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Study the relation for some pitfalls with the Kramers-Kronig

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Abstract
The properties of the Kramers-Kronig (KK) relationships relating the real and imaginary parts of the frequency-domain permittivity are well known, but not at every electrical engineer's fingertips. This tutorial presents some surprises (e.g., incorrect prediction of the imaginary part from the real part for a Drude-model cold plasma) and explains not only why but how these come about.

Keywords: pitfalls, Kramers-Kronig, electrical engineer's fingertips

Introduction

The Kramers-Kronig (KK) relationships [1-3] relate the imaginary part of the dielectric permittivity (in the frequency domain) to its real part, and vice versa. A form of these is the following:

$$\varepsilon'(\omega)-1=\frac{2}{\pi}P\int_{-\infty}^{\infty}dx\frac{x\varepsilon''(\omega)}{x^2-\omega^2},$$

$$\varepsilon''(\omega)=\frac{2\omega}{\pi}P\int_{-\infty}^{\infty}dx\frac{1-\varepsilon'(\omega)}{x^2-\omega^2}, \quad \ldots (1)$$

In which expressions, P indicates "principal value," and the prime and double-prime notation indicates real and imaginary parts, respectively. One will find a number of different Kramers-Kronig forms [4] in the literature, connecting related quantities. However, Equation (1) will suffice at present. In the time domain, one has

$$\mathbf{D}(t)=\int_{-\infty}^{\infty}dt'\varepsilon(t')\mathbf{E}(t-t'), \quad \ldots (2)$$

As the relationship between the electric displacement and field vectors in an isotropic medium. To ensure causality (i.e., that D(t) cannot depend on electric fields at times greater than t), the lower bound on this integral must be 0, not ∞ This implies [4] that ε(ω), as a function of a complex frequency ω, must be analytical in the upper complex-ω half-plane (if time-harmonic fields $\propto \exp(-i\omega t)$). This tutorial is heavily dependent upon that fact, which in turn implies that ε (ω) must have no poles for Im (ω) ≥ 0.

Consider the (Drude-model) permittivity of a cold plasma [5, 6] determined by a plasma frequency, ω_p and a collision frequency, v_c:

$$\varepsilon(\omega)=1-\frac{\omega_p{}^2}{\omega(\omega+iv_c)}. \quad \ldots (3)$$

Its real and imaginary parts are given by [7, 8]

$$1-\varepsilon'(\omega)=\frac{\omega_p{}^2}{\omega^2+v_c{}^2},$$

$$\varepsilon''(\omega)=\frac{\omega_p{}^2 v_c}{\omega\left(\omega^2+v_c{}^2\right)}. \quad \ldots (4)$$

It would appear from Equation (1) that

$$\varepsilon''(\omega)=\frac{2}{\pi}\int_{-\infty}^{\infty}dx\,\frac{\omega\omega_p^{\,2}}{\left(\omega^2+v_c^{\,2}\right)\left(x^2-\omega^2\right)}. \quad \ldots (5)$$

Evaluation of this integral with MATLAB® yields a surprising result: see Figure 1 (with ω_p = 12 GHz, v_c = 0.1 GHz). The dashed line represents ε"(a)) as from Equation (4), whereas the full line is the result of Equation (5). Clearly, this must be an erroneous result. Why this is the case follows from another way of expressing the Kramers-Kronig relationships:

$$\varepsilon(\omega)-1=\frac{1}{2\pi i}\oint dz\,\frac{\varepsilon(z)-1}{z-\omega}. \quad \ldots (6)$$

The fact that ε(z) is analytical in the upper complex-z half-plane renders this an obvious consequence of the Cauchy theorem. When Equation (4) is inserted into the right-hand side, one obtains.

$$\varepsilon(\omega)-1=-\frac{1}{2\pi i}\oint dz\,\frac{\omega_p^{\,2}}{z\left(z+iv_c\right)\left(z-\omega\right)}. \quad \ldots (7)$$

The problem becomes apparent: there is an extra pole at the origin, which therefore is not excluded from the upper half-plane. To see what the consequences of this are, one may replace l/z in the integrand by P(1/z)+iπδ(z). This amounts to doing the principal value of the integral, plus an integration on the infinitesimal half circle around the pole at the origin. The extra contribution to Equation (7) thus yields

$$\left[\varepsilon(\omega)-1\right]_{\text{extra}}=-\frac{i\omega_p^{\,2}}{\omega v_c}-\frac{1}{2\pi i}P\int_{-\infty}^{\infty}dx\,\frac{\omega_p^{\,2}}{\left(x+iv_c\right)\left(x-\omega\right)}. \quad \ldots (8a)$$

The consequence for the imaginary part is

$$\left[\varepsilon''(\omega)\right]_{\text{extra}}=-\frac{\omega_p^{\,2}}{\omega v_c}+\frac{1}{2\pi}P\int_{-\infty}^{\infty}dx\,\frac{x\omega_p^{\,2}}{\left(x^2+v_c^{\,2}\right)\left(x-\omega\right)}, \quad \ldots (8b)$$

and the sum of these two terms, together with the contribution from Equation (4), as calculated with MA TLAB is graphed in Figure 2 (also with ω_p= 12GHz, v $_c$= 0.1 GHz).

Comparison of Figure 2 with Figure 1 shows that the spurious-pole contribution accounts for the incorrect result of Equation (5). A reasonable question is whether such an incorrect result can be avoided. The answer is that a small correction to Equation (3) will suffice:

$$\varepsilon(\omega)=1-\lim_{\omega_0\to 0}\left[\frac{\omega_p^{\,2}}{\omega^2+\omega_0^{\,2}+iv_c\omega}\right]. \quad \ldots (9)$$

The poles of this ε(ω)-1 are given by the zeroes of the denominator in Equation (9), which are $\omega=-\frac{1}{2}iv_c\pm\frac{1}{2}\sqrt{-v_c^2+4\omega_0^2}$ Yielding approximately (for $\omega_0 \ll v_c$) (10).

$$\omega_1\approx -iv_c,$$

$$\omega_2\approx -\frac{i\omega_0^{\,2}}{2v_c}. \quad \ldots (10)$$

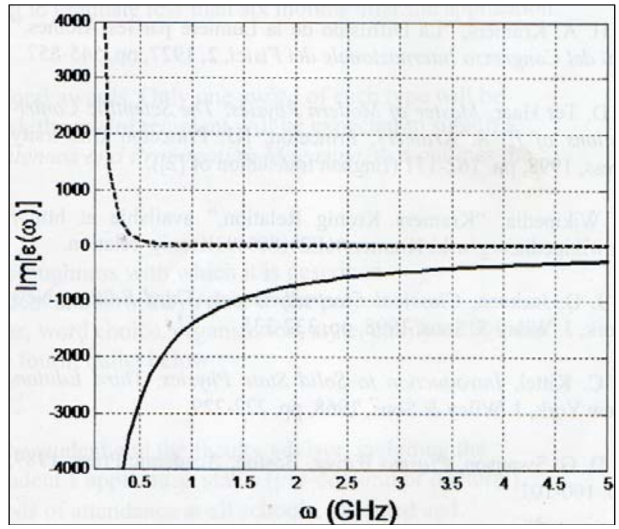

Fig 1: ε”(ω) as a function of ω

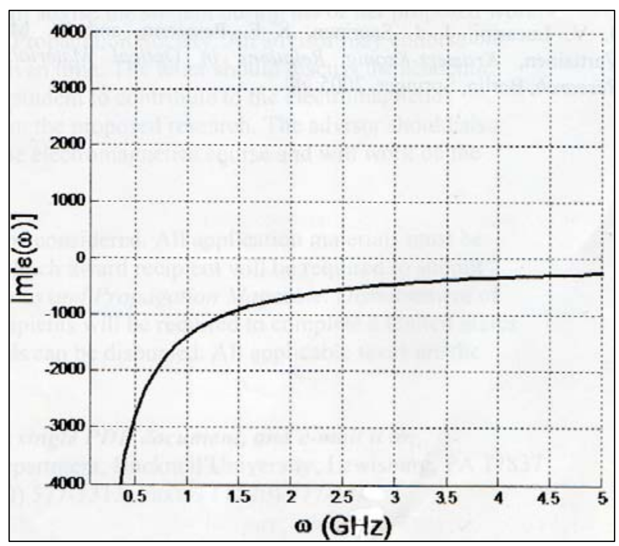

Fig 2: The consequence of the spurious pole for ω”(ω)

Conclusion

The ω pole is identical to what was found previously, but is still no problem, as it remains where it was in the lower half-plane. The offending pole at the origin, now ω_2, has moved (be it ever so slightly) into the lower half-plane, rand therefore is no longer a problem. Use of Equation (9) in thetight-hand side of Equation (1) yields the expected result shown by the dashed line in Figure 1. While Equation (4) may thus suffice for most applications, the above example shows that more caution is needed when using the Kramers-Kronig relationships to calculate the real or imaginary part of the permittivity from the other part.

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