Rozptylová funkce

Difrakce na apertuře (apertura v blízkosti optické osy)

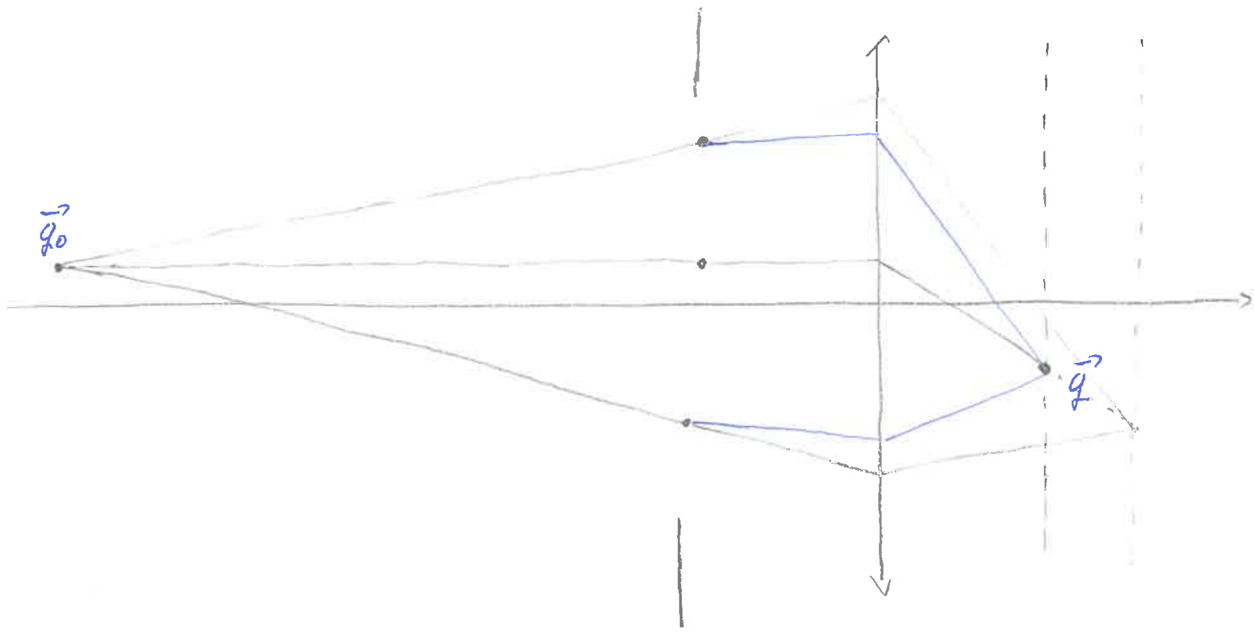
$$\psi = -ib(z) \iint_A \psi(x,y)\, e^{\frac{i}{k} S(\vec{r}, \vec{r}')} \, dx\, dy$$

V případě, že máme bodový zdroj, šíří se z něj kulová vlna, která difraktuje na apertuře. V tomto případě můžeme pro vlnovou funkci v apertuře psát

$$\psi(\vec{r}_a) \propto e^{\frac{i}{k} S(\vec{r}_0, \vec{r}_a)}$$

a pro vlnovou funkci za aperturou:

$$\psi \propto \iint_A e^{\frac{i}{k}(S(\vec{q}_0, \vec{q}_a) + S(\vec{q}_a, \vec{q}))} \, d^2\vec{q}_a$$



Rozptylová funkce - paraxiální aproximace

$\vec q$ - souřadnice v rovině obrazu

$$S(\vec q_0,\vec q_a)+S(\vec q_a,\vec q)\approx S^{(2)}(\vec q_0,\vec q_a)+S^{(2)}(\vec q_a,\vec q)$$

$$S^{(2)}(\vec q_0,\vec q_a)=\sqrt{2me}\int_{z_0}^{z_a}\left(-\frac{\Phi''+\eta^2B^2}{8\Phi^{*1/2}}\,q^{(1)2}(q_0,q_a,z)+\frac12\Phi^{*1/2}q^{(1)\prime 2}(\vec q_0,\vec q_a,z)\right)dz$$

$$=\sqrt{2me}\int_{z_0}^{z_a}\frac12\frac{d}{dz}\left(\Phi^{*1/2}q^{(1)\prime}(\vec q_0,\vec q_a,z)\,q^{(1)}(\vec q_0,\vec q_a,z)\right)=\sqrt{2me}\,\frac12\left[\Phi^{*1/2}q^{(1)\prime}(\vec q_0,\vec q_a,z)\,q^{(1)}(\vec q_0,\vec q_a,z)\right]_{z_0}^{z_a}$$

$$=\frac12\sqrt{2me}\left(\Phi_a^{*1/2}q^{(1)\prime}(q_0,q_a,z_a)\,\vec q_a-\Phi_0^{*1/2}q^{(1)\prime}(\vec q_0,\vec q_a,z_0)\,\vec q_0\right)=$$

$q^{(1)}(\vec q_0,\vec q_a,z)=\vec q_0\,s(z)+\vec q_a\,t(z)$; $s(z_0)=1$, $s(z_a)=0$, $t(z_0)=0$, $t(z_a)=1$; $\Rightarrow q^{(1)}(q_0,q_a,z_a)=$

$$=\frac12 g_a(\vec q_0 s_a'+\vec q_a t_a')\vec q_a-\frac12 g_0(\vec q_0 s_0'+\vec q_a t_0')\vec q_0=$$

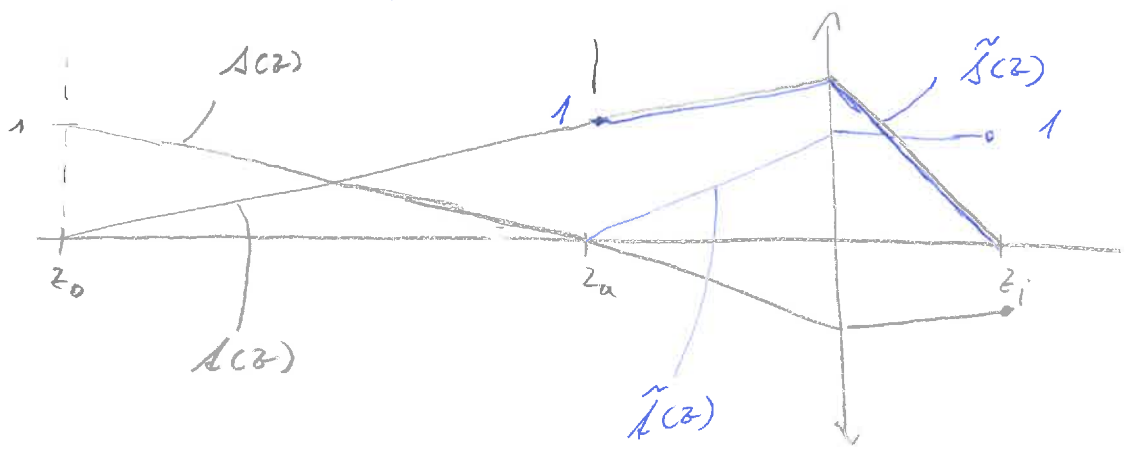
$$=\frac12 g_a t_a'\vec q_a^{\,2}+\frac12(g_a s_a'-g_0t_0')\vec q_0\vec q_a-\frac12 g_0 s_0'\vec q_0^{\,2}=$$

$$g_0(\underset{1}{s_0}t_0'-\overset{0}{t_0}s_0')=g_a(\overset{0}{s_a}t_a'-\underset{1}{t_a}s_a')\Rightarrow \underline{g_0t_0'=-g_as_a'}$$

$$=\frac12 g_a t_a'\vec q_a^{\,2}-g_0t_0'\vec q_0\vec q_a-\frac12 g_0 s_0'\vec q_0^{\,2}$$

$$S^{(2)}(\vec q_a,\vec q)=\frac12\sqrt{2me}\left(\Phi_i^{*1/2}\vec q^{(1)\prime}(q_a,\vec q,z_i)\,\vec q-\Phi_a^{*1/2}\vec q^{(1)\prime}(\vec q_0,\vec q_a,z_a)\,\vec q_a\right)=$$

$q^{(1)}(\vec q_a,\vec q,z)=\tilde s(z)\vec q_a+\tilde t(z)\vec q$: $\tilde s(z_a)=1$, $\tilde s(z_i)=0$, $\tilde t(z_a)=0$, $\tilde t(z_i)=1$



$\tilde s(z)=t(z)$

$\tilde t(z)=\frac{s(z)}{s(z_i)}$

$$=\frac12 g_i\tilde t_i'\vec q^{\,2}-g_a\tilde t_a'\vec q_a\vec q-\frac12 g_a\tilde s_a'\vec q_a^{\,2}=\frac12 g_i\frac{s_i'}{s_i}\vec q^{\,2}-g_a\frac{s_a'}{s_i}\vec q_a\vec q-\frac12 g_a t_a'\vec q_a^{\,2}$$

$$S^{(2)}(\vec{q}_o,\vec{q}_a) + S^{(2)}(q_a,\vec{q}) = -\frac{1}{2} g_o s_o' \vec{q}_o^{\,2} - g_o t_o' \vec{q}_o \vec{q}_a - g_a \frac{s_a'}{M}\vec{q}_a\vec{q} + \frac{1}{2} g_i \frac{s_i'}{M}\vec{q}^{\,2}$$

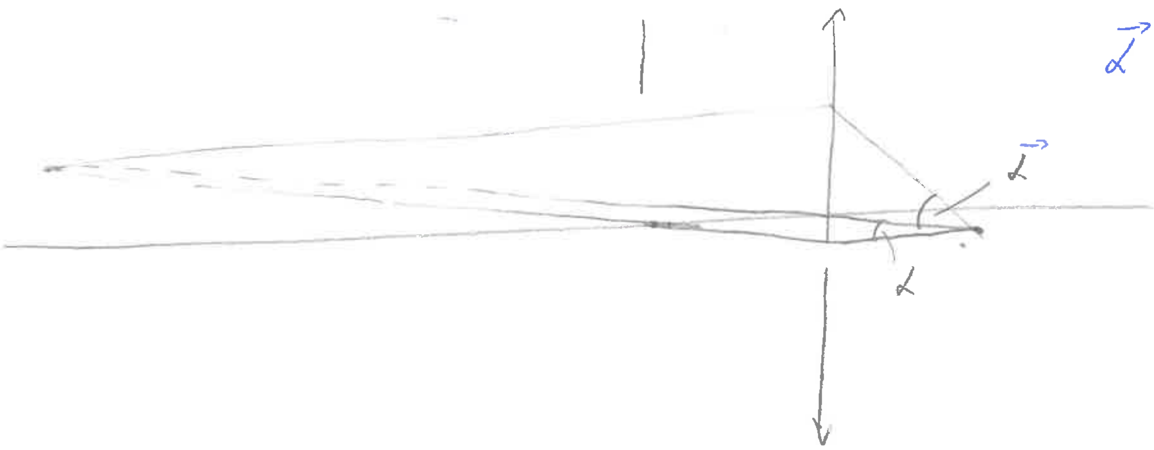
$$g_o(\underset{1}{s_o} t_o' - \underset{0}{t_o s_o'}) = g_i(\underset{M}{s_i} t_i' - \underset{0}{t_i s_i'}) \Rightarrow g_o t_o' = g_i M t_i'$$

$$g_a(\underset{0}{s_a t_a'} - s_a' \underset{1}{t_a}) = g_i(\underset{M}{s_i} t_i' - t_i \underset{0}{s_i'}) \Rightarrow g_a s_a' = M g_i t_i'$$

$$= -\frac{1}{2} g_o s_o' \vec{q}_o^{\,2} + g_i t_i' \vec{q}_a(\vec{q} - M\vec{q}_o) + \frac{1}{2} g_i \frac{s_i'}{M}\vec{q}^{\,2}$$

$$\psi \propto e^{-\frac{i}{k} g_o s_o' \vec{q}_o^{\,2}}\, e^{\frac{i}{k} g_i \frac{s_i'}{M}\vec{q}^{\,2}} \int_{Ap} e^{\frac{i}{k} g_i t_i' \vec{q}_a(\vec{q}-M\vec{q}_o)}\, d^2\vec{q}_a$$

$\vec{\alpha} = t_i' \vec{q}_a$



$$\psi \propto A \int_{Ap\,Ang} e^{\frac{i}{k} g_i \vec{\alpha}(\vec{q}-M\vec{q}_o)}\, d^2\vec{\alpha} = \iint A(\vec{\alpha})\, e^{\frac{2\pi i}{\lambda}\vec{\alpha}(\vec{q}-M\vec{q}_o)}$$

Fourierova transf. apertурní fce

Osově symetrická aperturní fce $A(\vec{\alpha}) = A(|\vec{\alpha}|) = A(\alpha)$

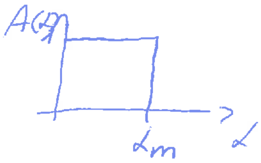
označíme $(\vec{q} - M\vec{q}_o) = \vec{d}$ – odchylka od paraxiálního obrazu

$$\vec{\alpha}\cdot\vec{d} = \alpha d(\cos\phi_1\cos\phi_2 + \sin\phi_1\sin\phi_2) = \alpha d\cos(\phi_1+\phi_2)$$

$$\psi \propto \iint A(\alpha)\, e^{\frac{2\pi i}{\lambda}\alpha d\cos(\phi_1+\phi_2)}\,\alpha\, d\phi_1\, d\alpha = \int A(\alpha)\alpha \int e^{\frac{2\pi i}{\lambda}\alpha d\sin(\phi_1+\phi_2+\frac{\pi}{2})}\, d\phi_1\, d\alpha$$

$$= \int A(\alpha)\,\alpha\, J_0\left(\frac{2\pi}{\lambda} d\alpha\right) d\alpha$$

Kruhová clona



$$\psi \propto \int_0^{\alpha_m} J_0\left(\frac{2\pi}{\lambda}\alpha d\right)\alpha\, d\alpha \quad \left| \begin{array}{l} x = \frac{2\pi}{\lambda}\alpha d \\ dx = \frac{2\pi}{\lambda} d\, d\alpha \\ \alpha = \frac{\lambda}{2\pi d} \\ \alpha\, d\alpha = \left(\frac{\lambda}{2\pi d}\right)^2 x\, dx \end{array} \right| = \int_0^{\frac{2\pi}{\lambda}\alpha_m d} J(x) \left(\frac{\lambda}{2\pi d}\right) x\, dx$$

$$= \left[x J_1(x) \left(\frac{\lambda}{2\pi d}\right)^2 \right]_0^{\frac{2\pi}{\lambda}\alpha_m d}$$

$$\frac{d}{dx}\left(x J_1(x)\right) = x J_0(x)$$

$$\psi \propto \frac{\lambda}{2\pi d}\alpha_m J_1\left(\frac{2\pi}{\lambda}\alpha_m d\right)$$

$$\rho = |\psi|^2 \sim \left| \frac{J_1\left(\frac{2\pi}{\lambda}\alpha_m d\right)}{\frac{2\pi}{\lambda}\alpha_m d} \right|^2$$

Efekt aberací na rozptylovou funkci

$$\psi \propto \iint_{Ap.Ang} e^{-\frac{i}{\hbar} g_i \chi(\vec{q}_0, \vec{q}_i')} e^{\frac{i}{\hbar} g_i \vec{q}_i' \vec{d}} \, d^2\vec{q}_i' =$$

$$= \iint A(\vec{\alpha}) \, e^{\frac{2\pi i}{\lambda} \chi(\vec{q}_0, \vec{\alpha})} e^{\frac{2\pi i}{\lambda} \vec{\alpha}\vec{d}} \, d^2\vec{\alpha}$$

$\chi(\vec{q}_0, \vec{\alpha})$ – deviace vlnoplochy

$$\Delta q_i = \frac{\partial \chi}{\partial \vec{\alpha}}$$

Dále přejdeme do komplexních souřadnic $w = x + iy$, $\alpha = \alpha_x + i\alpha_y$

$$\Delta w_i = 2 \frac{\partial \chi}{\partial \bar{\alpha}}$$

<u>aberace 3. řádu:</u> parametrizace pomocí pr. polohy a směrnice v obraze (odchylky o centr. traj.)

$$\Delta w_i = C_1 \alpha + C_3 \alpha^2 \bar{\alpha} + K_3 \alpha \bar{\alpha} w_i + K_3 \alpha^2 w_i + F_3 \alpha w_i \bar{w}_i + A_{3f} \bar{\alpha} w_i^2 + D_3 w_i^2 \bar{w}_i$$

$$\chi = \mathrm{Re}\left\{ \frac{1}{2} C_1 \alpha\bar{\alpha} + \frac{1}{4} C_3 (\alpha\bar{\alpha})^2 + \frac{1}{2} K_3 \alpha \bar{\alpha}^2 w_i + F_3 \alpha\bar{\alpha} w_i \bar{w}_i + A_{3f} \bar{\alpha}^2 w_i^2 + D_3 \bar{\alpha} w_i^2 \bar{w}_i \right\}$$

Osové aberace (osově nesymetrické)

$$\Delta w_i = A_0 + C_1 \alpha + A_1 \bar{\alpha} + B_2 \alpha^2 + 2\bar{B}_2 \alpha\bar{\alpha} + A_2 \bar{\alpha}^2 + C_3 \alpha^2 \bar{\alpha} + S_3 \alpha^3 + 3\bar{S}_3 \alpha \bar{\alpha}^2 + A_3 \bar{\alpha}^3 + \dots$$

$$\chi = \mathrm{Re}\left\{ A_0 \bar{\alpha} + \frac{1}{2} C_1 \alpha\bar{\alpha} + \frac{1}{2} A_1 \bar{\alpha}^2 + B_2 \alpha^2 \bar{\alpha} + \frac{1}{3} A_2 \bar{\alpha}^3 + \frac{1}{4} C_3 (\alpha\bar{\alpha})^2 + S_3 \alpha^3 \bar{\alpha} + \frac{1}{4} A_3 \bar{\alpha}^4 \right\}$$

Pokud má svazek nenulovou šířku

$$\Delta w_i = A_0 - C_{c0}\,\mathcal{K} + (C_1 - C_{c1}\mathcal{K} + C_{c2}\mathcal{K}^2)\alpha + (A_1 + A_{1c}\mathcal{K})\bar{\omega} + \dots$$

$\mathcal{K} = \frac{\Delta E}{E}$ - relativní deviace energie

vztahy jsou pak stejné jen je nutné změnit koef. na

$$A_0 \rightarrow A_0 - C_{c0}\,\mathcal{K}$$

$$C_1 \rightarrow C_1 - C_{c1}\,\mathcal{K} - C_{c2}\,\mathcal{K}^2$$

$$A_1 \rightarrow A_1 - A_{1c}\,\mathcal{K}$$

$$\vdots$$

Lze předpokládat, že dvě vlnové funkce o různých en. jsou nekoherentní výsledná intenzita vznikne integrací přes energiové spektrum ...

$$\rho(\vec{q}) = \int \rho(\vec{q}, \mathcal{K}) \cdot \rho(E)\, dE$$

- $\rho(\vec{q})$ – nekoherentní rozptylová funkce
- $\rho(\vec{q}, \mathcal{K})$ – intenzita vlnové fce pro dané $\mathcal{K}$ – koherentní rozptylová funkce
- $\rho(E)$ – energiové ~~~~ spektrum zdroje

– časová nekoherence

Velikost stopy svazku

Je nutné ještě uvažovat nenulovou velikost zdroje – – prostorová nekoherence

$$\rho(\vec{q}) = \iint \rho_{PSF}(\vec{q}, \vec{q}_0)\, \rho(\vec{q}_0)$$

$\rho(\vec{q}_0)$ – rozložení na zdroji elektronů