

Refractive index and wave vector in passive or active media

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Materials that exhibit loss or gain have a complex-valued refractive index n . Nevertheless, when considering the propagation of optical pulses, using a complex n is generally inconvenient—hence the standard choice of real-valued refractive index, i.e., $n_s = \text{Re}(\sqrt{n^2})$. However, an analysis of pulse propagation based on the second-order wave equation shows that use of n_s results in a wave vector *different* to that actually exhibited by the propagating pulse. In contrast, an alternative definition $n_c = \sqrt{\text{Re}(n^2)}$, always correctly provides the wave vector of the pulse. Although for small loss the difference between the two is negligible, in other cases it is significant; it follows that phase and group velocities are also altered. This result has implications for the description of pulse propagation in near resonant situations, such as those typical of metamaterials with negative (or otherwise exotic) refractive indices.

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I. INTRODUCTION

Recent work in metamaterials and negative refractive index media¹ [1–8] has focused attention on propagation in media with exotic values of permittivity ϵ and permeability μ , as well as those with significant loss or gain, where ϵ and μ are complex valued. These material properties (i.e., ϵ and μ) impact directly on the refractive index, and hence on the wave vector β and phase and group velocities [9,10].

When considering analytical solutions of the wave equation, it is often convenient to allow the propagation wave vector β and refractive index n to be complex valued, based on the definition $n^2 = c^2 \epsilon \mu$, so that $\beta = (\omega^2 n^2 / c^2)^{1/2}$. However, although this leads to many useful results, the approach also has some serious drawbacks. For example, the sign of the imaginary part of β , which determines whether the wave experiences gain or loss, needs to be specified according to the chosen direction of propagation. Worse, in the envelope and carrier description of pulse propagation, which is common in nonlinear optics (e.g., see [11]), the presence of a complex wave vector in the carrier function is very inconvenient, since it requires the nonlinear coefficients to be adjusted to compensate for the distance propagated. In addition, determining other parameters such as the group velocity under these circumstances is also a nontrivial task (see, e.g., [12]). For these and other reasons, it is often preferable to define a real-valued wave vector k and to treat the imaginary component separately.

The standard approach is to simply define k as the real part of β , i.e., $k = (\omega/c) \text{Re}(\sqrt{n^2}) = \omega n_s / c$. However, an alternative definition based on $k^2 = (\omega/c)^2 \text{Re}(n^2) = \omega^2 n_c^2 / c^2$ has been used with advantage in studies of causality-based constraints for negative refraction [13,14], although neither paper remarked on the nonstandard definition. In that context, this alternative definition is *required* because it keeps the real and imaginary parts of n^2 separate, and so ensures the Kramers-Kronig relations [15] continue to hold, linking the

two parts and enforcing causality. In contrast, the standard complex n is not required to be causal, although it is so in the case of passive (lossy) media (see, e.g., [16,17]).

In the present paper, the two definitions will be compared using the predictions of the second-order wave equation as the benchmark. It is shown that for field propagation in media with loss (“passive”) or gain (“active”), where the use of a complex wave vector is particularly problematic, the alternative definition has the clear advantage that it exactly matches the spatial oscillations of the field. In contrast, the standard definition gives an imperfect match, and the description only recovers the true propagation due to the presence (and inconvenience) of additional correction terms. Note that the alternative definition (for n_c) is not in any sense equivalent to one based on an effective refractive index, such as might occur in (e.g.) waveguides: it is an alternative choice of definition for the bulk refractive index.

Because I focus on the propagation of waves, in Sec. II, I present a short description of the second-order wave equation. Then, in Sec. III, I give some definitions required for the handling of both the standard case (Sec. IV) and the new alternative definition (Sec. V). After the discussion of the similarities and difference between the definitions in Sec. VI, I end by presenting my conclusions in Sec. VII.

II. SECOND-ORDER WAVE EQUATION

The second-order wave equation is commonly used in optics (at least as a starting point) in descriptions of propagation and results from the substitution of the $\nabla \times \vec{H}$ Maxwell’s equation into the $\nabla \times \vec{E}$ one in the source-free case (see, e.g., [11]). In homogeneous media, with $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ and $\partial_a \equiv \partial / \partial a$, the frequency space wave equation is

$$\nabla^2 \vec{E} + \beta^2 \vec{E} = 0. \quad (1)$$

Here $\beta^2 = \epsilon \mu \omega^2$ is the square of a complex propagation wave vector since both ϵ and μ can be complex. We can relate it to a complex refractive index squared quantity with

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¹Also commonly called negative phase velocity (NPV) media.

$$\beta^2 = n^2 \frac{\omega^2}{c^2}. \quad (2)$$

When considering the propagation of fields, it is convenient to split β^2 up into two parts (e.g., its real and imaginary parts). Here I write $\beta^2 = k^2 + i\gamma^2$ so that Eq. (1) becomes

$$\nabla^2 \vec{E} + k^2 \vec{E} + i\gamma^2 \vec{E} = 0. \quad (3)$$

When solving this wave equation, we will usually want the first two terms to give plane-wave solutions, with the rest component containing loss and nonlinearity.² This is an important step, since although we might solve linear problems using a complex valued n , realistic situations are not so easily handled.

The first two terms in Eq. (3), taken in isolation, have plane-wave solutions if k is real valued; I call this the “underlying propagation.” The third term in Eq. (3) is the “residual” component, which controls the discrepancy between the true propagation and the underlying propagation. Although in the case of small loss or gain the residual component will be only a weak perturbation, the theory presented here is valid for *any* strength.

As an aside, if we specialize to the case of fields propagating along the z direction, using the carrier and envelope models of pulse propagation [11,19–22], we would write $E(z,t) = A(z,t) \exp[i(\omega t - kz)] + \text{c.c.}$ to accommodate the rapidly oscillating behavior of the carrier frequency: this carrier represents the underlying propagation for a specific frequency. This then leaves only the (usually) slowly varying envelope $A(z,t)$, which would be affected only by the residual component.

Returning to the wave equation of Eq. (3) and taking propagation along the z axis, we can now factorize it using the Green’s functions [19,21,23] to give two first-order equations that are coupled only by the residual component. At the same time we can split the field into forward (E_+) and backward (E_-) parts (i.e., set $E = E_+ + E_-$), to give a pair of coupled, counterpropagating, first-order differential equations. These are

$$\partial_z E_{\pm} = \pm ik E_{\pm} \mp \frac{\gamma^2}{2k} (E_+ + E_-). \quad (4)$$

Here the underlying propagation is, as desired, plane-wave-like, since the first right-hand side (RHS) term just adds an ikz behavior onto the frequency dependent $i\omega t$. The propagation is then modified by the second RHS term, i.e., the γ^2 -dependent residual component. A feature of this approach is that we see that *any* contribution (whether linear or not) that is included in the residual component will couple the forward and backward fields together (see [19,21] for more discussion). Since such terms are scaled by k in Eq. (4), they change (but in a simple way) under my alternative form for the refractive index.

Here I consider only the one-dimensional linear case, where β^2 is independent of the field. This covers the cases of

both loss and/or gain (i.e., in passive and/or active media); however for simplicity I will often only refer to loss; nevertheless the case of gain is always allowed for (since gain can be seen as “negative loss”).

If we take the propagation to be of the form $E_{\pm} = E_0 \exp[i(\omega t - k'z)]$, with $E_- = 0$, then Eq. (4) gives us

$$-ik' = -ik + \frac{\gamma^2}{2k}, \quad (5)$$

so that $\gamma^2 < 0$ corresponds to loss for a forward propagating wave. Further, if we consider instead the oppositely propagating wave, Eq. (4) automatically ensures the necessary change in sign to ensure a loss stays loss, and a gain stays a gain. In contrast, when using a complex-valued n , care must be taken to ensure the correct sign (see e.g., [24]).

III. DEFINITIONS

We have that β^2 and n^2 are (in general) complex valued, and ω and c are strictly real valued. Thus when choosing the propagation wave vector we need to decide what to do about the imaginary parts. Our choice then affects the performance, utility, and convenience of the refractive index, phase velocity, and group velocity.

I now define some useful intermediate quantities to express the refractive index conveniently; I introduce $n_0^2 = |n^2|$ and the angle $\phi = \text{Arg}(n^2)$ so that

$$n^2 = n_0^2 e^{i\phi}, \quad (6)$$

$$n = n_0 e^{i\phi/2}. \quad (7)$$

Whether or not specific values of ϕ correspond to a negative refractive index or negative phase velocity can be determined from the criteria for ϵ and μ given in [25].³ I also define a reference wave vector k_n such that

$$k_n^2 = \frac{\omega^2}{c^2} n_0^2. \quad (8)$$

The standard form for a real-valued refractive index is

$$n_s = \text{Re}[\sqrt{(n^2)}] = n_0 \cos \frac{\phi}{2}. \quad (9)$$

I have already noted that many treatments leave n as a complex-valued quantity, leading to a complex wave vector k , and that while useful in many circumstances, in the context of pulse propagation it brings some significant disadvantages.

An alternative definition for the refractive index is

$$n_c = \sqrt{\text{Re}(n^2)} = n_0 \sqrt{\cos \phi}, \quad (10)$$

where n_c^2 satisfies the Kramers-Kronig relations [15] in partnership with the imaginary part $\text{Im}(n^2)$; this definition has already been used in the literature (e.g., see the recent [13,14]).

²We can even incorporate diffraction in the rest by including the transverse parts of ∇^2 ; see [18].

³Note that the ϕ used here corresponds to ϕ_+ in the summary in [26].

IV. STANDARD FORM

The standard form for the wave vector based on the standard form of refractive index [see Eq. (9)],

$$k_s^2 = \frac{\omega^2}{c^2} [\text{Re}(\sqrt{n^2})]^2 = k_n^2 \cos^2 \frac{\phi}{2}, \quad (11)$$

$$k_s = k_n \cos \frac{\phi}{2}. \quad (12)$$

Thus k_s is always real valued and can be negative in some circumstances. The phase velocity is then the usual $v_p = c/n_s$, and the (inverse) group velocity simply $v_g^{-1} = \frac{dk}{d\omega}$.

Let us now consider how this standard form of k_s^2 looks when substituted into the second-order wave equation. To do this let us express β^2 in terms of k_s^2 and k_n^2 ,

$$\beta^2 = k_s^2 + ik_n^2 \gamma_s^2, \quad (13)$$

with the residual behavior described by

$$i\gamma_s^2 = i \left[\sin \phi + i \sin^2 \frac{\phi}{2} \right]. \quad (14)$$

This standard choice of $k \equiv k_s$ leads to a second-order wave equation of the form

$$\partial_z^2 \vec{E} + k_s^2 \vec{E} + ik_n^2 \gamma_s^2 \vec{E} = 0. \quad (15)$$

When factorized, as briefly described in Sec. II, we get a pair of coupled, counterpropagating, first-order equations. These are

$$\partial_z E_{\pm} = \pm ik_s E_{\pm} \mp \frac{k_n^2}{2k_s} \gamma_s^2 (E_+ + E_-). \quad (16)$$

Since the residual component $i\gamma_s^2$ on the RHS of Eq. (16) contains a real part as well as an imaginary part, it is not pure loss. The real part will impose oscillations on the field as it propagates, thus altering the wave vector away from the assumed value k_s . However, the real part is quadratic in ϕ , being $\propto \sin^2 \frac{\phi}{2}$, so for small losses the correction to the underlying propagation will be small. If we rewrite Eq. (16) to incorporate the correction into the leading term, we get

$$\begin{aligned} \partial_z E_{\pm} = & \pm ik_s \left[1 - \frac{k_n^2}{2k_s^2} \sin^2 \frac{\phi}{2} \right] E_{\pm} \\ & \mp i \frac{k_n^2}{2k_s} \sin^2 \frac{\phi}{2} E_{\mp} \mp \frac{1}{2} \frac{k_n^2}{2k_s} [\sin \phi] (E_+ + E_-). \end{aligned} \quad (17)$$

As before, the first term on the RHS gives plane-wave-like propagation, but now with a wave vector that differs from k_s .

I will now express the effective propagation wave vector in terms of k_n and ϕ . To simplify the description, I apply the usually excellent [27] approximation that the effect of E_- on the propagation can be ignored (i.e., set $E_- = 0$). Hence,

$$\partial_z E_+ = +ik'_s E_+ - \frac{1}{2} \frac{k_n^2}{2k_s} \sin \phi E_+, \quad (18)$$

with

$$k'_s = k_n \cos \frac{\phi}{2} \left[1 - \frac{1}{2} \tan^2 \frac{\phi}{2} \right]. \quad (19)$$

For $\phi \ll 1$, we then find that

$$k'^2 \approx k_n^2 \cos \phi. \quad (20)$$

Thus although I began with the standard definition, which assumes that the (forwardlike) field will propagate with a wave vector $k \equiv k_s$, we see instead that it propagates with a wave vector $k \approx k_n \sqrt{\cos \phi}$. As we will see, this approximation to the effective propagation wave vector is usually close to that of the alternative form discussed below; the difference (for small loss) is of order ϕ^4 .

The standard phase velocity v_p is

$$v_p^2 = \frac{\omega^2}{k_s^2} = \frac{c^2}{n_0^2 \cos^2 \frac{\phi}{2}}. \quad (21)$$

However, if we were to use the effective propagation wave vector k'_s we would get a different answer; in the case of the approximate form of Eq. (20), it turns out the same as the alternate form given in Sec. V.

The standard group velocity v_g can be derived using

$$2k_s \partial_\omega k_s = k_s^2 \left[\frac{2}{n_0} (\partial_\omega n_0) - (\partial_\omega \phi) \tan \frac{\phi}{2} + \frac{2}{\omega} \right]. \quad (22)$$

Hence,

$$v_g^{-1} = \partial_\omega k_s = \frac{k_s}{\omega} \left[1 + \frac{\omega}{n_0} (\partial_\omega n_0) - \frac{\omega}{2} (\partial_\omega \phi) \tan \frac{\phi}{2} \right]. \quad (23)$$

Just as for phase velocity, if we were to use the effective propagation wave vector k'_s , we would get a different answer; in the case of the approximate form of Eq. (20), it turns out the same as the alternate form given in Sec. V.

V. ALTERNATIVE FORM

The alternative form for the wave vector, based on the product $\epsilon \mu$ [i.e., the square of the refractive index, see Eq. (10)], is

$$k_c^2 = \frac{\omega^2}{c^2} \text{Re}(n^2) = k_n^2 \cos \phi, \quad (24)$$

$$k_c = k_n \sqrt{\cos \phi}. \quad (25)$$

Thus k_c is either real valued or is pure imaginary. Real values of k_c correspond to a regime of propagating waves, imaginary values to that of evanescent waves. The phase velocity is then $u_p = c/n_c$, and the (inverse) group velocity simply $u_g^{-1} = \frac{dk_c}{d\omega}$; both will differ from the standard v_p and v_g and are given below. Note that k_c^2 is related to k_s^2 by

$$\frac{k_c^2}{k_s^2} = \frac{k_n^2 \cos \phi}{k_n^2 \cos^2 \frac{\phi}{2}} = 1 - \tan^2 \frac{\phi}{2}. \quad (26)$$

With this alternative choice, it is simple to express β^2 in terms of our wave vector k_c^2 ,

$$\beta^2 = k_c^2 + k_n^2 \gamma_c^2, \quad (27)$$

with the residual behavior described by

$$\iota \gamma_c^2 = \iota \sin \phi = \iota \gamma_s^2 + \sin^2 \frac{\phi}{2}. \quad (28)$$

For small $\phi \ll 1$, γ_s and γ_c differ only by terms of order ϕ^2 . Note that the losslike part of the residual component [i.e., of $\text{Im}(\gamma_s^2)$ or $\text{Im}(\gamma_c^2)$] is the same for either form; *but that only this alternative form of k (i.e., k_c) ensures that the residual component is purely lossy, and will not change the spatial oscillations of the field away from those of the propagation wave vector. However, the alternative form of k leads to the underlying propagation becoming evanescent if $\text{Re}(n^2) < 0$.*

With this choice of wave vector (i.e., $k \equiv k_c$), the second-order wave equation can be written as

$$\partial_z^2 \vec{E} + k_c^2 \vec{E} + \iota k_n^2 \gamma_c^2 \vec{E} = 0. \quad (29)$$

When factorized, as briefly described in Sec. II, we get

$$\partial_z E_{\pm} = \pm \iota k_c E_{\pm} \mp \frac{k_n^2}{2k_c} \gamma_c^2 [\sin \phi] (E_+ + E_-). \quad (30)$$

The phase velocity u_p is now *faster* than for the standard definition, being

$$u_p^2 = \frac{\omega^2}{k_c^2} = v_p^2 \left[1 - \tan^2 \frac{\phi}{2} \right]^{-1}. \quad (31)$$

The corresponding group velocity u_g can be derived using

$$2k_c \partial_{\omega} k_c = k_c^2 \left[\frac{2}{n_0} (\partial_{\omega} n_0) - (\partial_{\omega} \phi) \tan \phi + \frac{2}{\omega} \right]. \quad (32)$$

Hence,

$$u_g^{-1} = \partial_{\omega} k_c = \frac{k_c}{\omega} \left[1 + \frac{\omega}{n_0} (\partial_{\omega} n_0) - \frac{\omega}{2} (\partial_{\omega} \phi) \tan \phi \right]. \quad (33)$$

Here the comparison of u_g with the standard form v_g is less simple than for phase velocities: the prefactors are different [$\sqrt{\cos(\phi)}$ compared to $\cos \frac{\phi}{2}$]; also the bracketed terms differ slightly (with $\tan \phi$ not $\tan \frac{\phi}{2}$). However, for $\phi < \pi/2$, $\sqrt{\cos(\phi)} < \cos \frac{\phi}{2}$, so that the group velocity u_g is faster than the standard v_g .

VI. DISCUSSION

As already noted, for small losses the standard and alternative definitions of n (and also those of k) nearly coincide, but they diverge as the loss increases. Indeed, for (e.g., strongly resonant) situations where $\text{Re}(n^2) < 0$, the underlying propagation (i.e., that defined by k_s or k_c) can be of a completely different character. The simplest case is the trivial one where $\text{Im}(n^2) = 0$. Here $k_s^2 = k_c^2$, and both are always positive; both γ_s^2 and γ_c^2 are zero. The descriptions are identical.

Next we add a small imaginary part to n^2 , with $|\phi| \ll 1$, so that k_s and k_c no longer match. The losslike part of the residual component is (as always) the same in both cases, but a standard (k_s) description will be modified by an additional

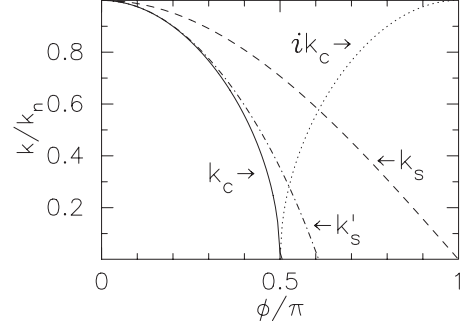


FIG. 1. Comparison of k values, as a function of $\phi = \text{Arg}(\epsilon\mu)$. The alternative choice k_c is shown using a solid line when it is real valued, and dotted when imaginary (“ ιk_c ”); the standard choice (k_s) is given by the dashed line, with the approximate corrected form (k'_s) from Eq. (20) as shown by the dot-dashed line.

oscillation, giving an effective wave vector comparable to k_c . This is perhaps the most typical regime for device operation; being either the low loss case of normal (positive phase velocity) propagation, or the low loss case of NPV propagation.

As ϕ increases, the two descriptions diverge, as summarized on Fig. 1. We see that the standard description ($k \equiv k_s$) gives qualitatively similar behavior for all $|\phi| \leq \pi$; being one of a wave vector k_s with added loss and a correction to achieve the true propagation wave vector. Obviously, the larger the ϕ , the larger the wave vector correction.

The alternative choice of $k \equiv k_c$ behaves differently. When $|\phi| = \pi/2$, i.e., when $n^2 = \text{Im}(n^2)$, the wave vector k_c vanishes, giving no underlying oscillatory evolution as the field propagates. The only evolution is that given by the residual component, i.e., the loss specified by $\text{Im}(n^2)$. Then, as $|\phi|$ increases further, so that $\text{Re}(n^2) = \text{Re}(c^2 \epsilon \mu) < 0$, we find that k_c takes on an imaginary value: this is just the case of plasmons, where $\text{Re}(\epsilon) \in (-\infty, 0]$, but $\text{Re}(\mu) \in [0, \infty)$. Here the imaginary k_c means that underlying propagation becomes evanescent; and any loss then acts in addition to that.

Note that the loss in the alternative description is simply $\text{Im}(n^2)$ —it differs from that used in the standard picture. In particular note that this is *not* identical to the sum of the permittivity-based “loss” [i.e., $\text{Im}(\epsilon)$] and the permeability-based “loss” [i.e., $\text{Im}(\mu)$]. Further, at least in the case of doubly passive media [26], $\text{Im}(n^2) < 0$ is in fact a criterion for NPV; i.e., *loss* is a criterion for NPV. More general statements on this relationship have been made when placing causality based constraints on negative refractive index media using the Kramers-Kronig relations [13,14].

Lastly, whichever choice of k or n we make, it depends only on the *sum* of the complex phases of ϵ and μ . In contrast, the summary given by [26] shows that the NPV criteria of [25] also depends on the *difference* of those phases. This sensitivity arises because the presence of NPV depends on the relative phases of the electric and magnetic fields; however the second-order wave equation does not distinguish between the electric and magnetic responses, considering only their net effect on the selected field (here, the electric field E).

VII. CONCLUSION

Here I have shown that the standard definition for a real-valued refractive index [i.e., $n \equiv n_s = \text{Re}(\sqrt{n^2})$] is only an ap-

proximation to the true real-valued refractive index seen by a propagating optical pulse. Instead, the true propagation wave vector is based on the alternate definition $n \equiv n_c = \sqrt{\text{Re}(n^2)}$. This conclusion was reached by examining how fields are actually propagated by the widely used electromagnetic second-order wave equation, in the case where loss (or gain) is treated as a modification to an underlying propagation based on a real-valued refractive index or wave vector. Treatments of pulse propagation that use this alternative n_c (and hence k_c) will not only be using wave vector that exactly matches the propagation, but adjustments to that propagation

will involve only gain or loss. In contrast, for the standard treatment based on n_s, k_s , corrections to the spatial oscillation of the fields must be applied along with those for gain or loss.

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