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Inward and outward integral equations and the KKR method for photons

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Abstract. In the case of electromagnetic waves it is necessary to distinguish between inward and outward on-shell integral equations. Both kinds of equation are derived. A correct implementation of the photonic KKR method then requires the inward equations and it follows directly from them. A derivation of the KKR method from variational principles is also outlined. Rather surprisingly, the variational KKR method cannot be entirely written in terms of surface integrals unless permeabilities are piecewise constant. Both kinds of photonic KKR method use the standard structure constants of the electronic KKR method and hence allow for a direct numerical application. As a by-product, matching rules are obtained for derivatives of fields on different sides of the discontinuity of permeabilities.

1. Introduction

This paper is the first in an intended series of papers devoted to problems of the photonic band gap and the propagation of electromagnetic waves in periodic dielectric structures. The question of the existence of a photonic band gap can be rephrased by asking whether it is possible to prepare a *perfect mirror from a transparent material* by drilling holes into it (in an appropriate way). The existence of a photonic band gap has been suggested theoretically [1] and has recently also been observed experimentally [2]. Nevertheless, there has been no calculations of band structure by more reliable methods, such as the KKR (Kohn–Korringa–Rostoker) or APW (augmented plane wave) methods. Even worse, a derivation of the photonic KKR method along the lines of [3] has not yet been given. Also, both theoretically and numerically, only a limited range of dielectric lattices has so far been considered: diamond-like, FCC and simple cubic lattices [4]. In all papers referred to, 'dielectric atoms' (a compact piece of dielectric in which (and only in which) permeabilities are allowed to differ from their host or average values) have been assumed to be spherically symmetric.

In attempting a calculation of the band structure of photons on various dielectric lattices with spherical atoms we have tried to generalize the scalar bulk KKR method [3] to a form appropriate for photons [5]. In the course of its derivation we have found that there persists some confusion in the photonic KKR method. This originates in the fact that, unlike the scalar case, in the case of photons fields can change *discontinuously* over *discontinuities* of electric and magnetic permeabilities. This is the essential difference between the Schrödinger and Maxwell equations. Consequently, derivatives of fields may be singular, and inward and

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outward limits of volume integrals over atoms may differ. Therefore, one has to carefully distinguish between 'inward' and 'outward' formulations, i.e. whether, in a given on-shell† surface integral, inward or outward limits of fields and their derivatives at the atom boundary are taken. In particular, we shall show that the photonic KKR method proposed in [6] does not serve the purpose. In [6], fields in integral equations are *outward* limits of fields with respect to the atom boundary, while the scalar product with *inward* limits of fields is taken.

These subtleties in the derivation of the photonic KKR method have stimulated us to write this paper. We hope that this derivation may be both instructive and interesting by itself. A more complete treatment of this subject, together with numerical results on the photonic band structure, will be given elsewhere [5].

2. Integral equations for electromagnetic potentials

2.1. Preliminaries

We shall first consider the *stationary macroscopic* Maxwell equations in a *non-conducting* medium with the current and charge densities equal to zero [7]. We shall only consider the simplest isotropic case, $\boldsymbol{D}(\boldsymbol{r}) = \epsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r})$ and $\boldsymbol{B}(\boldsymbol{r}) = \mu(\boldsymbol{r})\boldsymbol{H}(\boldsymbol{r})$ where $\boldsymbol{D}(\boldsymbol{r})$ ($\boldsymbol{B}(\boldsymbol{r})$) is the electric (magnetic) induction. We shall confine ourselves to monochromatic waves in order to avoid a non-local time relation between $\boldsymbol{D}(\boldsymbol{r})$ and $\boldsymbol{E}(\boldsymbol{r})$, or $\boldsymbol{B}(\boldsymbol{r})$ and $\boldsymbol{H}(\boldsymbol{r})$. We shall also allow for *complex* permeabilities, i.e. for absorption. In such a medium the Maxwell equations are symmetric under

$$\boldsymbol{E}(\boldsymbol{r}) \to \boldsymbol{H}(\boldsymbol{r}) \qquad \boldsymbol{H}(\boldsymbol{r}) \to -\boldsymbol{E}(\boldsymbol{r}) \qquad \epsilon(\boldsymbol{r}) \to \mu(\boldsymbol{r}). \tag{1}$$

They can be written as

$$\nabla \times \boldsymbol{H}(\boldsymbol{r}) + \mathrm{i}\frac{\omega}{c}\epsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) = 0 \tag{2}$$

$$\nabla \times \boldsymbol{E}(\boldsymbol{r}) - \mathrm{i}\frac{\omega}{c}\mu(\boldsymbol{r})\boldsymbol{H}(\boldsymbol{r}) = 0 \tag{3}$$

$$\nabla \cdot \boldsymbol{D}(\boldsymbol{r}) = \nabla \cdot \boldsymbol{B}(\boldsymbol{r}) = 0. \tag{4}$$

Now, by combining (2) and (3), one gets

$$\nabla \times [\nabla \times \boldsymbol{E}(\boldsymbol{r})] - (\omega/c)^2\epsilon(\boldsymbol{r})\mu(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) - \mu^{-1}(\boldsymbol{r})[\nabla\mu(\boldsymbol{r})] \times [\nabla \times \boldsymbol{E}(\boldsymbol{r})] = 0 \tag{5}$$

as well as

$$\nabla \times [\nabla \times \boldsymbol{H}(\boldsymbol{r})] - (\omega/c)^2\epsilon(\boldsymbol{r})\mu(\boldsymbol{r})\boldsymbol{H}(\boldsymbol{r}) - \epsilon^{-1}(\boldsymbol{r})[\nabla\epsilon(\boldsymbol{r})] \times [\nabla \times \boldsymbol{H}(\boldsymbol{r})] = 0. \tag{6}$$

Due to the symmetry (1) of the Maxwell equations, frequently only a single equation will be written from a conjugate pair. If $\mu(\boldsymbol{r})$ is set to be a constant, $\mu(\boldsymbol{r}) = \mu_0$, and one parametrizes $\mu_0\epsilon(\boldsymbol{r})$ into its constant uniform value $\mu_0\epsilon_0$ and a spatially varying part

† This notation is adopted from field theory. On-shell means that, starting from a given expression, the field or wavefunction are supposed to satisfy basic equations of motion, and this property is used at intermediate steps in the derivation of a resulting expression. For a free particle it means simply that the particle is on its mass-shell. On the other hand, off-shell assumes that a given expression can be derived without any additional recourse to basic equations of motion.

$v(r) = \mu_0[\epsilon(r) - \epsilon_0]$, one finds a striking resemblance between (5) and the Schrödinger equation, with $v(r)$ playing the role of a potential. Theoretically, this analogy serves as the main motivation for the search of a photonic band gap.

We shall see that to solve the Maxwell equations, even in the case when the potentials $\epsilon(r)$ and $\mu(r)$ can be written as a sum of functions of a single coordinate, is a *non-trivial* task because they *do not separate*. The reason is that any solution of, say, (5) has to satisfy the initial conditions (4) for the Maxwell equations in a dielectric. Provided that $\epsilon(r)$ is a non-trivial function of all coordinates then (4) mixes all components of $\boldsymbol{E}(r)$ together:

$$\nabla \cdot \boldsymbol{E}(r) = -\frac{1}{\epsilon(r)}[\nabla \epsilon(r) \cdot \boldsymbol{E}(r)]. \tag{7}$$

Similarly for $\boldsymbol{H}(r)$ in the case of non-trivial $\mu(r)$.

We shall now turn to the derivation of integral equations for electromagnetic fields. We shall consider either a finite or infinite region Ω with given boundary conditions imposed and with one dielectric atom V_s inside it. The generalization to several atoms is trivial. Since the group of lattice translations is Abelian, the Bloch theorem extends straightforwardly to vector wavefunctions. Hence, by setting Ω to be a primitive cell and with generalized periodic boundary conditions imposed, one can directly turn on to the study of electromagnetic wave propagation in dielectric lattices.

2.2. *'Outward' integral equations*

The first attempt to derive integral equations for electromagnetic fields in a dielectric in connection with the photonic KKR method is discussed in [6]. The derivation is basically due to Morse [3] and starts as follows. Provided r is restricted to the *interstitial* region, $r \in \Omega \backslash V_s$, the electric (magnetic) field $\boldsymbol{E}(r)$ ($\boldsymbol{B}(r)$) satisfies the equation

$$(\nabla^2 + \sigma^2)\boldsymbol{E}(r) = 0 \tag{8}$$

where $\sigma^2 = \omega^2 \epsilon_0 \mu_0$. Let $G_\sigma(r, r')$ be the Green function of the Helmholtz equation in Ω with suitable boundary conditions imposed, defined by

$$(\nabla^2 + \sigma^2)G_\sigma(r, r') = \delta(r - r'). \tag{9}$$

By using the defining equation (9) for $G_\sigma(r, r')$ one is tempted to write the following on-shell integral equation in the interstitial region:

$$\boldsymbol{E}(r) = \int_{\Omega \backslash V_s} \delta(r - r')\boldsymbol{E}(r')\,\mathrm{d}^3 r' = \int_{\Omega \backslash V_s} [\boldsymbol{E}(r')\nabla'^2 G_\sigma(r, r') - G_\sigma(r, r')\nabla'^2 \boldsymbol{E}(r')]\,\mathrm{d}^3 r' \tag{10}$$

which can be obviously rewritten as the surface integral

$$\boldsymbol{E}(r) = \oint_{\partial(\Omega \backslash V_s)} [\boldsymbol{E}(r')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')G_\sigma(r, r') - G_\sigma(r, r')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')\boldsymbol{E}(r')]. \tag{11}$$

Now, assuming Ω to be a primitive cell, then due to the periodicity of $G_\sigma(r, r')\,\boldsymbol{E}(r')$, the integral over the *cell* boundary vanishes and one is left with the surface integral over ∂V_s. The same equation also holds for $\boldsymbol{B}(r)$. Thus, formally, both $\boldsymbol{B}(r)$ and $\boldsymbol{E}(r)$ satisfy

the same integral equation (11) outside a dielectric atom V_s. What makes the difference between them are the matching conditions across a boundary of the atom.

However, there is one subtle point here. In (11) an *outward* limit of the electric field $\boldsymbol{E}(\boldsymbol{r})$ and its derivatives is taken. On the other hand, the KKR method requires knowledge of either interior or exterior solutions. However, the exterior problem is much more involved and *cannot* be solved usually. Only the *interior* solution can (sometimes) be obtained in an explicit form, supposing that there are some symmetries of the problem (such as spherical symmetry, for example). Therefore, despite the fact that in the surface integral (11) the *outward* limit of the electric field $\boldsymbol{E}(\boldsymbol{r})$ and its derivatives is taken, usually only the *inward* limit of the field and its derivatives is at our disposal. Now, our main task is to find integral equations for electromagnetic fields in Ω in terms of the *inward limit* of fields and their derivatives at the boundary of V_s. Provided that $\epsilon(\boldsymbol{r})$ is *discontinuous*, the discontinuity of the normal component $\boldsymbol{E}(\boldsymbol{r})$ at the atom boundary is

$$\boldsymbol{n} \cdot [\boldsymbol{E}_+(\boldsymbol{r}) - \boldsymbol{E}_-(\boldsymbol{r})] = \frac{v(\boldsymbol{r})}{\epsilon_0} \boldsymbol{E}_-(\boldsymbol{r}) \tag{12}$$

where $\boldsymbol{n}$ is the unit normal vector at the discontinuity. Thus, (5) and (6) inevitably contain *singular* terms. This makes a relation between inward and outward equations non-trivial. It is this point that was not taken into account in [6].

It what follows it will be assumed that on discontinuities of $\epsilon(\boldsymbol{r})$ the side limits of $\epsilon(\boldsymbol{r})$ and its derivatives are well defined. The same will be assumed for the limiting values of fields and their derivatives.

2.3. 'Inward' integral equations

In trying to find the '*inward*' integral equations one can try to establish a direct relation between fields and their derivatives on both sides of the atom boundary and rewrite (11) in terms of inward limits. It can be shown that like-side limits of $\epsilon(\boldsymbol{r})$ determine the relation of the side limits of $\boldsymbol{E}(\boldsymbol{r})$ (12), the side limits of *derivatives* of $\epsilon(\boldsymbol{r})$ do so for the side limits of derivatives of $\boldsymbol{E}(\boldsymbol{r})$ (see appendix 1). Before proceeding this way, the 'inward' integral equations will be derived by introducing electromagnetic potentials. This way seems to be easier and safer in treating the singularities that appear.

If the additive material relations are used

$$\boldsymbol{D}(\boldsymbol{r}) = \epsilon_0 \boldsymbol{E}(\boldsymbol{r}) + 4\pi \boldsymbol{P}(\boldsymbol{r}) \qquad \boldsymbol{B}(\boldsymbol{r}) = \boldsymbol{H}(\boldsymbol{r}) + 4\pi \boldsymbol{M}(\boldsymbol{r}) \tag{13}$$

the Maxwell equations take on the following form

$$\nabla \times \boldsymbol{B} + \mathrm{i}\omega\epsilon_0 \boldsymbol{E} = 4\pi \tilde{\boldsymbol{j}} \tag{14}$$

$$\nabla \times \boldsymbol{E} - \mathrm{i}\omega \boldsymbol{B} = 0 \tag{15}$$

$$\nabla \cdot \boldsymbol{E} = 4\pi\tilde{\rho} \tag{16}$$

$$\nabla \cdot \boldsymbol{B} = 0. \tag{17}$$

The current and charge density are defined by the relations

$$\tilde{\boldsymbol{j}} = -\mathrm{i}\omega \boldsymbol{P} + c\nabla \times \boldsymbol{M}(\boldsymbol{r}) \tag{18}$$

$$\tilde{\rho} = -\nabla \cdot \boldsymbol{P} \tag{19}$$

where $\boldsymbol{P}(\boldsymbol{r})$ ($\boldsymbol{M}(\boldsymbol{r})$) is the *electric (magnetic) polarization*:

$$\boldsymbol{P}(\boldsymbol{r}) = \frac{v(\boldsymbol{r})}{4\pi}\boldsymbol{E}(\boldsymbol{r}) \qquad \boldsymbol{M}(\boldsymbol{r}) = \frac{\mu(\boldsymbol{r})-1}{4\pi}\boldsymbol{H}(\boldsymbol{r}). \tag{20}$$

The equations (14)–(17) are formally identical to the equations for the electromagnetic field in a vacuum. By introducing a vector potential $\boldsymbol{A}(\boldsymbol{r})$ and a scalar potential $\phi(\boldsymbol{r})$ such that

$$\boldsymbol{B}(\boldsymbol{r}) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r}) \tag{21}$$

$$\boldsymbol{E}(\boldsymbol{r}) = \mathrm{i}\omega\boldsymbol{A}(\boldsymbol{r}) - \boldsymbol{\nabla}\phi(\boldsymbol{r}) \tag{22}$$

with the Lorentz gauge condition imposed

$$\boldsymbol{\nabla} \cdot \boldsymbol{A}(\boldsymbol{r}) = \mathrm{i}\omega\epsilon_0\phi(\boldsymbol{r}) \tag{23}$$

equations for $\boldsymbol{A}(\boldsymbol{r})$ and $\phi(\boldsymbol{r})$ can be *decoupled* [7].

In order to simplify our discussion the dielectric medium will be assumed to be *magnetically isotropic* and from now on we shall set $\mu(\boldsymbol{r}) = 1$ as well as $c = 1$. For the potentials one gets

$$\boldsymbol{\nabla}^2\boldsymbol{A}(\boldsymbol{r}) + \sigma^2\boldsymbol{A}(\boldsymbol{r}) = \mathrm{i}\omega v(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) \tag{24}$$

$$\boldsymbol{\nabla}^2\phi(\boldsymbol{r}) + \sigma^2\phi(\boldsymbol{r}) = -\boldsymbol{\nabla} \cdot \boldsymbol{E}(\boldsymbol{r}). \tag{25}$$

The integral equations for $\boldsymbol{A}(\boldsymbol{r})$ and $\phi(\boldsymbol{r})$ are

$$\boldsymbol{A}(\boldsymbol{r}) = \mathrm{i}\omega \int_{V_s} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')v(\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' \tag{26}$$

$$\phi(\boldsymbol{r}) = -\int_{V_s} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')[\boldsymbol{\nabla}' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'. \tag{27}$$

As we have mentioned above, due to the presence of a singular shell at the boundary of V_s the volume integrals over V_s have to be defined carefully as an *outward limit* through measurable sets Σ_n, $\Omega \supset \Sigma_n \supset V_s$, $\lim_{n\to\infty} \Sigma_n \searrow V_s$. The Gauss theorem requires the integrand to be at least a continuous function. Provided that a discontinuity appears in some region Σ to which it is going to be applied one proceeds as follows. The region Σ is split (if possible) into non-overlapping subregions Σ_j, $\Sigma = \cup_j \Sigma_j$, such that in any Σ_j the hypotheses of the Gauss theorem are satisfied. Then, the Gauss theorem is applied to each Σ_j separately. As mentioned above, inward and outward limits of volume integrals with a singular integrand at the boundary will differ in general. The first example provides (27). By using

$$\boldsymbol{\nabla} \cdot [v(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r})] = -\epsilon_0\boldsymbol{\nabla} \cdot \boldsymbol{E}(\boldsymbol{r}) \tag{28}$$

one finds

$$\begin{aligned}\phi(\boldsymbol{r}) &:= -\int_{V_{s+}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')[\boldsymbol{\nabla}' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}' \\ &= -\int_{V_{s-}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')[\boldsymbol{\nabla}' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}' - \frac{1}{\epsilon_0}\oint_{\partial V_{s-}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')v(\boldsymbol{r}')(\boldsymbol{E}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{S}')\end{aligned} \tag{29}$$

where V_{s+} (V_{s-}) means that the outward (inward) limit is taken. Here, the surface integral exactly corresponds to a delta function singularity which appears due to the discontinuity (12) of the normal component of $\boldsymbol{E}(\boldsymbol{r})$. Now, it is transparent that, provided the inward limit in (27) is taken, the resulting integral expressions (26) and (27) for the electromagnetic potentials do not satisfy the Lorentz condition (23).

The off-shell integral equation for $\boldsymbol{E}(\boldsymbol{r})$ can be directly written by using the defining relations (22), (26) and (27):

$$\boldsymbol{E}(\boldsymbol{r}) = -\omega^2 \int_{V_s} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')v(\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' - \int_{V_{s+}} [\nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}')][\nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'. \tag{30}$$

To find an on-shell integral equation for $\boldsymbol{E}(\boldsymbol{r})$ we shall make repeated use of (5) together with the identity (28) and with (9) satisfied by $G_\sigma(\boldsymbol{r}, \boldsymbol{r}')$. For a given region Σ, $\Sigma \subset V_s$, one finds in the limit $\Sigma \nearrow V_s$

$$\begin{aligned}\omega^2 \int_\Sigma G_\sigma(\boldsymbol{r}, \boldsymbol{r}')v(\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' \to & \\ - \oint_{\partial V_{s-}} \left[G_\sigma(\boldsymbol{r}, \boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')\boldsymbol{E}(\boldsymbol{r}') - \boldsymbol{E}(\boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\right] & \\ - \int_{V_s} \delta(\boldsymbol{r} - \boldsymbol{r}')\,\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' + \int_{V_{s-}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\nabla'[\nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'. & \end{aligned} \tag{31}$$

Here, the LHS of (31) is well defined as a both-side limit. Now, (30) can be rewritten on-shell as follows:

$$\begin{aligned}\boldsymbol{E}(\boldsymbol{r}) = \chi_{V_s}(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) + \oint_{\partial V_{s-}} \left[G_\sigma(\boldsymbol{r}, \boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')\boldsymbol{E}(\boldsymbol{r}') - \boldsymbol{E}(\boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\right] & \\ - \frac{1}{\epsilon_0} \oint_{\partial V_{s-}} [\nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}')]v(\boldsymbol{r}')(\boldsymbol{E}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{S}') - \oint_{\partial V_{s-}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')[\nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\,\mathrm{d}\boldsymbol{S}' & \end{aligned} \tag{32}$$

with $\chi_{V_s}(\boldsymbol{r})$ the characteristic function of V_s.

As for $\boldsymbol{B}(\boldsymbol{r})$, equations (21) and (26) together with (2) imply that

$$\boldsymbol{B}(\boldsymbol{r}) = \int_{V_{s+}} \frac{v(\boldsymbol{r}')}{\epsilon(\boldsymbol{r}')}[\nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}')] \times [\nabla' \times \boldsymbol{B}(\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'. \tag{33}$$

By repeated use of the Gauss theorem one finds the desired on-shell result:

$$\begin{aligned}\boldsymbol{B}(\boldsymbol{r}) = \chi_{V_s}(\boldsymbol{r})\boldsymbol{B}(\boldsymbol{r}) + \oint_{\partial V_{s-}} \frac{v(\boldsymbol{r}')}{\epsilon(\boldsymbol{r}')} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\,\mathrm{d}\boldsymbol{S}' \times [\nabla \times \boldsymbol{B}(\boldsymbol{r}')] & \\ + \oint_{\partial V_{s-}} \left[G_\sigma(\boldsymbol{r}, \boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')\boldsymbol{B}(\boldsymbol{r}') - \boldsymbol{B}(\boldsymbol{r}')(\mathrm{d}\boldsymbol{S}' \cdot \nabla')G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\right]. & \end{aligned} \tag{34}$$

We shall now compare outward (11) and inward (32), (34) integral equations. For simplicity, we shall confine ourselves to (32).

2.4. Relation between 'out' and 'in' formulations

Here, we would like to derive (32) from (11) (or vice versa) by a direct calculation of the relation between $\boldsymbol{E}(r)$ and its normal derivative on different sides of Σ (see appendix 1 for details). For simplicity, we shall confine ourselves to such Σ for which $(\partial_n \epsilon)_+ = (\partial_n \epsilon)_- = 0$. Then the last surface integral in (32) vanishes.

As can be found in any textbook, (3) or (4) imply the continuity of the normal component $D_n(r)$ of $\boldsymbol{D}(r)$ (i.e. a discontinuity of $E_n(r)$) or the tangential component $E_t(r)$ of $\boldsymbol{E}(r)$ on Σ, respectively:

$$E_n^+ - E_n^- = \frac{\epsilon_- - \epsilon_+}{\epsilon_+} E_n^- = \frac{v(r)}{\epsilon_0} E_n^- \qquad E_t^+ = E_t^-. \tag{35}$$

On the other hand, the normal derivative $\partial_n \boldsymbol{E}_t(r)$ of the tangential component of $\boldsymbol{E}(r)$ changes discontinuously across Σ:

$$\partial_n \boldsymbol{E}_t^+ - \partial_n \boldsymbol{E}_t^- = \left(\frac{1}{\epsilon_+} - \frac{1}{\epsilon_-}\right) \nabla_t D_n = \frac{v}{\epsilon_0} \nabla_t E_n^-. \tag{36}$$

Rather surprisingly, although the normal component $E_n(r)$ is discontinuous:

$$\partial_n E_n^+ = \partial_n E_n^-. \tag{37}$$

Now, by using (35) one can check directly the equivalence of (11) and (32) for normal components. As for the tangential components, one uses, assuming ∂V_s to have no boundary, that

$$-\frac{1}{\epsilon_0} \oint_{\partial V_{s-}} [\nabla' G_\sigma(r, r')] v(r') (\boldsymbol{E}(r') \cdot \mathrm{d}\boldsymbol{S}') = \frac{1}{\epsilon_0} \oint_{\partial V_{s-}} \mathrm{d}\boldsymbol{S}' \, G_\sigma(r, r') \nabla' [v(r') E_n(r')] \tag{38}$$

and

$$\nabla_t [v(r) E_n(r)] = v(r) \nabla_t E_n(r). \tag{39}$$

The use of (36) and (37) then gives the desired equivalence of (11) and (32), as expected.

3. Photonic KKR method

The KKR method is basically the method of rewriting *integral* equations like (32) and (34) into *algebraic* ones by using an appropriate basis (a basis of spherical harmonics in our case). In the case of electrons it is known to lead to a very compact scheme if the perturbing periodic potential $v(r)$ is *spherically symmetric* within inscribed spheres, and zero (constant) elsewhere [3]. The band structure of the problem is then determined by purely *geometrical structure constants*, characteristic of the type of lattice under consideration, and by *phase shifts* (logarithmic derivatives, at the surface of the inscribed sphere, of the s, p, d ... radial solutions of the corresponding radial equation), characteristic of the *scattering properties* of a given dielectric sphere.

In the case of photons the KKR method has been used only within the scalar approximation to the Maxwell equations [8]. Recently, a version of the KKR method has been given in the framework of *multiple-scattering theory* [9]. However, we have obtained

a different result [10]. Nevertheless, a derivation of the photonic KKR method in the spirit of [3] is still lacking.

Let us consider a dielectric lattice and look for Bloch wave-type solutions. In this case $G_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ possesses the standard expansion in terms of the eigenfunctions of the homogeneous boundary value problem

$$G_\sigma(\boldsymbol{r}, \boldsymbol{r}') = -\frac{1}{\tau} \sum_{\mathrm{n}} \frac{\exp[\mathrm{i}(\boldsymbol{K}_\mathrm{n} + \boldsymbol{k}) \cdot (\boldsymbol{r} - \boldsymbol{r}')]}{(\boldsymbol{K}_\mathrm{n} + \boldsymbol{k})^2 - \sigma^2} \tag{40}$$

where τ is the volume of the primitive cell Ω, $\boldsymbol{k}$ is the Bloch momentum, and the summation runs over all vectors $\boldsymbol{K}_\mathrm{n}$ of a reciprocal lattice.

To derive the photonic KKR method we shall turn back to either (32) or (34). There is one subtlety therein with the characteristic function $\chi_{V_\mathrm{s}}(\boldsymbol{r})$, as well as in (11). Depending on the order of the limits taken, $\chi(\boldsymbol{r})$ may be either one or zero for $\boldsymbol{r} \in \partial V_\mathrm{s}$. In order that $\chi(\boldsymbol{r})$ be zero for $\boldsymbol{r} \in \partial V_\mathrm{s}$, one takes as the first limit $\lim_{\boldsymbol{r} \to \partial V_\mathrm{s}}$, and then $\lim_{\Sigma \to V_\mathrm{s}-}$ in (32). In this case (32) and (34) give an integral equation for $\boldsymbol{E}(\boldsymbol{r})$ and $\boldsymbol{B}(\boldsymbol{r})$, respectively. For a dielectric lattice of *spherical* atoms with radius r_s it means that the expansion of $G_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ in spherical harmonics $Y_{lm}(\theta, \phi)$ with $r_\mathrm{s} > r > r'$ is used:

$$G_\sigma(\boldsymbol{r}, \boldsymbol{r}') = \sum_{lm} \sum_{l'm'} [A_{lm;l'm'}\, j_l(\sigma r')\, j_{l'}(\sigma r) + \sigma \delta_{ll'} \delta_{mm'} n_l(\sigma r)\, j_l(\sigma r')] \times Y_{lm}(\theta', \phi')\, Y^*_{l'm'}(\theta, \phi) \tag{41}$$

where $j_l(x)$ is the *spherical Bessel function* defined by

$$j_l(x) = \left(\frac{\pi}{2x}\right) J_{l+1/2}(x) \tag{42}$$

with $n_l(x) := (\pi/2x)^{1/2} J_{-l-1/2}(x)$, and θ, ϕ and θ', ϕ' are polar angles of $\boldsymbol{r}$ and $\boldsymbol{r}'$, relative to some fixed system of coordinates. This expansion follows by expanding the exponentials in (40) for $G_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ [3, 11]. The 'structure constants' $A_{lm;l'm'}$, $A_{l'm';lm} = A_{lm;l'm'}{}^*$, which are functions of σ and $\boldsymbol{k}$, are characteristic for the lattice under consideration. They are *exactly the same* as for the case of electrons, i.e. as in the case of the Schrödinger equation.

For $r < r_\mathrm{s}$ the true solution of our problem, for frequency ω, can be expanded in vectorial spherical harmonics [11]

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(\frac{\mathrm{i}}{\omega\epsilon} C^\mathrm{E}_{lm} \nabla \times [R^\mathrm{E}_l(r)\, \boldsymbol{X}_{lm}(\theta, \phi)] + C^\mathrm{M}_{lm}\, R^\mathrm{M}_l(r)\, \boldsymbol{X}_{lm}(\theta, \phi) \right) \tag{43}$$

where the coefficients C^E_{lm} and C^M_{lm} specify the amounts of *electric* (l, m) and *magnetic* (l, m) *multipole fields*. $R^\mathrm{A}_l(r)$, A = E, M, satisfies the corresponding radial part of equation (5) or (6) [5], with the boundary conditions

$$R^\mathrm{A}_l(0) = \text{finite} \qquad R^\mathrm{A}_l(r_\mathrm{s}) = 1. \tag{44}$$

R^M_l and R^E_l differ in general if $\epsilon(r) \neq$ constant. Now one takes scalar products of electric and magnetic multipoles with both sides of (32) and obtains a matrix equation. The condition of solvability, i.e. the vanishing of a corresponding determinant, then determines dispersion relation and eventually photonic bands.

On the other hand, the traditional variational derivation of the KKR method from a variational principle [3] uses the order of the limits which makes $\chi_{V_\mathrm{s}}(\boldsymbol{r})$ *zero* for $\boldsymbol{r} \in \partial V_\mathrm{s}$ (see (45) below).

3.1. Variational principle for the Maxwell equations

Let us formulate a general variational principle for the Maxwell equations which holds for an *arbitrary shape* of the basic 'atom' of a dielectric lattice. Taking into account the off-shell integral equation (30) for $\boldsymbol{E}(\boldsymbol{r})$ the off-shell photonic analogue of the scalar KKR functional is defined to be

$$\Lambda = \omega^2 \int_{V_s} \mathrm{d}^3 r\, v(\boldsymbol{r})\, \boldsymbol{E}^*(\boldsymbol{r}) \cdot \Big(\boldsymbol{E}(\boldsymbol{r}) + \omega^2 \int_{V_s} G_\sigma(\boldsymbol{r}, \boldsymbol{r}') v(\boldsymbol{r}') \boldsymbol{E}(\boldsymbol{r}')\, \mathrm{d}^3 r' + \int_{V_{s+}} \nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}') [\nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\, \mathrm{d}^3 r' \Big). \tag{45}$$

Here, the integral over r is well defined and exists as a *both-side* limit. Provided $\epsilon(\boldsymbol{r})$ is *real* (no absorption), and using the well known Hermitian properties of Green functions, $\partial_r G_\sigma(\boldsymbol{r}, \boldsymbol{r}') = -\partial_{r'} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ and $G^*_\sigma(\boldsymbol{r}, \boldsymbol{r}') = G_\sigma(\boldsymbol{r}', \boldsymbol{r})$, one can check that variations of Λ with respect to $\boldsymbol{E}(\boldsymbol{r})$ or $\boldsymbol{E}^*(\boldsymbol{r})$ reproduce correctly the equation for the electric field $\boldsymbol{E}(\boldsymbol{r})$ (30) or its complex conjugate $\boldsymbol{E}^*(\boldsymbol{r})$ within V_s, respectively. To deal properly with the singularities of G we must use a limiting procedure in evaluating Λ. In analogy with [3] we set

$$\Lambda := \lim_{\epsilon \to 0} \Lambda_\epsilon \tag{46}$$

where schematically

$$\Lambda_\epsilon := \omega^2 \int_{V_{s-2\epsilon}} \mathrm{d}^3 r\, v(\boldsymbol{r})\, \boldsymbol{E}^*(\boldsymbol{r}) \cdot \Big(\boldsymbol{E}(\boldsymbol{r}) + \omega^2 \int_{V_{s-\epsilon}} G_\sigma(\boldsymbol{r}, \boldsymbol{r}')\, v(\boldsymbol{r}')\, \boldsymbol{E}(\boldsymbol{r}')\, \mathrm{d}^3 r' + \int_{V_{s-\epsilon}} \nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}') [\nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\, \mathrm{d}^3 r' + \frac{1}{\epsilon_0} \oint_{\partial V_{s-\epsilon}} [\nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}')] v(\boldsymbol{r}') (\boldsymbol{E}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{S}') \Big). \tag{47}$$

Here, $V_{s-\epsilon}$ ($\partial V_{s-\epsilon}$) denotes the volume (boundary) of an atom up to a shell of a width of ϵ, one side of which is the boundary of the atom and another is formed by the boundary shifted by ϵ in the direction of the inward normal. Similarly for $V_{s-2\epsilon}$ and $\partial V_{s-2\epsilon}$.

Supposing that a complete set of interior solutions of (5) is known, it is more convenient to find the on-shell KKR functional. By using on-shell formulae (31) and (32) one finds the following on-shell form of the variational KKR functional:

$$\Lambda := \lim_{\epsilon \to 0} \Big(\oint_{\partial V_{s-2\epsilon}} \{ [(\mathrm{d}\boldsymbol{S} \cdot \nabla) \boldsymbol{E}^*(\boldsymbol{r})] - \boldsymbol{E}^*(\boldsymbol{r}) (\mathrm{d}\boldsymbol{S} \cdot \nabla) \} - \int_{V_{s-2\epsilon}} \nabla [\nabla \cdot \boldsymbol{E}^*(\boldsymbol{r})]\, \mathrm{d}^3 r \Big) \cdot \Big(\oint_{\partial V_{s-\epsilon}} [(\mathrm{d}\boldsymbol{S}' \cdot \nabla') \boldsymbol{E}(\boldsymbol{r}') - \boldsymbol{E}(\boldsymbol{r}') (\mathrm{d}\boldsymbol{S}' \cdot \nabla')] G_\sigma(\boldsymbol{r}, \boldsymbol{r}') - \frac{1}{\epsilon_0} \oint_{\partial V_{s-\epsilon}} [\nabla' G_\sigma(\boldsymbol{r}, \boldsymbol{r}')] v(\boldsymbol{r}') (\boldsymbol{E}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{S}') - \oint_{\partial V_{s-\epsilon}} [G_\sigma(\boldsymbol{r}, \boldsymbol{r}') \nabla' \cdot \boldsymbol{E}(\boldsymbol{r}')]\, \mathrm{d}\boldsymbol{S}' \Big). \tag{48}$$

Note that unless $\epsilon(\boldsymbol{r})$ is piecewise constant, i.e. the classical *muffin-tin potential*, it is *impossible* (at least for our variational principle) to write (45) on-shell in terms of surface

integrals only. Thus, when working with the variational KKR functional it is necessary to confine ourselves to the case when $\epsilon(r)$ is a *real muffin-tin potential*. Then the dielectric potential $v(r) = v$ can be moved in front of the integration sign, the terms which contain $\nabla \cdot \boldsymbol{E}(r)$ *vanish*, and (5) simplifies within V_s to

$$(\nabla^2 + \rho^2)\boldsymbol{E}(r) = 0 \tag{49}$$

where $\rho = \omega\sqrt{\epsilon}$.

In the case of spherically symmetric dielectric atoms, the general formula (48) can be simplified further:

$$\Lambda := \lim_{\epsilon \to 0} \oint_{r=r_s-2\epsilon} \mathrm{d}S \left[\partial_r \boldsymbol{E}^*(r) - \boldsymbol{E}^*(r)\partial_r\right] \cdot \left(\oint_{r'=r_s-\epsilon} \mathrm{d}S' \left[\partial_{r'} \boldsymbol{E}(r') - \boldsymbol{E}(r')\,\partial_{r'}\right] G_\sigma(r, r') \right.$$
$$\left. - \frac{1}{\epsilon_0} \oint_{r'=r_s-\epsilon} [\nabla' G_\sigma(r, r')] v(r') (\boldsymbol{E}(r') \cdot \mathrm{d}\boldsymbol{S}') \right). \tag{50}$$

The final expression (50) resembles the scalar case [3], the only difference being the last term.

From now on, a further treatment along the lines in [3] is straightforward, albeit more involved. The true solution of our problem, for frequency ω and for $r < r_s$, is approximated by finite sums of the form (43) with $R_l^{\mathrm{A}}(r)$ now being $R_l^{\mathrm{A}}(r) = a_l\, j_l(\rho r)$, a_l being a normalization constant (see for example [11]). Then, as in the previous case, bands are obtained from the condition of solvability which requires that the determinant of Λ be zero.

4. Conclusions

We have presented and discussed the relationship between the outward and inward integral equations for electromagnetic waves and we have outlined a derivation of the KKR method. For a correct implementation of the photonic KKR method in the spirit of [3], inward on-shell integral equations for electromagnetic fields are necessary. The photonic KKR method then follows from them either directly or through a variational principle. The 'direct' photonic KKR method has a wider region of applications: complex and non-constant $\epsilon(r)$ within atoms. Rather surprisingly, we have found that the variational KKR method has a rather limited range of applications. Unless $\epsilon(r)$ is piecewise constant the variational KKR method *cannot* be written in terms of surface integrals. Also, for complex $\epsilon(r)$, the variational KKR method cannot be used. However, being variational, it is expected to converge more rapidly within its range of application. Both of the photonic KKR methods presented make full use of the same structure constants as the electronic KKR method. We hope soon to report on numerical results [5].

In our formulation of the photonic KKR method singularities due to discontinuities of permeabilities are *safely* treated. Our results also imply that the photonic KKR method as proposed in [6] can be only used if, at the atom boundary, permeabilities are *continuous* and in addition side limits of their derivatives are identically zero. One's first thought might be to define the atom boundary to comprise discontinuities of permeabilities such that the photonic KKR method of [6] can be used. However, afterwards, singularities of delta function are moved into coefficients of corresponding radial equations.

Multiple-scattering theory for photons, which uses essentially outward integral equations, is presented in [10].

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Appendix 1. Derivatives of $E(r)$ on different sides of a normal discontinuity

Let Σ be some surface discontinuity of $\epsilon(r)$ and $\mu(r) = 1$ in Ω. We shall assume that near Σ only the normal derivative of $\epsilon(r)$ may be non-zero. In what follows, such a discontinuity will be called *normal*. In order to determine the discontinuity of $\partial_n E_t(r)$ we shall look carefully at the tangential components of (5)

$$\nabla^2 E_t(r) - \partial_n \epsilon(r)^{-1} \nabla_t D_n(r) + \omega^2 \epsilon(r) E_t(r) = 0 \tag{A1}$$

where we have used $\nabla \cdot E(r) = D(r) \cdot \nabla \epsilon(r)$. The most singular terms are given by the normal derivatives of $\epsilon(r)$. Obviously

$$\nabla \frac{1}{\epsilon(r)}\bigg|_\Sigma = \left(\frac{1}{\epsilon_+} - \frac{1}{\epsilon_-}\right)\delta(r - \Sigma)n. \tag{A2}$$

The requirement of cancellation of singular terms gives $\partial_n E_t(r) = \epsilon^{-1}(r)\nabla_t D_n(r)$, i.e.

$$(\partial_n E_t^+ - \partial_n E_t^-)\big|_\Sigma = \left(\frac{1}{\epsilon_+} - \frac{1}{\epsilon_-}\right)\nabla_t D_n = \frac{v}{\epsilon_0}\nabla_t E_n^-. \tag{A3}$$

Since $\nabla_t D_n(r)$ is continuous (see below) one also finds $\partial_n E_t^- = \nabla_t E_n^-$.

On the other hand, to determine the relation between normal derivatives of the normal component of $E(r)$ on different sides of the discontinuity, $E(r)$ is replaced by $(D(r)/\epsilon(r))$ in (5). After some manipulations one finds (for the normal component)

$$\nabla^2 D_n + \epsilon(r)\left(\partial_n \frac{1}{\epsilon(r)}\partial_n\right) D_n + \omega^2 \epsilon(r) D_n = 0. \tag{A4}$$

Note that terms proportional $\nabla^2(1/\epsilon(r))$ have cancelled. Now, the requirement of the cancellation of remaining singular terms in (A4) gives conditions on $\partial_n D_n(r)$ and $\nabla_t D_n(r)$. $\nabla_t D_n(r)$ changes continuously across Σ while $\partial_n D_n(r)$ has to be discontinuous. The discontinuity is such that $\partial_n D_n(r)/\epsilon(r)$ change continuously, i.e.

$$\frac{\partial_n D_n^+}{\epsilon_+} = \frac{\partial_n D_n^-}{\epsilon_-}. \tag{A5}$$

This in turn implies that

$$(\partial_n E_n^+ - \partial_n E_n^-)\big|_\Sigma = -\left(\frac{1}{\epsilon_+^2}(\partial_n \epsilon)_+ - \frac{1}{\epsilon_-^2}(\partial_n \epsilon)_-\right) D_n. \tag{A6}$$

Thus, although the normal component $E_n(r)$ of $E(r)$ is discontinuous, the side limits of $\partial_n E_n(r)$ *coincide* provided the side limits of the derivatives of $\epsilon(r)$ at Σ are zero.

Note that the above relations are a general consequence of the (non-stationary) Maxwell equations in a dielectric.

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