Generalization of Kramers-Kronig transforms and some approximations of relations between viscoelastic quantities

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Abstract: On the basis of some very plausible assumptions about the response of physical systems to stimuli, such as Boltzmann's superposition principle and the causality principle, Spence showed that the following characteristics obtain for the modulus and compliance functions: (i) They are analytic in the lower half of the complex frequency plane, (ii) they are limited if the frequency tends to infinity, and (iii) the real and imaginary parts are even and odd functions, respectively, of the frequency $\omega$. It can generally be demonstrated that the real and imaginary parts of every function satisfying these three requirements and (iv) without singularities on the real frequency axis, are interrelated by Kramers-Kronig transforms. Similar relations hold between the logarithm of the modulus and the argument of the function.

Under certain conditions the Kramers-Kronig relations may be approximated by rather simple equations. For linear viscoelastic materials, for instance, the following approximate relations were obtained for the components of the complex dynamic shear modulus, $G^*(i\omega) = G'(i\omega) + iG''(i\omega) = G_d(i\omega) \exp i\delta(\omega)$:

$$G''(\omega) \approx \frac{\pi}{2} \left( \frac{dG'(u)}{d\ln u} \right)_{u=\omega},$$

$$G'(\omega) - G'(\omega) \approx -\frac{\omega \pi}{2} \left( \frac{d[G''(u)/u]}{d\ln u} \right)_{u=\omega},$$

$$\delta(\omega) \approx \frac{\pi}{2} \left( \frac{d\ln G_d(u)}{d\ln u} \right)_{u=\omega}.$$

The first of these relations was published long ago by Staverman and Schwarzl and is useful over broad frequency ranges, as is the second relation. The last equation is the most general one, and also is better supported by experiment.

Key words: Kramers-Kronig relations, linear system functions, viscoelastic material, shear modulus, phase angle

1. Introduction

Many branches of science involve linear systems satisfying differential equations of the first degree with constant coefficients. The response of a linear system to two or more superposed inputs is the sum of the responses to the individual inputs, so that the principle of superposition applies to this type of systems. We may define a system function [1] as the complex ratio of output to input amplitudes for steady state sinusoidal excitation of radial frequency $\omega$. The integral transform relationships between the real and imaginary parts of this function are generally known among physicists as the Kramers-Kronig [2, 3] relations.
Traditionally, the proof of the Kramers-Kronig relations starts from the fact that the real and imaginary parts of system functions are the Fourier cosine and Fourier sine transforms of the response to unit impulse [4, 5]. Much more generally, however, they are a special case of relations which can be derived by methods borrowed from the theory of complex functions [6, 7, 8]. In this paper the derivation of these generalized relations will be recapitulated. The Kramers-Kronig relations, emphasizing that the frequency dependences of the real and the imaginary parts of a system function, respectively, are not independent of each other, have been known for a long time. They imply that also the absolute value (or modulus) and the argument (or amplitude) of the system function should be interrelated. It is astonishing that these relationships have not yet been studied in the literature. Bode [6] gave some relations for network systems and Dickinson and Witt [9] reported an approximate relation for the viscoelastic properties of paving asphalts, but complete Kramers-Kronig transforms between the modulus and argument of system functions have apparently not been given before. Therefore we extend the theory to these functions.

A final objective of this paper is to investigate some approximations of the Kramers-Kronig relations. Schwarzl and Brather [10] used these relations as a starting-point for very elaborate analyses of quantitative calculations of the one function from the other. This is not our present intention; rather, we are looking for simple qualitative relations applicable to a broad class of functions. The terminology will contain elements from viscoelasticity, but many of the relations may also be used for dielectrics, magnetism, optics, acoustics [11], quantum mechanics, scattering theories, etc.

2. Conditions for the relations

To Spence [7] we owe an illuminating function-theoretical analysis of relaxation phenomena and Kramers-Kronig relations. His theory rests on a minimum number of assumptions concerning the characteristics of a relaxation system, which assumptions are very general and are backed by experience. They are:

i) Boltzmann's superposition principle obtains, which means that a system's total response to all components of an excitation history is linear and therefore independent and additive.

ii) A real stimulus gives rise to a real response. From these two assumptions, Spence deduces that a) The real and the imaginary part of a system function are an even and an odd function of the frequency, respectively.

If, in addition, it is assumed that for the system

iii) The principle of causality obtains, i.e. the response follows the cause.

Then Spence further deduces that

b) The system function is analytic in the lower half of the complex frequency plane and can have singularities in the upper half only.

c) The system function converges to a constant value not equalling zero when the frequency in the lower half-plane tends to infinity.

Below, we will deal very generally with complex functions which meet conditions a – c. For the sake of simplicity, we further assume that

d) The function does not have singularities on the real frequency-axis either.

3. Derivation of the generalized Kramers-Kronig relations

Let \( \theta^*(u) \) be a complex function of the complex frequency \( u \) which meets conditions a – d. This function can be written as \( \theta^*(u) = A(u) + iB(u) = \theta(u) \exp i\delta(u) \), in which \( A(u) \) and \( B(u) \) are real, as well as the argument \( \delta(u) \). We now consider the integral

\[
\oint_{C} \frac{\theta^*(u) - A(\omega)}{u^2 - \omega^2} \, du
\]

\[
= \frac{1}{2\omega} \oint_{C} \left\{ \frac{\theta^*(u) - A(\omega)}{u - \omega} - \frac{\theta^*(u) - A(\omega)}{u + \omega} \right\} \, du.
\]

The integrals are analyti-

causal in the lower half-plane and have only poles on the real axis in \( u = \pm \omega \). Therefore, according to the Cauchy-Goursat theorem from the theory of complex functions, the integral along path \( C \) equals zero. We now let the radius \( R \) of the large semicircle round the origin tend to infinity, and the radii \( \epsilon \) of the small semicircles round \( \pm \omega \) to zero. Then with the aid of a theorem known from the theory of complex functions and with condition a it can be derived that