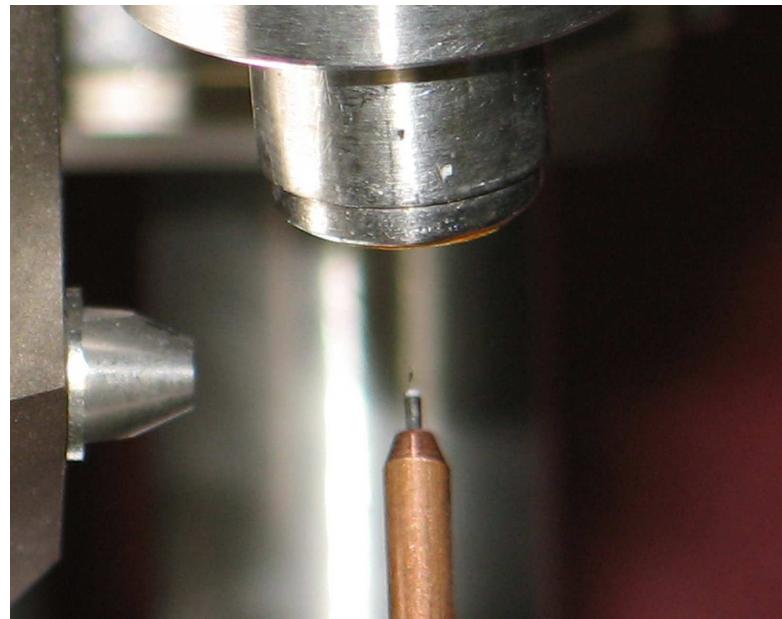
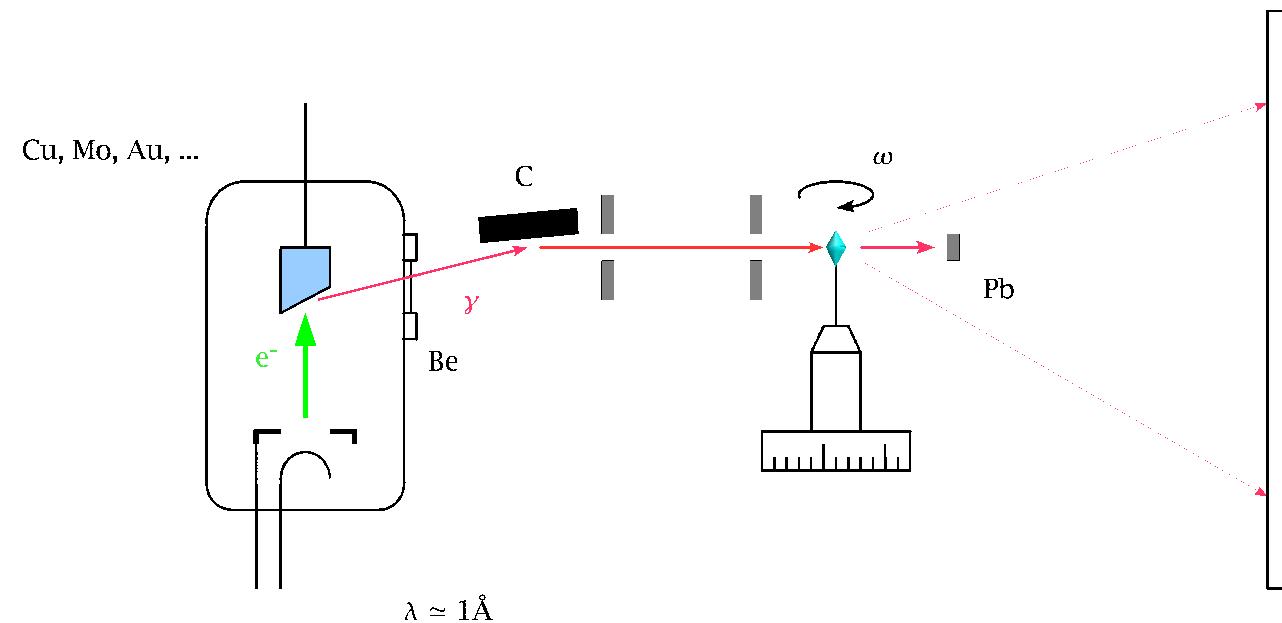

Tai, ką Jūs visada norėjote žinoti apie
rentgenostruktūrinę analizę

... bet nedrįsote paklausti

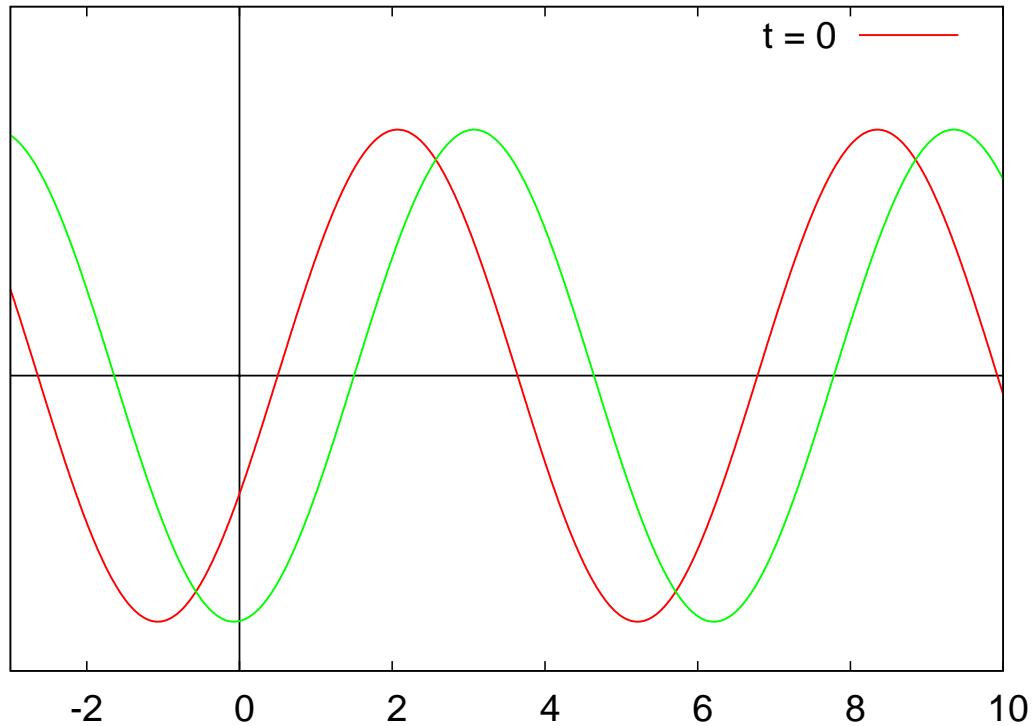
DIFRAKCIJOS EKSPERIMENTAS



DIFRAKCIJOS EKSPERIMENTO SCHEMA

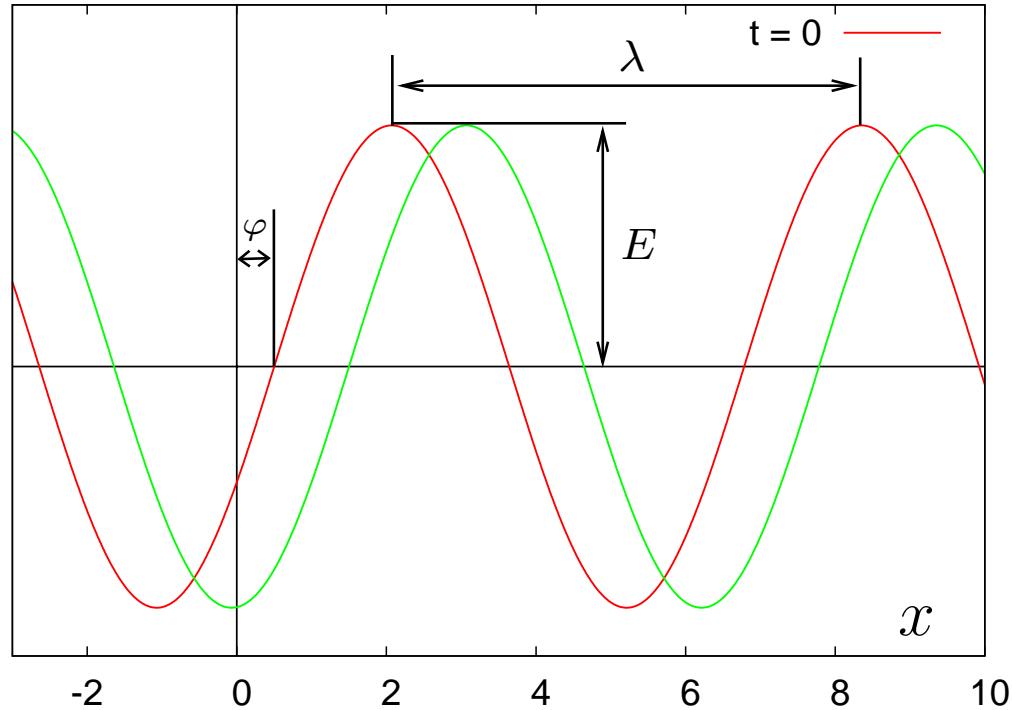


SIN BANGA



$$y = E \sin(kx - \omega t - \varphi) \quad (1)$$

SIN BANGOS ANATOMIJA



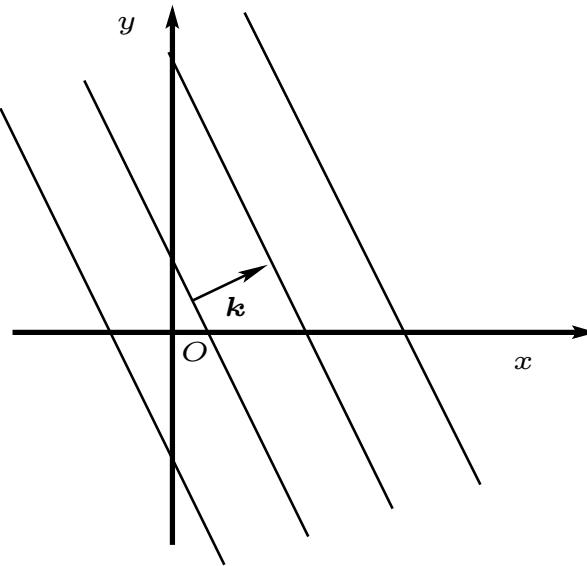
$$y = E \sin(kx - \omega t - \varphi) \quad (2)$$

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

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

PLOKŠČIOS MONOCHROMATINĖS BANGOS ERDVĖJE

Plokščia monochromatinė banga erdvėje gali būti aprašyta vectoriniu pavidalu:



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

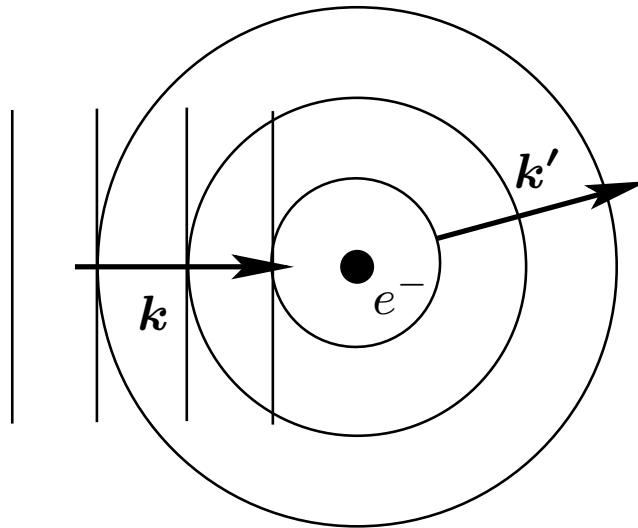
DVIEJŲ BANGŲ SUPERPOZICIJA

Elektromagnetinių bangų amplitudės sumuoja:

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

EL. M. BANGŲ SKLAIDYMAS ELEKTRONU

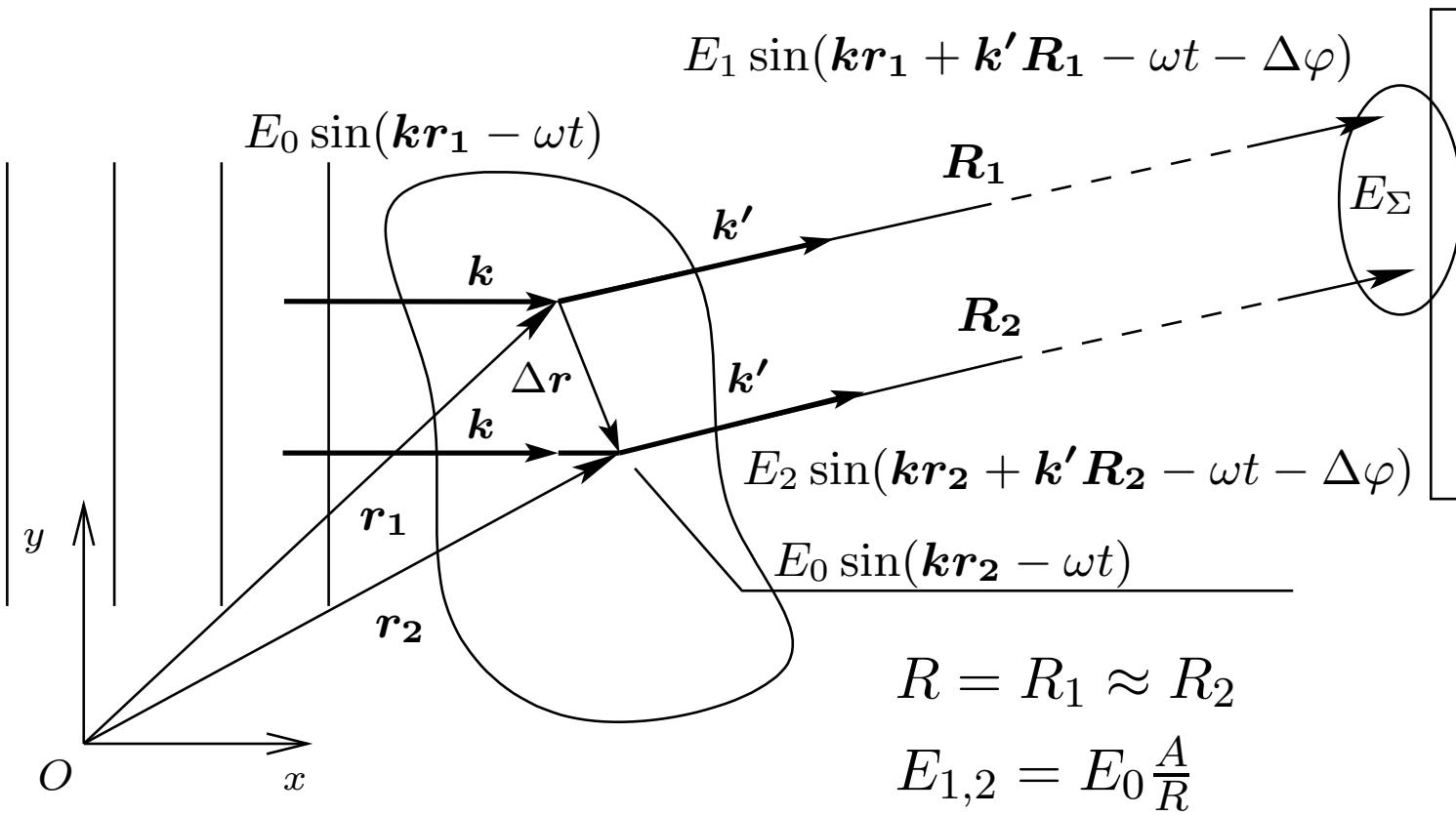
Thomsonas parodė, kad:



$$E_1(\mathbf{R}, t) = E_1 \sin(\mathbf{k}' \cdot \mathbf{R} - \omega t - \Delta\varphi) \quad (7) \quad m_{p^+} \approx 1800 \cdot m_{e^-}$$

$$E_1 = E_0 \frac{1}{R} \frac{e^2}{mc^2} \sin \phi = E_0 \frac{A}{R} \quad (8) \quad I_1 \approx 2\% \cdot I_0$$

EL. M. BANGŲ SKLAIDYMAS PAVYZDŽIU



$$E_{\Sigma} = E_1 \sin(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1 - \omega t - \Delta\varphi) + E_2 \sin(\mathbf{k}\mathbf{r}_2 + \mathbf{k}'\mathbf{R}_2 - \omega t - \Delta\varphi) \quad (9)$$



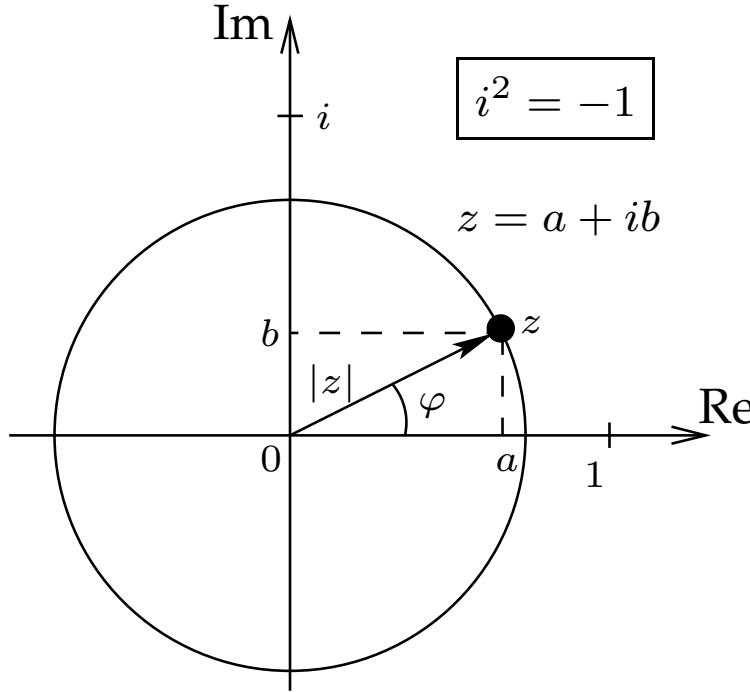
KOMPLEKSINĖS EKSPONENTĖS

Skaičiavimams patogiau naudoti ne sinusus ir kosinusus, o kompleksines eksponentes

$$e^{ix} = \cos x + i \sin x \quad (10)$$

Susitarkime vietoj sin rašyti kompleksinę eksponentę, atsimindami, kad mūsų "tikroji" banga yra šios eksponentės menamoji dalis. Arba realioji. Jeigu mums tai iš viso svarbu...

PRISIMINIMAI: KOMPLEKSINIAI SKAIČIAI ...



$$z = a + ib$$

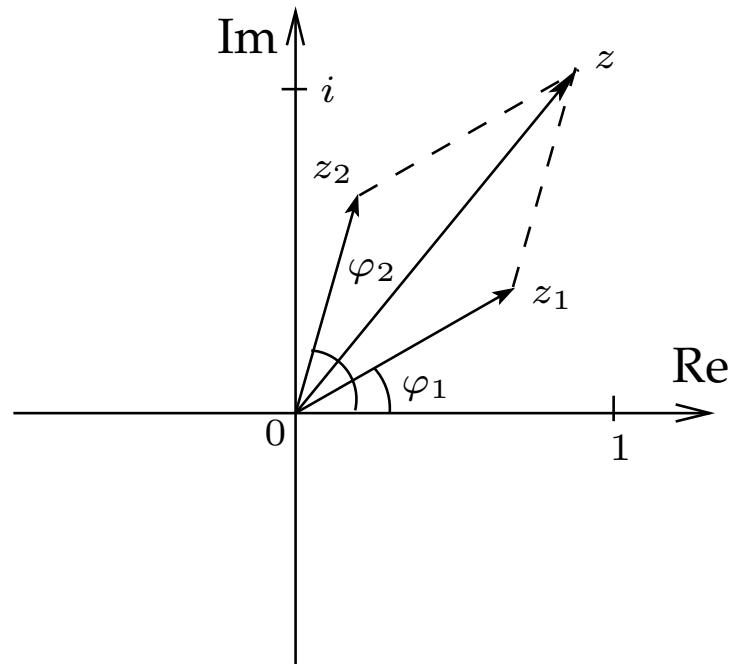
$$|z| = \sqrt{a^2 + b^2}$$

$$\tan \varphi = \frac{b}{a}$$

$$z^* = a - ib$$

$$|z|^2 = z \cdot z^*$$

PRISIMINIMAI: KOMPLEKSINIŲ SKAIČIUŲ VEKTORINIS PAVIDALAS ...



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

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

OILERIO (EULER) FORMULĖS IRODYMO ESKIZAS...

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

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

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

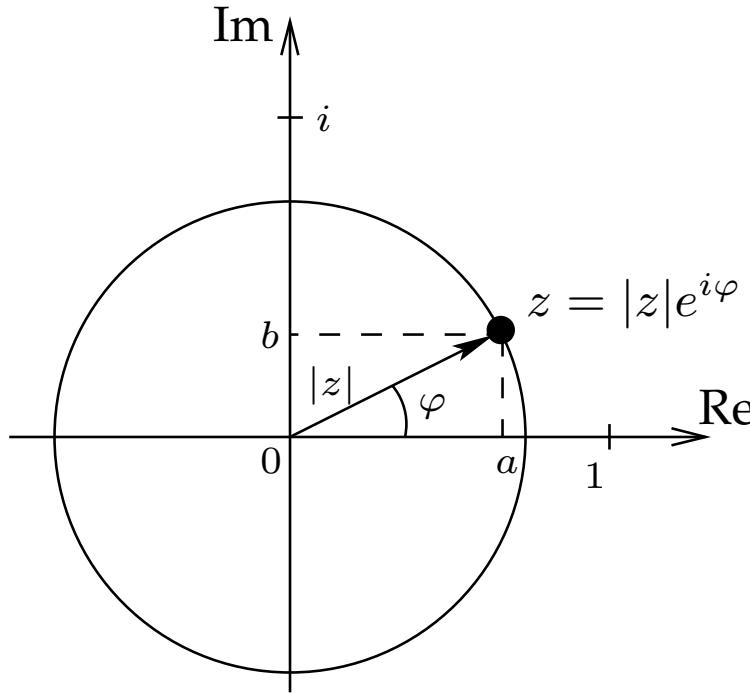
$$\cos x = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 - \cdots + (-1)^k \frac{1}{(2k)!}x^{2k} + \dots$$

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

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

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

KOMPLEKSINIŲ SKAIČIU UŽRAŠYMAS EKSPONENTĖMIS



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

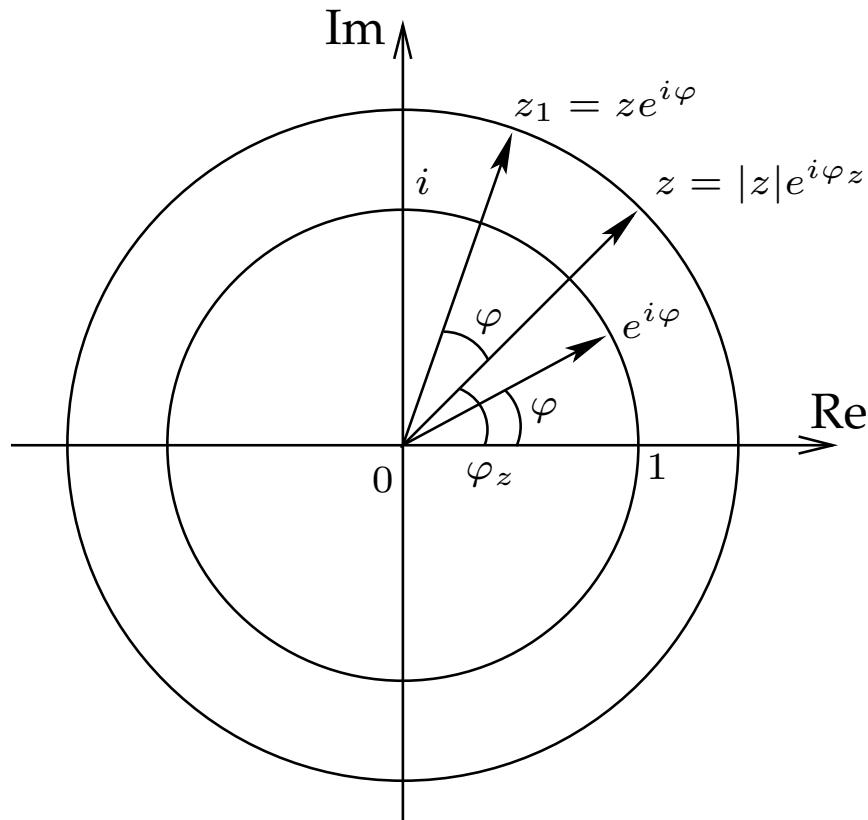
$$z = a + ib = |z| \cos \varphi + i|z| \sin \varphi = |z|(\cos \varphi + i \sin \varphi) = |z|e^{i\varphi}$$

NAUDINGOS EKSPONENČIŲ SAVYBĖS

$$e^a e^b = e^{a+b} \quad (13)$$

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

FAZĒS POSTŪMIS



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

DVIEJŲ EKSPONENČIŲ SUDĒTIS

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

AMPLITUDĒS KVADRATAS

let

$$z = |z|e^{i\varphi}, \quad (17)$$

then

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

BANGOS VAIZDAVIMAS EKSPONENTE

$$E \sin(\mathbf{k}\mathbf{r} - \omega t) = \text{Im}(E e^{i(\mathbf{k}\mathbf{r} - \omega t)}) \quad (19)$$

$$E \sin(\mathbf{k}\mathbf{r} - \omega t - \varphi) = \text{Im}(E e^{i(\mathbf{k}\mathbf{r} - \omega t - \varphi)}) \quad (20)$$

$$= \text{Im}(E e^{-i\varphi} e^{i(\mathbf{k}\mathbf{r} - \omega t)}) \quad (21)$$

$$E_1 \sin(\mathbf{k}\mathbf{r} - \omega t - \varphi_1) +$$

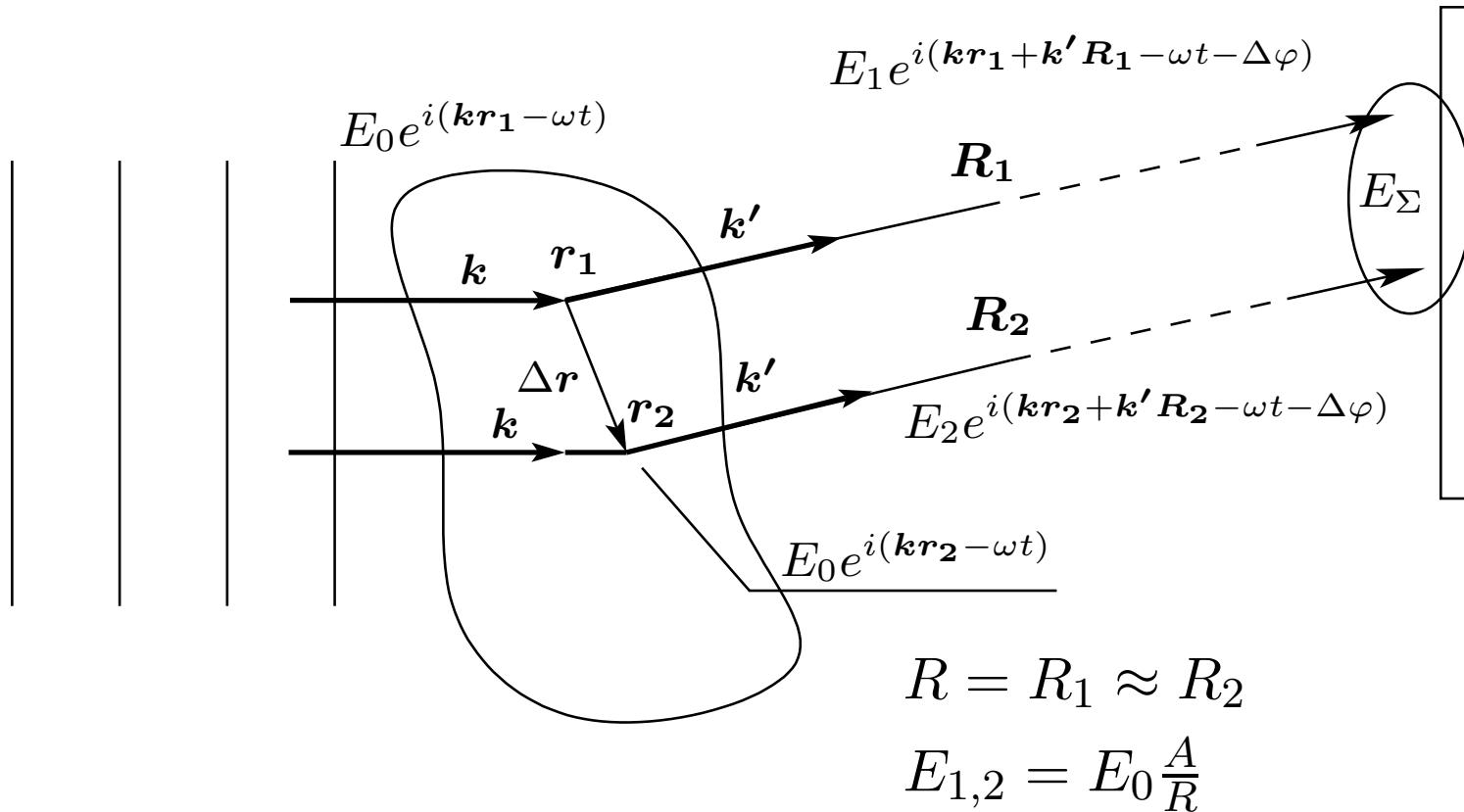
$$E_2 \sin(\mathbf{k}\mathbf{r} - \omega t - \varphi_2) = \text{Im}(E_1 e^{i(\mathbf{k}\mathbf{r} - \omega t - \varphi_1)} + E_2 e^{i(\mathbf{k}\mathbf{r} - \omega t - \varphi_2)})$$

$$= \text{Im}((E_1 e^{-i\varphi_1} + E_2 e^{-i\varphi_2}) e^{i(\mathbf{k}\mathbf{r} - \omega t)}) \quad (22)$$

$$(23)$$

VĖL PAVYZDŽIO SKLAIDYMAS

eksponentinis pavidalas:



$$E_\Sigma = E_1 e^{i(\mathbf{k} \cdot \mathbf{r}_1 + \mathbf{k}' \cdot \mathbf{R}_1 - \omega t - \Delta\varphi)} + E_2 e^{i(\mathbf{k} \cdot \mathbf{r}_2 + \mathbf{k}' \cdot \mathbf{R}_2 - \omega t - \Delta\varphi)} \quad (24)$$

DVIEJŲ MONOCHROMATINIŲ BANGŲ SUDĒTIS

$$\begin{aligned} E_1(\mathbf{R}_1, t) &= E_1 e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1 - \omega t - \Delta\varphi)} \\ &= \underbrace{E_0 \frac{A}{R} e^{-i\Delta\varphi} e^{-i\omega t}}_{\stackrel{\text{def}}{=} E'_0} e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1)} \\ &= E'_0 e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1)} \end{aligned} \tag{25}$$

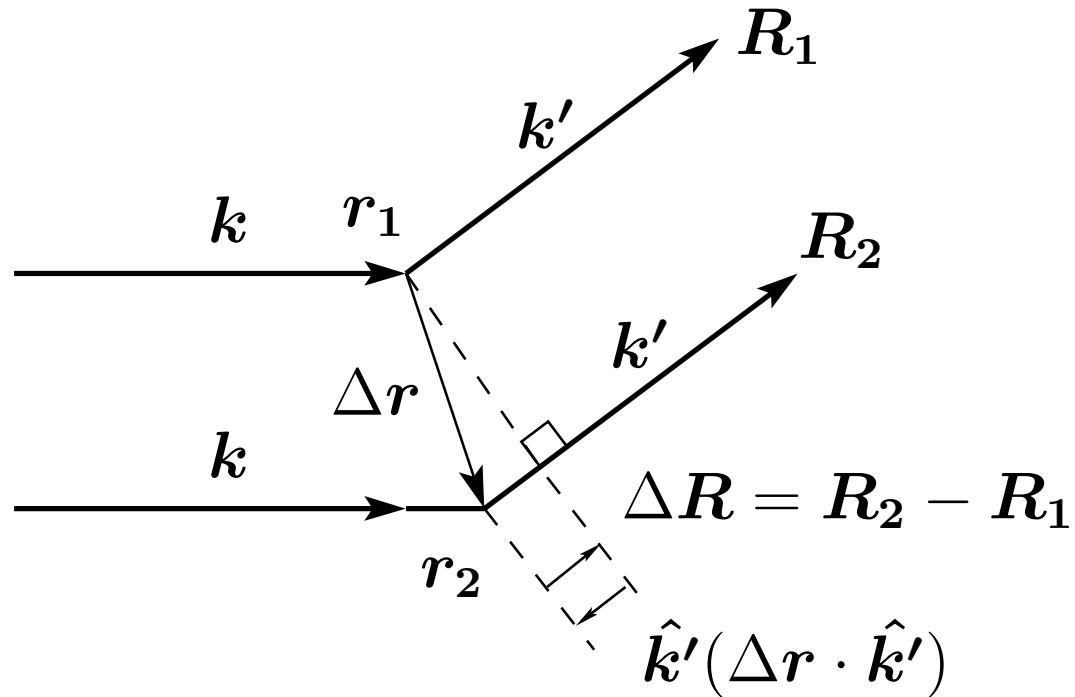
$$E_2(\mathbf{R}_2, t) = E'_0 e^{i(\mathbf{k}\mathbf{r}_2 + \mathbf{k}'\mathbf{R}_2)} \tag{26}$$

$$\begin{aligned} E_\Sigma &= E'_0 e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1)} + E'_0 e^{i(\mathbf{k}\mathbf{r}_2 + \mathbf{k}'\mathbf{R}_2)} \\ &= E'_0 [e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1)} + e^{i(\mathbf{k}\mathbf{r}_2 + \mathbf{k}'\mathbf{R}_2)}] \\ &= E'_0 e^{i(\mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_1)} [1 + e^{i(\mathbf{k}\mathbf{r}_2 - \mathbf{k}\mathbf{r}_1 + \mathbf{k}'\mathbf{R}_2 - \mathbf{k}'\mathbf{R}_1)}] \end{aligned} \tag{27}$$

DVIEJŲ MONOCHROMATINIŲ BANGŲ SUDĖTIS (2)

$$\begin{aligned} E_{\Sigma} &= \underbrace{E'_0 e^{i(\mathbf{k}r_1 + \mathbf{k}'R_1)}}_{=E''_0} [1 + e^{i(\mathbf{k}r_2 - \mathbf{k}r_1 + \mathbf{k}'R_2 - \mathbf{k}'R_1)}] \\ &= E''_0 [1 + e^{i(\mathbf{k}\Delta r + \mathbf{k}'\Delta R)}] \end{aligned} \quad (28)$$

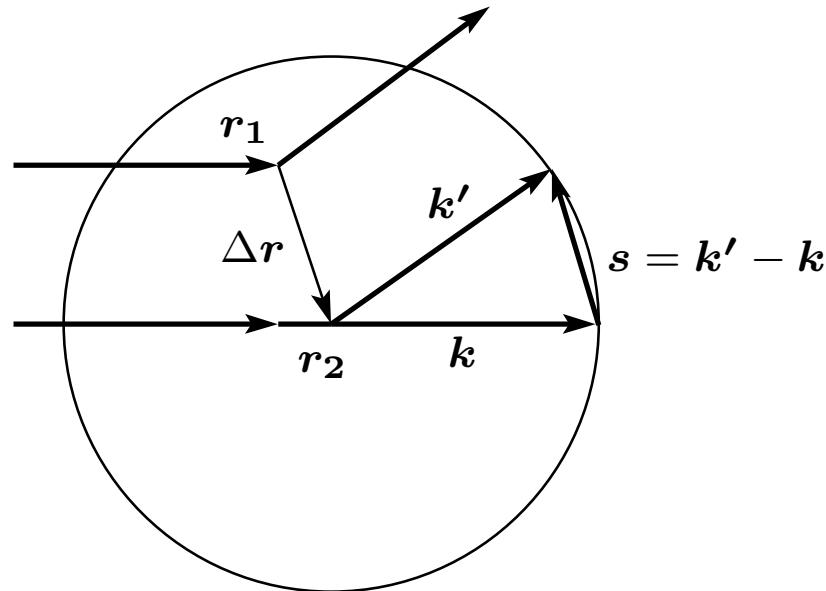
Δr PROJEKCIJA



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

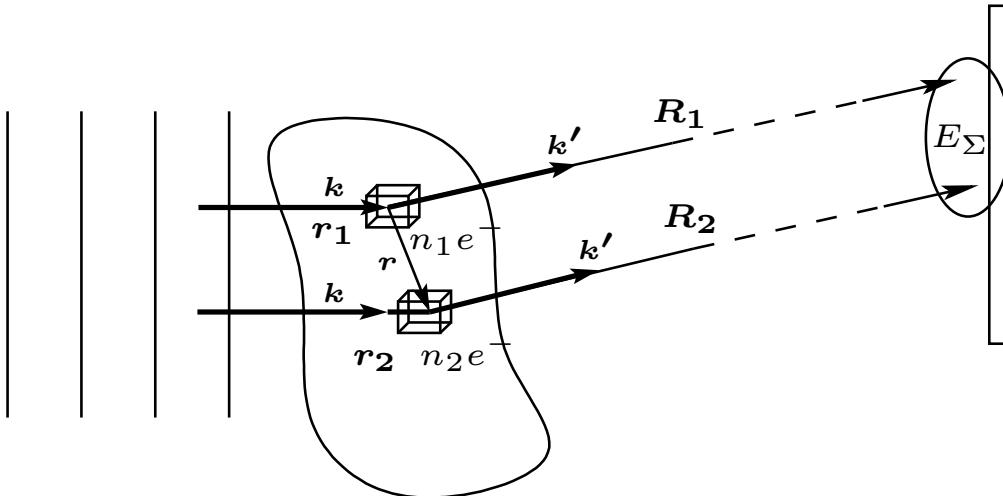
$$k' \Delta R = -k' \cdot \frac{k'}{k'} (\Delta r \cdot \frac{k'}{k'}) = -\frac{(k' \cdot k')}{k'^2} (\Delta r \cdot k') = -k' \Delta r$$

DVIEJŲ MONOCHROMATINIŲ BANGŲ SUDĒTIS (3)



$$\begin{aligned} E_{\Sigma} &= E_0''[1 + e^{i(\mathbf{k}\Delta\mathbf{r}-\mathbf{k}'\Delta\mathbf{r})}] \\ &= E_0''[1 + e^{i(\Delta\mathbf{r}(\mathbf{k}-\mathbf{k}'))}] \\ &= E_0''[1 + e^{i\Delta\mathbf{r}s}] \\ &= E_0''[1 \cdot e^{i\Delta\mathbf{r}_0 s} + e^{i\Delta\mathbf{r}s}] \end{aligned} \tag{29}$$

DVIEJŲ MONOCHROMATINIŲ BANGŲ SUDĒTIS (4)

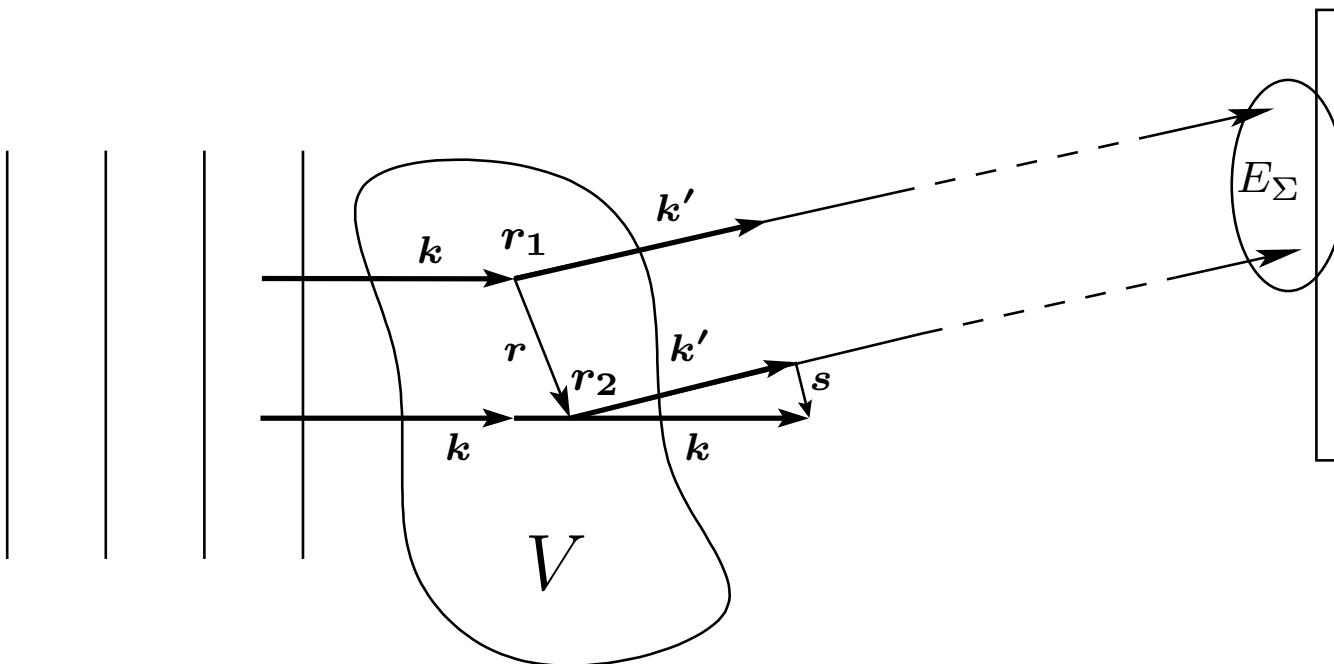


$$E_{1+2} = E_0'' [n_1 e^{i\mathbf{r}_0 s} + n_2 e^{i\mathbf{r}s}]$$

$$E_{\Sigma} = E_0'' \sum_{k=1}^N n_k e^{i\mathbf{r}_k s} \quad (30)$$

$$= E_0'' \sum_{k=1}^N \rho_k \Delta V_k e^{i\mathbf{r}_k s}$$

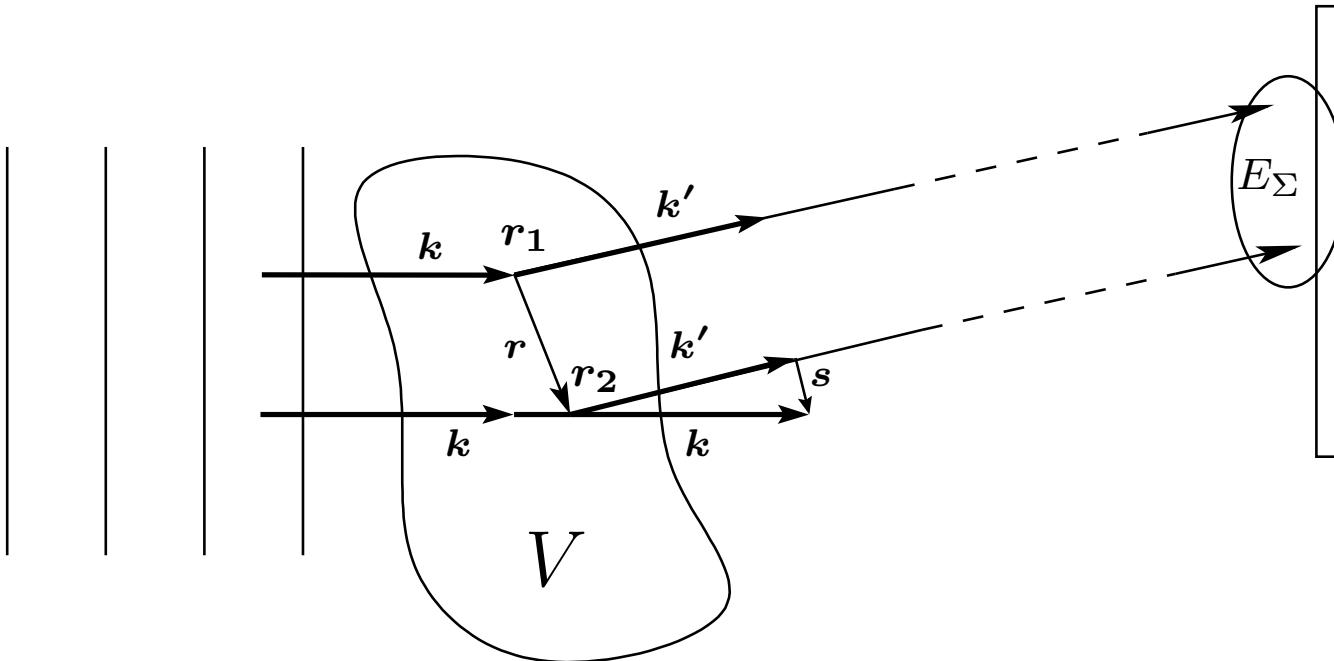
FURJE (FOURIER) TRANSFORMACIJA



$$E_{\Sigma} = \lim_{\substack{N \rightarrow \infty \\ \Delta V_k \rightarrow 0}} E_0'' \sum_{k=1}^N \rho_k \Delta V_k e^{i \mathbf{r}_k \cdot \mathbf{s}} \quad (31)$$

$$= E_0'' \int_V \rho(\mathbf{r}) e^{i \mathbf{r} \cdot \mathbf{s}} dV \quad (32)$$

FURJE TRANSFORMACIJA (2)



$$S = \frac{s}{2\pi} \quad (33)$$

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

STRUKTŪRINIAI FAKTORIAI

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

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

ATVIRKŠTINĖ FURJE TRANSFORMACIJA

let

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

then

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

FURJE TRANSFORMACIJOS SAVYBĖS

- Tiesiškumas

$$\mathcal{F}[\alpha\rho_1 + \beta\rho_2] = \alpha\mathcal{F}[\rho_1] + \beta\mathcal{F}[\rho_2] \quad (39)$$

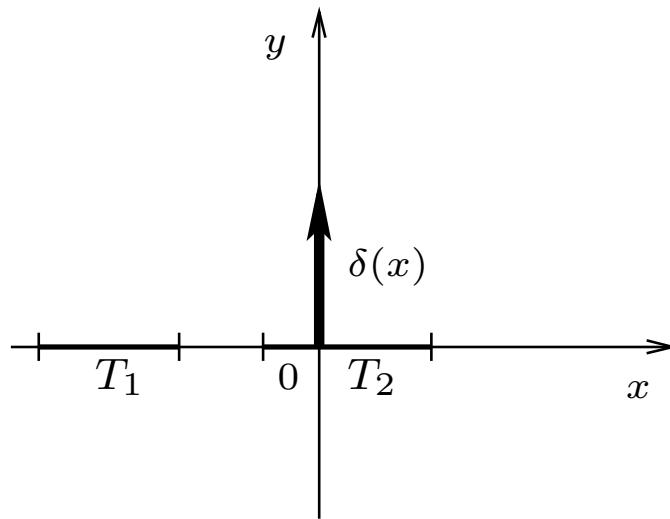
- Postūmis

$$\mathcal{F}[\rho(\mathbf{r} - \Delta\mathbf{r})] = e^{2\pi i(\Delta\mathbf{r}\cdot\mathbf{S})} \mathcal{F}[\rho(\mathbf{r})] \quad (40)$$

- Posūkis

$$\begin{aligned} \mathbf{r}' &= ||R||\mathbf{r} \\ \rho'(\mathbf{r}) &\stackrel{def}{=} \rho(\mathbf{r}') = \rho(||R||\mathbf{r}) \\ \mathcal{F}[\rho(||R||\mathbf{r})] &= F(||R||\mathbf{S}) \end{aligned} \quad (41)$$

DIRAKO (DIRAC) DELTA FUNKCIJA



$$\int_{T_1} \delta(x) f(x) dx \stackrel{\text{def}}{=} 0 \quad (42)$$

$$\int_{T_2} \delta(x) f(x) dx \stackrel{\text{def}}{=} f(0) \quad (43)$$

$$\int_{-\infty}^{+\infty} \delta(x) f(x) dx \stackrel{\text{def}}{=} f(0) \quad (44)$$

DELTA FUNKCIJOS SAVYBĖS

$$\delta(-x) = \delta(x) \quad (45)$$

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

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

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

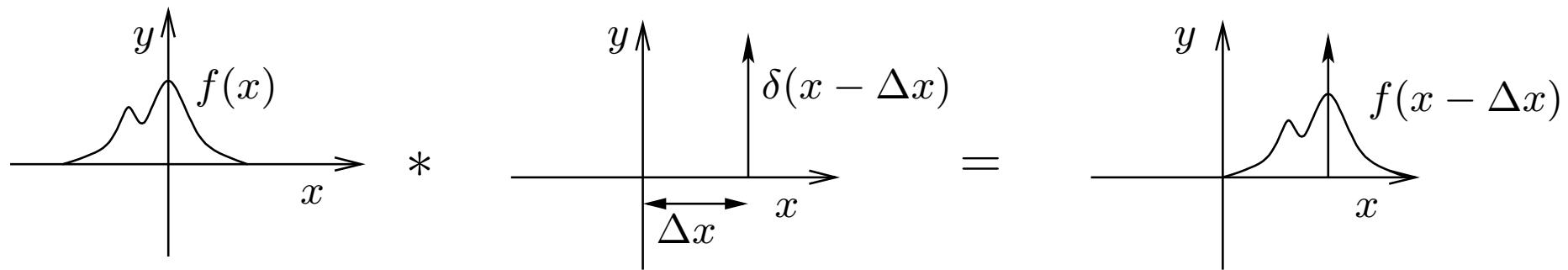
$$\mathcal{F}^{-1}[1] = \int_{-\infty}^{+\infty} e^{-2\pi i x S} dS = \delta(x) \quad (49)$$

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

KONVOLIUCIJA (SĄSŪKA)

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

KONVOLICIJA SU DELTA FUNKCIJA



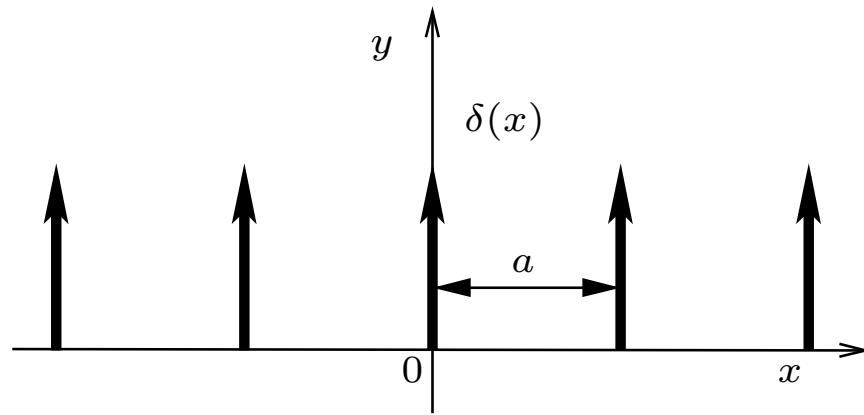
$$f(x) * \delta(x - \Delta x) = \int_{-\infty}^{+\infty} f(v)\delta(x - v - \Delta x)dv = f(x - \Delta x) \quad (52)$$

KONVOLIUCIJOS FURJE TRANSFORMACIJA

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

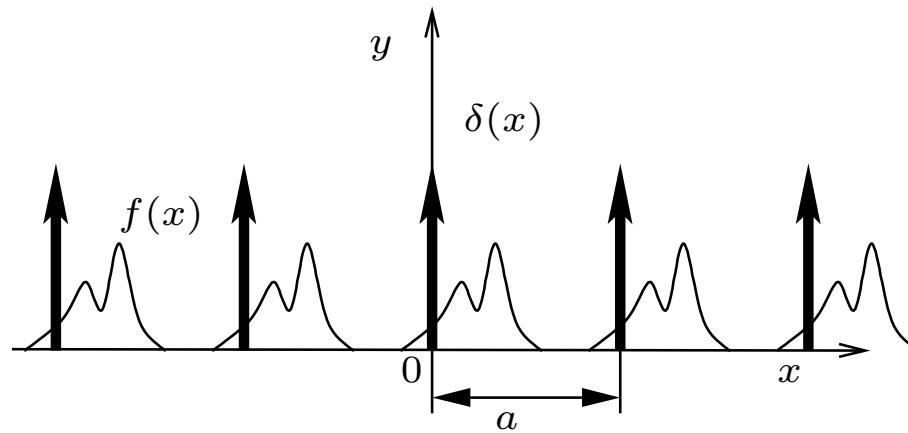
$$= \mathcal{F}[f] \cdot \mathcal{F}[g] \tag{54}$$

GARDELĒS FUNKCIJA



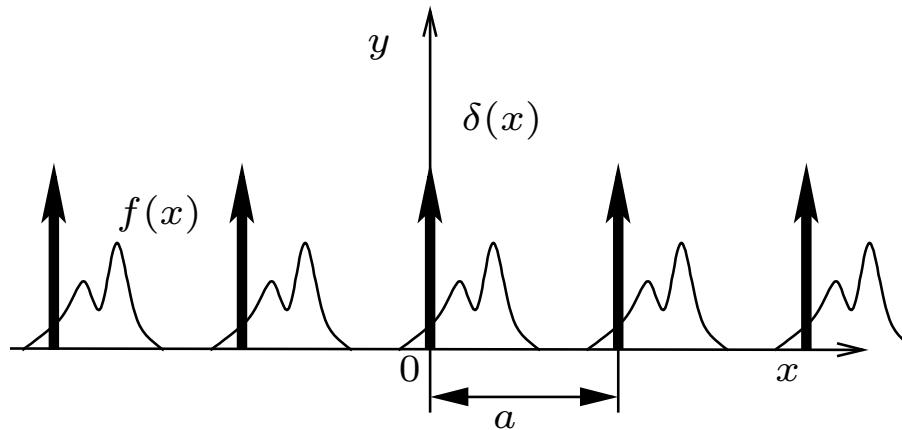
$$L(x) = \sum_{n=-\infty}^{+\infty} \delta(x - an) \quad (55)$$

KRISTALO APRAŠYMAS



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

KRISTALO EL. TANKIO FURJE TRANSFORMACIJA



$$\mathcal{F}[f * L] = \mathcal{F}[f] \cdot \mathcal{F}[L] \quad (57)$$

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

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

KRISTALO EL. TANKIO FURJE TRANSFORMACIJA (2)

$$\mathcal{F}[f * L] = \mathcal{F}[f] \cdot \mathcal{F}[L] \quad (60)$$

$$= F(S) \cdot \mathcal{F}[L] \quad (61)$$

$$= \mathcal{F}\left[\sum_{n=-\infty}^{+\infty} f(x - an)\right] \quad (62)$$

$$= \sum_{n=-\infty}^{+\infty} \mathcal{F}[f(x - an)] \quad (63)$$

$$= \sum_{n=-\infty}^{+\infty} F(S) e^{2\pi i S a n} \quad (64)$$

$$= F(S) \sum_{n=-\infty}^{+\infty} e^{2\pi i S a n} \quad (65)$$

KRISTALO EL. TANKIO FURJE TRANSFORMACIJA (3)

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

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

$$c_n = \frac{1}{a} \int_{-a/2}^{a/2} S(x) e^{2\pi i \cdot n \frac{x}{a}} dx \quad (68)$$

$$= \frac{1}{a} \int_{-a/2}^{a/2} \sum_{n=-\infty}^{\infty} f(x - an) e^{2\pi i \cdot n \frac{x}{a}} dx \quad (69)$$

$$= \frac{1}{a} \sum_{n=-\infty}^{\infty} \int_{-a/2}^{a/2} f(x - an) e^{2\pi i \cdot n \frac{x}{a}} dx \quad (70)$$

$$= \frac{1}{a} \int_{-\infty}^{\infty} f(x) e^{2\pi i \cdot x \frac{n}{a}} dx \quad (71)$$

$$= \frac{1}{a} F(n/a) \quad (72)$$

KRISTALO EL. TANKIO FURJE TRANSFORMACIJA (4)

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

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

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

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

GARDELĖS FURJE TRANSFORMACIJA

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

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

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

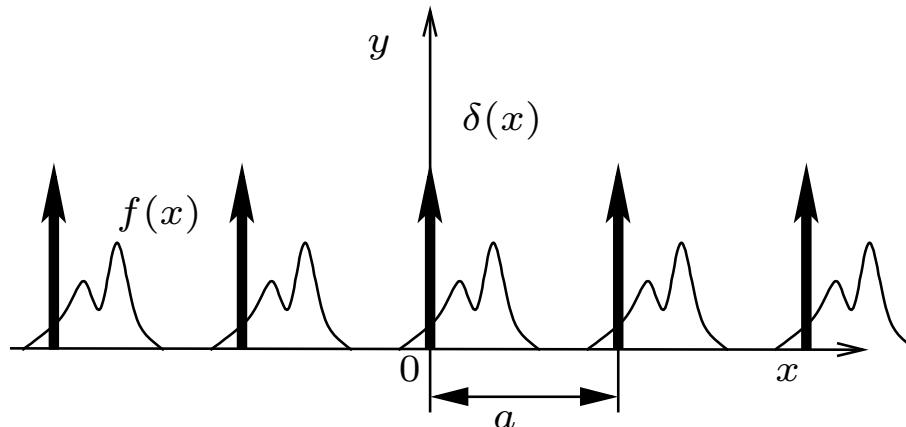
$$= \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta(x - an) e^{2\pi i x S} dx \quad (80)$$

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

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

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

ATVIRKŠTINĖ GARDELĖ, VIENMATĖ



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

$$\mathcal{F}[f * L] = \mathcal{F}[f] \cdot \mathcal{F}[L] \quad (85)$$

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

ATVIRKŠTINĖ GARDELĖ, TRIMATĖ

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

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

$$\mathbf{a}^* = \frac{[\mathbf{b} \times \mathbf{c}]}{V}, \quad \mathbf{b}^* = \frac{[\mathbf{c} \times \mathbf{a}]}{V}, \quad \mathbf{c}^* = \frac{[\mathbf{a} \times \mathbf{b}]}{V} \quad (89)$$

$$V = (\mathbf{a} \cdot [\mathbf{b} \times \mathbf{c}]) \quad (90)$$

LAUĖS (LAUE) SĄLYGOS

$$\mathcal{F}[\rho_{crys}] = \mathcal{F}[\rho * L] = \mathcal{F}[\rho] \cdot \mathcal{F}[L] \quad (91)$$

$$= F(\mathbf{S}) \cdot L^*(\mathbf{S}) \quad (92)$$

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

Matome, kad periodinio kristalo Furje transformacija nelygi nuliui tik tam tikroms vektoriaus \mathbf{S} reikšmėms

$$(\mathbf{S} \cdot \mathbf{a}) = h, \quad (\mathbf{S} \cdot \mathbf{b}) = k, \quad (\mathbf{S} \cdot \mathbf{c}) = l \quad (94)$$

$$h, k, l \in \mathbb{Z} \quad (95)$$

EVALDO (EWALD) KONSTRUKCIJA IR EVALDO SFERA

