

General constructs in condensed matter physics

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A. Proof of the Kramers-Kronig Relations

Let us take a look at deriving the Kramers-Kronig relations for the case of a susceptibility. We start with a susceptibility function which is analytic in the upper-half of the complex plane, $\chi(\omega)$. χ is a susceptibility and it must represent the Fourier transform of a time-dependent response in time, which is causal. The relationship between the field \mathbf{E} and the resulting polarization (or force) is given as follows : $\mathbf{F} = \chi \cdot \mathbf{E}$. Invoking the Cauchy theorem, we have the result for the integral :

$$\oint \frac{\chi(\omega') d\omega'}{\omega' - \omega} = 0 \quad (1)$$

This result relies on the assumption that the $\chi(\omega') \rightarrow 0$ faster than $1/(\omega' - \omega)$. In order to evaluate the integral above, we need to construct a contour in the complex plane, which is depicted in the plot of Figure 1.

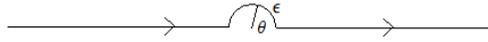


FIG. 1: (Color Online) Integration contour for evaluating the Kramers-Kronig relations.

We break up the Cauchy integral, in the following way :

$$\oint \frac{\chi(\omega') d\omega'}{\omega' - \omega} = \quad (2)$$

$$\int_{-R}^{\omega - \epsilon} \frac{\chi(\omega') d\omega'}{\omega' - \omega} \quad (3)$$

$$+ \int_{-\epsilon}^{\epsilon} \frac{\chi(\omega') d\omega'}{\omega' - \omega} \quad (4)$$

$$+ \int_{\omega + \epsilon}^R \frac{\chi(\omega') d\omega'}{\omega' - \omega} = 0 \quad (5)$$

In order to relax the integral path to the real axis, we can re-parameterize the frequency $\omega' - \omega = \epsilon e^{i\theta}$ we take the

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limit whereby $\epsilon \rightarrow 0$, $R \rightarrow \infty$ and we write :

$$\oint \frac{\chi(\omega') d\omega'}{\omega' - \omega} = \quad (6)$$

$$\int_{-\infty}^{\omega - \epsilon} \frac{\chi(\omega') d\omega'}{\omega' - \omega} \quad (7)$$

$$+ \int_0^{\pi} \frac{\chi(\omega') \epsilon i d\theta e^{i\theta}}{\epsilon e^{i\theta}} \quad (8)$$

$$+ \int_{\omega + \epsilon}^{\infty} \frac{\chi(\omega') d\omega'}{\omega' - \omega} = 0 \quad (9)$$

Rearranging this above expression, we have the following :

$$\pi i \chi(\omega) = \int_{-\infty}^{\infty} \frac{\chi(\omega') d\omega'}{\omega' - \omega} \quad (10)$$

Inserting the real and imaginary parts for the susceptibility function, we use the following :

$$\pi i (\chi_1(\omega) + i \chi_2(\omega)) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(\chi_1(\omega') + i \chi_2(\omega')) d\omega'}{\omega' - \omega} \quad (11)$$

from which come the Kramers-Kronig relations ;

$$\chi_2 = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \left(\frac{\chi_1(\omega')}{\omega' - \omega} \right) d\omega' \quad (12)$$

$$\chi_1 = \frac{1}{\pi} P \int_{-\infty}^{\infty} \left(\frac{\chi_2(\omega')}{\omega' - \omega} \right) d\omega' \quad (13)$$

$$(14)$$

We can multiply by the factor $(\omega' + \omega)/(\omega' + \omega)$, and use the property of the oddness of functions $\int_{-\infty}^{\infty} (\text{odd function}) = 0$. We have the more useful, semi-infinite

$$\chi_1(\omega) = \frac{1}{\pi} P \int_0^{\infty} d\omega' \left[\frac{\chi_2(\omega') \omega'}{\omega'^2 - \omega^2} \right] \quad (15)$$

B. Connection between the principal of causality, analyticity and the Kramers-Kronig relations

We start with a response function of a system in the time domain which is at the limit of a causal response, $\sigma(t) = \theta(t - t')$, where $\theta(t)$ is a Heaviside step function. The plot of $\sigma(t)$ is given below in the time domain We can

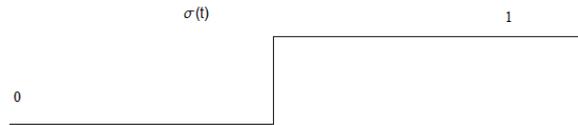


FIG. 2: (Color Online) Integration contour for evaluating the Kramers-Kronig relations.

take look at this response function in the frequency domain by taking the Fourier transform function.

$$\theta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \sigma(\omega) e^{-i\omega t} d\omega \quad (16)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \sigma(t) e^{i\omega t} dt \right) e^{-i\omega t} d\omega \quad (17)$$

We now go about using the integration by parts method ($\int u dv = uv - \int v du$) to perform the calculation for this Fourier integral and we write the integral as follows :

$$\frac{1}{2\pi} \int \theta(t) e^{i\omega t} dt = \frac{1}{2\pi} \left[\left(\frac{\theta(t) e^{i\omega t}}{i\omega} \right)_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{i\omega} \theta'(t) dt \right] \quad (18)$$

$$= \frac{1}{2\pi} \left[\left(\frac{\theta(t) e^{i\omega t}}{i\omega} \right)_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{i\omega} \delta(t) dt \right] \quad (19)$$

$$= \frac{1}{2\pi} \left(\frac{1}{i\omega} [\theta(t) e^{i\omega t}]_{-\infty}^{\infty} - \frac{e^{i\omega t}}{i\omega} \right) \quad (20)$$

$$= \frac{1}{2\pi} \left((\theta(t) - 1) \frac{e^{i\omega t}}{i\omega} \right) \quad (21)$$