Unit 5-6: The Kramers-Kronig Relation

For want of a better place to put this topic, I will put it here!

In our discussion of the frequency dependent atomic polarizability $\alpha(\omega)$ we saw that the response had to be *causal*, i.e. there is no response before the driving force begins. More mathematically,

$$\mathbf{p}(t) = \int_{-\infty}^{\infty} dt'\, \tilde{\alpha}(t-t')\, \mathbf{E}(t') \tag{5.6.1}$$

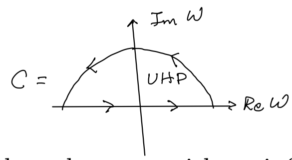
and the causality meant that we must have $\tilde{\alpha}(t) = 0$ for $t < 0$, so that $\mathbf{p}$ responds only to $\mathbf{E}$ at *earlier times.*

In terms of the Fourier transform $\alpha(\omega)$ we found that causality implied that $\alpha(\omega)$ could have no poles in the upper half of the complex ω plane.

This is a general feature of any causal response function, and it implies that there is a relation between the real and the imaginary parts of the response function. This is the Kramers-Kronig relation.

If $\alpha(\omega)$ is a causal response function, having no poles in the upper half of the complex ω plane (UHP), then for any complex valued $\bar{\omega}$ in the (UHP), we can write

$$\alpha(\bar{\omega}) = \frac{1}{2\pi i} \oint_C d\omega' \, \frac{\alpha(\omega')}{\omega' - \bar{\omega}} \tag{5.6.2}$$



where the contour C goes down the real axis, and then closes up with an infinite semicircle in the UHP.

The above result follows because, due to causality, $\alpha(\omega)$ has no poles in the UHP, and so the only pole of the integrand in the UHP is the pole at $\omega' = \bar{\omega}$.

Now the closing semicircular path of the contour in the UHP at infinity should give no contribution to the integral assuming that $\alpha(\omega)$ decays sufficiently quickly as $|\omega| \to \infty$. We thus have,

$$\alpha(\bar{\omega}) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \, \frac{\alpha(\omega')}{\omega' - \bar{\omega}} \tag{5.6.3}$$

Now consider $\bar{\omega} = \omega + i\delta$ where ω and δ are real valued, and $\delta \to 0$. Then

$$\alpha(\omega) = \lim_{\delta \to 0} \; \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \, \frac{\alpha(\omega')}{\omega' - \omega - i\delta} \tag{5.6.4}$$

Now

$$\frac{1}{\omega' - \omega - i\delta} = \mathbb{P}\left(\frac{1}{\omega' - \omega}\right) + i\pi\delta(\omega' - \omega) \qquad \text{where } \mathbb{P} \text{ stands for the principle part of the integral} \tag{5.6.5}$$

The principle part is defined by,

$$\mathbb{P}\int_{-\infty}^{\infty} d\omega' \frac{\alpha(\omega')}{\omega' - \omega} \equiv \lim_{\epsilon \to 0} \; \left[\int_{-\infty}^{\omega - \epsilon} d\omega' \frac{\alpha(\omega')}{\omega' - \omega} + \int_{\omega + \epsilon}^{\infty} d\omega' \frac{\alpha(\omega')}{\omega' - \omega}\right] \tag{5.6.6}$$

Substituting Eq. (5.6.5) into (5.6.4) then gives

$$\alpha(\omega) = \frac{1}{2\pi i}\, \mathbb{P}\int_{-\infty}^{\infty} d\omega' \, \frac{\alpha(\omega')}{\omega' - \omega} + \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \, i\pi\delta(\omega' - \omega)\alpha(\omega) = \frac{1}{2\pi i}\mathbb{P}\int_{-\infty}^{\infty} d\omega' \, \frac{\alpha(\omega')}{\omega' - \omega} + \frac{1}{2}\alpha(\omega) \tag{5.6.7}$$

This then gives

$$\alpha(\omega) = \frac{1}{\pi i}\, \mathbb{P}\int_{-\infty}^{\infty} d\omega' \, \frac{\alpha(\omega')}{\omega' - \omega} \tag{5.6.8}$$

Equating the real and the imaginary parts on both sides of the above then gives the Kramers-Kronig relations,

$$\boxed{\mathrm{Re}\,[\alpha(\omega)] = \frac{1}{\pi}\,\mathbb{P}\int_{-\infty}^{\infty} d\omega'\,\frac{\mathrm{Im}\,[\alpha(\omega')]}{\omega'-\omega} \qquad \text{and} \qquad \mathrm{Im}\,[\alpha(\omega)] = -\frac{1}{\pi}\,\mathbb{P}\int_{-\infty}^{\infty} d\omega'\,\frac{\mathrm{Re}\,[\alpha(\omega')]}{\omega'-\omega}} \tag{5.6.9}$$

So if a response function is causal, then if one knows the real part $\mathrm{Re}\,[\alpha]$, then one can reconstruct the imaginary part $\mathrm{Im}\,[\alpha]$, and vice-versa.