The 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. \( n_s = \Re(\sqrt{n^2}) \). 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 \( n_c = \sqrt{\Re(n^2)} \), 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.

I. INTRODUCTION

Recent work in metamaterials and negative refractive index media\(^1\) \([1, 2, 3, 4, 5, 6, 7, 8]\) has focused attention on propagation in media with exotic values of permittivity \( \epsilon \) and permeability \( \mu \), as well as those with significant loss or gain, where \( \epsilon \) and \( \mu \) are complex valued. These material properties (i.e. \( \epsilon, \mu \)) impact directly on the refractive index, and hence on the wave vector \( \beta \) and phase and group velocities\(^2\) \([3, 4]\).

When considering analytical solutions of the wave equation, it is often convenient to allow the propagation wave vector \( \beta \) 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 \( \beta \), 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 \([3]\)), 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 non-trivial task (see e.g. \([2]\)). 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 \( \beta \), i.e. \( k = (\omega/c) \Re(\sqrt{n^2}) = \omega n_s/c \). However, an alternative definition based on \( k^2 = (\omega/c)^2 \Re(n^2) = \omega^2 n_c^2/c^2 \) has been used with advantage in studies of causality-based constraints for negative refraction \([3, 4]\), although neither paper remarked on the non-standard 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\(^3\) 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. \([10, 17]\)).

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

II. THE 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. \([1]\)). 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

\[
\nabla^2 \vec{E} + \beta^2 \vec{E} = 0.
\]
Here $\beta^2 = \epsilon \omega^2 / c^2$ is the square of a complex propagation wave vector, since both $\epsilon$ and $\mu$ can be complex. We can relate it to a complex refractive index squared quantity with

$$\beta^2 = n^2 \omega^2 / c^2. \tag{2}$$

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

$$\nabla^2 \vec{E} + k^2 \vec{E} + \gamma^2 \vec{E} = 0. \tag{3}$$

When considering this wave equation, we will usually want the first two terms to give plane-wave solutions, with the rest component containing loss and nonlinearity. 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 eqn. (3), taken in isolation, have plane-wave solutions if $k$ is real-valued; I call this the “underlying propagation”. The third term in eqn. (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, we would write $E(z,t) = A(z,t) \exp[i(\omega t - kz)] + c.c.$ to accommodate the rapidly oscillating behaviour 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 eqn. (3), and taking propagation along the $z$-axis, we can now factorize it using Greens functions, 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, counter propagating, first order differential equations. These are

$$\partial_z E_\pm = \pm i k E_\pm + \gamma^2 / 2k (E_+ + E_-). \tag{4}$$

Here the underlying propagation is, as desired, plane-wave like, since the first RHS term just adds an $ikz$ behaviour onto the frequency dependent $\omega t$. The propagation is then modified by the second RHS term, i.e. the $\gamma^2$-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 eqn. (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 $\beta^2$ 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 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 $E_+ = E_0 \exp[i(\omega t - k'z)]$, with $E_- = 0$, then eqn. (4) gives us

$$-ik' = -ik + \gamma^2 / 2k; \tag{5}$$

so that $\gamma^2 < 0$ corresponds to loss for a forward propagating wave. Further, if we consider instead the oppositely propagating wave, eqn. (4) automatically ensures the necessary change of 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. [22]).

### III. DEFINITIONS

We have that $\beta^2$ and $n^2$ are (in general) complex valued, and $\omega$ 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 $\phi = \arg(n^2)$ so that

$$n^2 = n_0^2 e^{i\phi}, \tag{6}$$

$$n = n_0 e^{i\phi/2}. \tag{7}$$

Whether or not specific values of $\phi$ correspond to a negative refractive index or negative phase velocity can be determined from the criteria for $\epsilon$ and $\mu$ given in [23]. I also define a reference wave vector $k_n$ such that

$$k_n^2 = \omega^2 / c^2 n_0^2. \tag{8}$$

The standard form for a real valued refractive index is

$$n_s = \Re \left( \sqrt{(n^2)} \right) = n_0 \cos \phi / 2. \tag{9}$$

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

3 Note that the $\phi$ used here corresponds to $\phi_k$ in the summary in [24].
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 \[13, 14\]).

IV. THE STANDARD FORM

The standard form for the wave vector based on the standard form of refractive index (see eqn. \[1\]),

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

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

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 $v_g^{-1} = \frac{\partial v_p}{\partial \omega}$.  

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 $\beta^2$ in terms of $k_s^2$ and $k_n^2$,

$$\beta^2 = k_s^2 + i k_n^2 \gamma_s^2. \quad (13)$$

with the residual behaviour described by

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

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

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

When factorized, as briefly described in section \[1\] we get a pair of coupled, counter-propagating, first order equations. These are

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

Since the residual component $\gamma_s^2$ on the RHS of eqn. \[14\] 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 $\phi$, being $\propto \sin^2 \frac{\phi}{2}$, so for small losses the correction to the underlying propagation will be small.

If we rewrite eqn. \[16\] to incorporate the correction into the leading term, we get

$$\partial_z E_{\pm} = \pm i k_s E_{\pm} \mp \frac{k_n^2 \gamma_s^2}{2 k_s} (E_+ + E_-), \quad (17)$$

As before, the first term on the RHS is 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 $\phi$. To simplify the description, I apply the usually excellent \[21\] approximation that the effect of $E_-$ on the propagation can be ignored (i.e. set $E_- = 0$). Hence,

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

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

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

Thus although I began with the standard definition, which assumes that the (forward-like) 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 $\phi^4$.

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 eqn. \[20\], it turns out the same as the alternate form given in the next section. The standard group velocity $v_s$ can be derived using

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

Hence

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

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 eqn. \[21\], it turns out the same as the alternate form given in the next section.
V. THE ALTERNATIVE FORM

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

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

(24)

$$k_c = k_n \sqrt{\cos \phi}.$$  

(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 $u_g^{-1} = \frac{dk}{d\omega}$; both will differ from the standard $v_p, v_g$, and are given below. Note that $k_c^2$ is related to $k_s^2$ by

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

(26)

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

$$\beta^2 = k_c^2 + k_n^2 \gamma_c^2,$$

(27)

with the residual behaviour described by

$$v_{r_c}^2 = i \sin \phi = v_{r_s} + \sin^2 \frac{\phi}{2}. $$

(28)

For small $\phi \ll 1$, $\gamma_r$ and $\gamma_c$ differ only by terms of order $\phi^2$. Note that the loss-like 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

$$\partial^2_{zz} E + k_c^2 E + i k_n^2 \gamma_c^2 \partial_z E = 0$$

(29)

When factorized, as briefly described in section I we get

$$\partial_z E_{\pm} = \pm i k_c E_{\pm} + \frac{k_n^2 \gamma_c^2}{2k_c^2} \sin \phi \left( E_+ + E_- \right). $$

(30)

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

$$u_p^2 = \frac{\omega^2}{k_c^2} = \frac{v_p^2}{1 - \tan^2 \frac{\phi}{2}}.$$ 

(31)

The corresponding group velocity $u_g$ can be derived using

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

(32)

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 $\gamma_s^2$ and $\gamma_c^2$ 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 loss-like 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 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 $\phi$ increases, the two descriptions diverge, as summarized on fig. I. We see that the standard description ($k \equiv k_s$) gives qualitatively similar behaviour 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 $\phi$, the larger the wave vector correction.

The alternative choice of $k \equiv k_e$ behaves differently. When $|\phi| = \pi/2$, i.e. when $n^2 = \text{Im}(n^2)$, the wave vector $k_e$ 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 $\Re(n^2) = \Re(\sqrt{\epsilon\mu}) < 0$, we find that $k_e$ takes on an imaginary value: this is just the case of plasmons, where $\Re(\epsilon) \in (-\infty, 0]$, but $\Re(\mu) \in [0, \infty)$. Here the imaginary $k_e$ 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 [25], $\text{Im}(n^2) < 0$ 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 $\epsilon$ and $\mu$. In contrast, the summary given by [25] 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 nett 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. $n \equiv n_s = \sqrt{\epsilon\mu}$) is only an approximation 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 $n \equiv n_e = \sqrt{\Re(n^2)}$. This conclusion was reached by examining how fields are actually propagated by the widely used electromagnetic second order wave equation, in the case where when 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 $n_e$ (and hence $k_e$) 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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