Brachman, Malcolm K.
Macdonald, J. Ross
1954

Physica XX
266–1270

RELAXATION-TIME DISTRIBUTION FUNCTIONS AND THE KRAMERS-KRONIG RELATIONS

by MALCOLM K. BRACHMAN and J. ROSS MACDONALD

Texas Instruments Incorporated, Dallas 9, Texas, U.S.A.

Synopsis

A general proof is given that the real and imaginary parts of a network function representing a physically realizable network with a distribution of relaxation times satisfy the Kramers-Kronig relations. Conditions on the network function presented in the literature are shown by an example to be too stringent.

There has been considerable interest for some time in the subject of the relationships between the real and imaginary components of physically realizable network functions. These relationships have been employed in connection with complex dielectric constants [1] [2], complex magnetic susceptibilities [3] [4], network functions [5], and scattering matrices [6]. In the physical literature, the connection is frequently called the Kramers-Kronig relations, a usage we shall adopt.

The present work shows that a "network function" defined as a certain integral of a distribution function obeys the Kramers-Kronig relations. A simple relationship between the Mellin transforms of the real and imaginary parts of the network function suffices for the validity of the Kramers-Kronig relations on the basis of our treatment, which is essentially formal. The distribution function, $G(\tau)$, is assumed to represent a distribution of relaxation times. It is normalized so that

$$\int_0^\infty G(\tau)\,\mathrm{d}\tau = 1. \tag{1}$$

We now define the network function, $Q(\omega)$, as [7] [8]

$$Q(\omega) = \int_0^\infty [G(\tau)/(1 + i\omega\tau)]\,\mathrm{d}\tau. \tag{2}$$

For definiteness, we shall refer to Q as the reduced polarization, a quantity introduced by Fuoss and Kirkwood which obeys equation (2). We follow their notation by writing

$$Q(\omega) = J(\omega) - i\,H(\omega); \tag{3}$$

consequently,

$$J(\omega) = \int_0^\infty [G(\tau)/(1 + (\omega\tau)^2)]\,\mathrm{d}\tau, \tag{4}$$

and

$$H(\omega) = \int_0^\infty [(\omega\tau)\,G(\tau)/(1 + (\omega\tau)^2)]\,\mathrm{d}\tau. \tag{5}$$

We shall now show that $J(\omega)$ and $H(\omega)$ obey the Kramers-Kronig relationship, and that we may find a distribution function $G(\tau)$ related to a given $J(\omega)$ and $H(\omega)$ by equations (4) and (5) if it is known that $J(\omega)$ and $H(\omega)$ obey the Kramers-Kronig relations.

The most straightforward approach seems to be by way of the Mellin transform [9], as shown by the following considerations. Introduce the function

$$K(\tau) = (1 + \tau^2)^{-1}. \tag{6}$$

Equation (4) then takes the form

$$J(\omega) = \int_0^\infty K(\omega\tau)\, G(\tau)\, d\tau. \tag{7}$$

This is a standard form of integral equation [10] solvable by Mellin transform. The Mellin transform $j(s)$ of the function $J(\omega)$ is defined by the relation

$$j(s) = \int_0^\infty J(\omega)\, \omega^{s-1}\, d\omega. \tag{8}$$

The inverse of the Mellin transform is given by

$$J(\omega) = (2\pi i)^{-1} \int_{c-i\infty}^{c+i\infty} j(s)\, \omega^{-s}\, ds. \tag{9}$$

We shall not explicitly discuss the conditions for the validity of the Mellin transform and its inverse, nor shall we mention the L^2 theory [11] of the Mellin transform appropriate for the functions considered.

Equation (7) may be regarded as an integral equation for the function $G(\tau)$, if we assume that $J(\omega)$ and $K(\tau)$ are known functions. Multiplying both sides of equation (7) by ω^{s-1} and integrating over ω from zero to infinity gives

$$j(s) = k(s)\, g\,(1 - s). \tag{10}$$

Applying the same process to equation (5) yields

$$h(s) = k(1 + s)\, g\,(1 - s). \tag{11}$$

Since it is known that

$$\int_0^\infty [\tau^{s-1}/(1 + \tau^2)]\, d\tau = \frac{\pi}{2} \csc \frac{\pi}{2} s, \tag{12}$$

for our present case we therefore have

$$k(s) = \frac{\pi}{2} \csc \frac{\pi}{2} s, \tag{13}$$

and it is obvious that

$$k(1 \pm s) = \frac{\pi}{2} \sec \frac{\pi}{2} s. \tag{14}$$

Combining the preceding results, we obtain

$$h(s)/j(s) = \tan \frac{\pi}{2} s. \tag{15}$$

It is more interesting to write this result as

$$h(1-s)/j(1-s) = \tan\frac{\pi}{2}(1-s) = \cot\frac{\pi}{2}s. \tag{16}$$

Denoting the inverse Mellin transform of $\cot(\pi/2)s$ by $\varphi(x)$, we recognize from the similarity of equations (10) and (16) that we have obtained a solution of the integral equation,

$$H(\omega) = \int_0^\infty J(\omega x)\,\varphi(x)\,dx. \tag{17}$$

It is known that

$$\int_0^\infty \frac{2}{\pi}[x^{s-1}/(1-x^2)]\,dx = \cot\frac{\pi}{2}s; \tag{18}$$

therefore

$$\varphi(x) = 2\pi^{-1}(1-x^2)^{-1} \tag{19}$$

Inserting this result in equation (17), we obtain

$$H(\omega) = \frac{2}{\pi}\int_0^\infty J(\omega x)(1-x^2)^{-1}\,dx = \frac{2\omega}{\pi}\int_0^\infty [J(y)/(\omega^2-y^2)]\,dy \tag{20}$$

This is one of the Kramers-Kronig relations. To obtain the other, we take the reciprocal of equation (16),

$$\tan\frac{\pi}{2}s = j(1-s)/h(1-s), \tag{21}$$

and note that

$$\cot\frac{\pi}{2}(s+1) = -\tan\frac{\pi}{2}s. \tag{22}$$

Therefore,

$$\int_0^\infty 2\pi^{-1}[x^s/(x^2-1)]\,dx = \tan\frac{\pi}{2}s, \tag{23}$$

and we conclude that

$$J(\omega) = \frac{2}{\pi}\int_0^\infty \frac{H(\omega x)\,x}{x^2-1}\,dx = \frac{2}{\pi}\int_0^\infty \frac{H(y)\,y\,dy}{y^2-\omega^2}. \tag{24}$$

This equation is the other one of the Kramers-Kronig relations. We have thus shown that functions $J(\omega)$ and $H(\omega)$ defined by equations (1), (4), and (5) satisfy the Kramers-Kronig relations (20) and (24). It is obvious that we can obtain a distribution function $G(\tau)$ by solving equations (10) or (11) for $g(s)$ and inverting, if we are given $J(\omega)$ and $H(\omega)$ satisfying the Kramers-Kronig relations.

Bode [5]) gives a list of conditions to be satisfied by $Q(\omega)$. These conditions are that $J(\omega)$ be an even and $H(\omega)$ an odd function of frequency [12]); that there be no singularities in the interior of the lower half-plane; that singularities at any finite point ω_0 on the real frequency axis be of such a character that $(\omega-\omega_0)\,Q$ vanishes as ω approaches ω_0; and that Q be analytic at infinity. It may be of interest to point out that these requirements are unnecessarily restrictive. A good example is the $H(\omega)$ used by Fuoss-Kirkwood and Macdonald [13]),

$$H(\omega) = \operatorname{sech}\left[a \ln \frac{\omega_m}{\omega}\right] = \frac{2}{(\omega_m/\omega)^a + (\omega/\omega_m)^a}. \tag{25}$$

It is evident that this is an odd or even function only for a an odd or even integer, and in the range $0 \leqslant a \leqslant 1$ considered by these authors it undergoes a "transition" from one to the other. It is apparent that poles of this function occur for

$$\frac{\omega}{\omega_m} = e^{\pm i\pi/2a}, \tag{26}$$

so there are poles in the lower half-plane of the complex frequency plane.

By reading a table of Mellin transforms [14]), we can find pairs of functions satisfying equation (15); so we may make a brief list as follows:

$$\begin{array}{cc} \underline{H(\omega)} & \underline{J(\omega)} \\ \sin \omega & \cos \omega \\ \mathrm{Si}\,(\omega) - \frac{\pi}{2} & \mathrm{Ci}(\omega) \end{array} \tag{27}$$

A more extensive table than the one available to the authors might offer further examples.

The present work shows explicitly the reason for the equivalence of the methods of Macdonald [13]), who used the Kramers-Kronig relation to derive $J(\omega)$ from an $H(\omega)$ of the form (25), and Fuoss-Kirkwood [7]), who first derived a relation between Fourier transforms of $H(\omega)$ and $G(\tau)$, then used the resulting $G(\tau)$ consistent with (25) to obtain $J(\omega)$ from (4). It is perhaps worth mentioning that the present results hold in the limit of a single relaxation time as well as for a distribution of relaxation times. Thus, taking Q as the impedance of the parallel combination of a frequency-independent capacitor and resistor of time constant τ_0, the resulting distribution function is found to be $G(\tau) = \delta(\tau - \tau_0)$.

The principal result of this work is plausible on the basis of physical reasoning, since $Q(\omega)$ may be considered to be the sum of the network functions of a system of networks connected in series, each network containing a resistance and a capacitance in parallel. The Kramers-Kronig relations hold for each sub-network, and the system is linear, so we may expect these equations to be valid for the network as a whole.

Received 23-7-54.

REFERENCES

1) Kramers, H. A., Atti Congr. dei Fisici, Como (1927) 545.
2) Kronig, R., J. opt. Soc. Am. **12** (1926) 547.
3) Gorter, C. J. and Kronig, R., Physica **3** (1936) 1009.
4) Pake, G. E. and Purcell, E. M., Phys. Rev. **74** (1948) 1184.
5) Bode, H. W., Network Analysis and Feedback Amplifier Design (D. van Nostrand and Company, New York, 1945), Ch. XIII and XIV.
6) Schützer, W. and Tiomno, J., Phys. Rev. **83** (1951) 249.
7) Fuoss, R. M. and Kirkwood, J. G., J. Am. chem. Soc. **63** (1941) 385.
8) Fröhlich, H., Theory of Dielectrics (Clarendon Press, Oxford, England, 1949). Fröhlich uses $-i$ in place of our i.
9) Titchmarsh, E. C., Introduction to the Theory of Fourier Integrals, (Clarendon Press, Oxford, England, 1937), p. 7.
10) Reference 9, p. 315.
11) Reference 9, p. 94.
12) Bode's complex frequency p is equal to our ω multiplied by i.
13) Macdonald, J. R., J. chem. Phys. **20** (1952) 1107.
14) Sneddon, I. N., Fourier Transforms (McGraw-Hill Book Company, Inc., New York 1951). p. 527.