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Field representation inside arbitrary linear optical media by single surface currents

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Abstract

Recently a novel method has been proposed for the calculation of the scattering of an incoming electromagnetic wave by an arbitrarily shaped photonic crystal. The method rests on the representation of an arbitrary electromagnetic field inside a volume $V$ by a fictitious surface current distribution along the boundary of this volume which acts as a source for a point response tensor for the medium. The validity of such a representation is rigorously proven.

Keywords: Scattering; Maxwell theory; General field representation; Photonic crystals

1. Introduction

The appropriate analytical and numerical description of the scattering process of electromagnetic waves by photonic crystals is of great importance for our understanding of their behaviour and potential use. During the past decade, much theoretical effort in this field has been devoted to calculating photonic band structures and densities of states for ideal infinite crystals [1–10]. However, such calculations do not suffice to describe the optical response of real (finite) photonic materials, as they do not account for the scattering of the light at the crystal's surface. For instance, the proper reflection of light on a photonic crystal or a photonic coating on a waveguide clearly involve such a scattering phenomenon.

Existing methods that deal with this scattering problem, are e.g. the transfer-matrix method [11–13], the repeated-supercell method [14] and the generalised field-propagator method [15–18]. The transfer-matrix method assumes that the crystal can be built up from thin infinite layers whose scattering properties can be treated perturbatively (weak scattering). This leads to the calculation of a transfer matrix for each layer. Proper multiplication of the transfer matrices of all layers gives the transmission and reflection for a crystal slab. The repeated-supercell method applies the transfer concept for finite-size structures by artificially making them infinite by periodic repetition.
Finally, the generalised field-propagator method formulates the interaction problem in terms of the appropriate three-dimensional vector integral equations, which are then solved numerically. These numerical computations are very time-consuming as a result of the three-dimensional nature of the integral equations.

Recently we have proposed an alternative method to deal with the scattering of light on the boundary surface of photonic crystals, which takes full advantage of the existing infinite crystal bandstructure calculations [10]. This method was based on the property that any solution to Maxwell’s equations in an arbitrary linear medium may be considered as arising from one virtual current density distribution on the boundary surface of the medium. The main purpose of the present paper is to proof that such a representation actually exists; as far as we are aware, such a proof has not been given for an arbitrary linear medium.

The proposed representation by means of surface integrals (line integrals for two-dimensional crystals) is a non-trivial extension of a similar one valid for scattering by a perfect conductor, where the field is generated by a real surface current. Our representation clearly differs from the classical one, known as the equivalence principle [19,20], for two reasons. Classically, two virtual surface currents as well as two volume-current distributions are needed to represent the field, instead of only one surface current needed for our method. Moreover, our representation allows to represent the field either in terms of the Green’s tensor $\Gamma$ itself or, alternatively, in terms of $\nabla \times \Gamma$. We call this the equivalence of current- and dipole-layer representations, similarly to their electrostatically analogous [21,22].

The method put forward by us in [10] for scattering of light on three-dimensional (two-dimensional) systems, expresses the electromagnetic fields on either side of the boundary by means of surface integrals (line integrals). The integrands of these integrals are virtual surface-current density distributions times the appropriate point response (Green)tensor, generating the electromagnetic field. The continuity conditions of the electromagnetic field then lead to sets of linear equations for the virtual current densities on either side of the boundary with a two-dimensional (one-dimensional) nature. This is what makes our method numerically less time-consuming than the generalised field-propagator method.

We note that our method to describe scattering of light on an arbitrary linear medium may be considered related, to some extent, to the method of fictitious sources described by Boag et al. [23], by Zolla et al. [24] and Garcia de Abajo et al. [25]. Nevertheless, our method is essentially distinct from theirs, for various reasons. Firstly, they consider fictitious currents on the surface of every individual scatterer, which may consist of many separate scatterers arranged on a lattice, whereas we work with a virtual current distribution situated only on the boundary surface of the scattering medium (e.g. a photonic crystal). Secondly, in our method the scatterers do not need to be perfectly conducting, as assumed in [23]. Finally, the concept of Green’s functions in combination with the virtual surface currents is not an ingredient of the method employed in [23].

This paper is organised as follows: The proof of our key result, viz. the representation of an arbitrary electromagnetic field in terms of one surface current distribution is given in Section 2. The application of the proven representation to scattering problems (especially those for photonic crystals), is given in Section 3. Finally, in Section 4 we conclude.

2. The representation of the $H$ field by surface currents

In this section, we will present the proof of the representation of the electromagnetic field by a single current-density distribution at the surface of a medium. The proof is valid for fields in both two- and three-dimensional space. Our proof will be a generalisation of those given in [21,22] for scalar fields that obey the Laplace or Helmholtz equation, such that the theory becomes fully applicable to electromagnetic (vector) fields, satisfying Maxwell’s equations in an arbitrary dielectric medium with position dependent dielectric constant $\varepsilon(r)$. In such a medium of volume $V$ the magnetic field vector $\mathbf{H}(r)$ satisfies the vectorial wave equation:
∇′ × (η(r′)∇′ × H(r′)) = (ω/c)^2 H(r′)
(1)

and any point response dyadic Green function satisfies:

∇′ × (η(r′)∇′ × \vec{G}(r, r′))
= (ω/c)^2 \vec{G}(r, r′) + \vec{I} \delta(r - r′),
(2)

where η(r) = (ε(r))^{-1} and \vec{I} is the 3-dimensional unit tensor.

To be specific, our aim is to prove that electromagnetic fields inside the volume V, written in terms of their magnetic components H, can be expressed as an integral over the surface S of V of a dyadic Green’s function \vec{G}(r, r_0) times one effective surface current-density distribution J_{eff}(r_S):

\[ \vec{H}(r) = \int_S \vec{G}(r, r_s) \cdot J_{eff}(r_s) \, dr_s. \]
(3)

This will enable us to formulate the scattering problem in terms of one surface current-density distribution instead of two as would be needed when using the classical equivalence principle given in [19,20]. For the derivation of Eq. (3) we need the vector analogues of the two Green integral theorems. Using the vector identity \nabla \cdot (\vec{a} \times \vec{b}) = \vec{b} \cdot (\nabla \times \vec{a}) - \vec{a} \cdot (\nabla \times \vec{b}),
(4)

we can derive

\[ \int_V (\nabla′ × (η(r′)∇′ × \vec{G}(r, r′))) \cdot H(r′) \, dr′ = \int_V (η(r′)∇′ × \vec{G}(r, r′)) \cdot (∇′ × H(r′)) \, dr′ + \int_V (\nabla′ × (η(r′)∇′ × \vec{G}(r, r′)) \times H(r′)) \, dr′ \]
(5)

and

\[ \int_V \vec{G}(r, r′) \cdot (\nabla′ × (η(r′)∇′ × H(r′))) \, dr′ = \int_V (\nabla′ × \vec{H}(r′)) \cdot (\nabla′ × \vec{G}(r, r′)) \, dr′ - \int_V (\vec{G}(r, r′) ∙ (η(r′)∇′ × H(r′))) \, dr′ \]
(6)

Combining Eqs. (5) and (6) yields the vector form of Green’s second theorem:

\[ \int_V [(\nabla′ × (η(r′)∇′ × \vec{G}(r, r′))) \cdot H(r′) - \vec{G}(r, r′) \cdot (\nabla′ × (η(r′)∇′ × H(r′))) \, dr′ = \int_V \n′ \cdot [\vec{G}(r, r′) \cdot (\nabla′ × \vec{H}(r′))] \, dr′ + \vec{G}(r, r′) \cdot (\nabla′ × \vec{G}(r, r′)) \, dr′ \]
(7)

where, using Gauss’s theorem, the volume integral over a finite volume V is turned into a surface integral over a closed surface S, with the normal vector \n′ perpendicular to the surface and pointing outward. All position vectors with the subscript ‘S’, for example \vec{r}_S, refer to positions lying on the surface S. Position vectors with the superscript ‘+’ (‘−’), for example \vec{r}− (\vec{r}+) will be used to refer to position vectors inside (outside) the surface S.

Combination of Eqs. (1), (2) and (7) leads to

\[ \int_S \eta(\vec{r}_S)[(\nabla′ × \vec{G}(\vec{r}−, \vec{r}_S)) \cdot (\n′ × \vec{H}(\vec{r}_S−)) + \vec{G}(\vec{r}−, \vec{r}_S) \cdot (\n′ × (\nabla′ × \vec{H}(\vec{r}_S−)))] \, dr′ = -\vec{H}(\vec{r}−) \]
(8)

for \vec{r}− inside S and

\[ \int_S \eta(\vec{r}_S′)[(\nabla′ × \vec{G}(\vec{r}+, \vec{r}_S′)) \cdot (\n′ × \vec{H}(\vec{r}_S′−)) + \vec{G}(\vec{r}+, \vec{r}_S′) \cdot (\n′ × (\nabla′ × \vec{H}(\vec{r}_S−)))] \, dr′ = 0 \]
(9)

for \vec{r}+ outside S. Eqs. (8) and (9) are valid for any field H and dyadic Green’s function G that satisfy Eqs. (1) and (2). The representation (8) for the magnetic field inside S shows that this field is represented by a sheet of vector “dipoles” \n′ × \vec{G}(\vec{r}−, \vec{r}_S) with strength \n′ × \vec{H}(\vec{r}_S−) and a sheet of vector “charges” \vec{G}(\vec{r}−, \vec{r}_S′) with strength \n′ × (\nabla′ × \vec{H}(\vec{r}_S−))\vec{r}_S′. The terms ‘dipole’ and ‘charge’ originates from the analogy with the corresponding dipole- and charge-layer-induced fields arising in electrostatics, where a dipole dis-
tribution at the surface generates a field proportional to \( \mathbf{n} \cdot \nabla \mathbf{G} \) and a charge distribution at the surface generates a field proportional to \( \mathbf{G} \), where \( \mathbf{G} \) denotes any scalar Green function occurring in electrostatics. As our aim is to obtain a representation of the field in terms of a vector charge sheet distribution only (viz. Eq. (3)) we observe that we have obtained this goal if the dipole sheet distribution is transformed to a charge sheet distribution. To this end we define the function \( \mathbf{W} \), which is the “dipole sheet part” of Eq. (8):

\[
\mathbf{W}(\mathbf{r}) \equiv \int_S \eta(r'_S)(\nabla' \times \mathbf{G}(\mathbf{r}, \mathbf{r}'_S)) \cdot (\mathbf{n}' \times \mathbf{H}(\mathbf{r}'_S)) \, d\mathbf{r}'_S
\]

and prove the existence of a tangential current-density distribution function \( \mathbf{J}(\mathbf{r}_S) \) such that

\[
\mathbf{W}(\mathbf{r}^-) = \int_S \eta(r'_S)\mathbf{G}(\mathbf{r}^-, \mathbf{r}'_S) \cdot \mathbf{J}(\mathbf{r}'_S) \, d\mathbf{r}'_S \quad \text{for } \mathbf{r}^- \text{ inside } S.
\]

If Eq. (11) holds, it shows that every “dipole”-layer-induced field can also be represented by an equivalent “current”-layer-induced field, a result known in the literature of scalar fields as the equivalence of layers \([21,22]\).

For convenience we define

\[
\mathbf{V}(\mathbf{r}) \equiv \mathbf{W}(\mathbf{r}) - \mathbf{V}(\mathbf{r}) = \int_S \eta(r'_S)[(\nabla' \times \mathbf{G}(\mathbf{r}, \mathbf{r}'_S)) \cdot (\mathbf{n}' \times \mathbf{H}(\mathbf{r}'_S))]
\]

\[
- \mathbf{G}(\mathbf{r}, \mathbf{r}'_S) \cdot \mathbf{J}(\mathbf{r}'_S) \, d\mathbf{r}'_S.
\]

Eq. (13) shows that the transformation from a “dipole” layer to a “charge” layer distribution is accomplished once we have shown the existence of a tangential current-density distribution function \( \mathbf{J}(\mathbf{r}_S) \), such that \( \mathbf{X}(\mathbf{r}^-) = 0 \) for \( \mathbf{r}^- \) inside \( S \). Explicitly, if \( \mathbf{X}(\mathbf{r}^-) = 0 \), the representation Eq. (3) holds with \( \mathbf{J}(\mathbf{r}'_S) = \mathbf{J}(\mathbf{r}'_S) + \mathbf{n}' \times (\nabla' \times \mathbf{H}(\mathbf{r}'_S)) \).

For \( \mathbf{r}_S \) lying on the surface \( S \) and assuming that the normal derivative \( \mathbf{n} \times (\nabla \times \mathbf{W}(\mathbf{r}_S)) \) exists, we know that (see \([26]\) for the vectorial case and \([21,22]\) for the scalar case) there is a unique choice for the function \( \mathbf{J}(\mathbf{r}_S) \), such that

\[
\mathbf{n} \times (\nabla \times \mathbf{W}(\mathbf{r}_S)) = \mathbf{n} \times (\nabla \times \mathbf{W}(\mathbf{r}_S)).
\]

In other words, \( \mathbf{J}(\mathbf{r}_S) \) is fixed by imposing (14). The singular behaviour of the Green’s \(^1\) tensor \( \mathbf{G} \) is equal to the singular behaviour of the free-space Green’s tensor \( \mathbf{G} \), both inside and outside the surface \( S \). Let \( S_0 \subset S \) be a small area around the singularity of \( \mathbf{G}(\mathbf{r}, \mathbf{r}') \) at \( \mathbf{r}' = \mathbf{r} \). Then it follows from the standard theory of singular vector integral equations in \([27, pp. 243–244]\) that the normal derivative of \( \mathbf{V}(\mathbf{r}_S) \) possesses a discontinuity at the surface \( S \), whose size is equal to \( \mathbf{J}(\mathbf{r}_S) \):

\[
\mathbf{n} \times (\nabla \times (\mathbf{V}(\mathbf{r}_S))) = \mathbf{n} \times (\nabla \times \mathbf{W}(\mathbf{r}_S)) = \mathbf{n} \times (\nabla \times \mathbf{G}(\mathbf{r}^-, \mathbf{r}'_S))
\]

\[
- \mathbf{n} \times (\nabla \times \mathbf{G}(\mathbf{r}^+, \mathbf{r}'_S)) \cdot \mathbf{J}(\mathbf{r}'_S) \, d\mathbf{r}'_S = \mathbf{J}(\mathbf{r}_S).
\]

With this discontinuity of \( \mathbf{n} \times (\nabla \times \mathbf{V}(\mathbf{r}_S)) \), Eq. (14) now states that \( \mathbf{J}(\mathbf{r}_S) \) is fixed by imposing \( \mathbf{J}(\mathbf{r}_S) = \mathbf{n} \times (\nabla \times (\mathbf{W}(\mathbf{r}_S) - \mathbf{V}(\mathbf{r}_S))) \).

\[
= \mathbf{n} \times (\nabla \times (\mathbf{X}(\mathbf{r}_S))).
\]

From Eq. (13) it is verified immediately, that for both \( \mathbf{r}^+ \) outside \( S \) and \( \mathbf{r}^- \) inside \( S \), \( \mathbf{X}(\mathbf{r}^+) \) is a solution of the wave equation (1), with \( \mathbf{H} \equiv \mathbf{X} \). Therefore, we know that Eqs. (8) and (9), with \( \mathbf{H} \) replaced by \( \mathbf{X} \) and \( \mathbf{r}^+ \) interchanged by \( \mathbf{r}^- \), are valid:

\[
\int_S \eta(r'_S)[(\nabla' \times \mathbf{G}(\mathbf{r}^+, \mathbf{r}'_S)) \cdot (\mathbf{n}' \times \mathbf{X}(\mathbf{r}'_S))]
\]

\[
+ \mathbf{G}(\mathbf{r}^+, \mathbf{r}'_S) \cdot (\mathbf{n}' \times (\nabla' \times \mathbf{X}(\mathbf{r}'_S))) \, d\mathbf{r}'_S = -\mathbf{X}(\mathbf{r}^-)
\]

for \( \mathbf{r}^+ \) outside \( S \) and

\[
\int_S \eta(r'_S)[(\nabla' \times \mathbf{G}(\mathbf{r}^-, \mathbf{r}'_S)) \cdot (\mathbf{n}' \times \mathbf{X}(\mathbf{r}'_S))]
\]

\[
+ \mathbf{G}(\mathbf{r}^-, \mathbf{r}'_S) \cdot (\mathbf{n}' \times (\nabla' \times \mathbf{X}(\mathbf{r}'_S))) \, d\mathbf{r}'_S = 0
\]

\(^1\)This statement follows from the integral equation representation: \( \mathbf{G} = \mathbb{I} + \int \mathbb{I} \cdot (\mathbf{e} - 1) \mathbf{G} \) where \( \mathbb{I} \) denotes any free space Green tensor. As the second term involves integrations over \( \mathbb{I} \) only, the highest order singularity of \( \mathbf{G} \) is dictated by \( \mathbb{I} \).
for $r^-$ inside $S$. Adding Eqs. (13) and (17) gives

\[
\int_S \eta(r_S) \left[ (\nabla' \times \mathbf{G}(\mathbf{r}_S^+, \mathbf{r}_S^-)) \cdot (\mathbf{n} \times (\mathbf{X}(\mathbf{r}_S^+) + \mathbf{H}(\mathbf{r}_S^-))) \\
+ \mathbf{H}(\mathbf{r}_S^-) \right] \, d\mathbf{r}_S = 0
\]

(19)

for $r^+$ outside $S$.

Using the representation of $\mathbf{J}(\mathbf{r}_S)$ as in Eq. (16), Eq. (19) turns into

\[
\int_S \eta(r_S) (\nabla' \times \mathbf{G}(\mathbf{r}_S^+, \mathbf{r}_S^-)) \cdot (\mathbf{n} \times (\mathbf{X}(\mathbf{r}_S^+) - \mathbf{J}(\mathbf{r}_S^-))) \, d\mathbf{r}_S = 0
\]

(20)

for $r^+$ outside $S$. If the system is not at resonance, Eq. (20) can only be valid if

\[
\mathbf{n} \times \mathbf{X}(\mathbf{r}_S^-) = -\mathbf{n} \times \mathbf{H}(\mathbf{r}_S^-)
\]

(21)

for $\mathbf{r}_S$ lying on the surface $S$.

Substituting Eqs. (16) and (21) into (18), and using Eq. (13) we obtain:

\[
\mathbf{X}(\mathbf{r}^-) = 0
\]

(22)

for the unique choice of $\mathbf{J}(\mathbf{r}_S)$ imposed by Eq. (14). As argued below Eq. (13) this completes the proof of the representation Eq. (3).

3. The scattering problem for photonic crystals

We consider the scattering of monochromatic electromagnetic waves of frequency $\omega$ at the surface of a photonic crystal and use the above proven representation Eq. (3) for the fields. After having expressed the fields in terms of the virtual current densities at the surface, we solve the scattering problem by matching the fields across $S$, i.e. by imposing the continuity of the tangential components of the magnetic and the electric fields. This leads to a set of linear equations for the, hitherto unknown, current-density distributions. Solution of these equations suffices to obtain the fields everywhere. We note that for a $d$-dimensional photonic crystal, the equations for the surface-current densities have a dimensionality of only $d - 1$, which is an important computational advantage of our method.

Now we turn to the explicit formulation of the solution (cf. Fig. 1). First we would like to stress the point that the only requirement on the Green’s tensors involved is that they solve the field equations within the medium of interest (crystal or vacuum) for a point source, viz. Eq. (2). In particular, they do not need to satisfy any boundary conditions on the crystal surface, as these will be accounted for later in the calculation by fixing the virtual surface currents through the application of the continuity relations. For the example of light scattering on the interface between vacuum and a photonic crystal, we can take advantage of this freedom by using the dyadic Green’s tensors appropriate to infinite vacuum and to the infinite photonic crystal on the outside and inside of the crystal respectively. The latter can be expanded conveniently in terms of the solutions (the eigenfrequencies and eigenvectors) of the infinite-crystal photonic band-structure calculation.

On the vacuum side of the interface $S$, the magnetic field is expressed as

\[
\mathbf{H}_1(\mathbf{r}, t) = e^{i\omega t} \mathbf{H}_1(\mathbf{r})
\]

\[
= e^{i\omega t} \int_S \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}_S', \omega) \cdot \mathbf{J}_1(\mathbf{r}_S') \, d\mathbf{r}_S',
\]

(23)

where $\mathbf{J}_1$ is a virtual current-density distribution and $\mathbf{\Gamma}$ is the appropriate dyadic Green’s tensor needed for the description of electromagnetic fields in vacuum. In case we have an interface with a two-dimensional photonic crystal, the appropriate vacuum Green’s tensor reads:
\[ \tilde{G}(\mathbf{r}, \mathbf{r}', \omega) = \sum_n \frac{\mathbf{h}_n(\mathbf{r}; \mathbf{k}) \otimes \mathbf{h}_n(\mathbf{r}'; \mathbf{k})}{i\omega_n(\mathbf{k}) - \omega^2/c^2} \mathrm{d}\mathbf{k}, \]

where \( \mathbf{h}_n(\mathbf{r}; \mathbf{k}) \) are the Bloch modes, with dispersion relation \( \omega_n(\mathbf{k}) \), that follow from standard band structure calculations, and the integration runs over the first Brillouin zone.

We remind the reader that the current-density distributions \( \mathbf{J}_1 \) and \( \mathbf{J}_2 \) are unknown quantities initially. They can be solved from a set of coupled linear equations, which are obtained by imposing the continuity requirements on a discretized mesh across the interface \( S \).

One of the applications, for which we can use this method, is the calculation of the reflected far fields in the vacuum region from the current-density distribution \( \mathbf{J}_1 \), which actually involves the Fourier transformation of \( \mathbf{J}_1 \). Then we can plot an angular distribution of the intensity, i.e. the distribution of the energy flow over all outgoing directions, indicated by the angle \( \alpha \) with respect to the normal direction; \(-90^\circ < \alpha < 90^\circ\). For this angular distribution of the field intensity, we make use of the asymptotic behaviour of the Green’s tensor \( \Gamma \) at large distances from the crystal surface. Examples of such applications to two-dimensional photonic crystals have been presented in [10].

4. Discussion and conclusions

We have presented a method to calculate the scattering of light at the surface of a photonic crystal. The scattering problem is solved in terms of virtual surface-current distributions. These distributions generate together with any Green tensor valid for an arbitrary linear medium every electromagnetic field within this medium or in the outside free space using a free space Green tensor. The physical interpretation of this result is that a generalisation of Huygens principle for electromagnetic fields inside an arbitrary linear medium has been obtained: A superposition of Green tensor point response functions with appropriate strengths generate any electromagnetic field. This result is the generalisation of previously obtained results for the (scalar) case of the Helmholtz equation. In this case it was proven that any field inside a bounded domain always can be represented by a surface charge distribution. The use of surface currents reduces the dimensionality in the problem and thus also reduces the required computer time and memory. An important aspect of the method is that any Green tensor satisfying Eq. (2) is suitable for the field representation and that no a priori information concerning the shape of the boundary or boundary conditions has to be incorporated for the choice of the Green tensor to be used. Hence infinite-medium Green’s tensors can be used even if the scattering problem deals with finite-sized photonic crystals. We have given for the first time a detailed technical proof of the correctness of the concept of fictitious current distributions on which the method is based. We note that our method automatically accounts for
surface modes. These modes are localised near the surface of a photonic crystal due to exponential decay in both directions (into the crystal structure as well as into the vacuum). Our method does not require a special analysis of these modes, as given by Meade et al. [28] and by Robertson et al. [29].

First numerical results obtained by this method were given in a previous publication, [10], showing the feasibility of the method. Further results for transmission through photonic crystals slabs will be published elsewhere.

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