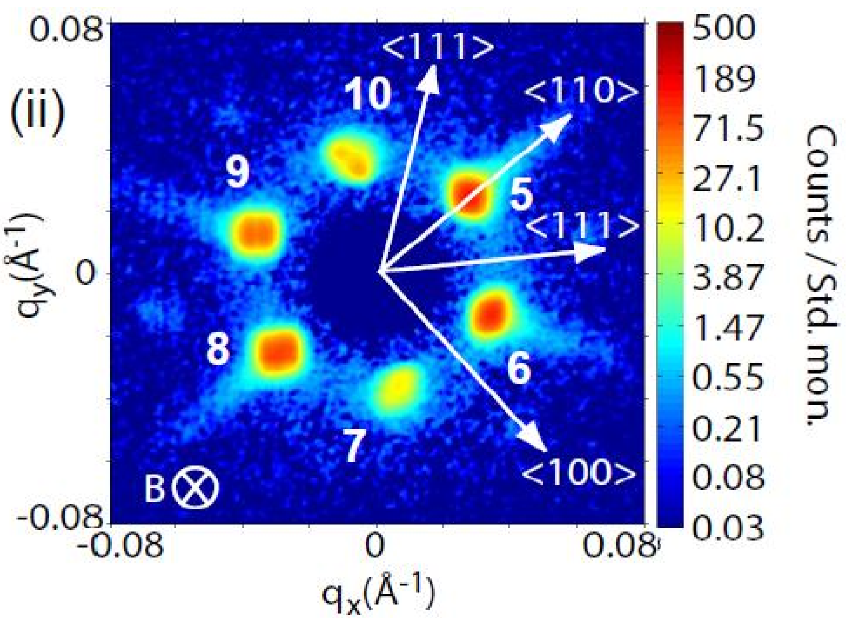
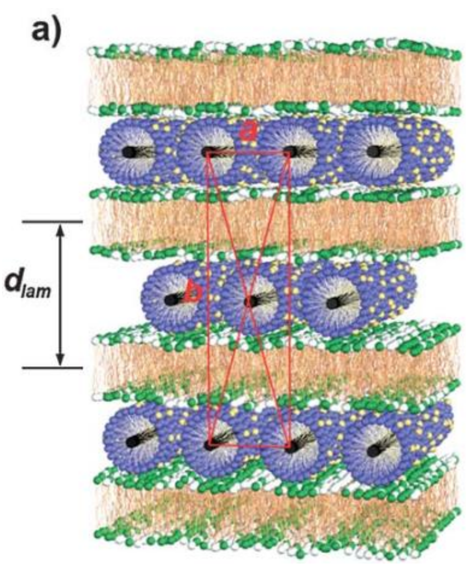
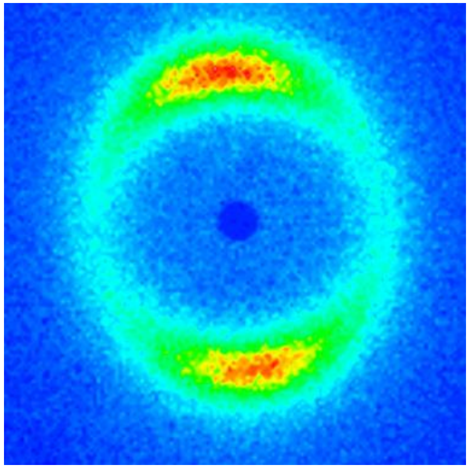
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons II, SS 2016



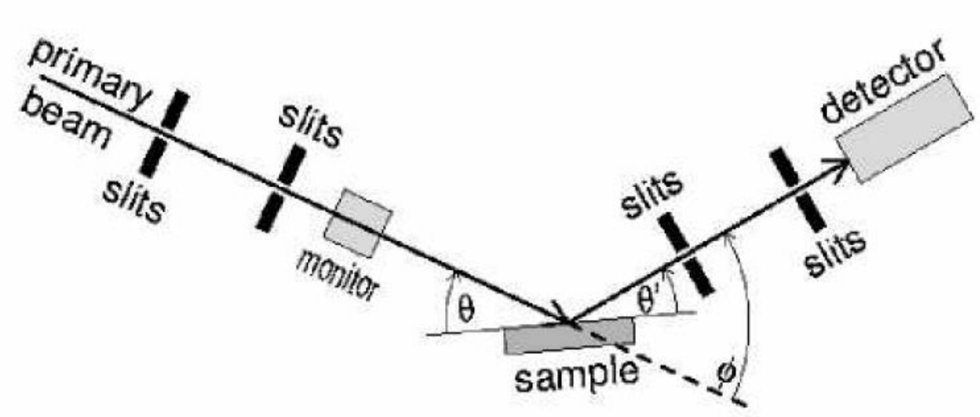




Lecture 4, 23.5.2016

Reflectometry

Basic geometry & layout



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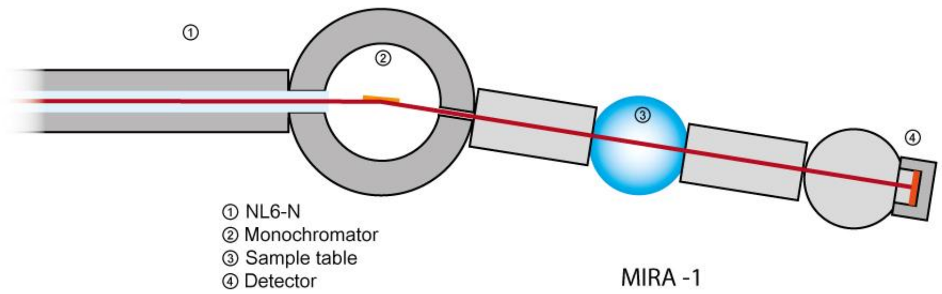
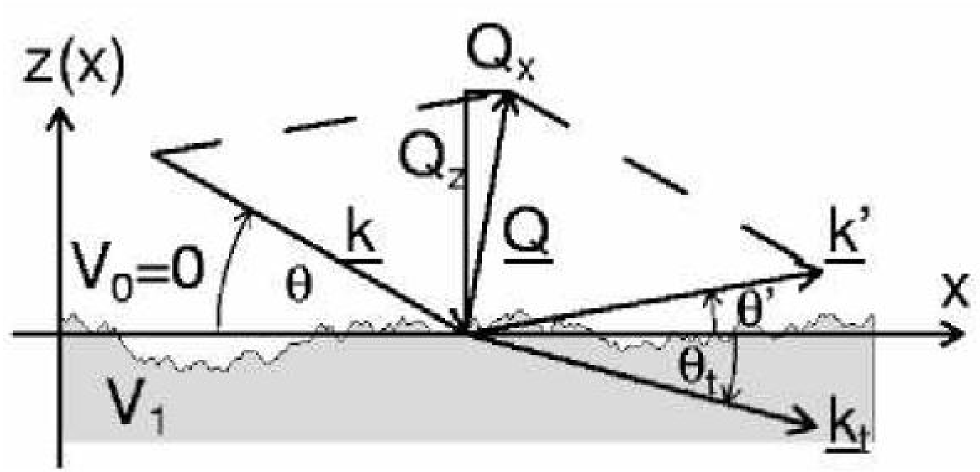
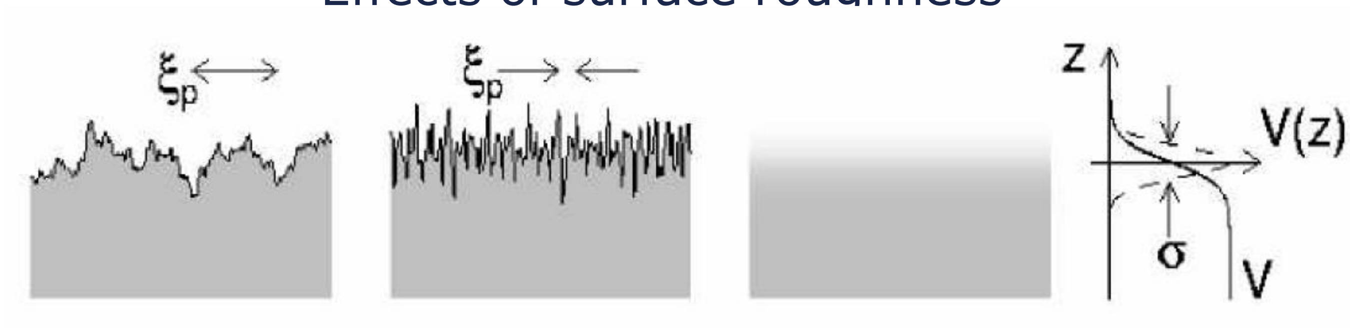




Reflectometry

Specular reflectivity in Born approximation Θ=Θ`

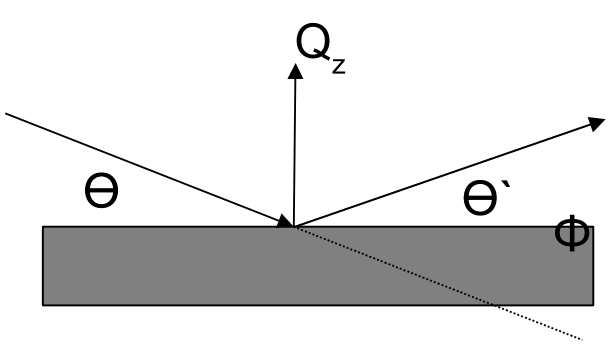
Effects of surface roughness

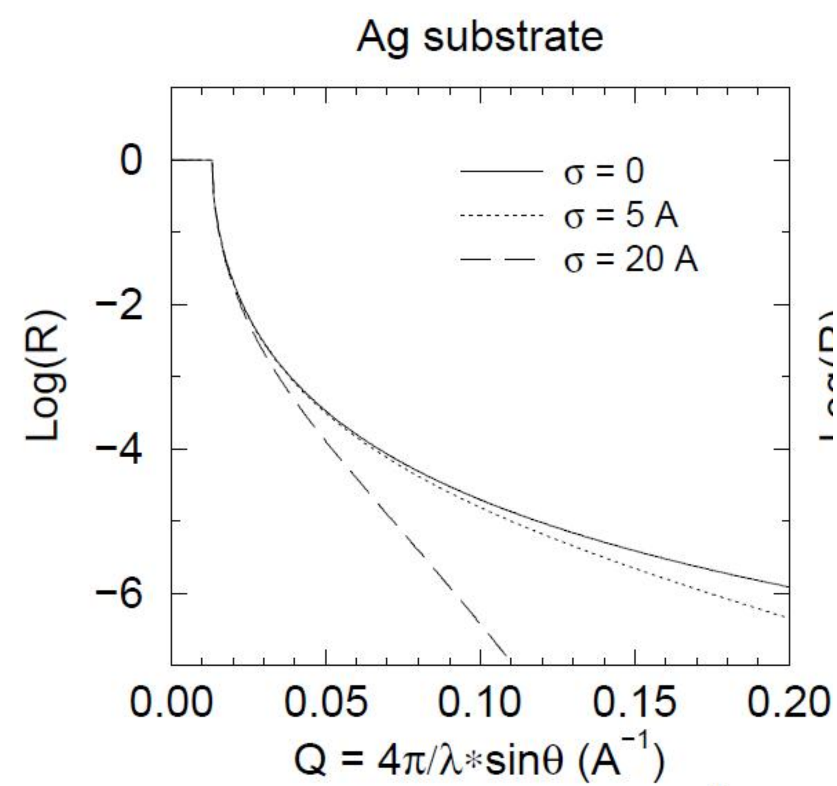


Reflectivity of a single, infinite layer

$$V(z) = \frac{2\pi\hbar^2 b\rho}{m_n}\left(\frac{1}{2} - \frac{1}{2}\Theta(z)\right) = \begin{cases} 0 & : \quad z > 0 \\ 2\pi\hbar^2 b\rho / m_n & : \quad z \leq 0 \end{cases}$$

$$I(Q_z) \sim \frac{1}{Q_z^4}\left|\int \frac{\mathrm{d}V(z)}{\mathrm{d}z} \exp(-iQ_z z)\mathrm{d}z\right|^2$$



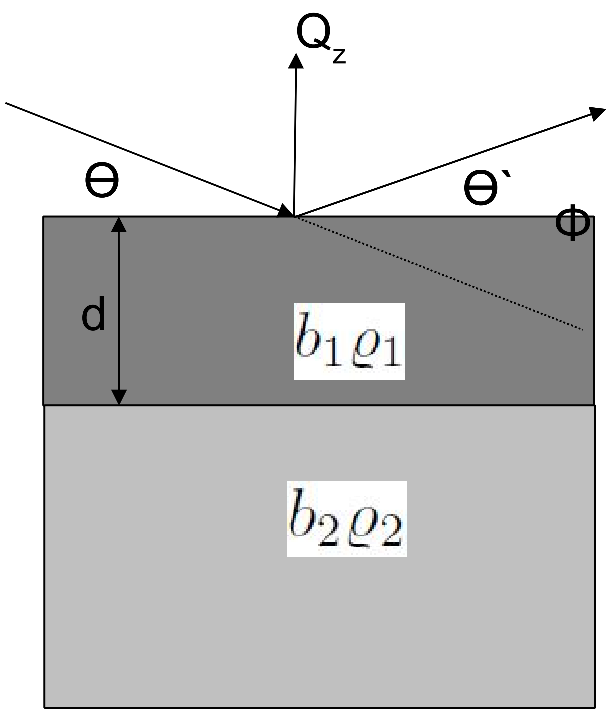


Reflectometry

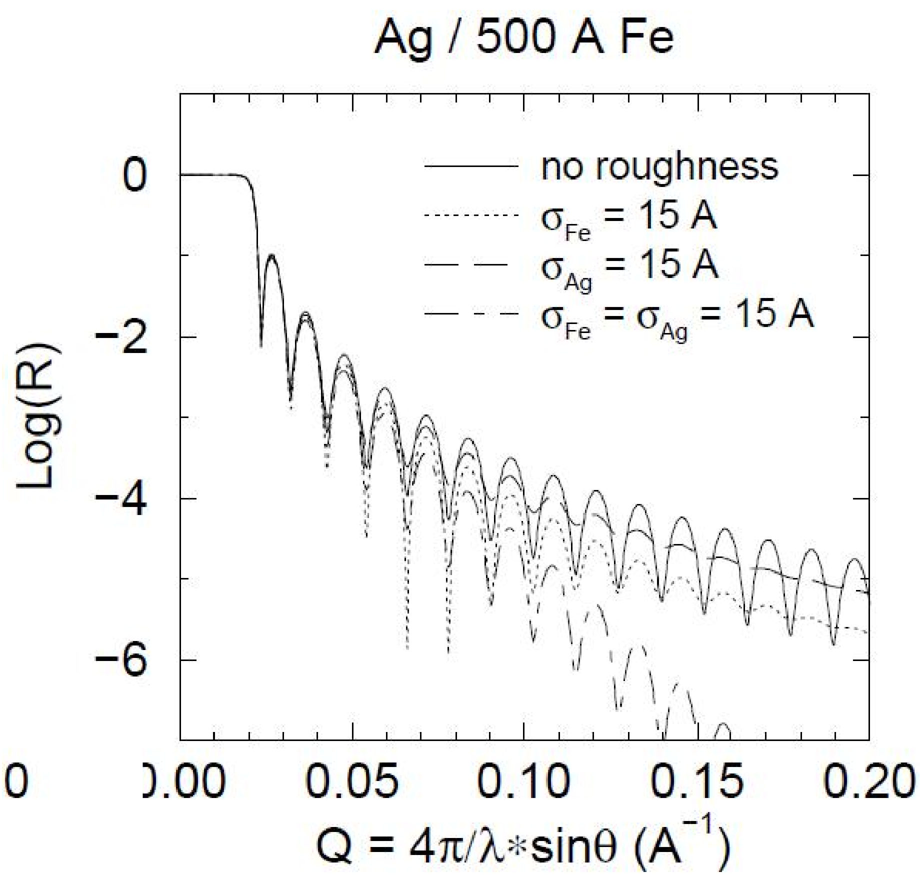
Specular reflectivity in Born approximation ϴ=ϴ`

$$I(Q_z) \approx \frac{1}{Q_z^4}\left[(b_2\varrho_2 - b_1\varrho_1)^2 + (b_1\varrho_1)^2 + 2(b_2\varrho_2 - b_1\varrho_1)(b_1\varrho_1)\cos(Q_z d)\right]$$

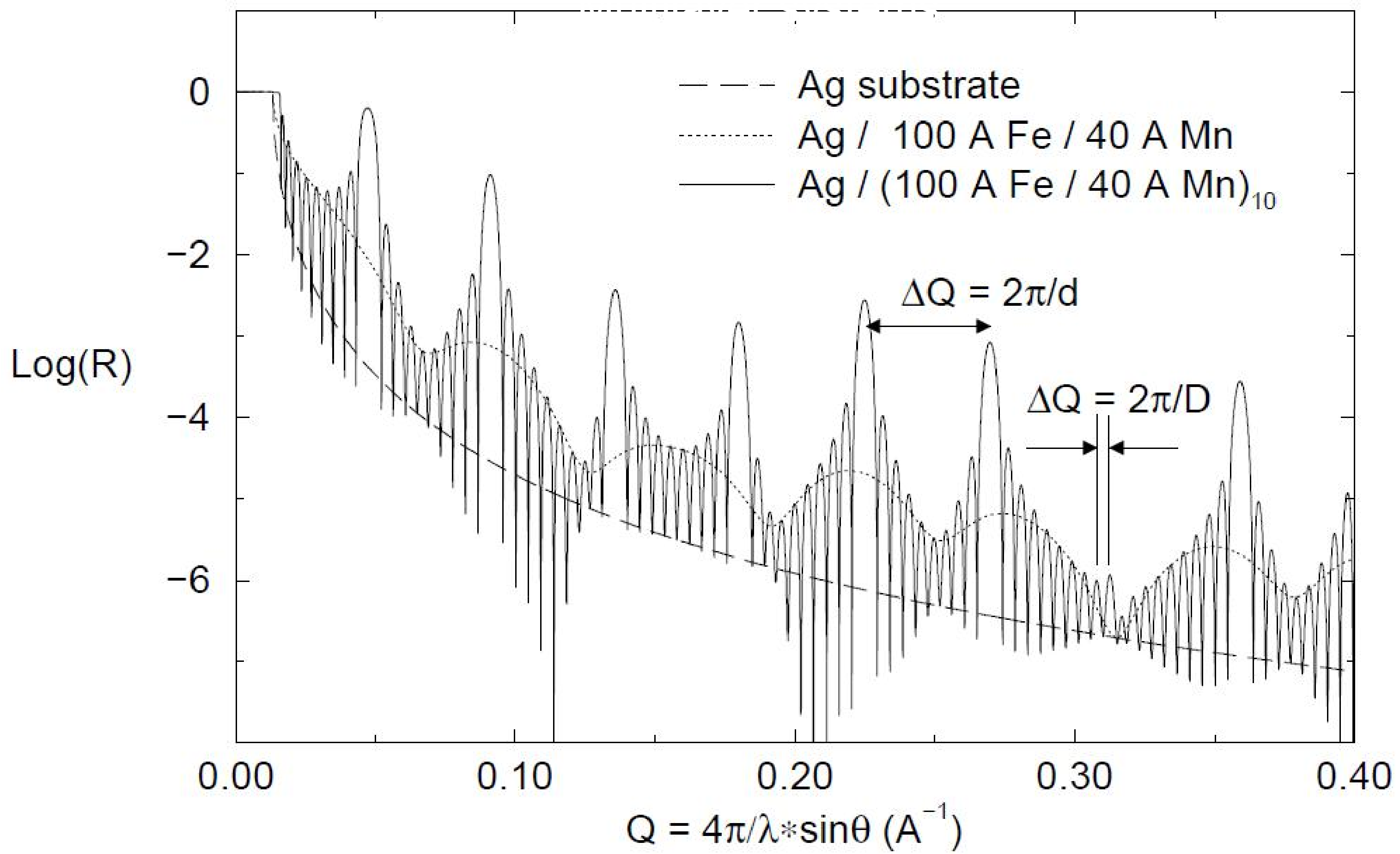
Reflectivity of a single, layer with thickness d

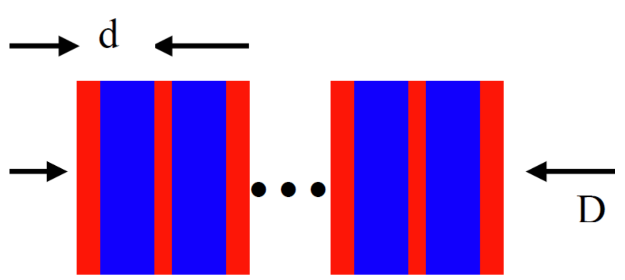


Effects of surface roughness and finite thickness



Multilayer systems





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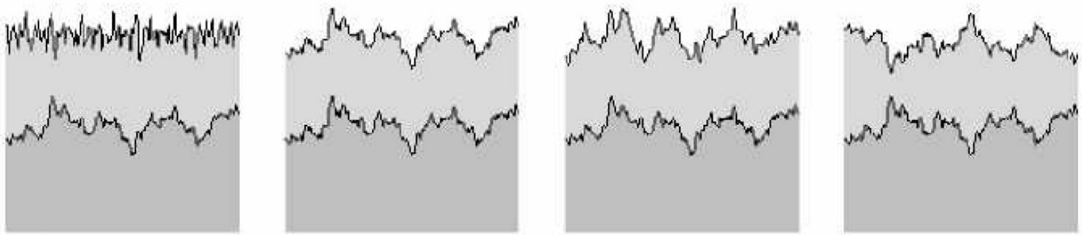
Reflectometry

Diffuse reflectivity in Born approximation Θ≠Θ`



Surface correlation function

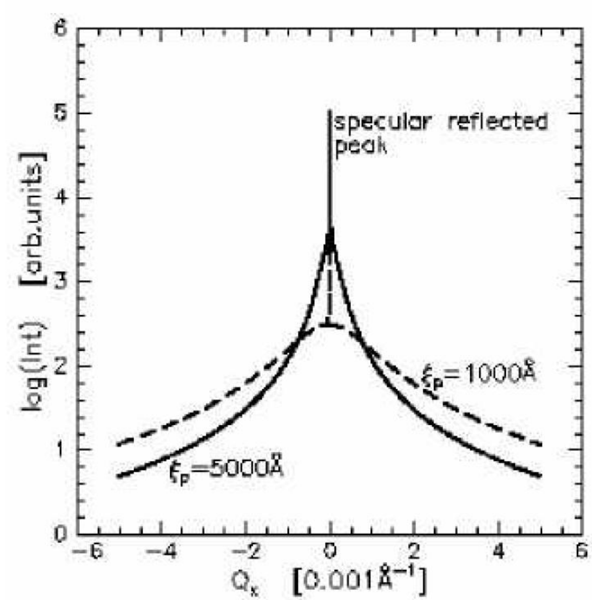
$$C_{jk}(R) = \int z_j(r) z_k(r+R) \mathrm{d}^2 r$$

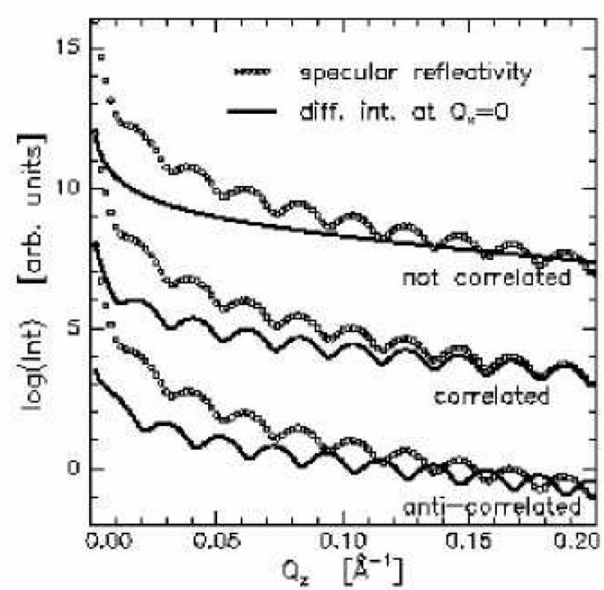
Diffuse offspecular intensity

$$I_{diff}(Q_x, Q_z) \approx \frac{1}{Q_z^2}[(b_2\varrho_2 - b_1\varrho_1)^2 e^{-Q_z^2\sigma_2^2} S_{22}(Q_x) + (b_1\varrho_1)^2 e^{-Q_z^2\sigma_1^2} S_{11}(Q_x) + 2(b_2\varrho_2 - b_1\varrho_1)(b_1\varrho_1) e^{\frac{-Q_z^2(\sigma_2^2+\sigma_1^2)}{2}} S_{12}(Q_x)\cos(Q_z d)$$

„Structure factor"

$$S_{jk}(Q_x) = \int (e^{Q_z^2 C_{jk}(x)} - 1) e^{-iQ_x x} \mathrm{d}x$$





Dynamical scattering theory: Index of refraction and reflectometry

Dynamical scattering theory

Born approximation: Intensity would diverge for Q->0 $I(Q_z) \sim \frac{1}{Q_z^4}\left|\int \frac{\mathrm{d}V(z)}{\mathrm{d}z} \exp(-iQ_z z)\mathrm{d}z\right|^2$

Complete description: Dynamical scattering theory

Derivation using Schrödinger equation for neutron wave in medium

Single, smooth layer using QM

$$\left[-\frac{\hbar^2}{2m_n}\Delta + V(r)\right]\Psi(r) = E\Psi(r)$$

Refractive index for neutrons (very small)

$$n_t = 1 - \frac{\lambda^2}{2\pi}\sum_j b_j \varrho_j = 1 - \delta_t$$

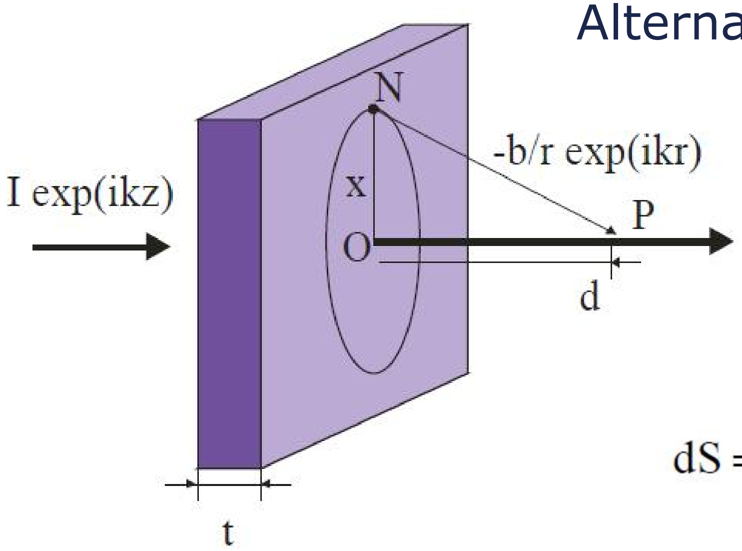
Transmitted and reflected wave

$$r_t = \frac{2k_z}{k_z + k_{t,z}} \qquad r_f = \frac{k_z - k_{t,z}}{k_z + k_{t,z}}$$

Absorption: Imaginary part

$$n_t = 1 - \delta_t + \mathrm{i}\beta_t$$

Dynamical scattering theory



Alternative derivation of refractice index

Amlitude at point P produced by spherical waves scattered from N

$$S_N = \frac{-b}{r}\exp(ikr)$$

Contribution of circle of radius x

$$dS = \frac{-\bar{b}}{r}\exp(ikr)\,\rho\; t2\pi x\,dx = -2\pi\bar{b}\rho t\exp\left(ik\sqrt{x^2+d^2}\right)\frac{x}{\sqrt{x^2+d^2}}dx$$

Amplitude of scattered wave at point P

$$S = -2\pi\bar{b}\rho t\int_0^\infty \exp\left(ik\sqrt{x^2+d^2}\right)\frac{x}{\sqrt{x^2+d^2}}dx = -i\frac{2\pi}{k}\bar{b}\rho t\exp(ikd)$$

Scattered and direct beam retarded with respect to incident beam

$$S + I = (1 - i\bar{b}\lambda\rho t)\exp(ikd) \approx \exp(ikd+\phi) \qquad \phi = -\bar{b}\lambda\rho t$$

Retardation can be expressed in terms of an refraction index

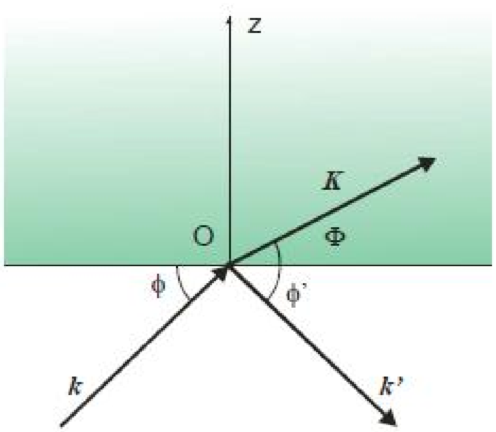
$$\phi = \frac{2\pi}{\lambda}(1-n)t \qquad \boxed{n = \frac{k_{medium}}{k_{vacuum}} = 1 - \frac{1}{2\pi}\rho\lambda^2\bar{b}}$$

Dynamical scattering theory

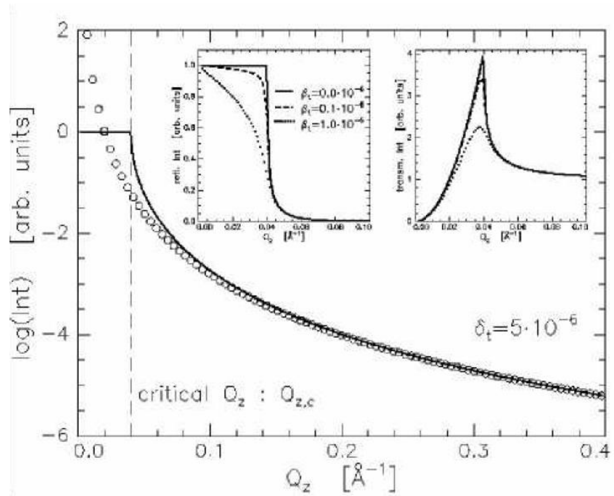
Consequences for neutron reflectivity

Fresnel formulas for reflected and transmitted beam

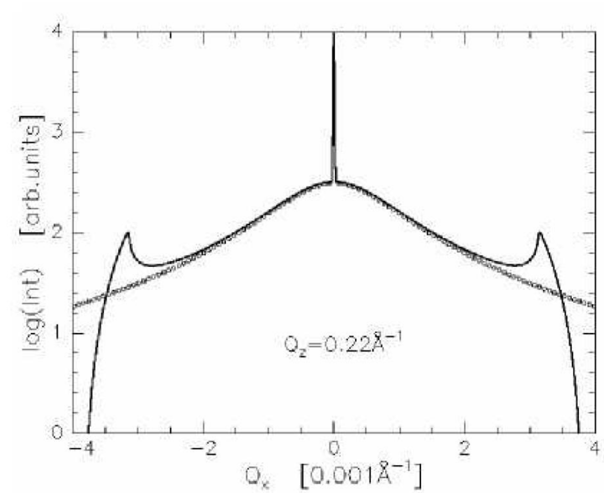
$$r_t = \frac{2k_z}{k_z + k_{t,z}} \qquad r_f = \frac{k_z - k_{t,z}}{k_z + k_{t,z}}$$



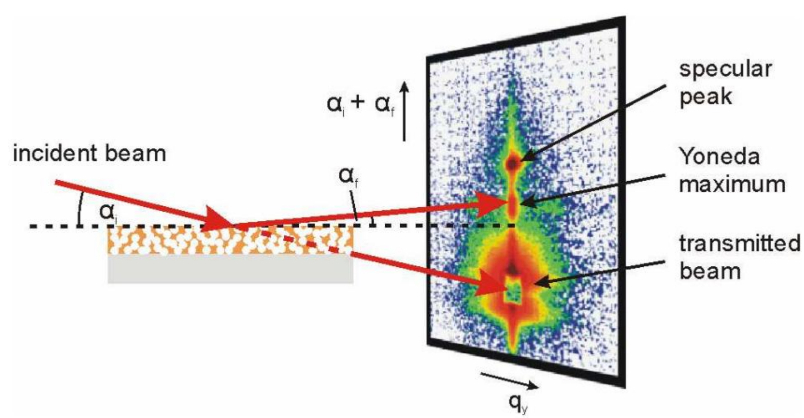
Plateau of total external reflection for Θ<Θ$_c$



Evanescent wave for Θ=Θ$_c$ (Yoneda peak)



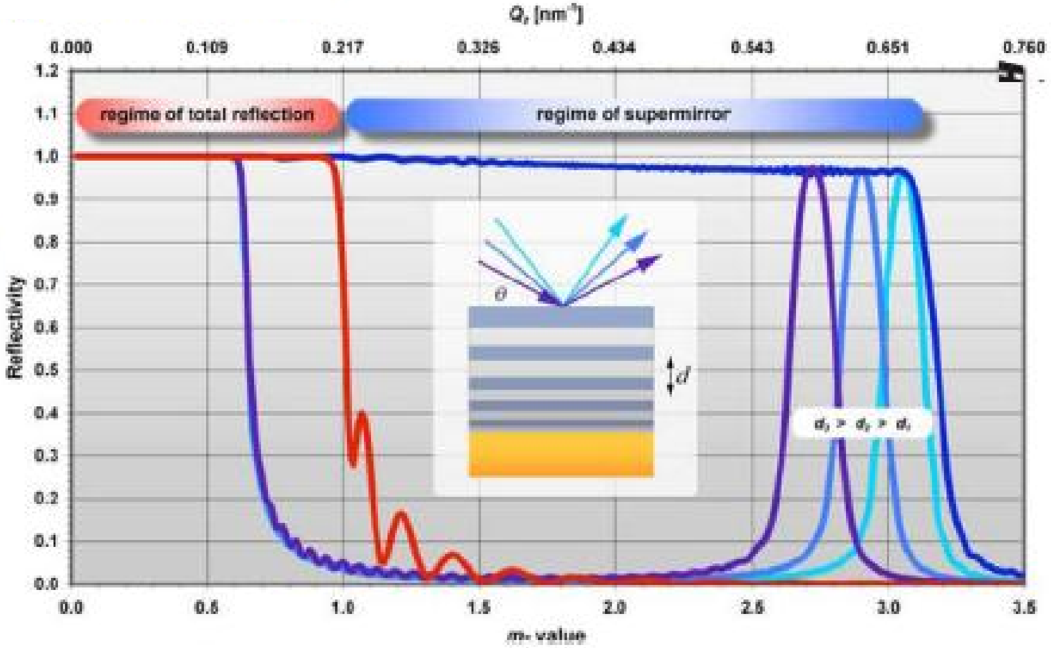
Full QM treatment only possible for specular reflectivity



Applications of Reflectometry

Neutron guides: Transporting neutrons via total external reflection

Supermirrors: Multilayer with varying spacing: Bragg peaks add up to reflection plateau



Regime of total reflection: $\Theta_c = \lambda\sqrt{\frac{\rho b}{\pi}}$

Regime of supermirror: $Q = \frac{4\pi}{\lambda}\sin(\Theta)$

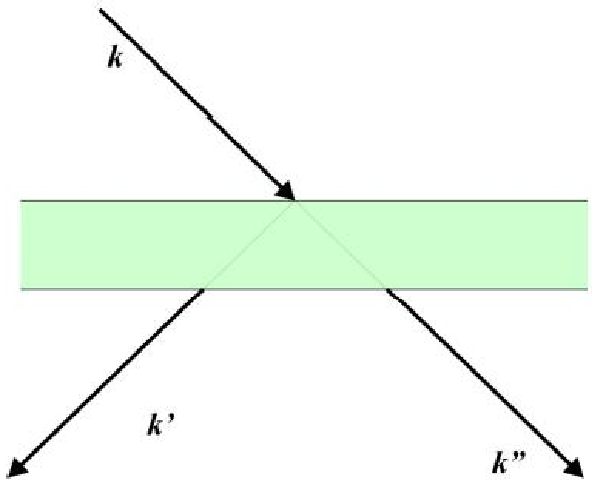
Refractive index smaller than 1 (unlike light)
Refractive index very small ($1-10^{-5}$, unlike light)

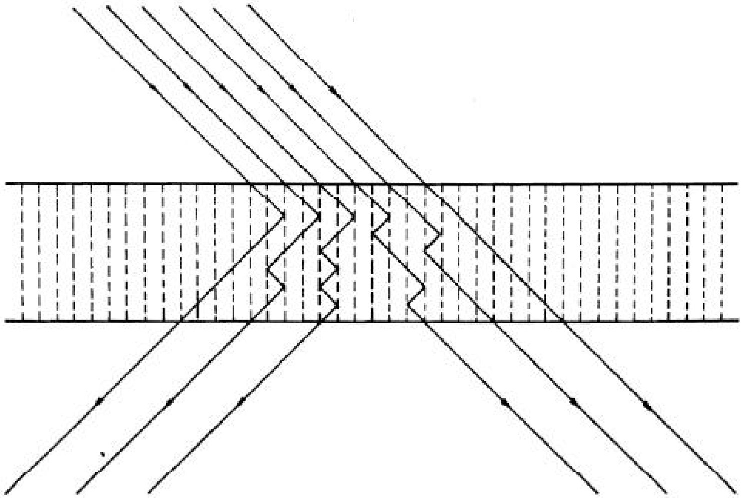
$$\left.\begin{array}{l}\rho = 0.09\text{Å}^{-1} \\ b = 10\text{fm} = 10^{-4}\text{Å}\end{array}\right\} \begin{array}{l}\lambda_c = 333\text{Å} \\ k_c = 0.019\text{Å}^{-1}\end{array} \quad \phi_c = 0.7^\circ \left(\lambda = 4\text{Å}\right)$$

Dynamical scattering theory: Modifications to diffraction

Dynamical scattering theory

Neutron conservation? Multiple scattering?





$$I_{hkl} \propto N \frac{(2\pi)^3}{V_0} |F_{hkl}|^2$$

Diffracted intensity proportional to sample thickness.

Transmission?

Rigorous treatment of multiple scatting

Dynamical scattering theory

Full treatment only using Schrödinger equation

Periodic potential $$V(r) = \frac{2\pi\hbar^2}{m_n}\langle\sum b_j \delta(r - R_j)\rangle$$ with $$R_j = l + d + u\binom{l}{d}$$

Use lattice sum identities to rewrite potential

$$\langle\sum b_j \delta(r - R_j)\rangle = \frac{1}{v_0}\sum_\tau F_\tau e^{-i\tau r}$$

$$F_\tau = \sum_d \bar{b}_d e^{i\tau d} e^{-W_d}$$

$$W_d = \frac{1}{2}\langle(\tau u\binom{l}{d})^2\rangle$$

Insert into Schrödinger equation:

$$\frac{\hbar^2}{2m_n}\nabla^2\Psi(E - V(r))\Psi = 0$$

Solution: Bloch waves $$\Psi = \sum_\tau a_\tau e^{i(k-\tau)r}$$

Coefficients: $$a_\tau(k_0^2 - (k-\tau)^2) = \sum_{\tau'} \frac{4\pi}{v_0} F_{\tau'} a_{\tau-\tau'}$$

Something happens close to Bragg peaks:

Dynamical scattering theory

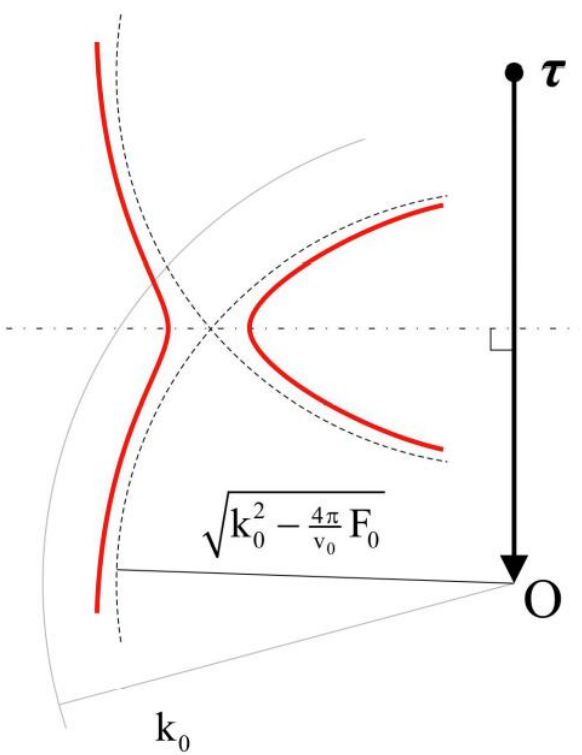
So far: Eigenstate of a neutron in a crystal is a plane wave

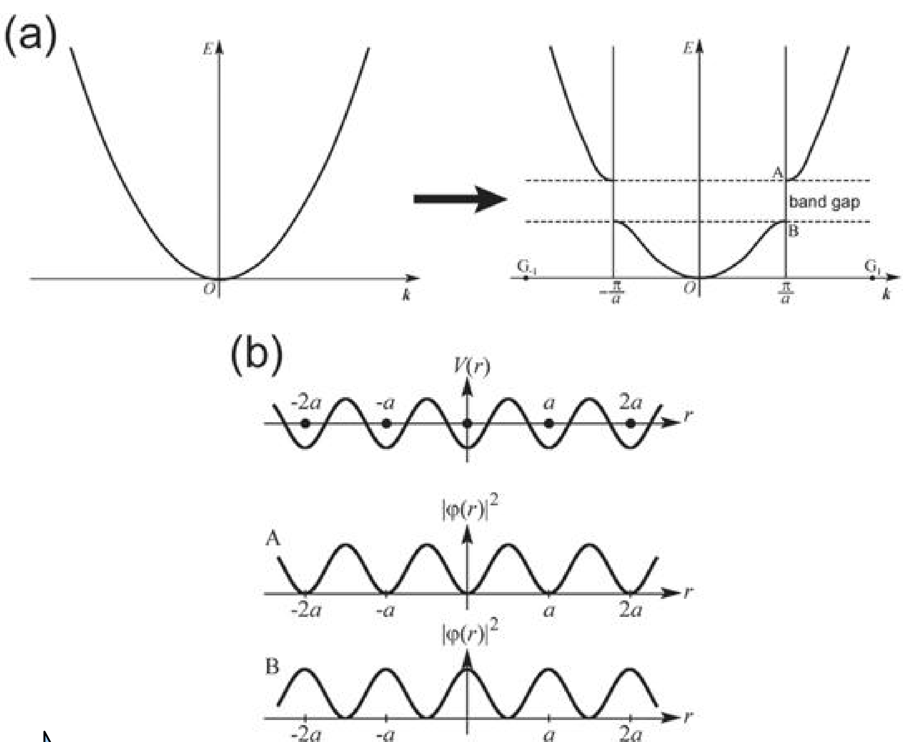
Rigorous treatment: Neutron as some kind of Bloch waves

Dispersion surfaces: Manifold of k-values of a Bloch wave where energy is equal to:

$$E = \frac{\hbar^2}{2m} k_0^2$$

Electrons in solids: Bloch waves

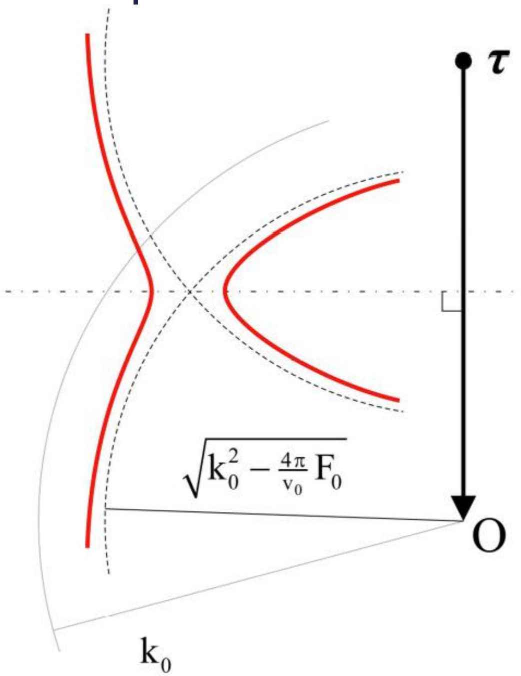




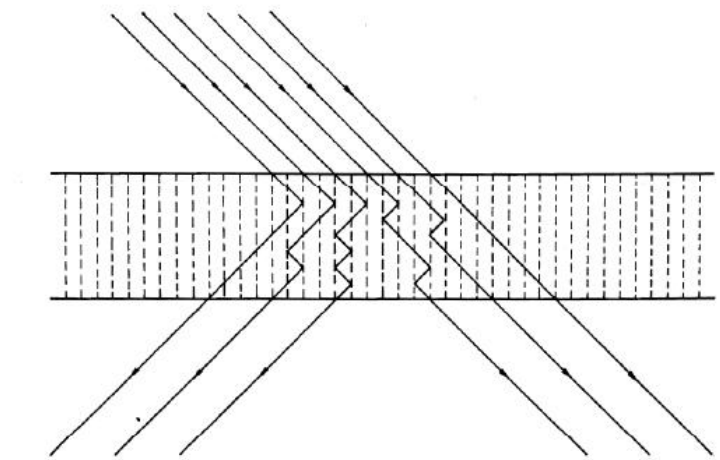
Band gap opens at the zone boundary

Dynamical scattering theory

Dispersion surfaces



Multiple scattering



Consequences of dynamical scattering theory:

Far away from Bragg peaks

Kinematic description (Born approximation) gives right result

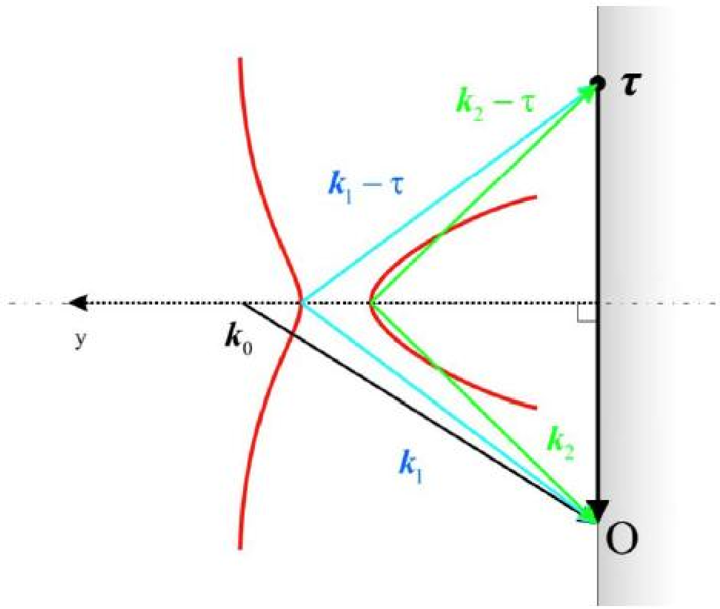
Close to Bragg peaks
in high quality single Xtals

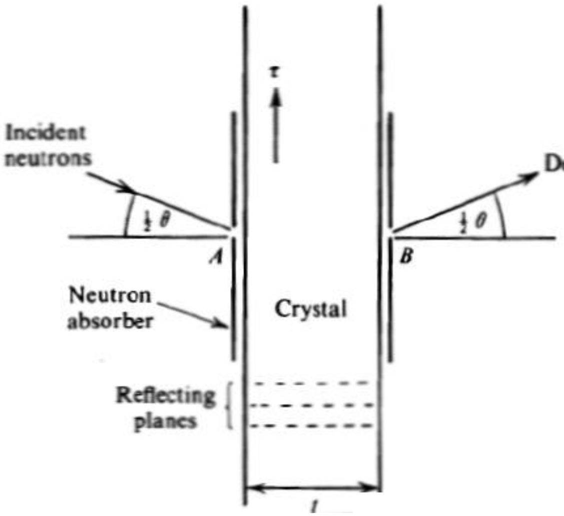
Kinematic description (Born approximation) is strongly modified

Dynamical scattering theory

Consequences of dynamical scattering theory:

Pendellösung oscillations (Kato fringes)



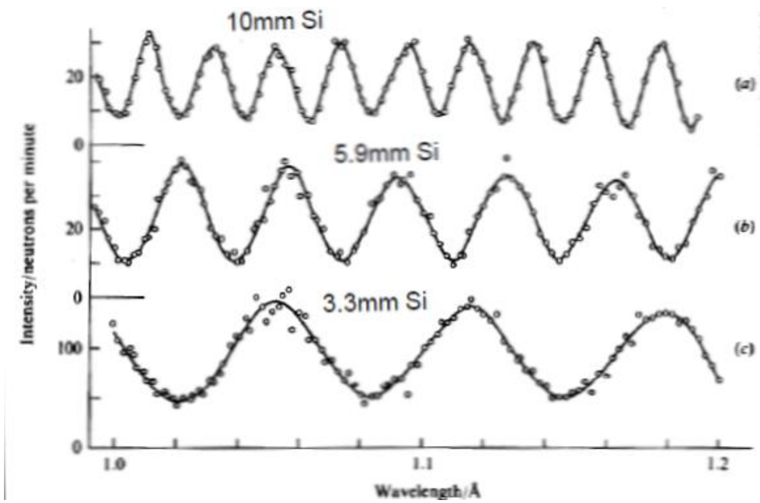


Interference fringes between k_1 and k_2:

➡ Intensity oscillations

Energy is constantly redistributed from one wave to the other.

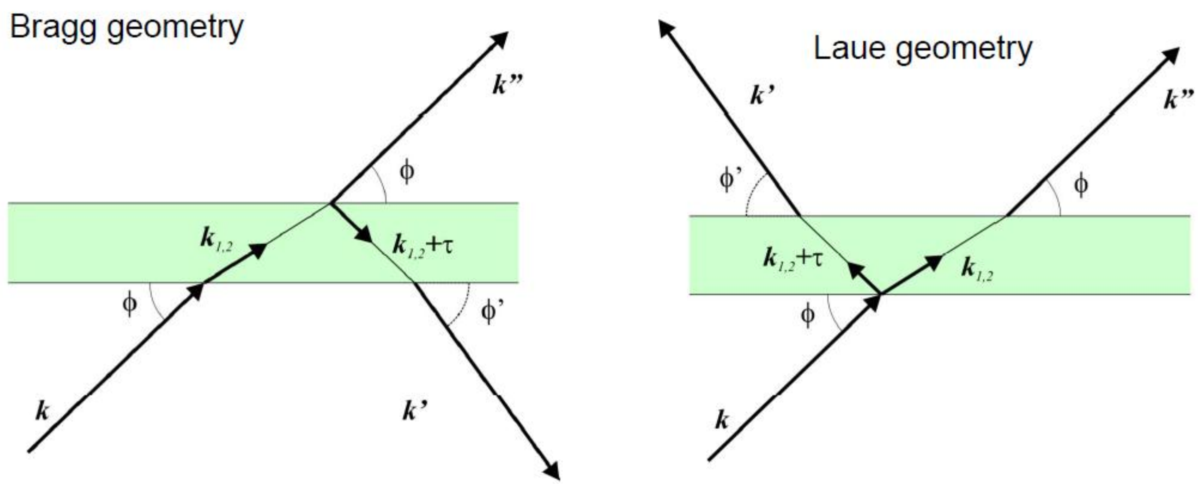
➡ Anomalous transmission

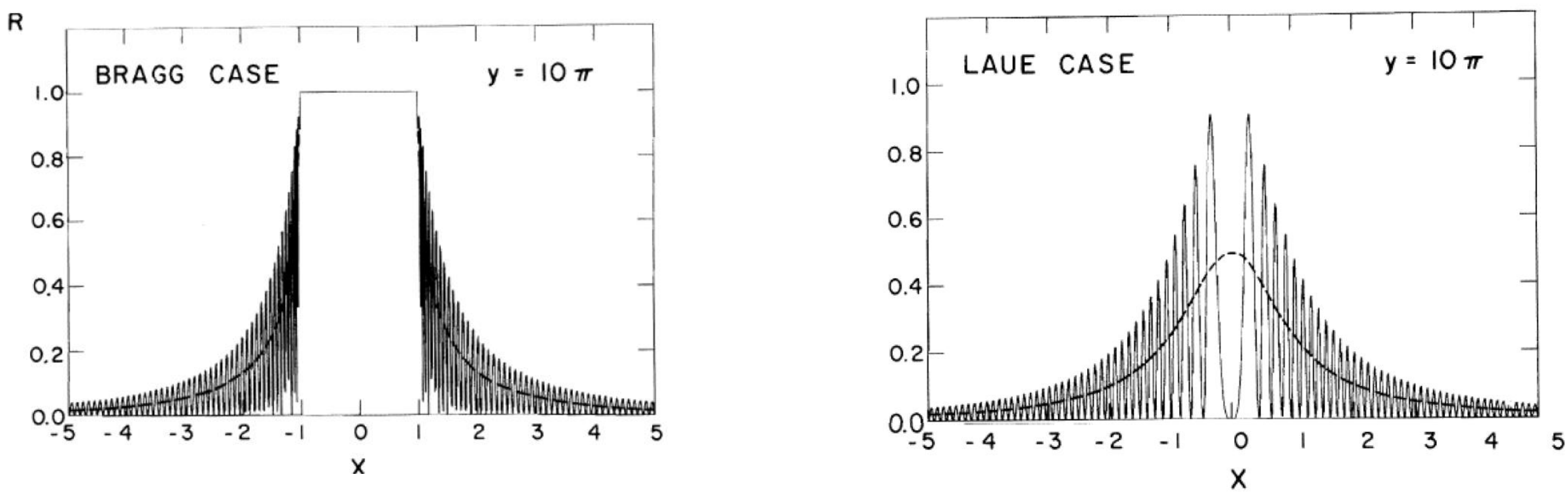


Dynamical scattering theory

Consequences of dynamical scattering theory:

Shape, width and intensity of Bragg peaks modified



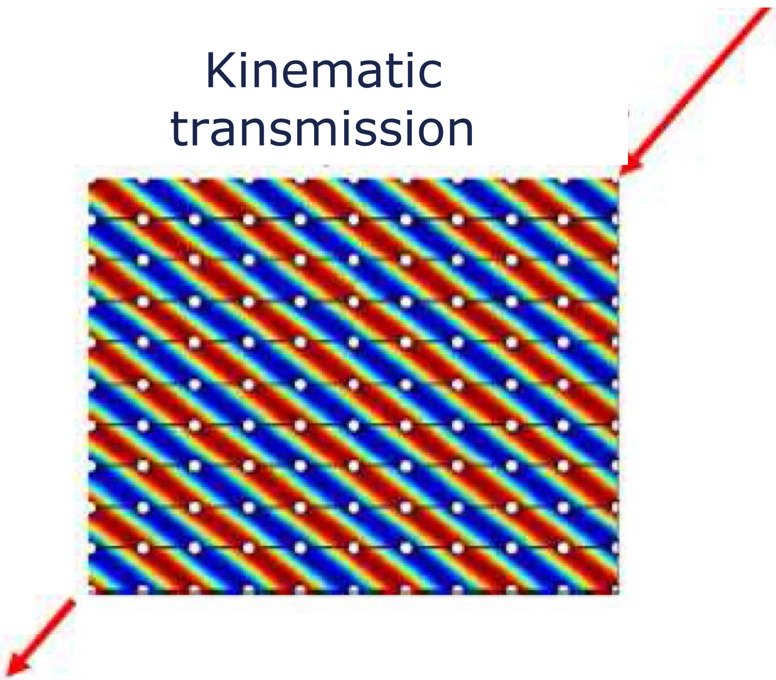


Dynamical scattering theory

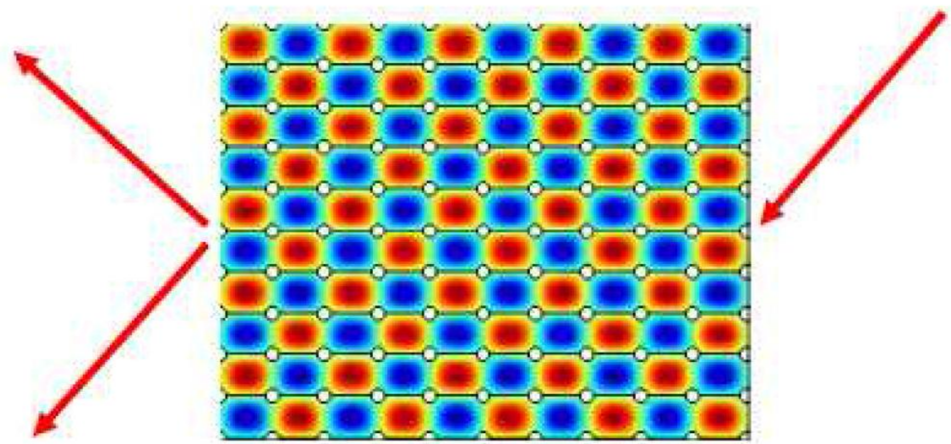
Consequences of dynamical scattering theory:

Anomalous transmission (Borrmann fan)

Kinematic transmission



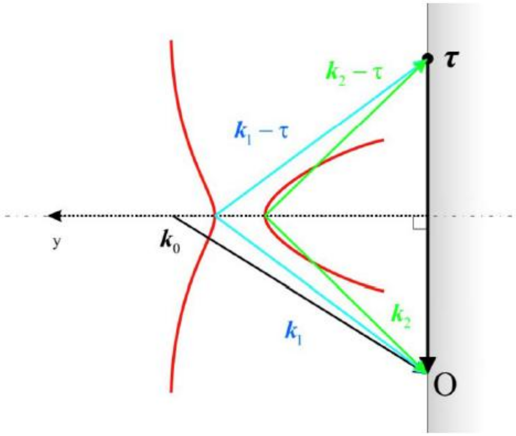
Anomalous transmission



Dynamical scattering theory

Consequences of dynamical scattering theory:

Primary extinction

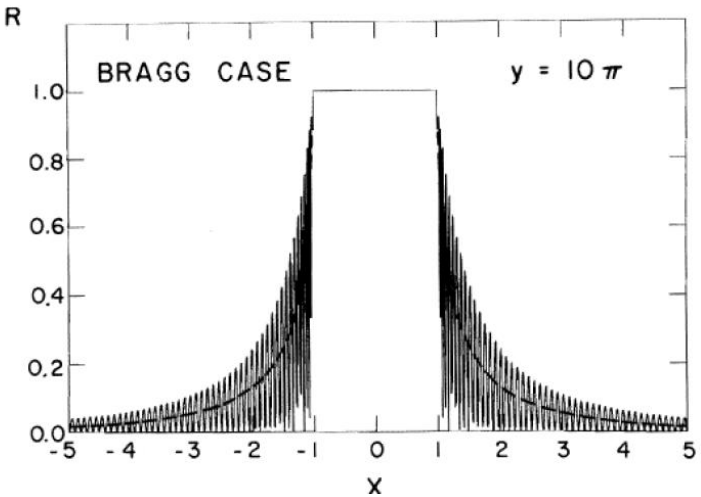


- Only the surface contritutes to Bragg reflections
- Intensity not given by structure factor (measurements are too low)

Define extinction length ξ

$$(k_1 - k_2)\frac{\xi}{\cos\frac{1}{2}\theta} = 1$$

Given by phase difference of k_1 and k_2



- Only several μm for good crystal samples
- Size ξ of the crystal reflects: Darwin width of peaks $\Delta\theta \approx \frac{1}{\tau\xi}$