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GENERALIZED IMMITTANCE KERNELS AND THE KRONIG-KRAMERS RELATIONS

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Synopsis

A general relation between the poles and residues of a Kronig-Kramers pair is established which enables one to prove that the generalized immittance kernel obtained as the solution of an Nth-order linear differential equation with constant coefficients and sinusoidal forcing must necessarily be consistent with the Kronig-Kramers relations. Finally, it is proved that the network or system function of a system exhibiting a distribution over any or all of the $(N + 1)$ arbitrary parameters of the Nth-order immittance kernel must itself be consistent with the Kronig-Kramers relations. The example of Lorentz dispersion is discussed.

Introduction. In a previous paper [1]), network functions representing physically realizable systems having a distribution of relaxation times were considered. These functions $Q(\omega)$ may represent such quantities as impedance, admittance, or complex electric or magnetic susceptibility. It was shown rigorously in the earlier paper that since the real and imaginary parts of the Debye network function $Q_D(\omega, \tau) \equiv (1 + i\omega\tau)^{-1}$ satisfied the Kronig-Kramers integral relations [2]), the corresponding network function $Q_1(\omega)$ obtained for a system having Debye-type response with a distribution of relaxation times rather than a single relaxation time, had real and imaginary parts also satisfying the Kronig-Kramers equations.

The Debye network function is obtained from the solution of a first-order linear differential equation with a sinusoidal driving term and involves the single parameter τ. Since many network functions important in both macroscopically continuous systems and in discontinuous systems such as lumped-parameter electric and mechanical circuits arise from higher-order linear differential equations with constant coefficients and involve more parameters, it becomes of interest to investigate the application of the Kronig-Kramers equations to such systems, especially in the case of distributions of some or all of the parameters of the elemental system. The present work is concerned with this matter. We see that there is a rough analogy here with the classical linear boundary-value problem

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where sums or integrals of solutions of the pertinent differential equations are combined by proper adjustment of the parameters (integration constants) occurring in the individual solutions. In the present work, our problem is to show that any linear combination of such solutions for sinusoidal forcing must yield a network function which is consistent with the Kronig-Kramers relations. Then, in practice, these relations may be employed to derive the real part of the network function from values of the imaginary part, measured for all pertinent frequencies, or *vice versa*.

The expansion theorem. If the network function $Q(\omega)$ is expressed as $[J(\omega) - iH(\omega)]$, the Kronig-Kramers relations may be written as [1])

$$J(\omega) = \frac{2}{\pi}\int_0^\infty \frac{H(y)y\mathrm{d}y}{y^2 - \omega^2}, \tag{1}$$

$$H(\omega) = \frac{2\omega}{\pi}\int_0^\infty \frac{J(y)\mathrm{d}y}{\omega^2 - y^2}. \tag{2}$$

The above integrals are understood to be Cauchy principal values when this concept is required. To ensure the proper direction of time's arrow, it is necessary that the response of a physical system not occur before the applied stimulus. Using this causality condition, it may be shown that $J(\omega)$ and $H(\omega)$ must be even and odd functions of ω, respectively. Functions which do not satisfy these conditions may still be consistent with one or the other Kronig-Kramers relation [1]), but they are usually of more mathematical than physical interest.

Let us denote the kth pole of $H(\omega)/\omega$ by ω_k and the corresponding residue by r_k. Then, for a $H(\omega)$ function representing a physical system, we may write

$$J(0) = \frac{2}{\pi}\int_0^\infty \frac{H(y)}{y}\,\mathrm{d}y = \frac{1}{\pi}\int_{-\infty}^\infty \frac{H(y)}{y}\,\mathrm{d}y = 2i\,\Sigma_k\, r_k, \tag{3}$$

where the sum is over the poles included in the appropriate contour. If we rewrite (1) as

$$J(\omega) = \frac{1}{\pi}\int_{-\infty}^\infty \frac{H(y)}{y}\cdot\frac{y^2}{y^2 - \omega^2}\,\mathrm{d}y \tag{1'}$$

and evaluate (1′) by the calculus of residues for a contour in the upper half plane which encircles the pole at $Z = \omega$ but is indented to skirt that at $Z = -\omega$, it is found that the contributions to the integral from these two regions cancel one another. Hence, from (3) and (1′) we obtain

$$J(\omega) = 2i\,\Sigma_k\, r_k \left\{\frac{\omega_k^2}{\omega_k^2 - \omega^2}\right\} \tag{4}$$

This equation shows that the poles of $J(\omega)$ are at $\pm\,\omega_k$ and the corresponding residues are

$$s_k = -\,2ir_k(\omega_k^2/2\omega_k) = -\,ir_k\omega_k. \tag{5}$$

Thus (4) may be written as

$$J(\omega) = 2\,\Sigma_k\, s_k\omega_k^2/(\omega^2 - \omega_k^2). \tag{6}$$

Equations (4) and (6) show that the poles and residues of $H(\omega)/\omega$ suffice to establish $J(\omega)$ uniquely; we shall refer to either equation as the expansion theorem and shall make use of this result in the next section. It should be especially noted that if the poles and residues of $H(\omega)/\omega$ are known, $J(\omega)$ can be obtained using the expansion theorem without the integration needed in applying the appropriate Kronig-Kramers relation. The expansion theorem and the above conclusion of course only apply to rational functions, as is tacitly assumed in equation (3), and do not include the case of integral functions such as $H(\omega)/\omega = (\sin\omega)/\omega$, for which, however, the Kronig-Kramers relations may still hold [3]).

Generalized network functions. Let us consider the Nth-order linear differential equation

$$\Sigma_{j=0}^{N}\,\tau_j\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^j x = e^{i\omega t}, \tag{7}$$

where the right-hand side represents a sinusoidal forcing term. On setting x equal to $Q_N(\omega)e^{i\omega t}$, we find

$$Q_N(\omega) = [\Sigma_{j=0}^{N}\,\tau_j(i\omega)^j]^{-1}. \tag{8}$$

This generalized network function (or immittance kernel of the Nth order) contains $(N+1)$ arbitrary constants τ_j assumed to be real and positive. We shall first show that its real and imaginary parts must satisfy the Kronig-Kramers relations. Note that $Q_N(\omega)$ may be made to correspond to any of the usual network functions which arise from linear differential equations with constant coefficients. For example, the Debye function Q_D is obtained on taking $N = 1$, $\tau_0 = 1$ and $\tau_1 = \tau$. The Lorentz network function Q_L, which is given by [4])

$$Q_L(\omega) = [\omega_0^2 - \omega^2 + i\gamma\omega]^{-1} = \frac{(\omega_0^2 - \omega^2) - i\gamma\omega}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}, \tag{9}$$

is obtained from Q_N by taking $N = 2$, $\tau_0 = \omega_0^2$, $\tau_1 = \gamma$, and $\tau_2 = 1$.

Let us rewrite (8) as

$$[Q_N(\omega)]^{-1} = \Sigma_{j=0}^{N}\,\tau_j(i\omega)^j = [J_N(\omega) - iH_N(\omega)]^{-1} \equiv A_N(\omega) + iB_N(\omega). \tag{10}$$

Then,

$$A_N(\omega) = \Sigma_{j=0}^{N_1}\,\tau_{2j}(-\,1)^j\omega^{2j}, \tag{11}$$

$$B_N(\omega) = \Sigma_{j=0}^{N_2}\,\tau_{2j+1}(-\,1)^j\omega^{2j+1}. \tag{12}$$

For N even, N_1 is $N/2$ and N_2 is $(N-2)/2$. When N is odd, both N_1 and N_2 are $(N-1)/2$. Next, we may write

$$P_N(\omega) \equiv A_N^2(\omega) + B_N^2(\omega), \tag{13}$$

and

$$Q_N(\omega) = \{A_N(\omega) - iB_N(\omega)\}/P_N(\omega). \tag{8'}$$

The quantity $P_N(\omega)$ is the sum of the $(N+1)$ terms involving even powers of ω from 0 to $2N$. It may be expressed in the alternative forms

$$P_N(\omega) = \Sigma_{j=0}^{2N} b_j\omega^j, \ b_{2j+1} = 0, \tag{13'}$$

and

$$P_N(\omega) = \Pi_{i=1}^{2N} (\omega - \omega_i). \tag{13''}$$

In writing equation (13″), we have taken $\tau_N = 1$ and have assumed that the $2N$ values of ω_i are the roots of $P_N(\omega) = 0$.

Next, it is desirable to express the b_j coefficients of equation (13′) in terms of the ω_i roots. The result is that b_k is $(-1)^k$ times the sum of $\binom{2N}{k}$ terms, where each k is composed of the product of $(2N-k)$ different ω_i's. A few such relations are found to be

$$b_0 = \omega_1\omega_2 \ldots \omega_{2N}, \tag{14}$$

$$b_1 = -[\omega_2\omega_3 \ldots \omega_{2N} + \omega_3\omega_4 \ldots \omega_{2N}\omega_1 + \ldots + \omega_1\omega_2 \ldots \omega_{2N-1}], \tag{15}$$

$$b_{2N-1} = -[\omega_1 + \omega_2 + \ldots + \omega_{2N}], \tag{16}$$

and

$$b_{2N} = 1. \tag{17}$$

The diagonal-sum method of quantum mechanics [5]) is related to equation (16). It is, of course, possible to express the b_j coefficients in terms of the τ_j parameters. The general relation is

$$b_{2j} = (-1)^j[\Sigma_{l=0}^{j} \tau_{2l}\tau_{2j-2l} - \Sigma_{l=0}^{j-1} \tau_{2l+1}\tau_{2j-2l-1}], \tag{18}$$

but we shall not need this expression for our present purposes.

We may now use the above results to show that $J_N(\omega)$ and $H_N(\omega)$ as defined in (10) satisfy the Kronig-Kramers relations. From (10), (8)′, (12), and (13″) we have

$$H_N(\omega) = B_N(\omega)/P_N(\omega) = \frac{\Sigma_{l=0}^{N_2} \tau_{2l+1}(-1)^l\omega^{2l+1}}{\Pi_{i=1}^{2N} (\omega - \omega_i)}. \tag{19}$$

It follows from (19) that the residue $r_k^{(N)}$ of $H_N(\omega)/\omega$ at $\omega = \omega_k$ is

$$r_k^{(N)} = B_N(\omega_k)/\omega_k \, \Pi_{i\neq k}^{2N} (\omega_k - \omega_i). \tag{20}$$

Substituting this result in (4) yields

$$J_N'(\omega) = 2i\,\Sigma \frac{\omega_k\, B_N\,(\omega_k)}{\omega_k^2 - \omega^2} \frac{1}{\Pi_{i\neq k}^{2N}(\omega_k - \omega_i)}, \tag{21}$$

where the prime designates that function which is obtained from $H_N(\omega)/\omega$ by applying the appropriate Kronig-Kramers relation.

In a similar fashion, it is readily demonstrated that the residue at $\omega = \omega_k$ of the $J_N(\omega)$ defined in (10) is given by

$$S_k^{(N)} = A_N(\omega_k)/\Pi_{i\neq k}^{2N} (\omega_k - \omega_i). \tag{22}$$

On combining (20) and (22), we find

$$S_k^{(N)}/r_k^{(N)} = A_N(\omega_k)\omega_k/B_N(\omega_k). \tag{23}$$

Now,

$$P(\omega_k) = [A_N(\omega_k) + iB_N(\omega_k)]\,[A_N(\omega_k) - iB_N(\omega_k)] = 0, \tag{24}$$

and we obtain

$$A_N(\omega_k)/B_N(\omega_k) = -\,i, \tag{25}$$

since only the term $[A_N(\omega_k) + iB_N(\omega_k)]$ produces a pole of $Q_N(\omega)$ as shown by (8'). From (23) and (25), it follows that

$$S_k^{(N)}/r_k^{(N)} = -\,i\omega_k. \tag{26}$$

Comparison of equations (5) and (26) now finally enables us to identify $J'_N(\omega)$ and $J_N(\omega)$. Thus, we have shown the validity of the Kronig-Kramers relations for $Q_N(\omega)$.

Although the function $Q_N(\omega)$ defined by (8) is rational for $N < \infty$, it is only positive real in the circuit analysis sense [6]) for $N = 1$. However, the function $(i\omega)^N Q_N(\omega)$ or $(i\omega)^{N-1} Q_N(\omega)$ will often be positive real for proper choice of the τ_j's and will satisfy the Kronig-Kramers relations. As an example, we may consider the Lorentz function defined by eq. 9. It is obviously not positive real since its real parts goes negative for sufficiently large ω. This function may be taken to represent the complex susceptibility of the Lorentz system. Since $(i\omega)Q_L(\omega)$ is positive real, this quantity may be used to represent (apart from a constant) the immittance function of the system, which is required to be positive real in a passive, realizable system [7]). In the present case, $(i\omega)Q_L(\omega)$ may be taken to respresent either the admittance of the system considered as a series RLC circuit or its impedance when considered as a parallel RLC circuit.

Distribution of parameters. In the last section, we showed that the generalized Nth-order network function or immittance kernel $Q_N(\omega)$ is necessarily consistent with the Kronig-Kramers relations. This result will now be extended to show explicitly that when a new function $Q(\omega)$ is obtained from $Q_N(\omega)$ by averaging $Q_N(\omega)$ over a distribution of any or all of its $(N + 1)$ parameters τ_j, the resulting function itself must also satisfy the Kronig-Kramers relations.

We wish to show explicitly that the functions

$$J(\omega) = \int J_N(\omega, \tau_0, \tau_1, \ldots, \tau_N)\, G(\tau_0, \tau_1, \ldots, \tau_N) \mathrm{d}\tau_0 \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_N \tag{27}$$

and

$$H(\omega) = \int H_N(\omega, \tau_0, \tau_1, \ldots, \tau_N)\, G(\tau_0, \tau_1, \ldots, \tau_N) \mathrm{d}\tau_0 \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_N \tag{28}$$

satisfy the Kronig-Kramers relations when J_N and H_N do so. Here $G(\tau_0, \tau_1, \ldots, \tau_N)$ is a $(N + 1)$-dimensional distribution function assumed normalized so that its integral over the range of the τ_i's is unity. To prove the validity of the Kronig-Kramers relations, we shall follow the methods of reference 1. The Mellin transform $j(s)$ of $J(\omega)$ is defined by

$$j(s) = \int_0^\infty \omega^{s-1} J(\omega) \mathrm{d}\omega. \tag{29}$$

It has been shown [1]) that the Mellin transforms of a Kramers-Kronig pair $J(\omega)$ and $H(\omega)$ satisfy the relation

$$h(s)/j(s) = \tan \frac{\pi}{2} s. \tag{30}$$

Let us abbreviate $\tau_0, \tau_1, \ldots, \tau_N$ by the vector $\boldsymbol{\tau}$. The Mellin transform of equation (27) becomes

$$\begin{aligned} j(s) &= \int_0^\infty \int J_N(\omega, \boldsymbol{\tau})\, G(\boldsymbol{\tau}) \omega^{s-1} \mathrm{d}\boldsymbol{\tau} \mathrm{d}\omega \\ &= \int [\int_0^\infty J_N(\omega, \boldsymbol{\tau}) \omega^{s-1} \mathrm{d}\omega]\, G(\boldsymbol{\tau}) \mathrm{d}\boldsymbol{\tau} \\ &= \int j_N(s, \boldsymbol{\tau})\, G(\boldsymbol{\tau}) \mathrm{d}\boldsymbol{\tau}, \end{aligned} \tag{31}$$

where $j_N(s, \boldsymbol{\tau})$ is the transform of $J_N(\omega, \boldsymbol{\tau})$. The corresponding result for equation (28) is

$$\begin{aligned} h(s) &= \int h_N(s, \boldsymbol{\tau})\, G(\boldsymbol{\tau}) \mathrm{d}\boldsymbol{\tau} = \int \left(\tan \frac{\pi}{2} s\right) j_N(s, \boldsymbol{\tau})\, G(\boldsymbol{\tau}) \mathrm{d}\boldsymbol{\tau} \\ &= \left(\tan \frac{\pi}{2} s\right) j(s). \end{aligned} \tag{32}$$

Comparison of (32) and (30) shows that $J(\omega)$ and $H(\omega)$ as defined in (27) and (28) do indeed satisfy the Kronig-Kramers relations and thus confirms the expectation of heuristic physical reasoning.

The results of the preceding work may be clarified by treating a concrete example such as the Lorentz function $Q_L(\omega)$ defined in equation (9). Examination of (9) shows that the Mellin transforms $j_L(s, \boldsymbol{\tau})$ and $h_L(s, \boldsymbol{\tau})$ may be computed from the integral

$$\xi(a) = \int_0^\infty \omega^{a-1} [(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2]^{-1} \mathrm{d}\omega. \tag{34}$$

Let us introduce the quantities

$$\sigma = [\omega_0^2 - \gamma^2/4]^{1/2} \tag{34}$$

$$\mu = (i\gamma/2) + \sigma \tag{35}$$

and

$$\nu = (i\gamma/2) - \sigma. \tag{36}$$

Then,

$$j_L(s) = \omega_0^2 \xi(s) - \xi(s + 2) = - [\mu\nu\xi(s) + \xi(s + 2)], \tag{37}$$

and

$$h_L(s) = \gamma\xi(s + 1) = - i(\mu + \nu)\, \xi(s + 1). \tag{38}$$

It may be shown by contour integration [8]) that

$$\xi(a) = \frac{\pi}{4i\gamma\sigma} \csc a\pi \,\{(-1)^{a-1} - 1\}\, \{\mu^{a-2} - \nu^{a-2}\}. \tag{39}$$

There is some ambiguity in the interpretation of $(-1)^{a-1}$. By considering the limit of the function

$$f(a) = - i \csc a\pi\{(-1)^{a-1} - 1\} \tag{40}$$

as a tends to an odd integer $(2n + 1)$ and by then comparing with the value obtained by direct contour integration *without* employing the result of Whittaker and Watson used in obtaining (39), we can establish that one is to take (-1) as $\exp(-i\pi)$. We thus readily find that

$$\frac{h_L(s)}{j_L(s)} = \frac{i(\mu + \nu)\xi(s + 1)}{\mu\nu\xi(s) + \xi(s + 2)} = \frac{i\{1 - (-1)^s\}}{\{(-1)^{s-1} - 1\}}$$

$$= \frac{-i\{1 - e^{-i\pi s}\}}{1 + e^{-i\pi s}} = \tan \tfrac{1}{2}\pi s. \tag{41}$$

Equation (41) shows that the Kronig-Kramers relations hold between the real and imaginary parts of the Lorentz function $Q_L(\omega)$. This function contains the arbitrary parameters ω_0 and γ. We have shown in the present section that any system exhibiting a continuous or discontinuous distribution of ω_0 and/or γ must have a network function consistent with the Kronig-Kramers relations provided the distribution function $G(\omega_0, \gamma)$ is normalizable.

In summary, we have (*a*) discussed a general expansion theorem relating the poles and residues of a Kronig-Kramers pair; (*b*) shown that the Nth-order immittance kernel $Q_N(\omega, \tau_0, \tau_1, \ldots, \tau_N)$ obtained from a linear differential equation with constant coefficients with a sinusoidal forcing term is consistent with the Kronig-Kramers equations; and (*c*), finally established that a system exhibiting a normalizable but otherwise arbitrary distribution over any or all of the $(N + 1)$ τ_j parameters of $Q_N(,\omega\, \boldsymbol{\tau})$ has itself a system function $Q(\omega)$ which is consistent with the Kronig-Kramers relations.

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