Today’s Outline - February 05, 2015

- Reflection from a thin slab
- Kiessig fringes
- Kinematical approximation for a thin slab
- Multilayers in the Kinematical Regime
- Parratt’s exact recursive calculation
- Reflection from a graded index

Reading Assignment: Chapter 3.5–3.8

Homework Assignment #02: Problems on Blackboard due Thursday, February 12, 2015

No class on Tuesday, February 10, 2015
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Homework Assignment #02:
Problems on Blackboard
due Thursday, February 12, 2015

No class on Tuesday, February 10, 2015
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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\[ n_0 \rightarrow \text{reflection} \rightarrow n_1 \]

\[ n_0 \rightarrow \text{transmission} \rightarrow n_1 \]

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.
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.

\[
\begin{align*}
\mathbf{n}_0 & \quad \mathbf{n}_1 \\
\end{align*}
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\[
n_0 \quad \text{\small \begin{array}{c} n_0 \end{array}} \quad n_1 \quad \text{\small \begin{array}{c} n_1 \end{array}}
\]

\[
r = \frac{Q - Q'}{Q + Q'}
\]

\[
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Reflection and Transmission Coefficients

For a slab of thickness $\Delta$ on a substrate, the transmission and reflection coefficients at each interface are labeled:
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Reflection and Transmission Coefficients

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

\[ r_{12} \] reflection in $n_1$ off $n_2$
\[ t_{12} \] transmission from $n_1$ into $n_2$

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- $t_{12}$ – transmission from $n_1$ into $n_2$
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- $t_{12}$ – transmission from $n_1$ into $n_2$
- $r_{10}$ – reflection in $n_1$ off $n_0$
- $t_{10}$ – transmission from $n_1$ into $n_0$

Build the composite reflection coefficient from all possible events.
The composite reflection coefficient for each ray emerging from the top surface is computed

\[ r_01 + t_01 r_{12} t_{10} \cdot p_2 + t_01 r_{12} r_{10} r_{12} t_{10} \cdot p_4 \]

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

\[ p_2 = e^{i2(k_1 \sin \alpha_1)\Delta} = e^{iQ_1\Delta} \]

which multiplies the reflection coefficient with each pass through the slab.
Overall Reflection from a Slab

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

\[ r_{01} \]

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Overall Reflection from a Slab

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\[ n_0 \]

\[ n_1 \]

\[ n_2 \]

\[ \Delta \]

\[ r_{01} \]

\[ + \]

\[ t_{01} r_{12} t_{10} \]

\[ + \]

\[ t_{01} r_{12} r_{10} r_{12} t_{10} \]

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

\[ r_{01} \]

\[ + \]

\[ t_{01} r_{12} t_{10} \cdot p^2 \]

\[ + \]

\[ t_{01} r_{12} r_{10} r_{12} t_{10} \cdot p^4 \]

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

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

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

\[ r_{\text{slab}} = r_{01} + t_{01}r_{12}t_{10}p_2 + t_{01}r_{10}r_{21}t_{10}p_4 + \cdots + \sum_{m=0}^{\infty} \left( r_{10}r_{12}p_2 \right)^m \]

Factoring out second term from all the rest.

Summing the geometric series as previously.

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

\[ r = Q - Q', \quad t = 2QQ' + Q' \]
Composite Reflection Coefficient

The composite reflection coefficient can now be expressed as a sum

\[ r_{slab} = r_0 + t_0 r_{12} t_{10} p^2 + t_0 r_{10} r_{12} t_{10} p^4 + t_0 r_{10} r_{12} t_{10} p^6 + \cdots \]
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\[ r = Q - Q' Q + Q', \]
\[ t = 2 Q Q + Q'. \]
The composite reflection coefficient can now be expressed as a sum

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\[ r_{slab} = r_0 + t_{01} t_{10} r_{12} p^2 \sum_{m=0}^{\infty} (r_{10} r_{12} p^2)^m \]

= \[ r_0 + t_{01} t_{10} r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

factoring out second term from all the rest

summing the geometric series as previously
The composite reflection coefficient can now be expressed as a sum

\[ r_{\text{slab}} = r_{01} + t_{01} r_{12} t_{10} p^2 + t_{01} r_{10} r_{12}^2 t_{10} p^4 + t_{01} r_{10}^2 r_{12}^3 t_{10} p^6 + \cdots \]

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

\[ r = \frac{Q - Q'}{Q + Q'} \]

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The composite reflection coefficient can now be expressed as a sum

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

Factoring out the second term from all the rest and summing the geometric series as previously, we get:

$$r_{slab} = r_{01} + t_{01} t_{10} r_{12} p^2 \sum_{m=0}^{\infty} \left( r_{10} r_{12} p^2 \right)^m$$

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

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

\[ r = \frac{Q - Q'}{Q + Q'}, \quad t = \frac{2Q}{Q + Q'} \]
Applying the Fresnel equations to the top interface

\[
\begin{align*}
    r_{01} &= Q_0 - Q_1 \\
    r_{10} &= Q_1 - Q_0 \\
    t_{01} &= 2Q_0 + Q_1 \\
    t_{10} &= 2Q_1 + Q_0
\end{align*}
\]

we can, therefore, construct the following identity

\[
\begin{align*}
    r_{201} + t_{01} t_{10} &= (Q_0 - Q_1)^2 (Q_0 + Q_1)^2 + 2Q_0 Q_0 + Q_1 2Q_1 Q_1 + Q_0^2 = Q_2 + 2Q_0 Q_1 + Q_2^2
\end{align*}
\]

\[
\begin{align*}
    (Q_0 + Q_1)^2 (Q_0 + Q_1)^2 &= 1
\end{align*}
\]
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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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

\[ r_{01} = \frac{Q_0 - Q_1}{Q_0 + Q_1} \quad t_{01} = \frac{2Q_0}{Q_0 + Q_1} \]

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\[ = \frac{Q_0^2 + 2Q_0Q_1 + Q_1^2}{(Q_0 + Q_1)^2} \]
Fresnel Equation Identity

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\[ = \frac{Q_0^2 + 2Q_0Q_1 + Q_1^2}{(Q_0 + Q_1)^2} = \frac{(Q_0 + Q_1)^2}{(Q_0 + Q_1)^2} = 1 \]
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

$$r_{\text{slab}} = r_{01} + t_{01} t_{10} r_{12}$$

Using the identity $t_{01} t_{10} = 1 - r_{201}$

Expanding over a common denominator and recalling that $r_{10} = -r_{01}$.

In the case of $n_0 = n_2$ there is the further simplification of $r_{12} = -r_{01}$.
Starting with the reflection coefficient of the slab obtained earlier

\[ r_{slab} = r_{01} + t_{01} t_{10} r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

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

Using the identity

\[ t_{01} t_{10} = 1 - r_{01}^2 \]
Reflection Coefficient of a Slab

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

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In the case of \( n_0 = n_2 \) there is the further simplification of \( r_{12} = -r_{01} \).

Using the identity \( t_{01} t_{10} = 1 - r_{01}^2 \).
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

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

\[ = r_{01} + \left( 1 - r_{01}^2 \right) r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

Using the identity

\[ t_{01} t_{10} = 1 - r_{01}^2 \]

Expanding over a common denominator and recalling that \( r_{10} = -r_{01} \).
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Starting with the reflection coefficient of the slab obtained earlier

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

\[ = r_{01} + \left(1 - r_{01}^2\right) r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

\[ = r_{01} + r_{01}^2 r_{12} p^2 + \left(1 - r_{01}^2\right) r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

Using the identity

\[ t_{01} t_{10} = 1 - r_{01}^2 \]

Expanding over a common denominator and recalling that \( r_{10} = -r_{01} \).
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

\[ r_{slab} = r_0 + t_{01} t_{10} r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

\[ = r_0 + (1 - r_{01}^2) r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

\[ = \frac{r_0 + r_{01}^2 r_{12} p^2 + (1 - r_{01}^2) r_{12} p^2}{1 - r_{10} r_{12} p^2} \]

\[ r_{slab} = \frac{r_0 + r_{12} p^2}{1 + r_{01} r_{12} p^2} \]

Using the identity

\[ t_{01} t_{10} = 1 - r_{01}^2 \]

Expanding over a common denominator and recalling that \( r_{10} = -r_{01} \).
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

\[ r_{slab} = r_0 + t_0 t_1 r_1 \frac{p^2}{1 - r_0 r_1 p^2} \]

\[ = r_0 + \left(1 - r_{01}^2\right) r_1 \frac{p^2}{1 - r_0 r_1 p^2} \]

\[ = \frac{r_0 + r_{01}^2 r_1 p^2 + \left(1 - r_{01}^2\right) r_1 p^2}{1 - r_0 r_1 p^2} \]

Using the identity

\[ t_0 t_1 = 1 - r_{01}^2 \]

Expanding over a common denominator and recalling that \( r_1 = -r_{01} \).

In the case of \( n_0 = n_2 \) there is the further simplification of \( r_{12} = -r_{01} \).
Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

\[ r_{slab} = r_0 + t_0 t_{10} r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

\[ = r_0 + \left( 1 - r_{01}^2 \right) r_{12} p^2 \frac{1}{1 - r_{10} r_{12} p^2} \]

\[ = \frac{r_0 + r_{01}^2 r_{12} p^2 + \left( 1 - r_{01}^2 \right) r_{12} p^2}{1 - r_{10} r_{12} p^2} \]

Using the identity

\[ t_0 t_{10} = 1 - r_{01}^2 \]

Expanding over a common denominator and recalling that \( r_{10} = -r_{01} \).

In the case of \( n_0 = n_2 \) there is the further simplification of \( r_{12} = -r_{01} \).
Kiessig Fringes

\[ p^2 = e^{iQ_1 \Delta} \]

\[ r_{slab} = \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \]

If we plot the reflectivity

\[ R_{slab} = |r_{slab}|^2 \]

These are Kiessig fringes which arise from interference between reflections at the top and bottom of the slab. They have an oscillation frequency

\[ 2\pi/\Delta = 0.092 \text{Å}^{-1} \]
Kiessig Fringes

\[ p^2 = e^{iQ_1 \Delta} \]

\[ r_{slab} = \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \]

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\[ 2\pi / \Delta = 0.092 \text{Å}^{-1} \]
Kinematical Reflection from a Thin Slab

Recall the reflection coefficient for a thin slab.

\[ r_{\text{slab}} = \frac{r_{01}}{(1 - r_{01}^2) - \rho^2} \approx r_{01} \left(1 - \rho^2\right) \]

\[ r_{\text{slab}} \approx \left(\frac{Qc}{Q0}\right)^2 \left(1 - e^{iQ\Delta}\right) \]

\[ q \gg 1 \quad |r_{01}| \ll 1 \]

\[ \alpha > \alpha_c \]

\[ r_{01} = q_0 - q_1 \]

\[ q_0 + q_1 = q_2 \]

\[ r_{\text{slab}} \approx -\frac{16\pi r_0}{Q^2} e^{iQ\Delta/2} / \left( e^{iQ\Delta/2} - e^{-iQ\Delta/2} \right) \]

\[ -i \left(4\pi r_0 \Delta Q \sin(\alpha) \right) = r_{\text{thin slab}} \]

Since \( Q\Delta \ll 1 \) for a thin slab.
Recall the reflection coefficient for a thin slab.

\[ r_{slab} = \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \]
Kinematical Reflection from a Thin Slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle

\[ r_{slab} = \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \]
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Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

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\[ r_{slab} = \frac{r_0 (1 - p^2)}{1 - r_0^2 p^2} \]

\[ q \gg 1 \]

\[ |r_0| \ll 1 \quad \alpha > \alpha_c \]
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\begin{align*}
    r_{slab} &= \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \\
    &\approx r_{01} (1 - p^2)
\end{align*}
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r_{slab} = \frac{r_{01}(1 - p^2)}{1 - r_{01}^2 p^2} \approx r_{01}(1 - p^2) \approx r_{01}(1 - e^{iQ\Delta})
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\[ r_{01} = \frac{q_0 - q_1}{q_0 + q_1} \]
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\[ r_{01} = \frac{q_0 - q_1}{q_0 + q_1} \frac{q_0 + q_1}{q_0 + q_1} \]

\[ \approx -i \left(4\pi \rho r_{01} \Delta Q \right) \sin\left(Q \Delta / 2\right) Q \Delta / 2 \]

\[ \approx -i \lambda \rho r_{01} \Delta \sin \alpha = r_{thin\ slab} \]
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\]

\[
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\[
r_{01} = \frac{q_0 - q_1}{q_0 + q_1} \frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2}
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    q &\gg 1 \\
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 r_{slab} \approx \left( \frac{Q_c}{2 Q_0} \right)^2 \left( 1 - e^{iQ\Delta} \right)
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\[ r_{slab} = \frac{r_{01} (1 - p^2)}{1 - r_{01}^2 p^2} \approx r_{01} (1 - p^2) = r_{01} \left(1 - e^{iQ\Delta}\right) \]

\[ r_{slab} \approx \left(\frac{Q_c}{2Q_0}\right)^2 \left(1 - e^{iQ\Delta}\right) \]

\[ r_{slab} = -\frac{16\pi \rho r_o}{4Q^2} e^{iQ\Delta/2} \left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right) \]

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Where

- \( q \gg 1 \)
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Since \( Q\Delta \ll 1 \) for a thin slab
$N$ repetitions of a bilayer of thickness $\Lambda$ composed of two materials, $A$ and $B$ which have a density contrast ($\rho_A > \rho_B$).
Multilayers in the Kinematical Regime

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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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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.
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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 and assuming that material A is a fraction $\Gamma$ of the bilayer thickness

\[ \rho \rightarrow \rho_{AB} = \rho_A - \rho_B \]

\[ r_1(\zeta) = -i \frac{\lambda r_o \rho_{AB}}{\sin \theta} \int_{-\Gamma\Lambda/2}^{+\Gamma\Lambda/2} e^{i2\pi \zeta z/\Lambda} dz \]
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$$e^{ix} - e^{-ix} = 2i \sin x$$

$$Q = 4\pi \sin \theta / \lambda = 2\pi \zeta / \Lambda$$
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$$r_1 = -2i r_o \rho_{AB} \left( \frac{\Lambda^2 \Gamma}{\zeta} \right) \frac{\sin (\pi \Gamma \zeta)}{\pi \Gamma \zeta}$$
Absorption Coefficient of a Bilayer

The total reflectivity for the multilayer is therefore:

\[ r_N = -2i r_o \rho_{AB} \left( \frac{\Lambda^2 \Gamma}{\zeta} \right) \frac{\sin (\pi \Gamma \zeta)}{\pi \Gamma \zeta} \frac{1 - e^{i2\pi \zeta N} e^{-\beta N}}{1 - e^{i2\pi \zeta} e^{-\beta}} \]
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The incident x-ray has a path length $\Lambda / \sin \theta$ in a bilayer, a fraction $\Gamma$ through $n_A$ and a fraction $(1 - \Gamma)$ through $n_B$. 
The total reflectivity for the multilayer is therefore:

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The incident x-ray has a path length \( \Lambda / \sin \theta \) in a bilayer, a fraction \( \Gamma \) through \( n_A \) and a fraction \( (1 - \Gamma) \) through \( n_B \). The amplitude absorption coefficient, \( \beta \) is
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\[ \beta = 2 \left[ \frac{\mu_A}{2} \frac{\Gamma \Lambda}{\sin \theta} + \frac{\mu_B}{2} \frac{(1 - \Gamma)\Lambda}{\sin \theta} \right] \]
Absorption Coefficient of a Bilayer

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\[ \beta = 2 \left[ \frac{\mu_A}{2} \frac{\Gamma \Lambda}{\sin \theta} + \frac{\mu_B}{2} \frac{(1 - \Gamma) \Lambda}{\sin \theta} \right] = \frac{\Lambda}{\sin \theta} [\mu_A \Gamma + \mu_B (1 - \Gamma)] \]
Reflectivity Calculation

When \( \zeta = \frac{Q \Lambda}{2 \pi} \) is an integer, we have peaks.

As \( N \) becomes larger, these peaks would become more prominent.

This is effectively a diffraction grating for x-rays.

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

C. Segre (IIT)  
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10 bilayers of W/Si
$\Delta_W / \Delta_{Si} = 10\text{Å} / 40\text{Å}$
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10 bilayers of W/Si

$Q (\text{Å}^{-1})$

$10^0$

$10^{-2}$

$10^{-4}$

$0$ 0.2

C. Segre (IIT)
Slab - Multilayer Comparison

Δ = 68 Å

10 bilayers of W/Si

Δ_w/Δ_{Si} = 10Å/40Å
Parratt’s Recursive Method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.
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\[
\begin{align*}
\vec{k}_z & = k_z \\
\vec{k}_j & = \sqrt{Q_j^2 - 8k^2\delta_j + 8ik^2\beta_j}
\end{align*}
\]
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Because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$k_{zj}^2 = (n_jk)^2 - k_x^2$$
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$$k_{zj}^2 = (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2$$
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$$k_{zj}^2 = (n_jk)^2 - k_x^2$$
$$= (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2$$
$$\approx k_z^2 - 2\delta_jk^2 + 2i\beta_jk^2$$

\[Q_j = 2k_j\sin \alpha_j = 2k_zj = \sqrt{Q_j^2 - 8k^2\delta_j + 8i\beta_jk^2} \]
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and the wavevector transfer in the $j^{th}$ layer.
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\[
\begin{align*}
    k^2_{zj} &= (n_jk)^2 - k_x^2 \\
    &= (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2 \\
    &\approx k^2_z - 2\delta_jk^2 + 2i\beta_jk^2
\end{align*}
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and the wavevector transfer in the $j^{th}$ layer
Parratt Reflectivity Calculation

The reflectivity from the interface between layer $j$ and $j + 1$, not including multiple reflections is

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

$$r_{N-2}, N-1 = r'_{N-2}, N-1 + r_{N-1}, N p_2^{N-1} + r'_{N-2}, N-1 r_{N-1}, N p_2^{N-1}$$
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The reflectivity from the interface between layer $j$ and $j + 1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$
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Now start calculating the reflectivity from the bottom of the $N^{th}$ layer, closest to the substrate, where multiple reflections are not present.
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\]

\[
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\[ r_{N-1,N} = \frac{r'_{N-1,N} + r'_{N,\infty}p_N^2}{1 + r'_{N-1,N}r'_{N,\infty}p_N^2} \]
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$$r_{N-2,N-1} = \frac{r'_{N-2,N-1} + r_{N-1,N}p_{N-1}^2}{1 + r'_{N-2,N-1}r_{N-1,N}p_{N-1}^2}$$
Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions. Parratt calculation gives $R_{\text{Par}} = 1$ as $Q \to 0$ while kinematical diverges ($R_{\text{Kin}} \to \infty$).

Parratt peaks shifted to slightly higher values of $Q$. Peaks in kinematical calculation are somewhat higher reflectivity than true value.
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Graded Interfaces

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The density profile of the interface can be described by the function $f(z)$ which approaches 1 as $z \to \infty$. 
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The reflectivity of this kind of interface can be calculated best in the kinematical limit \((Q > Q_c)\).

The density profile of the interface can be described by the function \(f(z)\) which approaches 1 as \(z \to \infty\).

The reflectivity can be computed as the superposition of the reflectivity of a series of infinitesimal slabs of thickness \(dz\) at a depth \(z\).
The differential reflectivity from a slab of thickness $dz$ at depth $z$ is:

$$
\delta r(Q) = -i Q^2 c^4 Q f(z) dz.
$$

Calculating the full reflection coefficient relative to the Fresnel reflection coefficient $R(Q)$:

$$
R(Q) = \left| \int_{-\infty}^{\infty} \left( \frac{df}{dz} \right) e^{iQz} dz \right|^2.
$$
Reflectivity of a Graded Interface

\[ \delta r(Q) = -i \frac{Q^2}{4Q} f(z) dz \]

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integrating, to get the entire reflectivity
Reflectivity of a Graded Interface

\[ \delta r(Q) = -i \frac{Q^2_c}{4Q} f(z) dz \]

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Reflectivity of a Graded Interface

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\[ r(Q) = -i \frac{Q_c^2}{4Q} \int_{-\infty}^{\infty} f(z) e^{iQz} dz \]

\[ = i \frac{1}{iQ} \frac{Q_c^2}{4Q} \int_{-\infty}^{\infty} f'(z) e^{iQz} dz \]

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integrating by parts simplifies the term in front is simply the Fresnel reflectivity for an interface, \( r_F(Q) \) when \( q \gg 1 \).
Reflectivity of a Graded Interface

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Calculating the full reflection coefficient relative to the Fresnel reflection coefficient

\[ \frac{R(Q)}{R_F(Q)} = \left| \int_{-\infty}^{\infty} \left( \frac{df}{dz} \right) e^{iQz} \, dz \right|^2 \]
The Error Function - a Specific Case

The error function is often chosen as a model for the density gradient

\[ f(z) = \text{erf}\left(\frac{z}{\sqrt{2\sigma}}\right) = \frac{1}{\sqrt{\pi}} \int_0^{z/\sqrt{2\sigma}} e^{-t^2} dt \]

Or more accurately,

\[ R(Q) = R_F(Q) e^{-Q^2/\sigma^2} = R_F(Q) e^{-QQ'/\sigma^2} \]

\[ Q = k \sin \theta, \quad Q' = k' \sin \theta' \]
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whose Fourier transform is also a Gaussian, which when squared to obtain the reflection coefficient, gives.

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