Kramers-Kronig Relations

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In the following pages, we will examine the mathematical properties of the dielectric permittivity as a function of the frequency for rapidly variable fields and we will derive the Kramers-Kronig relations, which mutually relate the real and imaginary part of the permittivity.

I. RELATION BETWEEN THE E FIELD AND THE INDUCTION D

Let us consider a medium in presence of an electric field, which varies in time. For rapidly variable fields, the amplitudes of the fields involved are pratically always fairly small. Therefore, the relation between $\mathbf{D}$ and $\mathbf{E}$ can be always taken to be linear. The most generic linear relation between $\mathbf{D}(t)$ and the values of $\mathbf{E}(t)$ at every previous instant can be written in the integral form:

$$\mathbf{D}(t) = \mathbf{E}(t) + \int_0^t f(\tau)\mathbf{E}(t-\tau)\mathrm{d}\tau \tag{1}$$

$f(\tau)$ is a function of time and of the properties of the medium. In analogy with the electrostatic relation $\mathbf{D} = \epsilon\mathbf{E}$, we can write equation (1) in the symbolic form $\mathbf{D} = \hat{\epsilon}\mathbf{E}$, where $\hat{\epsilon}$ is a linear integral operator whose effect is the one shown in (1).
Any variable field can be expanded into a series of single-frequency components (*Fourier series*), in which all quantities depend on time through the factor $e^{-i\omega t}$. For these field, relation (1) can be rewritten as

$$\mathbf{D} = \hat{\epsilon}(\omega)\mathbf{E} \tag{2}$$

where the function $\hat{\epsilon}(\omega)$ is defined, as

$$\hat{\epsilon}(\omega) \equiv \frac{\epsilon(\omega)}{\epsilon_0} = 1 + \int_0^{+\infty} f(\tau)e^{i\omega\tau}\mathrm{d}\tau \tag{3}$$

ϵ_0 being the dielectric constant in vacuum. From now on, we will omit the hat sign. Hence, for variable fields, we can regard the electric permittivity as a function of the frequency and of the properties of the medium. The dependence of ϵ on the frequency is called *dispersion law*.
In general, the function $\epsilon(\omega)$ is complex. We shall denote its real and imaginary parts by respectively ϵ' and ϵ'': $\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$. From equation (3), it follows immediately that

$$\epsilon(-\omega) = \epsilon^*(\omega) \tag{4}$$

Separating real and imaginary parts, we obtain

$$\epsilon'(-\omega) = \epsilon'(\omega), \qquad \epsilon''(-\omega) = -\epsilon''(\omega) \tag{5}$$

Thus, ϵ' is an even function of the frequency, while ϵ'' is odd. In the limit $\omega \to 0$, the function $\epsilon(\omega)$ tends naturally to the dielectric constant $\epsilon_r > 1$. For dielectrics, therefore, the Taylor expansion of ϵ' begins with the constant term ϵ_r, while the Taylor expansion of ϵ'' begins with a term in ω.
In the limit $\omega \to \infty$, $\epsilon(\omega)$ tends to unity: this is due to the fact that when the fields vary too rapidly, the polarization processes responsible of the difference between the field $\mathbf{E}$ and the induction $\mathbf{D}$ cannot occur. We shall assume that the frequency of the field is greater compared to the frequencies that characterize the motion of the electrons of the atoms of the medium. When this condition is satisfied, we can calculate the polarization of the medium regarding the electrons as free and neglecting any other interaction. The velocities v of the motion of the electrons are far smaller than the speed of light c, so the distances travelled v/ω by the electrons in one period of the electromagnetic wave are small compared to the wavelenght c/ω. For this reason, we can assume that the field is uniform in order to determine the velocity acquired by one electron in that field.
The equation of motion is therefore

$$m\frac{\mathrm{d}\mathbf{v}'}{\mathrm{d}t} = -e\mathbf{E} = -e\mathbf{E}_0 e^{-i\omega t} \tag{6}$$

where $-e$ and m are the charge and the mass of the electron. Solving the equation we obtain $\mathbf{v}' = -ie\mathbf{E}/m\omega$. The displacement $\mathbf{r}$ is given by $\dot{\mathbf{r}} = \mathbf{v}'$, that is $\mathbf{r} = e\mathbf{E}/m\omega^2$. The polarization is the dipole moment per unit volume: if N is the total number of electrons per unit volume, we have

$$\mathbf{P} = -Ne\mathbf{r} = -\frac{Ne^2\mathbf{E}}{m\omega^2} \tag{7}$$

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From the definition of induction[?], $\mathbf{D} = \epsilon(\omega)\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}$, it follows

$$\epsilon(\omega) = 1 - \frac{4\pi N e^2}{m\omega^2} \tag{8}$$

II. RELATION BETWEEN REAL PART AND IMAGINARY PART OF $\epsilon(\omega)$

The function $f(\tau)$ which appears in equation (1) is finite for every value of τ, including zero. For dielectrics, it tends to zero as $\tau \to \infty$. This merely expresses the fact that the value of $\mathbf{D}(t)$ at some instant cannot be appreciably affected by the values of $\mathbf{E}(t)$ at remote instants. The physical concept underlying equation (1) is the establishment of electric polarization; therefore, the range of values for which $f(\tau)$ is significantly different from zero is of the order of the relaxation time that characterizes these processes.
We have defined the function $\epsilon(\omega)$ as

$$\epsilon(\omega) = 1 + \int_0^{+\infty} e^{i\omega\tau} f(\tau) \mathrm{d}\tau$$

It is possible to derive some general properties involving this function by using the methods of complex analysis. In order to do so, we regard ω as a complex variable ($\omega = \omega' + i\omega''$) and study the properties of the function $\epsilon(\omega)$ in the upper-half plane ($\omega'' > 0$).
For the definition (1), together with the properties mentioned above, it follows that $\epsilon(\omega)$ is an one-valued regular function everywhere in the upper-half plane. Matter of fact, for $\omega'' > 0$, the integrand in (1) contains the exponentially-decreasing factor $e^{-\omega''\tau}$; hence, since $f(\tau)$ is finite throughout the region of integration, the integral converges. The permittivity $\epsilon(\omega)$ for dielectrics has no singularities on the real axis ($\omega'' = 0$). The physical meaning of $\epsilon(\omega)$ in the upper-half plane is the relation between $\mathbf{D}$ and $\mathbf{E}$ for fields whose amplitude decreases as $e^{-\omega'' t}$. The conclusion that $\epsilon(\omega)$ is regular on the upper-half plane is, physically, a consequence of the casualty principle.
It is also evident from definition (1) that

$$\epsilon(-\omega^*) = \epsilon^*(\omega) \tag{9}$$

This relation generalizes the one expressed in equation (4) to complex ω. In particular, for purely imaginary ω we have $\epsilon(i\omega'') = \epsilon^*(i\omega'')$, that means that $\epsilon(\omega)$ is real on the imaginary axis:

$$\Im(\epsilon) = 0 \qquad \text{for } \omega = i\omega'' \tag{10}$$

Equation (9) simply expresses the fact that the operator relation $\mathbf{D} = \hat{\epsilon}\mathbf{E}$ must give real values of $\mathbf{D}$ for real values of $\mathbf{E}$. If the field $\mathbf{E}(t)$ is given by the real expression

$$\mathbf{E} = \mathbf{E}_0 e^{-i\omega t} + \mathbf{E}_0^* e^{i\omega^* t}$$

then, applying the operator $\hat{\epsilon}$ we have

$$\mathbf{D} = \epsilon(\omega)\mathbf{E}_0 e^{-i\omega t} + \epsilon(-\omega^*)\mathbf{E}_0^* e^{i\omega^* t}$$

and the condition for this to be real is indeed the condition (9).

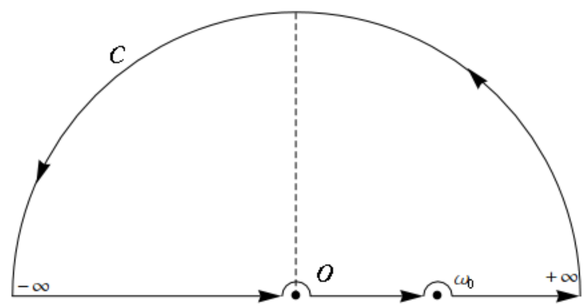
The imaginary part of $\epsilon(\omega)$ is positive for real positive $\omega = \omega' > 0$, that is the right-half plane. Since from equation (9) we have $\Im(\epsilon(-\omega')) = -\Im(\epsilon(\omega'))$, the imaginary part of $\epsilon(\omega)$ is negative in the left-half plane. In compact form

$$\Im(\epsilon) \lesseqgtr 0 \qquad \text{for } \omega = \omega' \lesseqgtr 0 \tag{11}$$

For $\omega = 0$, $\Im(\epsilon)$ changes sign passing through zero: the origin is the only point on the real axis in which $\Im(\epsilon)$ might vanish.
As ω approaches to ∞ in any manner in the upper-half plane, $\epsilon(\omega)$ tends to unity: if $\omega \to \infty$ in such a way that $\omega'' \to \infty$, the integral in equation (1) vanishes due to the factor $e^{-\omega''\tau}$ in the integrand, while if ω'' remains finite but $|\omega'| \to \infty$, the integral vanishes because of the oscillating factor $e^{i\omega'\tau}$ (*Riemann-Lebesgue lemma*).
The properties seen of $\epsilon(\omega)$ are sufficient to demonstrate the following

Theorem 1.
The function $\epsilon(\omega)$ takes no real values at any finite point in the upper-half plane, except on the imaginary axis, where it decreases monotonically from $\epsilon_0 > 1$ (for dielectrics) for $\omega = i0$ to 1 for $\omega = i\infty$. In particular, it follows that $\epsilon(\omega)$ has no zeroes on the upper-half plane.

Let us now choose a real value ω_0 of ω and integrate the function $(\epsilon(\omega) - 1)/(\omega - \omega_0)$ along the contour C given by:



The contour C includes the whole real axis, indented upwards at $\omega = \omega_0$ and it is completed by a semi-circle of infinite radius. At infinities, $\epsilon \to 1$ and the function $(\epsilon - 1)/(\omega - \omega_0)$ tends to zero more rapidly than $1/\omega$. Therefore the integral

$$\oint_C \frac{\epsilon(\omega) - 1}{\omega - \omega_0} \mathrm{d}\omega \tag{12}$$

converges; since $\epsilon(\omega)$ is regular in the upper-half plane and the point $\omega = \omega_0$ has been excluded from the region of integration, the function $(\epsilon-1)/(\omega-\omega_0)$ is analytic everywhere inside the contour C and therefore the integral is zero for Cauchy's theorem. The integral over the semi-circle of infinite radius is also zero. We pass round the point ω_0 along a semi-circle whose radius $\rho \to 0$. The direction of integration is clockwise, and the contribution to the integral is $-i\pi[\epsilon(\omega_0) - 1)]$. Hence we have

$$\lim_{\rho \to 0} \left[\int_{-\infty}^{-\rho+\omega_0} \frac{\epsilon - 1}{\omega - \omega_0} \mathrm{d}\omega + \int_{\rho+\omega_0}^{\infty} \frac{\epsilon - 1}{\omega - \omega_0} \mathrm{d}\omega \right] - i\pi[\epsilon(\omega_0) - 1] = 0$$

The limit represents the integral from $-\infty$ to $+\infty$, taken as principal value. Thus

$$\mathrm{PV} \int_{-\infty}^{+\infty} \frac{\epsilon - 1}{\omega - \omega_0} \mathrm{d}\omega - i\pi[\epsilon(\omega_0) - 1] = 0 \tag{13}$$

The variable of integration ω takes now only real values. We replace it with x, call ω the chosen real value ω_0 and write the function $\epsilon(\omega)$ as $\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$. Separating the real and imaginary parts in equation (13) we obtain at last the following two formulae:

$$\epsilon'(\omega) - 1 = \frac{1}{\pi} \mathrm{PV} \int_{-\infty}^{+\infty} \frac{\epsilon''(x)}{x - \omega} \mathrm{d}x \tag{14}$$

$$\epsilon''(\omega) = -\frac{1}{\pi} \mathrm{PV} \int_{-\infty}^{+\infty} \frac{\epsilon'(x) - 1}{x - \omega} \tag{15}$$

first derived by H.A. Kramers and R. de L. Kronig in 1927. It is important to notice that the only property of the function $\epsilon(\omega)$ used in the derivation is the regularity on the upper-half plane. Therefore, we can assert that Kramers-Kronig formulae are a direct consequence of the casualty principle.
Using the fact that $\epsilon''(x)$ is an odd function, we can rewrite equation (14) as

$$\begin{aligned} \epsilon'(\omega) - 1 &= \frac{1}{\pi} \mathrm{PV} \int_0^{+\infty} \frac{\epsilon''(x)}{x - \omega} \mathrm{d}x + \frac{1}{\pi} \mathrm{PV} \int_0^{+\infty} \frac{\epsilon''(x)}{x + \omega} \mathrm{d}x \\ &= \frac{2}{\pi} \mathrm{PV} \int_0^{+\infty} \frac{x\epsilon''(x)}{x^2 - \omega^2} \mathrm{d}x \end{aligned} \tag{16}$$

Equation (16) has an important significance: it makes possible to calculate the function $\epsilon'(\omega)$ even if the function $\epsilon''(\omega)$ is known approximately (i.e. empirically). We notice that for every function $\epsilon''(\omega)$ satisfying $\epsilon'' > 0$ for $\omega > 0$, formula (16) gives a function ϵ' which is coherent with all the physical requirements. On the other side, that is not true for equation (15), because for any arbitrary choice of $\epsilon'(\omega)$, it might be not true that the condition $\epsilon''(\omega) > 0$ for $\omega > 0$ is satisfied.
In dispersive theory, the expression of $\epsilon'(\omega)$ is usually written as

$$\epsilon'(\omega) - 1 = -\frac{4\pi e^2}{m} \mathrm{PV} \int_0^{+\infty} \frac{f(x)}{\omega^2 - x^2} \mathrm{d}x \tag{17}$$

where e and m are the charge and the mass of the electron and $f(\omega)\mathrm{d}\omega$ is called the *oscillator strength* in frequency range $\mathrm{d}\omega$. A comparison with equation (16) shows us that the relation that occurs between $f(\omega)$ and $\epsilon''(\omega)$ is

$$f(\omega) = \frac{m}{2\pi^2 e^2} \omega \epsilon''(\omega) \tag{18}$$

For very large values of ω, x^2 can be neglected in the integrand of (16), thus

$$\epsilon'(\omega) - 1 = -\frac{2}{\pi\omega^2} \int_0^{+\infty} x\epsilon''(x)\mathrm{d}x \tag{19}$$

For the dielectric constant at high frequencies, relation (8) holds and the comparison shows that

$$\frac{m}{2\pi^2 e^2} \int_0^{+\infty} \omega\epsilon''(\omega)\mathrm{d}\omega = \int_0^{+\infty} f(\omega)\mathrm{d}\omega = N \tag{20}$$

If $\epsilon''(\omega)$ is regular in $\omega = 0$, we can take the limit for $\omega \to 0$ in equation (16), obtaining

$$\epsilon'(0) - 1 = \frac{2}{\pi} \int_0^{+\infty} \frac{\epsilon''(x)}{x} \mathrm{d}x \tag{21}$$

For a dielectric, equation (21) can be rewritten as

$$\epsilon_r - 1 = \frac{4\pi N e^2}{m} \overline{\omega^{-2}} \tag{22}$$

where the bar denotes the average over the number of oscillators:

$$\overline{\omega^{-2}} \equiv \frac{1}{N}\int_0^{+\infty}\frac{f(\omega)}{\omega^2}\mathrm{d}\omega \qquad (23)$$

Equation (22) might be used to estimate the value of ϵ_r.
At last, the following formula relates the values of $\epsilon(\omega)$ on the upper-half of the imaginary axis to the ones of $\epsilon''(\omega)$ on the real axis:

$$\epsilon(i\omega) - 1 = \frac{2}{\pi}\int_0^{+\infty}\frac{x\epsilon''(x)}{x^2+\omega^2}\mathrm{d}x \qquad (24)$$

Integrating over all frequencies, we obtain

$$\int_0^{+\infty}[\epsilon(i\omega)-1]\mathrm{d}\omega = \int_0^{+\infty}\epsilon''(\omega)\mathrm{d}\omega \qquad (25)$$

III. APPENDIX

In this appendix, we shall prove theorem 2.1. We report the statement:

Theorem 1.
The function $\epsilon(\omega)$ takes no real values at any finite point in the upper-half plane, except on the imaginary axis, where it decreases monotonically from $\epsilon_r > 1$ (for dielectrics) for $\omega = i0$ to 1 for $\omega = i\infty$. In particular, it follows that $\epsilon(\omega)$ has no zeroes on the upper-half plane.

Proof. Let $\alpha(\omega) = \epsilon(\omega) - 1$. We prove the theorem for dielectrics. From complex analysis it is known that the integral

$$\frac{1}{2\pi i}\oint_C \frac{\mathrm{d}\alpha(\omega)}{\mathrm{d}\omega}\frac{\mathrm{d}\omega}{\alpha(\omega)-a} \qquad (26)$$

taken over a certain close curve C is equal to the difference between the number of zeroes and the number of poles of the function $\alpha(\omega) - a$ in the region bounded by C. We choose $a \in \mathbb{R}$ and let C be the curve formed by the whole real axis, closed by an infinite semicircle in the upper-half plane. Since in the upper-half plane the function $\alpha(\omega)$ has no pole, so $\alpha(\omega) - a$ has no pole and the integral (26) simply gives the number of zeroes of the function $\alpha(\omega) - a$. In order to evaluate the integral, we write it as

$$\frac{1}{2\pi i}\oint_{C'}\frac{\mathrm{d}\alpha}{\alpha - a} \qquad (27)$$

where C' is the curve which maps the curve C in the ω-plane in the plane of the complex variable α. The infinite semicircle is mapped on to the point $\alpha = 0$, while the origin $\omega = 0$ is mapped on to the point $\alpha_0 \equiv \epsilon_r - 1$. The right and left halves of the real axis are mapped in the α-plane on to some very complicated curves, which entirely lie in the upper-half plane and in the lower-half plane, respectively. It is important to note that these curves do not cross the real axis (except in the points $\alpha = 0, \alpha = \alpha_0$), since α does not take real values for any real value of ω except $\omega = 0$. Because of this property of C', the total variation in argument of the complex number $\alpha - a$ passing round C' is 2π if $a \in [0, \alpha_0]$, or zero if $a \notin [0, \alpha_0]$. It follows that the integral (26) is equal to 1 if $0 < a < \alpha_0$, zero for any other value of a. We therefore conclude that $\alpha(\omega)$ takes in the upper-half plane each real value of a in the range $[0, \alpha_0]$ only once and the values outside the range not at all. Hence, on the imaginary axis, where $\alpha(\omega)$ is real, $\alpha(\omega)$ can not have neither a maximum nor a minimum, otherwise it will assume twice some value. Consequently, $\alpha(\omega)$ varies monotonically on the imaginary axis, taking on that axis and nowhere else each real value from α_0 to zero only once.

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IV. REFERENCES

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