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Multiply subtractive Kramers-Kronig relations for impedance function of concrete

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Abstract

The impedance function of concrete is considered and multiply subtractive Kramers-Kronig relations and sum rules are given for the impedance function. It is proposed that multiply subtractive Kramers-Kronig relations provide better convergence, and thus increase the reliability of numerical analysis of impedance of concrete than the conventional Kramers-Kronig relations.

Keywords: Kramers-Kronig relations; Impedance; Concrete

1. Introduction

Recently, the utilization of Kramers-Kronig (K-K) relations, which were originally derived for data inversion of optical spectra [1–3], has attracted attention in the investigation of the impedance function of concrete [4,5]. Unfortunately, K-K relations require the knowledge of real or imaginary part of the impedance function at the whole semi-infinite frequency range of the applied external electric field. However, by experiments it is possible to get data only at a finite frequency range. Thus the reliability of the numerical inversion related to K-K relations becomes problematic and a source of errors. Traditionally a solution offered for the problem is to extrapolate the real or imaginary part beyond the measured range. Unfortunately, this is usually not a good solution but a source of serious error in data inversion [6]. For practical data analysis a method to estimate the average error of data inversion has been proposed [7].

The purpose of this paper is to draw attention of the society of concrete and cement research to the progress made in optical spectroscopy especially in the utilization of the K-K relations and their reliability. The problem of the reliability of data inversion by K-K relations using data at finite range has been solved both in linear [8] and nonlinear [9,10] optical spectroscopy. The solution is based on so-called multiply subtractive K-K relations, which have much stronger convergence than conventional K-K relations.

2. Multiply subtractive Kramers-Kronig relations for the complex impedance of concrete

The basic property for the existence of the K-K relations for any physical quantity is the principle of causality. Rigorous mathematical treatment of the causality and K-K relations can be found, e.g. in Refs. [3,11]. We next concentrate only on the concept of impedance (Z), which is a complex function of real frequency (ω) as follows:

$$Z(\omega) = Z'(\omega) + iZ''(\omega), \tag{1}$$

where i is the imaginary unit. Note that K-K relations can be derived defining the complex impedance function either as $Z=Z'+iZ''$ or $Z=Z'-iZ''$. The derivation is based on a crucial property that the impedance function is an analytic function in the upper-half of complex frequency plane, and that it has strong enough asymptotic fall off as the frequency tends to

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infinity [3]. Thus one can employ the complex contour integration and the theorem of residues to obtain so-called Hilbert-transforms [3]. Hilbert transforms are integrals where the integration is from minus infinity to plus infinity. K-K relations are obtained from Hilbert transformations by the assumption that the impedance function has a parity property i.e. $Z(-\omega)=[Z(\omega)]^*$, where "*" denotes the complex conjugate. Thus we have

$$Z'(-\omega) = Z'(\omega)$$

$$Z''(-\omega) = -Z''(\omega). \qquad (2)$$

The message of Eq. (2) is that Z' is an even and Z'' is an odd function of the variable ω. Under the assumptions mentioned above we can express the K-K relations as follows:

$$Z'(\omega') - Z(\infty) = \frac{2}{\pi} P \int_0^\infty \frac{\omega Z''(\omega)}{\omega^2 - \omega'^2} \mathrm{d}\omega$$

$$Z''(\omega') = \frac{-2\omega'}{\pi} P \int_0^\infty \frac{Z'(\omega) - Z'(\infty)}{\omega^2 - \omega'^2} \mathrm{d}\omega \qquad (3)$$

where P denotes the Cauchy principal value. Cauchy principal value means that the singular point ω is approached in a symmetric manner both from left and right side in the numerical integration. Note that the first K-K relation in Eq. (3) yields a DC-impedance relation, which is called in optical physics a "sum rule"

$$Z'(0) - Z(\infty) = \frac{2}{\pi} P \int_0^\infty \frac{Z''(\omega)}{\omega} \mathrm{d}\omega, \qquad (4)$$

and which gives the real part of the impedance at zero frequency. Another sum rule for the even real part of the impedance can be derived using complex contour integration. Then we can write [3]

$$\int_0^\infty [Z'(\omega) - Z'(\infty)] \mathrm{d}\omega = 0. \qquad (5)$$

The message of Eq. (5) is that the average impedance is zero.

The problem with Eqs. (3) and (4) (in the case of Eq. (5) the problem is more serious) is the integration that ranges from zero to infinity. Fortunately, in impedance spectroscopy of concrete and other materials it is possible to measure both the real and imaginary parts of the complex impedance. This fact makes it possible to utilize multiply subtractive K-K relations (MS K-K) that provide much faster convergence of the integrals, but they require so-called "anchor points". Indeed, then one has to know either real part or imaginary at some discrete frequencies Ω_1, $\Omega_2, \ldots, \Omega_Q$, which belong to the frequency range of measured data. The derivation [8] of the MS K-K follow similar guide lines as those of conventional K-K. Here we give the results for the complex impedance function as follows

$$\begin{aligned}
&Z'(\omega') - Z'(\infty) \\
&= \frac{(\omega'^2 - \Omega_2^2)(\omega'^2 - \Omega_3^2)\ldots\left(\omega'^2 - \Omega_Q^2\right)}{(\Omega_1^2 - \Omega_2^2)(\Omega_1^2 - \Omega_3^2)\ldots\left(\Omega_1^2 - \Omega_Q^2\right)}[Z'(\Omega_1) - Z'(\infty)] + \ldots \\
&+ \frac{(\omega'^2 - \Omega_1^2)\ldots\left(\omega'^2 - \Omega_{j-1}^2\right)\left(\omega'^2 - \Omega_{j+1}^2\right)\ldots\left(\omega'^2 - \Omega_Q^2\right)}{\left(\Omega_j^2 - \Omega_1^2\right)\ldots\left(\Omega_j^2 - \Omega_{j-1}^2\right)\left(\Omega_j^2 - \Omega_{j+1}^2\right)\ldots\left(\Omega_j^2 - \Omega_Q^2\right)} \\
&\times \left[Z'(\Omega_j) - Z'(\infty)\right] + \ldots \\
&+ \frac{(\omega'^2 - \Omega_1^2)(\omega'^2 - \Omega_2^2)\ldots\left(\omega'^2 - \Omega_{Q-1}^2\right)}{\left(\Omega_Q^2 - \Omega_1^2\right)\left(\Omega_Q^2 - \Omega_2^2\right)\ldots\left(\Omega_Q^2 - \Omega_{Q-1}^2\right)}\left[Z'(\Omega_Q) - Z'(\infty)\right] \\
&+ \frac{2}{\pi}\left[(\omega'^2 - \Omega_1^2)(\omega'^2 - \Omega_2^2)\ldots\left(\omega'^2 - \Omega_Q^2\right)\right] \\
&\times P \int_{\omega_1}^{\omega_2} \frac{\omega Z''(\omega)\mathrm{d}\omega}{(\omega^2 - \omega'^2)\ldots\left(\omega^2 - \omega_Q^2\right)}
\end{aligned} \qquad (6)$$

and

$$\begin{aligned}
\frac{Z''(\omega)}{\omega'} &= \frac{(\omega'^2 - \Omega_2^2)(\omega'^2 - \Omega_3^2)\ldots\left(\omega'^2 - \Omega_Q^2\right)}{(\Omega_1^2 - \Omega_2^2)(\Omega_1^2 - \Omega_3^2)\ldots\left(\Omega_1^2 - \Omega_Q^2\right)} \frac{Z''(\Omega_1)}{\Omega_1} + \ldots \\
&+ \frac{(\omega'^2 - \Omega_1^2)\ldots\left(\omega'^2 - \Omega_{j-1}^2\right)\left(\omega'^2 - \Omega_{j+1}^2\right)\ldots\left(\omega'^2 - \Omega_Q^2\right)}{\left(\Omega_j^2 - \Omega_1^2\right)\ldots\left(\Omega_j^2 - \Omega_{j-1}^2\right)\left(\Omega_j^2 - \Omega_{j+1}^2\right)\ldots\left(\Omega_j^2 - \Omega_Q^2\right)} \frac{Z''(\Omega_j)}{\Omega_j} \\
&+ \ldots + \frac{(\omega'^2 - \Omega_1^2)(\omega'^2 - \Omega_2^2)\ldots\left(\omega'^2 - \Omega_{Q-1}^2\right)}{\left(\Omega_Q^2 - \Omega_1^2\right)\left(\Omega_Q^2 - \Omega_2^2\right)\ldots\left(\Omega_Q^2 - \Omega_{Q-1}^2\right)} \frac{Z''(\Omega_Q)}{\Omega_Q} \\
&- \frac{2}{\pi}\left[(\omega'^2 - \Omega_1^2)(\omega'^2 - \Omega_2^2)\ldots\left(\omega'^2 - \Omega_Q^2\right)\right] \\
&\times P \int_{\omega_1}^{\omega_2} \frac{\omega[Z'(\omega) - Z'(\infty)]\mathrm{d}\omega}{(\omega^2 - \omega'^2)\ldots\left(\omega^2 - \omega_Q^2\right)}
\end{aligned} \qquad (7)$$

where $[\omega_1,\omega_2]$ is the frequency range used in the measurement. If we compare the K-K relations of Eq. (3) and the MS K-K relations of Eqs. (6) and (7) we observe that the integrands in Eqs. (6) and (7) have much faster convergence than the integrands in Eq. (3). Our experience in optical spectroscopy has shown that already one anchor point is usually sufficient for reliable data inversion or testing the validity of the measured data. In such a case also the mathematical expressions, which are obtained from Eqs. (6) and (7) by allowing only one anchor point Ω_1, become much simpler. In the case of one anchor point we have singly subtractive K-K relations (SS K-K), which are

$$\begin{aligned}
&Z'(\omega') - Z'(\Omega_1) \\
&= \frac{2\left(\omega'^2 - \Omega_1^2\right)}{\pi} P \int_{\omega_1}^{\omega_2} \frac{\omega Z''(\omega)}{(\omega^2 - \omega'^2)\left(\omega^2 - \Omega_1^2\right)} \mathrm{d}\omega.
\end{aligned} \qquad (8)$$

and

$$\frac{Z''(\omega')}{\omega'} - \frac{Z''(\Omega_1)}{\Omega_1} = -\frac{2(\omega'^2 - \Omega_1^2)}{\pi} P \int_{\omega_1}^{\omega_2} \frac{Z'(\omega) - Z'(\infty)}{(\omega^2 - \omega'^2)(\omega^2 - \Omega_1^2)} \mathrm{d}\omega. \quad (9)$$

Naturally the accuracy of inversion is better whenever a relatively broad spectral range is measured. Another method to have a strong convergence of the K-K relations is based on the relations for the powers of the impedance. Such a method has been employed in practical data analysis of nonlinear optical polymers [12].

Finally we mention that if only the modulus of the impedance is known at finite frequency range then another effective method for phase retrieval is based on so-called maximum entropy method [3].

3. Conclusion

The full potential of K-K relations in data inversion can be improved by the the so-called subtractive Kramers-Kronig relations. Their advantage is the better convergence of integrals. I hope that this paper would stimulate the application of MS K-K also in the studies related to complex impedance of concrete and dynamic change of systems involving concrete or cement. The sum rules presented in this paper may also turn out useful in such investigations.

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