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A Fourier series method for numerical Kramers–Kronig analysis

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Abstract. Using a time domain method, the Kramers–Kronig integrals are derived without recourse to complex analysis (except in evaluating the Fourier transform of sgn (t)) From the time domain result, a Fourier series method for numerical evaluation of causality relations is derived. This method eliminates the need to use numerical integration, the use of logarithms in evaluating the function and the consideration of Cauchy principal parts. Through the use of the fast Fourier transform algorithm the calculation can be very rapid. The accuracy of the technique is considered.

1. Introduction

The Kramers–Kronig relations give the connection between the real and imaginary parts of the frequency dependent response function of a causal physical system. Since the relations are normally expressed as integrals, the practical calculation of one part from the other (eg derived from experimental data) requires the use of numerical integration. By considering the even and odd parts of the corresponding temporal response function, relations can be found which connect the Fourier coefficients of the real and imaginary parts of the frequency function.

2. Relation between time functions

In optical studies a response function often used is the complex dielectric function $\epsilon(\omega)-1$. Although the following derivation will be written in terms of $\epsilon(\omega)-1$, the analysis applies to all causal response functions which are finite for all time. The temporal function $f(t)$ is found from the corresponding frequency function $F(\omega)$ by applying the inverse Fourier transform:

$$f(t) = \mathscr{F}^{-1}(F(\omega)) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)\exp(-\mathrm{i}\omega t)\,\mathrm{d}\omega. \tag{1}$$

The temporal function corresponding to $\epsilon(\omega)-1$ is therefore $\epsilon(t)-\delta(t)$.

Letting $p(t)$ and $q(t)$ be the even and odd contributions to the real function $\epsilon(t)-\delta(t)$ respectively,

$$\epsilon(t)-\delta(t) = p(t)+q(t). \tag{2}$$

Since the dielectric function is causal,

$$\epsilon(t)-\delta(t) = 0, \qquad t < 0. \tag{3}$$

By considering positive and negative t separately, equations (2) and (3) yield

$$p(t) = \operatorname{sgn}(t)q(t), \qquad t \neq 0. \tag{4}$$

It remains to connect p and q for $t = 0$. Since $q(t)$ is odd, $q(0) = 0$. In order to determine $p(0)$, assume that (4) does *not* apply at $t = 0$, ie

$$p(t) = \operatorname{sgn}(t)q(t)+z(t), \qquad \text{(all } t\text{)}, \tag{5}$$

where $z(t) = 0$ for $t \neq 0$, in order that (4) be true for $t \neq 0$. If $z(0)$ were finite, the Fourier transform $P(\omega)$ of $p(t)$ would be no different from that for $z(0) = 0$. Thus, the only forms for $z(t)$ which affect $P(\omega)$ are $\delta(t)$ or a derivative of $\delta(t)$. However, the derivation of the Kramers–Kronig integral requires that $p(t)$ be finite for all values of t (Landau and Lifshitz 1960) or that $\epsilon(\omega)-1$ be square integrable (Toll 1956). Both these conditions preclude $z(t)$ from being a delta function or one of its derivatives. Therefore (5) can only be true if $z(t) = 0$, ie

$$p(0) = 0.$$

Thus for causal functions which are finite for all t,

$$p(t) = \operatorname{sgn}(t)q(t), \qquad \text{(all } t\text{)}. \tag{6}$$

However, since $(\epsilon(t)-\delta(t))$, $p(t)$ and $-\mathrm{i}q(t)$ are the inverse Fourier transforms of $\epsilon(\omega)-1$ $(=\epsilon_1(\omega)-1+\mathrm{i}\epsilon_2(\omega))$, $\epsilon_1(\omega)-1$ and $\epsilon_2(\omega)$ respectively, equation (6) can be used to relate $\epsilon_1(\omega)-1$ to $\epsilon_2(\omega)$. The Fourier transform of $\operatorname{sgn}(t)$ can be written:

$$\operatorname{sgn}(t) = \frac{1}{2\pi}\mathrm{P}\int_{-\infty}^{\infty} \frac{2\mathrm{i}}{\omega}\exp(-\mathrm{i}\omega t)\,\mathrm{d}\omega, \tag{7}$$

where P represents the Cauchy principal part of the integral. In cases where it is necessary to take the principal part of the transform integral, the familiar convolution theorem incorporates the principal part in the following way. For

$$h(t) = f(t)g(t)$$

then

$$H(\omega) = \frac{1}{2\pi}\mathrm{P}\int_{-\infty}^{\infty} F(\omega-\omega')G(\omega')\,\mathrm{d}\omega', \tag{8}$$

where

$$h(t) = \mathscr{F}^{-1}(H(\omega))$$
$$f(t) = \mathscr{F}^{-1}(F(\omega))$$
$$g(t) = \mathrm{P}\mathscr{F}^{-1}(G(\omega)).$$

By applying (8) to (6) the familiar Kramers–Kronig relation is obtained:

$$\epsilon_1(\omega)-1 = \frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty} \frac{\epsilon_2(\omega')}{\omega'-\omega}\,\mathrm{d}\omega'. \tag{9}$$

This derivation of the Kramers–Kronig integral is based on the usual initial assumptions (which lead to analyticity of $\epsilon(\omega)$ (Toll 1956)). The complex analysis however, is only required in order to find (7). The remaining analysis uses standard Fourier theory.

3. Use of Fourier series

Equation (6) cannot be applied directly to experimental data since the temporal function is not know. The appropriate tool for practical application of (6) is the Fourier series. In order to use Fourier series, $\epsilon_1(\omega)-1$ and $\epsilon_2(\omega)$ must be band-limited (ie significantly nonzero only within the frequency range $-\omega_1 < \omega < \omega_1$). Under these conditions they can be represented within the range $(-\omega_1, \omega_1)$ by the Fourier exponential series:

$$\begin{aligned} \epsilon_1(\omega)-1 &= \sum_{k=-\infty}^{\infty} p_k \exp\left(\frac{ik\pi\omega}{\omega_1}\right) \\ \epsilon_2(\omega) &= \sum_{k=-\infty}^{\infty} -iq_k \exp\left(\frac{ik\pi\omega}{\omega_1}\right) \end{aligned} \tag{10}$$

where the Fourier coefficients p_k and q_k are given by π/ω_1 times the inverse Fourier transforms $p(t)$ and $q(t)$ at time $t = k\pi/\omega_1$. Thus equation (6) can be applied to the Fourier coefficients:

$$p_k = \operatorname{sgn}(k) q_k. \tag{11}$$

The relationship given by (10) and (11) can also be written using Fourier sine–cosine series:

$$\epsilon_1 - 1 = 2\sum_{k=1}^{\infty} p_k \cos\left(\frac{k\pi\omega}{\omega_1}\right) \tag{12}$$

$$\epsilon_2(\omega) = 2\sum_{k=1}^{\infty} p_k \sin\left(\frac{k\pi\omega}{\omega_1}\right). \tag{13}$$

By finding values of p_k which satisfy (13) and then substituting these into (12), the function $\epsilon_1(\omega)-1$ may be found from $\epsilon_2(\omega)$.

4. Errors in use of series causal relations

Although relations (6), (10), (11), (12) and (13) are exact, there are errors associated with applying the series to practical data. For gathering data such as $\epsilon_2(\omega)$ it is normal to sample the function at a finite number of discrete frequencies. If the function is sampled at $(2N+1)$ points ω_j, equally spaced in the range $(-\omega_1, \omega_1)$, there is no justification in using more than $(2N+1)$ Fourier coefficients to represent this data, ie

$$\begin{aligned} \epsilon_2(\omega_j) &= \sum_{k=-N}^{N} -iq'_k \exp\left(\frac{ik\pi\omega_j}{\omega_1}\right) \\ \omega_j &= \frac{2j\omega_1}{2N+1}, \qquad j = -N \text{ to } +N. \end{aligned} \tag{14}$$

The usual method (eg in the fast Fourier transform, Christiansen and Hockney 1971, Cooley and Tukey 1965) of determining the coefficients q'_k in (14) is to solve the $(2N+1)$ equations. This yields

$$-\mathrm{i}q'_k = \frac{1}{2N+1}\sum_{j=-N}^{N} \epsilon_2(\omega_j)\exp\left(\frac{-2\pi ijk}{2N+1}\right). \tag{15}$$

However, had the function $\epsilon_2(\omega)$ been available in full the correct coefficients would have been given by:

$$-\mathrm{i}q_k = \frac{1}{2\omega_1}\int_{-\omega_1}^{\omega_1} \epsilon_2(\omega)\exp\left(\frac{-ik\pi\omega}{\omega_1}\right)\mathrm{d}\omega. \tag{16}$$

Equation (15) can be viewed as evaluating the integral in (16) by means of the trapezium rule.

Consequently the $(2N+1)$ coefficients q'_k are not identical to the first $(2N+1)$ true coefficients of the full function $\epsilon_2(\omega)$. (This full function is of course not available.) In order to assess the error in this process, the sampled function values $\epsilon_2(\omega_j)$ obtained from the infinite series (10) are substituted into the expression (15) for the coefficients of the finite series, with the result:

$$q'_k = \sum_{m=-\infty}^{\infty} q_{k+m(2N+1)}, \qquad k = -N \text{ to } N. \tag{17}$$

Since equation (17) shows an infinite set of 'true' coefficients q_k, and equation (11) only applies to 'true' coefficients, it is not possible to obtain an exact expression for the relationship between the $(4N+2)$ calculated coefficients p'_k, q'_k of the finite series. However, it is possible to derive an expression for the error involved in applying (11) to calculated coefficients, ie in using

$$p'_k = \mathrm{sgn}(k)q'_k. \tag{18}$$

Let p''_k be the value of the kth coefficient of the finite series for $\epsilon_1(\omega_j)-1$. The coefficients p''_k are 'correct' in the sense that their use in the finite series gives the exact values of $\epsilon_1(\omega_j)-1$.

The error in the Fourier coefficients is

$$e'_k = p''_k - p'_k$$

where p'_k is the kth coefficient given by (18).

By use of (17), (18) and (11) the error can be shown to be:

$$\begin{aligned} e'_k &= -2\sum_{m=1}^{\infty} q_{k-m(2N+1)}, \qquad k>0 \\ e'_k &= 2\sum_{m=1}^{\infty} q_{k+m(2N+1)}, \qquad k\leqslant 0. \end{aligned} \tag{19}$$

The error at ω_j may be found by substituting (19) into the series:

$$E(\omega_j) = \sum_{k=-N}^{N} e'_k \exp\left(\frac{2\pi ijk}{2N+1}\right).$$

Since $q(t)$ is odd, q_k is also odd. Using this fact, the error in the calculation of $\epsilon_1(\omega_j)-1$ is

$$E(\omega_j) = 4 \sum_{k=0}^{N}{}' \sum_{m=1}^{\infty} q_{m(2N+1)-k} \cos\left(\frac{2\pi kj}{2N+1}\right)$$

where Σ' means add the $k = 0$ term into the sum with half weight. Since $q_k \to 0$ as $k \to \infty$ the major contribution to the error will be the $m = 1$ term:

$$E(\omega_j) \simeq 4 \sum_{k=0}^{N}{}' q_{2N+1-k} \cos\left(\frac{2\pi jk}{2N+1}\right). \tag{20}$$

Thus, as could be expected, the error depends on those Fourier coefficients, of the full function, which are not used in the analysis. This gives a criterion for the spacing of data points—the points should be close enough so that the Nth Fourier coefficient is small. For example, if a peak is covered by P points in the range where its amplitude exceeds h (assuming unit peak height), then the value of the Nth coefficient is approximately

$$\frac{f_N}{f_0} = \exp-\left(\frac{\pi(P-1)}{4\sqrt{\ln 1/h}}\right)^2 \qquad \text{Gaussian peak} \tag{21}$$

$$\frac{f_N}{f_0} = \exp-\left[\frac{\pi(P-1)}{2}\left(\frac{h}{1-h}\right)^{1/2}\right] \qquad \text{Lorentzian peak.} \tag{22}$$

For $h = 0{\cdot}1, f_N = 0{\cdot}01 f_0$, these give $P = 5{\cdot}1$ and $P = 9{\cdot}8$ respectively.

5. Summary and discussion

For a causal system the real and imaginary parts of the frequency dependent response function are related to each other by the Kramers–Kronig integrals. By beginning with the causal temporal response functions it is possible to derive a corresponding relationship between the even and odd parts of the time function. This relationship may be applied to Fourier series to provide a method of analysis which does not require the use of numerical integration.

The features of this method are:

(i) The calculation does not involve the Cauchy principal part since there are no infinities on the real time axis.

(ii) The speed of calculation is high since the fast Fourier transform (Christiansen and Hockney 1971, Cooley and Tukey 1965) algorithm can be used to calculate Fourier coefficients. The speed is also enhanced because the logarithms required in other methods are not needed for this technique.

(iii) Equation (6) allows the following insight into the use of the analysis on experimental data. In practice, limited instrument resolution results in the analysis being applied to a function $f(t)q(t)$ (ie $\epsilon_2(\omega)$ is convoluted with the instrument response function $F(\omega)$, whose transform is $f(t)$). When $f(t)q(t)$ is used instead of $q(t)$ in (6), the result is $f(t)p(t)$. Thus the resulting frequency function $\epsilon_1(\omega)-1$ is also convoluted with the same instrument response function $F(\omega)$.

(iv) Equation (20) provides a simple expression for the accuracy of the technique. Expressions like (21) and (22) may be used in conjunction with (20) to indicate the spacing of sampling points required to provide a given accuracy.

It is important to note that the Fourier series derivation requires the functions $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ to be band-limited. In general this can be satisfied since they both tend to zero as $\omega \to \infty$. However, the Kramers–Kronig integral, and hence the Fourier series technique, can be used to determine the canonical phase shift from the absolute value of the frequency response function (Toll 1956). This requires the use of

$$\ln(\epsilon(\omega)-1) = \ln(A(\omega)\exp \mathrm{i}\phi(\omega)) = \ln A(\omega)+\mathrm{i}\phi(\omega).$$

Since $\epsilon(\omega)-1 \to 0$ as $\omega \to \infty$, then $\ln A(\omega) \to -\infty$, as $\omega \to \infty$ and so the real part of $\ln(\epsilon(\omega)-1)$ is not band-limited. In order to use the Fourier series method to calculate the phase shift, $\epsilon(\omega)$ must be modified at high frequencies in some way without destroying causality.

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