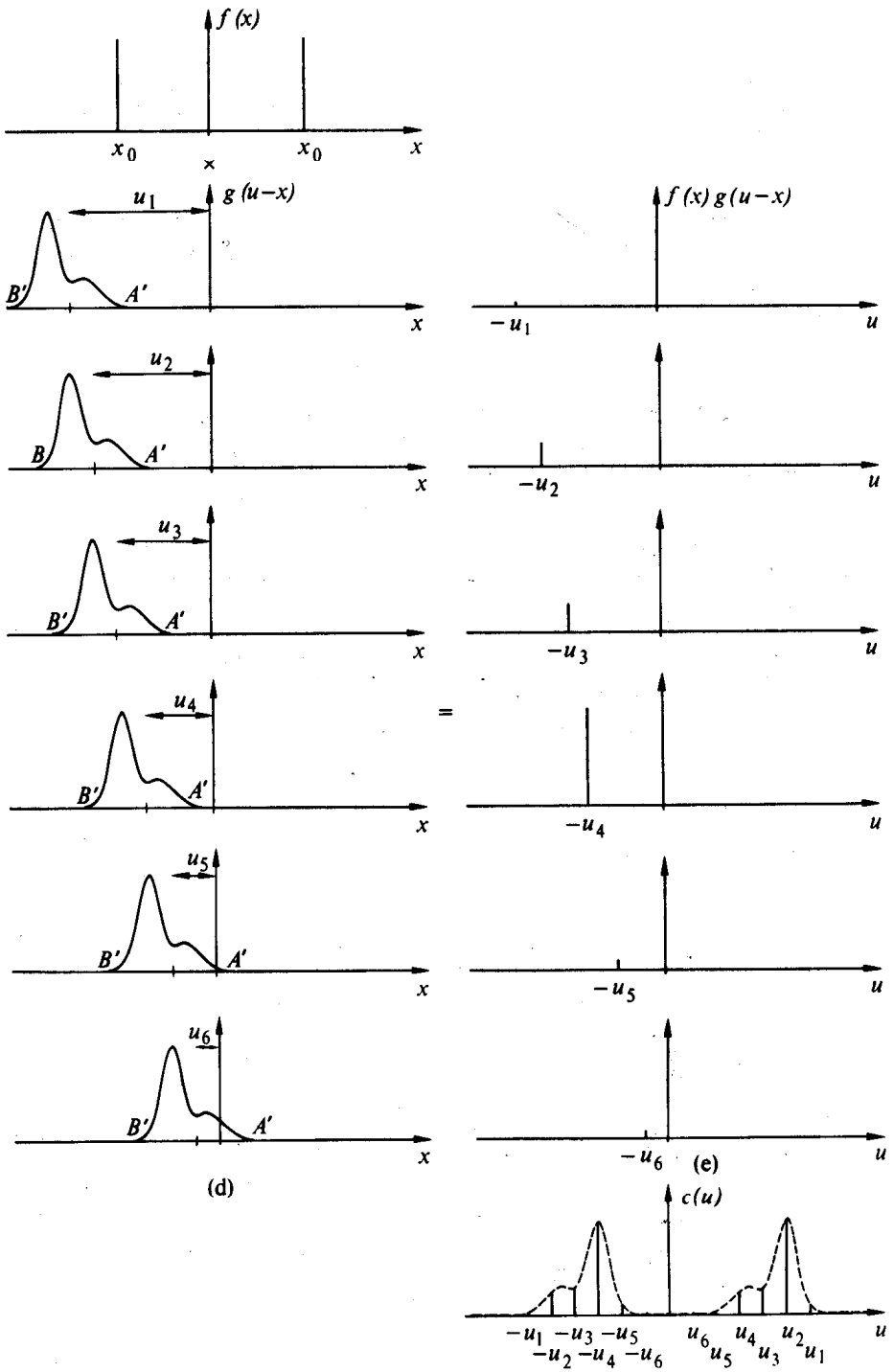
  $$= g(u + x_0) + g(u - x_0)$$

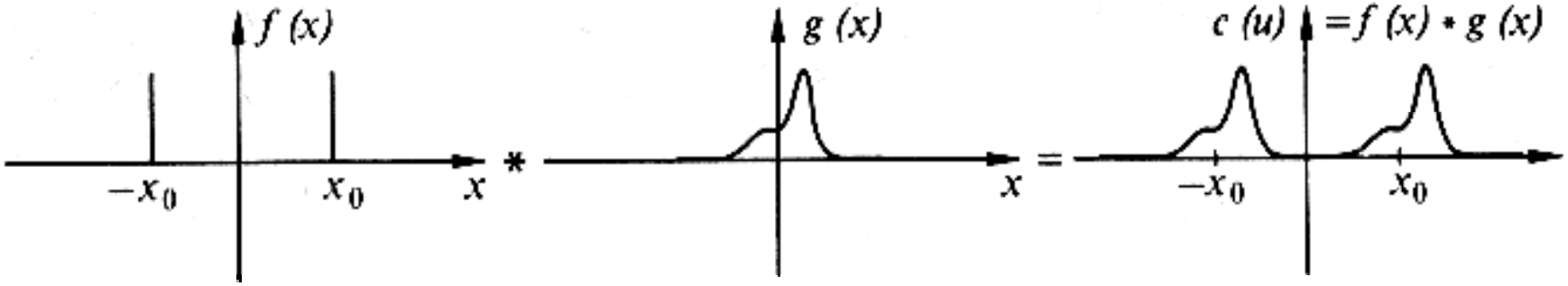


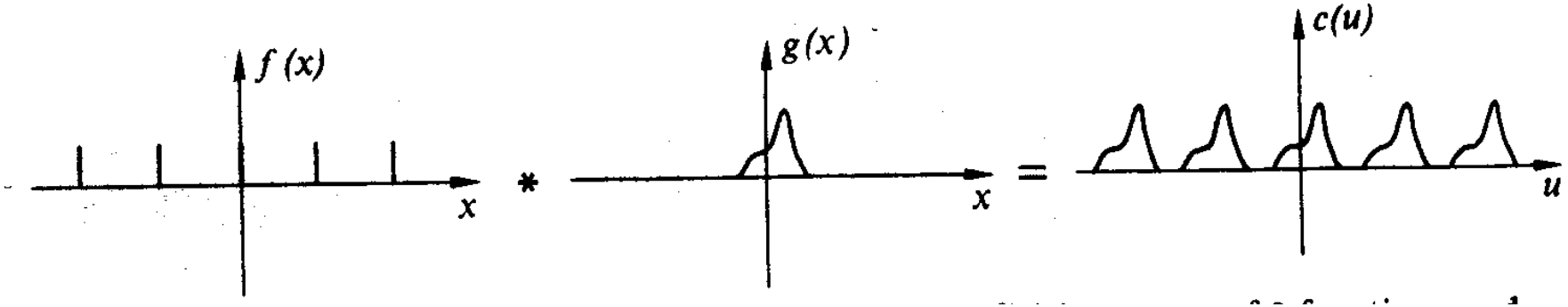
inversion in 3-D


f (x)
$-x_0$
x_0
x
*
g (x)
x


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


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


f (x)
$-x_0$
x_0
x
*
g (x)
x
=
c (u)
=f (x) * g (x)
$-x_0$
x_0


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

Diffraction by 1-D Obstacles

- two wide slit

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

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

  $1 \quad if \quad -(x_0 + X_0) < x < -(x_0 - X_0)$

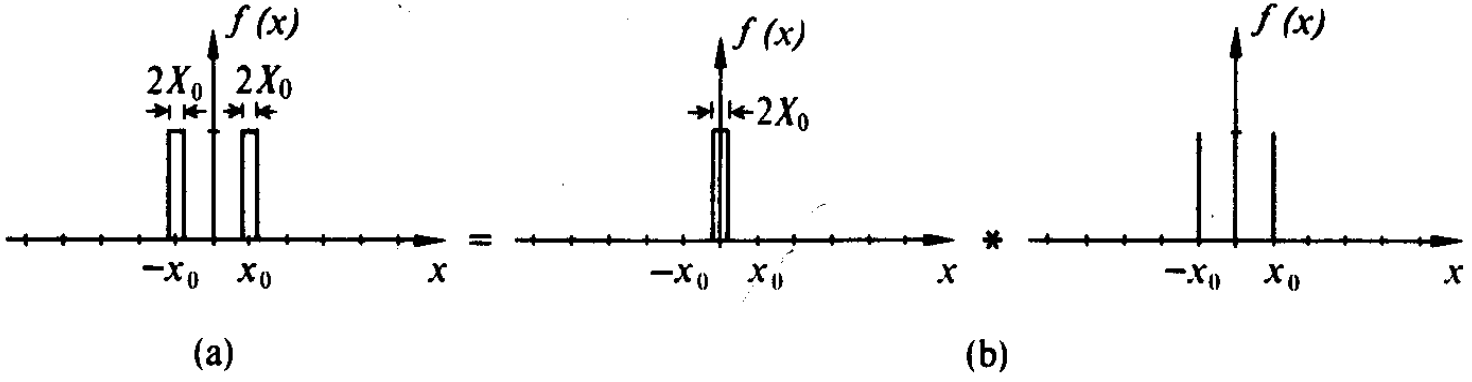
  $0 \quad if \quad -(x_0 - X_0) < x < (x_0 - X_0)$

  $1 \quad if \quad (x_0 - X_0) < x < (x_0 + X_0)$

  $0 \quad if \quad (x_0 + X_0) < x < \infty$

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

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



Diffraction by 1-D Obstacles

- Fourier transform

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

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

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

- one wide slit

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

- two narrow slit

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

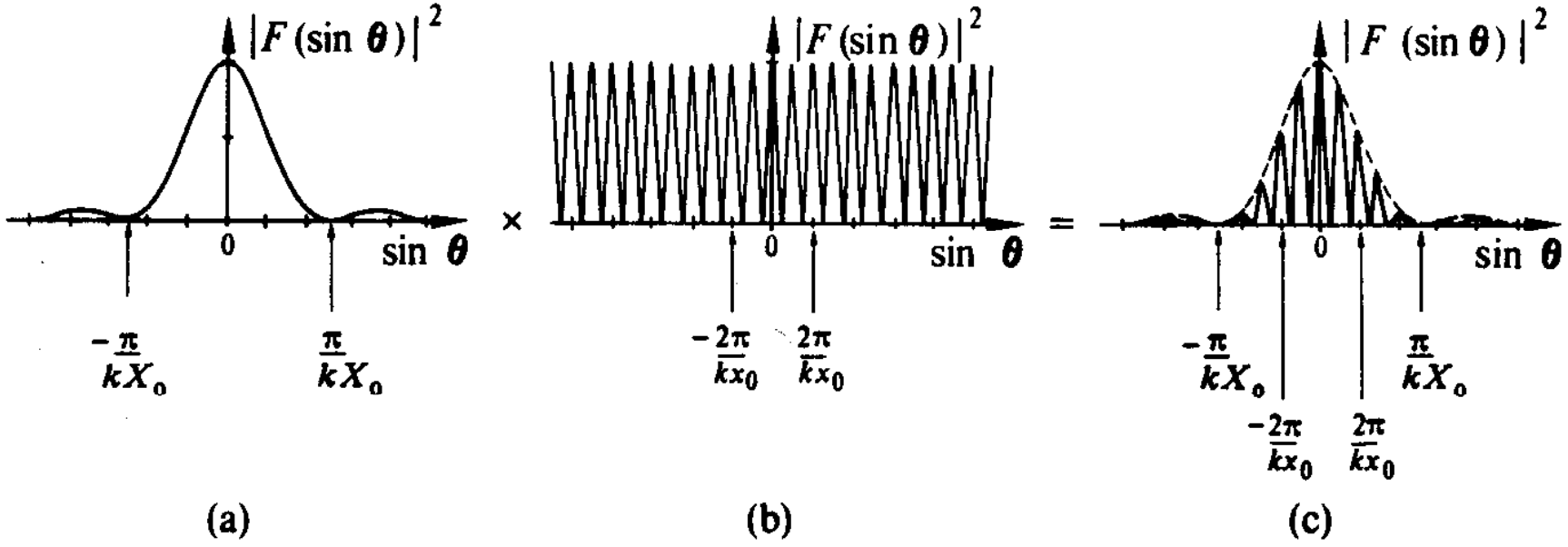
Diffraction by 1-D Obstacles

- 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

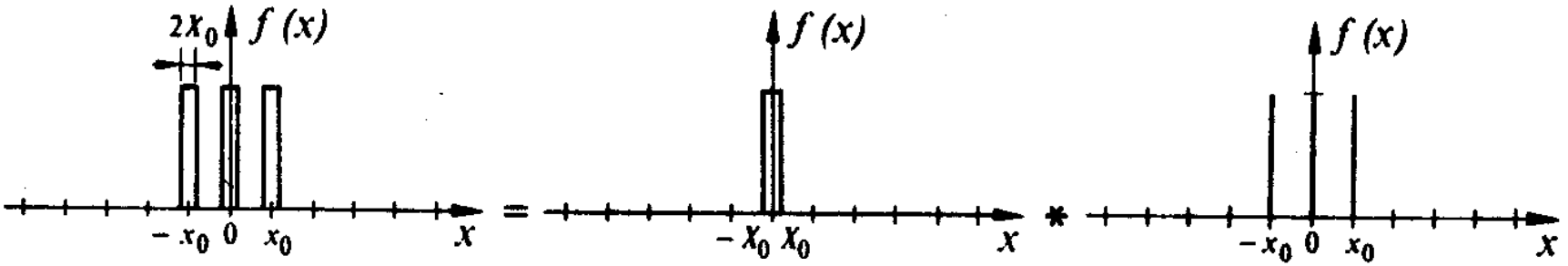
- amplitude function

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

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

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

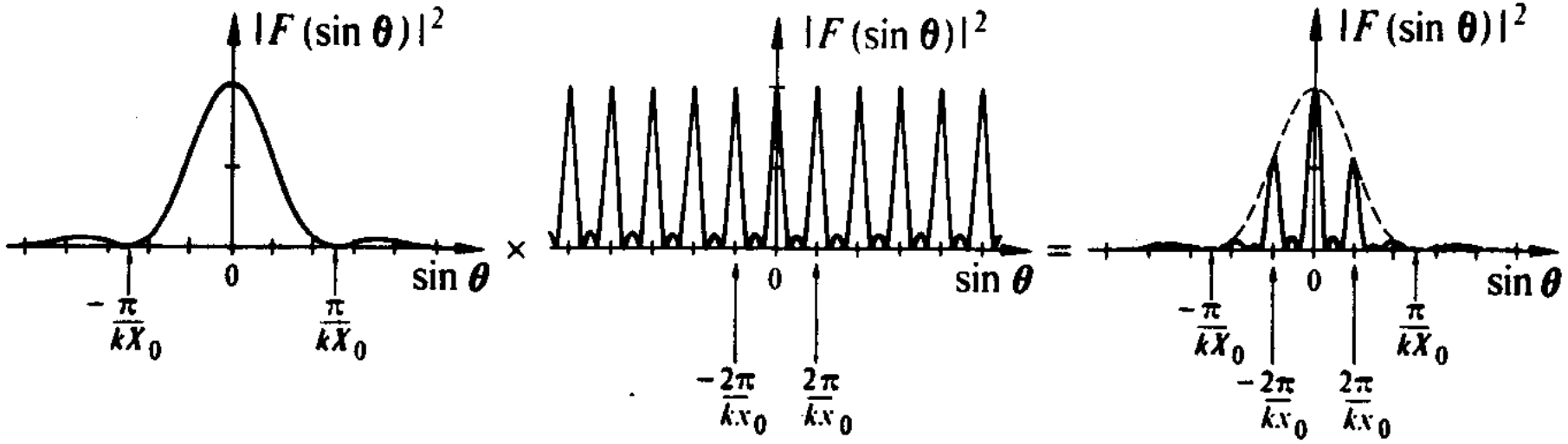
- $F(\sin\theta) = 2X_0 \dfrac{\sin(kX_0 \sin\theta)}{kX_0 \sin\theta}[1 + 2\cos(kx_0 \sin\theta)]$



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

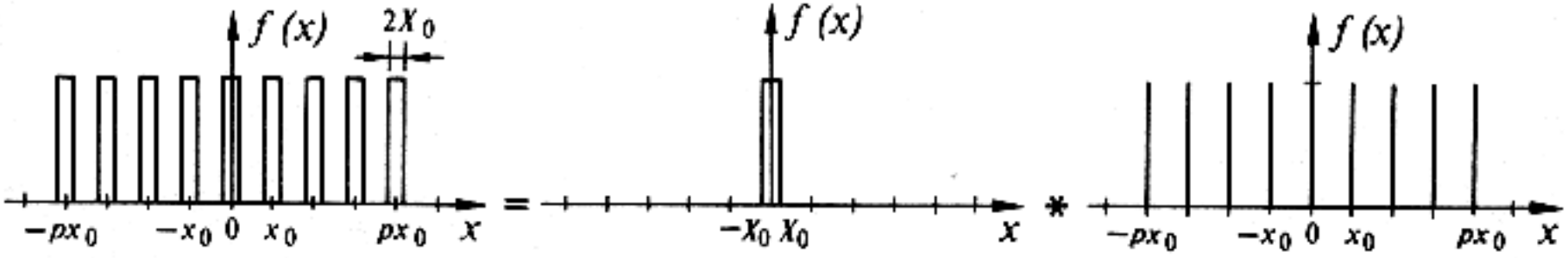
  width of $2X_0$, centered on a δ function

- amplitude function

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

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

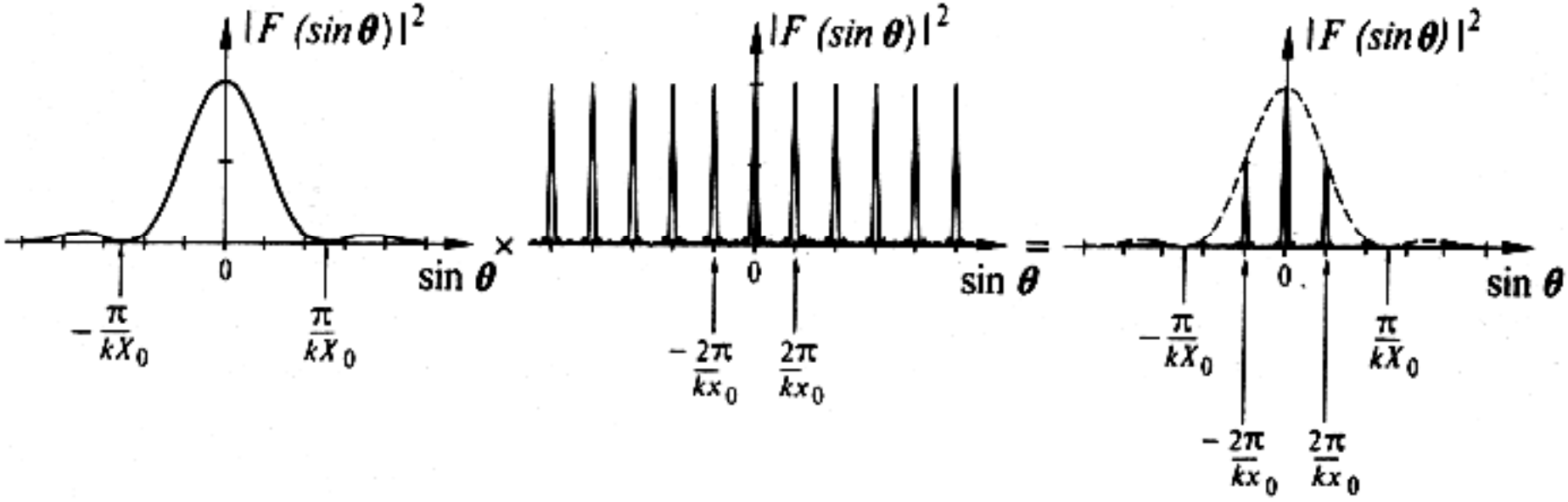
$$Tf(N\ wide\ slit) = Tf(one\ wide\ slit) * Tf(N\ narrow\ slits)$$



Diffraction by 1-D Obstacles

- N wide slits
- intensity

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



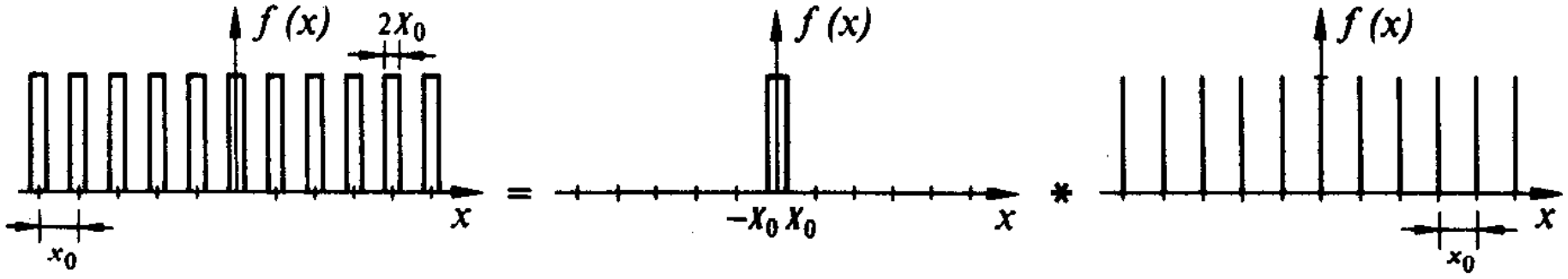
Diffraction by 1-D Obstacles

- infinite wide slits
- amplitude function

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

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

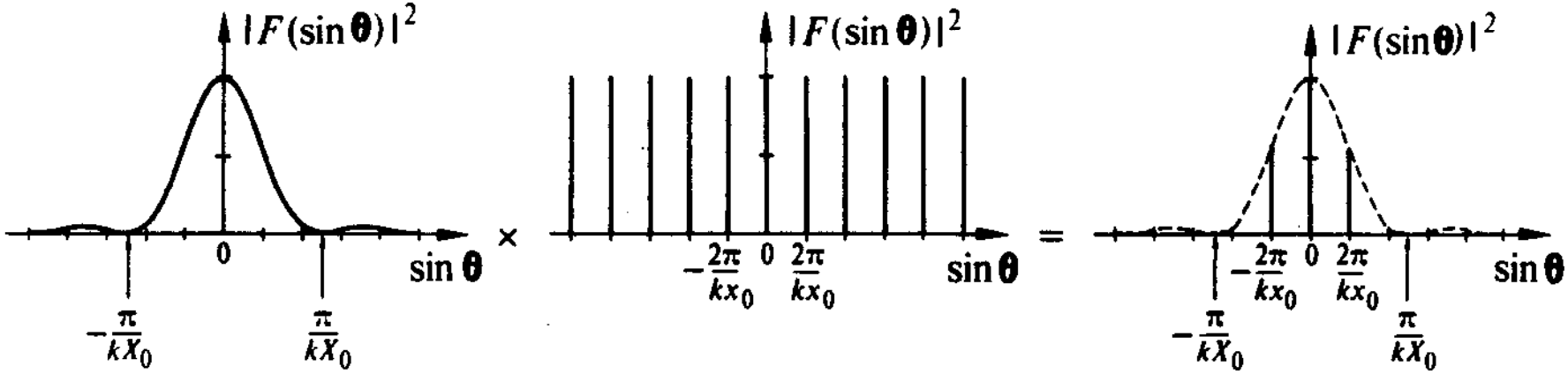
$$Tf(\infty\ wide\ slit) = Tf(one\ wide\ slit) * Tf(\infty\ narrow\ slits)$$



Diffraction by 1-D Obstacles

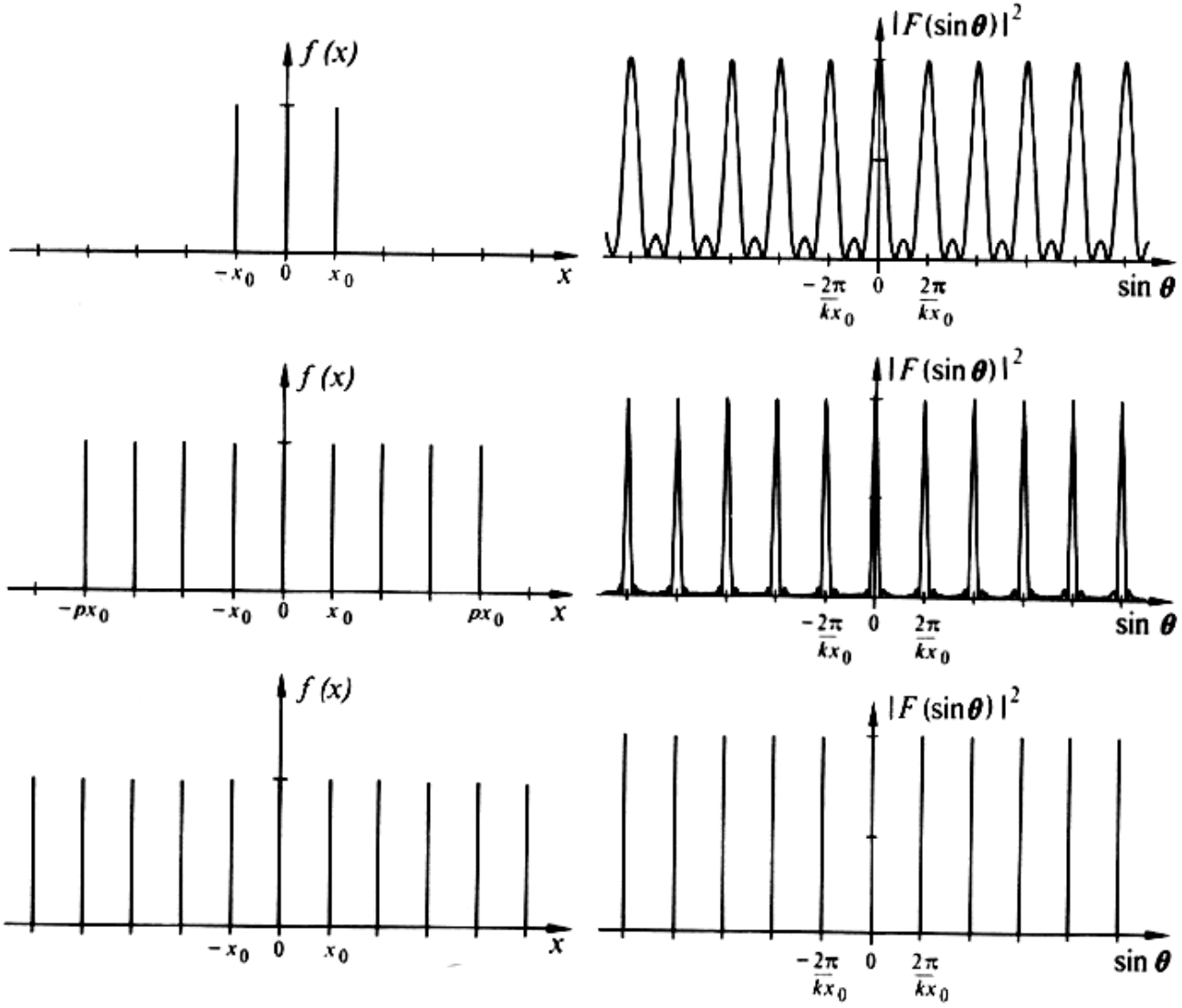
- infinite number of wide slits
- intensity

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



Diffraction by 1-D Obstacles

- significance of the diffraction pattern



Diffraction by 1-D Obstacles

- narrow slits

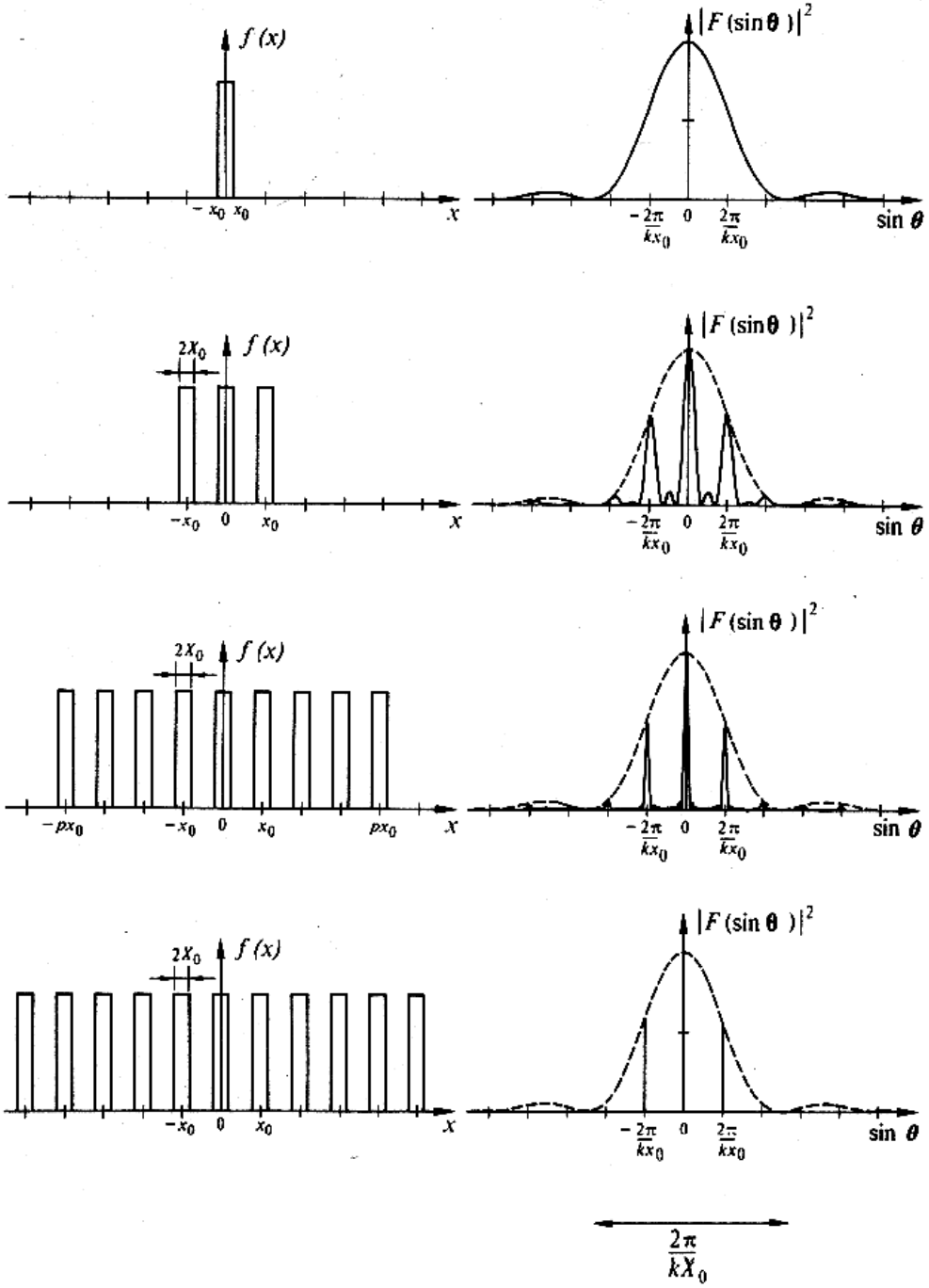
1. As the number of slits increases, the main peaks become sharper and narrower, whilest the subsidiary peaks become rapidly less intense
2. The position and separation of the main peaks is constant independent of the number of peaks. The man peaks are separated by an angular deflection given by

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

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

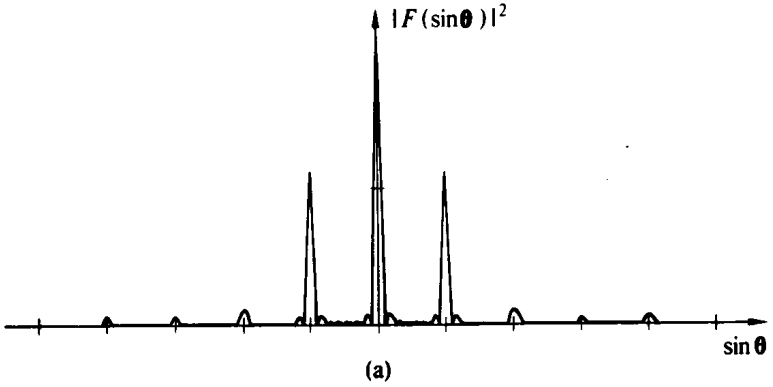
Diffraction by 1-D Obstacles

- 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.

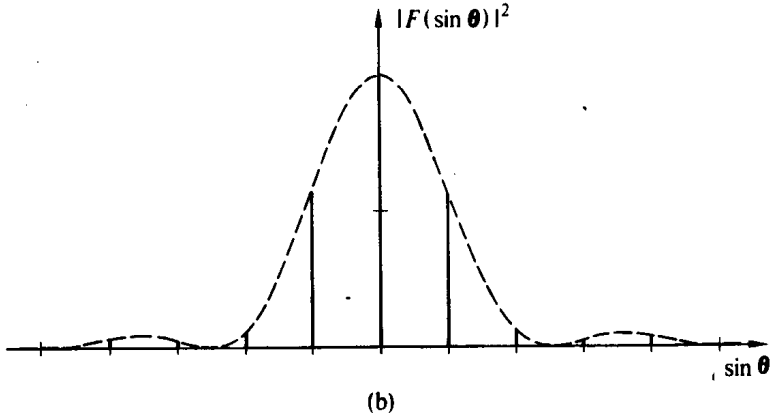

f (x)
$|F(\sin\theta)|^2$
$-x_0$ x_0
x
$-\frac{2\pi}{kx_0}$ 0 $\frac{2\pi}{kx_0}$
sin θ
$2X_0$
$-x_0$ 0 x_0
$-px_0$ px_0
$\frac{2\pi}{kX_0}$

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
  → structure of motif



(a)



(b)

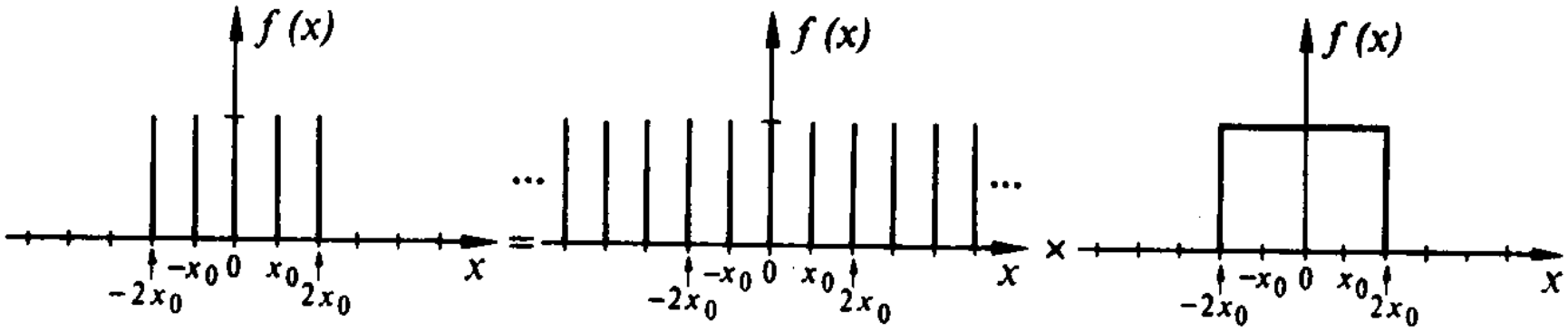
Diffraction by 1-D Obstacles

- 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

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

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

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

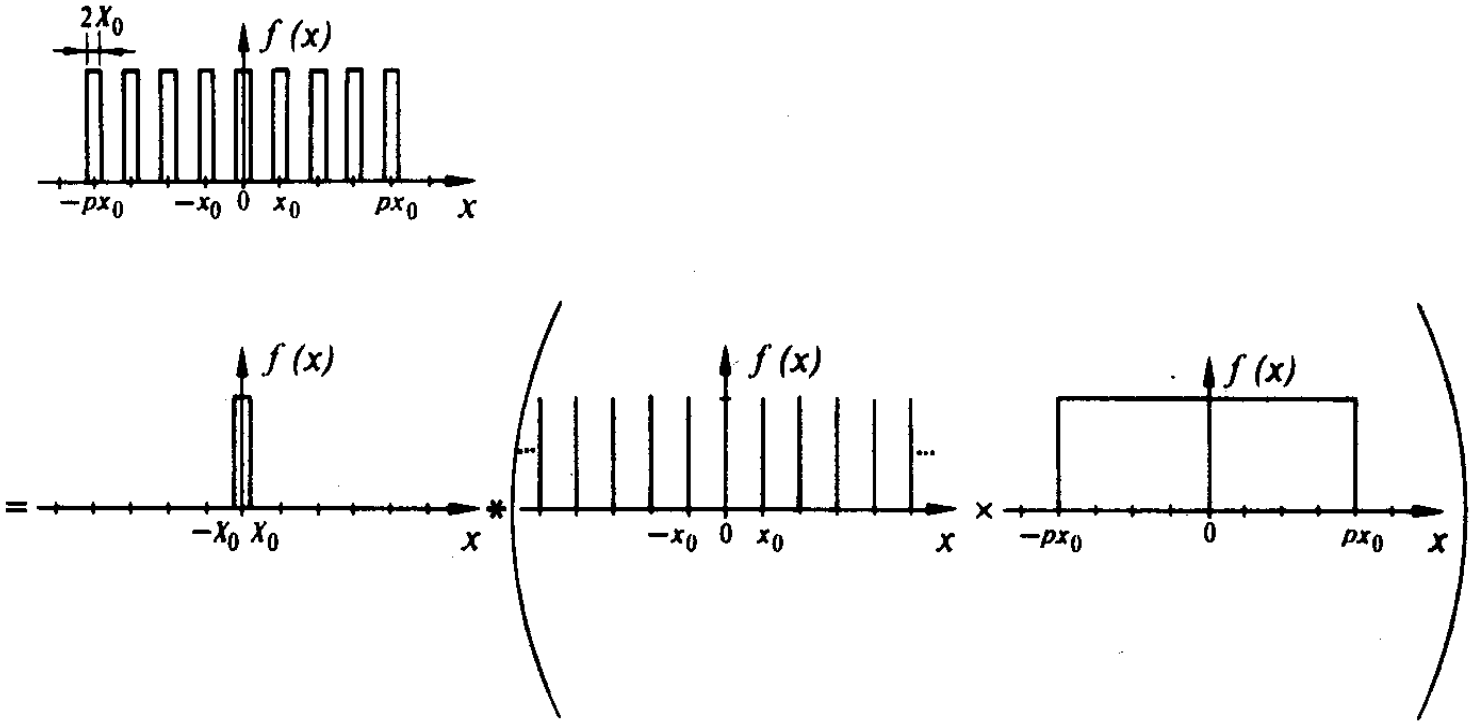
$$= Tf(\textit{motif}) \bullet [Tf(\textit{infinite lattice}) * Tf(\textit{shape function})]$$

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

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

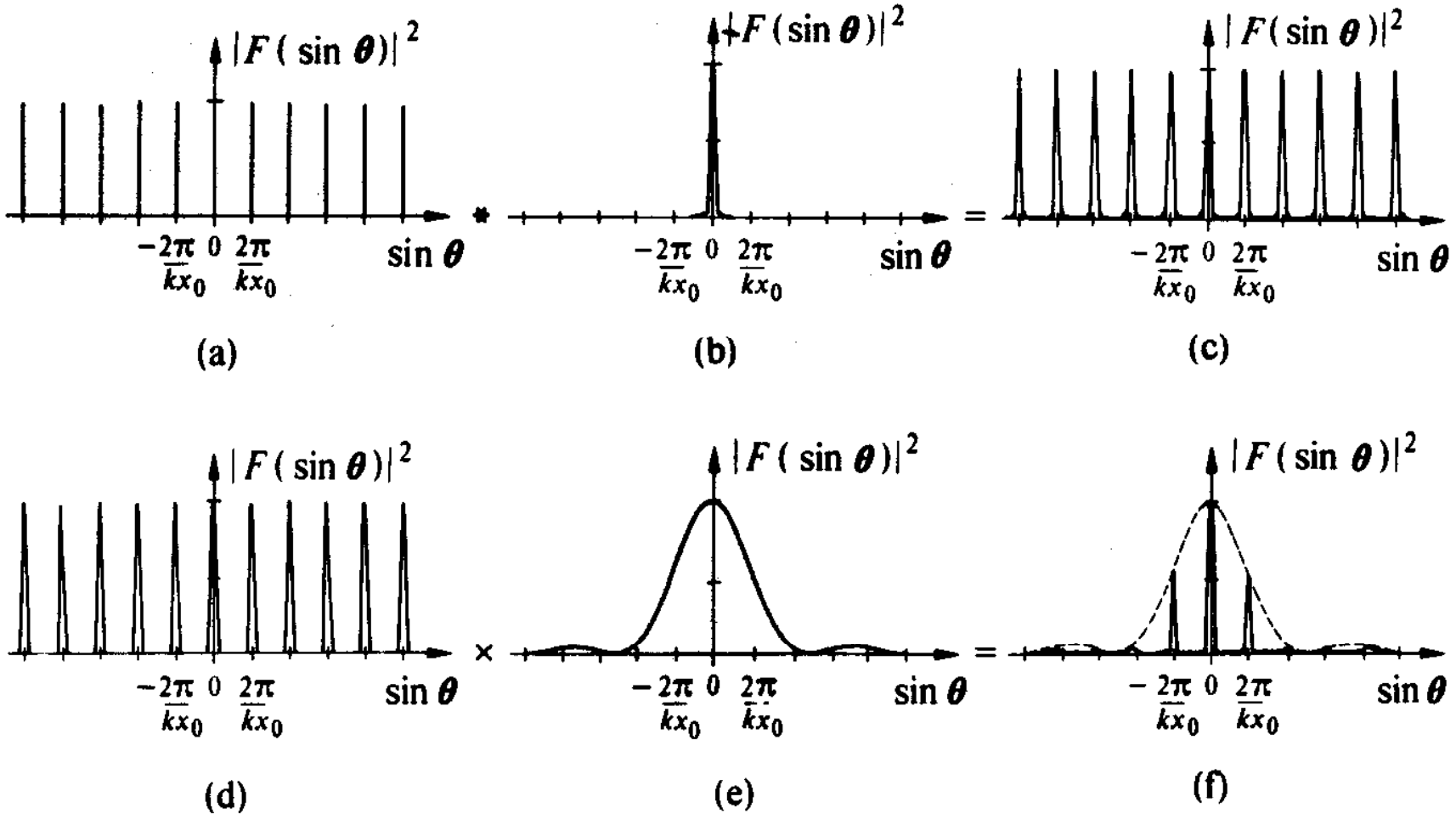
- three types of structural information

that concerning the lattice

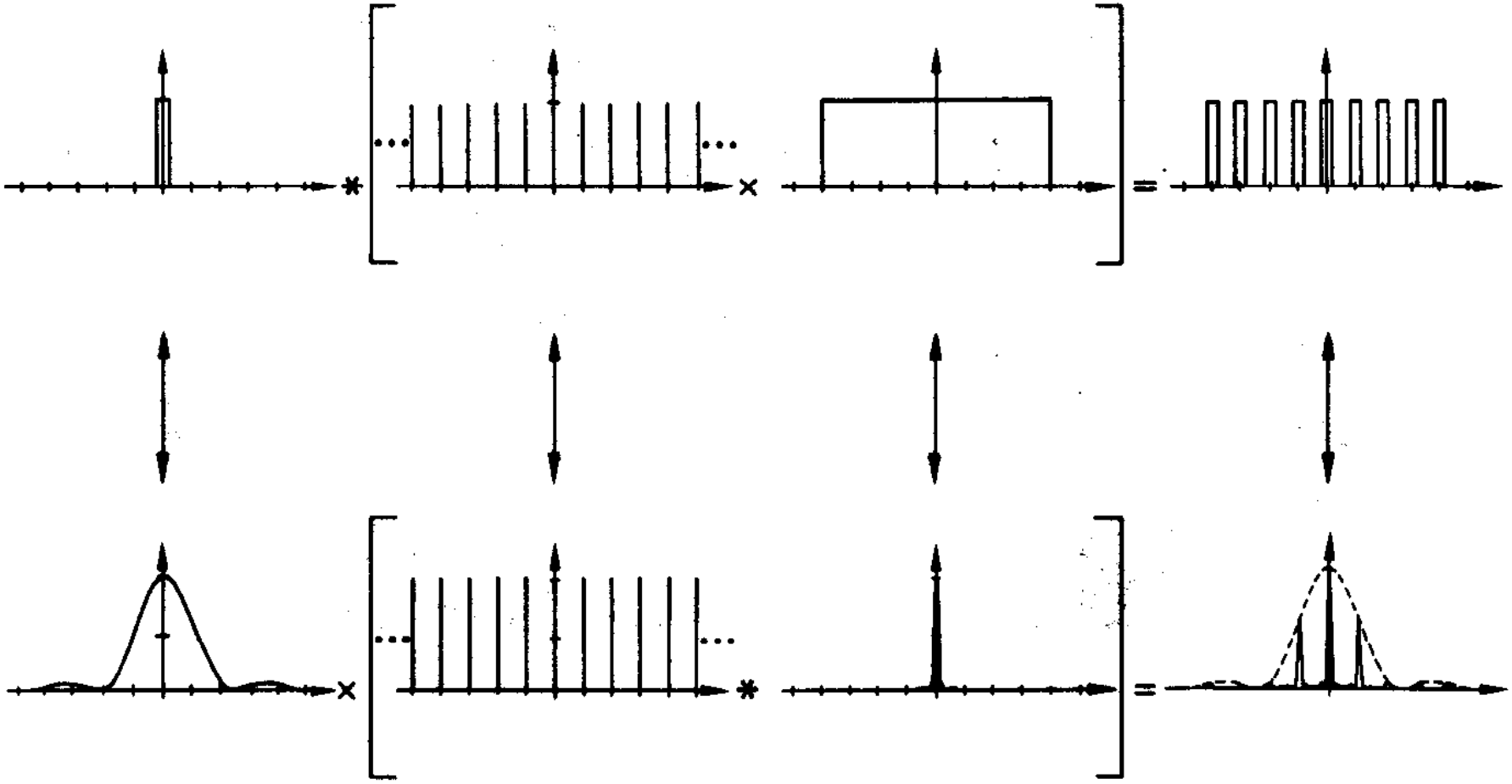
that concerning the motif

that concerning the shape of the entire crystal

Diffraction by 1-D Obstacles



Diffraction by 1-D Obstacles



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