Today's outline - October 19, 2021

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Reading Assignment: Chapter 6.3-6.4

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Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Thursday, October 21, 2021

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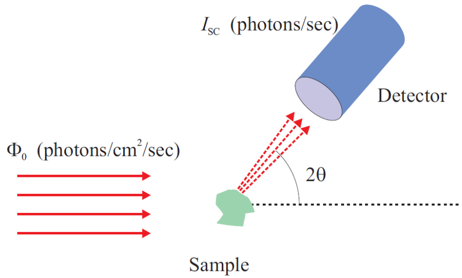
Reading Assignment: Chapter 6.3-6.4

Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Thursday, October 21, 2021

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

Scattering intensity from a crystallite

A small crystal fully illuminated by a monochromatic x-ray beam has differential scattering cross-section



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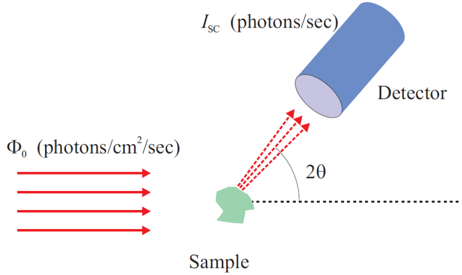

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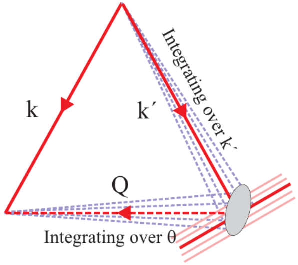

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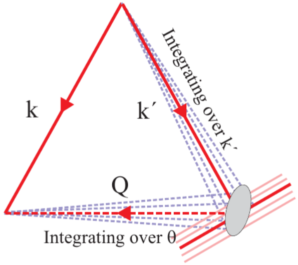

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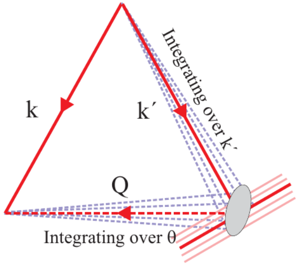

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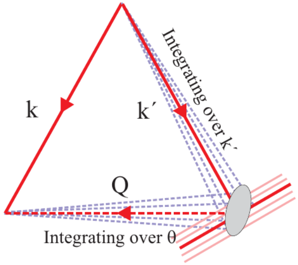

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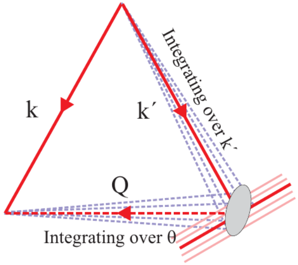

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$$\int \delta(\vec{Q} - \vec{G}) d\vec{k}' = \int \delta(\vec{k} - \vec{k}' - \vec{G}) d\vec{k}' = \cdots = \frac{2}{k}\delta(G^2 - 2kG\sin\theta)$$

Lorentz factor

After the integration over $\vec{k}'$, the differential scattering cross section must still be integrated over θ

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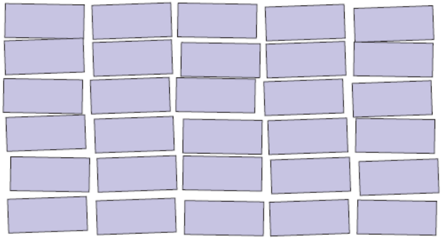
scattering by each electron is given by $r_0^2 P$ while The scattering from each of N unit cells is ${}_0^2 P|F(\vec{Q})|^2$ and the last term is the Lorentz factor

Extinction

Most small crystals are not “perfect” but can be seen as composed of small blocks with misalignments of the order of $\leq 0.1^\circ$



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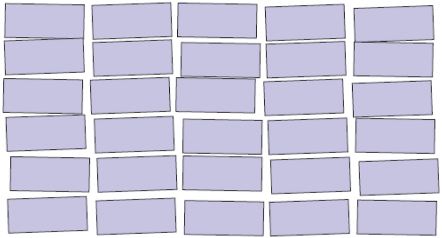

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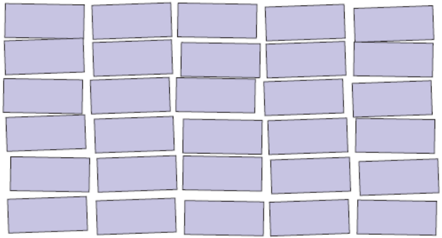

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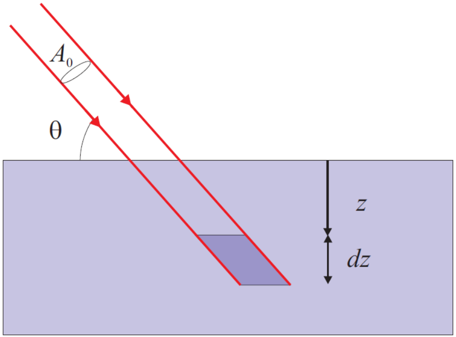
Primary extinction effects arise when there is a large perfect crystal as will be seen later on

Absorption

Absorption effects have been ignored so far but can have a significant effect



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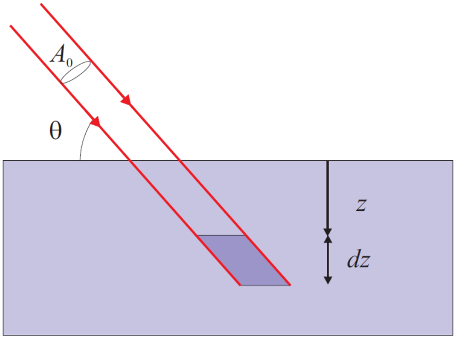

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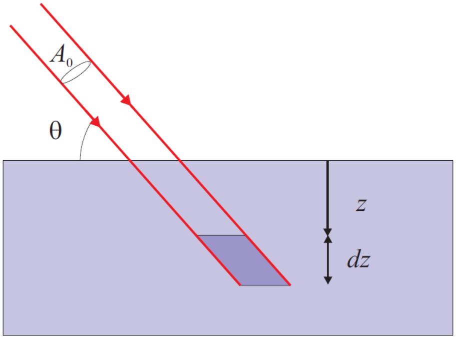

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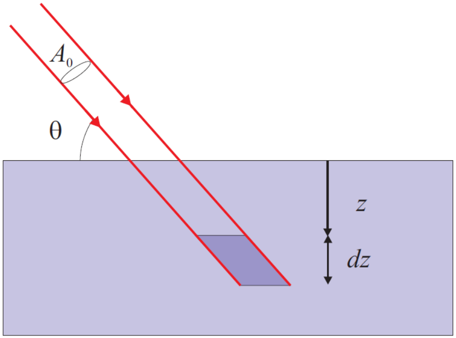

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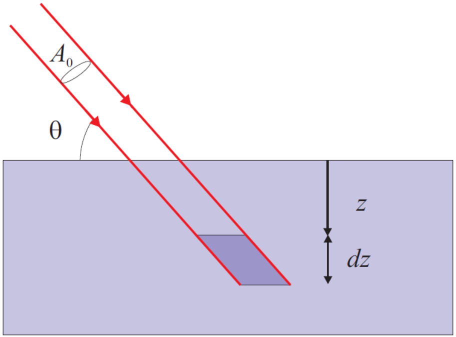

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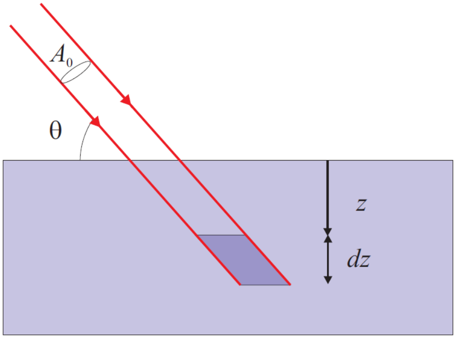

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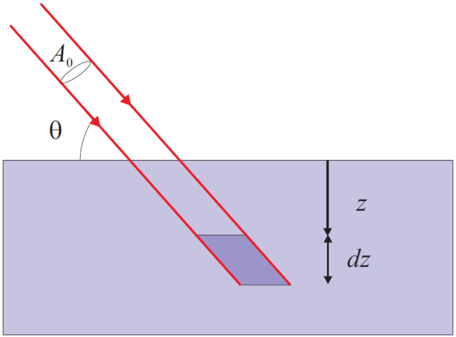

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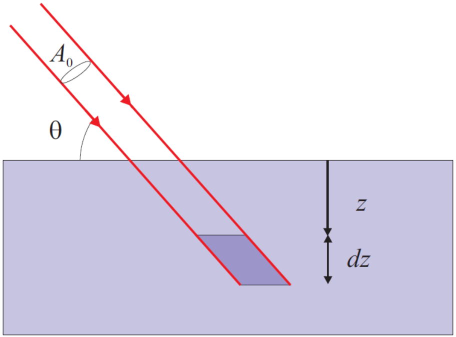

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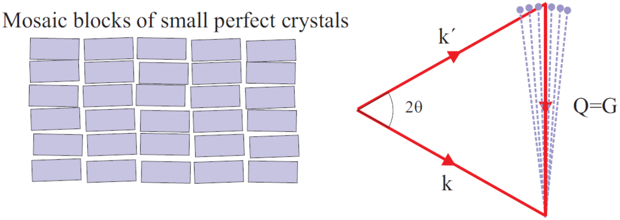
Kinematical vs. dynamical diffraction



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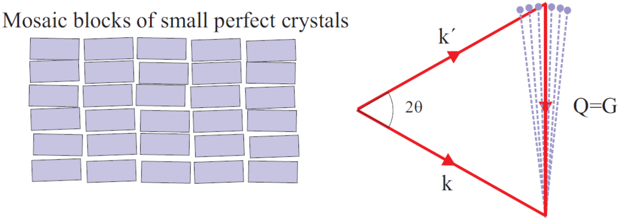

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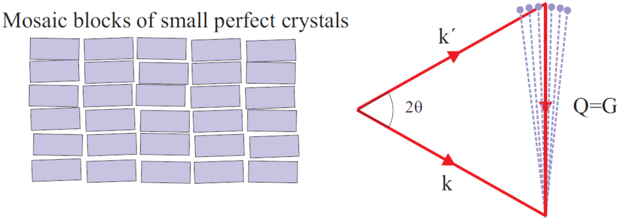

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This theory takes into account multiple reflections, and attenuation of the x-ray beam as it propagates through the perfect crystal.

Bragg & Laue geometries

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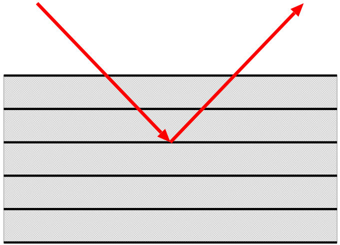
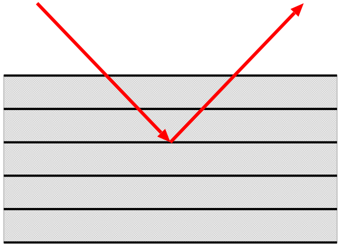


symmetric

$\longleftarrow$ Bragg

Bragg & Laue geometries



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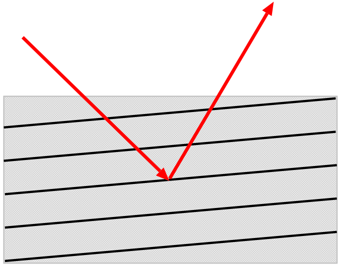

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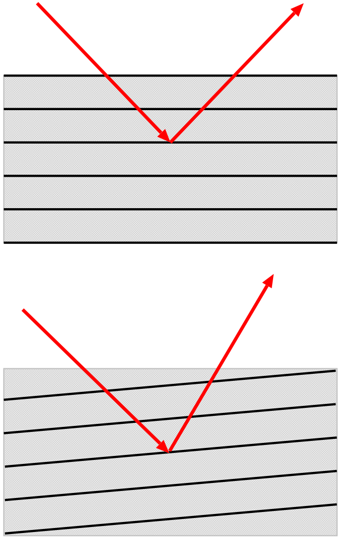

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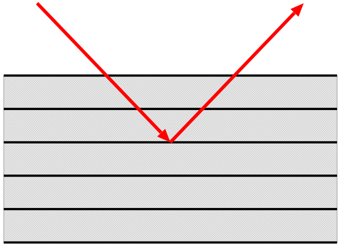

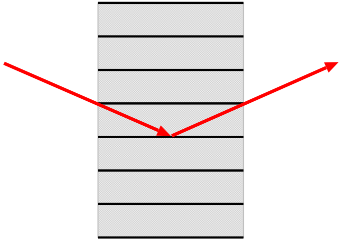

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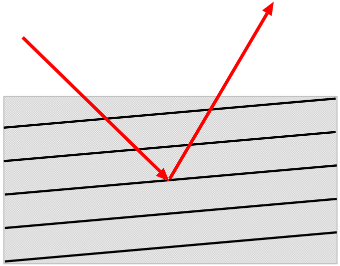

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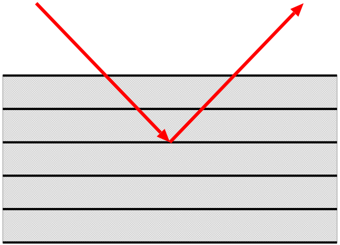

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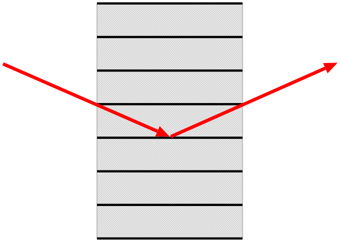
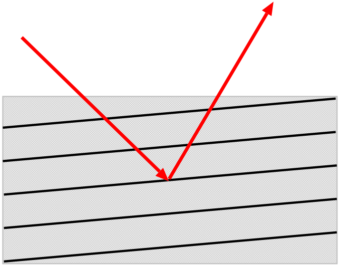


$\longleftarrow$ Bragg Laue $\longrightarrow$



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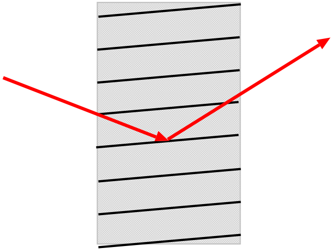

Scattering geometry

Consider symmetric Bragg geometry

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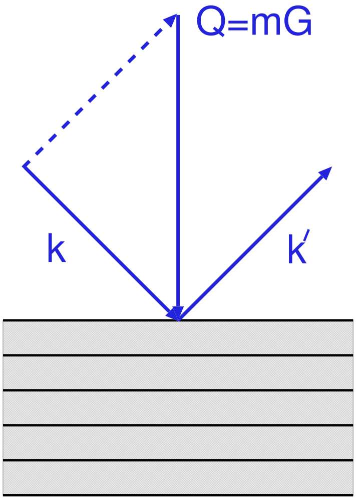

Scattering geometry

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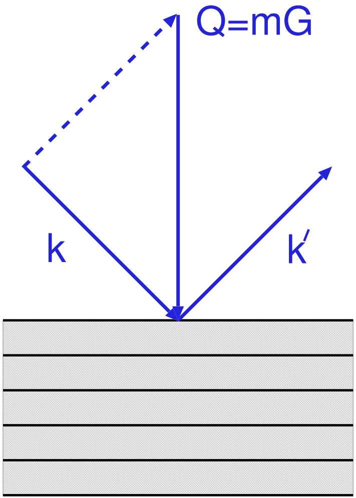
We expect the crystal to diffract in an energy bandwidth defined by Δk



Scattering geometry

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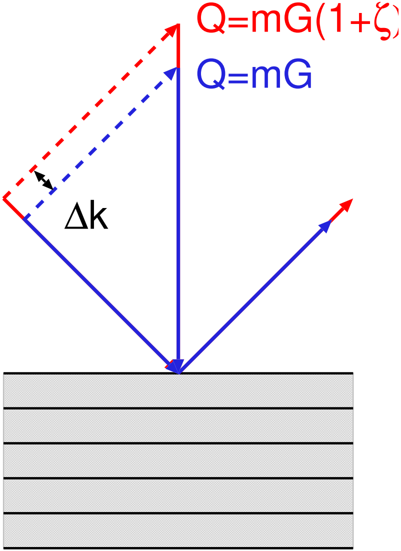
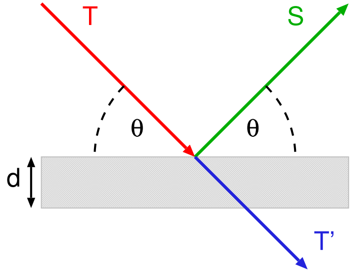
This defines a spread of scattering vectors such that

$$\zeta = \frac{\Delta Q}{Q} = \frac{\Delta k}{k}$$

called the relative energy or wavelength bandwidth

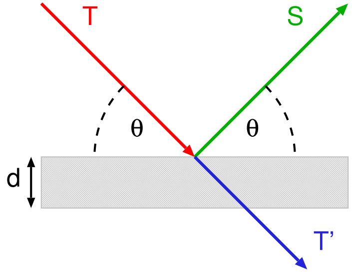


Darwin approach – single layer reflectivity



Darwin approach – single layer reflectivity

Consider a single thin slab with electron density ρ and thickness $d \ll \lambda$, the reflected and transmitted waves are functions of the incident wave



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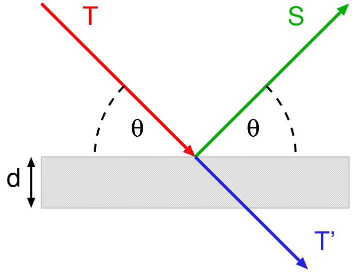

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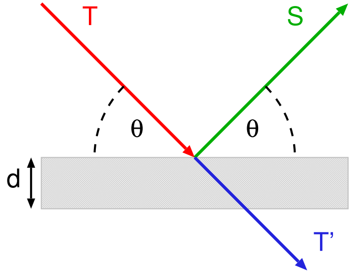

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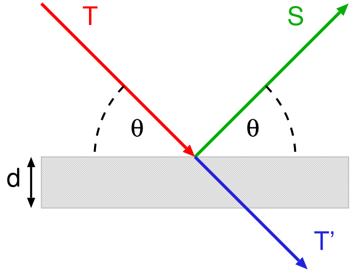

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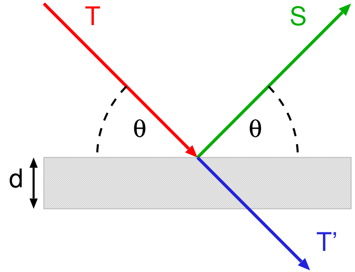

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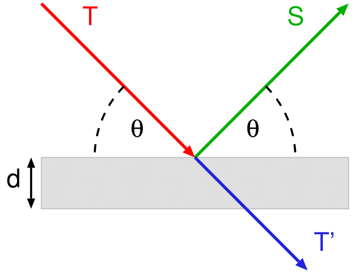

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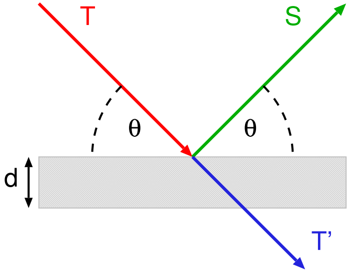

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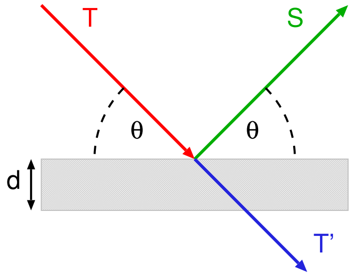

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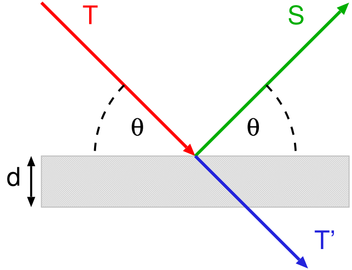

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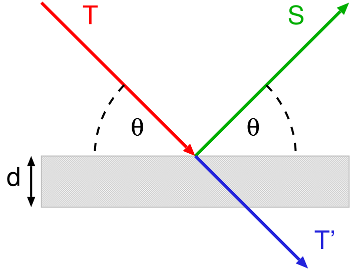

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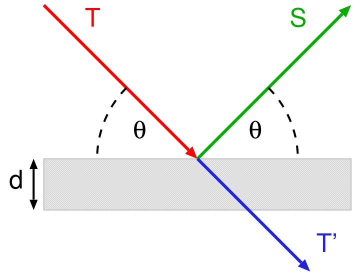

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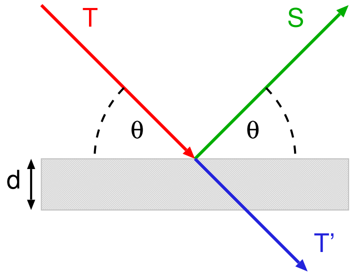

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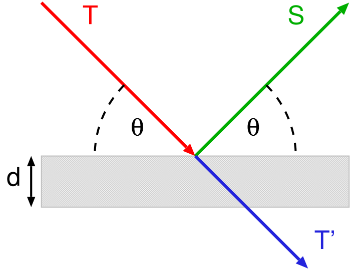

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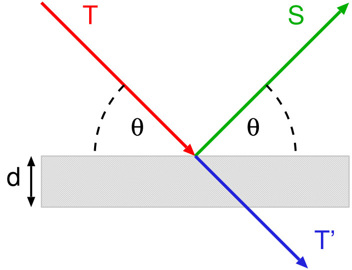

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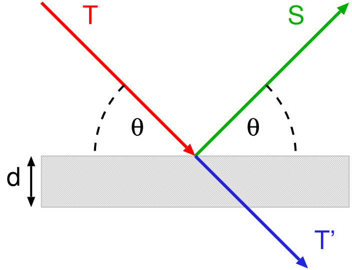

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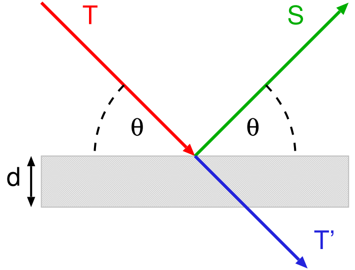

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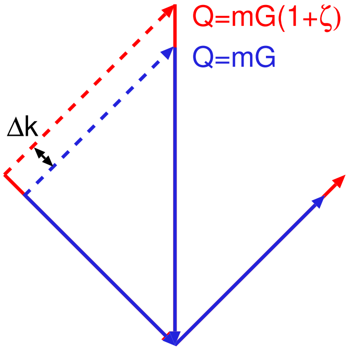

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$$\zeta = \frac{\Delta Q}{Q} = \frac{\Delta k}{k} = \frac{\Delta \mathcal{E}}{\mathcal{E}} = \frac{\Delta \lambda}{\lambda}$$

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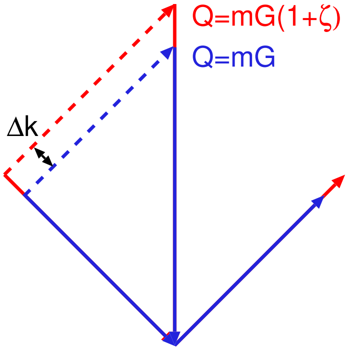

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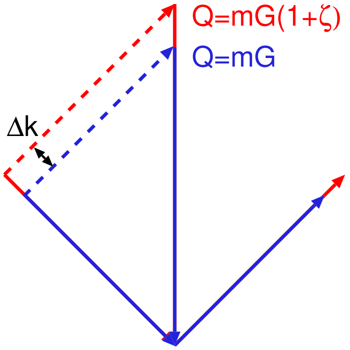

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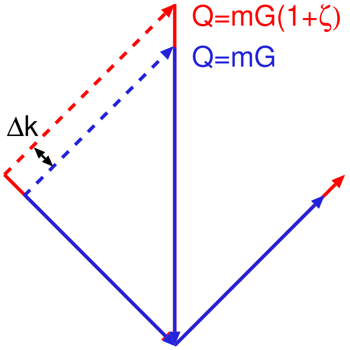

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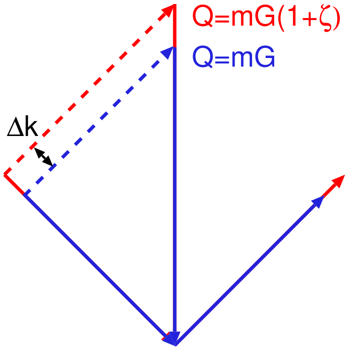

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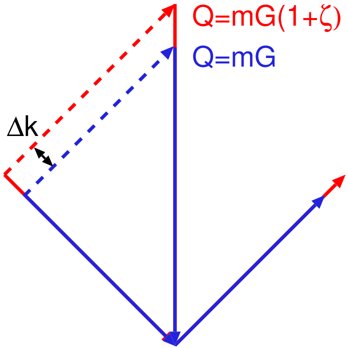

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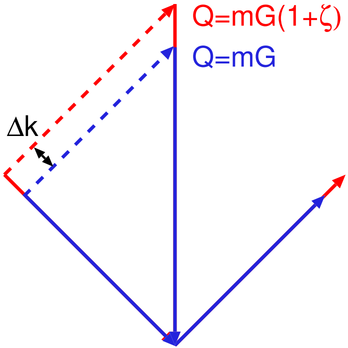

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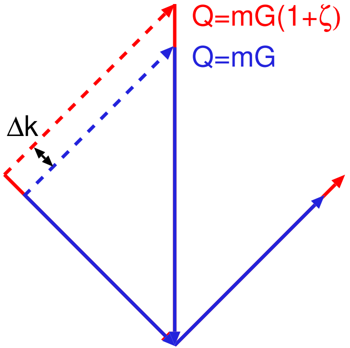

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As the crystal becomes infinite ($N \to \infty$) this kinematical approximation breaks down because $gN \sim 1$

Diffraction in the kinematical limit

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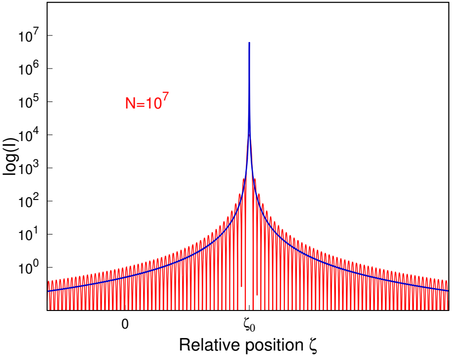

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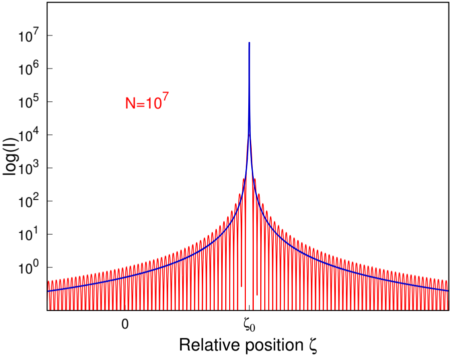

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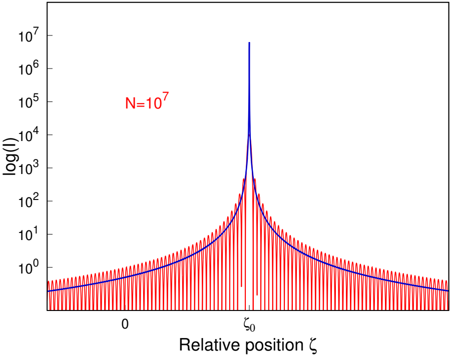

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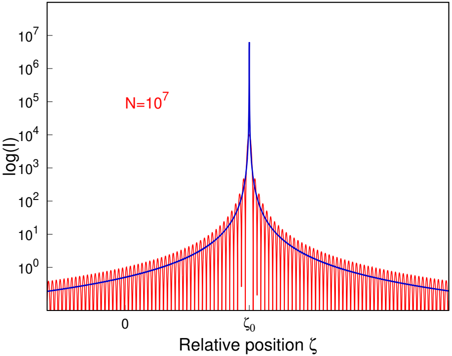

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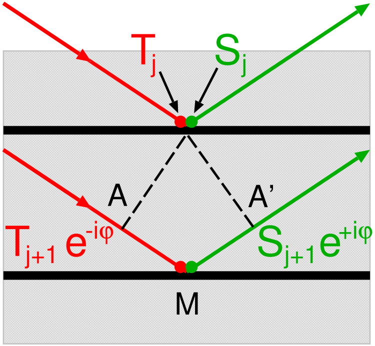
The kinematical limit clearly breaks down near ζ_0 so we need a dynamical diffraction theory

Reflectivity of a perfect crystal

In a perfect crystal, there are always two wavefields, the T wave which propagates in the direction of the incident beam and the S wave in the direction of the reflected wave



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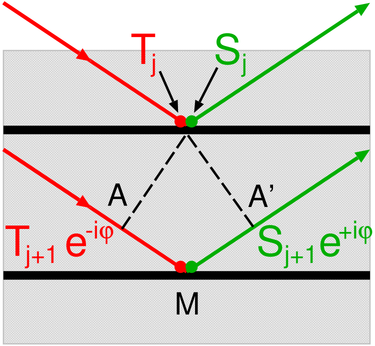

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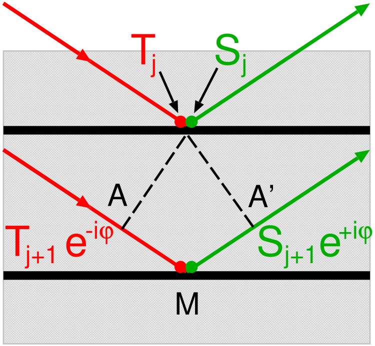

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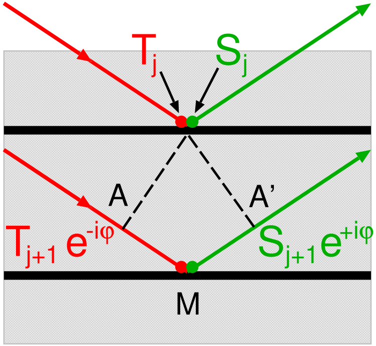

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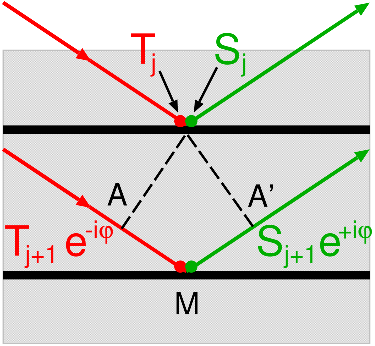

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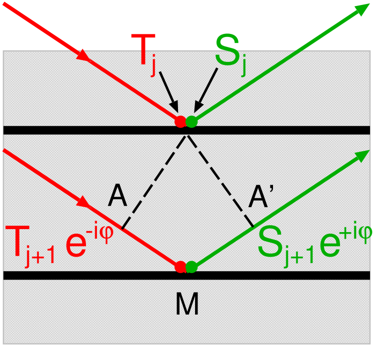

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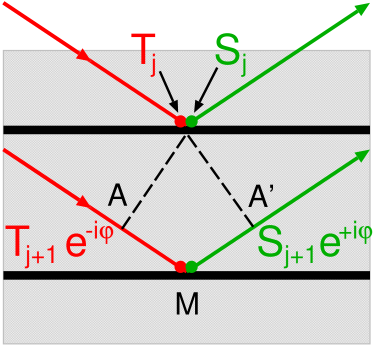

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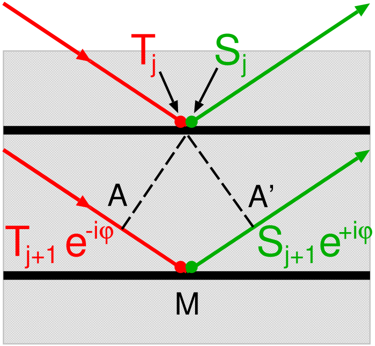

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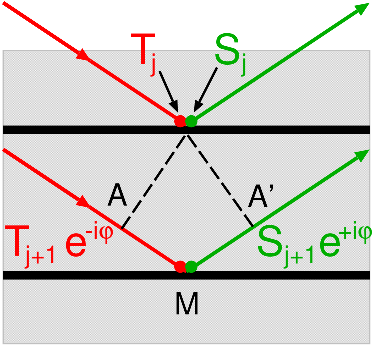
Difference equation

Let T_j and S_j be the fields just above layer j.



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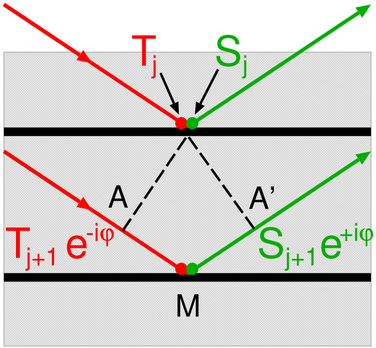

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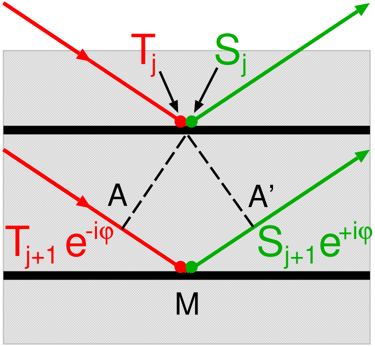

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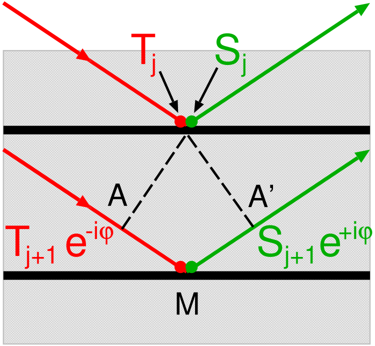

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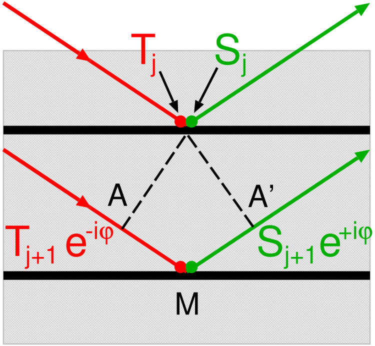

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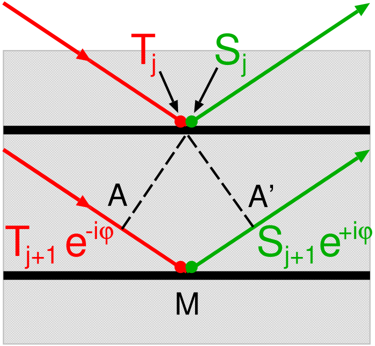

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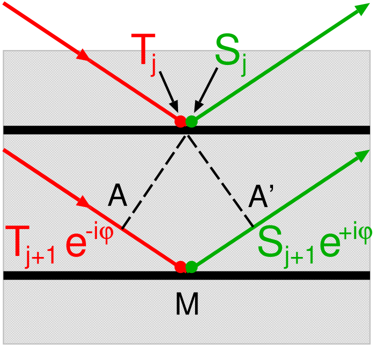

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these coupled equations must be solved for an infinite stack of atomic layers

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With the trial solution $T_{j+1} = e^{-\eta}e^{im\pi}\,T_j, \qquad T_{j-1} = e^{\eta}e^{-im\pi}\,T_j$

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Solving for the T field

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assuming that g, g_0, and Δ are very small quantities, we can expand

$$(1-ig_0)(1-i\Delta-\frac{\Delta^2}{2})\left[(1-\eta+\frac{\eta^2}{2})+(1+\eta+\frac{\eta^2}{2})\right]$$
$$\approx g^2+(1-2ig_0-g_0^2)+(1-i2\Delta-2\Delta^2)$$

Solving for the T field

$$(1 - ig_0)(1 - i\Delta - \frac{\Delta^2}{2})\left[(1 - \eta + \frac{\eta^2}{2}) + (1 + \eta + \frac{\eta^2}{2})\right]$$
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Cancelling and expanding all products keeping only second order terms

Solving for the T field

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$$(1 - ig_0 - i\Delta - g_0\Delta - \frac{\Delta^2}{2})(2 + \eta^2) \approx g^2 + 2 - 2ig_0 - 2i\Delta - g_0^2 - 2\Delta^2$$

Solving for the T field

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Cancelling and expanding all products keeping only second order terms

$$(1-ig_0-i\Delta-g_0\Delta-\frac{\Delta^2}{2})(2+\eta^2)\approx g^2+2-2ig_0-2i\Delta-g_0^2-2\Delta^2$$
$$2-2ig_0-2i\Delta-2g_0\Delta-\Delta^2+\eta^2\approx g^2+2-2ig_0-2i\Delta-g_0^2-2\Delta^2$$

Solving for the T field

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The solution for the attenuation factor of the transmitted field is thus

Solving for the T field

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Solving for the T field

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Solving for the T field

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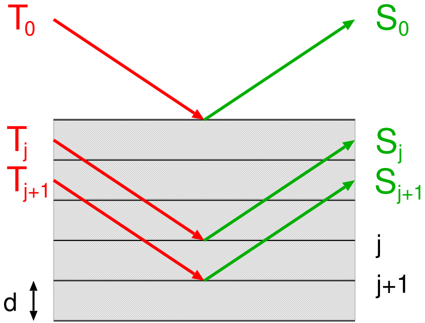
$$T_{j+1} = e^{-\eta} e^{im\pi} T_j, \qquad S_{j+1} = e^{-\eta} e^{im\pi} S_j$$

Reflectivity of a perfect crystal

In order to calculate the absolute reflectivity curve, solve for S_0 and T_0 using the solution and the recursive relations.



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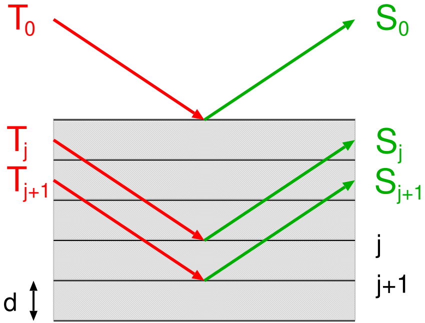

$$S_{j+1} = e^{-\eta} e^{im\pi} S_j$$

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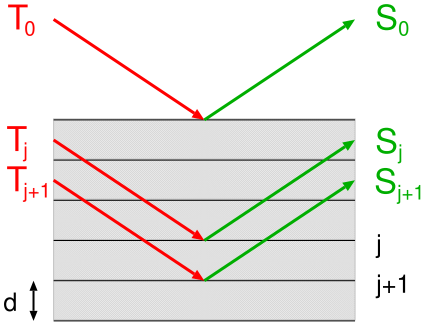

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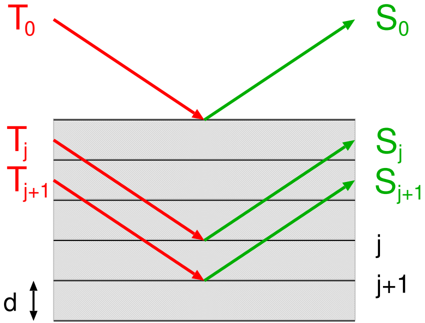

$$S_1 = e^{-\eta} e^{im\pi} S_0$$

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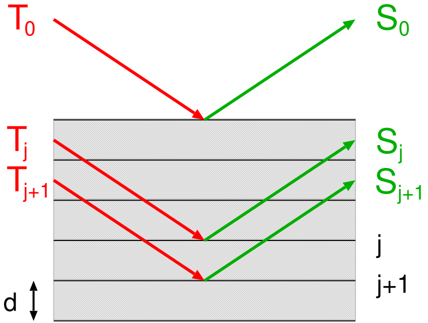

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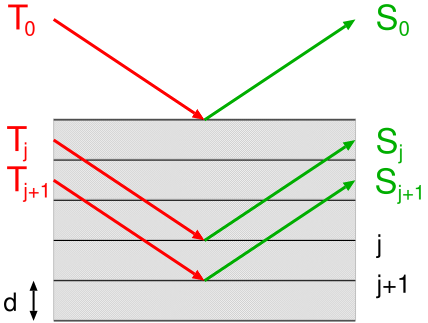

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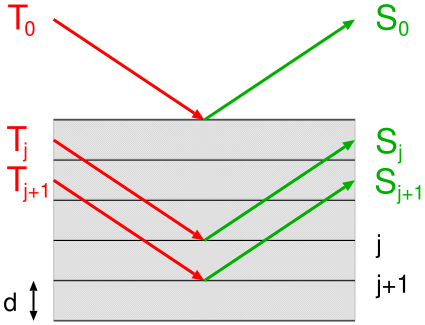

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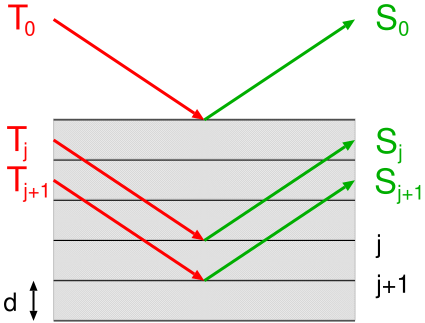

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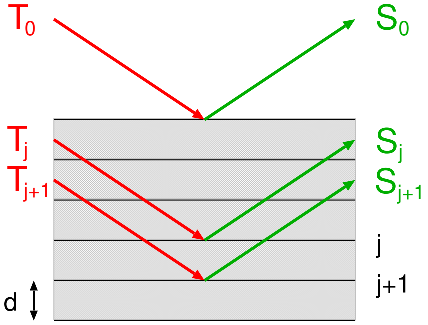

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$$\frac{S_0}{T_0} \approx \frac{-ig}{1 - (1 - ig_0)(1 - \eta)(1 + i\Delta)} \approx \frac{-ig}{ig_0 + \eta - i\Delta} = \frac{g}{i\eta + (\Delta - g_0)}$$

Darwin reflectivity curve

$$r = \frac{S_0}{T_0} = \frac{g}{i\eta + (\Delta - g_0)}$$

It is convenient to express the reflection coefficient in terms of reduced units using

$\epsilon = \Delta - g_0,$,

Darwin reflectivity curve

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It is convenient to express the reflection coefficient in terms of reduced units using

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Darwin reflectivity curve

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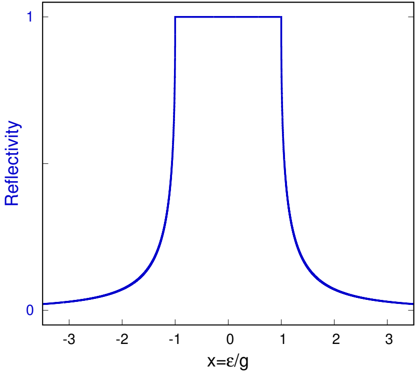

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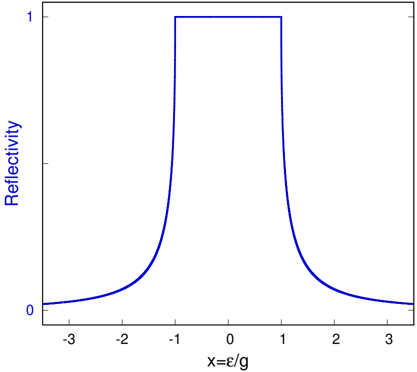

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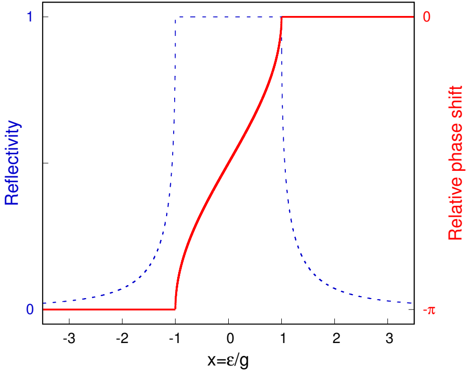

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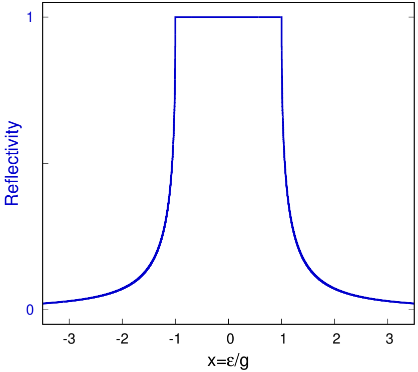
Darwin width



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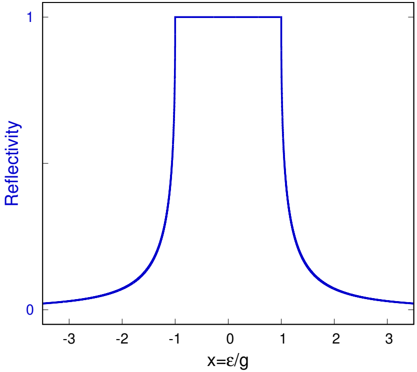

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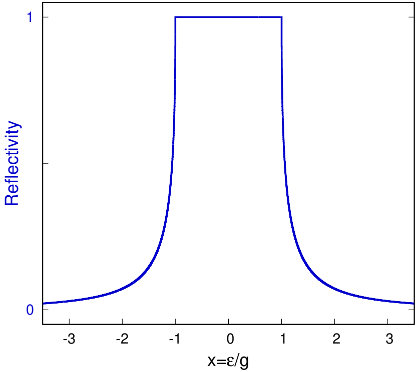

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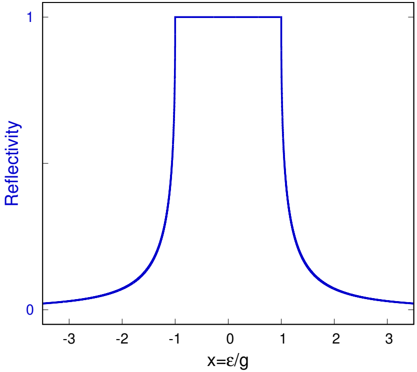

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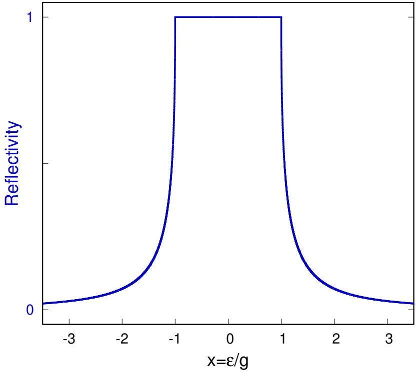

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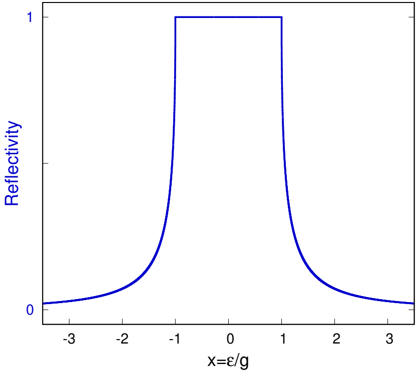

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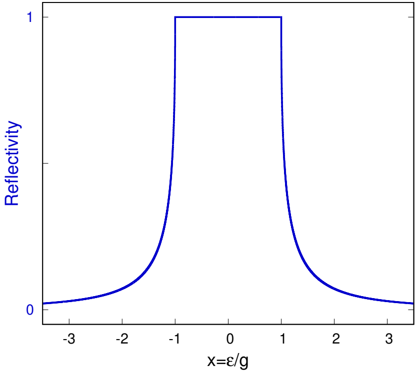

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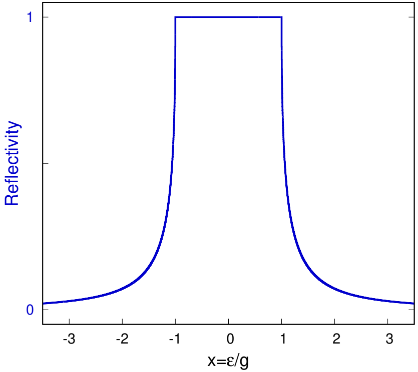

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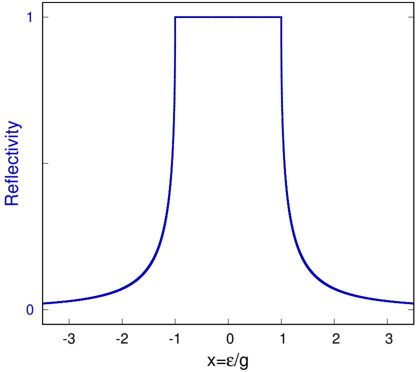

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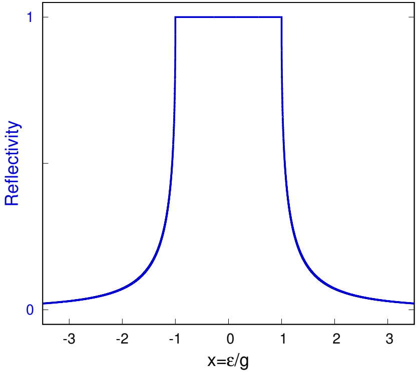

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