Kramers–Kronig in two lines

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Citation: American Journal of Physics **57**, 821 (1989); doi: 10.1119/1.15901
View online: https://doi.org/10.1119/1.15901
View Table of Contents: https://aapt.scitation.org/toc/ajp/57/9
Published by the American Association of Physics Teachers

conclusions are very much the same. Clausius–Mossotti effects, i.e., the removal of the dipole–dipole on-site interaction, are implicitly included when we consider the energy bands of the solid.

IV. CONCLUSIONS

Clausius–Mossotti effects in dielectrics arise when we take into account the fact that the polarizable centers of the solid do not see their own field. When the polarizable centers are located with cubic symmetry, the local field at a given site of the lattice produced by the rest of the system is exactly the same as the average over the unit cell of that field. Thus the difference between these two fields produces no extra contribution to the Clausius–Mossotti effect.

In a quantum mechanical treatment for crystalline solids, the removal of the dipole–dipole on-site interaction is automatically taken into account if we consider the energy gap of the solid rather than the atomic energy gap.

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(Received 21 September 1988; accepted for publication 28 October 1988)

A short derivation of the Kramers–Kronig relations is presented.

The Kramers–Kronig relations relate the real and imaginary parts of the frequency-dependent linear response function $\chi(\omega)$,

$$\mathrm{Im}[\chi(\omega)] = -\frac{1}{\pi} P \int d\omega' \frac{\mathrm{Re}[\chi(\omega')]}{\omega' - \omega} \quad (1a)$$

$$\mathrm{Re}[\chi(\omega)] = \frac{1}{\pi} P \int d\omega' \frac{\mathrm{Im}[\chi(\omega')]}{\omega' - \omega}, \quad (1b)$$

where P means principal part. These relations are a consequence of causality and have found applications in many branches of physics, ranging from electrical network theory to elementary particle theory. The traditional method of proving these relations is to continue $\chi(\omega)$ to complex frequencies and then to exploit its analyticity in the upper half ω plane.[1,2] More elementary but slightly lengthier approaches can also be used to obtain these relations.[3] The purpose of this article is to present a derivation of the Kramers–Kronig relations that is both quick and simple.

The prerequisites for the derivation are two well-known results. The first is that the Fourier transform of the step function,

$$\theta(t) = \begin{cases} 1, & t > 0; \\ 0, & t < 0, \end{cases}$$

is given by[4]

$$\int_{-\infty}^{\infty} dt\, \theta(t) e^{i\omega t} = \lim_{\epsilon \to 0^+} \frac{i}{\omega + i\epsilon} = P\frac{i}{\omega} + \pi\delta(\omega). \quad (2)$$

The second is the Fourier transform convolution theorem[5]

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t} \hat{f}(t) \hat{g}(t) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega - \omega') g(\omega'). \quad (3)$$

Because of causality, the response function $\hat{\chi}(t)$ must have the form

$$\hat{\chi}(t) = \theta(t) \hat{Y}(t), \quad (4)$$

where $\hat{Y}(t) = \hat{\chi}(t)$ for $t > 0$. We are free to choose $\hat{Y}(t)$ for $t < 0$. On Fourier transforming Eq. (4) and using Eq. (2) and the convolution theorem, we obtain

$$\chi(\omega) = \frac{1}{2\pi} P \int \frac{iY(\omega')}{\omega - \omega'} d\omega' + \frac{Y(\omega)}{2}. \quad (5)$$

Now we exploit our freedom to choose $\hat{Y}(t)$ for $t < 0$.

(i) Choose $\hat{Y}(-|t|) = \hat{Y}(|t|)$. Then $Y(\omega)$ is pure real, and, hence, Eq. (5) gives $Y(\omega) = (2)\mathrm{Re}[\chi(\omega)]$. Substituting this into the integrand in Eq. (5) yields Eq. (1a).

(ii) Choose $\hat{Y}(-|t|) = -\hat{Y}(|t|)$. Then $Y(\omega)$ is pure imaginary, and, hence, Eq. (5) gives $iY(\omega) = -(2)\mathrm{Im}[\chi(\omega)]$. Substituting this into the integrand in Eq. (5) yields Eq. (1b).

ACKNOWLEDGMENT

This work is supported by the U.S. Office of Naval Research.

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