KRAMERS-KRONIG COMPUTATIONS IN LOGARITHMIC FREQUENCY DOMAIN

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ABSTRACT

The Kramers-Kronig transformation has been extensively applied in optical spectroscopy to calculate the real component of an optical quantity from the imaginary component, such as the determination of the dispersive mode from a measurement of the absorptive mode and vice versa. In this paper some methods for Kramers-Kronig transform computation are presented, without employing numerical integration and extrapolation or assumptions about the behavior of the tested signals outside the measured range, and the obtained results are compared.

Keywords: *Kramers-Kronig relation, logarithmic sampling.*

1. INTRODUCTION

Hilbert transforms arise in many applications from optics and they are often called by different names such as dispersion relations, Kramers-Kronig (KK) transforms, and Cauchy principal value integrals. According to KK theory, the attenuation/amplification of light is always connected with a phase shift. The interaction between a light wave and matter can be described with a complex susceptibility of the material, whose real and imaginary parts are connected with the phase shift and the amplitude variation of the wave, respectively [1]. Usually the susceptibility is investigated as a function of the optical frequency, and strong variations occur near the excitation frequencies [2]. Since the susceptibility must be an analytical function, its real and imaginary parts are related by the KK relations (they are not independent). The KK relations are more general, however, since their origin is purely mathematical and is not related to a specific effect in physics. Therefore, they can be used with any variable as long as the susceptibility as a function of this variable fulfills the mathematical conditions.

A main problem in KK computation is that it requires information over the entire frequency range, while any set of experimental data covers only a finite range.

The goal of this paper is to compare some numerical methods for KK relations in the logarithmic frequency domain, without employing numerical integration and extrapolation or assumptions about the behavior of the tested signals outside the measured range. For this purpose we remind the needed KK transform background in Section 2, where we also describe some techniques for KK evaluation: an algorithm based on logarithmic derivative, some algorithms based on logarithmic difference (first, second and fourth order), Newton-Cotes approach and, Simpson approach. The testing signal and simulation results are presented in Section 3. Related results have been reported in [3, 4].

2. LOGARITHMIC FREQUENCY DOMAIN TECHNIQUES FOR KRAMERS-KRONIG COMPUTATION

2.1 Kramers-Kronig Transform

Let us consider $F(j\omega)$ the Fourier transform of a causal function $f(t)$:

$$F(j\omega) = \int_0^{\infty} f(t)e^{-j\omega t}dt = R(\omega) + jI(\omega), \quad (1)$$

then we have [5]:

$$R(\omega) = R(\infty) - \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{I(\omega)}{y-\omega}dy, \quad (2)$$

$$I(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{R(y)}{y-\omega}dy, \quad (3)$$

which establish the KK pair. Directly by taking logarithms, after fulfilling the requirements needed to satisfy the right half plane analyticity conditions of the Hilbert transform, the imaginary part $I(\omega)$ can be uniquely determined from the real part (in nepers) $R(\omega)$:

$$I(\omega) = \frac{2\omega}{\pi}\int_0^{\infty}\frac{R(y)-R(\omega)}{y^2-\omega^2}dy. \quad (4)$$

Because of the important applications of Hilbert transforms, considerable effort has been devoted to the numerical evaluation of Cauchy principal value integrals and there is also an extensive body of work devoted to the application of KK transforms to experimental data. Some strategies have been focused on avoiding the principal value integrals altogether. A primary area of application is the analysis of optical data. There are two principal issues involved in optical data analysis [2]:

1. Fitting measurements to some particular functional form, including a resolution of the extrapolation problem to regions outside which spectral measurements have been made;
2. Solving the KK inversion either analytically or numerically.

Other applications of KK transform includes computation of the imaginary or real part of complex frequency response of a passive linear system, from the other known component.

We consider as sampling points $\{ \omega_j | \omega_j = \omega_c \Delta^j, j \in \mathbb{Z} \}$ with $\Delta > 1$ (on these points is defined the logarithmic sampling on positive real axis). The imaginary part can be expressed as:

$$I(\omega_c) \approx \sum_{n \in \mathbb{N}} \Gamma(n, \Delta, \omega_c) \left[R(\omega_c \Delta^n) - R(\omega_c \Delta^{-n}) \right], \quad (5)$$

where $\Gamma(n, \Delta, \omega_c)$ is the function to be determined.

2.2 Logarithmic Approximation

A popular way for imaginary part evaluation, very used in circuits analysis and control theory, consists in using the logarithmic derivative of the real part:

$$I(\omega_c) \approx \frac{\pi}{2} \frac{\partial R(\omega_c, \Delta)}{\partial \Delta}. \quad (6)$$

Another method for imaginary part computation uses an approximative formula (with first order logarithmic difference):

$$I(\omega_c) \approx \frac{\pi}{2} \frac{R(\omega_c \Delta) - R(\omega_c \Delta^{-1})}{\Delta - \Delta^{-1}}. \quad (7)$$

The relationship using four terms was proposed in [6]:

$$I(\omega_c) = \sum_{n=-2}^{2} a_n R(\omega_c \Delta^n), \quad (8)$$

with the coefficients $a_n = \frac{(1, -6, 0, 6, -1)}{8 \ln \Delta}$. The division factor $8 \ln \Delta$ modifies the coefficients according to the chosen sample rate [7]. For $\Delta = 2$ the following values were considered in [6]:

$$a_n = [0.44688, 0.14195, 0.0, -0.14195, -0.44688]. \quad (9)$$

Parameters from (9) will be denoted Set I (Wübbenhorst and Turnhout [6] parameters). Equation (8) can be rewritten as (using second order logarithmic difference):

$$I(\omega_c) = \sum_{n=1}^{2} a_n \left[R(\omega_c 2^{-n}) - R(\omega_c 2^n) \right]. \quad (10)$$

Other methods implement the imaginary part evaluation using forth order logarithmic difference:

$$I(\omega_c) = \sum_{n=1}^{4} a_n \left[R(\omega_c 2^{-n}) - R(\omega_c 2^n) \right]. \quad (11)$$

Parameters values a_n are given in Table 1: Set II (Steeman and Turnhout [8] parameters) and Set III (Shtrauss [7] parameters).

2.3 Approximation by Use of Quadrature Formulae

First a general approximation formula in the logarithmic frequency domain [9] will be shown, then two quadrature formulae using Newton-Cotes and Simpson algorithms will be presented.

$$I(\omega) \approx \frac{1}{\pi}[R(\omega\Delta) - R(\omega/\Delta)] + \frac{2\ln\Delta}{\pi} \int_1^k \frac{R(\omega\Delta^z) - R(\omega\Delta^{-z})}{\Delta^z - \Delta^{-z}} dz, \quad (12)$$

n	a_n Set II	a_n Set III
−4	0.13458	0.13432
−3	−0.11000	−0.09418
−2	0.22726	0.18538
−1	0.44530	0.48499
0	0.00000	0.00000
1	−0.44530	−0.48499
2	−0.22726	−0.18538
3	0.11000	0.09418
4	−0.13458	−0.13432

Table 1: Values for a_n parameters.

where $\Delta > 1$ and $k \in \mathbb{N}$, $k \geq 1$ satisfy certain conditions [9].

For numerical computational support, it is of interest to develop a quadrature formula where the imaginary part function will be determined from the samples corresponding to the real part. Unfortunately the convergence of the series is slower. Also, the numerical evaluation of the higher order derivatives are likely to have sizeable errors [10].

The condition of equally spaced abscissas leads to one of the Newton-Cotes or Simpson's quadrature formulae [10]. At the beginning we select the trapezoidal formula (Newton-Cotes) and we obtain the first approximation $I_T(\omega)$ of the imaginary part:

$$I_T(\omega) = \sum_{p \in \mathbb{Z}} T_p R(\omega \Delta^p), \quad (13)$$

where $T_p = T_{-p}$

$$T_p = \begin{cases} \frac{1}{\pi}\left(1 + \frac{\ln\Delta}{\Delta - \Delta^{-1}}\right), & p = 1; \\ \frac{2\ln\Delta}{\pi(\Delta^p - \Delta^{-p})}, & p = \overline{2, k-1}; \\ \frac{\ln\Delta}{\pi(\Delta^p - \Delta^{-p})}, & p = k; \\ 0, & \text{otherwise.} \end{cases} \quad (14)$$

The parabolic rule (Simpson), for $k = 2m + 1$ gives the second proposed quadrature approach $I_S(\omega)$:

$$I_S(\omega) = \sum_{p \in \mathbb{Z}} S_p R(\omega \Delta^p), \quad (15)$$

where $S_p = S_{-p}$

$$S_p = \begin{cases} \frac{1}{\pi}\left(1 + \frac{2/3\ln\Delta}{\Delta - \Delta^{-1}}\right), & p = 1; \\ \frac{8\ln\Delta}{3\pi(\Delta^p - \Delta^{-p})}, & p = \pm 2, \ldots, \pm 2m; \\ \frac{4\ln\Delta}{3\pi(\Delta^p - \Delta^{-p})}, & p = \pm 3, \ldots, \pm(2m-1); \\ \frac{2\ln\Delta}{3\pi(\Delta^p - \Delta^{-p})}, & p = \pm(2m+1); \\ 0, & \text{otherwise.} \end{cases} \quad (16)$$

Remarks:

1. From the previous estimations it seems that the two quadrature formulae are comparable in performance

according to the number of samples. However, the multiplying constants and the level of derivatives differ a lot. Sometimes the parabolic rule outperforms the trapezoidal formula, sometimes not;
2. The formulae developed above are both easy to implement;
3. We did not assume special conditions for the frequency ω, and consequently the imaginary part can be approximated for every frequency within the conditions mentioned above;
4. The coefficients T_p and S_p do not depend on the frequency.

3. SIMULATION RESULTS

3.1 Testing Signal

As testing function we consider the attenuation coefficient of a transmitted beam in a thick holographic grating. The functions that appear in the case of a transmitted beam in a thick holographic grating near the Bragg mismatch angle, can be evaluated using KK relationships [11]. The diffraction efficiency and the effective attenuation coefficient are rapidly modifying according to the Bragg angle [12]. The diffraction efficiency is:

$$\Psi(\omega) = \frac{\sin^2 \omega}{\omega^2}, \tag{17}$$

respectively the corresponding real part:

$$\phi(\omega) = \frac{1}{\omega}\left[\frac{\sin(2\omega)}{2\omega} - 1\right]. \tag{18}$$

Consequently, the whole transmission is modeled by:

$$\overline{\phi}(\omega) = \phi(\omega) - j\Psi(\omega) = \frac{j}{2\omega^2}[\exp(2j\omega) + 2j\omega - 1].$$

3.2 Kramers-Kronig Approximation Examples

The KK transform of the imaginary part corresponding to a transmitted beam in a thick holographic grating, together with its approximations are presented in Figures 1÷ 4. The approximations use the logarithmic difference method, the logarithmic derivative technique, the Newton-Cotes approximation, respectively the Simpson rule.

In order to compare the results given by the different KK approximation methods, we have used the L_1, L_2 and respectively L_∞ norms. Where the value of norm is lower, the approximation is better. The values obtained for each norm are presented in Table 2. For Newton-Cotes and Simpson approaches we have taken into account the case $k = 17$ [13]; as it can be seen in Figures 3 and 4, same results for the KK transform approximation is obtained using 17, 33 or 65 points.

In Table 2, we have used next notations for the KK computation: LD - algorithm based on logarithmic derivative, LD1 - algorithm based on first order logarithmic difference, LD2 - method based on second order logarithmic difference, LD4-II - method based on fourth order logarithmic difference, with the parameters a_n from Set II, LD4-III - method

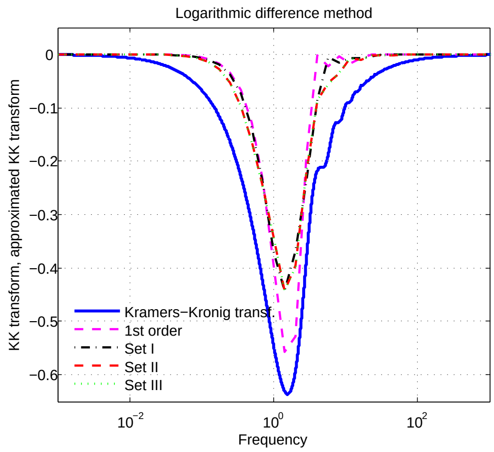

Figure 1: *Kramers-Kronig transform vs. approximated Kramers-Kronig transform using logarithmic difference.*

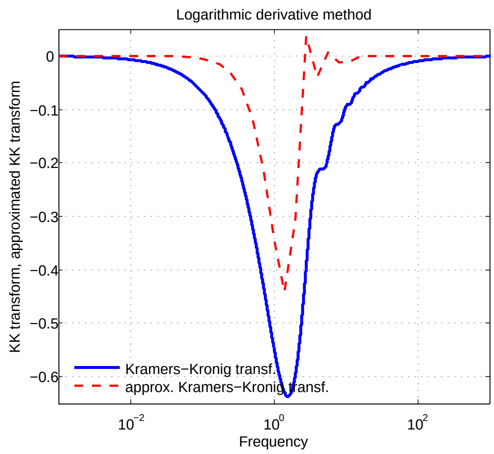

Figure 2: *Kramers-Kronig transform vs. approximated Kramers-Kronig transform using logarithmic derivative.*

based on fourth order logarithmic difference, with the parameters a_n from Set III, NC - trapezoidal approach, S - parabolic approach.

Method	L_1	L_2	L_∞
LD	$4.3878579e-002$	$9.3304185e-002$	$4.2286100e-001$
LD1	$3.4167457e-002$	$6.7700649e-002$	$2.1651730e-001$
LD2	$3.6406583e-002$	$7.1340620e-002$	$2.2492219e-001$
LD4-II	$3.4244494e-002$	$6.7018717e-002$	$2.0196802e-001$
LD4-III	$3.4174345e-002$	$6.6867465e-002$	$2.0293856e-001$
NC	$1.5460832e-003$	$3.6323305e-003$	$1.8913794e-002$
S	$1.8025268e-003$	$4.3675589e-003$	$2.1469917e-002$

Table 2: Methods comparison – attenuation coefficient of a transmitted beam in a thick holographic grating.

From the results presented in this paper and also from the results reported in [3, 4, 13] we can conclude that the best approximations in the logarithmic frequency domain for the attenuation coefficient of a transmitted beam in a thick holographic grating, are obtained using quadrature formulas. As it can be seen in Table 2 the lowest values for each norm are obtained for the approximation of KK transform using

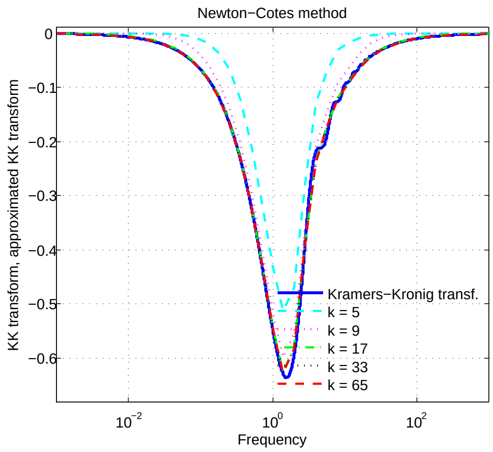

Figure 3*: Kramers-Kronig transform vs. approximated Kramers-Kronig transform using Newton-Cotes algorithm.*

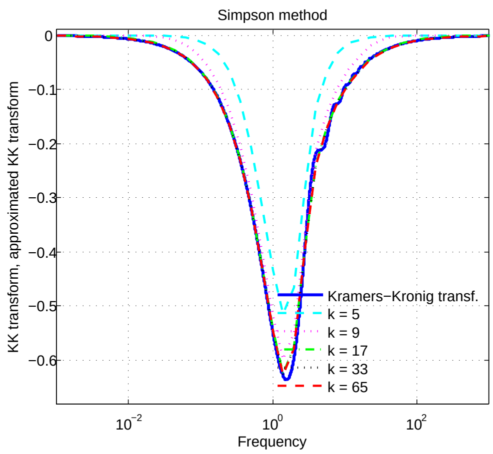

Figure 4*: Kramers-Kronig transform vs. approximated Kramers-Kronig transform using Simpson approach.*

the Newton-Cotes technique.

4. CONCLUSIONS

In this paper we present some methods that computes the KK transform without using numerical integration and extrapolation.

Simulations results show that the KK transform approximations are relatively accurate and the complexity of implementation is not large.

The KK transform approximation is not justified to be evaluated using more than 17 points, in the case of Newton-Cotes or Simpson approaches because the computational complexity increases by increasing the number of points used for approximation. Some problems can appear when the function is rapidly changing in a relatively narrow frequency range; but an approximation using 17 points is adequate even if the function presents a large number of minima and maxima in a narrow frequency range.

REFERENCES

[1] K. Diethelm, "Peano Kernels and Bounds for the Error Constants of Gaussian and Related Quadrature Rules for Cauchy Principal Value Integrals," *Journal of Numerische Mathematik*, vol. 73, pp. 53–63, Nov. 1996.

[2] F. W. King, "Efficient Numerical Approach to the Evaluation of Kramers-Kronig Transforms," *Journal of Optical Society of America B*, vol. 19, n0. 10, pp. 2427–2436, Oct. 2002.

[3] L. Grama and A. Dişcant, "Kramers-Kronig Relationship Computation by Gaussian Quadrature," *International Journal of Computers, Communications and Control*, vol. 1, no. Supplement, pp. 239–244, June 2006.

[4] L. Grama, "Logarithmic Gain Altered Data and Phase Computation," in *Proceedings of ICCC 2009 10th International Carpathian Control Conference*, Zakopane, Poland, May 24-26 2009, pp. 313–316.

[5] H. W. Bode, *Network Analysis and Feedback Amplifier Design*. New Jersy, Princeton: D. Van Nostrand, 1945.

[6] M. Wübbenhorst and J. van Turnhout, "Analysis of Complex Dielectric Spectra. I. One-Dimensional Derivative Technique and Three-Dimensional Modelling," *Journal of Non-Crystal. Solids*, vol. 305, no. 1-3, pp. 40–49, July 2002.

[7] V. Shtrauss, "FIR Kramers-Kronig Transformers for Relaxation Data Conversion," *Signal Processing*, vol. 86, no. 10, pp. 2887–2900, 2006.

[8] P. A. M. Steeman and J. van Turnhout, "A Numerical Kramers-Kronig Transform for the Calculation of Dielectric Relaxation Losses free from Ohmic Conduction Losses," *Journal of Colloid and Polymer Science*, vol. 275, pp. 106–115, 1997.

[9] C. Rusu, "Several Approaches to Cost Function Adaptation and Phase Approximation," Ph.D. dissertation, Tampere University of Technology, Tampere, Finland, 2000.

[10] A. Ralston, *A First Course in Numerical Analysis*. New-York: McGraw-Hill, 1965.

[11] B. E. A. Saleh and M. C. Teich, *Fundamentals of Photonics*. New-York: Wiley, 2007.

[12] M. Häckel, L. Kador, C. Frenz and H. W. Schmidt, "Consequences of the Kramers-Kronig Relations for Light Diffraction on Thick Gratings," *Optics Letters*, vol. 29, no. 15, pp. 1721–1723, Aug. 2004.

[13] L. Grama, "Researches Regarding Phase Approximation from Frequency Response Gain Samples," Ph.D. dissertation (in Romaniam), Technical University of Cluj-Napoca, Cluj-Napoca, Romania, 2009.

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