Derived the wave equation

\[ \nabla^2 \mathbf{E}(\mathbf{r}, t) = \rho_0 \varepsilon_0 \frac{\partial^2 \mathbf{E}(\mathbf{r}, t)}{\partial t^2} + \mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t} \]

with solutions of the form

\[ \mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} + c.c. \]

We found that the polarization of the material affects wave propagation, and found the dispersion relation \( \omega(k) \)

\[ k^2 = \frac{\omega^2}{c^2} \left( 1 + \chi_e(\omega) \right) \]

with the corresponding refractive index given by

\[ n \approx \sqrt{1 + \chi_e} \]

(approximately because: ignores magnetization, assumes low frequency)
Found that polarization of materials (atoms) has finite response time.

Harmonic fields will give harmonic response, but with finite phase lag. 
⇒ Electric susceptibility must contain imaginary contribution:

\[ \chi(\omega) = \chi'(\omega) + i\chi''(\omega) \]

This in turn implied that the refractive index contains an imaginary component:

\[ \eta(\omega) = n(\omega) + ik(\omega) = \sqrt{1 + \chi'(\omega) + i\chi''(\omega)} \]

which was found to lead to a complex wavevector that describes attenuation \( \alpha \)

\[ \alpha = 2 \text{Im}(k) = 2k \frac{\omega}{c} \]

**In short:** finite polarization response time (related to \( n \)) \( \Rightarrow \) attenuation

refractive index \( n(\omega) \) must be linked to attenuation \( \alpha(\omega) \)
Derive **Kramers-Kronig relations** linking

- real refractive index $n$ to an absorption spectrum $\alpha$

$$n(\omega) = 1 + \frac{C}{\pi} \int_0^\infty \frac{\alpha(\omega')}{\omega' \omega^2 - \omega'^2} \, d\omega'$$

- real susceptibility $X'$ to a spectrum of the imaginary susceptibility $X''$

$$X'(\omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega' X''(\omega')}{\omega' \omega^2 - \omega'^2} \, d\omega'$$

- a phase shift upon reflection $\phi$ to a reflectivity spectrum $R$

$$\phi(\omega) = \frac{\omega}{\pi} \int_0^\infty \frac{\ln \left( \frac{R(\omega')}{R(\omega)} \right)}{\omega' \omega^2 - \omega'^2} \, d\omega'$$
A simple truth  – and an essential trick!

\( X(t) \) doesn’t change if you multiply it by a step function :

\[ X(t) = X(t) \Theta(t) \]

This has implications about the symmetry of the frequency dependence (Fourier Tr.)
A simple consequence – and some simple math

If \( X(t) = X(t) \Theta(t) \) then also

\[
\mathcal{F}[X(t)] = \mathcal{F}[X(t) \Theta(t)]
\]

with \( \mathcal{F}[X(t)] \) the Fourier transform of \( X(t) \), given by

\[
\mathcal{F}[X(t)] = X(\omega) = \int_{-\infty}^{\infty} X(t) e^{i\omega t} dt
\]

If you delve deep into your memory for Fourier theory, you’ll remember (yes?)

\[
\mathcal{F}[a \cdot b] = \mathcal{F}[a] \ast \mathcal{F}[b]
\]

where the symbol \( \ast \) denotes convolution, which is defined as:

\[
p \ast q = \int_{-\infty}^{\infty} p(\omega') q(\omega - \omega') d\omega'
\]
We now have found the relation

\[ \mathcal{F}[x(t)] = \mathcal{F}[x(t) \theta(t)] = \mathcal{F}[x(t)] * \mathcal{F}[\theta(t)] \]

The left side of the equation is simply given by

\[ \mathcal{F}[x(t)] = \int x(t) e^{-j\omega t} dt \]

In the following slides, we will work out the right side of the equation.

First: look at \( \mathcal{F}[\theta(t)] \), then convolute with \( \mathcal{F}[x(t)] \).
Fourier transform of the step function around t=0

\[ \mathcal{F}[\Theta(t)] = \frac{1}{2} \delta(\omega) + \frac{i}{2\pi \omega} \]

Note that sine waves have the correct symmetry around t=0.
Getting ready to convolute ...

We now have

\[ F[\theta(t)] = \frac{1}{2} \delta(w) + \frac{i}{2\pi w} \]

and

\[ F[X(t)] = \int X(t) e^{jwt} dt \]

as well as the relation

\[ F[X(t) \theta(t)] = F[X(t)] \ast F[\theta(t)] \]

we'll now write this convolution in terms of the known Fourier components above.
Using the known Fourier components, we find \( \mathcal{F}[x(t)] \times \mathcal{F}[\Theta(t)] \) is equal to

\[
\int \int x(t) e^{i\omega t} dt \left( \frac{1}{2} \delta(\omega - \omega') + \frac{i}{2\pi(\omega - \omega')} \right) d\omega',
\]

which we can split into two components – one relating to the real part of \( \mathcal{F}[\Theta(t)] \) and one related to the imaginary part of \( \mathcal{F}[\Theta(t)] \):

\[
\frac{1}{2} \int x(t) e^{i\omega t} dt + \frac{i}{2\pi(\omega - \omega')} \int x(t) e^{i\omega t} dt d\omega',
\]

which we can in turn write as

\[
\frac{1}{2} X(\omega) + \frac{i}{2\pi} \int \frac{1}{\omega - \omega'} X(\omega') d\omega'.
\]
Using the result derived on the previous slide, we found that the relation

\[ \mathcal{F} [X(t)] = \mathcal{F} [X(t) \Theta(t)] \]

corresponds to the relation

\[ X(\omega) = \frac{1}{2} X(\omega) + \frac{i}{2\pi} \int \frac{X(\omega')}{\omega - \omega'} \, d\omega' \]

which after some serious math magically turns into

\[ X(\omega) = \frac{i}{\pi} \int \frac{X(\omega')}{\omega - \omega'} \, d\omega' \]

*Time to scratch your head!* Taking an infinite integral of \( X \) with a frequency dependent imaginary weighing factor gives you... \( X \) again!

\[ \Rightarrow \text{ we can link imaginary parts of } X \text{ to real parts of } X \text{ and vice versa} \]
Separating imaginary and real parts

Final steps: with

\[ X(\omega) = \frac{i}{\pi} \int \frac{X'(\omega')}{\omega - \omega'} d\omega' \quad \text{and} \quad X(\omega) = X'(\omega) + iX''(\omega) \]

we find that

\[ X'(\omega) + iX''(\omega) = \frac{i}{\pi} \int \frac{X'(\omega')}{\omega - \omega'} d\omega' + \frac{i}{\pi} \int \frac{iX''(\omega')}{\omega - \omega'} d\omega' \]

Grouping real and imaginary terms yields

\[ X'(\omega) = -\frac{1}{\pi} \int \frac{X''(\omega')}{\omega - \omega'} d\omega' \]
\[ X''(\omega) = \frac{1}{\pi} \int \frac{X'(\omega')}{\omega - \omega'} d\omega' \]

These **Kramers-Kronig relations for** \( X(\omega) \) **relate** \( X'(\omega) \) **to** \( X''(\omega) \) **and vice versa**
Rewrite to positive frequencies only

Reality condition: \( X'(\omega) \) is an even function, \( X''(\omega) \) is an odd function

This allows Kramers-Kronig relations to be written as: (see homework)

\[
X'(\omega) = \frac{2}{\pi} \int_{0}^{\infty} \frac{\omega' X''(\omega')}{\omega'^2 - \omega^2} \, d\omega'
\]

\[
X''(\omega) = -\frac{2\omega}{\pi} \int_{0}^{\infty} \frac{X'(\omega)}{\omega'^2 - \omega^2} \, d\omega'
\]

Note that these integrals run over positive angular frequencies only
Simplifications for dilute media

Previously we derived the frequency dependent complex refractive index:

$$\eta(\omega) = \sqrt{1 + X'(\omega) + i X''(\omega)}$$

For dilute media or weak susceptibility: \(X'\) and \(X''\) are small.

Using the approximation \(\sqrt{1+x} \approx 1 + \frac{1}{2}x\) for small \(x\) this leads to

$$\eta(\omega) = n(\omega) + i k(\omega) \approx 1 + \frac{X'(\omega)}{2} + i \frac{X''(\omega)}{2}$$

Comparing real and imaginary terms respectively, this gives

$$n(\omega) \approx 1 + \frac{X'(\omega)}{2} \quad \text{and} \quad k(\omega) \approx \frac{X''}{2}$$

We also derived

$$\alpha = 2 \Im(k) = 2k \frac{\omega}{c} \quad \text{so} \quad \alpha = \frac{\omega}{c} X''(\omega)$$
Kramers-Kronig relations for $n$ and $\alpha$

With

$$n(\omega) = 1 + \frac{X'(\omega)}{2}$$

and

$$X''(\omega) = \alpha \frac{c}{\omega}$$

the relation

$$X'(\omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega' X''(\omega')}{\omega'^2 - \omega^2} \, d\omega'$$

can be written as

$$n(\omega) = 1 + \frac{c}{\pi} \int_0^\infty \frac{\alpha(\omega')}{\omega'^2 - \omega^2} \, d\omega'$$

One can get the **frequency dependent refractive index** from an **absorption spectrum**

We simplified the math by assuming dilute media, but the result is true in general!
Example for a single absorption line 1/3

To get \( n(\omega) \) at a specific frequency, integrate the entire absorption spectrum with a frequency dependent weighing factor \( \frac{1}{(\omega')^2 - \omega^2} \)

\[
n(\omega) = 1 + \frac{C}{\pi} \int_{0}^{\infty} \frac{\alpha(\omega')}{(\omega')^2 - \omega^2} \, d\omega'
\]

If \( \omega < \omega_{\text{res}} \) then:

Below \( \omega \)
- \( \alpha \) small and positive
- Weighing factor negative
- "small negative contribution"

Above \( \omega \)
- \( \alpha \) large and positive
- Weighing factor positive
- "large positive contribution"

For frequencies below resonance, KK relations yield large \( n(\omega) \)
Example for a single absorption line 2/3

To get \( n(\omega) \) at a specific frequency, integrate the entire absorption spectrum with a frequency dependent weighing factor \( \frac{1}{(\omega'^2 - \omega^2)} \)

\[
n(\omega) = 1 + \frac{C}{\pi} \int_{0}^{\infty} \frac{\alpha(\omega')}{\omega'^2 - \omega^2} \, d\omega'
\]

If \( \omega > \omega_{\text{res}} \) then:

**Below \( \omega \)**
- \( \alpha \) large and positive
- weighing factor negative
- “large negative contribution”

**Above \( \omega \)**
- \( \alpha \) small and positive
- weighing factor positive
- “small positive contribution”

For frequencies above resonance, KK relations yield small \( n(\omega) \)
Example for a single absorption line 3/3

Repeating this integration for many $\omega$ yields $n(\omega)$:

\[ -4 \leq 50 [n(\omega) - 1] \leq 4 \]
\[ \alpha(\omega') \]

Between resonances: $n$ slowly *increases* = “normal dispersion”

Close to resonances: $n$ rapidly *decreases* = “anomalous dispersion”

At high frequencies (~ x-ray wavelengths) $n$ can become slightly smaller than 1
A quicker but less intuitive route - Cauchy

We can also use Cauchy’s integral theorem to derive the KK relations for $X(\omega)$

$$X(\omega) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{X(\omega')}{\omega - \omega'} d\omega'$$

This is equivalent to proving (with apologies for the parameter changes!)

$$i\pi X(\Omega) = \int_{-\infty}^{\infty} \frac{X(\omega)}{\omega - \Omega} d\omega$$

We will show this by solving the integral using Cauchy’s integral theorem
Cauchy’s integral theorem (“CIT”): the closed path integral of an analytic function yields zero. (with some caveats) More info, see e.g. MathWorld

If we make $\omega$ complex, the CIT still holds. We now have a closed path of which

- the value of the integrand goes to zero for large $|\omega|$  
- the integration is tricky around $\Omega$  
- the integration is over real frequencies and very familiar looking.
Integration at large values of $|\omega|$

Half-circle section: the value of the integrand goes to zero for large $|\omega|$

This can be seen by looking at $X(\omega)$ at **fixed** complex and large $\omega$

$$X(\omega) = \int_{0}^{\infty} X(t) e^{i\omega t} dt$$

For large real part of $\omega$, this term oscillates fast over small $\Delta t$
Integration around a pole

That leaves us with $\boxed{\text{blue} + \text{red} = 0}$

\[
\int_{\gamma} \frac{X(\omega)}{\omega - \Omega} \, d\omega = 0
\]

where $\ell_\varepsilon$ is the vanishingly small length of the half circle around $\Omega$

That leaves us with $\boxed{i\pi X(\Omega)}$

We can calculate the small path integral around $\Omega$ using the residue theorem:

http://mathworld.wolfram.com/ResidueTheorem.html

(the essential step)
The final result

We have found

\[ - \begin{array}{c} 3 \\ \text{2} \end{array} = \begin{array}{c} 3 \\ \text{2} \end{array} \]

We found: integration over real \( \omega \) (except small \( \mathbb{M} \) region) = \( i\pi X(\Omega) \)

We set out to prove:

\[ i\pi X(\Omega) = \int_{-\infty}^{\infty} \frac{X(\omega)}{\omega - \Omega} \, d\omega \]

\( \sim \) DONE!

It turns out that avoiding the infinitely small section around omega is ‘reasonable’ (recall the example integrations earlier this lecture)
Kramers-Kronig relations relating reflectivity to phase shift 1/3

A light wave incident on a planar surface of a dispersive material

\[ E(t,z) = E_0 \cos(\omega t - k z) \]

generates a reflected wave with a frequency dependent amplitude and phase shift

The fraction of reflected irradiance scales with the reflectance \( R \):

\[ R(\omega) = r(\omega) r^*(\omega) \]

with \( r(\omega) \) the amplitude reflection coefficient:

\[ r(\omega) = \frac{1-n(\omega)-iK(\omega)}{1+n(\omega)-iK(\omega)} \]

Note that for a low absorption situation (e.g. glass at visible frequencies) this gives:

\[ R = \left(\frac{1-n}{1+n}\right)^2 \]
Kramers-Kronig relations relating reflectivity to phase shift 2/3

It is difficult to measure $\varphi$ vs. $\omega$, but we can derive a KK relation for $\varphi$ and $R$

First step: express $r(\omega)$ as a complex exponent:

$$r(\omega) = \rho(\omega) e^{i \varphi(\omega)}$$

We want to arrive at a relation of the form

$$X(\omega) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{X'(\omega')}{\omega - \omega'} d\omega'$$

with $X$ of the form $X' + i X''$ (this linked the $X''$ integral to $X'$ and vice versa)

To enable this, we will derive a KK relation for $\ln(r(\omega))$

$$\ln(r(\omega)) = \ln(\rho(\omega)) + i \varphi(\omega)$$
Using the Cauchy Integral Theorem and the residue theorem we find

\[
\ln(p(w)) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\varphi(w')}{w' - w} \, dw'
\]

\[
\varphi(w) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\ln(p(w'))}{w' - w} \, dw'
\]

The latter integral can be (see handouts) written in the form

\[
\varphi(w) = \frac{1}{\pi} \int_{0}^{\infty} \frac{\ln(R(w')/R(w))}{w'^2 - w^2} \, dw'
\]

⇒ we can find the frequency dependent phase shift upon reflection by measuring a reflection spectrum!
Using reality condition OR Cauchy, found **Kramers-Kronig relations** linking

- real refractive index $n$ to an absorption spectrum $\alpha$

\[
n(w) = 1 + \frac{C}{\pi} \int_0^\infty \frac{\alpha(w')}{w'^2 - w^2} \, dw'
\]

- real susceptibility $X'$ to a spectrum of the imaginary susceptibility $X''$

\[
X'(w) = \frac{2}{\pi} \int_0^\infty \frac{w' X''(w')}{{w'}^2 - w^2} \, dw'
\]

- a phase shift upon reflection $\phi$ to a reflectivity spectrum $R$

\[
\phi(w) = \frac{\omega}{\pi} \int_0^\infty \frac{\ln(R(w')/RC(w))}{w'^2 - w^2} \, dw'
\]
Next week

Show that oscillating electrons radiate, and show that this can slow down light
⇒ ‘microscopic view’ of refractive index

Lecture 5: model dipole radiation
Lecture 6: derive simple model for oscillating dipoles (Lorentz model)

Low frequency ⇒ Amplitude in phase with $E_{\text{in}}$

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