## Today's Outline - February 05, 2015

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- Reflection from a thin slab


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- Kiessig fringes


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Reading Assignment: Chapter 3.5-3.8

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- 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

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- 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

## Review of Interface Effects

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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$r_{01}-$ reflection in $n_{0}$ off $n_{1}$
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$$
\begin{aligned}
& r_{12}-\text { reflection in } n_{1} \text { off } n_{2} \\
& t_{12}-\text { transmission from } n_{1} \text { into } n_{2}
\end{aligned}
$$

## Reflection and Transmission Coefficients

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


```
r01 - reflection in nofoff n
t01 - transmission from no into n1
r12 - reflection in n
t12 - transmission from n}\mp@subsup{n}{1}{}\mathrm{ into }\mp@subsup{n}{2}{
r r10 - reflection in n}\mp@subsup{n}{1}{}\mathrm{ off n
t10 - transmission from n}\mp@subsup{n}{1}{}\mathrm{ into no
```


## Reflection and Transmission Coefficients

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


```
ro1 - reflection in no off n
t01 - transmission from no into n1
r12 - reflection in n}\mp@subsup{n}{1}{}\mathrm{ off n}\mp@subsup{n}{2}{
t12 - transmission from n}\mp@subsup{n}{1}{}\mathrm{ into }\mp@subsup{n}{2}{
r r10 - reflection in n}\mp@subsup{n}{1}{}\mathrm{ off n
t10 - transmission from n}\mp@subsup{n}{1}{}\mathrm{ into }\mp@subsup{n}{0}{
```

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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$n_{0} \quad \downarrow$
$r_{01}$

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

## Overall Reflection from a Slab

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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which multiplies the reflection coefficient

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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_{\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 second term from all the rest

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& \text { factoring out second term } \\
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} & \text { from all the rest }
\end{array}
$$

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& \begin{array}{l}
\text { summing the geometric series } \\
\\
\text { as previously }
\end{array}
\end{array}
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## Fresnel Equation Identity

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

## Reflection Coefficient of a Slab

Starting with the reflection coefficient of the slab obtained earlier

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t_{01} t_{10}=1-r_{01}^{2} \\
& =r_{01}+\left(1-r_{01}^{2}\right) r_{12} p^{2} \frac{1}{1-r_{10} r_{12} p^{2}} &
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Expanding over a common denominator and recalling that $r_{10}=-r_{01}$.

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

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In the case of $n_{0}=n_{2}$ there is the further simplification of $r_{12}=-r_{01}$.

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& =\frac{r_{01}+r_{01}^{2} r_{12} p^{2}+\left(1-r_{01}^{2}\right) r_{12} p^{2}}{1-r_{10} r_{12} p^{2}} \\
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}}
\end{aligned}
$$

Using the identity

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t_{01} t_{10}=1-r_{01}^{2}
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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

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\begin{gathered}
p^{2}=e^{i Q_{1} \Delta} \\
r_{s l a b}=\frac{r_{01}\left(1-p^{2}\right)}{1-r_{01}^{2} p^{2}}
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If we plot the reflectivity

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R_{\text {slab }}=\left|r_{s l a b}\right|^{2}
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These are Kiessig fringes which arise from interference between reflections at the top and bottom of the slab.


## Kiessig Fringes

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If we plot the reflectivity

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R_{s l a b}=\left|r_{s l a b}\right|^{2}
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These are Kiessig fringes which arise from interference between reflections at the top and bottom of the slab. They have an oscillation frequency

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

Kinematical Reflection from a Thin Slab
Recall the reflection coefficient for a thin slab.

## Kinematical Reflection from a Thin Slab

Recall the reflection coefficient for a thin slab.

$$
r_{\text {slab }}=\frac{r_{01}\left(1-p^{2}\right)}{1-r_{01}^{2} p^{2}}
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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_{o} \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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## Reflectivity Calculation



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


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- 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


## Slab - Multilayer Comparison




## Parratt's Recursive Method

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& \approx k_{z}^{2}-2 \delta_{j} k^{2}+2 i \beta_{j} k^{2}
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## Parratt's Recursive Method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate. Take $\Delta_{j}$ as the thickness of each layer and $n_{j}=1-\delta_{j}+i \beta_{j}$ as the index of refraction of each layer.
Because of continuity, $k_{x j}=k_{x}$ and therefore, we can compute the z-component of $\vec{k}_{j}$

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k_{z j}^{2} & =\left(n_{j} k\right)^{2}-k_{x}^{2} \\
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$$
r_{N-1, N}=\frac{r_{N-1, N}^{\prime}+r_{N, \infty}^{\prime} p_{N}^{2}}{1+r_{N-1, N}^{\prime} r_{N, \infty}^{\prime} p_{N}^{2}}
$$ now calculated (note no prime!)

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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Parratt peaks shifted to slightly higher values of $Q$

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

## Graded Interfaces

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

The reflectivity can be computed as the superposition of the reflectivity of a series of infinitesmal slabs of thickness $d z$ at a depth $z$.

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integrating by parts simplifies the term in front is simply the Fresnel reflectivity for an interface, $r_{F}(Q)$ when $q \gg 1$, the integral is the Fourier transform of the density gradient, $\phi(Q)$

Calculating the full reflection coefficient relative to the Fresnel reflection coefficient

$$
\frac{R(Q)}{R_{F}(Q)}=\left|\int_{-\infty}^{\infty}\left(\frac{d f}{d z}\right) e^{i Q z} d z\right|^{2}
$$

## The Error Function - a Specific Case

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

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f(z)=\operatorname{erf}\left(\frac{z}{\sqrt{2} \sigma}\right)=\frac{1}{\sqrt{\pi}} \int_{0}^{z / \sqrt{2} \sigma} e^{-t^{2}} d t
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\begin{gathered}
R(Q)=R_{F}(Q) e^{-Q^{2} \sigma^{2}}=R_{F}(Q) e^{-Q Q^{\prime} \sigma^{2}} \\
Q=k \sin \theta, \quad Q^{\prime}=k^{\prime} \sin \theta^{\prime}
\end{gathered}
$$

