Finite Frequency Range Kramers Kronig Relations: Bounds on the Dispersion

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Dispersion inequalities are presented to check for the self-consistency of experimentally obtained complex moduli, such as the complex dielectric constant, magnetic permeability, and complex bulk and shear moduli of viscoelastic materials. Unlike the Kramers-Kronig dispersion relations, they only require measurements over a finite frequency range. They can provide highly accurate interpolation formulas for the real part, given its value at a few selected frequencies and given the imaginary part over a range of frequencies. [S0031-9007(97)04253-1]

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Dispersion relations are prevalent throughout physics and derive from the causal nature of the response of materials, bodies, or particles to electromagnetic, elastic, or other fields. The classic example of a dispersion relation is the Kramers-Kronig (KK) relation [1,2] that couples the real and imaginary parts of the complex dielectric constant $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ of a material by

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{(\omega')^2 - \omega^2} \, d\omega', \qquad (1)$$

where P denotes the principle value of the integral. [Another KK relation expresses $\epsilon_2(\omega)$ in terms of $\epsilon_1(\omega)$ is not discussed here.] The chief obstacle to the practical application of the KK relation is that one needs to know $\epsilon_2(\omega)$ over all frequencies to determine $\epsilon_1(\omega)$, whereas a given experiment yields values of $\epsilon_2(\omega)$ only over a finite frequency range. This is typically handled in a crude manner which is only sometimes effective: Some approximation for $\epsilon_2(\omega)$ is used outside the measured frequency range. When the measured and computed function $\epsilon_1(\omega)$ disagree, one is left in doubt as to whether the measurements of $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are compatible with each other, or whether the data set violates what is known about the analytic properties of $\epsilon(\omega)$. In this paper we overcome these problems in a systematic and mathematically justified manner [assuming *only* the standard analytic properties of $\epsilon(\omega)$ including the positivity of $\epsilon_2(\omega)$ for $\omega > 0$], by deriving rigorous bounds on the function $\epsilon_1(\omega)$ for $\omega \in (\omega_-, \omega_+)$ given $\epsilon_2(\omega)$ over the same frequency interval. The appearance of bounds is natural and reflects the incompleteness of our knowledge of $\epsilon_2(\omega)$.

Analogous KK relations exist which give the real part of the complex magnetic permeability and the complex bulk and shear moduli in terms of their positive imaginary parts. Therefore, our bounds apply equally well to testing the compatibility of experimental data for these magnetic and viscoelastic moduli. With appropriate normalization (to capture the correct high frequency limit) they apply to the frequency dependent response of electrical networks and elastic structures. They are also applicable (with minor modification) in particle physics [3–5], specifically to testing the compatibility of measurements of the complex forward scattering amplitude collected over a finite range of energies.

Our bounds have potentially greater utility than the KK relation Eq. (1), being valid when the data have been measured only over a *finite frequency range*. They provide a simple series of tests to self-consistently analyze the compatibility of measured real and imaginary dielectric constants. Each successive bound is more strict, but requires more experimental data. Specifically, it is assumed the imaginary part is known over an entire interval of frequencies and bounds are obtained that correlate the values of the real part at N selected frequencies *within the interval*. These bounds are called M point bounds, where $M = N - 1$, because the bound on the real part at one of the selected frequencies incorporates information about the real part at the M remaining selected frequencies.

The bounds are the *sharpest possible* within the class of functions compatible with the required analytic constraints. Moreover, they provide *analytically admissible approximants* to the experimental data within the measured frequency range. Outside this range, the approximants may be poor predictors of the behavior. See [5–7] for discussions of the hazards and methods of extrapolating experimental data using analyticity.

Additional information about the high frequency behavior (assuming the plasma frequency is known) could easily be incorporated to yield even tighter bounds. Also the bounds are easily generalized to allow one to test the compatibility of measurements taken over two disjoint frequency ranges. This is particularly useful when a different experimental apparatus is used to take the measurement over the second frequency range.

Figures 1–3 illustrate the practical utility of the bounds as applied to high frequency transmission line measurements of the complex relative magnetic permeability of

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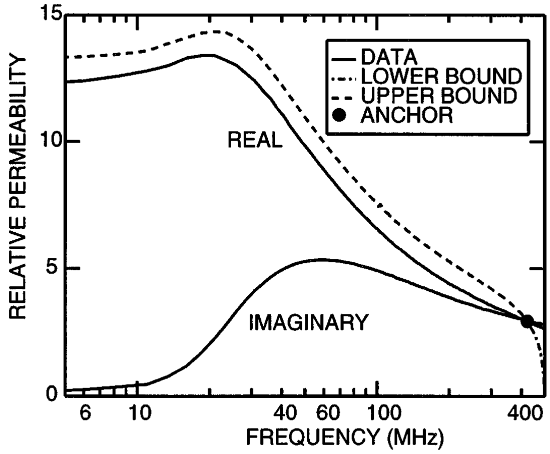

FIG. 1. Measurements of the real and imaginary parts of the complex relative magnetic permeability of a composite made with equal parts of barium titanate ($BaTiO_3$) and a magnesium-copper-zinc ferrite ($Cu_{0.2}Mg_{0.4}Zn_{0.4}Fe_2O_4$). Also graphed are the one-point bounds.

a composite made with equal parts (by volume) of barium titanate ($BaTiO_3$) and a magnesium-copper-zinc ferrite ($Cu_{0.2}Mg_{0.4}Zn_{0.4}Fe_2O_4$). The measurements were taken over the frequency range 1–500 MHz. Further information about the material and the experiments which supplied the data can be found in the paper by Mantese *et al.* [8]. As these examples demonstrate, the bounds provide a highly useful tool for judging the reliability of experimental data, and for earmarking frequency ranges over which the data need to be reexamined. Moreover, Fig. 3 shows that the bounds can be very tight. Therefore, if one has a high degree of certainty about the imaginary part, then these data can sometimes be used to construct the real part if one knows the values at a few selected frequencies [9].

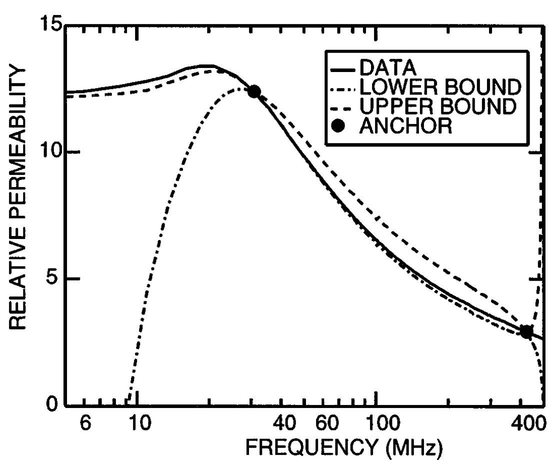

FIG. 2. The two-point bounds applied to the data are shown. The violation of the two-point bounds below 26 MHz indicates an error in the real part below 26 MHz or an error in the imaginary part, possibly at frequencies greater than 26 MHz. Thus the measurements below 26 MHz, if not unreliable, are at least inconsistent with the measurements above 26 MHz.

The basis for our compatibility tests are the following well-known properties of the complex dielectrical constant ϵ as a function of frequency: (i) $\epsilon(-\omega) = \epsilon^*(\omega^*)$, where $*$ denotes complex conjugation; (ii) the function $\epsilon(\omega)$ is analytic in the upper half plane; (iii) $\epsilon_2(\omega') \geq 0$ when ω' is real and $\omega' > 0$; (iv) $\lim_{\omega\to\infty} \epsilon(\omega) \equiv \epsilon(\infty) = 1$. For technical reasons, the last constraint (iv) will be replaced by the *relaxed constraint* (iv′) $\epsilon(\infty) \geq 1$. Any function $\epsilon(\omega)$ satisfying (iv′) can be converted to a function satisfying (iv), while maintaining properties (i), (ii), and (iii), by adding $[\epsilon(\infty) - 1]\omega^2/(\omega_0^2 - \omega^2)$ to $\epsilon(\omega)$. Provided ω_0 is chosen sufficiently large, this produces negligible change in the function except at very high frequencies.

The bounds and a brief description of their derivation are now given. It is convenient to introduce the variable $z = \omega^2$ and to study the function

$$g(z) = \epsilon(\sqrt{z}) - 1\,, \tag{2}$$

where $g(z) = g_1(z) + ig_2(z)$. It follows from the properties of $\epsilon(\omega)$ that (i) $g(z) = g^*(z^*)$. (ii) $g(z)$ is an analytic function in the plane, except on the real positive axis. (iii) $g_2(z' + i\delta) \geq 0$ for positive infinitesimal values of δ when z' is real and positive, and (iv′) $g(\infty) \geq 0$. Thus $g(z) - g(\infty)$ is a Stieltjes function of $-z$.

The dispersion relation for $g_1(z)$ given $g_2(z)$ is

$$g_1(z) = g(\infty) + \frac{1}{\pi} P \int_0^\infty \frac{g_2(z')}{z' - z}\, dz'. \tag{3}$$

If $g_2(z) = \epsilon_2(\sqrt{z})$ is known for an interval of frequencies $z \in (z_-, z_+)$, then a computable estimate for $g_1(z) = \epsilon_1(\sqrt{z}) - 1$ is

$$g_0(z) = \frac{1}{\pi} P \int_{z_-}^{z_+} \frac{g_2(z')}{z' - z}\, dz'. \tag{4}$$

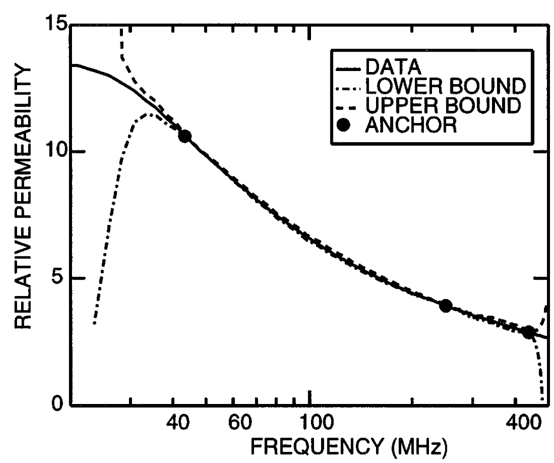

FIG. 3. The three-point bounds applied the data, disregarding those measurements taken at frequencies less than 26 MHz. These data were substantiated by an independent set of measurements. There is good agreement between the data and the bounds.

Both $g_1(z)$ and $g_0(z)$ are real when z is real. The difference between them defines a *discrepancy function*, $f(z) = g_1(z) - g_0(z)$ or

$$f(z) = g(\infty) + \frac{1}{\pi} P \int_0^{z_-} \frac{g_2(z')}{z' - z} dz' + \frac{1}{\pi} P \int_{z_+}^{\infty} \frac{g_2(z')}{z' - z} dz'. \quad (5)$$

The discrepancy function $f(z)$ has the same basic properties (i), (ii), (iii), and (iv′) as the function $g(z)$. In addition it is analytic along the interval (z_-, z_+) on the positive real axis. Rational functions have these properties if and only if they have (a) an equal number of poles and zeros which are all simple and located along the non-negative real axis, (b) their poles and zeros interlaced with a pole near (or at) the origin and a zero near (or at) infinity, (c) no poles lie in the interval (z_-, z_+), (d) each pole has a negative real residue.

Known bounds on Stieltjes functions due to Baker [10] can be used to generate bounds on $f(z)$ incorporating the known values $f(z_1), f(z_2), \ldots, f(z_M)$. However, the resulting bounds are generally suboptimal because they incorporate only the analyticity of $f(z)$ along a single interval on the real axis, and not along two disjoint intervals.

Our optimal bounds on $f(z)$ for all real $z \in (z_-, z_+)$ provide a quantitative compatibility test for experimental data. The one-point bound requires knowledge of the discrepancy function at a single point z_1. It states that

$$f(z) \geq \max\{f(z_1), z_1 f(z_1)/z\} \quad \text{when } z \geq z_1, \quad \text{and}$$
$$f(z) \leq \min\{f(z_1), z_1 f(z_1)/z\} \quad \text{when } z \leq z_1. \quad (6)$$

While crude, this is the best possible one-point bound. For example, in the case where $f(z_1) > 0$ the function $f(z) = f(z_1) + c(1/z_1 - 1/z)$ takes every value permitted by the bound as c ranges between 0 and ∞. The bound in this case is equivalent to stating that $f(z)$ is monotone increasing in z for all $z \in (z_-, z_+)$. This monotonicity can be proved by calculating $df(z)/dz$ and using the positivity of $g_2(z)$. [The positivity of $g_2(z)$ is needed to prove not just this bound but also the higher order bounds.]

The two-point bounds require knowledge of the discrepancy function at two distinct points z_1 and z_2. The bounds are constructed by considering the simplest possible rational functions that interpolate the known points, and that do not have any free parameters. More specifically, the candidate bounding functions $f_b(z)$ are constructed so that only one pole or zero remains, not counting poles at $0, z_-$, and z_+, and not counting any zero at ∞. The amplitude of the function and the position of this pole or zero is determined by the constraints that $f_b(z_1) = f(z_1)$ and $f_b(z_2) = f(z_2)$.

The seven rational functions listed below are the only rational functions consistent with these criteria for the two-point bound.

Candidate 1—Set

$$f_b(z) = \frac{(z_1 - z_2)}{(z - z_2)/f(z_1) + (z_1 - z)/f(z_2)}. \quad (7)$$

Candidates 2–4—Take a pole ζ_1 at $0, z_-$, or z_+, set

$$f_b(z;\zeta_1) = \frac{(z_1 - \zeta_1)(z - z_2)f(z_1) + (z_2 - \zeta_1)(z_1 - z)f(z_2)}{(z - \zeta_1)(z_1 - z_2)} \quad (8)$$

Candidates 5–7—Take poles $\zeta_1 > \zeta_2$ at $0, z_-$, or z_+, set

$$f_b(z;\zeta_1,\zeta_2) = \frac{[(z_1 - \zeta_1)(z_1 - \zeta_2)(z - z_2)f(z_1) + (z_2 - \zeta_1)(z_2 - \zeta_2)(z_1 - z)f(z_2)]}{(z - \zeta_1)(z - \zeta_2)(z_1 - z_2)}. \quad (9)$$

Of these seven candidate rational functions, we discard those functions that do not meet the required analytic constraints (a), (b), and (c). The remaining functions necessarily satisfy the constraint (d) because the interlacing of the poles and zeros automatically ensures that the poles have negative residues. [Assuming $f(z_1)$ and $f(z_2)$ satisfy the monotonicity requirement that $(z_1 - z_2)[f(z_1) - f(z_2)] \geq 0$.] At a given value of z between z_- and z_+ the bounds are then the minimum and maximum values taken by the accepted candidate functions. Which pair of functions gives the bounds turns out to depend on the value of $q = [z_1 f(z_1) - z_2 f(z_2)]/[f(z_1) - f(z_2)]$, which is necessarily positive when the one-point bounds are satisfied. We find that $f(z)$ lies between $f_b(z; z_-, 0)$ and $f_b(z; z_+, 0)$ when $z_- \geq q \geq 0$; between $f_b(z; z_-)$ and $f_b(z; z_+, 0)$ when $z_+ \geq q \geq z_-$; and between $f_b(z; z_-)$ and $f_b(z; z_+)$ when $q \geq z_+$. These bounds on $f(z) = \epsilon_1(\sqrt{z}) - 1 - g_0(z)$ are translated back into bounds on $\epsilon_1(\omega)$ (where $\omega = \sqrt{z}$) and the measured real and imaginary dielectric data are deemed incompatible if the real part lies outside the bounds.

In the limit as z_- approaches zero and z_+ approaches infinity our two-point bounds tighten and reduce to the familiar Kramers-Kronig relations. This is because both $f(z_1)$ and $f(z_2)$ approach zero, which forces each candidate function to approach zero (except possibly at $z = 0, z_-$, or z_+.) By letting z_2 approach z_1 one obtains bounds which incorporate $f(z_1)$ and the derivative $df(z_1)/dz_1$. Bounds on Stieltjes functions incorporating the value of the function and its derivatives, or equivalently the moments of the associated positive measure, are well known from the theory of moments [11]. Our bounds are tighter because they incorporate the additional fact that the measure is supported on two disjoint intervals.

The construction of the multipoint bounds is similar. Suppose that $f(z)$ is known at z_i for $i = 1, 2, \ldots, M$ with

$M > 2$. In the candidate rational functions one chooses to either position a pole or not position a pole at each of the three points 0, z_-, or z_+. This step generates eight possibilities. Additional poles and zeros, totaling $M - 1$ in number (or M in number if one of the zeros is at ∞) are placed along the real axis, so the overall number of poles equals the overall number of zeros. This latter constraint determines whether or not we place a zero at ∞. The amplitude of the function and the positions of the additional poles and zeros are determined by the M constraints that $f_b(z_i) = f(z_i)$ for $i = 1, 2, \ldots, M$. (If this is impossible then we move on to consider the next of the eight possibilities.) Of the eight candidate functions we discard those that do not meet the required analytic constraints (a), (b), and (c). At a given value of z between z_- and z_+ the bounds are the minimum and maximum values taken by the accepted candidate functions (of which there is at least one and generally at least two.) These bounds are translated back to the original variables, and the measured real and imaginary dielectric data are deemed incompatible if the real part lies outside the bounds. One cautionary remark: Before applying the M-point bounds one must first check the compatibility of the M known values $f(z_1), \ldots, f(z_m)$, i.e., that $f(z_2)$ satisfies the one-point bound when $f(z_1)$ is given, that $f(z_3)$ satisfies the two-point bound when $f(z_1)$ and $f(z_2)$ are given, and so forth. If the bounds are violated at any stage, the data set is deemed incompatible.

The proof of these bounds rests on an extension of the analysis of Milton [12]: See, in particular, formula (12). Briefly, $f(z)$ can be approximated by a rational function of very high degree satisfying (a), (b), and (c). The positions of the poles and zeros of this function can then be varied to maximize or minimize $f(z)$ at the given value of z while maintaining its known values $f(z_i)$ and the properties (a), (b), and (c). An examination of first-order variations shows that a necessary condition for a maximum or minimum to occur is that the total number of poles and zeros, not counting the poles at the endpoints $z = 0$, $z = z_-$, $z = z_+$ and the zero at $z = \infty$, must not exceed $M - 1$.

In actual experiments $\epsilon_2(\omega)$ is measured not over an interval of frequencies, but rather at a discrete set of finely spaced frequencies $\omega_1 < \omega_2 < \omega_3 < \cdots < \omega_k$. In this case nothing can be rigorously said about the values $\epsilon_1(\omega_1)$,$\epsilon_1(\omega_2) \ldots, \epsilon_1(\omega_k)$ can take: By considering the effect of very small amplitude delta-function resonances, resonant at frequencies very near $\omega_1, \omega_2, \ldots,$ and ω_k, it is clear that any combination of values is possible. Nevertheless, one can smoothly interpolate the measured $\epsilon_2(\omega)$ to all frequencies between ω_1 and ω_k and apply our bounds. If inconsistencies occur and if one has complete confidence in the measured values, then the interpolation must be poor. This itself is useful information, likely indicating the presence of undiscovered resonances at intermediate frequencies.

Experimental measurements will also have errors associated with them. Errors in $\epsilon_1(\omega)$ are easily treated. The bounds define a region $\mathcal{R}$ in a $(N + 1)$-dimensional space where the point $[\epsilon_1(\omega), \epsilon_1(\omega_1), \epsilon_1(\omega_2), \ldots, \epsilon_1(\omega_N)]$ must lie. Allowing for known errors the measurements define a box in this space where $[\epsilon_1(\omega), \epsilon_1(\omega_1), \epsilon_1(\omega_2), \ldots, \epsilon_1(\omega_N)]$ must lie. The data are deemed incompatible if the box does not intersect the region $\mathcal{R}$. Since the bounds may be very narrow for modest values of N, the transverse dimensions of R are small. In this case, a slight underestimation of the experimental errors can lead to a possibly erroneous conclusion that for a given N, the data are incompatible. This is not a difficult problem to overcome in practice because one must compute the one-point bound, the two-point bound, etc., before the N-point bounds. From this sequence it is logical to stop computing tighter bounds when the width of the current bounds is comparable to the known experimental error. Errors in $\epsilon_2(\omega)$ are not as easy to treat. However, if the errors are not systematic then $g_0(z)$ and hence also the bounds should be fairly insensitive to these errors because of the convolution appearing in Eq. (4). See also [13] and [14], and references therein, for a discussion of how errors can be handled.

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