enter

The Kramers-Kronig Relations

Section 7.10

"Causality and the KK relations"

$$\mathrm{Re}\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{2}{\pi\epsilon_0}\mathcal{P}\int_0^\infty \frac{\omega'\,\mathrm{Im}\,\epsilon(\omega')}{(\omega')^2-\omega^2}\,d\omega'$$

$$\mathrm{Im}\frac{\epsilon(\omega)}{\epsilon_0} = -\frac{2\omega}{\pi\epsilon_0}\mathcal{P}\int_0^\infty \frac{\mathrm{Re}\,\epsilon(\omega')-\epsilon_0}{(\omega')^2-\omega^2}\,d\omega'$$

Today we'll show that the Kramers-Kronig relations are true specifically for the Lorentz model of dispersion.

Next time we will show that the KK relations are completely general, i.e., they must be true for any theory of $\epsilon(\omega)$.

Review the the Lorentz dispersion model; define $K(\omega) \equiv \epsilon(\omega)/\epsilon_0$ =

$$K(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

Real and imaginary parts of $K(\omega)$

$$\mathrm{Re}\,K(\omega) = 1 + \frac{\omega_p^2(\omega_0^2-\omega^2)}{(\omega_0^2-\omega^2)^2 + (\gamma\omega)^2}$$

$$\mathrm{Im}\,K(\omega) = \frac{\omega_p^2\,\gamma\,\omega}{(\omega_0^2-\omega^2)^2 + (\gamma\omega)^2}$$

$K(\omega)$ is holomorphic in the upper half ω plane. There are two poles in the lower half ω plane.

```
poles = Solve[ω0^2 - ω^2 - I*ω*γ == 0, ω];
poles[[1]] // Expand
poles[[2]] // Expand
```

$$\left\{\omega \to -\frac{i\gamma}{2} - \frac{1}{2}\sqrt{-\gamma^2 + 4\,\omega 0^2}\right\}$$

$$\left\{\omega \to -\frac{i\gamma}{2} + \frac{1}{2}\sqrt{-\gamma^2 + 4\,\omega 0^2}\right\}$$

Therefore, by Cauchy's integral theorem,

$$K(\omega) - 1 = \frac{1}{2\pi i}\oint_{UHP} \frac{K(z) - 1}{z - \omega - i\epsilon}\, dz$$

in the limit $\epsilon \longrightarrow 0$.

This ϵ is not permittivity!
This ϵ is a positive infinitesimal.

Now, the integral over the semicircle at infinity is 0. (K(z)–1 ~ R^{-2})
So the integration region is the real axis.

The Plemelj Formulae

$$\frac{1}{x \pm i\epsilon} = \mathcal{P}\,\frac{1}{x} \mp i\,\pi\,\delta(x)$$

$\mathcal{P}$ = Cauchy Principal Value

(If you are not familiar with the Plemelj formulae, Google it.)
Applying the Plemelj formula

$$K(\omega)-1 = \frac{1}{2\pi i}\,\mathcal{P}\int_{-\infty}^{\infty} \frac{K(z)-1}{z-\omega}\, dz + \frac{1}{2\pi i}(i\pi)\,(K(\omega)-1)$$

$$K(\omega)-1 = \frac{1}{\pi i}\,\mathcal{P}\int_{-\infty}^{\infty} \frac{K(z)-1}{z-\omega}\, dz$$

Separate the real and imaginary parts ...

$$\text{Re } K(\omega) - 1 = \frac{1}{\pi} \mathcal{P}\int_{-\infty}^{\infty} \frac{\text{Im } K(z)}{z-\omega}\, dz$$

$$\text{Im } K(\omega) = -\frac{1}{\pi} \mathcal{P}\int_{-\infty}^{\infty} \frac{\text{Re } K(z) - 1}{z-\omega}\, dz$$

These are one one form of the Kramers-Kronig relations.

They relate *absorption* (the imaginary part) to *dispersion* (the real part).

Real part, Imaginary part, index of refraction and attenuation coefficient

- $\epsilon(\omega)$ is complex.
- From Maxwell's equations, the plane wave solution $\propto$ exp(i kz – i ωt) where k is complex;
- $\frac{\omega}{k} = \text{“ } v_{\text{phase}} \text{ ”} = \frac{1}{\sqrt{\mu_0\, \epsilon(\omega)}} = \text{c}\sqrt{\frac{\epsilon_0}{\epsilon(\omega)}}$
- $\text{k} = \beta + \text{i}\alpha/2 \implies e^{\text{ikz}} = e^{\text{i}\beta\text{z}}\, e^{-\text{z}\alpha/2}$
- attenuation coefficient = α
- index of refraction = n = $\frac{c}{\omega/\beta} = \frac{\text{c}\beta}{\omega}$
- $k^2 = \frac{\omega^2}{c^2} \frac{\epsilon(\omega)}{\epsilon_0} = \beta^2 - \frac{\alpha^2}{4} + \text{i}\,\alpha\,\beta$

  $= \frac{\omega^2}{c^2} (\text{Re } K + i \text{ Im } K)$

Another integral relation

Recall, for the Lorentz model of dispersion,

$$\mathrm{Im}\,K(z) = \frac{\gamma\, z\, \omega_p^2}{(\omega_0^2 - z^2)^2 + \gamma^2 z^2}$$

Note that Im K(–z) = – Im K(z).
Therefore we can write the integral relations in another way ...

$$\int_{-\infty}^{\infty} \frac{A(z)}{z-\omega} dz = \int_0^{\infty} \frac{A(z)}{z-\omega} dz + \int_{-\infty}^{0} \frac{A(z)}{z-\omega} dz$$

$$= \int_0^{\infty} \left\{ \frac{A(z)}{z-\omega} + \frac{A(-z)}{-z-\omega} \right\} dz$$

$$= \int_0^{\infty} \left\{ \frac{2\, z\, A(z)}{z^2-\omega^2} \right\} dz$$

Use this in the integral for Re K(ω) ...

$$\mathrm{Re}\,K(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{z\, \mathrm{Im}\,K(z)}{z^2-\omega^2} dz \quad \text{▫ (7.120)}$$

So far, we have shown that the Kramers-Kronig relations are true for the Lorentz model of dispersion.

But the Lorentz model is only based on a crude phenomenological model,

$$m\,(\ddot{x} + \gamma\,\dot{x} + \omega_0{}^2\, x = -\,e\,E\,)$$

and $\quad P_x = N\,(-e\,x)$

a two-parameter model (γ and ω_0).

In fact, an atomic theory of polarization must require quantum mechanics.

Friday: The Kramers-Kronig relations must be true for any theory of complex permittivity.

Applications of the Kramers-Kronig relations ⇒ optical materials research

There exist experimental methods to measure the absorption coefficient,

$$\alpha = \frac{\omega^2}{\beta c^2} \operatorname{Im} K$$

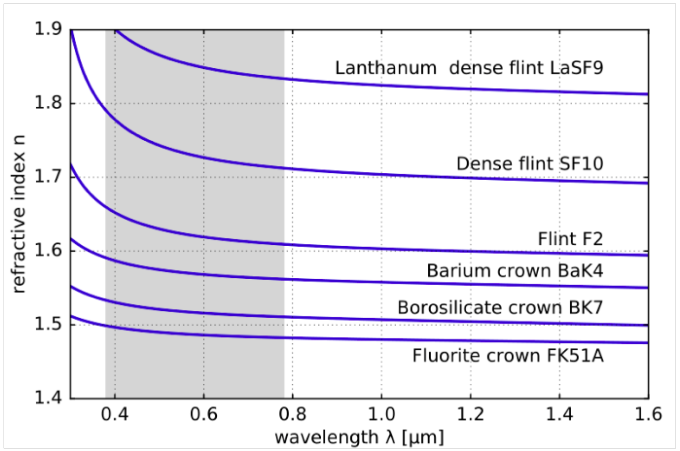
and the index of refraction

$$n = \frac{c\beta}{\omega} = \sqrt{\frac{c^2}{\omega^2}\left(\frac{\alpha^2}{4} + \frac{\omega^2}{c^2} \operatorname{Re} K\right)}$$

Because Im K and Re K are related by the KK relations, the measurements can be verified.

"The refractive index and extinction coefficient, n and κ, cannot be measured directly. They must be determined indirectly from measurable quantities that depend on them, such as reflectance, R, or transmittance, T. The determination of n and κ from such measured quantities will involve developing a theoretical expression for R or T, in terms of a valid physical model for n and κ. By fitting the theoretical model to the measured R or T, using regression analysis, n and κ can be deduced."

gl



Sum Rules

Here is an example.
For any material we may *define* the ***plasma frequency*** ω_p by

$$\omega_p = \lim_{\omega \longrightarrow \infty} \{ \omega^2 [1 - \epsilon(\omega)/\epsilon_0] \}$$

Then it can be shown that

$$\omega_p^2 = \frac{2}{\pi} \int_0^\infty \omega \, \mathrm{Im} \, \epsilon(\omega) \, / e_0 \, d\omega$$

which relates absorption to the plasma frequency.