Causal determination of acoustic group velocity and frequency derivative of attenuation with finite-bandwidth Kramers-Kronig relations

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Kramers-Kronig (KK) analyses of experimental data are complicated by the extrapolation problem, that is, how the unexamined spectral bands impact KK calculations. This work demonstrates the causal linkages in resonant-type data provided by acoustic KK relations for the group velocity (c_g) and the derivative of the attenuation coefficient (α') (components of the derivative of the acoustic complex wave number) without extrapolation or unmeasured parameters. These relations provide stricter tests of causal consistency relative to previously established KK relations for the phase velocity (c_p) and attenuation coefficient (α) (components of the undifferentiated acoustic wave number) due to their shape invariance with respect to subtraction constants. For both the group velocity and attenuation derivative, three forms of the relations are derived. These relations are equivalent for bandwidths covering the entire infinite spectrum, but differ when restricted to bandlimited spectra. Using experimental data from suspensions of elastic spheres in saline, the accuracy of finite-bandwidth KK predictions for c_g and α' is demonstrated. Of the multiple methods, the most accurate were found to be those whose integrals were expressed only in terms of the phase velocity and attenuation coefficient themselves, requiring no differentiated quantities.

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I. INTRODUCTION

Fundamentally rooted in causality, Kramers-Kronig (KK) relations provide linkages between the physical properties that govern the response of matter and materials to external stimuli. Due to their general foundations [1], KK relations have applications across a broad range of physical frameworks, from continuum mechanics to elementary particle phenomenology. As tools for the analysis of physical systems, these relations are employed to perform a wide array of tasks that include measuring fundamental material parameters, establishing the consistency of laboratory data, and building causally consistent physical models. When applying KK relations to data, a knowledge gap exists between the infinite bandwidth required by the KK integrals and the inherently bandlimited measurements. The impact of this gap on KK calculations, also referred to as the extrapolation problem, depends on many factors, both general and system dependent. In some cases the gaps are filled in via extrapolation [2] while in others the potential influences of the unknown bands are reduced through subtractions [2,3]. One can also estimate analytically admissible approximants to a conjugate KK parameter given finite data [4].

Previously, we established the consistency of finite-bandwidth acoustic KK relations of the twice-subtracted form between the ultrasonic attenuation coefficient $\alpha(\omega)$ and phase velocity $c_p(\omega)$ using data from suspensions of encapsulated microbubbles that exhibit an isolated resonance [5]. Using only information from within the measurement spectrum, finite-bandwidth KK relations provided for accurate transformations between the two quantities $\alpha(\omega)$ and $c_p(\omega)$ with the proper selection of the subtraction frequency. The choice of subtraction frequency ω_0 determines the slope and intercept of a linear contribution to the calculation that is critical to the accuracy of the prediction. In the ideal case, in which the entire spectrum is available for the calculation, the results are independent of the subtraction frequency. However, for the finite-bandwidth case the result is highly sensitive to this choice of ω_0. Furthermore, it is not clear that objective criteria can be established to favor the best-fitting choices for ω_0 over other values. As a result, the subtraction frequency is effectively a tuning parameter which makes this approach somewhat unsatisfactory.

In this work we derive KK relations for the inverse group velocity $1/c_g(\omega)$ and frequency derivative of attenuation $\alpha'(\omega)=d\alpha(\omega)/d\omega$, which are the real and imaginary components of the first derivative (with respect to frequency) of the acoustic complex wave number. We find three specific expressions for each relation that are equivalent when integrated over the entire spectrum but distinct over a limited bandwidth. These include relations for determining $1/c_g(\omega)$ directly from the attenuation coefficient, and for determining $\alpha'(\omega)$ directly from the phase velocity. Furthermore, these two specific formulations, which involve no differentiated quantities in the integrals, are found to provide the most accurate predictions for the data examined in this paper.

For finite-bandwidth analysis, an important general property of these KK relations is that the shapes of the predicted curves are independent of the subtraction frequency. As a result these relations for c_g and α' permit a more stringent test of causal consistency for dispersive acoustic data than the twice-subtracted KK relations for the primary quantities c_p and α. It should also be noted that the group velocity can be directly (i.e., without differentiation) determined in the properly designed experiment and so, in principle, can be known to the same precision as the phase velocity. Consequently, the use of $c_g(\omega)$ in these relations does not necessarily decrease the precision of a calculation relative to $c_p(\omega)$ and $\alpha(\omega)$ even though it is technically defined as a differentiated quantity.

Following the derivations of these KK relations, we use their direct forms $[\alpha(\omega)\to c_g(\omega)$ and $c_p(\omega)\to\alpha'(\omega)]$ to demonstrate the close agreement between experimental determinations and finite-bandwidth KK predictions for data exhibiting multiple resonant structures. The consistency between the data and predictions for group velocity and derivative of attenuation under our relations clearly establishes the causal link between attenuation and dispersion for these data over a finite bandwidth without extrapolation.

II. THEORY

A. Subtracted relations in the expanded form

The transfer function for a passive, linear isotropic medium can be written

$$H(\omega,D)=\exp[iK(\omega)D], \tag{1}$$

where

$$K(\omega)=\omega/c_p(\omega)+i\alpha(\omega) \tag{2}$$

is the complex wave number, $\alpha(\omega)$ is the attenuation coefficient, $c_p(\omega)$ is the phase velocity, and D is the thickness. The transfer function $H(\omega,D)$ is the Fourier transform of a causal, square-integrable function [i.e., the impulse response $h_D(t)$], which implies via Titchmarsh's theorem [6] that its real and imaginary parts form a Hilbert transform pair. Since $h_D(t)$ is real, the components of $H(\omega,D)$ exhibit definite parity, which in turn permits the mapping of the negative frequency components of the Hilbert integrals to positive frequencies. The resulting transforms are labeled as Kramers-Kronig relations. Using the method of subtractions, one can also derive KK relations for the components of $K(\omega)$. Based on both empirical and analytic evidence [5,7,8] two subtractions appear to be sufficient for establishing a Hilbert transform pair from the acoustic complex wave number. The twice-subtracted relations in the expanded form are

$$\frac{\omega}{c_p(\omega)}=\frac{\omega_0}{c_p(\omega_0)}+(\omega-\omega_0)\left.\frac{d}{d\omega}\frac{\omega}{c_p(\omega)}\right|_{\omega=\omega_0}+\lim_{\substack{\sigma\to0\\ \Omega\to\infty}}\left[I_\alpha(\omega,\sigma,\Omega)-I_\alpha(\omega_0,\sigma,\Omega)-(\omega-\omega_0)\left.\frac{d}{d\omega}I_\alpha(\omega,\sigma,\Omega)\right|_{\omega=\omega_0}\right], \tag{3}$$

where

$$I_\alpha(\omega,\sigma,\Omega)=\frac{1}{\pi}\int_\sigma^\Omega\frac{\alpha(x)-\alpha(\omega)}{x-\omega}dx-\frac{1}{\pi}\int_\sigma^\Omega\frac{\alpha(x)-\alpha(\omega)}{x+\omega}dx, \tag{4}$$

and

$$\alpha(\omega)=\alpha(\omega_0)+(\omega-\omega_0)\alpha'(\omega_0)+\lim_{\substack{\sigma\to0\\ \Omega\to\infty}}\left[I_c(\omega,\sigma,\Omega)-I_c(\omega_0,\sigma,\Omega)-(\omega-\omega_0)\left.\frac{d}{d\omega}I_c(\omega,\sigma,\Omega)\right|_{\omega=\omega_0}\right], \tag{5}$$

where

$$I_c(\omega,\sigma,\Omega)=-\frac{1}{\pi}\int_\sigma^\Omega\frac{x/c_p(x)-\omega/c_p(\omega)}{x-\omega}dx-\frac{1}{\pi}\int_\sigma^\Omega\frac{x/c_p(x)+\omega/c_p(\omega)}{x+\omega}dx, \tag{6}$$

and ω_0 is the subtraction frequency. By evaluating the integrals in Eqs. (3) and (5) before taking the limit of $\Omega\to\infty$, the divergences of the individual integrals will cancel. Although it is conventional to combine the remapped negative frequency contribution [the second integrals in Eqs. (4) and (6), respectively] with the positive frequency part, keeping them separate has some advantages for computational and analytical work. Note that the local variations in the quantities $\omega/c_p(\omega)$ and $\alpha(\omega)$ on the left-hand sides of Eqs. (3) and (5) are largely generated by the first terms [i.e., $I_\alpha(\omega,\sigma,\Omega)$ and $I_c(\omega,\sigma,\Omega)$] on the respective right-hand sides. The remaining terms in both relations define linear contributions whose slopes and intercepts are functions of ω_0.

The group velocity and derivative of attenuation are components of the differentiated complex wave number,

$$\frac{d}{d\omega}K(\omega)=\frac{d}{d\omega}\frac{\omega}{c_p(\omega)}+i\frac{d}{d\omega}\alpha(\omega) \tag{7a}$$

$$=1/c_g(\omega)+i\alpha'(\omega). \tag{7b}$$

The KK relations for $1/c_g(\omega)$ and $\alpha'(\omega)$ are of the once-subtracted type and can each be written in one of three ways depending on the method used for their derivation. The general form for all three expressions of the group velocity relation is

$$1/c_g(\omega)=1/c_g(\omega_0)+\lim_{\substack{\Omega\to\infty\\ \sigma\to0}}[I_\alpha^{(V)}(\omega,\sigma,\Omega)-I_\alpha^{(V)}(\omega_0,\sigma,\Omega)]. \tag{8}$$

where the explicitly defined integral sets $I_\alpha^{(V)}(\omega,\sigma,\Omega)$ are distinguished by the label $V=$ "sub", "diff", or "pv" ("sub" is derived directly from the method of subtractions; "diff" is derived by differentiation of an earlier relation; "pv" contains a principal value integral). $I_\alpha^{(\mathrm{sub})}(\omega,\sigma,\Omega)$ is derived by applying the method of subtractions directly to Eq. (7b):

$$I_\alpha^{(\mathrm{sub})}(\omega,\sigma,\Omega)=\frac{1}{\pi}\int_\sigma^\Omega \frac{\alpha'(x)-\alpha'(\omega)}{x-\omega}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{\alpha'(x)+\alpha'(\omega)}{x+\omega}dx. \tag{9}$$

Alternatively, one can differentiate Eq. (3) with respect to frequency to obtain $I_\alpha^{(\mathrm{diff})}(\omega,\sigma,\Omega)$,

$$I_\alpha^{(\mathrm{diff})}(\omega,\sigma,\Omega)=\frac{1}{\pi}\int_\sigma^\Omega \frac{\alpha(x)-\alpha(\omega)-(x-\omega)\alpha'(\omega)}{(x-\omega)^2}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{\alpha(x)-\alpha(\omega)+(x+\omega)\alpha'(\omega)}{(x+\omega)^2}dx. \tag{10}$$

Finally, using the fact that the Hilbert transform of a constant is zero, the third set of integrals can be taken from Eq. (10)

$$I_\alpha^{(\mathrm{pv})}(\omega,\sigma,\Omega)=\frac{1}{\pi}P\int_\sigma^\Omega \frac{\alpha(x)-\alpha(\omega)}{(x-\omega)^2}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{\alpha(x)-\alpha(\omega)}{(x+\omega)^2}dx \tag{11}$$

where P denotes integration in the principal value sense. This form has the advantage of containing no explicit differentiated quantities in its integrands.

As implied by Eq. (8), in the limits $\sigma\to 0$, $\Omega\to\infty$ these three formulations are equivalent. This work is concerned with finite limits of integration, however, and when σ and Ω are confined to the finite limits of the measured spectra, the three forms will produce different results. More details regarding the differences among Eqs. (9)–(11) will be discussed in Sec. IV.

As with the group velocity, the relation for the frequency derivative of attenuation can be expressed in three ways, with the general form

$$\alpha'(\omega)=\alpha'(\omega_0)+\lim_{\substack{\Omega\to\infty\\ \sigma\to 0}}\lfloor I_c^{(V)}(\omega,\sigma,\Omega)-I_c^{(V)}(\omega_0,\sigma,\Omega)\rfloor, \tag{12}$$

and the three specific integral forms

$$I_c^{(\mathrm{sub})}(\omega,\sigma,\Omega)=-\frac{1}{\pi}\int_\sigma^\Omega \frac{1/c_g(x)-1/c_g(\omega)}{x-\omega}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{1/c_g(x)-1/c_g(\omega)}{x+\omega}dx, \tag{13}$$

$$I_c^{(\mathrm{diff})}(\omega,\sigma,\Omega)=-\frac{1}{\pi}\int_\sigma^\Omega \frac{x/c_p(x)-\omega/c_p(\omega)-(x-\omega)/c_g(\omega)}{(x-\omega)^2}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{x/c_p(x)+\omega/c_p(\omega)-(x+\omega)/c_g(\omega)}{(x+\omega)^2}dx, \tag{14}$$

and

$$I_c^{(\mathrm{pv})}(\omega,\sigma,\Omega)=-\frac{1}{\pi}P\int_\sigma^\Omega \frac{x[1/c_p(x)-1/c_p(\omega)]}{(x-\omega)^2}dx + \frac{1}{\pi}\int_\sigma^\Omega \frac{x[1/c_p(x)-1/c_p(\omega)]}{(x+\omega)^2}dx. \tag{15}$$

Note that Eq. (15) is derived by rewriting the numerators in Eq. (14) as follows:

$$\frac{x}{c_p(x)}\pm\frac{\omega}{c_p(\omega)}-\frac{x\pm\omega}{c_g(\omega)}=x\left(\frac{1}{c_p(x)}-\frac{1}{c_p(\omega)}\right) + (x\pm\omega)\omega\frac{c_p'(\omega)}{c_p(\omega)^2}. \tag{16}$$

In summary, each of the parameters $c_g(\omega)$ and $\alpha'(\omega)$ has three possible KK formulations that are distinguished by their integrands. The first type ("sub") contains only the differentiated quantities themselves, the second form ("diff") contains a mixture of primary (i.e., undifferentiated) and differentiated quantities, and the third type ("pv") contains only the primary quantities. In this work, we have found that the third types, the "pv" forms (11) and (15), produce the most accurate results. This is a significant finding since the most accurate $1/c_g(\omega)$ and $\alpha'(\omega)$ predictions result from integrals containing only the primary quantities $c_p(\omega)$ and $\alpha(\omega)$. Also, in contrast to the determinations of $c_p(\omega)$ and $\alpha(\omega)$ given in Eqs. (3) and (5), the choice of subtraction frequency ω_0 in Eqs. (8) and (12) defines only an offset and so the shapes of the $1/c_g(\omega)$ and $\alpha'(\omega)$ curves are completely independent of the choice for ω_0.

III. RESULTS

The data examined in this work are from transmission measurements of agitated suspensions of polymer microspheres in saline [9,10]. The two suspensions used in this work contain spheres distributed narrowly in size about mean radii of 50.8 and 34.8 μm, respectively. The measurements exhibit several attenuation peaks and rapid dispersive sweeps, covering the spectrum from 3 to 30 MHz and the circumference-to-wavelength (ka) spectrum from 0.64 to 6.4 and 0.44 to 4.4, respectively. The four panels of Fig. 1 show the finite-bandwidth KK predictions of $c_g(f)$ and $\alpha'(f)$ in comparison with the experimental data for these two suspensions. The calculations of $c_g(f)$ and $\alpha'(f)$ (where $f=\omega/2\pi$) were performed with the general relations (8) and (12) using the specific integral forms (11) and (15), respectively. The limits of integration were fixed to $\sigma=3$ MHz and $\Omega=30$ MHz, the spectral extent of the data. In all four panels, excellent agreement is apparent, especially in the first two-thirds of the spectrum. At the higher frequencies, the attenuation and dispersion of the suspensions exhibit small-scale rapid oscillations that are not well resolved by the frequency step size of the data. The rapid variations in the KK results at high frequency do represent the underlying behavior of data, although the detailed correspondence is not as precise at this end of the spectrum.

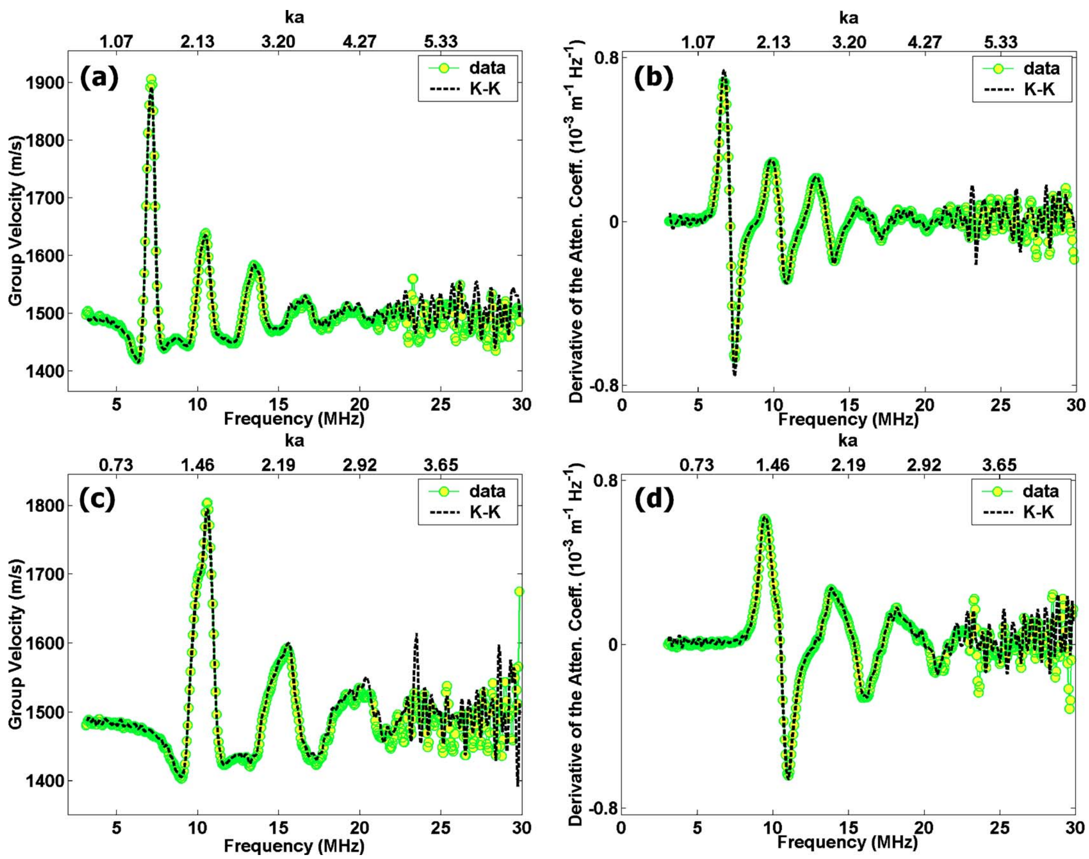

FIG. 1. (Color online) Comparisons between the experimentally determined and Kramers-Kronig (KK) predicted quantities for (a) group velocity and (b) frequency derivative of the attenuation coefficient for the 50.8 μm suspension. (c) and (d) show these same comparisons for the 34.8 μm suspension. In all four panels, the circles are the experimental data and the dotted curves are the finite-bandwidth KK predictions. The KK calculations were performed using the integral formulations in Eqs. (11) and (15), respectively.

IV. DISCUSSION

A. Role of subtraction frequency

In previous work, the phase velocity and attenuation coefficient data from Albunex[1] microbubble suspensions have been shown to be consistent with finite-bandwidth KK relations (3) and (5) with the limits of integration fixed to $\sigma=1$ MHz and $\Omega=15$ MHz [5]. These twice-subtracted relations can also accurately transform between $c_p(f)$ and $\alpha(f)$ for the microsphere data used in this work. However, for both the Albunex and microsphere suspensions the accuracies of the $c_p(f)$ and $\alpha(f)$ predictions depend critically on the choice of subtraction frequency $f_0=\omega_0/2\pi$ used in the calculations, where in the ideal case of $\sigma=0$ and $\Omega\rightarrow\infty$ the outcomes should be independent of this choice. About 20% of the frequencies contained in the discrete data sets can produce reasonably good agreement when used as f_0's, while a similar fraction produces strongly divergent results. [Finding an objective physical justification for choosing f_0 in the $c_p(f)$ and $\alpha(f)$ predictions is the subject of an ongoing investigation.] In contrast, the agreement for each of $c_g(f)$ and $\alpha'(f)$ clearly demonstrates the causal link in the microsphere data in a more satisfying manner, since the KK calculations produce shape-invariant predictions of the two quantities. One can also go to the next order of derivative and eliminate the subtraction frequency f_0 completely. However, the higher-order differentiation of discrete data can be problematic because it amplifies noise and becomes increasingly delocalized.

B. Use of differentiated quantities

A significant aspect of the methods developed here is that accurate transforms are obtained for the two derivative components of the complex wave number without requiring any differentiated quantities in the integrals. Of these derivative quantities of the complex wave number, the group velocity is a highly relevant physical parameter that can be clearly demonstrated to be the velocity of the peak in the modulation envelope of the properly constructed wave packet (e.g., a narrowband, Gaussian-gated continuous wave [11]). The group velocity itself can be determined by the direct measurement of group delay, and so, in principle, it can be known to the same precision as the phase velocity. This im-

[1]Certain commercial equipment, instruments, or materials are identified in this paper only in order to specify the experimental procedure adequately. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

plies that the group velocity is not necessarily saddled with the increase in noise that is associated with the differentiation of experimental data. Consequently, it is possible to use $c_g(\omega)$ in these KK calculations without causing any loss of precision relative to the primary quantities $c_p(\omega)$ and $\alpha(\omega)$.

The relations for the derivative of the attenuation coefficient are of interest mainly to provide a conjugate relation as a further demonstration of causal consistency. As an independent physical quantity, $\alpha'(\omega)$ is not widely used outside of biomedical ultrasonics where it is known as the "slope of attenuation" and used as a parameter in tissue characterization. It is not clear if there is a way to determine $\alpha'(\omega)$ directly through an amplitude measurement to a similar precision as one can determine $\alpha(\omega)$. Consequently, it may not be possible to circumvent the introduction of noise due to differentiation with respect to this parameter.

C. Issues in determining the optimum method

As mentioned earlier, the three individual integral formulations (9)–(11) of the group velocity relation are equivalent when evaluated from 0 to ∞. The same holds true for the three forms (13)–(15) of the relation for the attenuation derivative. When σ is nonzero and/or Ω is finite each of the integrals produces artifacts of the bandwidth restriction that are unique to the integrand and integration limits, as well as the type of behavior exhibited by the system (e.g., resonant, monotonic power law) [5,7]. These artifacts can manifest themselves as scaling factors of the desired result and/or as terms additive to the desired result. In some cases multiple artifacts may partially cancel one another, or alternatively they could overwhelm the target quantity. Without analytically modeling the system beforehand, it is not clear that one can *a priori* choose the optimal form of the integrals for a given data set. Still, one can obtain analytical, model-independent expressions for the differences among the three forms of each relation. These derived expressions were found to be in close agreement with the numerically calculated differences. For this work, the differences between the methods were small, and each method produced a reasonably accurate result on its own. For the $c_g(f)$ prediction the worst discrepancies between Eqs. (9)–(11) (occurring near the largest peak in each suspension) were less than 3% of the value of the quantity itself. For $\alpha'(f)$, the three methods produced quite similar predictions with the only significant differences occurring near the largest peak in each data set.

V. CONCLUSION

In this work, KK relations for determining the group velocity and frequency derivative of attenuation have been derived. For finite-bandwidth predictions with data exhibiting multiple resonant structures, these relations for $c_g(\omega)$ and $\alpha'(\omega)$ were shown to produce accurate results. A significant finding is that the best $c_g(\omega)$ and $\alpha'(\omega)$ predictions were determined from integrals over the primary quantities $\alpha(\omega)$ and $c_p(\omega)$, respectively, without any differentiated parameters in the integrands. As tools for finite-bandwidth analysis, the predictions of these relations for $c_g(\omega)$ and $\alpha'(\omega)$ are morphologically independent of the subtraction frequency and thus provide more satisfactory methods for confirming the causal consistency of dispersion data in comparison with KK relations for $c_p(\omega)$ and $\alpha(\omega)$. Furthermore, accurate predictions are achieved without using any unmeasured or extrapolated parameters.

The underlying framework used to derive these relations is not specific to acoustics and can be applied to other types of wave propagation. For example, a similar relation for group velocity (or group index of refraction) can be derived for the propagation of electromagnetic waves. Such a relation could be especially useful in the optical range, where phase measurements can be much more challenging than absorption measurements and pulses are typically narrowband.

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