

GENERALIZATION OF THE KRAMERS-KRONIG FORMULAS TO MEDIA WITH SPATIAL DISPERSION

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A condition that must be satisfied by the complex electric permittivity of a medium with spatial dispersion, and that generalizes the Kramers-Kronig formulas, is derived by requiring satisfaction of the causality principle in a form following from the theory of relativity. The conditions obtained, in contrast to the Kramers-Kronig formulas, not only relate the real and imaginary parts of the permittivity to each other but also impose restrictions on each of them separately.

As is known, the complex dielectric permittivity $\epsilon(\omega)$ of a medium, as a function of ω , must satisfy the integral equation

$$\epsilon(\omega) - 1 = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\epsilon(\xi) - 1}{\xi - \omega} d\xi + \frac{4\pi\sigma_0 i}{\omega} \quad (1)$$

(here P indicates that the integral at the point $\xi = \omega$ is to be interpreted as the principal value; σ_0 is the conductivity at $\omega = 0$). This equation is equivalent to equations for the real and imaginary parts of $\epsilon(\omega)$ that are known as the Kramers-Kronig formulas (cf., for example, reference 1, Sec. 62). If instead of the complex permittivity we use the complex conductivity $\sigma(\omega) = -i\omega \times (\epsilon(\omega) - 1)/4\pi$, then instead of (1) we get for $\sigma(\omega)$ the equation

$$\sigma(\omega) = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\sigma(\xi)}{\xi - \omega} d\xi, \quad (2)$$

which can also be written in the form

$$\sigma(\omega) = \frac{1}{i\pi} \int_0^{\infty} \{\sigma(\omega + \eta) - \sigma(\omega - \eta)\} \frac{d\eta}{\eta}, \quad (2')$$

equivalent to (2). On setting $\sigma = \sigma' - \sigma''$, we get from (2) the Kramers-Kronig formulas

$$\sigma'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\sigma''(\xi)}{\xi - \omega} d\xi, \quad \sigma''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\sigma'(\xi)}{\xi - \omega} d\xi. \quad (3)$$

One of the functions, $\sigma'(\omega)$ or $\sigma''(\omega)$, may be given; then the other is determined by (3). It must be remembered that either of the equations (3) implies the other as a consequence.

These formulas are obtained from a condition imposed by the principle of causality. Namely, since the field is the cause of the current, the linear integral operator that connects the total

current $j(t)$ with the field $E(t)$ must have the form

$$j(t) = \int_0^{\infty} S(\tau) E(t - \tau) d\tau,$$

where the integration extends only over instants of time $t - \tau$ preceding the instant t . Accordingly, the complex conductivity $\sigma(\omega)$, which relates the current and the field [$j = \sigma(\omega) E$] when the field varies according to the factor $e^{-i\omega t}$, is expressed by the one-sided Fourier integral (between limits 0 and ∞)

$$\sigma(\omega) = \int_0^{\infty} S(\tau) e^{i\omega\tau} d\tau. \quad (4)$$

Equation (2) or (2') is the condition that the Fourier transform $s(\tau)$ of the function $\sigma(\omega)$ vanish for negative τ , so that the Fourier expansion of $\sigma(\omega)$ may be a one-sided integral (cf., for example, reference 2, Secs. 5.1 - 5.4).

In a medium with spatial dispersion, the current at a given point is determined by the field not just at that point but at neighboring points as well. The relation between the current and the field in this case is expressed by an integral both over time and over space. In this case the requirement imposed by the causality principle, with attention to the requirements of the theory of relativity, leads to the result that in this integral the integration must be extended over the region inside a cone of light facing the past. For our purpose it is sufficient to consider the case in which the field depends only on the coordinate x . Then for a homogeneous medium the requirement mentioned clearly leads to the following expression relating the current to the field:

$$j(t, x) = \int_0^{\infty} d\tau \int_{-\tau}^{\tau} S(\tau, \xi) E(t - \tau, x - \xi) d\xi.$$

Here the unit of time has been so chosen that $c = 1$. On setting $E(t, x) = \exp[-i(\omega t + kx)]$, we get $j = \sigma(\omega, k) E$, with the complex conductivity

$$\sigma(\omega, k) = \int_0^\infty e^{i\omega\tau} d\tau \int_{-\tau}^\tau S(\tau, \xi) e^{ik\xi} d\xi. \quad (5)$$

From the fulfillment of this necessary condition of relativity theory it follows, in particular, that the leading wave front is propagated with the speed of light. This conclusion is quite natural, since now the equations of electrodynamics (including even the equation that relates the current to the field) satisfy the requirements of relativity theory. An analytic proof of this conclusion is also quite simple. (This conclusion, obviously, is correct also for media without spatial dispersion, when the causality requirement is fulfilled in the form indicated above; and it implies that in the limit $\sigma(\omega) \rightarrow 0$ as $\omega \rightarrow \infty$.)

As is known,^{3,4} the complex conductivity of isotropic media, which we are here considering, is described by a tensor of the form

$$\sigma_{ij} = \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right) \sigma^t(\omega, k) + \frac{k_i k_j}{k^2} \sigma^l(\omega, k).$$

Although we have not explicitly taken account of this circumstance, we obviously may consider separately transverse and longitudinal waves; thus the quantity $\sigma(\omega, k)$ may be either the transverse conductivity σ^t or the longitudinal one σ^l . The conductivity $\sigma(\omega, k)$ depends only on the absolute value k of the vector \mathbf{k} .* Furthermore, since the function $S(\tau, \xi)$ is real, the real part of $\sigma(\omega, k)$ is an even function of ω , and the imaginary part is an odd function.

It is obvious that for fixed k , the conductivity $\sigma(\omega, k)$, Eq. (5), as a function of ω can be expressed as a semi-infinite Fourier integral over τ , and reduces to the form (4) if we set

$$S(\tau) = \int_{-\tau}^\tau S(\tau, \xi) e^{ik\xi} d\xi.$$

Therefore $\sigma(\omega, k)$ as a function of ω must (for arbitrary fixed k) satisfy Eq. (2'), i.e.,

$$\sigma(\omega, k) = \frac{1}{i\pi} \int_0^\infty \left\{ \sigma(\omega + \eta, k) - \sigma(\omega - \eta, k) \right\} \frac{d\eta}{\eta}. \quad (6)$$

*It is not difficult to show that the possibility of expressing the function $\sigma(\omega, k)$ in the form (5) is equivalent to the possibility of expressing it in the form of an integral over space:

$$\sigma(\omega, k) = \int_0^\infty e^{i\omega\tau} d\tau \int_{r<\tau} Q(\tau, r) e^{ikr} dr.$$

where

$$Q(\tau, r) = (1/2\pi r) \partial S(\tau, r) / \partial r.$$

We may, however, write a more general equation for $\sigma(\omega, k)$ if we notice that Eq. (5) preserves its form when the variables τ and ξ undergo a Lorentz transformation (with transformation of the scale of both variables). In fact, under this transformation the light cone is transformed into itself. At the same time σ goes over into a function of variables ω' and k' , related to ω and k also by a Lorentz transformation (inverse to the transformation of τ and ξ):

$$\omega = \gamma(\omega' - \beta k'), \quad k = \gamma(k' - \beta \omega'), \quad |\beta| \leq 1. \quad (7)$$

From this it follows that $\sigma(\gamma(\omega' - \beta k'), \gamma(k' - \beta \omega'))$, as a function of ω' (for fixed k'), will also satisfy condition (6), i.e.,

$$\begin{aligned} &\sigma(\gamma(\omega' - \beta k'), \gamma(k' - \beta \omega')) \\ &= \frac{1}{i\pi} \int_0^\infty \left\{ \sigma(\gamma(\omega' + \eta' - \beta k'), \gamma(k' - \beta \omega' - \beta \eta')) \right. \\ &\quad \left. - \sigma(\gamma(\omega' - \eta' - \beta k'), \gamma(k' - \beta \omega' + \beta \eta')) \right\} \frac{d\eta'}{\eta'}. \end{aligned}$$

By transforming now to the variables ω and k and setting $\eta = \gamma \eta'$, we get

$$\sigma(\omega, k) = \frac{1}{i\pi} \int_0^\infty \left\{ \sigma(\omega + \eta, k - \beta \eta) - \sigma(\omega - \eta, k + \beta \eta) \right\} \frac{d\eta}{\eta}, \quad (8)$$

where β has an arbitrary value in the interval $|\beta| \leq 1$.

We shall now show that in order that $\sigma(\omega, k)$ may be expressible in the form of a Fourier integral (5) extended over the quadrant $|\xi| < \tau$, it is sufficient that condition (8) be satisfied for $\beta = +1$ and for $\beta = -1$. For this purpose we find the Fourier transform of a function $\sigma(\omega, k)$ satisfying condition (8).

This will be

$$S(\tau, \xi) = \frac{1}{4\pi^2} \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-i(\omega\tau + k\xi)} \sigma(\omega, k) d\omega dk.$$

Here τ and ξ may take all values from $-\infty$ to $+\infty$. On inserting $\sigma(\omega, k)$ from (8), changing the order of integration, and making the transformation of variables $\omega \pm \eta = \omega_1$, $k \mp \beta \eta = k_1$, we get

$$\begin{aligned} S(\tau, \xi) &= \frac{1}{2\pi^2} \int_0^\infty \frac{\sin(\tau - \beta \xi) \eta}{\eta} d\eta \\ &\times \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-i(\omega_1 \tau + k_1 \xi)} \sigma(\omega_1, k_1) d\omega_1 dk_1. \end{aligned}$$

By noting that

$$\int_0^\infty \sin \alpha \eta \frac{d\eta}{\eta} = \frac{\pi}{2} \operatorname{sgn} \alpha,$$

we get

$$S(\tau, \xi) = S(\tau, \xi) \operatorname{sgn}(\tau - \beta\xi)$$

or
$$S(\tau, \xi) [1 - \operatorname{sgn}(\tau - \beta\xi)] = 0. \quad (9)$$

Hence it is clear that $S(\tau, \xi)$ can be different from zero only where $\tau - \beta\xi$ is positive.

This means that for fixed β the function $S(\tau, \xi)$ can be different from zero to the right of the straight line $\xi = \tau/\beta$ (in the unshaded half-plane in the figure). When β varies from -1 to $+1$, this straight line rotates clockwise, taking all positions between the straight lines $\xi = -\tau$ and $\xi = \tau$ (which bound the quadrant of interest to us, $|\xi| < \tau$). It is clear that from condition (9) merely for $\beta = -1$ and $\beta = +1$ it follows that $S(\tau, \xi)$ is different from zero only in this quadrant; and this means that the Fourier expansion of $\sigma(\omega, k)$ has the form (5). Satisfaction of condition (8) for $\beta = +1$ and for $\beta = -1$ is thus sufficient. Since (5) follows from this, satisfaction of condition (8) for other values of β ($|\beta| \leq 1$) is a consequence of satisfaction of it for $\beta = +1$ and for $\beta = -1$.

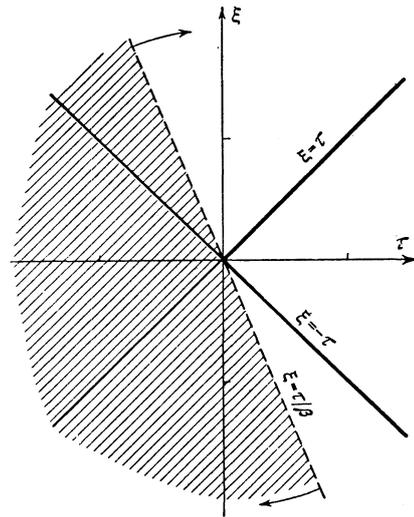
The complex conductivity $\sigma(\omega, k)$, which is of interest to us, is an even function of k . It is easy to show that for an even function, the conditions (8) written for $\beta = +1$ and for $\beta = -1$ coincide. Therefore our function $\sigma(\omega, k)$ needs to satisfy a single condition, which is obtained from (8) by setting $\beta = 1$. If we now go over to the usual units of time, k must be replaced by kc ; then on transforming (8) to a form analogous to (2), we get

$$\sigma(\omega, k) = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\sigma(\zeta, k + \beta(\zeta - \omega)/c)}{\zeta - \omega} d\zeta. \quad (10)$$

It is sufficient that $\sigma(\omega, k)$ satisfy this condition for $\beta = 1$; then $\sigma(\omega, k)$ will satisfy it for arbitrary β ($|\beta| \leq 1$).

Equation (10) gives the generalization of the Kramers-Kronig formulas for a medium with spatial dispersion. As $c \rightarrow \infty$, (10) becomes usual Kramers-Kronig equation (2).

It is necessary, however, to pay attention to the following important difference in the conditions imposed on $\sigma(\omega, k)$. In the usual case, without spatial dispersion, one of the functions, $\sigma'(\omega)$ or $\sigma''(\omega)$ ($\sigma = \sigma' - i\sigma''$), may be specified arbitrarily, whereas the other is determined by a Kramers-Kronig formula. The two formulas (3), relating $\sigma'(\omega)$ and $\sigma''(\omega)$, are not independent, one being a consequence of the other (for example, substitution in the first formula of $\sigma''(\omega)$ from the second leads to an equality containing only $\sigma'(\omega)$ and satisfied identically). Whereas $\sigma(\omega)$ is expressed in the form of the semi-infinite Fourier integral (4), $\sigma'(\omega)$ and $\sigma''(\omega)$ are expressed in the form



of the general Fourier integral, extended from $-\infty$ to $+\infty$, but their Fourier transforms can be expressed in terms of each other in a known fashion:

$$\begin{aligned} \sigma'(\omega) &= \frac{1}{2} \int_{-\infty}^{\infty} S(\tau) e^{i\omega\tau} d\tau, \\ \sigma''(\omega) &= \frac{1}{2i} \int_{-\infty}^{\infty} S(\tau) e^{i\omega\tau} \operatorname{sgn} \tau \cdot d\tau, \\ S'(-\tau) &= S(\tau). \end{aligned}$$

In contrast to this, condition (10) not only relates the real and imaginary parts of $\sigma(\omega, k)$, but also imposes restrictions on each of them separately. For since [by (5)] $\sigma(\omega, k)$ is expressed by a Fourier integral extended only over the single quadrant $|\xi| < \tau$ therefore $\sigma'(\omega, k)$ and $\sigma''(\omega, k)$ will be expressed by Fourier integrals extended only over two quadrants ($|\xi| < \tau$ and the one opposite it), and not over the whole (ξ, τ) plane. This imposes a condition on each of the functions $\sigma'(\omega, k)$ and $\sigma''(\omega, k)$.

It is still necessary to add the following. Whereas the longitudinal conductivity $\sigma^l(\omega, k)$ must always satisfy condition (10), the transverse conductivity $\sigma^t(\omega, k)$ satisfies this condition only for a nonmagnetic medium; more accurately, for a medium whose static magnetic permeability is unity. In the general case we have^{3,4}

$$\sigma^t(\omega, k) = \sigma^l(\omega, k) - \frac{ik^2c^2}{\omega} \left(1 - \frac{1}{\mu(\omega, k)}\right), \quad (11)$$

where $\mu(\omega, k)$ is the magnetic permeability, dependent on ω and k . Whereas $\sigma^l(\omega, k)$, describing the electrical properties of the medium, has no singularity at $\omega = 0$, the function $\sigma^t(\omega, k)$, as is clear from (11), has a singular point (pole) there if $\mu(0, k) \neq 1$.

To generalize Eq. (10) to this case, it is necessary to proceed in the following manner.

The quantity $\partial j/\partial t$ will be related to the field E by an integral operator of the same type as that relating j to E ; and, clearly, this operator will also satisfy the requirements of relativistic causality. For a monochromatic plane transverse wave

$$\partial j/\partial t = -i\omega\sigma^t(\omega, k)E.$$

Consequently $\omega\sigma^t(\omega, k)$ must satisfy an equation of the form (10) (since $\omega\sigma^t$ no longer has a singular point at $\omega = 0$), i.e., the equation

$$\omega\sigma^t(\omega, k) = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\zeta\sigma^t(\zeta, k + \beta(\zeta - \omega)/c)}{\zeta - \omega} d\zeta. \quad (12)$$

Hence after some transformations we get

$$\begin{aligned} \sigma^t(\omega, k) &= \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\sigma^t(\zeta, k + \beta(\zeta - \omega)/c)}{\zeta - \omega} d\zeta \\ &+ \frac{1}{i\pi\omega} P \int_{-\infty}^{\infty} \sigma^t\left(\zeta, k + \frac{\beta}{c}(\zeta - \omega)\right) d\zeta. \end{aligned} \quad (13)$$

Here the integrals are to be interpreted as principal values at the points $\zeta = 0$ and $\zeta = \omega$. From (12) we get

$$\frac{1}{i\pi} P \int_{-\infty}^{\infty} \sigma^t\left(\zeta, k + \frac{\beta}{c}(\zeta - \omega)\right) d\zeta = \lim_{\omega' \rightarrow 0} \omega' \sigma^t\left(\omega', k - \frac{\beta}{c}\omega\right),$$

and from (11) we find

$$\begin{aligned} \lim_{\omega' \rightarrow 0} \omega' \sigma^t\left(\omega', k - \frac{\beta}{c}\omega\right) \\ = -i\left(k - \frac{\beta}{c}\omega\right)^2 c^2 \left(1 - \frac{1}{\mu(0, k - \beta\omega/c)}\right). \end{aligned}$$

On substituting this value in (13), we get

$$\begin{aligned} \sigma^t(\omega, k) &= \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{\sigma^t(\zeta, k + \beta(\zeta - \omega)/c)}{\zeta - \omega} d\zeta \\ &- \frac{i(kc - \beta\omega)^2}{\omega} \left(1 - \frac{1}{\mu(0, k - \beta\omega/c)}\right). \end{aligned} \quad (14)$$

In closing, it should be indicated how the conclusions deduced above carry over to an anisotropic medium, with spatial dispersion described by a complex conductivity tensor $\sigma_{ij}(\omega, \mathbf{k})$ whose components depend both on the absolute value of k and on the direction of the vector \mathbf{k} . It is easy to show that the requirements of relativistic causality impose restrictions not on the dependence of σ_{ij} on the direction of \mathbf{k} , but only on its dependence on the absolute value k . Thus in this case each component σ_{ij} , as a function of ω and k , satisfies the previous equation (10) [or, in the general case, (14)].

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