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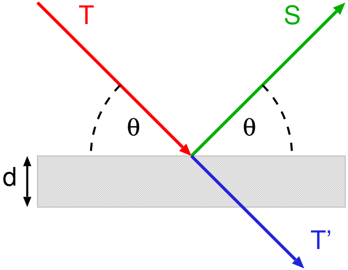
Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Thursday, April 02, 2020

Darwin approach – single layer reflectivity



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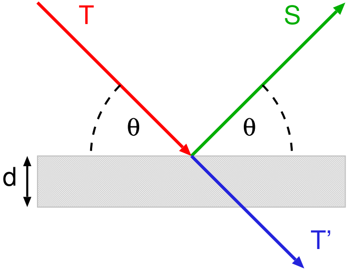

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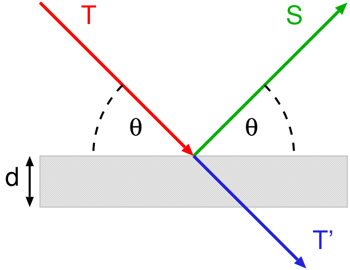

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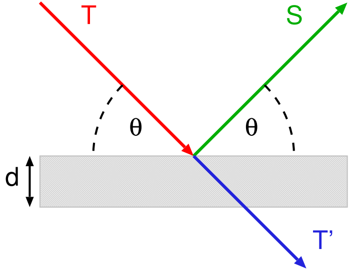

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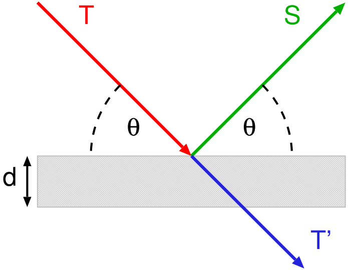

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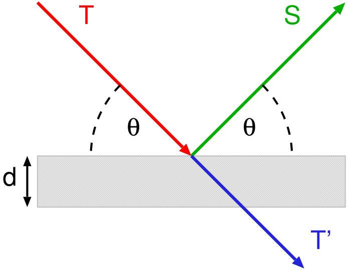

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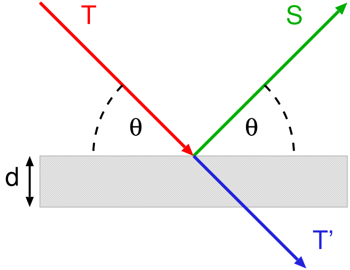

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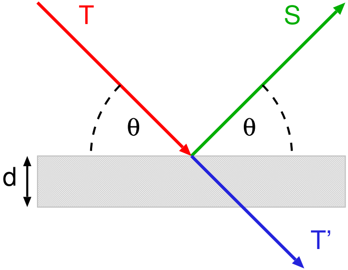

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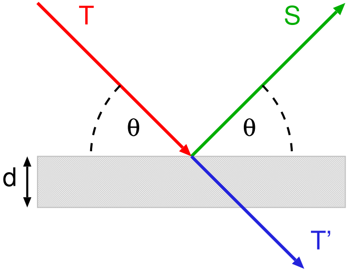

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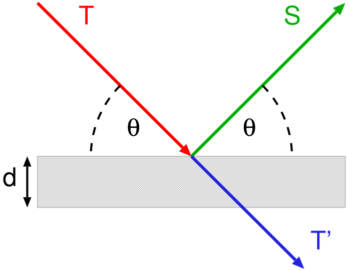

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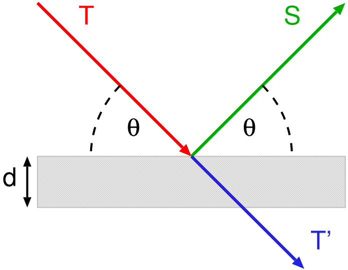

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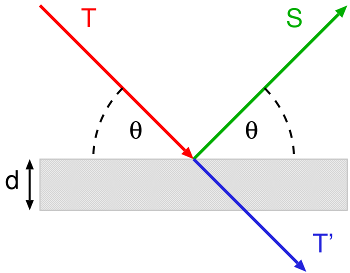

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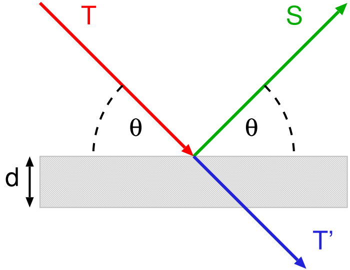

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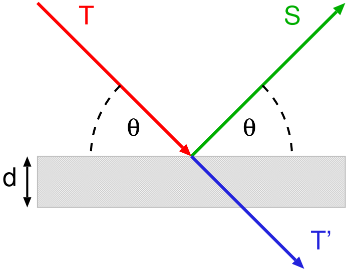

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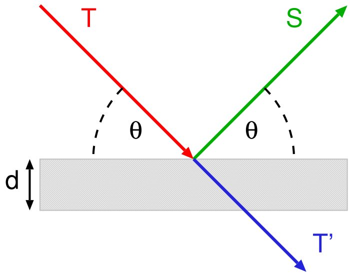

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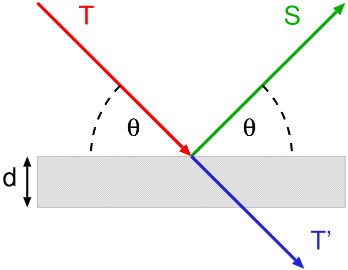

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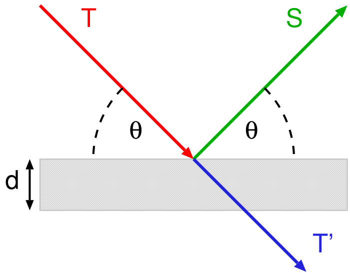

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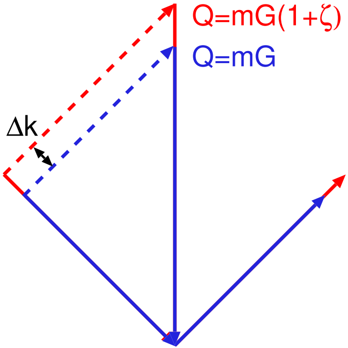

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these N unit cell layers will give a reciprocal lattice with points at multiples of $G = 2\pi/d$ we are interested in small deviations from the Bragg condition:

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

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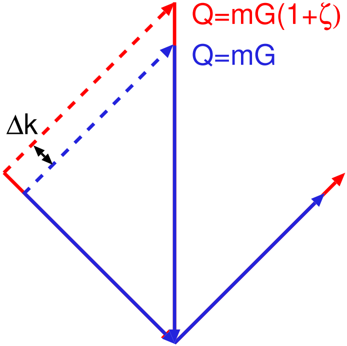

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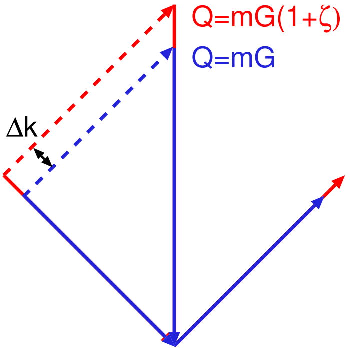

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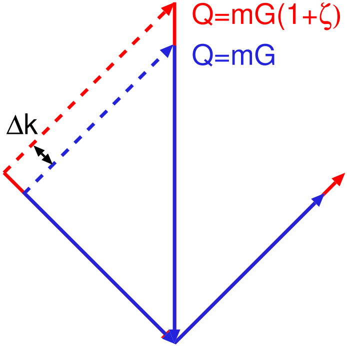

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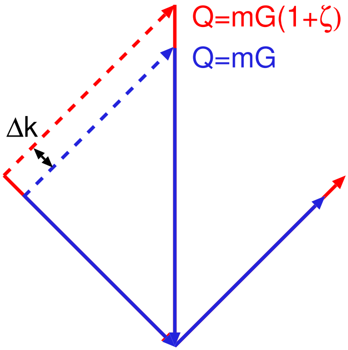

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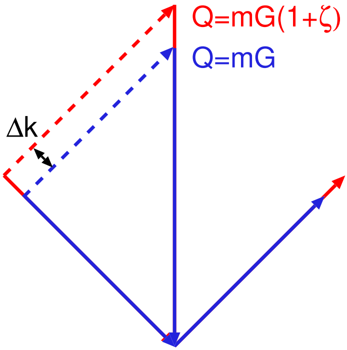

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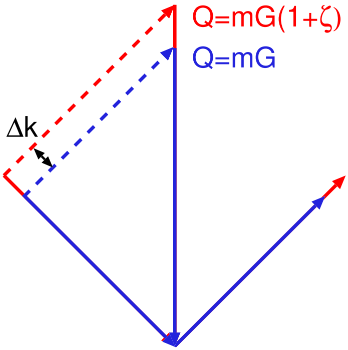

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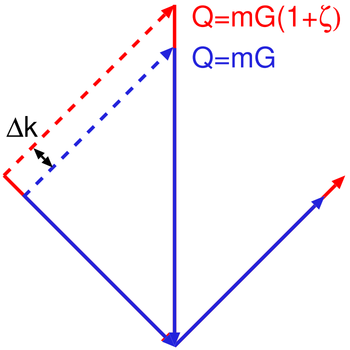

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This describes a shift of the Bragg peak *away from the reciprocal lattice point*, the maximum being at $\zeta = \zeta_0/m$

As $\zeta \to \zeta_0/m$, the modulus of the reflectivity becomes

$$|r_N(\zeta_0/m)| \approx g \frac{\pi N}{\pi} = gN$$

The shift in the peak is due to refraction inside the crystal and varies as the reciprocal of the order, $1/m$

Multiple layer reflection

This geometric series can be summed as usual

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

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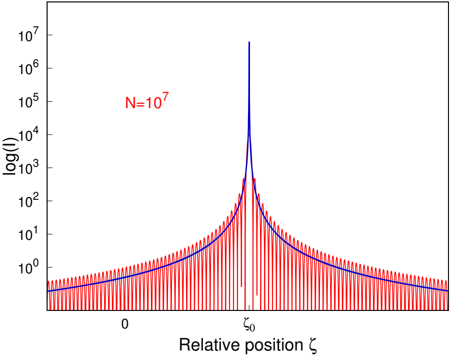

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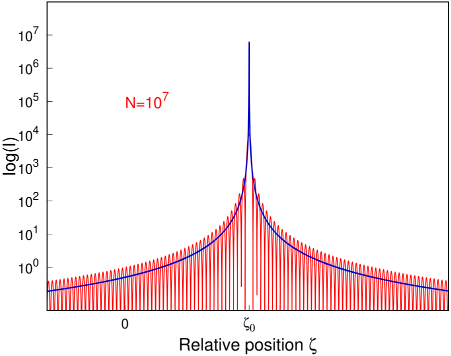

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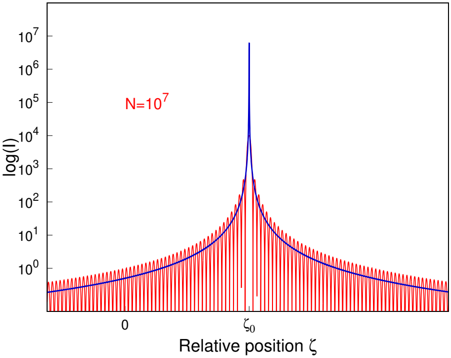

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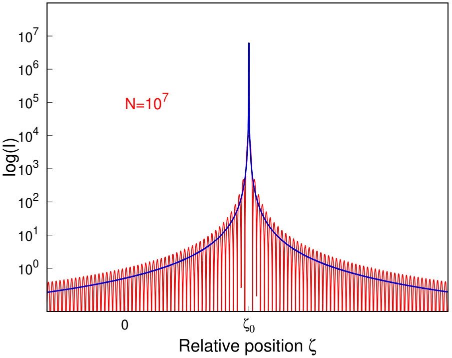

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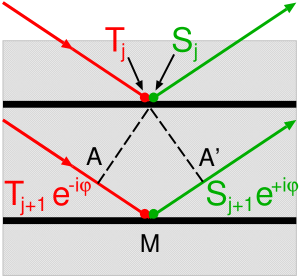
The kinematical limit clearly breaks down near ζ_0 so we need a dynamical diffraction theory

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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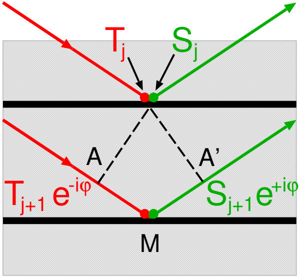

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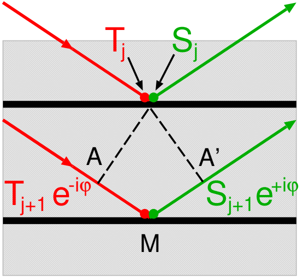

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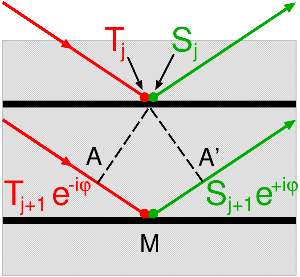

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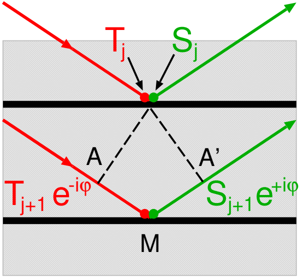

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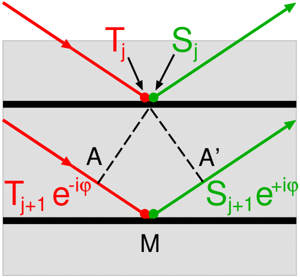

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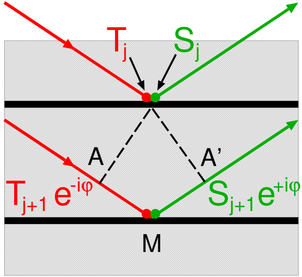

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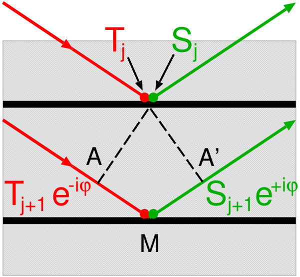

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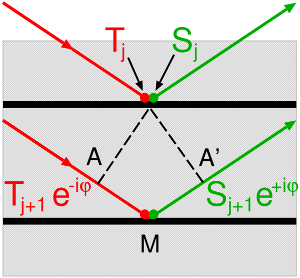
Difference equation

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



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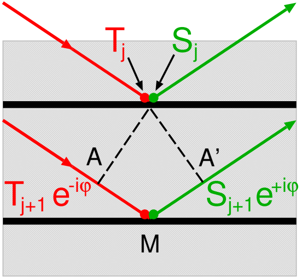

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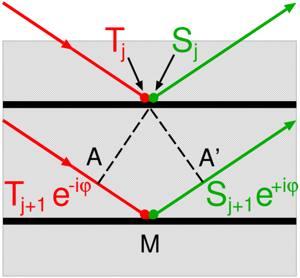

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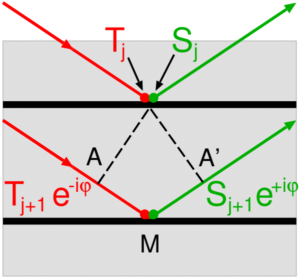

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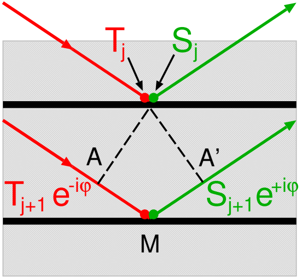

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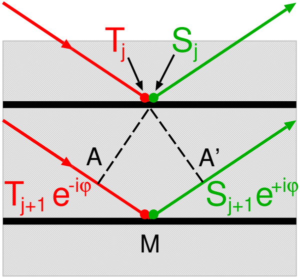

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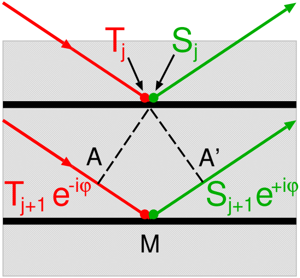

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these coupled equations must be solved for an infinite stack of atomic layers

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the fields T_j and T_{j+1} are out of phase by nearly $m\pi$ (top right equation) since g and g_0 are very small and the T wave field must attenuate as it penetrates deeper into the crystal so our trial solution is

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now substitute into the equation for S_j above

$$(1-ig_0)\,T_{j-1}e^{-i\phi} - T_j e^{-i2\phi} = g^2\,T_j + (1-ig_0)\left[(1-ig_0)\,T_j - T_{j+1}e^{-i\phi}\right]$$

$$(1-ig_0)e^{-i\phi}\left[T_{j+1} + T_{j-1}\right] = \left[g^2 + (1-ig_0)^2 + e^{-i2\phi}\right]T_j$$

the fields T_j and T_{j+1} are out of phase by nearly $m\pi$ (top right equation) since g and g_0 are very small and the T wave field must attenuate as it penetrates deeper into the crystal so our trial solution is

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

Solving for the T field

$$(1 - ig_0)e^{-i\phi}\left[T_{j+1} + T_{j-1}\right] = \left[g^2 + (1 - ig_0)^2 + e^{-i2\phi}\right] T_j$$

,

Solving for the T field

$$(1 - ig_0)e^{-i\phi}\left[T_{j+1} + T_{j-1}\right] = \left[g^2 + (1 - ig_0)^2 + e^{-i2\phi}\right] T_j$$

With the trial solution ,

Solving for the T field

$$(1 - ig_0)e^{-i\phi}\left[T_{j+1} + T_{j-1}\right] = \left[g^2 + (1 - ig_0)^2 + e^{-i2\phi}\right] T_j$$

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Solving for the T field

$$(1 - ig_0)e^{-i\phi}\left[T_{j+1} + T_{j-1}\right] = \left[g^2 + (1 - ig_0)^2 + e^{-i2\phi}\right] T_j$$

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Solving for the T field

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

and substituting this solution into the defining equation for T

Solving for the T field

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$$(1 - ig_0)e^{-i\phi}\left[e^{-\eta} e^{im\pi} T_j + e^{\eta} e^{-im\pi} T_j\right] = \left[g^2 + (1 - ig_0)^2 + e^{-i2\phi}\right] T_j$$

Solving for the T field

$$(1-ig_0)e^{-i\phi}\left[T_{j+1}+T_{j-1}\right]=\left[g^2+(1-ig_0)^2+e^{-i2\phi}\right]T_j$$

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

and substituting this solution into the defining equation for T and noting that $\phi\equiv m\pi+\Delta$

$$(1-ig_0)e^{-i\phi}\left[e^{-\eta}e^{im\pi}T_j+e^{\eta}e^{-im\pi}T_j\right]=\left[g^2+(1-ig_0)^2+e^{-i2\phi}\right]T_j$$

Solving for the T field

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$$(1-ig_0)e^{-im\pi}e^{-i\Delta}\left[e^{-\eta}e^{im\pi}+e^{\eta}e^{-im\pi}\right]=g^2+(1-ig_0)^2+e^{-i2m\pi}e^{-i2\Delta}$$

Solving for the T field

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

Solving for the T field

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

Solving for the T field

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$$(1 - ig_0)\cancel{e^{-im\pi}} e^{-i\Delta}\left[e^{-\eta}\cancel{e^{im\pi}} + e^{\eta}\cancel{e^{-im\pi}}\right] = g^2 + (1 - ig_0)^2 + \cancel{e^{-i2m\pi}} e^{-i2\Delta}$$

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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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Solving for the T field

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Cancelling and expanding all products keeping only second order terms

Solving for the T field

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

Cancelling and expanding all products keeping only second order terms

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

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

Solving for the T field

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

Cancelling and expanding all products keeping only second order terms

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

$$\cancel{2}-\cancel{2ig_0}-\cancel{2i\Delta}-2g_0\Delta-\Delta^2+\eta^2\approx g^2+\cancel{2}-\cancel{2ig_0}-\cancel{2i\Delta}-g_0^2-2\Delta^2$$

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

$$i\eta = \pm\sqrt{(\Delta - g_0) - g^2}$$

Solving for the T field

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with fields

Solving for the T field

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

Solving for the T field

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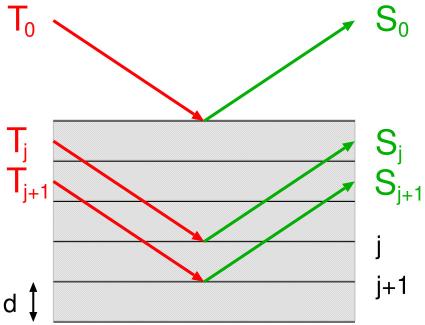
with fields

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

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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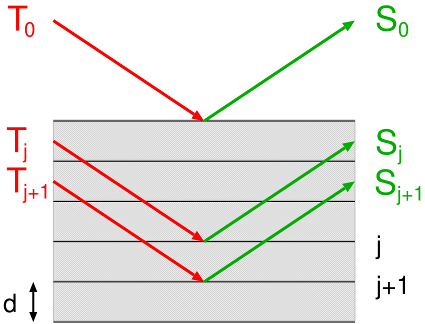

$$S_{j+1} = e^{-\eta} e^{im\pi} S_j$$

$$S_j = -igT_j + (1 - ig_0) S_{j+1} e^{i\phi}$$

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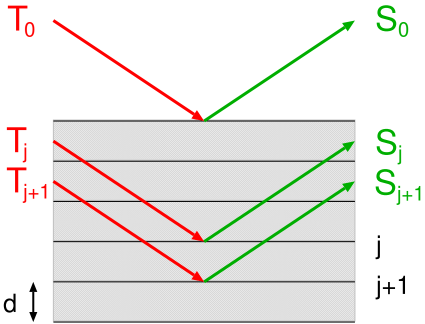

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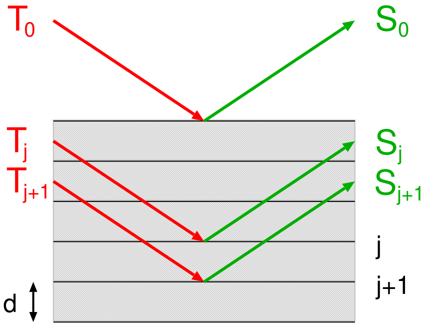

$$S_1 = e^{-\eta} e^{im\pi} S_0$$

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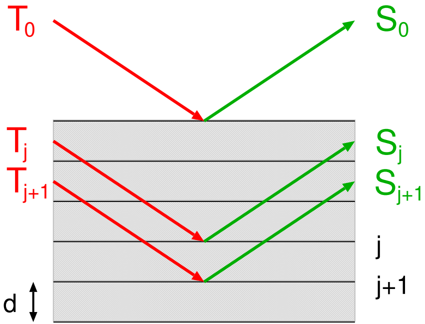

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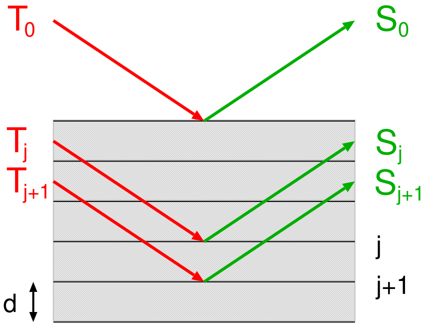

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$$S_0 \left[1 - (1 - ig_0) e^{-\eta} e^{i2m\pi} e^{i\Delta} \right] = -ig\,T_0$$

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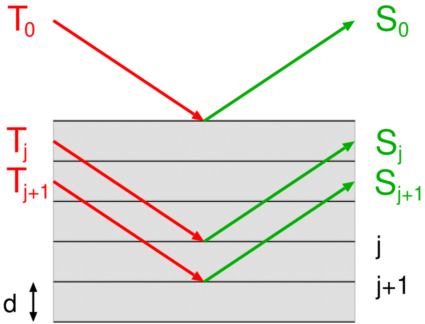

$$S_1 = e^{-\eta} e^{im\pi} S_0$$

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

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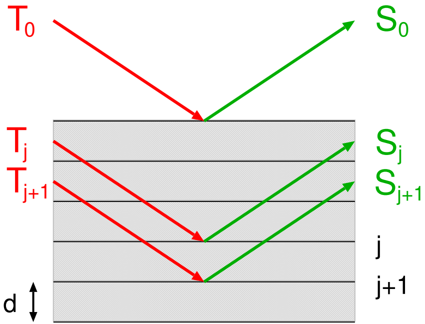

$$S_1 = e^{-\eta} e^{im\pi} S_0$$

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$$S_0 = -ig\, T_0 + (1 - ig_0) S_0 e^{-\eta} e^{im\pi} e^{im\pi} e^{i\Delta}$$

$$S_0 \left[1 - (1 - ig_0) e^{-\eta} e^{i2m\pi} e^{i\Delta} \right] = -ig\, T_0$$

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

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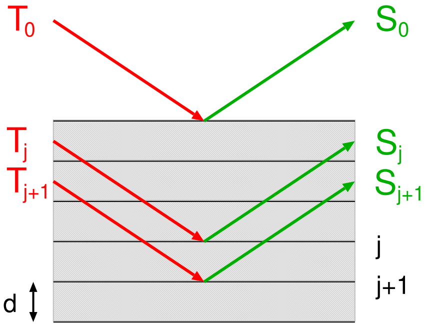

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$$S_0 = -ig\,T_0 + (1 - ig_0) S_1 e^{i\phi}$$

$$S_0 = -ig\,T_0 + (1 - ig_0) S_0 e^{-\eta} e^{im\pi} e^{im\pi} e^{i\Delta}$$

$$S_0 \left[1 - (1 - ig_0) e^{-\eta} e^{i2m\pi} e^{i\Delta}\right] = -ig\,T_0$$

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

Darwin reflectivity curve

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

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

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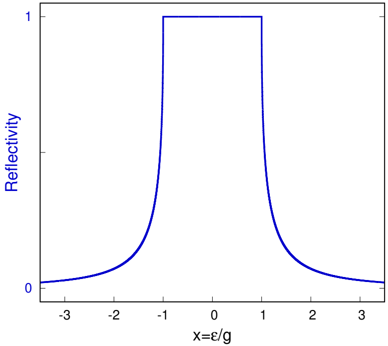

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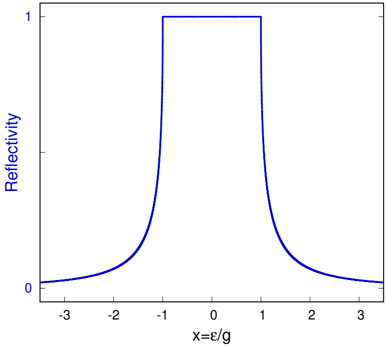

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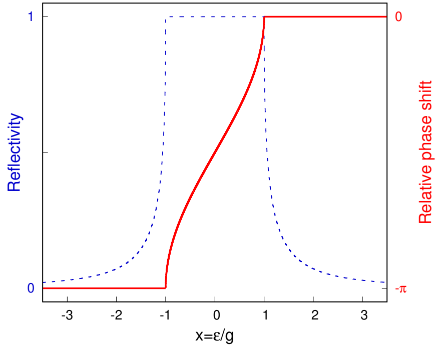

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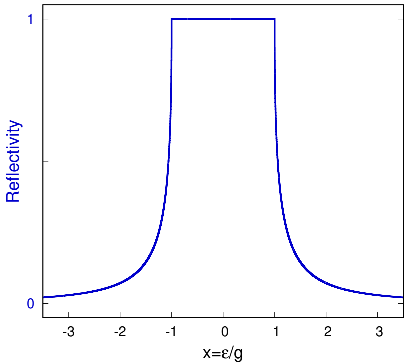
the relative phase between the scattered and transmitted waves varies from out of phase at $x = -1$ to in phase at $x = +1$

Darwin width



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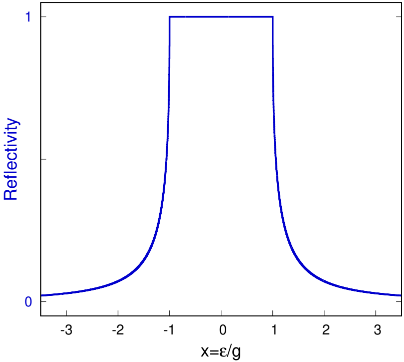

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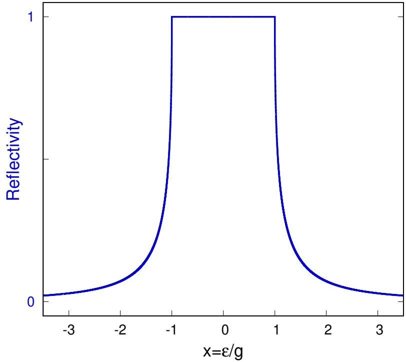

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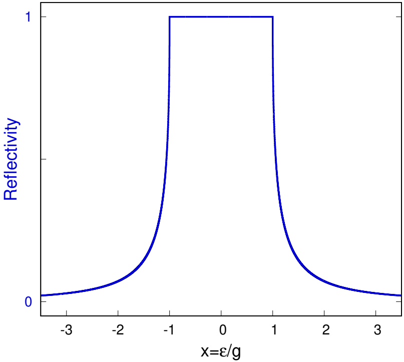

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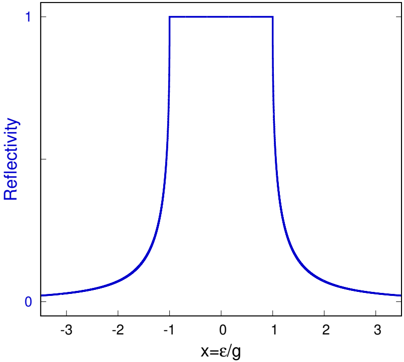

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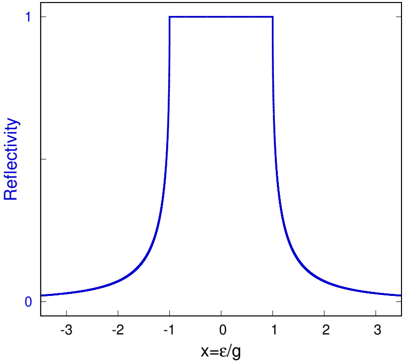

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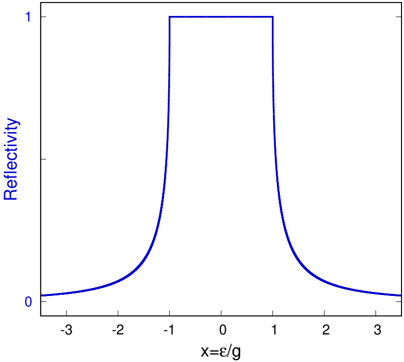

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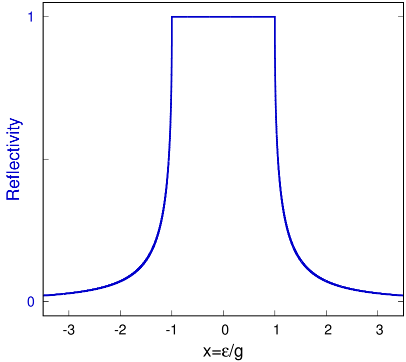

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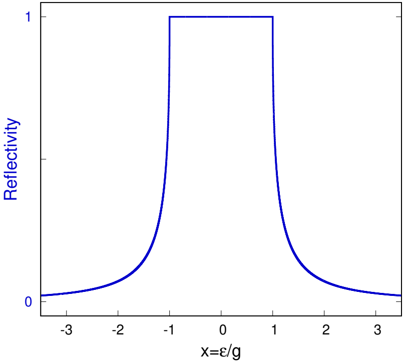

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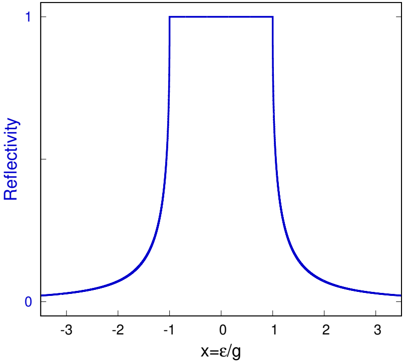

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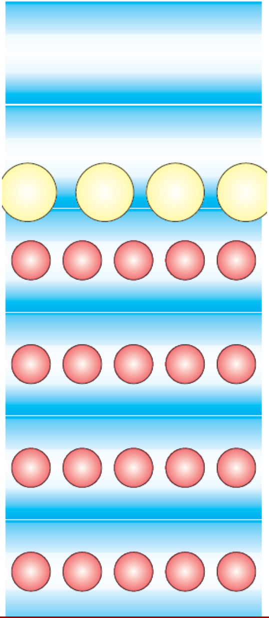
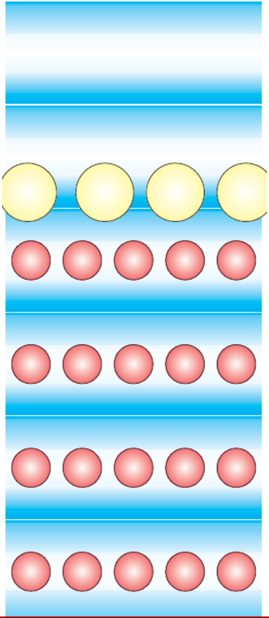
Standing waves



$\longleftarrow x = -1$

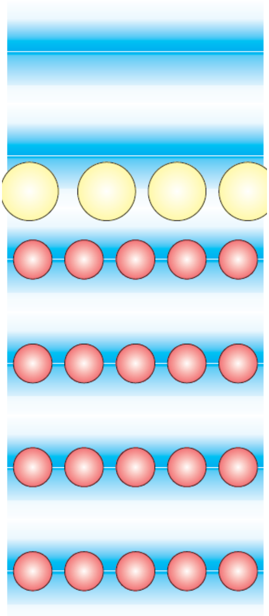
out of phase

Standing waves

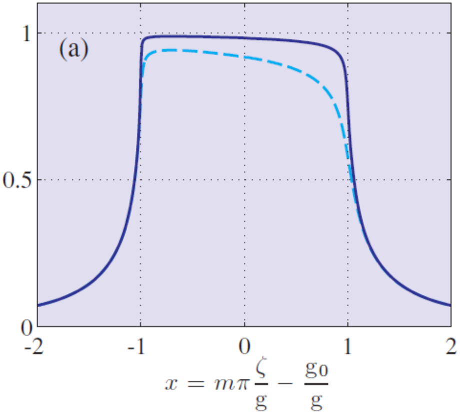


$\longleftarrow x = -1$
out of phase

$x = +1 \longrightarrow$
in phase



Absorption effects



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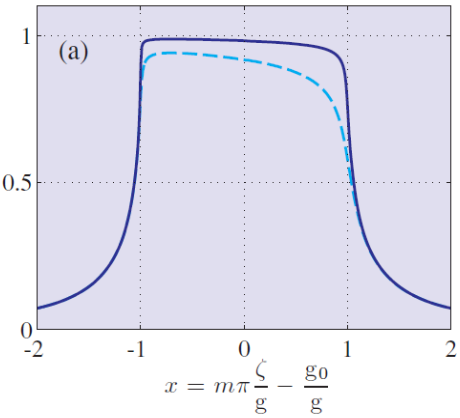
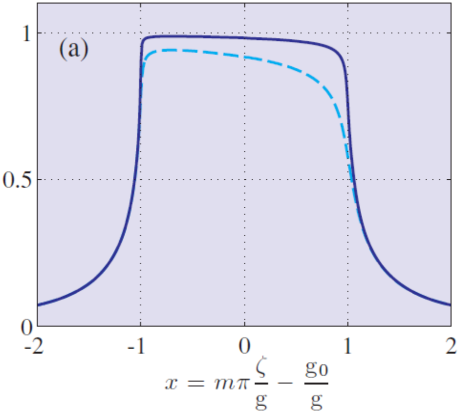


Silicon (111) Darwin curves

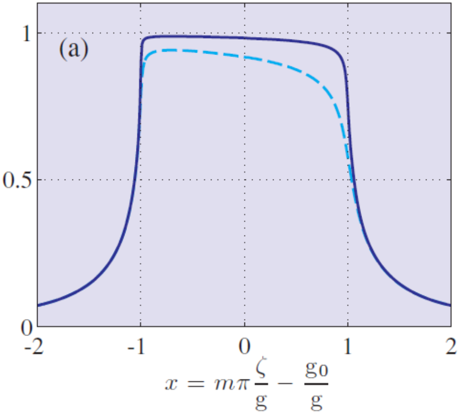
Absorption effects



Silicon (111) Darwin curves

solid line is for $\lambda = 0.70926$ Å

Absorption effects

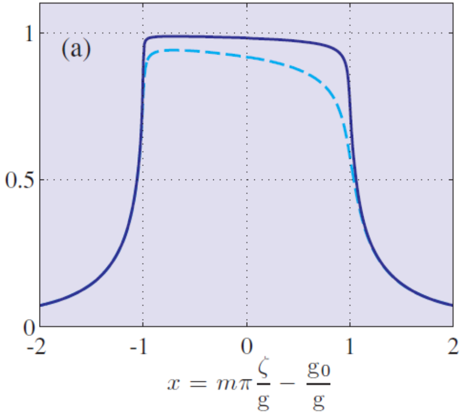


Silicon (111) Darwin curves

solid line is for $\lambda = 0.70926$ Å

dashed line is for $\lambda = 0.1.5405$ Å

Absorption effects



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solid line is for $\lambda = 0.70926$ Å

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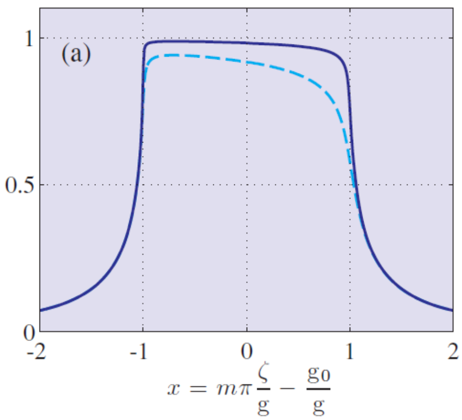
absorption is highest at $x = +1$ since the standing wave field is in phase with the atomic planes

Absorption effects



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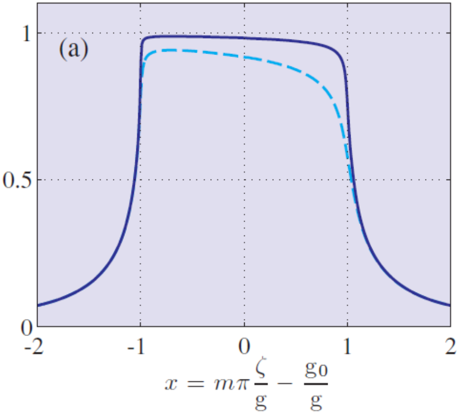

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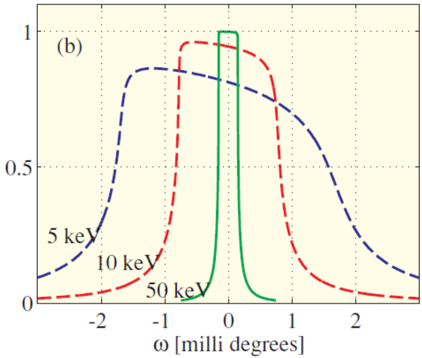
note that width of Darwin curve is independent of wavelength

Energy dependence



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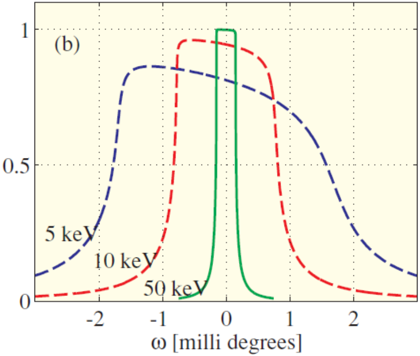
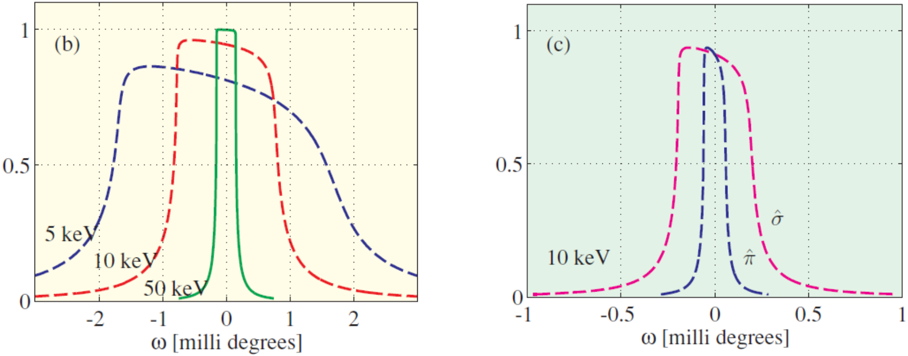


The angular Darwin width, w_D does depend on energy

Energy dependence



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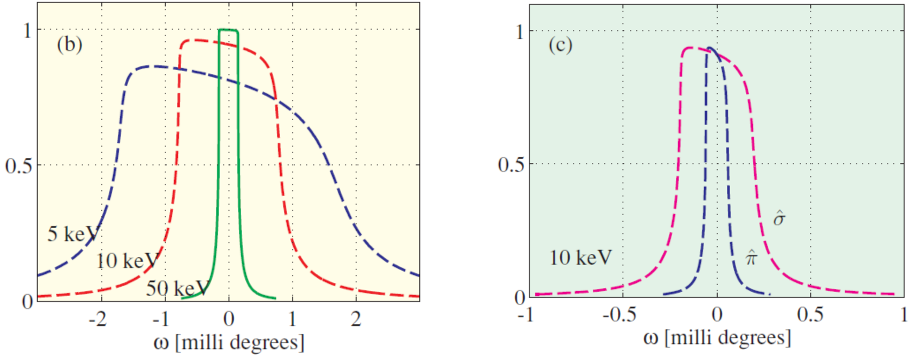
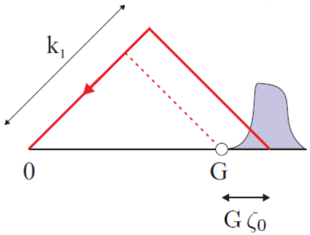


The angular Darwin width, w_D does depend on energy and polarization of the beam

Harmonic suppression

The displacement of the Darwin curve varies inversely as the order, m, of the reflection.



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The displacement of the Darwin curve varies inversely as the order, m, of the reflection.

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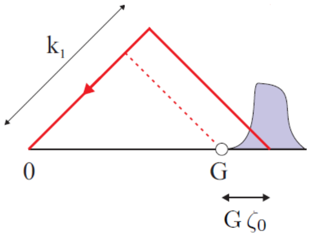
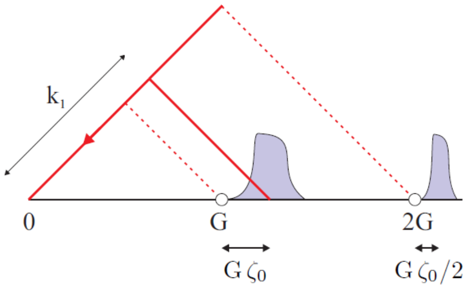


Harmonic suppression

The displacement of the Darwin curve varies inversely as the order, m, of the reflection. The width varies as the inverse squared.



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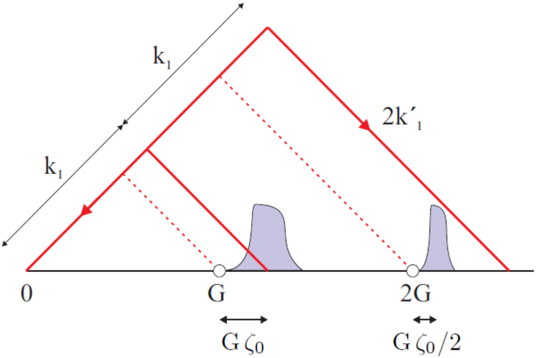

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By tuning to the center of a lower order reflection, the high orders can be effectively suppressed.

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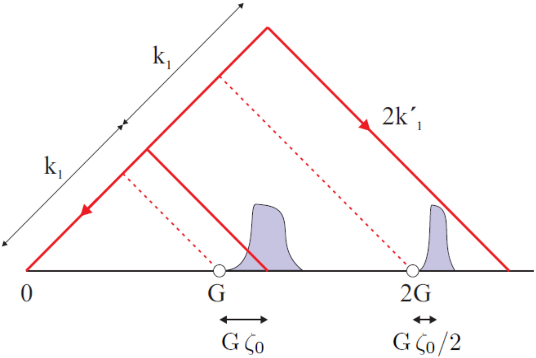

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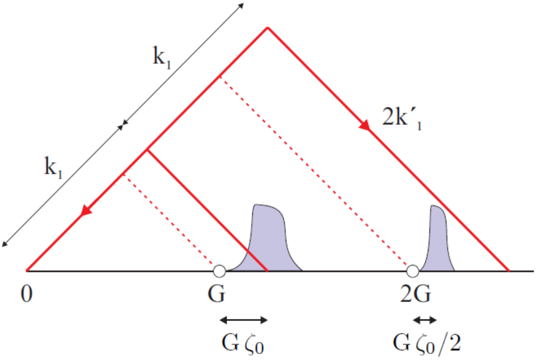
By tuning to the center of a lower order reflection, the high orders can be effectively suppressed.

By tuning a bit off on the "high" side we get even more suppression. This is called "detuning".

Angular offset

We can calculate the angular offset by noting that the offset and width have many common factors.



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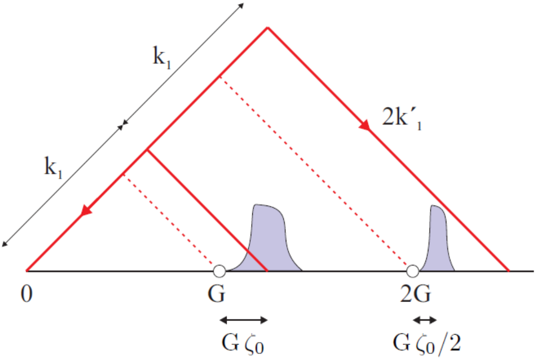

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$$\zeta^{off} = \frac{\zeta_0}{m} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}$$

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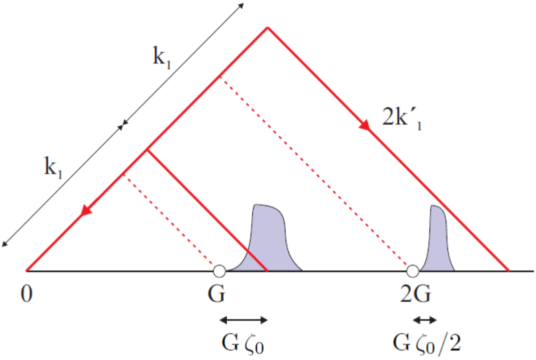

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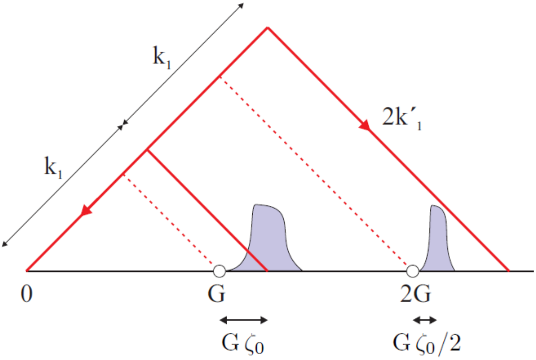
$$\Delta\theta^{off} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}\tan\theta$$

Angular offset

We can calculate the angular offset by noting that the offset and width have many common factors. Converting this to an angular offset.



$$\zeta_0 = \frac{2d^2|F_0|r_0}{\pi m v_c}$$

$$\zeta_D = \frac{4d^2|F|r_0}{\pi m^2 v_c}$$

$$\zeta^{off} = \frac{\zeta_0}{m} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}$$

$$\Delta\theta^{off} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}\tan\theta$$

For the Si(111) at $\lambda = 1.54056$Å

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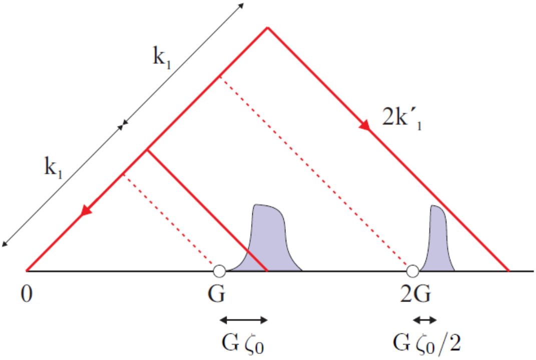

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For the Si(111) at $\lambda = 1.54056$Å

$$\omega_D^{total} = 0.0020^\circ$$

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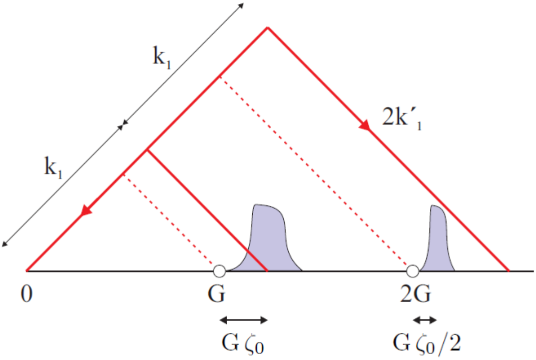

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For the Si(111) at $\lambda = 1.54056$Å

$$\omega_D^{total} = 0.0020^\circ \qquad \Delta\theta^{off} = 0.0018^\circ$$

Darwin widths

	$\zeta_D^{FWHM} \times 10^6$								
	(111)			(220)			(400)		
Diamond a= 3.5670 Å	61.0			20.9			8.5		
	3.03	0.018	-0.01	1.96	0.018	-0.01	1.59	0.018	-0.01
Silicon a= 5.4309 Å	139.8			61.1			26.3		
	10.54	0.25	-0.33	8.72	0.25	-0.33	7.51	0.25	-0.33
Germanium a= 5.6578 Å	347.2			160.0			68.8		
	27.36	-1.1	-0.89	23.79	-1.1	-0.89	20.46	-1.1	-0.89

the quantities below the widths are $f^0(Q)$, f', and f'' (for $\lambda = 1.5405\,\text{Å}$). For an angular width, multiply times $\tan\theta$ and for π polarization, multiply by $\cos(2\theta)$.