Theory of the propagation of coupled waves in arbitrarily-inhomogeneous stratified media

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Abstract. – We generalize the invariant imbedding theory of the wave propagation and derive new invariant imbedding equations for the propagation of arbitrary number of coupled waves of any kind in arbitrarily-inhomogeneous stratified media, where the wave equations are effectively one-dimensional. By doing this, we transform the original boundary value problem of coupled second-order differential equations to an initial value problem of coupled first-order differential equations, which makes the numerical solution of the coupled wave equations much easier. Using the invariant imbedding equations, we are able to calculate the matrix reflection and transmission coefficients and the wave amplitudes inside the inhomogeneous media exactly and efficiently. We establish the validity and the usefulness of our results by applying them to the propagation of circularly-polarized electromagnetic waves in one-dimensional photonic crystals made of isotropic chiral media. We find that there are three kinds of bandgaps in these structures and clarify the nature of these bandgaps by exact calculations.

Introduction. – The phenomena of the coupling of two or more wave modes in inhomogeneous media and mode conversion between them are ubiquitous in various branches of science, including plasma physics, optics, condensed matter physics and electrical engineering [1–6]. In this Letter, we develop a generalization of the powerful invariant imbedding method [6–13] to the case of several coupled waves in stratified media. Starting from a very general wave equation of a matrix form, we derive a new version of the invariant imbedding equations for calculating the reflection and transmission coefficients and the field amplitudes. By doing this, we transform the original boundary value problem of coupled second-order differential equations to an initial value problem of coupled first-order differential equations. This makes the numerical solution of the coupled wave equations much easier. Furthermore, our equations have a great advantage that there is no singular coefficient even in the cases where the material parameters change discontinuously at the boundaries and inside the inhomogeneous medium. We check the validity and the usefulness of our invariant imbedding equations by applying them to the propagation of electromagnetic waves in stratified chiral media. By calculating

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the matrix reflection and transmission coefficients exactly, we clarify the nature of the three different photonic bandgaps that can exist in photonic crystals made of chiral media.

Theory. – We consider a system of $N$ coupled waves propagating in a stratified medium, where all parameters may depend on only one spatial coordinate. We take this coordinate as the $z$ axis and assume the inhomogeneous medium of thickness $L$ lies in $0 \leq z \leq L$. We also assume that all $N$ waves propagate in the $xz$ plane. The $x$ component of the wave vector, $q$, is a constant and the dependence on $x$ of all wave functions can be taken as being through a factor $e^{iqx}$. In a large class of interesting problems, the wave equation of $N$ coupled waves in the present situation has the form

\[
\frac{d^2 \psi}{dz^2} - \frac{dE}{dz}E^{-1}(z) \frac{d\psi}{dz} + [E(z)K^2M(z) - q^2I] \psi = 0,
\]

where $\psi = (\psi_1, \cdots, \psi_N)^T$ is an $N$-component vector wave function and $E$ and $M$ are $N \times N$ matrix functions that depend on $z$ in an arbitrary manner inside the inhomogeneous medium. We assume that the waves are incident from the vacuum region where $z > L$ and transmitted to another vacuum region where $z < 0$. $I$ is a unit matrix and $K$ is a diagonal matrix such that $K_{ij} = k_i \delta_{ij}$, where $k_i$ is the magnitude of the vacuum wave vector for the $i$-th wave. $E$ and $M$ are unit matrices in the vacuum region. The nonsingular functions $E(z)$ and $M(z)$, which specify the material properties of the medium and/or the external conditions, can change discontinuously at the boundaries and at discrete $z$ values inside the medium. By assigning $E(z)$ and $M(z)$ suitably, eq. (1) is able to describe many different kinds of waves in a large number of stratified media.

There are numerous examples where the effective wave equations have precisely the same form as eq. (1). Later in this Letter, we will apply our theory to the propagation of electromagnetic waves of two different polarizations in layered chiral media, where $\psi$ is a two-component vector and $E$, $M$ and $K$ are $2 \times 2$ matrices. Another interesting example is the propagation of the probe and phase-conjugate waves in layered phase-conjugating media [14, 15]. A wide variety of mode conversion phenomena observed in space and laboratory plasmas can also be studied using eq. (1) [1, 2, 13, 16].

Following Gryanik and Klyatskin [6], we generalize eq. (1) slightly, by replacing the vector wave function $\psi$ by an $N \times N$ matrix wave function $\Psi$, the $j$-th column vector $(\Psi_{1j}, \cdots, \Psi_{Nj})^T$ of which represents the wave function when the incident wave consists only of the $j$-th wave. We are interested in the $N \times N$ reflection and transmission coefficient matrices $r = r(L)$ and $t = t(L)$. Let us introduce a matrix

\[
g(z, z') = \begin{cases} T \exp \left[ i \int_{z'}^{z} \frac{dz''}{2} E(z'') P \right], & z > z' \\ \tilde{T} \exp \left[ -i \int_{z}^{z'} \frac{dz''}{2} E(z'') P \right], & z < z' \end{cases}
\]

where $T$ and $\tilde{T}$ are the time-ordering and anti-time-ordering operators respectively. $P$ is a diagonal matrix satisfying $P_{ij} = p_i \delta_{ij}$ and $p_i$ is the negative $z$ component of the vacuum wave vector for the $i$-th wave. It is straightforward to prove that $g(z, z')$ satisfies the differential equations

\[
\frac{\partial}{\partial z} g(z, z') = i \operatorname{sgn}(z - z') E(z)P g(z, z'), \quad \frac{\partial}{\partial z'} g(z, z') = -i \operatorname{sgn}(z - z') g(z, z')E(z')P.
\]

Using eqs. (2) and (3), the wave equation (1) is transformed to an integral equation

\[
\Psi(z, L) = g(z, L) \left. \frac{\partial}{\partial z'} \int_0^L dz' g(z, z') \left[ E(z')P - PM(z') - q^2P^{-1}M(z') + q^2P^{-1}E^{-1}(z') \right] \Psi(z', L) \right|_{z'=0}.
\]
where we consider $\Psi$ as a function of both $z$ and $L$. We take a partial derivative of this
equation with respect to $L$ and obtain
\[ \frac{\partial \Psi(z, L)}{\partial L} = i \Psi(z, L) \alpha(L) + \Phi(z, L), \]  
(5)
where
\[ \alpha(L) = \mathcal{E}(L)P - \frac{1}{2} [\mathcal{E}(L)P - PM(L) - q^2P^{-1}M(L) + q^2P^{-1}\mathcal{E}^{-1}(L)] \Psi(L, L), \]  
(6)
and $\Phi(z, L)$ satisfies an equation similar to eq. (4) except that there is no source term (that
is, $g(z, L)$). This implies $\Phi(z, L) = 0$ and then we have
\[ \frac{\partial \Psi(z, L)}{\partial L} = i \Psi(z, L) \alpha(L). \]  
(7)
Taking now the derivative of $\Psi(z, L)$ with respect to $L$, we obtain
\[ \frac{d \Psi(z, L)}{dL} = \frac{\partial \Psi(z, L)}{\partial z} \bigg|_{z=L} + \frac{\partial \Psi(z, L)}{\partial L} \bigg|_{z=L} = i \mathcal{E}(L)P [r(L) - I] + i \Psi(z, L) \alpha(L). \]  
(8)
Since $\Psi(z, L) = I + r(L)$, we easily find the $(N \times N)$ matrix invariant imbedding equation
satisfied by $r(L)$:
\[ \frac{dr}{dL} = i [r(L)\mathcal{E}(L)P + \mathcal{E}(L)Pr(L)] \]  
\[ - \frac{i}{2} [r(L) + I] [\mathcal{E}(L)P - PM(L) - q^2P^{-1}M(L) + q^2P^{-1}\mathcal{E}^{-1}(L)] [r(L) + I]. \]  
(9)
Similarly by setting $z = 0$ in eq. (7), we find the invariant imbedding equation for $t(L)$
($= \Psi(0, L)$):
\[ \frac{dt}{dL} = it(L)\mathcal{E}(L)P \]  
\[ - \frac{i}{2} t(L) [\mathcal{E}(L)P - PM(L) - q^2P^{-1}M(L) + q^2P^{-1}\mathcal{E}^{-1}(L)] [r(L) + I]. \]  
(10)
These invariant imbedding equations are supplemented with the initial conditions, $r(0) = 0$
and $t(0) = I$. For given values of $P$ and $q$ and for arbitrary matrix functions $\mathcal{E}(L)$ and $M(L)$,
we solve the coupled nonlinear ordinary differential equations (9) and (10) numerically using
the initial conditions, and obtain the reflection and transmission coefficient matrices $r$ and $t$
as functions of $L$. The invariant imbedding method can also be used in calculating the field
amplitude $\Psi(z)$ inside the inhomogeneous medium. Rewriting eq. (7), we get
\[ \frac{\partial \Psi(z, l)}{\partial l} = i \Psi(z, l)\mathcal{E}(l)P \]  
\[ - \frac{i}{2} \Psi(z, l) [\mathcal{E}(l)P - PM(l) - q^2P^{-1}M(l) + q^2P^{-1}\mathcal{E}^{-1}(l)] [r(l) + I]. \]  
(11)
For a given $z$ ($0 < z < L$), the field amplitude $\Psi(z, L)$ is obtained by integrating this equation
from $l = z$ to $l = L$ using the initial condition $\Psi(z, z) = I + r(z)$.
Application. – Eqs. (9), (10) and (11), which have never been derived before to the best of our knowledge, will be the starting point in our future analysis of a variety of wave coupling and mode conversion phenomena. In the rest of this Letter, we establish the validity and the utility of our invariant imbedding equations by applying them to the problem of the electromagnetic wave propagation in stratified chiral media.

Isotropic chiral media are those where the appropriate constitutive relations are given by

\[
D = \epsilon \mathbf{E} + i\gamma \mathbf{H}, \quad B = \mu \mathbf{H} - i\gamma \mathbf{E}.
\] (12)

The parameters \(\epsilon, \mu\) and \(\gamma\) are the dielectric permittivity, the magnetic permeability and the chiral index respectively [17–19]. Some researchers use alternative constitutive relations [20,21]

\[
D = \tilde{\epsilon} \mathbf{E} + i\xi \mathbf{B}, \quad H = B/\mu + i\xi \mathbf{E}.
\] (13)

The two relations give identical results if the parameters are identified by

\[
\tilde{\epsilon} = \epsilon - \gamma^2/\mu, \quad \xi = \gamma/\mu.
\] (14)

We will use eq. (12) from now on. In recent years, there have been a large number of theoretical [17, 19–24] and experimental [18, 25–28] studies on the wave propagation in various kinds of chiral media.

From the Maxwell’s equations and the constitutive relations, we are able to derive the wave equations satisfied by the electric field in inhomogeneous chiral media:

\[
\mu \nabla \times \left( \frac{1}{\mu} \nabla \times \mathbf{E} \right) = (\epsilon \mu - \gamma^2) \frac{\omega^2}{c^2} \mathbf{E} + \frac{\omega}{c} \left[ \gamma \nabla \times \mathbf{E} + \mu \nabla \times \left( \frac{\gamma}{\mu} \mathbf{E} \right) \right].
\] (15)

In the uniform case, right- and left-circularly-polarized waves are eigenmodes of this equation with the effective refractive indices \(\sqrt{\epsilon \mu + \gamma}\) and \(\sqrt{\epsilon \mu - \gamma}\) respectively. In inhomogeneous media, these two modes are no longer eigenmodes and are coupled to each other. The equation satisfied by the magnetic field \(\mathbf{H}\) is similar except that the roles of \(\epsilon\) and \(\mu\) are reversed. In media stratified in the \(z\) direction, \(\epsilon, \mu\) and \(\gamma\) are functions of \(z\) only. For plane waves propagating in the \(xz\)-plane, the \(x\) dependence of all field components is contained in the factor \(e^{iqx}\). In this situation, we can eliminate \(E_x, E_z, H_x\) and \(H_z\) from eq. (15) and obtain two coupled wave equations satisfied by \(E_y = E_y(z)\) and \(H_y = H_y(z)\), which turn out to have precisely the same form as eq. (1) with

\[
\psi = \begin{pmatrix} E_y \\ H_y \end{pmatrix}, \quad K = \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix}, \quad \mathcal{E} = \begin{pmatrix} \mu & i\gamma \\ -i\gamma & \epsilon \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} \epsilon & i\gamma \\ -i\gamma & \mu \end{pmatrix},
\] (16)

where \(k = \omega/c\).

We have used eqs. (12), (10) and (14) in calculating the reflection and transmission coefficients in various situations. In all cases where exact solutions by other methods are available, our theory gives the same results. In our notation, \(r_{11}(r_{21})\) is the reflection coefficient when the incident wave is \(s\)-polarized and the reflected wave is \(s(p)\)-polarized. Similarly, \(r_{22}(r_{12})\) is the reflection coefficient when the incident wave is \(p\)-polarized and the reflected wave is \(p(s)\)-polarized. Similar definitions are applied to the transmission coefficients. By a suitable linear combination of these coefficients, we are able to obtain a new set of the reflection and transmission coefficients \(r_{ij}\) and \(t_{ij}\), where \(i\) and \(j\) are either \(+\) or \(−\) [19]. For instance, \(r_{++}(r_{--})\) represents the reflection coefficient when the incident wave is right-circularly-polarized and the reflected wave is right(left)-circularly-polarized. The reflectances and transmittances are defined by \(R_{ij} = |r_{ij}|^2\) and \(T_{ij} = |t_{ij}|^2\).
As an example, we consider a uniform chiral layer of finite thickness with the parameters \( \epsilon, \mu \) and \( \gamma \), placed between uniform achiral media of infinite thicknesses. In this case, the electromagnetic wave equations can be solved analytically, following the methods used in elementary quantum mechanics. Lekner has presented an exact analytical solution of this problem \([19]\)\(^1\). In defining the reflection and transmission coefficients, \( r_{ss}, r_{sp}, r_{ps}, r_{pp} \), \( t_{ss}, t_{sp}, t_{ps} \) and \( t_{pp} \), Lekner uses different conventions from ours. In order to compare his solution with ours, we need to identify the expressions for the reflection and transmission coefficients satisfying our invariant imbedding equations exactly.

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In fig. 1 we plot the reflectances \( R_{++}, R_{--} \) and \( R_{+-} \) and the transmittances \( T_{++} \) and \( T_{--} \), when a wave is incident at \( \theta = 45^\circ \) on a one-dimensional photonic crystal made of alternating chiral and dielectric layers of the same thicknesses \( \Lambda / 2 \). It can be proved easily that \( R_{12} = R_{21} \) and \( R_{+-} = R_{-+} \). The chiral layer has the parameter values of \( \epsilon = 4, \mu = 1 \) and \( \gamma = 0.3 \) and the dielectric layer has \( \epsilon = 2, \mu = 1 \) and \( \gamma = 0 \). The total number of periods is 50. The \( x \) component of the wave vector, \( q \), is given by \( q = \omega \sin \theta / c \) and the \( z \) component of the vacuum wave vector matrix, \( P \), is given by \( P = pI \), where \( p = \omega \cos \theta / c \). Also plotted is the imaginary part of the Bloch wave number \( \kappa \) for an infinitely large photonic crystal. This quantity was obtained using an exact analytical expression for the dispersion relation of infinitely large photonic crystals made of two different kinds of alternating chiral layers, which we have derived recently \([29]\). The frequency region where the imaginary part of \( \kappa \) is nonzero corresponds to a photonic bandgap.

We find an excellent agreement between the analytical result on the dispersion relation and the reflectance and transmittance spectra. In general, there are three kinds of bandgaps, two of which are so-called co-polarization bandgaps and one of which is called a cross-polarization bandgap. Unlike in previous studies of this phenomenon \([23, 24]\), our theory is free of any approximation and provides exact band structures. For large values of \( \gamma \) and \( \theta \), these three bandgaps can be well-separated, as demonstrated in fig. 1 where we show the second group of bandgaps. The \( R_{+-} \) spectrum clearly displays a cross-polarization bandgap and the \( R_{++} \) and \( R_{--} \) spectra show co-polarization bandgaps. The transmittance spectra show that a right(left)-circularly-polarized wave, the frequency of which lies in the co-polarization bandgap of left(right)-circularly-polarized waves, is freely transmitted.

It is straightforward to apply our method to more general situations where the parameters \( \epsilon, \mu \) and \( \gamma \) are arbitrary functions of \( z \). For example, we can easily study the effects of defects and randomness on the wave propagation in chiral media using eqs. (9), (10), (11) and (16). Our equations can also be applied to the cases where both \( \epsilon \) and \( \mu \) take negative values with no modification. A detailed study of this so-called negative refractive index medium \([30]\), which is also chiral, is of great interest and will be presented elsewhere. We have also applied our method successfully to a number of other coupled wave problems, such as the phase-conjugate reflection of light from nonlinear phase-conjugating media, the light propagation in uniaxial and biaxial media and the mode conversion phenomena in both unmagnetized and magnetized plasmas \([31]\). In these studies, we solve the full wave equations exactly, without using common approximations such as the slowly varying envelope approximation and the WKB approximation. These results will be presented in a near future.

\(^1\)There are three typos in Lekner’s solution. In the expressions of \( G_1^+ \) and \( G_2^- \) in eq. (A2), \( c_1^2 + c_\epsilon c_- \) and \( c_2^2 + c_\epsilon c_- \) have to be replaced by \( c_1^2 - c_\epsilon c_- \) and \( c_2^2 - c_\epsilon c_- \) respectively. The expression \( Z_+ Z_-^2 \) appearing at the end of the equation for \( t_{ps} \) in eq. (A5) has to be replaced by \( Z_+^2 Z_- \).
Fig. 1 – (a) Imaginary part of the Bloch wave number $\kappa$ for an infinitely large photonic crystal made of alternating layers of chiral and dielectric materials of the same thicknesses $\Lambda/2$. The chiral layer has the parameter values of $\epsilon = 4$, $\mu = 1$ and $\gamma = 0.3$ and the dielectric layer has $\epsilon = 2$, $\mu = 1$ and $\gamma = 0$. The transverse component of the wave vector, $q$, is given by $q = \omega \sin \theta/c$, where $\theta = 45^\circ$. The $z$ component of the vacuum wave vector matrix, $P$, is given by $P = pI$, where $p = \omega \cos \theta/c$. The frequency region where $\text{Im} \kappa$ is nonzero corresponds to a bandgap. (b-f) Reflectance and transmittance spectra for a one-dimensional photonic crystal made of alternating layers of chiral and dielectric materials. The parameter values and the values of $\theta$, $p$ and $q$ are the same as in (a) and the number of periods is 50.
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