IOSR Journal of VLSI and Signal Processing (IOSR-JVSP)
Volume 11, Issue 6 (Nov. - Dec. 2021), pp.16-24
e-ISSN: 2319-4200, p-ISSN: 2319-4197
www.iosrjournals.org

On Numerical Strategy for Kramers-Kronig Relations via the Impulse Response Function Approach

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Abstract
In this work, the well-known Kramers–Kronig (K-K) relation is reviewed in the context of the frequency domain response function of a linear and causal medium. K-K relation is a bidirectional mathematical expression which relates the real and imaginary parts of a given complex function analytic in the upper half plane. The Fourier integral can be applied to the complete frequency response of a physical system to yield a causal time-domain impulse response. The frequency response of the system being invariant is described under the Hilbert transform. One of the pairs of the K-K relation expresses the real part of a complex function in terms of an infinite integral involving the imaginary part. The resulting real part of the K-K is a singular function and requires a careful evaluation. Fast Fourier transformation (FFT) algorithm was used to evaluate the real part of the K-K relation which can be applied in a realistic semiconductor optical spectra. Matlab program was used to implement the resulting FFT and its inverse transform algorithms. The classical optical dielectric function is discussed to illustrate the algorithm at different normalised frequencies. Results obtained exhibited a good agreement in the oscillator example, though the imaginary path of the oscillator spectrum may require some paddings in the FFT treatment to fit correctly the tail of the spectrum. However, the major artefacts and basic physics in our results are preserved, making it applicable in real materials spectroscopic methods.
Keywords: *K-K relation, FFT, Oscillator model, Optical spectroscopy, Hilbert transform*

I. Introduction

K-K relations refers to a bidirectional mathematical expression which relates the real and imaginary parts of a given complex function that is analytic in the upper half plane [1,2,3]. These relations are special functions coined from the generalised Hilbert transform. It is used to calculate the real part from the imaginary part (or vice versa) of a response function in a physical system. It is pertinent to know that any system whose present response does not depend on future values of the input is called a causal system and such system is practically realizable. The analyticity of a causal system obeys the complex mathematical rule [2]

$$\chi(\omega) = \chi_1(\omega) + i\chi_2(\omega) \quad \textbf{(1)}$$

where the variables χ_1 and χ_2 are real parameters, the symbol ω is the causal parameter. This creates dispersions relations, which are supposedly one of the few important topics where the causality paradigm plays an important role [4] and have a wide application in elasto-dynamics and electromagnetism [3]. If we suppose that this function is analytic in the upper half plane of ω and vanishes as the absolute value of the response parameter $|\omega| \to \infty$. Then the K-K relations implies the following for an example [1, 2, 5]

$$\chi_1(\omega) = \frac{1}{\pi} \wp \int_{-\infty}^{\infty} \frac{\chi_2(\omega)}{\omega' - \omega} d\omega' \quad \textbf{(2)}$$

$$\chi_2(\omega) = \frac{1}{\pi} \wp \int_{-\infty}^{\infty} \frac{\chi_1(\omega)}{\omega' - \omega} d\omega' \quad \textbf{(3)}$$

where symbol *p* appearing in equation (2) and (3) represent the Cauchy principal value. The real and imaginary part of such a function are not independent, and the full function can be reconstructed given just one of its parts [1,6] In principle, application of the Fourier integral to the complete frequency response of any physical network should always yield a causal time domain impulse response. In practice, the frequency response information is often complete on a discrete- frequency point and can contain some measurement errors. K-K formalism can be applied to the response functions of linear systems such as signal processing [1]. For an example, it can be used to explain the relationship between the absorption and refractive index of transparent media. K-K relation implies that observing the dissipative response of a system is sufficient to determine its phase response and vice versa. The integral running from the range -∞ to +∞ implies that we know the response at negative frequencies. In most systems, the positive frequency response determines the negative frequency response because $\chi(\omega)$ is the Fourier transform of a real quantity $\chi(t-t')$, hence it can be written

$$\chi(-\omega) = \chi^{*}(\omega) \qquad \textbf{(4)}$$

This means that $\chi_1(\omega)$ is an even function of frequency and $\chi_2(\omega)$ is odd. Using these properties, the integral can be transformed into one of definite parity by multiplying the numerator and denominator of the integrand by $(\omega' + \omega)$ and separating, we obtain;

$$\chi_1(\omega) = \frac{1}{\pi}\wp\int_{-\infty}^{\infty}\frac{\omega'\chi_2(\omega)}{\omega'^{2'} - \omega^2}d\omega' +$$

$$\frac{1}{\pi}\wp\int_{-\infty}^{\infty}\frac{\omega'\chi_1(\omega)}{\omega'^{2'} - \omega^2}d\omega' \qquad \textbf{(5)}$$

Since $\chi_2(\omega)$ is odd, the second integral necessarily vanishes and we are left with

$$\chi_1(\omega) = \frac{2}{\pi}\wp\int_{-\infty}^{\infty}\frac{\omega'\chi_2(\omega)}{\omega'^{2'} - \omega^2}d\omega' \qquad \textbf{(6)}$$

The same derivative for imaginary parts also gives

$$\chi_2(\omega) = -\frac{2\omega}{\pi}\wp\int_{-\infty}^{\infty}\frac{\omega'\chi_2(\omega)}{\omega'^{2'} - \omega^2}d\omega' \qquad \textbf{(7)}$$

Equation (6) and (7) are the so called K-K relation in a form that is generally applied for a physically realistic response function [1,2]

II. Theoretical Formulation

2.1. K-K relation from response function

For a non-linear and time invariant system, the property of a causal function requires a vanishing impulse response in time domain directed to the K-K relation in frequency domain [7]. The simplest causal function is the Heaviside step function which can simply be defined by the integrals,

$$u(t) = \begin{cases} \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\omega)e^{-i\omega t}d\omega, \\ \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\omega)e^{-i\omega(t-t')}d\omega \end{cases} \qquad (8)$$

Where $t = (t - t')$ and $u(t) = u(t - t') = 0$ such that $t < 0$ or $(t - t') < 0$.

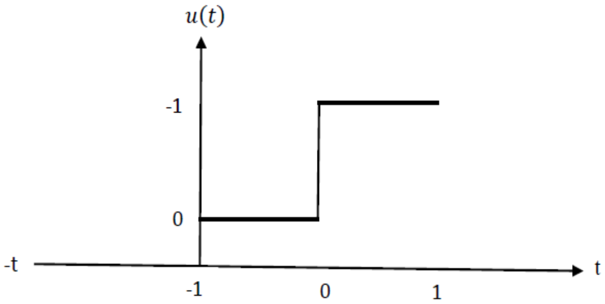

Figure 1: A typical representation of the Heaviside step function.

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Given $h(t)$ as the impulse response of a linear system, $H(\omega)$ of the frequency response, then the Fourier transform of the frequency response is given by:

$$H(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} h(t)e^{-j\omega t}dt \qquad \textbf{(9)}$$

If we assume the impulse function, $h(t) = 0$ such that $t < 0$, then it follows that

$$H(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0} h(t)e^{-j\omega t}dt \qquad \textbf{(10)}$$

$$H(\omega) = -\frac{1}{\sqrt{2\pi}}\int_{\infty}^{0} h(t)e^{-j\omega t}dt \qquad \textbf{(11)}$$

$$H(\omega) = \frac{1}{\sqrt{2\pi}}\int_{0}^{\infty} h(t)e^{-j\omega t}dt \qquad \textbf{(12)}$$

Equation (12) as derived above is the frequency domain and the right hand side can be multiplied with the Heaviside step function $u(t)$ to obtain the convolution equivalence;

$$H(\omega) = F\{h(t) * u(t)\} \qquad \textbf{(13)}$$

Hence the convolution theorem one obtains

$$F\{h(t) * u(t)\} = \frac{H(\omega) * F\{u(t)\}}{2\pi} \qquad \textbf{(14)}$$

The Fourier transform of the Heaviside function can be expressed as

$$F\{u(t)\} = H(t) = \frac{1}{2} + \frac{1}{2}\{\text{sgn}(t)\} \qquad \textbf{(15)}$$

Where the sigmoid function $\text{sgn}(t)$ is depicted in figure 2 and is expressed as

$$\text{sgn}(t) = \begin{cases} 1, t > 0 \\ 0, t = 0 \\ -1, t < 0 \end{cases} \qquad \textbf{(16)}$$

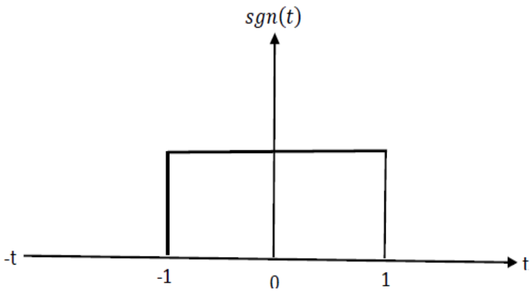

Figure 2: A typical representation of the sigmoid function.

Its Fourier transform of $\mathrm{sgn}(t)$ is given by
Thus,

$$f\{\mathrm{sgn}(t)\} = \begin{cases} \dfrac{2}{j\omega}, \omega \neq 0 \\ 0, \omega = 0 \end{cases} \quad \textbf{(17)}$$

Finding the Fourier function equation (15) one obtains the following;

$$F\{H(t)\} = f\left\{\frac{1}{2}\right\} + \frac{1}{2} f\{\mathrm{sgn}(t)\} \quad \textbf{(18)}$$

But $f\left\{\frac{1}{2}\right\} = \frac{1}{2}\int_0^{\infty} e^{-j\omega t} dt$, where the integral represents the Dirac Delta function which is denoted by $\delta(\omega)$, from this one obtains that

$$f\left\{\frac{1}{2}\right\} = \pi\delta(\omega) \quad \textbf{(19)}$$

Substituting equations (17) and (19) into (18) and putting (19) into equation (14) gives yields the simple equation,

$$F\{h(t) * u(t)\} = H(t) * \left\{\frac{1}{2\pi}\left(\frac{1}{j\omega} + \pi\delta(\omega)\right)\right\} \quad \textbf{(20)}$$

Also from equation (13), one obtains

$$H(\omega) = H(\omega) * \left\{\frac{1}{2\pi}\left(\frac{1}{j\omega} + \pi\delta\omega\right)\right\} \quad \textbf{(21)}$$

From equation (20), performing the convolution gives, and knowing that ω is invariant, the equation becomes

$$H(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{H(\omega')}{j(\omega - \omega')} d\omega' \quad \textbf{(22)}$$

Considering two different conditions for the frequency responses at $\omega < 0$ and $\omega > 0$, hence equation (22) can be written as

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{H(\omega')}{j(\omega-\omega')}d\omega' = \frac{1}{\pi}\int_{-\infty}^{0}\frac{H(\omega')}{j(\omega-\omega')}d\omega' + \frac{1}{\pi}\int_{0}^{\infty}\frac{H(\omega')}{j(\omega-\omega')}d\omega' \quad \textbf{(23)}$$

From the right hand side, we have that

$$\frac{1}{\pi}\int_{0}^{\infty}\frac{H(\omega')}{j(\omega-\omega')}d\omega' = \frac{1}{\pi}\int_{-\infty}^{0}\frac{H(\omega')}{j(\omega-\omega')}d\omega' \quad \textbf{(24)}$$

But since $H(\omega) = -H(\omega')$ or $H(\omega) = -H(\omega'')$,

We may obtain from the following equation,

$$\int_{0}^{\infty}\frac{H(\omega')}{j(\omega-\omega')}d\omega' = \int_{-\infty}^{0}\frac{H(\omega'')}{j(\omega+\omega')}d\omega'' \quad \textbf{(25)}$$

Also the Fourier integral definition, $H(-\omega'') = H^{*}(\omega'')$ from equation (22)

$$H(\omega) = \frac{1}{\pi}\int_{-\infty}^{0}\frac{H(\omega')}{j(\omega-\omega')}d\omega' + \frac{1}{\pi}\int_{0}^{\infty}\frac{H^{*}(\omega'')}{j(\omega+\omega'')}d\omega''$$
$$= \frac{1}{j\pi}\int_{0}^{\infty}\frac{H(\omega')}{(\omega-\omega')}d\omega' + \int_{0}^{\infty}\frac{H^{*}(\omega'')}{(\omega+\omega'')}d\omega'' \quad \textbf{(26)}$$

If we let the frequency $\omega'' = \omega'$, we find that

$$H(\omega) = \frac{1}{j\pi}\left[\int_{0}^{\infty}\frac{(\omega+\omega')H(\omega')d\omega'}{(\omega^{2}-\omega'^{2})} + \frac{(\omega-\omega')H^{*}(\omega')d\omega'}{(\omega^{2}-\omega'^{2})}\right] \quad \textbf{(27)}$$

Separating equation (27) into its real and imaginary parts, we may obtain the following

$$H(\omega) = \frac{2}{j\pi}\left[\int_{0}^{\infty}\frac{H_{\mathrm{Im}}(\omega')d\omega' - jH_{i\,\mathrm{Re}}(\omega')}{(\omega^{2}-\omega'^{2})}d\omega \quad \textbf{(28)}\right.$$

One can readily obtain the real and imaginary part of the K-K relation from equation (28) as

$$H_{\mathrm{Re}}(\omega) = \frac{2}{\pi}\int_{0}^{\infty}\frac{\omega' H_{\mathrm{Im}}(\omega')}{(\omega^{2}-\omega'^{2})}d\omega' \quad \textbf{(29)}$$

And

$$H_{\mathrm{Im}}(\omega) = -\frac{2}{\pi}\int_{0}^{\infty}\frac{\omega H_{\mathrm{Re}}(\omega')}{(\omega^{2}-\omega'^{2})}d\omega' \quad \textbf{(30)}$$

Where the transfer function $H(\omega)$ is defined by the Fourier transform of the Greens function of a system $h(t)$, which is the system's response to an impulsive perturbation. Since $h(t)$ is a real function, $H(\omega)$ is a complex function whose real and imaginary parts are even and odd functions of the frequency, respectively. Hence the real and imaginary parts are not independent of each other. For the equation obtained above to be programmable we apply the form;

$$H_{\mathrm{Re}}(\omega) = \frac{1}{\pi} \wp \int_{-\infty}^{\infty} \frac{\omega' H_{\mathrm{Im}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(31)}$$

$$H_{\mathrm{Im}}(\omega) = -\frac{2}{\pi} \wp \int_{-\infty}^{\infty} \frac{\omega H_{I\,\mathrm{Re}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(32)}$$

Where P is the Cauchy principal value of the integrals. A simple multiplication of the denominator and numerator of equation (30) the integrals by $(\omega + \omega')$ gives back the K-K relation of equation (29). This will be based on the two conditions [8] (i) that the integral over the frequency domain of an odd function is equal to zero. (ii) That the integral over the whole frequency domain of even function is equal to two times the integral from zero to infinity. Then the equations (31) and (32) above can be written using positive frequencies as:

$$H_{\mathrm{Re}}(\omega) = \frac{2\omega'}{\pi} \wp \int_{-\infty}^{\infty} \frac{H_{\mathrm{Im}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(31)}$$

$$H_{\mathrm{Im}}(\omega) = -\frac{2}{\pi} \wp \int_{-\infty}^{\infty} \frac{\omega H_{I\,\mathrm{Re}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(32)}$$

where symbol $\wp$ represents the Cauchy principal value of the integral. A simple multiplication of the denominator and numerator of equation (30) the integrals by $(\omega + \omega')$ gives back the K-K relation of equation (29). This will be based on the two conditions [8] (i) that the integral over the frequency domain of an odd function is equal to zero. (ii) That the integral over the whole frequency domain of even function is equal to two times the integral from zero to infinity. Then the equations (31) and (32) above can be written using positive frequencies as:

$$H_{\mathrm{Re}}(\omega) = \frac{2\omega'}{\pi} \wp \int_{-\infty}^{\infty} \frac{H_{\mathrm{Im}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(33)}$$

$$H_{\mathrm{Im}}(\omega) = -\frac{2\omega}{\pi} \wp \int_{-\infty}^{\infty} \frac{\omega H_{I\,\mathrm{Re}}(\omega')}{(\omega^2 - \omega'^2)} d\omega' \quad \textbf{(34)}$$

This will result to the numerical solution of the Kramers-Kronig relation.

2.2. Numerical Implementation of K-K Relation Using the Discrete Fourier Transformation (DFT) Algorithm

A numerical recipe of the discrete Fourier transform is actualized using the FFT algorithm. This can be developed allowing the K-K relation to be calculated for half of the frequencies at the same time. The fast Fourier transform method is based on the fact that both real and imaginary parts of the K-K integrals are proportional to the convolution products between the real and imaginary components and the function $1/\omega$. Applying Fourier transform to both sides of the equations (33) and (34) using the Time-Convolution Theory yields,

$$f\{H_{\mathrm{Re}}(\omega)\} = \frac{1}{\pi} f\{H_{\mathrm{Im}}(\omega)\} f\left[\frac{1}{\omega}\right] \quad \textbf{(35)}$$

$$f\{H_{\mathrm{Im}}(\omega)\} = \frac{1}{\pi} f\{H_{\mathrm{Re}}(\omega)\} f\left[\frac{1}{\omega}\right] \quad \textbf{(36)}$$

The Fourier transform for real and imaginary parts can be calculated numerically, while that of the is already analytically to be, $f\left[\frac{1}{\omega}\right] = -j$ only if $f\left[\frac{1}{\omega}\right]$ and $\tau > 0$ and $f\left[\frac{1}{\omega}\right] = j$ if $\tau < 0$

Where τ is equal to the conjugate variable of ω and $j = \sqrt{-1}$. The real and imaginary parts for all the frequencies is then obtained by taking into account the inverse Fourier transform upon the products of these two functions. To make a numerical calculation of the convolution of equation (30), it must be reorganized in order to fulfil the requirements of this calculus. Due to parity of the functions, integrals in (30) are completely solved by splitting them into two integrals and calculation just the positive frequency domain. Interchanging the limits of the first integral removes the negative sign. But the frequency ω' can be swapped with ($-\omega$), noting that $H_{\text{Im}}(\omega) = -H_{\text{Im}}(-\omega')$. Substituting equation (35) into (34) and after a little algebra, one obtains the real and the imaginary parts of the K-K relations for the frequency domain namely;

$$H_{\text{Re}}(\omega) = -\frac{1}{\pi}\wp\int_0^{\infty}\frac{H_{\text{Im}}(\omega')}{(\omega-\omega')}d\omega' \qquad \textbf{(37)}$$

$$H_{\text{Im}}(\omega) = -\frac{1}{\pi}\wp\int_0^{\infty}\frac{\omega H_{\text{Re}}(\omega')}{(\omega-\omega')}d\omega' \qquad \textbf{(38)}$$

III. Results And Discussion

The resulting equations of the K-K relation which are numerically programmable were implemented in MATLAB's Discrete Fourier Transform (DFT). The DFT is a complex invertible linear transform. If we have a vector, x it can be transformed into another vector X in the fast Fourier transform. MATLAB application for the DFT is quite simple since it has in-built libraries for the FFT and its inverse fast Fourier transform component (iFFT) having vector of length N. The function fft(x) and its corresponding inverse ifft(X) transforms are numerically implemented as the following [9,10,11]:

$$X_k = \sum_{k=1}^{N} x_k \omega_N^{(j-1)(k-1)} \qquad \textbf{(39)}$$

$$x_k(X) = \frac{1}{N}\sum_{k=1}^{N} X_k \omega_N^{(-j-1)(k-1)} \qquad \textbf{(40)}$$

Where $\omega_N = e^{-2\pi i/N}$. Equations (38) and (39) can readily be programmed or obtained directly from Matlab libraries as functions usage fft(x) and iff(x) respectively.

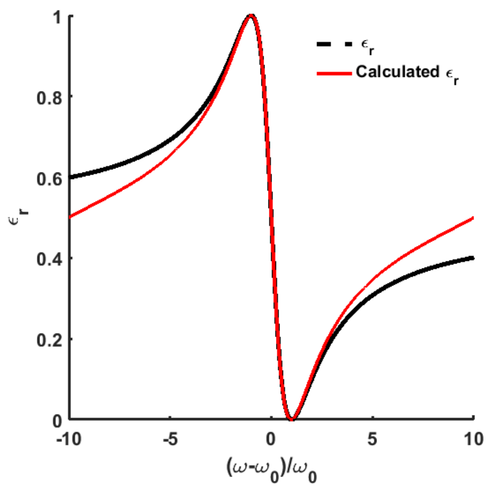

Figure 3: Plots of real part of the optical dielectric function $\varepsilon_r(\omega)$ as a function of frequency detuning $(\omega-\omega_0)/\omega$ for the calculated (red) and analytical (black).

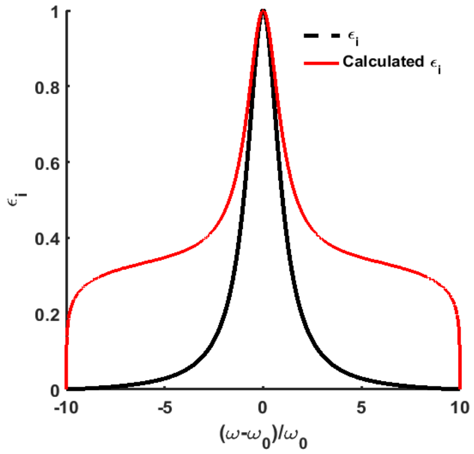

Figure 4: Plots of imaginary part of the optical dielectric function $\varepsilon_i(\omega)$ as a function of frequency detuning $(\omega - \omega_0)/\omega$ for the calculated (red) and analytical (black) spectra.

As an example in this paper to illustrate the algorithm at different normalised frequencies. Let us consider the well-known classical dielectric function emanating from the Fourier transform of the retarded Green's [2].

$$\varepsilon(\omega) = 1 - \omega_{\rho l}^2 \delta(\omega - \omega_0) \quad \textbf{(41)}$$

The symbols $\omega_{\rho l}$ and ω_0 are respectively the plasma frequency, critical frequency and photon frequency. It is convenient to simply approximate the delta function appearing in equation (42) as the well-known Lorentzian linewidth. $\delta(\omega - \omega_0) = 1/\omega + i\gamma$. The symbol γ represents the materials broadening parameter which approximates the level of scattering or relaxation of quasi-particles in the real semiconductor material medium. Hence one obtains after some algebra the closed form solution of both the real $\epsilon_r(\omega)$ and $\epsilon_i(\omega)$ the imaginary parts given respectively as

$$\varepsilon_r(\omega) = 1 - \frac{\omega_{\rho l}^2}{2\omega_0} \frac{1}{((\omega - \omega_0)^2 + \gamma^2)} \quad \textbf{(42)}$$

$$\varepsilon_i(\omega) = \frac{\omega_{\rho l}^2}{2\omega_0} \frac{1}{((\omega - \omega_0)^2 + \gamma^2)} \quad \textbf{(43)}$$

The plots of the classical optical dielectric function and their corresponding KKT obtained by MATLAB FFT algorithm are depicted as shown in figures 3 and figure 4 above. In figure 2 above, the calculated (FFT) real dielectric function $\varepsilon_r(\omega)$ show a good agreement with the analytical dielectric function (black). In figure 4, the calculated and analytically obtained imaginary dielectric function $\varepsilon_i(\omega)$ show good agreement at the resonant peak. The little deviation in the calculated $\varepsilon_i(\omega)$ within the vicinity of the normalised resonant frequency may be compensated by frequency padding. However, the accurate estimate of the amplitude and their corresponding resonance frequencies are genuinely guaranteed (Haug and Koch, 2004).This thus paves a way for a wide application in material data analysis such as in absorption and photoluminescence spectroscopy.

IV. Conclusion

In this study, we have reviewed the derivation of the dispersions relations arising from the K-K transformation via the frame work of the causal time-domain impulse response function. This approach was seen to exhibit a resonant behavior for the K-K relations over finite frequency bands. Using the algorithmic approach for the implementation of the K-K relation in MATLAB, well and consist results were reproduced when applied to the simple case of the dielectric function of a simple oscillator model. The results obtained offer a promising spectroscopic estimates in materials data analysis with the prior knowledge of the real or imaginary part of any complex material spectroscopic property and vice versa. Though, the methods of our calculation show somewhat a lower precision in the frequency tails of the imaginary part of the real dielectric function, the major artifacts and resonance signatures are genuinely preserved, showing its validity in material spectroscopy.

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