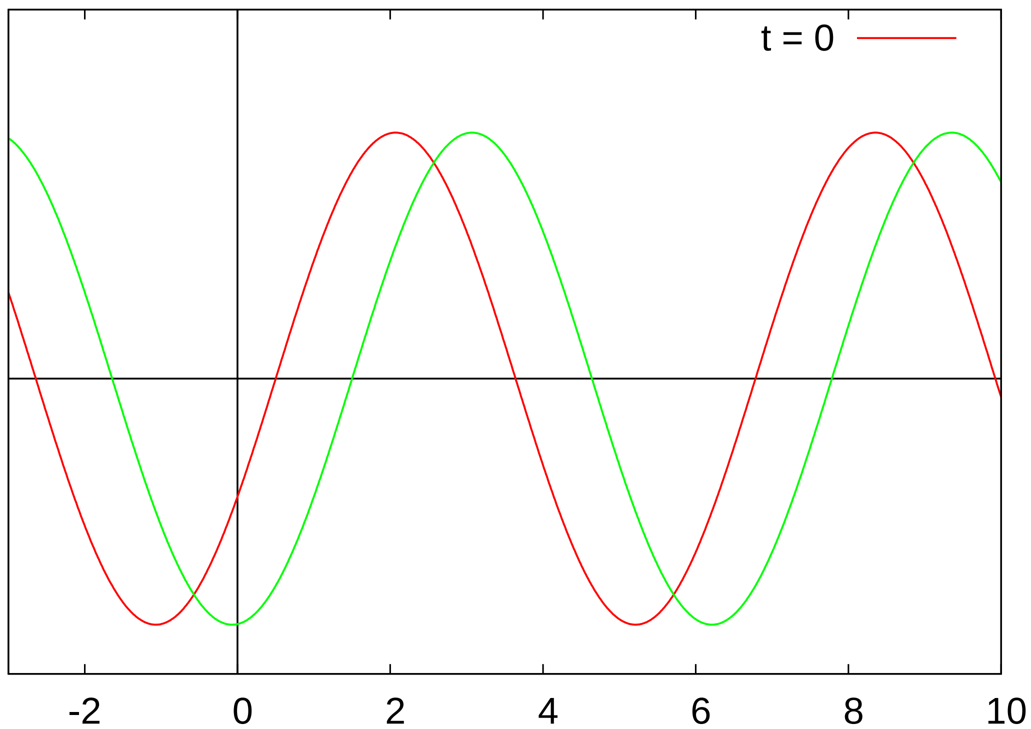
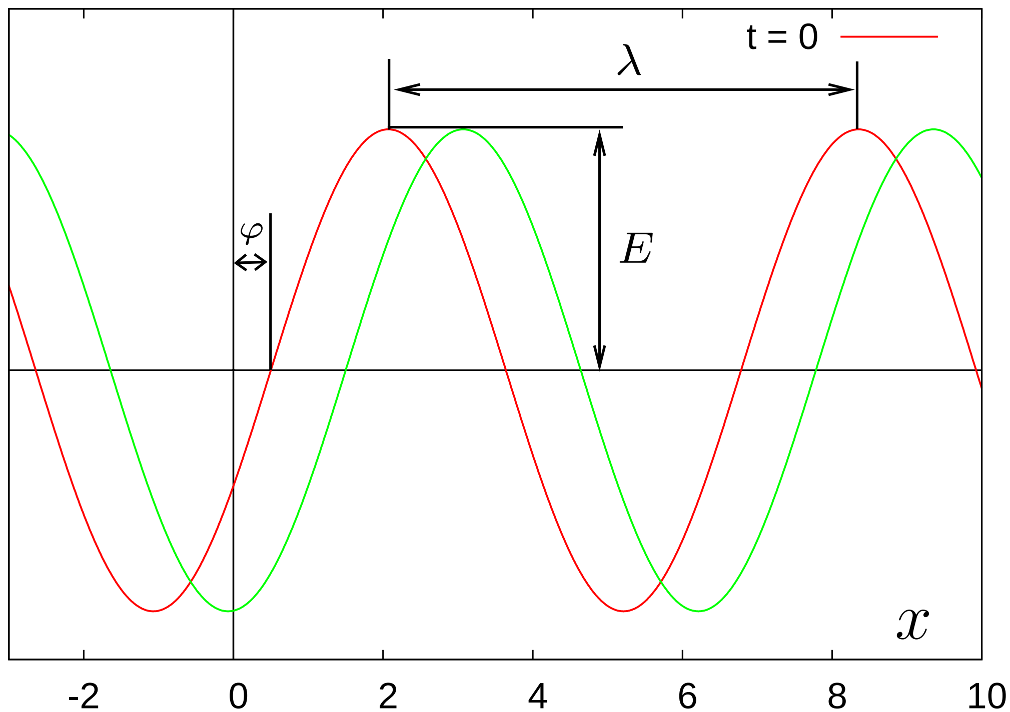
Sin wave



$$y = E\sin(kx - \omega t - \varphi) \tag{1}$$

Sin wave and its parameters



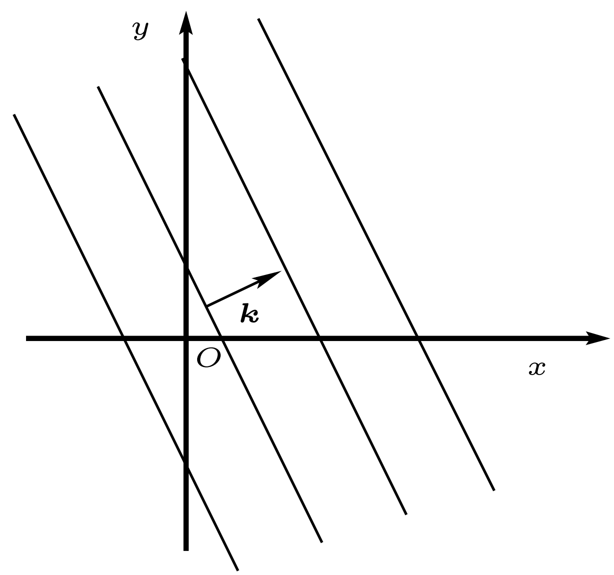
$$y = E\sin(kx - \omega t - \varphi) \quad (2)$$

$$k \underset{def}{=} \frac{2\pi}{\lambda} \quad (3)$$

$$\omega \underset{def}{=} \frac{2\pi}{T} \quad (4)$$

Flat monochromatic wave in space

A flat monochromatic wave in space can be given by the following vector equation:



$$E(\boldsymbol{r}, t) = E_0 \sin(\boldsymbol{k}\boldsymbol{r} - \omega t - \varphi) \tag{5}$$

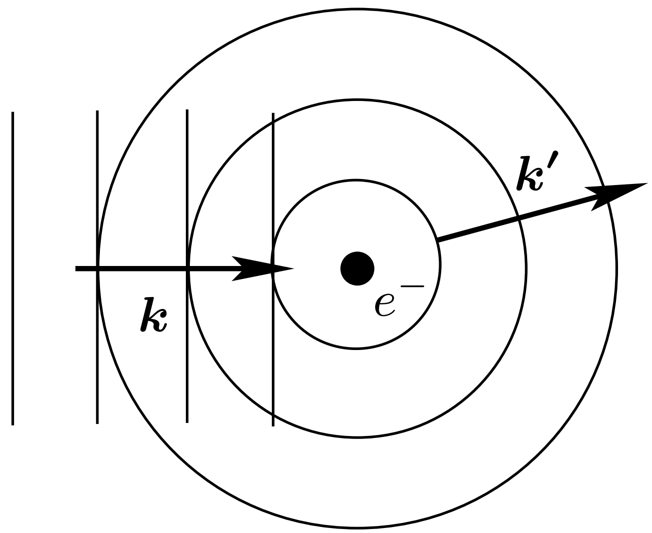
Superposition of two monochromatic waves

Amplitutes of two elecromagnetic waves add up:

$$E = E_1 + E_2 \tag{6}$$

Scattering by an electron

Thomson showed that:



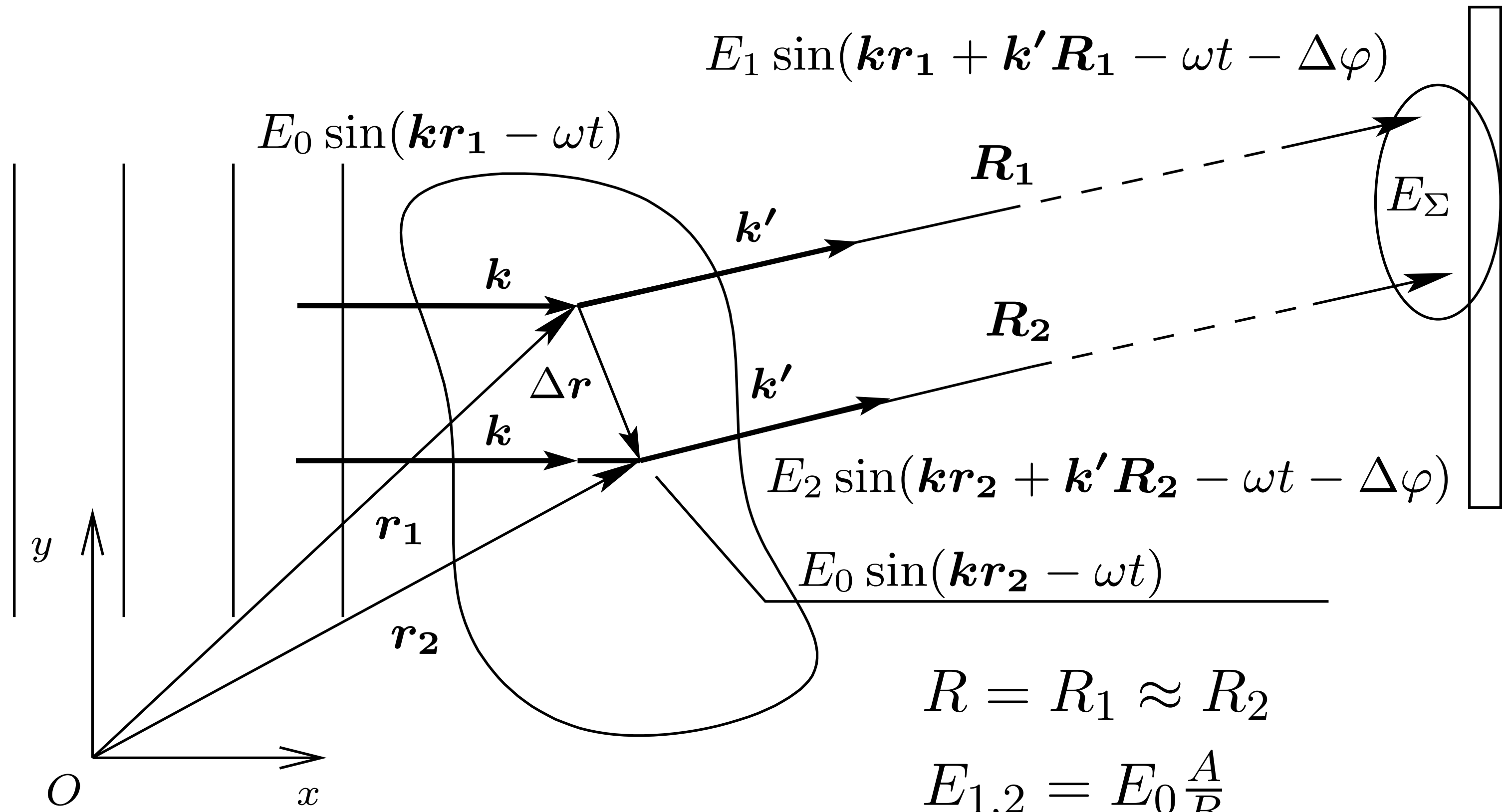
$$E_1(\boldsymbol{R}, t) = E_1 \sin(\boldsymbol{k'R} - \omega t - \Delta\varphi) \quad (7)$$

$$E_1 = E_0 \frac{1}{R} \frac{e^2}{mc^2} \sin\phi = E_0 \frac{A}{R} \quad (8)$$

$$m_{p^+} \approx 1800 \cdot m_{e^-}$$

$$I_1 \approx 2\% \cdot I_0$$

Scattering by a specimen



$$R = R_1 \approx R_2$$

$$E_{1,2} = E_0 \frac{A}{R}$$

$$E_\Sigma = E_1 \sin(\boldsymbol{kr_1} + \boldsymbol{k'R_1} - \omega t - \Delta\varphi) + E_2 \sin(\boldsymbol{kr_2} + \boldsymbol{k'R_2} - \omega t - \Delta\varphi) \tag{9}$$

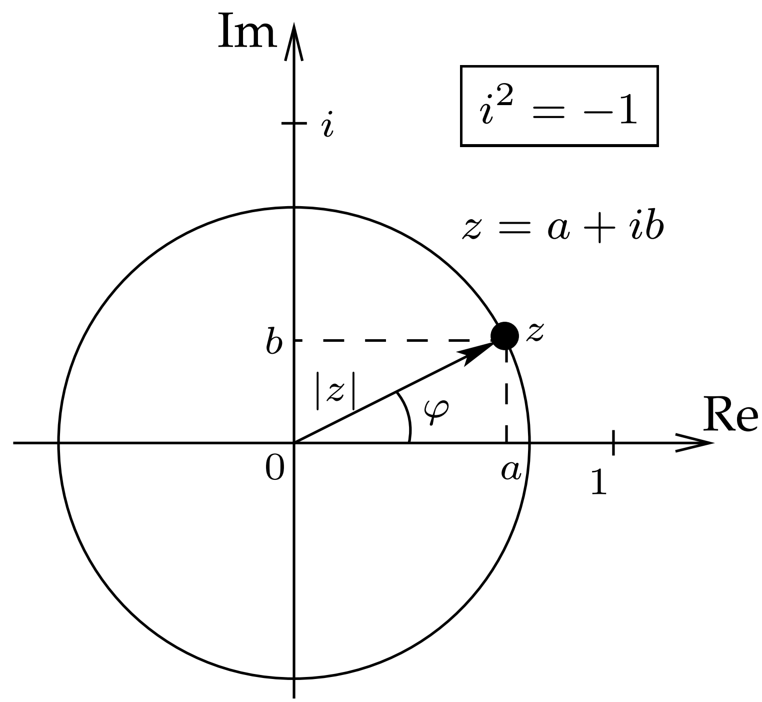
COMPLEX EXPONENTS

It is more convenient in physics to represent waves by complex exponents, using Euler's formula:

$$e^{ix} = \cos x + i \sin x \tag{10}$$

We just agree that instead of $\sin$ function, we write a complex exponent and always keep in mind that our real wave is just the imaginary part. Or real. If we care... :)

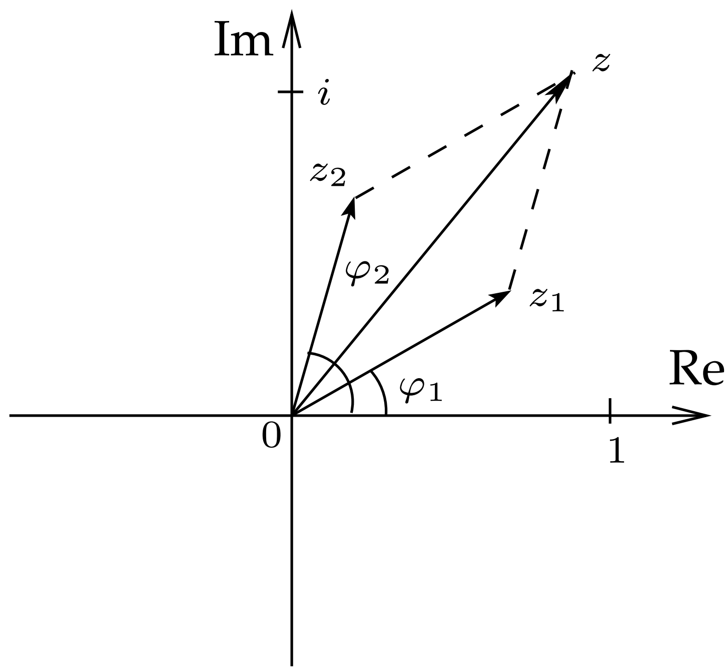
REMINESCENCES: COMPLEX NUMBERS ...



$$z = a + ib \qquad |z| = \sqrt{a^2 + b^2} \qquad \tan\varphi = \frac{b}{a}$$

$$z^* = a - ib \qquad |z|^2 = z \cdot z^*$$

REMINESCENCES: COMPLEX NUMBERS AS VECTORS ...



$$z = z_1 + z_2 = a + ib = (a_1 + a_2) + i(b_1 + b_2) \tag{11}$$

$$z_1 z_2 = (a_1 + ib_1)(a_2 + ib_2) = (a_1 a_2 - b_1 b_2) + i(a_1 b_2 + a_2 b_1) \tag{12}$$

Outline of Euler's formula proof...

$$e^{ix} = \cos x + i \sin x$$

$$\sin x = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \cdots + (-1)^k \frac{1}{(2k+1)!}x^{2k+1} + \ldots$$

$$i \sin x = ix + \frac{1}{3!}(ix)^3 + \frac{1}{5!}(ix)^5 + \cdots + \underbrace{(-1)^k i^{-2k-1} i}_{=1} \frac{1}{(2k+1)!}(ix)^{2k+1} + \ldots$$

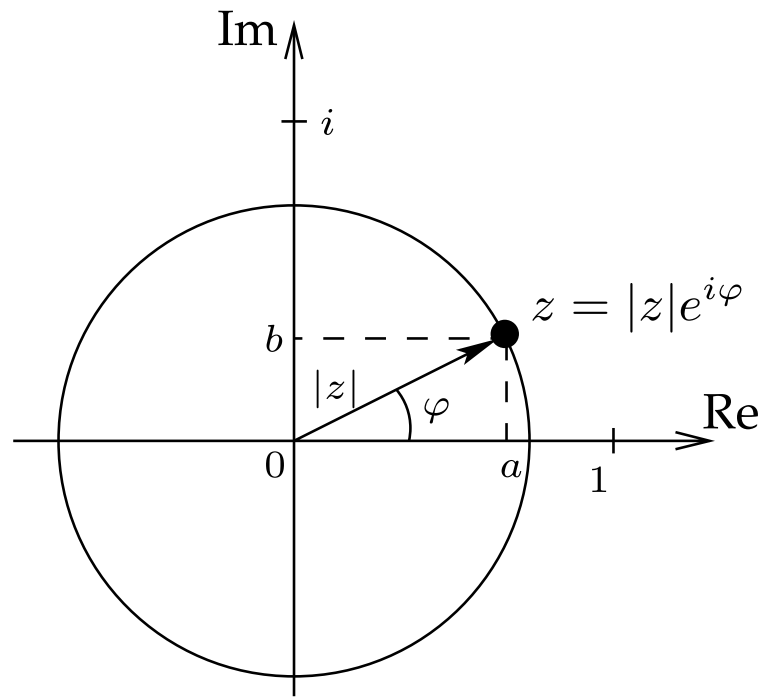
$$\cos x = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 - \cdots + (-1)^k \frac{1}{(2k)!}x^{2k} + \ldots$$

$$= 1 + \frac{1}{2!}(ix)^2 + \frac{1}{4!}(ix)^4 + \cdots + \underbrace{(-1)^k i^{-2k}}_{=1} \frac{1}{(2k)!}(ix)^{2k} + \ldots$$

$$e^x = 1 + \frac{1}{1!}x + \frac{1}{2!}x^2 + \cdots + \frac{1}{k!}x^k + \ldots$$

$$e^{ix} = 1 + ix + \frac{1}{2!}(ix)^2 + \frac{1}{3!}(ix)^3 + \frac{1}{4!}(ix)^4 + \cdots + \frac{1}{k!}(ix)^k + \ldots$$

COMPLEX NUMBER AS EXPONENTS



$$|z| = \sqrt{a^2 + b^2} \qquad a = |z|\cos\varphi \qquad b = |z|\sin\varphi$$

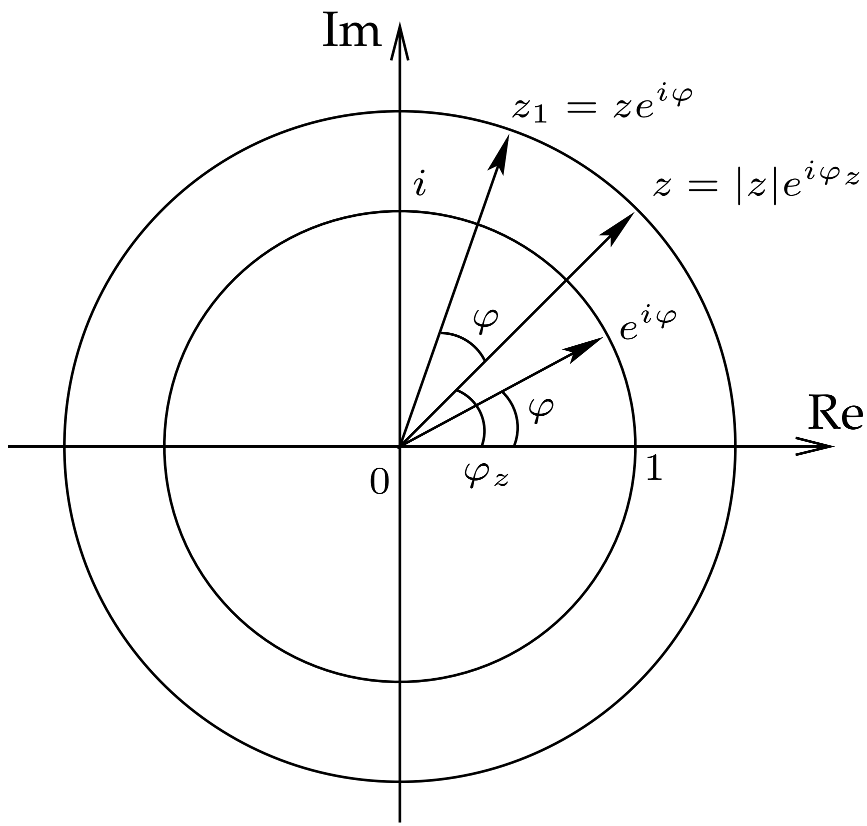
$$z = a + ib = |z|\cos\varphi + i|z|\sin\varphi = |z|(\cos\varphi + i\sin\varphi) = |z|e^{i\varphi}$$

Useful properties of exponents

$$e^a e^b = e^{a+b} \tag{13}$$

$$e^{ix} e^{i\varphi} = e^{i(x+\varphi)} \tag{14}$$

Phase shift



$$z_1 = ze^{i\varphi} = |z|e^{i\varphi_z}e^{i\varphi} = |z|e^{i(\varphi_z+\varphi)} \tag{15}$$

Adding two exponents

$$
\begin{aligned}
e^{ix} + e^{iy} &= e^{ix}(1 + e^{i(y-x)}) \\
&= e^{ix} e^{i\frac{y-x}{2}} (e^{-i\frac{y-x}{2}} + e^{i\frac{y-x}{2}}) \\
&= e^{i2\frac{x}{2}} e^{i\frac{y-x}{2}} (\cos\frac{y-x}{2} - i\sin\frac{y-x}{2} + \cos\frac{y-x}{2} + i\sin\frac{y-x}{2}) \\
&= e^{i\frac{x+y}{2}} \cdot 2\cos\frac{y-x}{2} \qquad (16)
\end{aligned}
$$

Square of the amplitude

let

$$z = |z| e^{i\varphi} \,, \tag{17}$$

then

$$\begin{aligned} z \cdot z^* &= |z| e^{i\varphi} \cdot |z| e^{-i\varphi} \\ &= |z|^2 \underbrace{e^{\overbrace{i(\varphi - \varphi)}^{=0}}}_{=1} \\ &= |z|^2 \end{aligned} \tag{18}$$

Representing waves by exponents

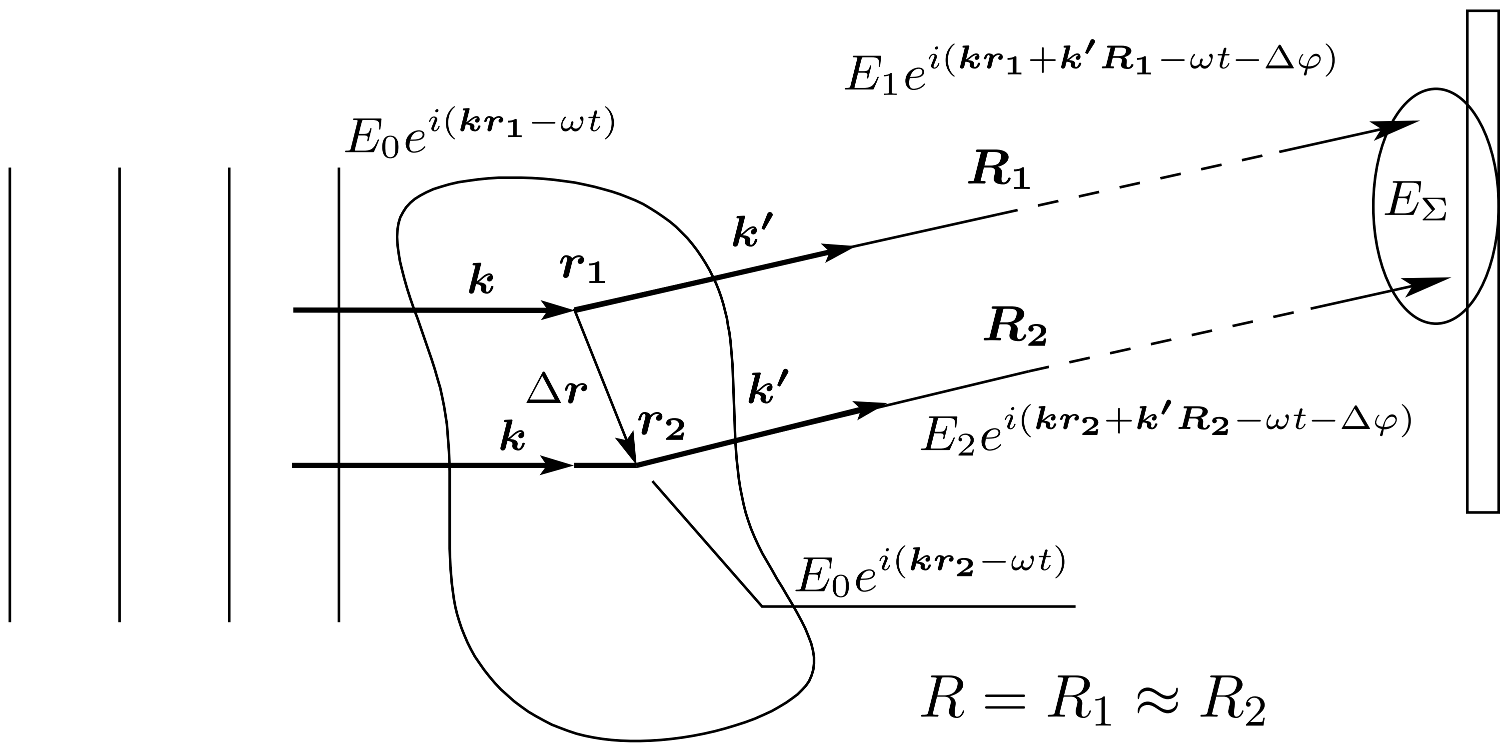
$$E\sin(\boldsymbol{kr}-\omega t)=\mathrm{Im}(Ee^{i(\boldsymbol{kr}-\omega t)}) \tag{19}$$

$$\begin{aligned}E\sin(\boldsymbol{kr}-\omega t-\varphi)&=\mathrm{Im}(Ee^{i(\boldsymbol{kr}-\omega t-\varphi)}) &(20)\\ &=\mathrm{Im}(Ee^{-i\varphi}e^{i(\boldsymbol{kr}-\omega t)}) &(21)\end{aligned}$$

$$\begin{aligned}&E_1\sin(\boldsymbol{kr}-\omega t-\varphi_1)+\\ &E_2\sin(\boldsymbol{kr}-\omega t-\varphi_2)=\mathrm{Im}(E_1e^{i(\boldsymbol{kr}-\omega t-\varphi_1)}+E_2e^{i(\boldsymbol{kr}-\omega t-\varphi_2)})\\ &\qquad=\mathrm{Im}((E_1e^{-i\varphi_1}+E_2e^{-i\varphi_2})e^{i(\boldsymbol{kr}-\omega t)}) &(22)\\ & &(23)\end{aligned}$$

Scattering by a specimen revisited

exponential form:



$$R = R_1 \approx R_2$$

$$E_{1,2} = E_0 \frac{A}{R}$$

$$E_\Sigma = E_1 e^{i(\boldsymbol{k r_1}+\boldsymbol{k' R_1}-\omega t-\Delta\varphi)} + E_2 e^{i(\boldsymbol{k r_2}+\boldsymbol{k' R_2}-\omega t-\Delta\varphi)} \qquad (24)$$

Adding two monochromatic waves

$$
\begin{aligned}
E_1(\boldsymbol{R_1}, t) &= E_1 e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1} - \omega t - \Delta\varphi)} \\
&= \underbrace{E_0 \frac{A}{R} e^{-i\Delta\varphi} e^{-i\omega t}}_{\underset{def}{=} E_0'} e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1})} \\
&= E_0' e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1})} \qquad (25)
\end{aligned}
$$

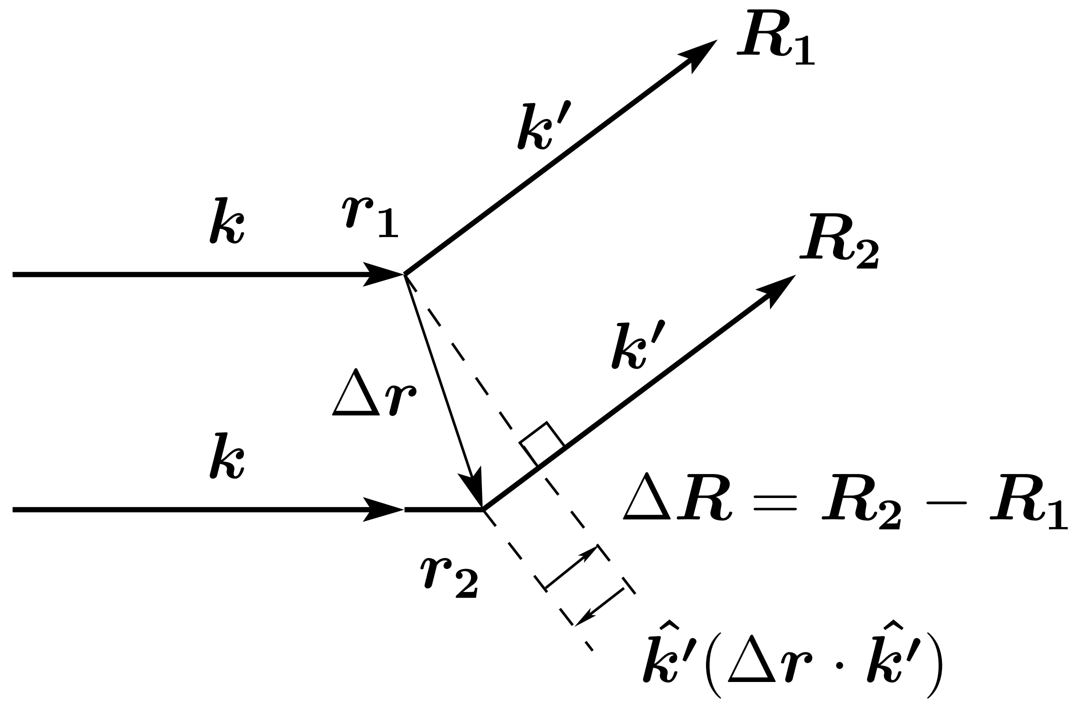
$$
E_2(\boldsymbol{R_2}, t) = E_0' e^{i(\boldsymbol{kr_2} + \boldsymbol{k'R_2})} \qquad (26)
$$

$$
\begin{aligned}
E_\Sigma &= E_0' e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1})} + E_0' e^{i(\boldsymbol{kr_2} + \boldsymbol{k'R_2})} \\
&= E_0' [e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1})} + e^{i(\boldsymbol{kr_2} + \boldsymbol{k'R_2})}] \qquad (27) \\
&= E_0' e^{i(\boldsymbol{kr_1} + \boldsymbol{k'R_1})} [1 + e^{i(\boldsymbol{kr_2} - \boldsymbol{kr_1} + \boldsymbol{k'R_2} - \boldsymbol{k'R_1})}]
\end{aligned}
$$

Adding two monochromatic waves (2)

$$
\begin{aligned}
E_\Sigma &= \underbrace{E_0' e^{i(\boldsymbol{k r_1} + \boldsymbol{k' R_1})}}_{=E_0''} [1 + e^{i(\boldsymbol{k r_2} - \boldsymbol{k r_1} + \boldsymbol{k' R_2} - \boldsymbol{k' R_1})}] \\
&= E_0'' [1 + e^{i(\boldsymbol{k} \Delta \boldsymbol{r} + \boldsymbol{k'} \Delta \boldsymbol{R})}]
\end{aligned}
\tag{28}
$$

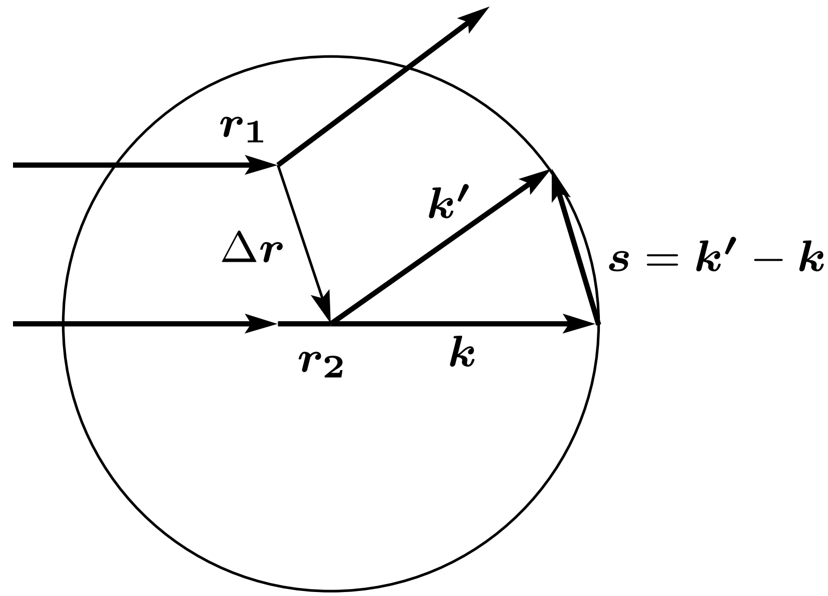
PROJECTION OF Δr



$$\hat{\boldsymbol{k}}' = \frac{\boldsymbol{k}'}{k'} \qquad \Delta \boldsymbol{R} = -\hat{\boldsymbol{k}}'(\Delta \boldsymbol{r} \cdot \hat{\boldsymbol{k}}')$$

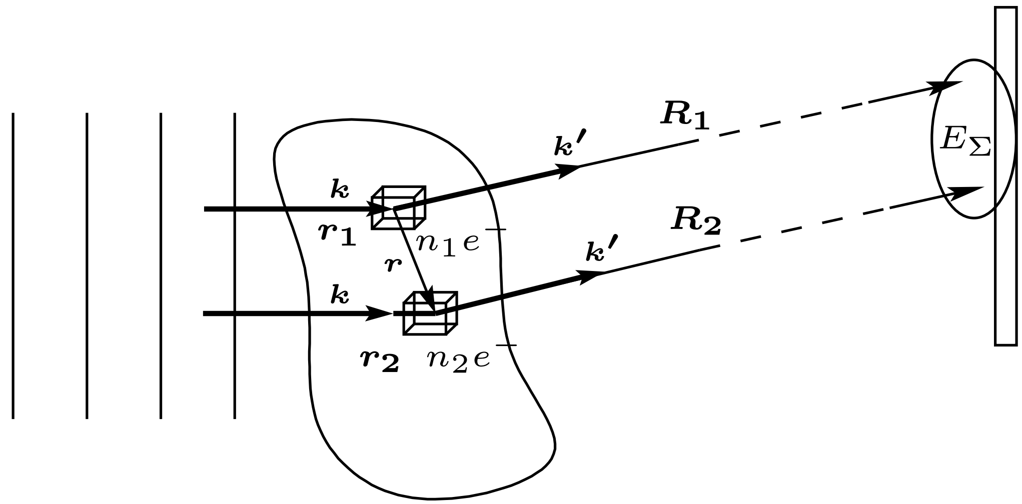
$$\boldsymbol{k}' \Delta \boldsymbol{R} = -\boldsymbol{k}' \cdot \frac{\boldsymbol{k}'}{k'}\left(\Delta \boldsymbol{r} \cdot \frac{\boldsymbol{k}'}{k'}\right) = -\frac{(\boldsymbol{k}' \cdot \boldsymbol{k}')}{k'^2}(\Delta \boldsymbol{r} \cdot \boldsymbol{k}') = -\boldsymbol{k}' \Delta \boldsymbol{r}$$

ADDING TWO MONOCHROMATIC WAVES (3)



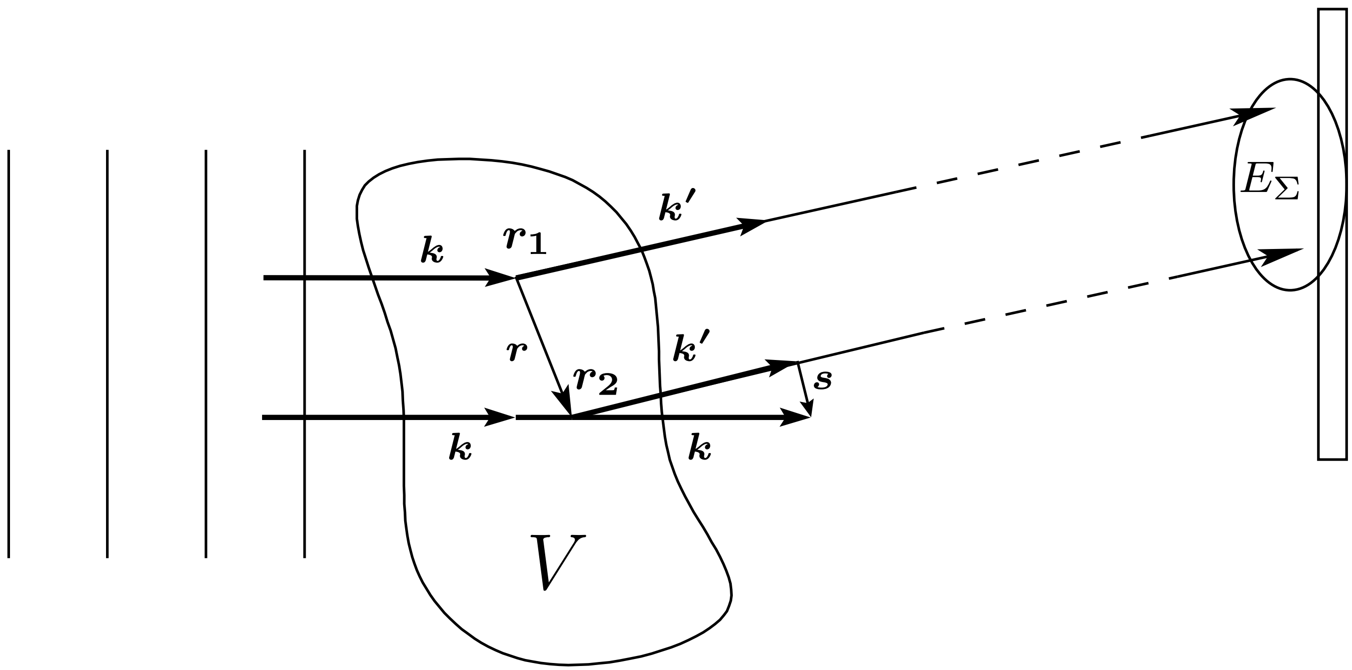
$$
\begin{aligned}
E_\Sigma &= E_0''[1 + e^{i(\boldsymbol{k}\Delta\boldsymbol{r} - \boldsymbol{k'}\Delta\boldsymbol{r})}] \\
&= E_0''[1 + e^{i(\Delta\boldsymbol{r}(\boldsymbol{k}-\boldsymbol{k'}))}] \\
&= E_0''[1 + e^{i\Delta\boldsymbol{r}\boldsymbol{s}}] \\
&= E_0''[1 \cdot e^{i\Delta\boldsymbol{r_0}\boldsymbol{s}} + e^{i\Delta\boldsymbol{r}\boldsymbol{s}}]
\end{aligned}
\tag{29}
$$

Adding two monochromatic waves (4)



$$
\begin{aligned}
E_{1+2} &= E_0''[n_1 e^{i\boldsymbol{r_0 s}} + n_2 e^{i\boldsymbol{rs}}] \\
E_\Sigma &= E_0'' \sum_{k=1}^{N} n_k e^{i\boldsymbol{r}_k \boldsymbol{s}} \\
&= E_0'' \sum_{k=1}^{N} \rho_k \Delta V_k e^{i\boldsymbol{r}_k \boldsymbol{s}}
\end{aligned}
\tag{30}
$$

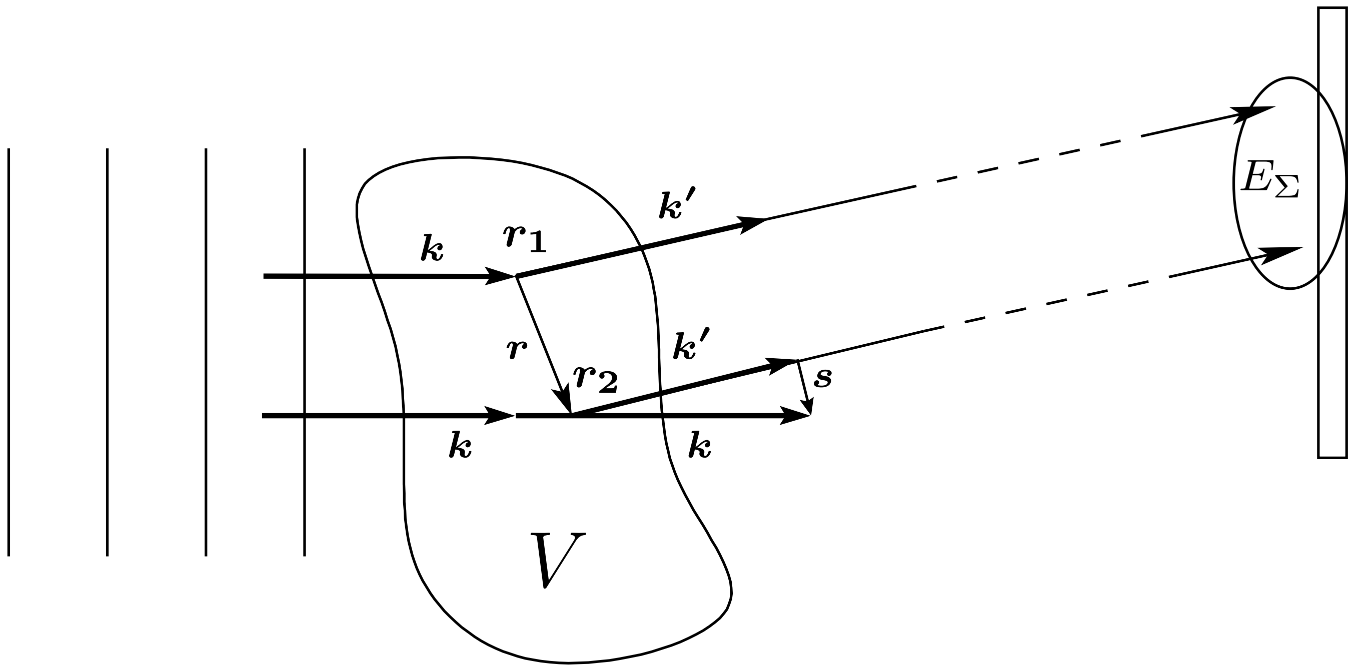
FOURIER TRANSFORM



$$E_\Sigma = \lim_{\substack{N\to\infty \\ \Delta V_k \to 0}} E_0'' \sum_{k=1}^{N} \rho_k \Delta V_k e^{i\boldsymbol{r}_k \boldsymbol{s}} \tag{31}$$

$$= E_0'' \int_V \rho(\boldsymbol{r}) e^{i\boldsymbol{r}\boldsymbol{s}} dV \tag{32}$$

Fourier transform (2)



$$\boldsymbol{S} = \frac{\boldsymbol{s}}{2\pi} \tag{33}$$

$$E_\Sigma = E_0'' \int_V \rho(\boldsymbol{r}) e^{2\pi i \boldsymbol{r}\boldsymbol{S}} dV \tag{34}$$

Structure factor

$$E_\Sigma = E_0'' \underbrace{\int_V \rho(\boldsymbol{r}) e^{2\pi i \boldsymbol{r}\boldsymbol{S}} dV}_{F(\boldsymbol{S})} \qquad (35)$$

$$\boxed{\mathcal{F}[\rho()](\boldsymbol{S}) = F(\boldsymbol{S}) = \int_V \rho(\boldsymbol{r}) e^{2\pi i \boldsymbol{r}\boldsymbol{S}} dV} \qquad (36)$$

Inverse Fourier transform

let

$$F(\boldsymbol{S}) = \int_{-\infty}^{+\infty} \rho(\boldsymbol{r}) e^{2\pi i \boldsymbol{r}\boldsymbol{S}} dV \tag{37}$$

then

$$\rho(\boldsymbol{r}) = \int_{-\infty}^{+\infty} F(\boldsymbol{S}) e^{-2\pi i \boldsymbol{r}\boldsymbol{S}} d\boldsymbol{S} \tag{38}$$

Properties of the Fourier transform

- Linearity

$$\mathcal{F}[\alpha\rho_1 + \beta\rho_2] = \alpha\mathcal{F}[\rho_1] + \beta\mathcal{F}[\rho_2] \tag{39}$$

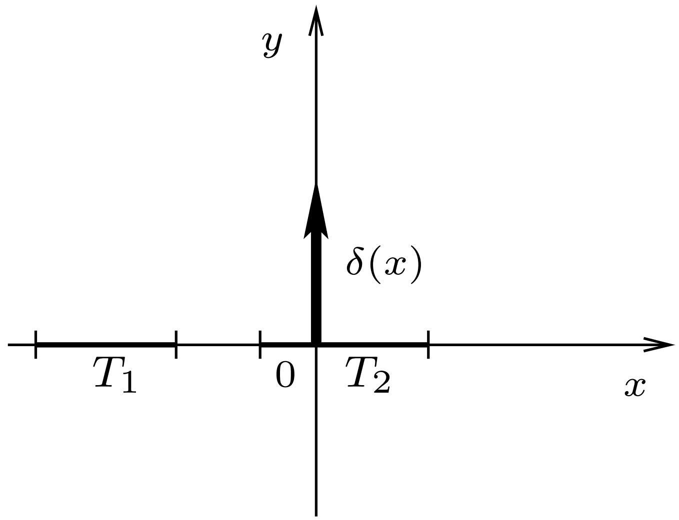
- Shift

$$\mathcal{F}[\rho(\boldsymbol{r} - \Delta\boldsymbol{r})] = e^{2\pi i(\Delta\boldsymbol{r}\boldsymbol{S})}\,\mathcal{F}[\rho(\boldsymbol{r})] \tag{40}$$

- Rotation

$$\begin{aligned} \boldsymbol{r}' &= ||R||\boldsymbol{r} \\ \rho'(\boldsymbol{r}) \underset{def}{=} \rho(\boldsymbol{r}') &= \rho(||R||\boldsymbol{r}) \\ \mathcal{F}[\rho(||R||\boldsymbol{r})] &= F(||R||\boldsymbol{S}) \end{aligned} \tag{41}$$

DIRAC DELTA FUNCTION



$$\int_{T_1} \delta(x) f(x) dx \underset{def}{=} 0 \tag{42}$$

$$\int_{T_2} \delta(x) f(x) dx \underset{def}{=} f(0) \tag{43}$$

$$\int_{-\infty}^{+\infty} \delta(x) f(x) dx \underset{def}{=} f(0) \tag{44}$$

PROPERTIES OF THE DELTA FUNCTION

$$\delta(-x) = \delta(x) \tag{45}$$

$$\int_{-\infty}^{+\infty} \delta(x)dx = 1 \tag{46}$$

$$\int_{-\infty}^{+\infty} \delta(x - x_0)f(x)dx = f(x_0) \tag{47}$$

$$\mathcal{F}[\delta] = \int_{-\infty}^{+\infty} \delta(x)e^{2\pi ixS}dx = e^0 = 1 \tag{48}$$

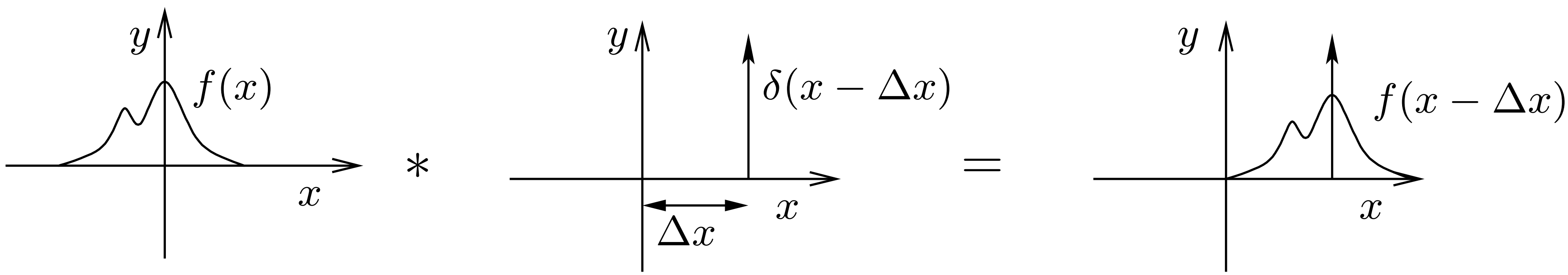
$$\mathcal{F}^{-1}[1] = \int_{-\infty}^{+\infty} e^{-2\pi ixS}dS = \delta(x) \tag{49}$$

$$\mathcal{F}[1] = \int_{-\infty}^{+\infty} e^{2\pi ixS}dx = \delta(S) \tag{50}$$

Convolution

$$(f * g)(x) \underset{def}{=} \int_{-\infty}^{+\infty} f(v)g(x-v)dv \tag{51}$$

CONVOLUTION WITH DELTA FUNCTION

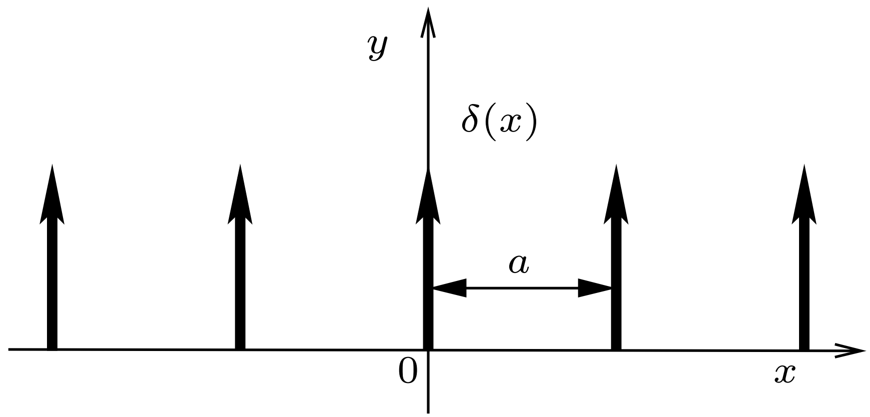


$$f(x) * \delta(x - \Delta x) = \int_{-\infty}^{+\infty} f(v)\delta(x - v - \Delta x)dv = f(x - \Delta x) \quad (52)$$

Fourier transform of the convolution

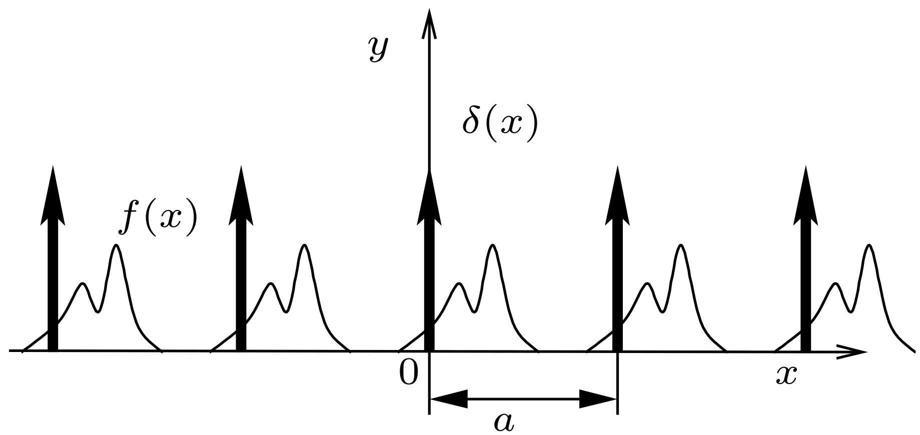
$$
\begin{aligned}
\mathcal{F}[f * g] &= \int_{-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} f(v) g(x-v) dv \right) e^{2\pi i S x} dx \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(v) g(x-v) e^{2\pi i S(x-v)} e^{2\pi i S v} dv dx \\
&= \int_{-\infty}^{+\infty} f(v) e^{2\pi i S v} dv \cdot \\
&\int_{-\infty}^{+\infty} g(x-v) e^{2\pi i S(x-v)} d(x-v) \qquad (53) \\
&= \mathcal{F}[f] \cdot \mathcal{F}[g] \qquad (54)
\end{aligned}
$$

Lattice function



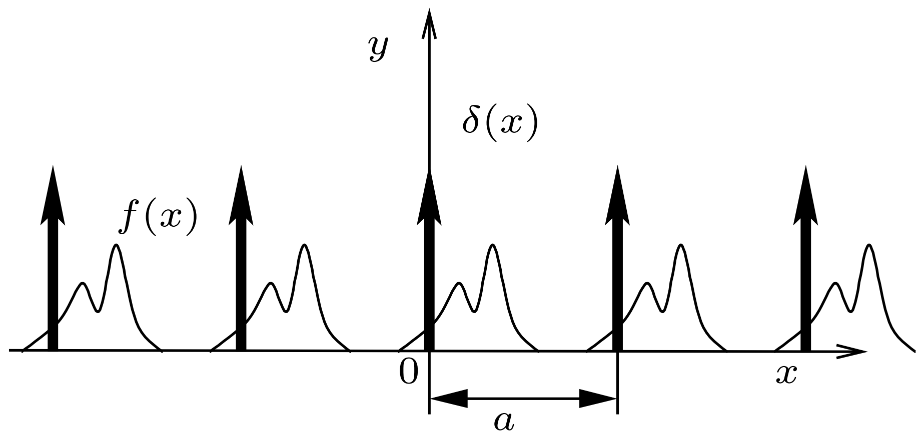
$$L(x) = \sum_{n=-\infty}^{+\infty} \delta(x - an) \tag{55}$$

Crystal function



$$f * L = \sum_{n=-\infty}^{+\infty} f(x - an) \tag{56}$$

Crystal Fourier transform



$$\mathcal{F}[f * L] = \mathcal{F}[f] \cdot \mathcal{F}[L] \tag{57}$$

$$= \mathcal{F}[\sum_{n=-\infty}^{+\infty} f(x - an)] \tag{58}$$

$$= \sum_{n=-\infty}^{+\infty} \mathcal{F}[f(x - an)] \tag{59}$$

Crystal Fourier transform (2)

$$\begin{aligned}
\mathcal{F}[f * L] &= \mathcal{F}[f] \cdot \mathcal{F}[L] && (60)\\
&= F(S) \cdot \mathcal{F}[L] && (61)\\
&= \mathcal{F}[\sum_{n=-\infty}^{+\infty} f(x - an)] && (62)\\
&= \sum_{n=-\infty}^{+\infty} \mathcal{F}[f(x - an)] && (63)\\
&= \sum_{n=-\infty}^{+\infty} F(S) e^{2\pi i S a n} && (64)\\
&= F(S) \sum_{n=-\infty}^{+\infty} e^{2\pi i S a n} && (65)
\end{aligned}$$

Crystal Fourier transform (3)

$$\sum_{n=-\infty}^{\infty} f(x-an) \underset{def}{=} S(x) \tag{66}$$

$$= \sum_{n=-\infty}^{\infty} c_n e^{-2\pi i \cdot n \frac{x}{a}} \tag{67}$$

$$
\begin{aligned}
c_n &= \frac{1}{a}\int_{-a/2}^{a/2} S(x)e^{2\pi i\cdot n\frac{x}{a}}dx && (68)\\
&= \frac{1}{a}\int_{-a/2}^{a/2}\sum_{n=-\infty}^{\infty} f(x-an)e^{2\pi i\cdot n\frac{x}{a}}dx && (69)\\
&= \frac{1}{a}\sum_{n=-\infty}^{\infty}\int_{-a/2}^{a/2} f(x-an)e^{2\pi i\cdot n\frac{x}{a}}dx && (70)\\
&= \frac{1}{a}\int_{-\infty}^{\infty} f(x)e^{2\pi i\cdot x\frac{n}{a}}dx && (71)\\
&= \frac{1}{a}F(n/a) && (72)
\end{aligned}
$$

Crystal Fourier transform (4)

$$c_n = \frac{1}{a} F(n/a) \tag{73}$$

$$\sum_{n=-\infty}^{\infty} f(x - an) = \sum_{n=-\infty}^{\infty} c_n e^{-2\pi i \cdot n \frac{x}{a}} \tag{74}$$

$$= \frac{1}{a} \sum_{n=-\infty}^{\infty} F(n/a) e^{-2\pi i \cdot n \frac{x}{a}} \tag{75}$$

$$\sum_{n=-\infty}^{\infty} \delta(x - an) = \frac{1}{a} \sum_{n=-\infty}^{\infty} e^{-2\pi i \cdot n \frac{x}{a}} \tag{76}$$

Lattice Fourier transform

$$\sum_{n=-\infty}^{\infty} \delta(x - an) = \frac{1}{a} \sum_{n=-\infty}^{\infty} e^{2\pi i \cdot n \frac{x}{a}} \tag{77}$$

$$\sum_{n=-\infty}^{\infty} \delta(x - n/a) = a \sum_{n=-\infty}^{\infty} e^{-2\pi i \cdot nax} \tag{78}$$

$$\mathcal{F}[L] = \mathcal{F}[\sum_{n=-\infty}^{\infty} \delta(x - an)] \tag{79}$$

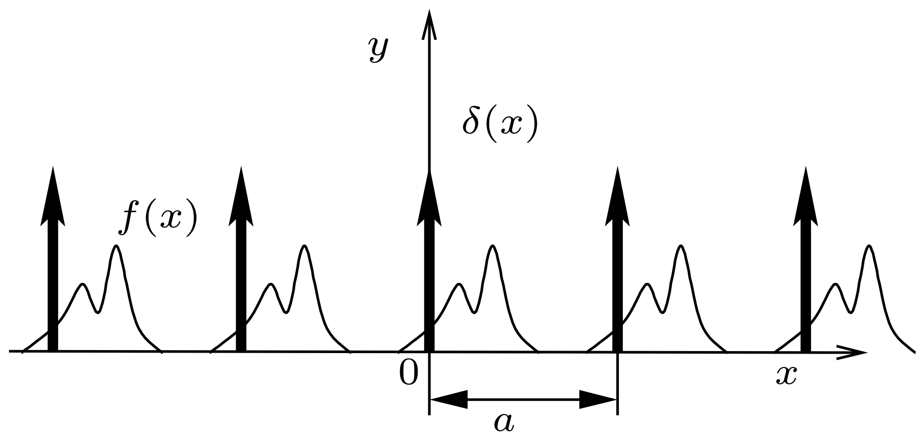
$$= \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta(x - an) e^{2\pi i x S} dx \tag{80}$$

$$= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x - an) e^{2\pi i x S} dx \tag{81}$$

$$= \sum_{n=-\infty}^{\infty} e^{2\pi i a n S} \tag{82}$$

$$= \frac{1}{a} \sum_{n=-\infty}^{\infty} \delta(S - n/a) \tag{83}$$

Reciprocal lattice, 1D case



$$L(x) = \sum_{n=-\infty}^{+\infty} \delta(x - an) \tag{84}$$

$$\mathcal{F}[f * L] = \mathcal{F}[f] \cdot \mathcal{F}[L] \tag{85}$$

$$= F(S) \cdot \frac{1}{a} \sum_{n=-\infty}^{\infty} \delta(S - n/a) \tag{86}$$

Reciprocal lattice, 3D case

$$L(x) = \sum_{m,n,p=-\infty}^{+\infty} \delta(\boldsymbol{r} - \boldsymbol{a}m - \boldsymbol{b}n - \boldsymbol{c}p) \tag{87}$$

$$L^*(\boldsymbol{S}) = \mathcal{F}[L] = \frac{1}{V} \sum_{h,k,l=-\infty}^{+\infty} \delta(\boldsymbol{S} - h\boldsymbol{a}^* - k\boldsymbol{b}^* - l\boldsymbol{c}^*) \tag{88}$$

$$\boldsymbol{a}^* = \frac{[\boldsymbol{b} \times \boldsymbol{c}]}{V}, \qquad \boldsymbol{b}^* = \frac{[\boldsymbol{c} \times \boldsymbol{a}]}{V}, \qquad \boldsymbol{c}^* = \frac{[\boldsymbol{a} \times \boldsymbol{b}]}{V} \tag{89}$$

$$V = (\boldsymbol{abc}) = (\boldsymbol{a} \cdot [\boldsymbol{b} \times \boldsymbol{c}]) \tag{90}$$

Laue conditions

$$\mathcal{F}[\rho_{cryst}] = \mathcal{F}[\rho * L] = \mathcal{F}[\rho] \cdot \mathcal{F}[L] \tag{91}$$

$$= F(\boldsymbol{S}) \cdot L^{\star}(\boldsymbol{S}) \tag{92}$$

$$= F(\boldsymbol{S}) \cdot \frac{1}{V} \sum_{h,k,l=-\infty}^{+\infty} \delta(\boldsymbol{S} - h\boldsymbol{a}^* - k\boldsymbol{b}^* - l\boldsymbol{c}^*) \tag{93}$$

We see that the transformant of the crystal is non-vanishing only for a certain values of $\boldsymbol{S}$

$$(\boldsymbol{S} \cdot \boldsymbol{a}) = h, \qquad (\boldsymbol{S} \cdot \boldsymbol{b}) = k, \qquad (\boldsymbol{S} \cdot \boldsymbol{c}) = l \tag{94}$$

$$h, k, l \in \mathbb{Z} \tag{95}$$

Evald construct and Evald sphere