

Today's outline - September 16, 2024





- Limiting cases of Fresnel equations

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- Reflection from a thin slab

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- Parratt's exact recursive calculation

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Reading Assignment: Chapter 3.7–3.8

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- Reflection from a thin slab
- Kiessig fringes
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation

Reading Assignment: Chapter 3.7–3.8

Homework Assignment #03:

Chapter 3: 1,3,4,6,8

due Monday, September 30, 2024



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- Reflection from a thin slab
- Kiessig fringes
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation

Reading Assignment: Chapter 3.7–3.8

Homework Assignment #03:

Chapter 3: 1,3,4,6,8

due Monday, September 30, 2024

Homework Assignment #04:

Chapter 4: 2,4,6,7,10

due Monday, October 14, 2024

Fresnel equation review



The scattering vector (or momentum transfer)
is given by

Fresnel equation review



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$$Q = \frac{4\pi}{\lambda} \sin \alpha$$

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and for small angles

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The scattering vector (or momentum transfer) is given by

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$$Q = \frac{4\pi}{\lambda} \sin \alpha = 2k \sin \alpha \approx 2k\alpha$$

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similarly for the critical angle we define

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using the reduced scattering vectors, the three defining optical equations become

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$$q^2 = q'^2 + 1 - 2ib_\mu, \quad b_\mu = \frac{2k}{Q_c^2} \mu$$

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Limiting cases - $q \gg 1$



Starting with Snell's Law

$$q^2 = q'^2 + 1 - 2ib_\mu$$



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$$q^2 = q'^2 + 1 - 2ib_\mu$$

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rearrange and simplify for $q \gg 1$ and real

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this implies $Re(q') \approx q$,



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this implies $Re(q') \approx q$, while the imaginary part can be computed by assuming



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$$q' = q + i Im(q')$$



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$$q'^2 = q^2 \left(1 + i \frac{Im(q')}{q} \right)^2$$



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$$Im(q')q \approx b_\mu$$



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the reflected wave is in phase with the incident wave, almost total transmission

Limiting cases - $q \ll 1$



Starting with Snell's Law again

$$q^2 = q'^2 + 1 - 2ib_\mu$$

Limiting cases - $q \ll 1$



Starting with Snell's Law again

when $q \ll 1$

$$q^2 = q'^2 + 1 - 2ib_\mu$$

$$q'^2 = q^2 - 1 + 2ib_\mu$$

Limiting cases - $q \ll 1$



Starting with Snell's Law again

when $q \ll 1$, q' is mostly imaginary with magnitude 1 since b_μ is very small

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Limiting cases - $q \ll 1$

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$$\Lambda \approx \frac{1}{Q_c}$$



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$$\Lambda \approx \frac{1}{Q_c}$$

The reflected wave is out of phase with the incident wave, there is only small transmission in the form of an evanescent wave, and the penetration depth is very short.

Limiting cases - $q \sim 1$



Using Snell's Law, with $q \sim 1$,

$$q^2 = q'^2 + 1 - 2ib_\mu$$



Limiting cases - $q \sim 1$

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$$q'^2 \approx 2ib_\mu$$



Limiting cases - $q \sim 1$

Using Snell's Law, with $q \sim 1$,

adding and subtracting b_μ ,

$$q^2 = q'^2 + 1 - 2ib_\mu$$

$$q'^2 = q^2 - 1 + 2ib_\mu$$

$$q'^2 \approx 2ib_\mu = b_\mu(1 + 2i - 1)$$



Limiting cases - $q \sim 1$

Using Snell's Law, with $q \sim 1$,

adding and subtracting b_μ ,

q' is complex with real and imaginary parts of equal magnitude.

$$q^2 = q'^2 + 1 - 2ib_\mu$$

$$q'^2 = q^2 - 1 + 2ib_\mu$$

$$q'^2 \approx 2ib_\mu = b_\mu(1 + 2i - 1) = b_\mu(1 + i)^2$$



Limiting cases - $q \sim 1$

Using Snell's Law, with $q \sim 1$,

adding and subtracting b_μ ,

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Limiting cases - $q \sim 1$

Using Snell's Law, with $q \sim 1$,

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The reflected wave is in phase with the incident, there is significant (larger amplitude than the reflection) transmission with a large penetration depth.

Review of interface effects

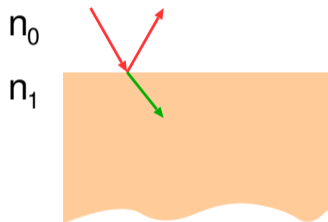


We have covered the interface boundary conditions which govern the transmission and reflection of waves at a change in medium.

Review of interface effects



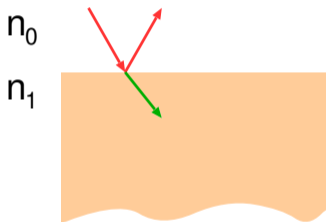
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Review of interface effects



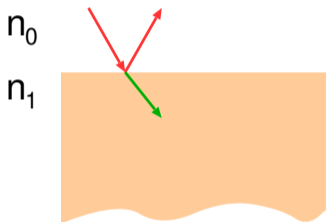
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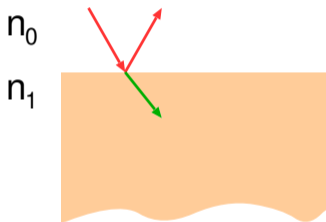


$$r = \frac{Q - Q'}{Q + Q'}$$

Review of interface effects



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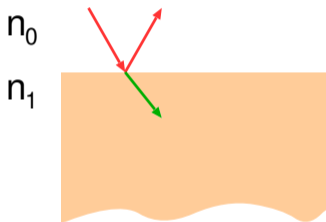
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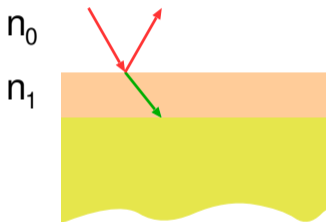
$$t = \frac{2Q}{Q + Q'}$$

We have assumed that the transmitted wave eventually attenuates to zero in all cases due to absorption.

Review of interface effects



We have covered the interface boundary conditions which govern the transmission and reflection of waves at a change in medium. These result in the Fresnel equations which we rewrite here in terms of the momentum transfer.



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$$t = \frac{2Q}{Q + Q'}$$

We have assumed that the transmitted wave eventually attenuates to zero in all cases due to absorption. We now consider what happens if there is a second interface encountered by the transmitted wave before it dies away. That is, a thin slab of material on top of an infinite substrate

Reflection and transmission coefficients

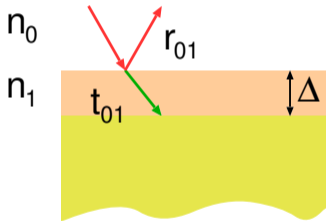


For a slab of thickness Δ on a substrate, the transmission and reflection coefficients at each interface are labeled:

Reflection and transmission coefficients



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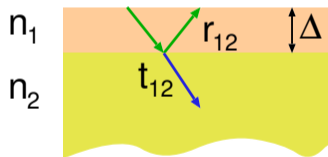
r_{01} – reflection in n_0 off n_1

t_{01} – transmission from n_0 into n_1

Reflection and transmission coefficients



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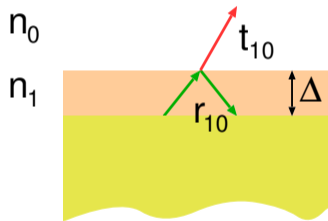
r_{12} – reflection in n_1 off n_2

t_{12} – transmission from n_1 into n_2

Reflection and transmission coefficients



For a slab of thickness Δ on a substrate, the transmission and reflection coefficients at each interface are labeled:



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r_{12} – reflection in n_1 off n_2

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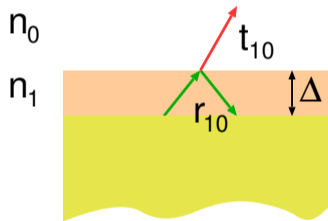
r_{10} – reflection in n_1 off n_0

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Reflection and transmission coefficients



For a slab of thickness Δ on a substrate, the transmission and reflection coefficients at each interface are labeled:



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t_{12} – transmission from n_1 into n_2

r_{10} – reflection in n_1 off n_0

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Build the composite reflection coefficient from all possible events

Overall reflection from a slab

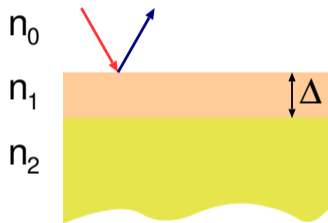


The composite reflection coefficient for each ray emerging from the top surface is computed

Overall reflection from a slab



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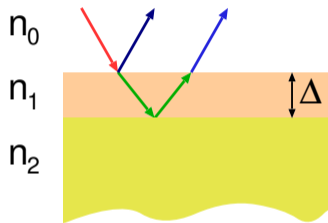


r_{01}

Overall reflection from a slab



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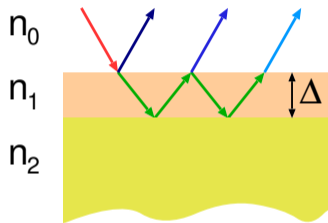


$$r_{01} + t_{01} r_{12} t_{10}$$

Overall reflection from a slab



The composite reflection coefficient for each ray emerging from the top surface is computed

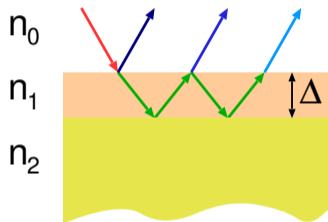


$$\begin{aligned} & r_{01} \\ & + \\ & t_{01} r_{12} t_{10} \\ & + \\ & t_{01} r_{12} r_{10} r_{12} t_{10} \end{aligned}$$

Overall reflection from a slab



The composite reflection coefficient for each ray emerging from the top surface is computed



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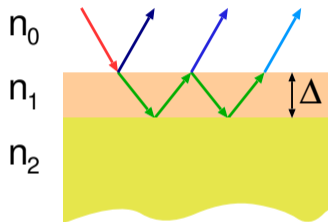
Inside the medium, the x-rays are travelling an additional 2Δ per traversal. This adds a phase shift of

$$p^2 = e^{i2(k_1 \sin \alpha_1)\Delta}$$

Overall reflection from a slab



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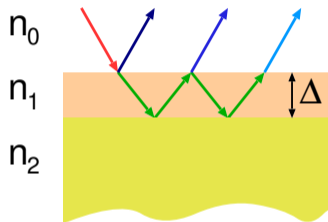
Inside the medium, the x-rays are travelling an additional 2Δ per traversal. This adds a phase shift of

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Overall reflection from a slab



The composite reflection coefficient for each ray emerging from the top surface is computed



$$\begin{aligned} & r_{01} \\ & + \\ & t_{01} r_{12} t_{10} \cdot p^2 \\ & + \\ & t_{01} r_{12} r_{10} r_{12} t_{10} \end{aligned}$$

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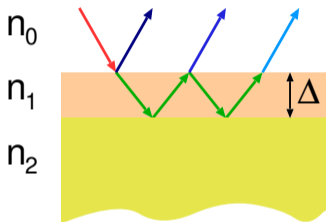
$$p^2 = e^{i2(k_1 \sin \alpha_1)\Delta} = e^{iQ_1\Delta}$$

which multiplies the reflection coefficient

Overall reflection from a slab



The composite reflection coefficient for each ray emerging from the top surface is computed



$$\begin{aligned} & r_{01} \\ & + \\ & t_{01} r_{12} t_{10} \cdot p^2 \\ & + \\ & t_{01} r_{12} r_{10} r_{12} t_{10} \cdot p^4 \end{aligned}$$

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$$p^2 = e^{i2(k_1 \sin \alpha_1)\Delta} = e^{iQ_1\Delta}$$

which multiplies the reflection coefficient with each pass through the slab

Composite reflection coefficient



The composite reflection coefficient can now be expressed as a sum

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$$r_{slab} = r_{01} + t_{01}r_{12}t_{10}p^2 + t_{01}r_{10}r_{12}^2t_{10}p^4 + t_{01}r_{10}^2r_{12}^3t_{10}p^6 + \dots$$

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factoring out the second term from
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$$\begin{aligned} r_{slab} &= r_{01} + t_{01}t_{10}r_{12}p^2 \sum_{m=0}^{\infty} (r_{10}r_{12}p^2)^m \\ &= r_{01} + t_{01}t_{10}r_{12}p^2 \frac{1}{1 - r_{10}r_{12}p^2} \end{aligned}$$

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The individual reflection and transmission coefficients can be determined using the Fresnel equations. Recall

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Composite reflection coefficient



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The individual reflection and transmission coefficients can be determined using the Fresnel equations. Recall

$$r = \frac{Q - Q'}{Q + Q'}, \quad t = \frac{2Q}{Q + Q'}$$

Fresnel equation identity

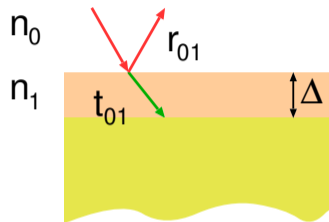


Applying the Fresnel equations to the top interface



Fresnel equation identity

Applying the Fresnel equations to the top interface

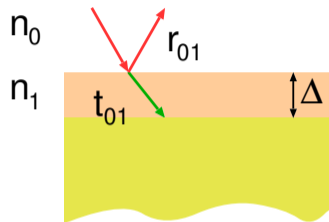


$$r_{01} = \frac{Q_0 - Q_1}{Q_0 + Q_1}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



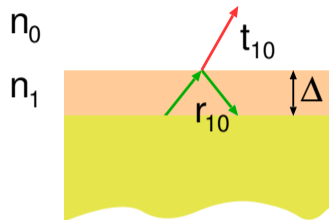
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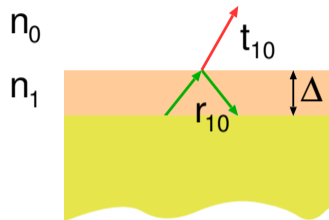
$$t_{01} = \frac{2Q_0}{Q_0 + Q_1}$$

$$r_{10} = \frac{Q_1 - Q_0}{Q_1 + Q_0} = -r_{01}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



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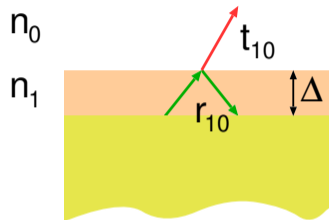
$$r_{10} = \frac{Q_1 - Q_0}{Q_1 + Q_0} = -r_{01}$$

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Fresnel equation identity

Applying the Fresnel equations to the top interface



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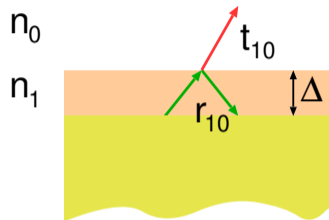
we can, therefore, construct the following identity

$$r_{01}^2 + t_{01}t_{10}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



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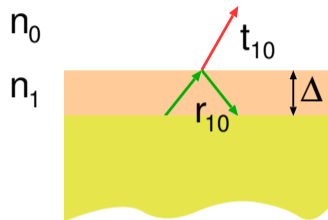
we can, therefore, construct the following identity

$$r_{01}^2 + t_{01}t_{10} = \frac{(Q_0 - Q_1)^2}{(Q_0 + Q_1)^2} + \frac{2Q_0}{Q_0 + Q_1} \frac{2Q_1}{Q_1 + Q_0}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



$$r_{01} = \frac{Q_0 - Q_1}{Q_0 + Q_1}$$

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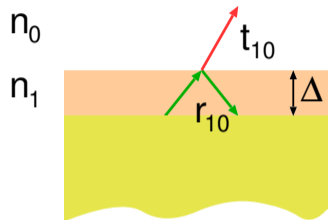
we can, therefore, construct the following identity

$$r_{01}^2 + t_{01}t_{10} = \frac{(Q_0 - Q_1)^2}{(Q_0 + Q_1)^2} + \frac{2Q_0}{Q_0 + Q_1} \frac{2Q_1}{Q_1 + Q_0} = \frac{Q_0^2 - 2Q_0Q_1 + Q_1^2 + 4Q_0Q_1}{(Q_0 + Q_1)^2}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



$$r_{01} = \frac{Q_0 - Q_1}{Q_0 + Q_1}$$

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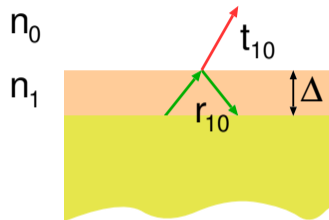
we can, therefore, construct the following identity

$$\begin{aligned} r_{01}^2 + t_{01}t_{10} &= \frac{(Q_0 - Q_1)^2}{(Q_0 + Q_1)^2} + \frac{2Q_0}{Q_0 + Q_1} \frac{2Q_1}{Q_1 + Q_0} = \frac{Q_0^2 - 2Q_0Q_1 + Q_1^2 + 4Q_0Q_1}{(Q_0 + Q_1)^2} \\ &= \frac{Q_0^2 + 2Q_0Q_1 + Q_1^2}{(Q_0 + Q_1)^2} \end{aligned}$$



Fresnel equation identity

Applying the Fresnel equations to the top interface



$$r_{01} = \frac{Q_0 - Q_1}{Q_0 + Q_1}$$

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Reflection coefficient of a slab



Starting with the reflection coefficient of the slab obtained earlier

Reflection coefficient of a slab



Starting with the reflection coefficient of the slab obtained earlier

$$r_{slab} = r_{01} + t_{01} t_{10} r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2}$$

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Kiessig fringes



$$p^2 = e^{iQ_1\Delta}$$

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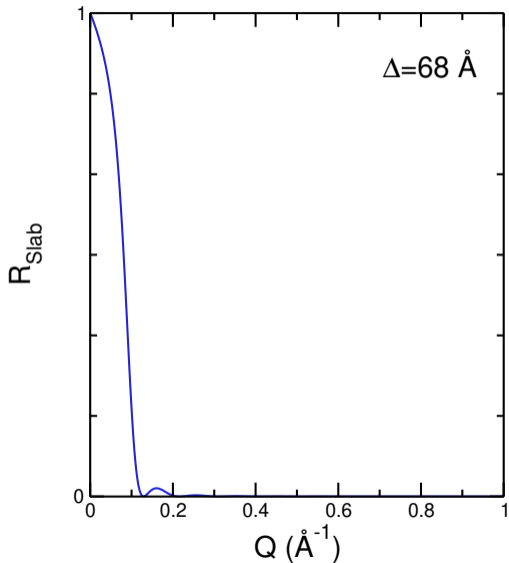


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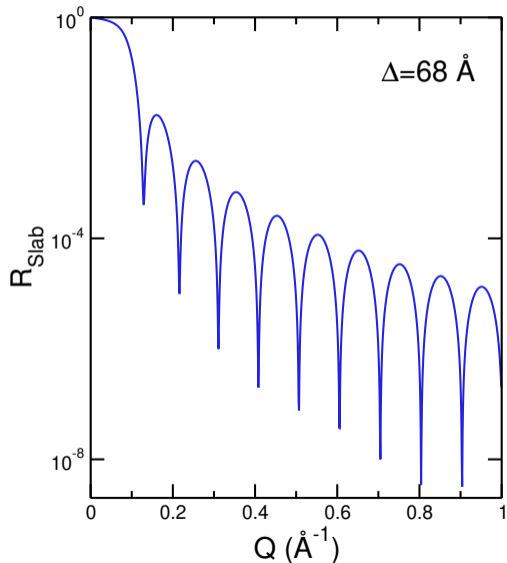


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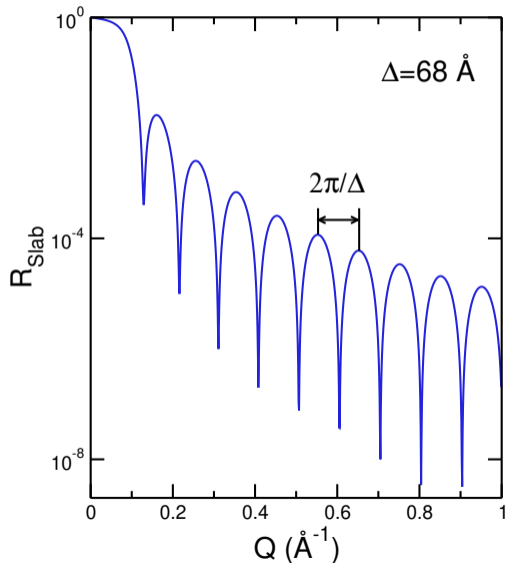
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$$2\pi/\Delta = 0.092\text{\AA}^{-1}$$



Kinematical reflection from a thin slab



Recall the reflection coefficient for a thin slab.

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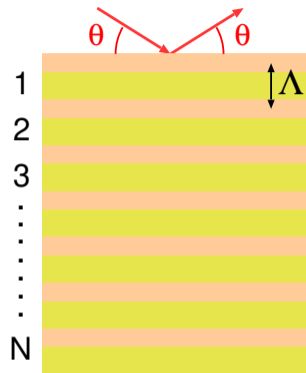
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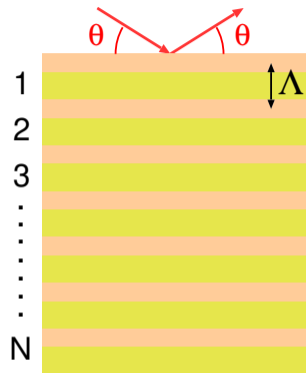
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Multilayers in the kinematical regime



N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast ($\rho_A > \rho_B$).

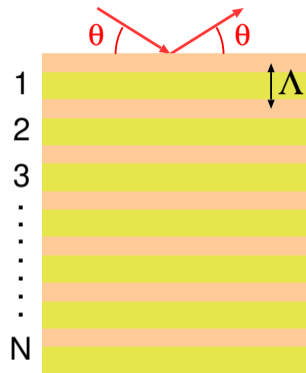
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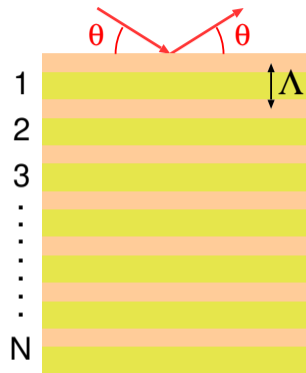


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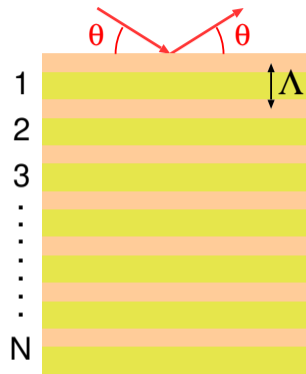
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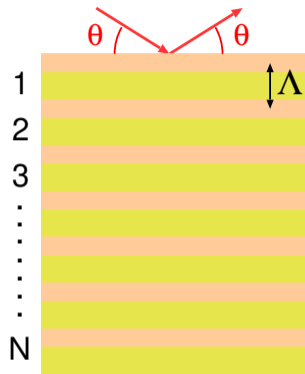
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Form a stack of N bilayers

$$r_N(\zeta) = \sum_{\nu=0}^{N-1} r_1(\zeta) e^{i2\pi\zeta\nu} e^{-\beta\nu}$$

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Form a stack of N bilayers

$$r_N(\zeta) = \sum_{\nu=0}^{N-1} r_1(\zeta) e^{i2\pi\zeta\nu} e^{-\beta\nu} = r_1(\zeta) \frac{1 - e^{i2\pi\zeta N} e^{-\beta N}}{1 - e^{i2\pi\zeta} e^{-\beta}}$$

Reflectivity of a bilayer



The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components

Reflectivity of a bilayer



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Absorption coefficient of a bilayer



The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB} \left(\frac{\Lambda^2\Gamma}{\zeta} \right) \frac{\sin(\pi\Gamma\zeta)}{\pi\Gamma\zeta} \frac{1 - e^{i2\pi\zeta N} e^{-\beta N}}{1 - e^{i2\pi\zeta} e^{-\beta}}$$

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Absorption coefficient of a bilayer



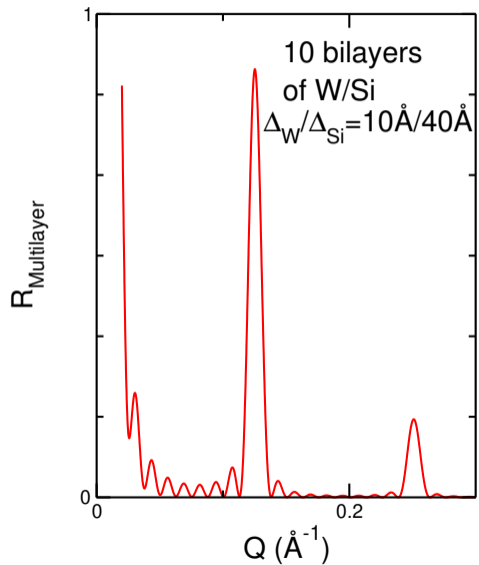
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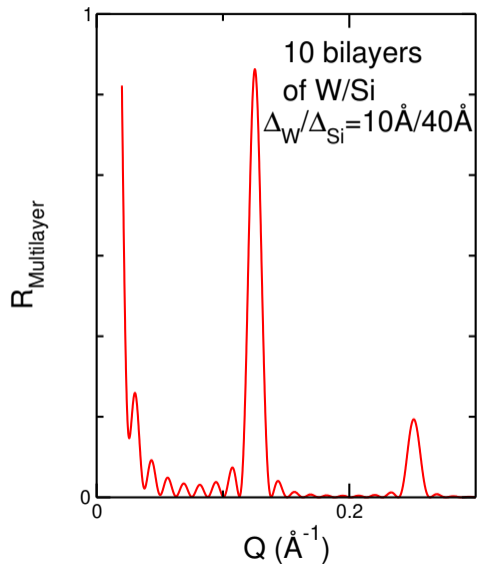
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Reflectivity calculation

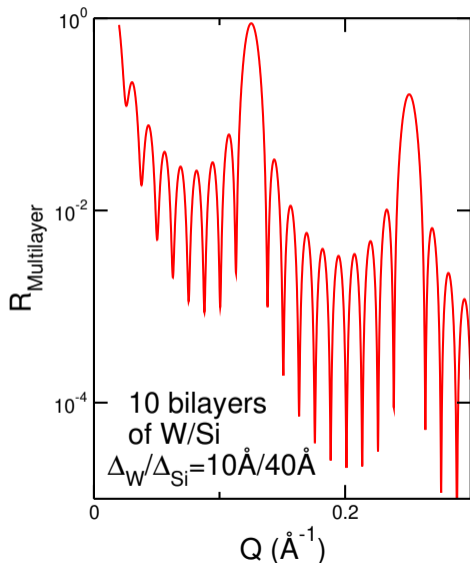


Reflectivity calculation



When $\zeta = Q\Lambda/2\pi$ is an integer, we have peaks

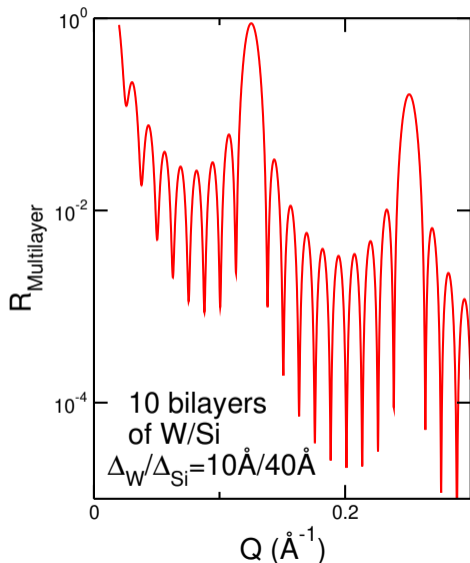
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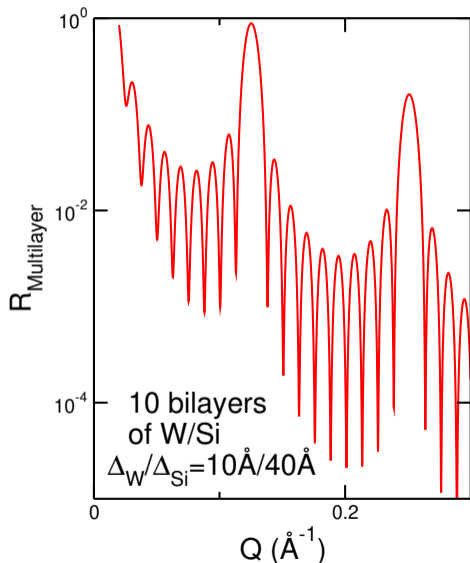


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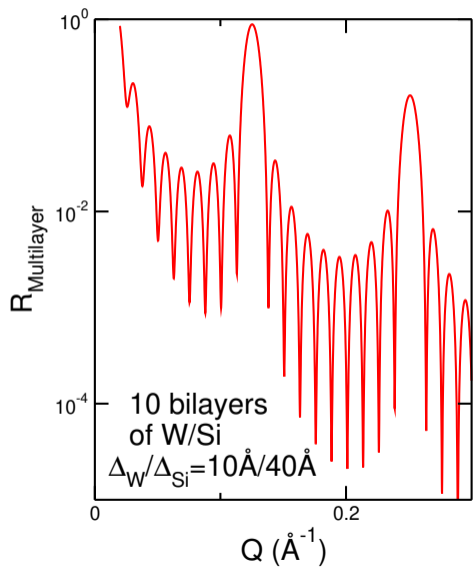
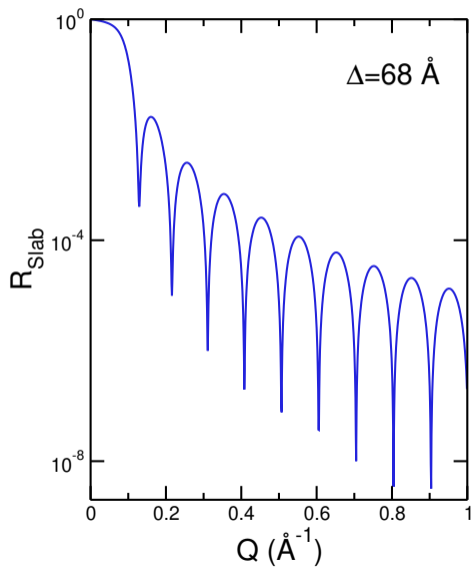
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Multilayers are used commonly on laboratory sources as well as at synchrotrons as mirrors

Slab - multilayer comparison



Parratt's recursive method



Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

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take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

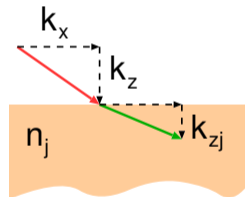
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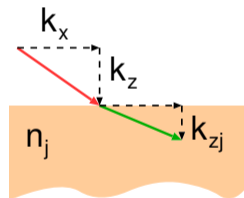


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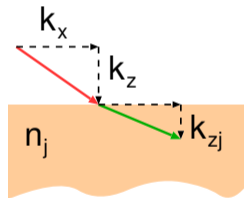


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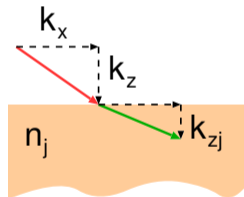


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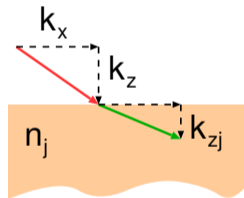


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and the wavevector transfer in the j^{th} layer

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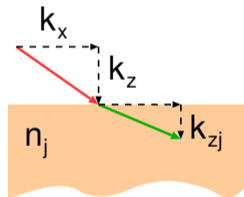
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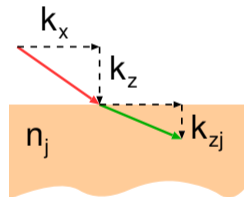


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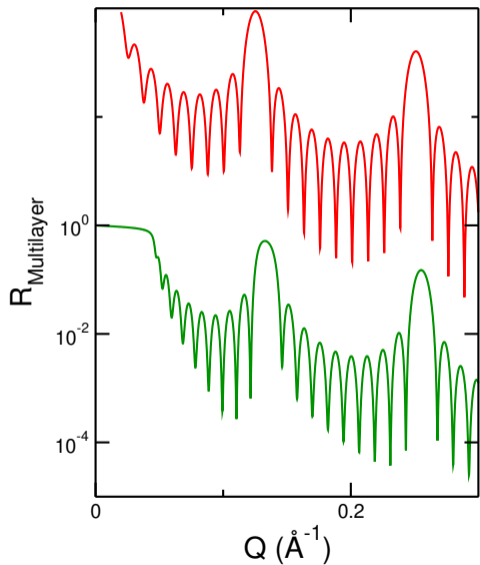
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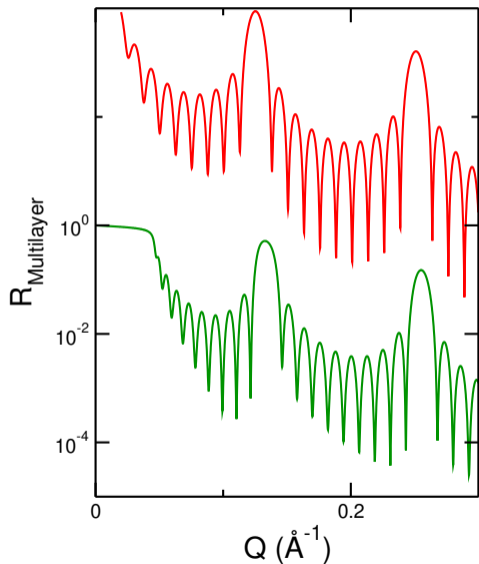
The recursive relation can be seen from the calculation of reflectivity of the next layer up

$$r_{N-2,N-1} = \frac{r'_{N-2,N-1} + r_{N-1,N} p_{N-1}^2}{1 + r'_{N-2,N-1} r_{N-1,N} p_{N-1}^2}$$

Kinematical - Parratt comparison

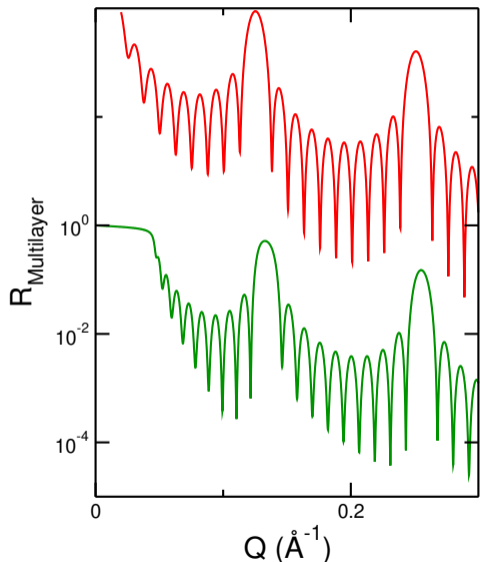


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Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions.

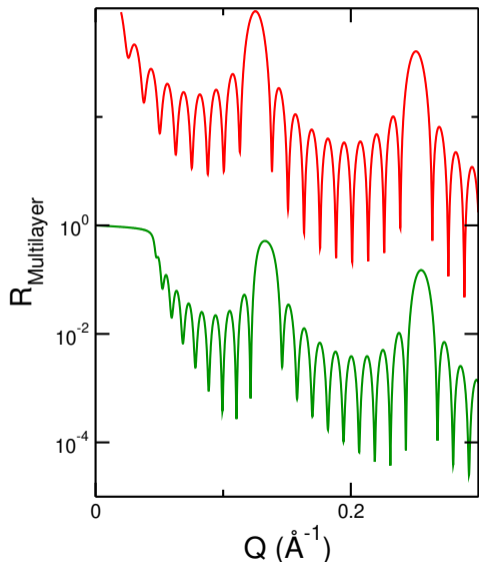
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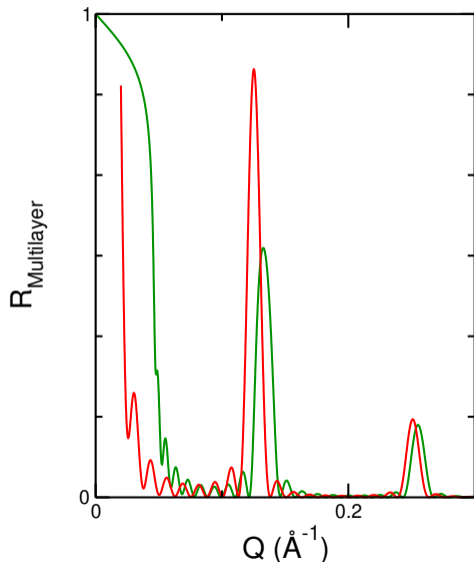


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Peaks in kinematical calculation are somewhat higher reflectivity than true value.