## Today's outline - February 04, 2020

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- 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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- Multilayers in the kinematical regime
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Reading Assignment: Chapter 3.5-3.8

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- Reflection from a thin slab
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- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation

Reading Assignment: Chapter 3.5-3.8
Homework Assignment \#02:
Problems on Blackboard
due Tuesday, February 18, 2020

## Fresnel equation review

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## Limiting cases - $q \gg 1$

Start by rearranging Snell's Law

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q^{2}=q^{2}+1-2 i b_{\mu}
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## Limiting cases $-q \gg 1$

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Start by rearranging Snell's Law and since $q$ is real by definition, when $q \gg 1$
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reflected wave in phase with incident, almost total transmission

## Limiting cases - $q \ll 1$

When $q \ll 1$

$$
q^{2}=q^{\prime 2}+1-2 i b_{\mu}
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## Limiting cases $-q \ll 1$

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## Limiting cases $-q \ll 1$

When $q \ll 1, q^{\prime}$ is mostly imaginary with magnitude 1 since $b_{\mu}$ is very small

$$
\begin{aligned}
& q^{2}=q^{\prime 2}+1-2 i b_{\mu} \\
& q^{\prime 2}=q^{2}-1+2 i b_{\mu} \\
& q^{\prime 2} \approx-1
\end{aligned}
$$

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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.

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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.

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

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

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\begin{aligned}
& r_{12}-\text { reflection in } n_{1} \text { off } n_{2} \\
& t_{12} \text { - transmission from } n_{1} \text { into } n_{2}
\end{aligned}
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t12 - transmission from n}\mp@subsup{n}{1}{}\mathrm{ into }\mp@subsup{n}{2}{
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& r_{10} \text { - reflection in } n_{1} \text { off } n_{0} \\
& t_{10} \text { - transmission from } n_{1} \text { into } n_{0}
\end{aligned}
$$

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

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r_{01} \\
+ \\
t_{01} r_{12} t_{10} \\
+ \\
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The composite reflection coefficient for each ray emerging from the top surface is computed


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

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p^{2}=e^{i 2\left(k_{1} \sin \alpha_{1}\right) \Delta}
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## Composite reflection coefficient

The composite reflection coefficient can now be expressed as a sum

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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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factoring out the second term
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r_{\text {slab }}=r_{01}+t_{01} t_{10} r_{12} p^{2} \sum_{m=0}^{\infty}\left(r_{10} r_{12} p^{2}\right)^{m}
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\text { from all the rest }
\end{array} \quad \begin{array}{ll}
\text { summing the geometric series } \\
& =r_{01}+t_{01} t_{10} r_{12} p^{2} \frac{1}{1-r_{10} r_{12} p^{2}}
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& \text { as previously }
\end{aligned}
$$

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

$$
r=\frac{Q-Q^{\prime}}{Q+Q^{\prime}}, \quad t=\frac{2 Q}{Q+Q^{\prime}}
$$

## Fresnel equation identity

Applying the Fresnel equations to the top interface

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we can, therefore, construct the following identity
$r_{01}^{2}+t_{01} t_{10}=\frac{\left(Q_{0}-Q_{1}\right)^{2}}{\left(Q_{0}+Q_{1}\right)^{2}}+\frac{2 Q_{0}}{Q_{0}+Q_{1}} \frac{2 Q_{1}}{Q_{1}+Q_{0}}$

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& r_{01}^{2}+t_{01} t_{10}=\frac{\left(Q_{0}-Q_{1}\right)^{2}}{\left(Q_{0}+Q_{1}\right)^{2}}+\frac{2 Q_{0}}{Q_{0}+Q_{1}} \frac{2 Q_{1}}{Q_{1}+Q_{0}} \\
& =\frac{Q_{0}^{2}-2 Q_{0} Q_{1}+Q_{1}^{2}+4 Q_{0} Q_{1}}{\left(Q_{0}+Q_{1}\right)^{2}}
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& =\frac{Q_{0}^{2}-2 Q_{0} Q_{1}+Q_{1}^{2}+4 Q_{0} Q_{1}}{\left(Q_{0}+Q_{1}\right)^{2}}=\frac{Q_{0}^{2}+2 Q_{0} Q_{1}+Q_{1}^{2}}{\left(Q_{0}+Q_{1}\right)^{2}}
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\end{aligned}
$$

## Reflection coefficient of a slab

Starting with the reflection coefficient of the slab obtained earlier

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r_{s l a b}=r_{01}+t_{01} t_{10} r_{12} p^{2} \frac{1}{1-r_{10} r_{12} p^{2}}
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r_{\text {slab }} & =r_{01}+t_{01} t_{10} r_{12} p^{2} \frac{1}{1-r_{10} r_{12} p^{2}} & \text { Using the identity } \\
& =t_{01} t_{10}=1-r_{01}^{2} \\
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Expanding over a common denominator and recalling that $r_{10}=-r_{01}$.

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r_{\text {slab }} & =\frac{r_{01}+r_{12} p^{2}}{1+r_{01} r_{12} p^{2}}=\frac{r_{01}\left(1-p^{2}\right)}{1-r_{01}^{2} p^{2}}
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## Kiessig fringes

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\begin{gathered}
p^{2}=e^{i Q_{1} \Delta} \\
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These are Kiessig fringes which arise from interference between reflections at the top and bottom of the slab.


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



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Recall the reflection coefficient for a thin slab.

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& \approx \frac{1}{\left(2 q_{0}\right)^{2}}
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\approx \\
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r_{\text {slab }} & \approx\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2}\left(1-e^{i Q \Delta}\right) & \approx \frac{1}{\left(2 q_{0}\right)^{2}}=\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2} \\
r_{\text {slab }} & =-\frac{16 \pi \rho r_{0}}{4 Q^{2}} e^{i Q \Delta / 2}\left(e^{i Q \Delta / 2}-e^{-i Q \Delta / 2}\right)
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&=r_{01}\left(1-e^{i Q \Delta}\right) \quad \approx \frac{1}{\left(2 q_{0}\right)^{2}}=\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2} \\
& r_{\text {slab }} \approx\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2}\left(1-e^{i Q \Delta}\right) \quad \\
& r_{\text {slab }}=-\frac{16 \pi \rho r_{0}}{4 Q^{2}} e^{i Q \Delta / 2}\left(e^{i Q \Delta / 2}-e^{-i Q \Delta / 2}\right) \\
&=-i\left(\frac{4 \pi \rho r_{0} \Delta}{Q}\right) \frac{\sin (Q \Delta / 2)}{Q \Delta / 2} e^{i Q \Delta / 2}
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Since $Q \Delta \ll 1$ for a thin slab

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& r_{\text {slab }} \approx\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2}\left(1-e^{i Q \Delta}\right) \quad \approx \frac{1}{\left(2 q_{0}\right)^{2}}=\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2} \\
& r_{\text {slab }}=-\frac{16 \pi \rho r_{0}}{4 Q^{2}} e^{i Q \Delta / 2}\left(e^{i Q \Delta / 2}-e^{-i Q \Delta / 2}\right) \\
& =-i\left(\frac{4 \pi \rho r_{0} \Delta}{Q}\right) \frac{\sin (Q \Delta / 2)}{Q \Delta / 2} e^{i Q \Delta / 2}
\end{aligned}
$$

Since $Q \Delta \ll 1$ for a thin slab

## 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 refraction effects can be ignored and we are in the "kinematical" regime.

$$
\begin{aligned}
r_{\text {slab }} & =\frac{r_{01}\left(1-p^{2}\right)}{1-r_{01}^{2} p^{2}} \\
& \approx r_{01}\left(1-p^{2}\right) \quad q \gg 1 \\
& =r_{01}\left(1-e^{i Q \Delta}\right) \quad\left|r_{01}\right| \ll 1 \quad \alpha>\alpha_{c} \\
r_{\text {slab }} & \approx\left(\frac{Q_{c}}{2 Q_{0}}\right)^{2}\left(1-e^{i Q \Delta}\right) \quad \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}}{\left(q_{0}+q_{1}\right)} \\
r_{\text {slab }} & =-\frac{16 \pi \rho r_{0}}{4 Q^{2}} e^{i Q \Delta / 2}\left(e^{i Q \Delta / 2}-e^{-i Q \Delta / 2}\right) \\
& \left.=-i\left(\frac{4 \pi \rho r_{0} \Delta}{Q}\right) \frac{\sin (Q \Delta / 2)}{Q \Delta / 2} e^{i Q \Delta / 2} \approx-i \frac{Q_{c}}{2 Q_{0}}\right)^{2} \\
\sin \alpha & =r_{\text {thin slab }}
\end{aligned}
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## Multilayers in the kinematical regime



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# $N$ repetitions of a bilayer of thickness $\Lambda$ composed of two materials, $A$ and $B$ which have a density contrast $\left(\rho_{A}>\rho_{B}\right)$. 

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& =-i \frac{\lambda r_{0} \rho_{A B}}{\sin \theta} \frac{\Lambda}{i 2 \pi \zeta}\left[e^{i \pi \zeta \Gamma}-e^{-i \pi \zeta \Gamma}\right] & & e^{i x}-e^{-i x}=2 i \sin x \\
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r_{1}=-2 i r_{0} \rho_{A B}\left(\frac{\Lambda^{2} \Gamma}{\zeta}\right) \frac{\sin (\pi \Gamma \zeta)}{\pi \Gamma \zeta}
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## Absorption coefficient of a bilayer

The total reflectivity for the multilayer is therefore:

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r_{N}=-2 i r_{0} \rho_{A B}\left(\frac{\Lambda^{2} \Gamma}{\zeta}\right) \frac{\sin (\pi \Gamma \zeta)}{\pi \Gamma \zeta} \frac{1-e^{i 2 \pi \zeta N} e^{-\beta N}}{1-e^{i 2 \pi \zeta} e^{-\beta}}
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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}\left[\mu_{A} \Gamma+\mu_{B}(1-\Gamma)\right]
$$

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- This is effectively a diffraction grating for x-rays
- Multilayers are used commonly on laboratory sources as well as at synchrotrons as mirrors


## Slab - multilayer comparison




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Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

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This is Parratt's recursive approach and needs to be computed numerically

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Q_{j} & =2 k_{j} \sin \alpha_{j}=2 k_{z j} \\
& =\sqrt{Q^{2}-8 k^{2} \delta_{j}+8 i k^{2} \beta_{j}}
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The recursive relation can be seen from the calculation of reflectivity of the next layer up

$$
r_{N-2, N-1}=\frac{r_{N-2, N-1}^{\prime}+r_{N-1, N} p_{N-1}^{2}}{1+r_{N-2, N-1}^{\prime} r_{N-1, N} p_{N-1}^{2}}
$$

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

