# Boundary conditions for interfaces of electromagnetic crystals and the generalized Ewald-Oseen extinction principle

Pavel A. Belov
*Queen Mary College, University of London, Mile End Road, London E1 4NS, United Kingdom*
*and Photonics and Optoinformatics Department, St. Petersburg State University of Information Technologies, Mechanics and Optics, Sablinskaya 14, 197101 St. Petersburg, Russia*

Constantin R. Simovski
*Photonics and Optoinformatics Department, St. Petersburg State University of Information Technologies, Mechanics and Optics, Sablinskaya 14, 197101 St. Petersburg, Russia*

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The problem of plane-wave diffraction on semi-infinite orthorhombic electromagnetic (photonic) crystals of a general kind is considered. Boundary conditions are obtained in the form of infinite system of equations relating amplitudes of incident wave, eigenmodes excited in the crystal, and scattered spatial harmonics. The generalized Ewald-Oseen extinction principle is formulated on the base of deduced boundary conditions. The knowledge of properties of infinite crystal's eigenmodes provides an option to solve the diffraction problem for the corresponding semi-infinite crystal numerically. In the case when the crystal is formed by small inclusions which can be treated as point dipolar scatterers with fixed direction the problem admits complete rigorous analytical solution. The amplitudes of excited modes and scattered spatial harmonics are expressed in terms of the wave vectors of the infinite crystal by closed-form analytical formulas. The result is applied for the study of reflection properties of metamaterial formed by cubic lattice of split-ring resonators.

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## I. INTRODUCTION

Electromagnetic crystals are artificial periodical structures operating at the wavelengths comparable with their periods.[1–3] At the optical frequencies such structures are called photonic crystals. The inherent feature of these materials is the existence of frequency bands where the crystal does not support propagating waves. The band gaps are caused by spatial resonances of the crystal lattice and strongly depend on the direction of propagation. It means that electromagnetic crystals are media with spatial dispersion.[4–6] The material parameters; permittivity and permeability for such materials, if they can be introduced at all, depend on the wave vector as well as on the frequency. Notice that the homogenization approach is not the most convenient way for the description of electromagnetic crystals even at low frequencies. It often requires the introduction of additional boundary conditions in order to describe boundary problems correctly, and this involves related complexities. The photonic and electromagnetic crystals are usually studied with the help of numerical methods.[1–3] Analytical models exist only for a very narrow class of the crystals. Some types of the crystals can be studied analytically under a certain approximation, but the strict analytical solution for a photonic crystal is an exception.

The goal of the present paper is to demonstrate how boundary problems for electromagnetic crystals can be effectively studied using analytical methods. The paper is separated into two parts. In the first part the boundary conditions for electromagnetic crystals of a general kind are deduced in the form of an infinite system of equations relating amplitudes of the incident wave, excited eigenmodes of the crystal, and scattered spatial harmonics. This system can be interpreted as a generalization of the well-known Ewald-Oseen extinction principle (Refs. 7–9) which states that the polarization of the dielectric is distributed so that it cancels out the incident wave and produces the propagating wave. For the electromagnetic crystals, inherently periodic structures, the generalized Ewald-Oseen principle states that the polarization of the dielectric is distributed so that it cancels out the incident wave as well as all spatial harmonics associated with periodicity of the boundary. This principle expressed in the form of the infinite system of boundary conditions provides an opportunity to solve the boundary problem for semi-infinite crystal of a certain kind numerically if the eigenmode problem for corresponding infinite crystal is already solved. In the second part of the paper the proposed approach is applied for the case of electromagnetic crystals formed by

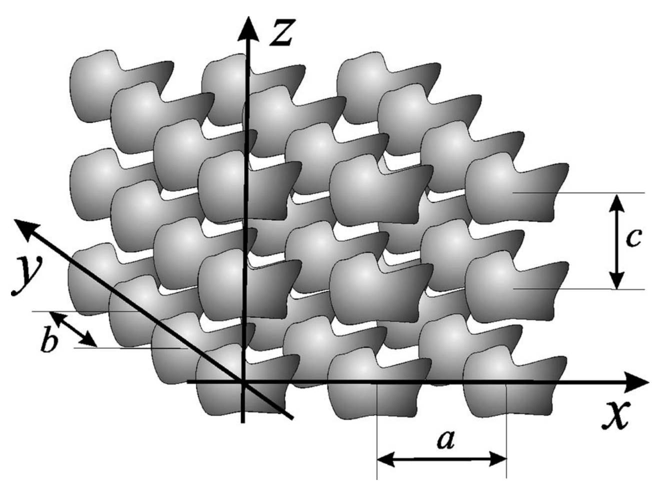


FIG. 1. Geometry of an infinite electromagnetic crystal.

 

small inclusions which can be treated as point dipolar scatterers with fixed direction. In this case the system of boundary conditions admits a complete rigorous analytical solution. The amplitudes of excited eigenmodes and scattered spatial harmonics are expressed in terms of wave vectors of eigenmodes using closed-form analytical formulas. These results are unique extension and generalization of the known Mahan-Obermair theory (Ref. 10) for the case when the period of the crystal is compared with the wavelength. At the end of the paper it is demonstrated how reflection from the semi-infinite cubic lattice of resonant scatterers (split-ring resonators) can be modeled in the regime of strong spatial dispersion observed in such crystals.[11]

## II. PROOF OF THE GENERALIZED EWALD-OSEEN EXTINCTION PRINCIPLE

In this section we provide proof of the generalized Ewald-Oseen extinction principle for an arbitrary semi-infinite electromagnetic crystal with an orthorhombic elementary cell. First, let us consider an infinite orthorhombic electromagnetic crystal with geometry schematically presented in Fig. 1 and characterized by three-periodical permittivity distribution:

$$\bar{\bar{\varepsilon}}(\mathbf{r}) = \bar{\bar{\varepsilon}}(\mathbf{r} + \mathbf{a}n + \mathbf{b}s + \mathbf{c}l). \tag{1}$$

In this expression and following in the text the two lines over a quantity designate that the quantity is dyadic (tensor of second rank in a three-dimensional space). It means that we consider the most general kind of electromagnetic crystals formed by dielectrics.

In this paper we are using a local field approach, an unconventional method for description of fields inside dielectrics. We will operate with local parameters like polarization density $\mathbf{P}$ and local electrical field $\mathbf{E}_{\rm loc}$, but not with average electric field $\mathbf{E}$ and displacement $\mathbf{D}$ as usual. The similar approach was used in Ref. 9 for rigorous derivation of the Ewald-Oseen extinction theorem and in Ref. 6. The dielectric can be treated as a very dense cubic lattice of point scatterers with ceratin local polarizability. In this formulation the dielectric permittivity $\bar{\bar{\varepsilon}}(\mathbf{r})$ has to be replaced (see Fig. 2 for an illustration) by the local polarizability $\bar{\bar{\alpha}}(\mathbf{r})$ relating the bulk polarization density $\mathbf{P}(\mathbf{r})$ to the local electric field $\mathbf{E}_{\rm loc}(\mathbf{r})$,

$$\mathbf{P}(\mathbf{r}) = \bar{\bar{\alpha}}(\mathbf{r})\mathbf{E}_{\rm loc}(\mathbf{r}). \tag{2}$$

The expression for local polarizability in terms of dielectric permittivity has the following form:

$$\bar{\bar{\alpha}}^{-1}(\mathbf{r}) = [\bar{\bar{\varepsilon}}(\mathbf{r}) - \varepsilon_0\bar{\bar{I}}]^{-1} + \bar{\bar{I}}/(3\varepsilon_0), \tag{3}$$

where $\varepsilon_0$ is the permittivity of free space and $\bar{\bar{I}}$ is unit dyadic. This expression follows from the Lorentz-Lorenz formula (Ref. 9)

$$\mathbf{E}_{\rm loc}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) + \mathbf{P}(\mathbf{r})/(3\varepsilon_0) \tag{4}$$

and material equation

$$\mathbf{D}(\mathbf{r}) = \varepsilon_0\mathbf{E}(\mathbf{r}) + \mathbf{P}(\mathbf{r}) = \bar{\bar{\varepsilon}}(\mathbf{r})\mathbf{E}(\mathbf{r}). \tag{5}$$

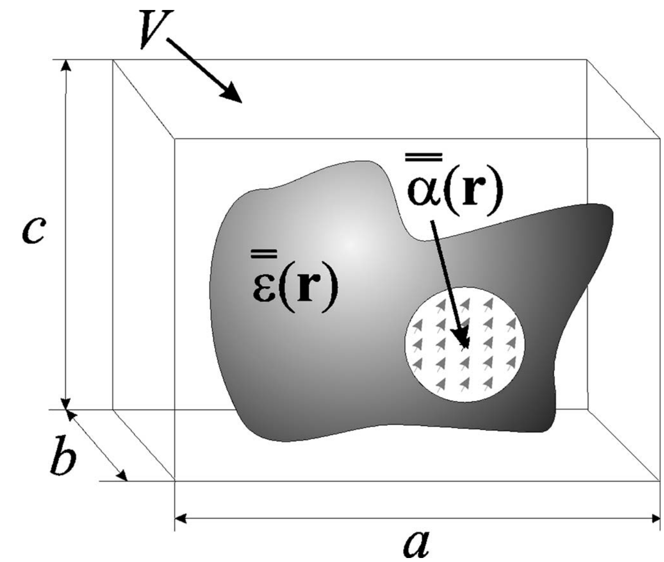


FIG. 2. Illustration for the replacement of the dielectric permittivity by the local polarizability.

### A. Dispersion equation

Following the local field approach one can write down the dispersion equation for the crystal under consideration in the next integral form

$$\mathbf{P}(\mathbf{r}) = \bar{\bar{\alpha}}(\mathbf{r})\int_V' \bar{\bar{G}}_3(\mathbf{r}-\mathbf{r}',\mathbf{q})\mathbf{P}(\mathbf{r}')d\mathbf{r}', \quad \forall\, \mathbf{r} \in V, \tag{6}$$

where $V=V(\mathbf{a},\mathbf{b},\mathbf{c})$ is the volume of the elementary lattice cell, $\bar{\bar{G}}_3(\mathbf{r},\mathbf{q})$ is the lattice dyadic Green's function,

$$\bar{\bar{G}}_3(\mathbf{r},\mathbf{q}) = \sum_{n,s,l} \bar{\bar{G}}(\mathbf{r}-\mathbf{a}n-\mathbf{b}s-\mathbf{c}l)e^{-j(q_x an+q_y bs+q_z cl)}, \tag{7}$$

which takes into account the cell-to-cell polarization distribution determined by wave vector $\mathbf{q}=(q_x,q_y,q_z)^T$,

$$\mathbf{P}(\mathbf{r}+\mathbf{a}n+\mathbf{b}s+\mathbf{c}l) = \mathbf{P}(\mathbf{r})e^{-j(q_x an+q_y bs+q_z cl)}, \tag{8}$$

$\bar{\bar{G}}(\mathbf{r})$ is dyadic Green's function of free space,

$$\bar{\bar{G}}(\mathbf{r}) = (k^2\bar{\bar{I}} + \nabla\nabla)\frac{e^{-jkr}}{4\pi\varepsilon_0 r}, \tag{9}$$

$n,s,l$ are integer indices, and $k$ is the wave number of free space. The integral in (6) is singular if the point corresponding to vector $\mathbf{r}$ is located inside of some polarized dielectric. It has to be evaluated in the meaning of the principal value by excluding a small spherical region around the singular point and tending the radius of this region to zero.[12]

The dispersion equation (6) relates the distribution of polarization density $\mathbf{P}(\mathbf{r})$ and wave vector $\mathbf{q}$ corresponding to the eigenmodes of the electromagnetic crystal. If the distribution of the average electric field $\mathbf{E}(\mathbf{r})$ of a crystal eigenmode is known then the polarization density $\mathbf{P}(\mathbf{r})$ can be found directly using material equation (5),

$$\mathbf{P}(\mathbf{r}) = [\bar{\bar{\varepsilon}}(\mathbf{r}) - \varepsilon_0]\mathbf{E}(\mathbf{r}). \tag{10}$$

The reverse operation is possible only for space regions filled by dielectric with $\bar{\bar{\varepsilon}}(\mathbf{r}) \neq \varepsilon_0$. The distribution of the electric field in free space regions, if required, has to be calculated using the next integral representation

$$\mathbf{E}(\mathbf{r}) = \int_V \bar{\bar{G}}_3(\mathbf{r}-\mathbf{r}',\mathbf{q})\mathbf{P}(\mathbf{r}')d\mathbf{r}'. \tag{11}$$

For our proof of the generalized Ewald-Oseen extinction principle we have to transform dispersion equation (6) into the form corresponding to summation by layers in the $x$ direction. The expression for the lattice dyadic Green's function $\bar{\bar{G}}_3(\mathbf{r},\mathbf{q})$ (7) can be rewritten using a summation over planes in the form

$$\bar{\bar{G}}_3(\mathbf{r},\mathbf{q}) = \sum_{n=-\infty}^{+\infty} \bar{\bar{G}}_2(\mathbf{r}-\mathbf{a}n)e^{-jq_x an}, \tag{12}$$

where $\bar{\bar{G}}_2(\mathbf{r})$ is the grid dyadic Green's function

$$\bar{\bar{G}}_2(\mathbf{r}) = \sum_{s,l} \bar{\bar{G}}(\mathbf{r}-\mathbf{b}s-\mathbf{c}l)e^{-j(q_y bs+q_z cl)}. \tag{13}$$

Applying Poisson summation formula by both indices $s$ and $l$ one can express the grid dyadic Green's function in terms of the spatial Floquet harmonics. This expansion is also called a spectral representation

$$\bar{\bar{G}}_2(\mathbf{r}) = \sum_{s,l} \bar{\bar{\gamma}}_{s,l}^{\mathrm{sgn}(x-a)} e^{-j(\mathbf{k}_{s,l}^{\mathrm{sgn}(x)}\cdot\mathbf{r})}, \tag{14}$$

where

$$\bar{\bar{\gamma}}_{s,l}^{\pm} = \frac{j}{2bc\varepsilon_0 k_{s,l}}[\mathbf{k}_{s,l}^{\pm}\times[\mathbf{k}_{s,l}^{\pm}\times\bar{\bar{I}}]], \quad \mathbf{k}_{s,l}^{\pm} = (\pm k_{s,l}^x, k_s^y, k_l^z)^T,$$

$$k_s^y = q_y + \frac{2\pi s}{b}, \quad k_l^z = q_z + \frac{2\pi l}{c}, \quad k_{s,l}^x = \sqrt{k^2-(k_s^y)^2-(k_l^z)^2}.$$

The square root in the expression for $k_{s,l}$ should be chosen so that $\mathrm{Im}(\sqrt{\cdot})<0$. The sign $\pm$ corresponds to half spaces $x>a$ and $x<a$, respectively.

Using (12) the dispersion equation (6) can be rewritten in the following form which will be used later on:

$$\mathbf{P}(\mathbf{r}) = \bar{\bar{\alpha}}(\mathbf{r}) \sum_{n=-\infty}^{+\infty} \int_V \bar{\bar{G}}_2(\mathbf{r}-\mathbf{r}'-\mathbf{a}n)\mathbf{P}(\mathbf{r}')e^{-jq_x an}d\mathbf{r}'. \tag{15}$$

### B. Semi-infinite crystal

Now let us consider a semi-infinite crystal (half space $x \geqslant a$, see Fig. 3) excited by a plane electromagnetic wave with wave vector $\mathbf{k}=(k_x,k_y,k_z)^T$ coming from free space

$$\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) = \mathbf{E}_{\mathrm{inc}}e^{-j(\mathbf{k}\cdot\mathbf{r})}. \tag{16}$$

The origin of our coordinate system is intentionally shifted by one period into the free space since it simplifies rather cumbersome calculations which are presented below and causes exponential convergence of the series in the final expressions.

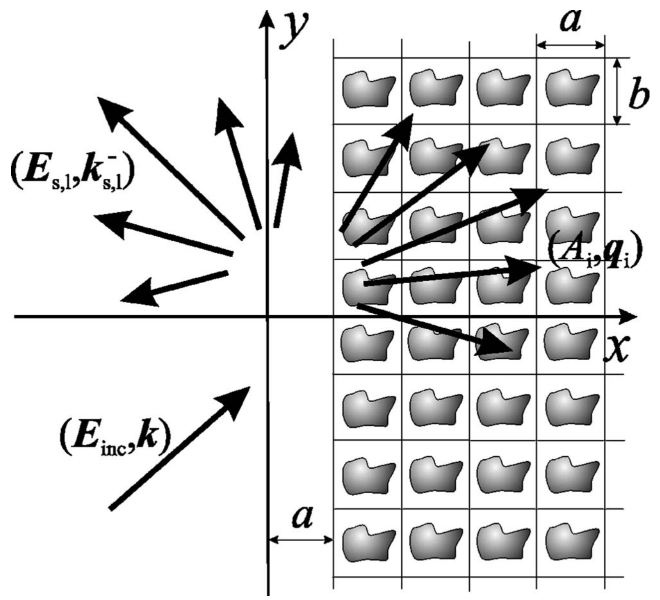


FIG. 3. Geometry of an semi-infinite electromagnetic crystal.

Due to the periodicity of the semi-infinite structure along $y$ and $z$ axes the distribution of the excited polarization along these directions is determined by the phase of the incident wave

$$\mathbf{P}(\mathbf{r}+\mathbf{a}m+\mathbf{b}s+\mathbf{c}l) = \mathbf{P}(\mathbf{r}+\mathbf{a}m)e^{-j(k_y bn+k_z cl)}, \tag{17}$$

for any $\mathbf{r}\in V$ and $m \geqslant 1$.

The electric field produced by the polarized semi-infinite crystal has the form

$$\mathbf{E}_{\mathrm{scat}}(\mathbf{r}) = \sum_{n=1}^{+\infty} \int_V \bar{\bar{G}}_2(\mathbf{r}-\mathbf{r}'-\mathbf{a}n)\mathbf{P}(\mathbf{r}'+\mathbf{a}n)d\mathbf{r}'. \tag{18}$$

The total local electric field is the sum of incident and scattered (produced by polarization of crystal) fields. Following the local field approach we can write

$$\mathbf{P}(\mathbf{r}) = \bar{\bar{\alpha}}(\mathbf{r})[\mathbf{E}_{\mathrm{inc}}(\mathbf{r})+\mathbf{E}_{\mathrm{scat}}(\mathbf{r})]. \tag{19}$$

Combining (18) and (19) we obtain an integral equation for the polarization in the semi-infinite crystal excited by an incident wave

$$\mathbf{P}(\mathbf{r}) = \bar{\bar{\alpha}}(\mathbf{r})\left[\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) + \sum_{n=1}^{+\infty}\int_V \bar{\bar{G}}_2(\mathbf{r}-\mathbf{r}'-\mathbf{a}n)\mathbf{P}(\mathbf{r}'+\mathbf{a}n)d\mathbf{r}'\right]. \tag{20}$$

Now let us suppose that the dispersion equation (6) is solved under the condition that a wave vector has the form $\mathbf{q}=(q_x,k_y,k_z)^T$ with unknown $x$ component $q_x$, and the set of eigenmodes $\{(\mathbf{P}_i(\mathbf{r}),q_x^{(i)})\}$, characterized by the $x$ component of wave vector $q_x^{(i)}$ and polarization distribution $\mathbf{P}_i(\mathbf{r})$, is found. In addition, we include in this set only the eigenmodes which either transfer energy into the half-space $x\geqslant a$ $[dq_x^{(i)}/d\omega>0]$ or decay in the $x$ direction $[\mathrm{Im}(q_x^{(i)})<0]$. In such a case the polarization of the semi-infinite crystal excited by the incident wave (16) can be expanded by the eigenmodes of the infinite crystal as follows:

$$\mathbf{P}(\mathbf{r}+\mathbf{a}m)=\sum_i A_i\mathbf{P}_i(\mathbf{r})e^{-jq_x^{(i)}am},\quad \forall\,\mathbf{r}\in V, m\geqslant 1. \tag{21}$$

Substituting (21) into (20) and using (16) we obtain

$$\sum_i A_i\mathbf{P}_i(\mathbf{r})e^{-jq_x^{(i)}am}=\bar{\bar{\alpha}}(\mathbf{r})\left[\mathbf{E}_{\mathrm{inc}}e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)}+\sum_{n=1}^{+\infty}\sum_i A_i\int_V \bar{\bar{G}}_2[\mathbf{r}-\mathbf{r}'-\mathbf{a}(n-m)]\mathbf{P}_i(\mathbf{r}')e^{-jq_x^{(i)}an}d\mathbf{r}'\right]. \tag{22}$$

Splitting the series in the dispersion equation (15) one can derive the following auxiliary relation:

$$\mathbf{P}_i(\mathbf{r})e^{-jq_x^{(i)}am}=\bar{\bar{\alpha}}(\mathbf{r})\sum_{n=1}^{+\infty}\int_V \bar{\bar{G}}_2[\mathbf{r}-\mathbf{r}'-\mathbf{a}(n-m)]\mathbf{P}_i(\mathbf{r}')e^{-jq_x^{(i)}an}d\mathbf{r}'+\bar{\bar{\alpha}}(\mathbf{r})\sum_{n=-\infty}^{0}\int_V \bar{\bar{G}}_2[\mathbf{r}-\mathbf{r}'-\mathbf{a}(n-m)]\mathbf{P}_i(\mathbf{r}')e^{-jq_x^{(i)}an}d\mathbf{r}'. \tag{23}$$

Substituting (23) into (22) and following the fact that $\det\{\bar{\bar{\alpha}}(\mathbf{r})\}\neq 0$ we obtain

$$\sum_i A_i\sum_{n=-\infty}^{0}\int_V \bar{\bar{G}}_2[\mathbf{r}-\mathbf{r}'-\mathbf{a}(n-m)]\mathbf{P}_i(\mathbf{r}')e^{-jq_x^{(i)}an}d\mathbf{r}' =\mathbf{E}_{\mathrm{inc}}e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)}. \tag{24}$$

Further, substituting (14) into (24), changing the summation order, and evaluating the sum of the geometrical progression by index $n$, we get

$$\sum_{s,l}\left(\sum_i A_i\frac{\bar{\bar{\gamma}}_{s,l}^{+}\int_V \mathbf{P}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{+}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}-k_{s,l}^{x})a}}\right)e^{-j[\mathbf{k}_{s,l}^{+}\cdot(\mathbf{r}+\mathbf{a}m)]} =\mathbf{E}_{\mathrm{inc}}e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)}. \tag{25}$$

### C. The generalized Ewald-Oseen extinction principle

The left part of Eq. (25) represents an expansion of the right part into a spatial spectrum of Floquet harmonics. The right part represents an incident spectrum of Floquet harmonics containing only the single incident plane wave (16) with $\mathbf{k}=\mathbf{k}_{0,0}^{+}$. Equating coefficients in the left and right parts of (25) we obtain

$$\bar{\bar{\gamma}}_{s,l}^{+}\sum_i A_i\frac{\int_V \mathbf{P}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{+}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}-k_{s,l}^{x})a}}=\begin{cases}\mathbf{E}_{\mathrm{inc}}, & (s,l)=(0,0),\\ 0, & (s,l)\neq(0,0).\end{cases} \tag{26}$$

The values in the right side of (26) are the amplitudes of the incident spatial harmonics (all harmonics except fundamental one have zero amplitudes), and the series in the left side are the amplitudes of the spatial harmonics produced by the whole semi-infinite crystal polarization in order to cancel these incident harmonics. It means that Eq. (26) represents the generalization of Ewald-Oseen extinction principle [see Refs. 7–9 for classical formulation in the case of dielectrics]: the polarization in a semi-infinite electromagnetic crystal excited by a plane wave is distributed in such a way that it cancels the incident wave together with all high-order spatial harmonics associated with periodicity of the boundary (even if they have zero amplitudes as in the present case). The additional words related to high-order Floquet harmonics is the main and principal difference of the Ewald-Oseen extinction principle formulation for electromagnetic crystals as compared to the classical case of isotropic dielectrics.

Substitution of (21) and (14) into (18) allows us to express the scattered field in the half space $x<a$ in terms of spatial Floquet harmonics

$$\mathbf{E}_{\mathrm{scat}}=\sum_{s,l}\mathbf{E}_{\mathrm{scat}}^{s,l}e^{-j(\mathbf{k}_{s,l}^{-}\cdot\mathbf{r})}, \tag{27}$$

$$\mathbf{E}_{\mathrm{scat}}^{s,l}=\bar{\bar{\gamma}}_{s,l}^{-}\sum_i A_i\frac{\int_V \mathbf{P}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{-}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}+k_{s,l}^{x})a}}. \tag{28}$$

Note that the formula for the amplitudes of scattered Floquet harmonics (28) contains series which have the same form as (26) and differs only by the sign of the $x$ components of wave vectors $\mathbf{k}_{s,l}^{\pm}=(\pm k_{s,l}^{x},k_y,k_z)^T$ corresponding to the spatial harmonics propagating into the half spaces $x<a$ and $x>a$, respectively.

If the eigenmodes of the crystal $\{q_x^{(i)},\mathbf{P}_i(\mathbf{r})\}$ are known then one can solve the system of linear equations (26) and find amplitudes of excited eigenmodes $\{A_i\}$. With the use of these amplitudes the scattered field can be found by (28).

This provides a numerical method which allows one to solve the problem of plane-wave diffraction by a semi-infinite electromagnetic crystal using the knowledge of eigenmodes of the infinite crystal. This fact is very important since at the moment the reflection and dispersion problems for electromagnetic crystals are usually solved by separate numerical approaches. The expressions (26) and (28) create a link between these two problems and show how results of dispersion studies can be used in order to describe reflection properties of electromagnetic crystals.

Until this point we considered only one incident wave with wave vector $\mathbf{k}=\mathbf{k}_{0,0}^{+}$, but from (25) it is clear that we could consider also other incident spatial harmonics with wave vectors $\mathbf{k}_{s,l}^{+}$ and get similar results as (26), but the nonzero terms at the right side of the equation would correspond to the respective incident spatial harmonic. Using the principles of superposition we obtain that if the semi-infinite crystal is excited by the whole spectrum of incident spatial harmonics with amplitudes $\mathbf{E}_{\text{inc}}^{s,l}$ and wave vectors $\mathbf{k}_{s,l}^{+}$, then the following system of linear equations is valid:

$$\bar{\bar{\gamma}}_{s,l}^{+}\sum_i A_i \frac{\int_V \mathbf{P}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{+}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}-k_{s,l}^{x})a}} = \mathbf{E}_{\text{inc}}^{s,l}. \tag{29}$$

The scattered field is given by (28) as in the case of one incident wave. Equation (29) represents the cancellation of all incident spatial spectra by induced polarization of the crystal in accordance with the above formulated generalized Ewald-Oseen extinction principle.

### D. Formulation of boundary conditions

In the preceding section we proved the generalized Ewald-Oseen extinction principle for the case of semi-infinite electromagnetic crystal described by certain periodic permittivity distribution $\bar{\bar{\varepsilon}}(\mathbf{r})$ excited by a plane wave coming from free space. In order to extend this theory to the case when the incident wave comes from a homogeneous isotropic dielectric with permittivity $\varepsilon$ it is enough to change $\varepsilon_0$ in all formulas to $\varepsilon$. Physically it means that we have to consider the polarization of the crystal with respect to the host material with permittivity $\varepsilon$, but not free space. In the model of a dense cubic lattice of point dipoles it means that the lattice is located inside this host material. This approach is very unusual since it can lead to results which are strange at first. For example, free space happens to have a negative polarization density with respect to dielectrics with $\varepsilon > \varepsilon_0$. This can be simply explained since free space with respect to these dielectrics is like real materials with $\varepsilon < \varepsilon_0$ with respect to free space; they indeed have negative polarization density.

The meaning of polarization density becomes relative automatically when the replacement of $\varepsilon_0$ to $\varepsilon$ is made. In order to avoid the use of this ambiguous polarization in the final formulae it is possible to express the polarization density in terms of the average field using (5). The resulting expressions provide a complete set of boundary conditions for interface between a semi-infinite electromagnetic crystal and isotropic dielectric

$$\mathbf{E}(\mathbf{r}) = \begin{cases} \sum_{s,l} (\mathbf{E}_{\text{inc}}^{s,l} e^{-j\mathbf{k}_{s,l}^{-}\mathbf{r}} + \mathbf{E}_{\text{scat}}^{s,l} e^{-j\mathbf{k}_{s,l}^{+}\mathbf{r}}), & x < a, \\ \sum_i A_i \mathbf{E}_i e^{-j\mathbf{q}_i\mathbf{r}}, & x \geqslant a, \end{cases} \tag{30}$$

$$\bar{\bar{\gamma}}_{s,l}^{+}\sum_i A_i \frac{\int_V [\bar{\bar{\varepsilon}}-\varepsilon_0\bar{\bar{I}}]\mathbf{E}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{+}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}-k_{s,l}^{x})a}} = \mathbf{E}_{\text{inc}}^{s,l}, \tag{31}$$

$$\bar{\bar{\gamma}}_{s,l}^{-}\sum_i A_i \frac{\int_V [\bar{\bar{\varepsilon}}-\varepsilon_0\bar{\bar{I}}]\mathbf{E}_i(\mathbf{r}')e^{j(\mathbf{k}_{s,l}^{-}\cdot\mathbf{r}')}d\mathbf{r}'}{1-e^{j(q_x^{(i)}+k_{s,l}^{x})a}} = \mathbf{E}_{\text{scat}}^{s,l}, \tag{32}$$

where we use following notations:

$$\bar{\bar{\gamma}}_{s,l}^{\pm} = \frac{j}{2bc\varepsilon k_{s,l}}[\mathbf{k}_{s,l}^{\pm}\times[\mathbf{k}_{s,l}^{\pm}\times\bar{\bar{I}}]], \quad \mathbf{k}_{s,l}^{\pm} = (\pm k_{s,l}^{x}, k_s^{y}, k_l^{z})^T,$$

$$k_s^y = q_y + \frac{2\pi s}{b}, \quad k_l^z = q_z + \frac{2\pi l}{c}, \quad k_{s,l}^x = \sqrt{k^2-(k_s^y)^2-(k_l^z)^2}.$$

$k$ is the wave number in the dielectric with permittivity $\varepsilon$, $\mathbf{q}_i=(q_i^x,k_y,k_z)^T$ and the square root in the expression for $k_{s,l}$ should be chosen so that $\text{Im}(\sqrt{\cdot})<0$.

The expressions (31) and (32) relate amplitudes of incident $\mathbf{E}_{\text{inc}}^{s,l}$ and scattered $\mathbf{E}_{\text{scat}}^{s,l}$ spatial harmonics corresponding to tangential wave vector $\mathbf{k}_t=(k_y,k_z)^T$ and the periodicity of the boundary (rectangular lattice with periods $b$ and $c$) with amplitudes $A_i$ of eigenmodes $(\mathbf{E}_i,q_i^x)$ excited in the semi-infinite crystal.

The presented set of boundary conditions is complete; these equations are enough to determine amplitudes of excited eigenmodes and scattered spatial harmonics if the eigenmodes $\{(\mathbf{E}_i,q_i^x)\}$ of infinite crystal corresponding to tangential wave vector $\mathbf{k}_t$ are known. But this set is not unique. One can immediately suggest using classical boundary conditions (the continuous tangential component of an electric field and a normal component of electric displacement at any point of the boundary $x=a$) which being expanded into the Fourier series will also grant a complete set of linear equations relating amplitudes of incident, scattered, and excited modes.

The advantage of Eqs. (31) and (32) as compared to any other boundary conditions is such that they have a very special form which can admit an analytical solution. We will demonstrate it in the next section for the special case of electromagnetic crystals formed by small scatterers which can be treated as point dipole with fixed orientation. But this is not the only case when an analytical solution of (31) and (32) can be obtained. Recently, Silveirinha (Ref. 13) demonstrated that the method proposed by ourselves can be successfully applied for studies of reflection from semi-infinite wire medium, material with strong low-frequency spatial dispersion.[14] Unfortunately, we cannot provide solutions of Eqs. (31) and (32) for the general case. However, we can give some recommendations and an example as to how these equations can be solved using the method of characteristic

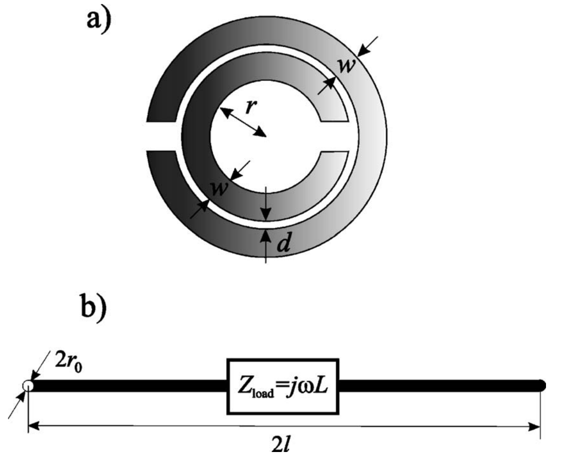


FIG. 4. Geometries of scatterers which can be modeled as dipoles with fixed orientation: (a) split-ring resonator, (b) inductively loaded wire.

function. We hope that with some modification this method can be used for other special cases as well.

## III. LATTICE OF UNIAXIAL DIPOLAR SCATTERERS

If the scatterers which form electromagnetic crystal are small as compared to the wavelength then sometimes they can be effectively replaced by point dipoles. It is assumed that the dipole moment of such a dipole is determined by a local field acting to the scatterer and the field produced by the scatterer is equal to the field created by the dipole. The polarizability which relates the induced dipole moment and the local field acting to the scatterer is the only parameter which depends on the shape of the scatterer in such a local field approach.

Generally, the field produced by any scatterer can be presented using expansion by multipoles. The electric and magnetic dipoles are first and second order multipoles. For some scatterers, the electric or magnetic dipole moments dominate over high-order multipoles. It means that some scatterers behave as electrical dipoles, some others as magnetic. Below we will only consider such scatterers. The scatterers which have both electric and magnetic dipole moments of the same order or whose quadrupole or other high-order multipoles can not be neglected are out of the scope of our consideration. Moreover, below we will consider only scatterers which can be replaced by dipoles with fixed orientation.

The typical example of the scatterer which behaves as an electric dipole with fixed orientation at microwave frequencies is a short metallic cylinder or piece of wire which can be loaded by some inductance in order to increase its polarizability (Ref. 15) [see Fig. 4(b)]. At optical frequencies it can be a prolate metallic cylinder which has strong plasmonic resonance. The typical magnetic scatterer at microwave frequencies is a split-ring resonator (Ref. 16) [see Fig. 4(a)] if the bianisotropic properties of this scatterer are neglected or canceled using the method suggested in (Ref. 17). At optical frequencies the split metallic rings (Refs. 18 and 19) behave as magnetic scatterers with a fixed orientation of dipole moment. Metallic spheres which also can be replaced by point dipoles are out of the scope of our consideration since the orientation of their dipole moments depends on the direction of the external field.

### A. History of the problem

Later in this section we present an analytical solution for the problem of plane-wave diffraction on semi-infinite electromagnetic crystals formed by point scatterers with known polarizabilites, but before that we have to describe the history of this problem. An attempt to obtain such an analytical solution was made by Mahan and Obermair in a seminal work.[10] Analytical expressions for reflection coefficients and amplitudes of excited modes for a semi-infinite crystal were obtained in terms of wave vectors of the infinite crystal eigenmodes. However, this theory is not free from drawbacks. Mahan and Obermair treated the interaction between a reference crystal plane of a semi-infinite crystal and its $N$ nearest-neighbors exactly, neglecting the other crystal planes. That is why this approximation is called the "nearest-neighbor approximation." Such an approach allows one to introduce fictitious zero polarization at the imaginary crystal planes in free space over the semi-infinite crystal. This manipulation gave a set of equations which were treated in Ref. 10 as additional boundary conditions. It will be shown below that if the interaction between planes is taken into account exactly but not restricted to a finite number of neighboring planes then the fictitious polarization of imaginary planes turns out to be nonzero. In the work of Mead[20,21] it was already shown that the nearest-neighbor approximation appears to not be a strict one. Mead states that if serious disagreement appears in the cases then the interaction between crystal planes falls off not sufficiently fast with distance. In other words, the results of Mahan and Obermair are valid only when the high-order spatial Floquet harmonics produced by the planes rapidly decay with distance. Mahan and Obermair considered only the normal incidence of the plane wave. Within such a restriction their approach is valid in the case when the periods of the structure are small as compared with the wavelength in the host medium. The strong disagreement with the exact solution appears when one high-order Floquet harmonic happens to be propagating one. This fact is illustrated below by a numerical comparison.

The work[10] caused numerous extensions.[22–24] The Mahan and Obermair approach was generalized for the cases of oblique incidence,[22] both possible polarizations of the incident wave,[24] various lattice structures of the crystal,[22] tensorial polarizability of scatterers,[24] and even diffraction of the finite-size slabs of the crystals were considered.[23] Note that all the listed works use the same nearest-neighbor approximation and their applicability is restricted as described above. In order to avoid this trouble one needs to use another model for interaction between crystal planes. The simplest one is the so-called "exp model" suggested by Mead[20,25] which assumes that interaction can be described by a single decaying exponent. In terms of spatial Floquet harmonics this approach is equivalent to neglecting all high-order Floquet harmonics, except the one with the slowest decay. The exp model as well as the nearest-neighbor approximation allow us to solve the problem of excitation analytically for both normal[20] and oblique[25] incidences. The exp model of Mead gives a set of two equations which correspond to the generalized Ewald-Oseen extinction principle formulated in the present paper. The first equation of Mead is the same as one of the equations given by the nearest-neighbor approximation. It describes the fact that the incident electromagnetic wave (fundamental Floquet harmonic) inside the semi-infinite crystal is canceled by induced polarization of the crystal. This fact was pointed out in the (Refs. 10, 20, and 24). The second equation clearly expresses the fact that induced polarization also cancels the second Floquet harmonic (taken into account in the exp model) of the incident wave which has zero amplitude, but unfortunately it was not noted by the authors. The system of these two equations is solved in Ref. 20 and the amplitudes of excited eigenmodes and an expression for reflection coefficient are obtained.

It is possible to modify the exp model in order to obtain an exact solution. For that purpose one simply should take into account all Floquet harmonics in the interaction between the crystal planes. This has been done by authors of the present paper and the results are presented below. As it was shown above, it turns out that every incident Floquet harmonic (even if it has zero amplitude) is canceled by the induced polarization following the generalized Ewald-Oseen extinction principle. It provides an infinite system of equations relating amplitudes of excited eigenmodes. This system can be truncated and then the number of equations in the system turns out to be equal to the number of Floquet harmonics taken into account. Such a finite system can be easily solved analytically for the case when only two Floquet harmonics are taken into account [this is the exp model of Mead[20]], but in the case when one would like to take into account more Floquet harmonics this approach requires numerical calculations. We avoid the truncation of the system of equations and offer a closed-form rigorous analytical solution which is simple and explicit.

Note, that a "formally closed solution" for the problem under consideration was proposed by Mead in Ref. 21. In this solution there is a contour integral of a certain function given in the form of infinite series. However, the calculation with the help of such a formally closed solution requires serious numerical efforts. The main idea of the work[21] is based on the introduction of a characteristic analytical function which allows one to determine all parameters entering the expression for the reflection coefficient. It is shown that knowledge of its roots allows one to recover this function and obtain analytical expressions for all amplitudes of excited eigenmodes and for the reflection coefficient, consequently. Unfortunately, these roots were not found in Ref. 21. That is why the contour integration was used in Ref. 21 in order to bypass the problem of these roots finding. In fact, as it is shown below, the roots of this characteristic analytical function are determined by the wave vectors of Floquet harmonics and can be easily expressed analytically. This fact is a consequence of the generalized Ewald-Oseen extinction principle.

One could directly apply general results (26) and (28) to the problem under consideration. It is enough to replace polarization density of eigenmodes by the three-dimensional delta function corresponding to the point of location of the dipolar scatterer in the unit cell and one could obtain the system of linear Eqs. (26) and (28) which correspond to the boundary conditions in the present case as it is shown below. However, we prefer to re-deduce all the expressions by making the same steps as in the previous section but for the case of point scatterers. We suppose that it is a very useful step in order to demonstrate the physical background of the computations undertaken in the previous section as a specific example.

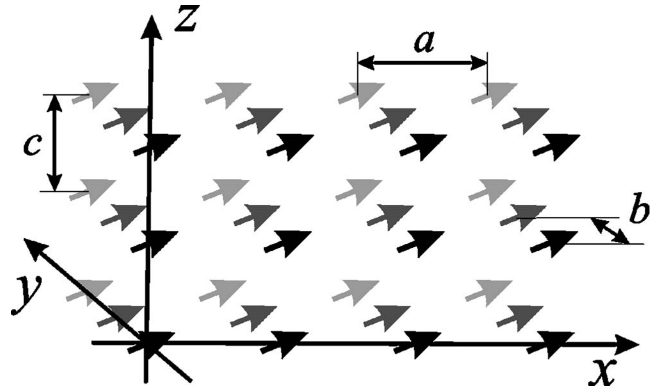


FIG. 5. Geometry of an infinite electromagnetic crystal formed by uniaxial dipolar scatterers.

### B. Dispersion equation

Let us consider an infinite crystal formed by point dielectric dipoles with some known polarizability $\alpha$ along a fixed direction given by unit vector $\mathbf{d}$, $\bar{\bar{\alpha}}=\alpha\mathbf{dd}$. The case of magnetic dipoles can be easily obtained from the theory for dielectric ones using the duality principles. The scatterers are arranged in the nodes of the three-dimensional lattice with an orthorhombic elementary cell $a\times b\times c$ located in free space, see Fig. 5.

The distribution of dipole moments corresponding to an eigenmode with wave vector $\mathbf{q}=(q_x,q_y,q_z)^T$ is described as $\mathbf{p}_{n,s,l}=\mathbf{p}e^{-j(q_xan+q_ybs+q_zcl)}$, where $n,s,l$ are integer indices of scatterers along the $x$-, $y$-, and $z$-axes, respectively, and $\mathbf{p}$ is a dipole moment of the scatterer located at the center of coordinate system. Following the local field approach $\mathbf{p}$ can be expressed as $\mathbf{p}=\alpha(\mathbf{E}_{\rm loc}\cdot\mathbf{d})\mathbf{d}$, where $\mathbf{E}_{\rm loc}$ is a local electric field acting to the scatterer. The local field is produced by all other scatterers which form the infinite crystal and can be given by the formula

$$\mathbf{E}_{\rm loc}=\sum_{n,s,l}{}'\,\bar{\bar{G}}(\mathbf{R}_{n,s,l})\mathbf{p}_{n,s,l}, \tag{33}$$

where $\bar{\bar{G}}(\mathbf{r})$ is the three-dimensional dyadic Green's function of the free space (9) and the summation is taken over all triples of indices except the zero one. Accordingly the following dispersion equation for the crystal under consideration is obtained [compare with (6)]:

$$\alpha^{-1}=\left[\sum_{n,s,l}{}'\,\bar{\bar{G}}(\mathbf{R}_{n,s,l})e^{-j(q_xan+q_ybs+q_zcl)}\mathbf{d}\right]\cdot\mathbf{d}. \tag{34}$$

In order to evaluate sums of series in (34) we use a planewise approach.[26] According to this approach the dispersion equation takes the following form:

$$\alpha^{-1} = \sum_{n=-\infty}^{+\infty} \beta_n e^{-jq_x an}. \quad (35)$$

The coefficients $\beta_n$ describe the interaction between planes and include the information on transverse wave vector components $q_y$, $q_z$ as well as on a geometry of a single plane (lattice periods $b$, $c$). For $n \neq 0$ coefficients $\beta_n$ can be expressed using expansion by Floquet harmonics. For $n=0$ the calculation of coefficient $\beta_0$ (describing the interaction inside a plane and expressed in the form of a two-dimensional series without the zero term) requires additional efforts [see Refs. 11, 26, and 27 for details].

The electric field produced by a single plane (namely a two-dimensional grid $b \times c$ of point dipoles with the distribution $\mathbf{p}_{s,l}=\mathbf{p}e^{-j(q_y bs+q_z cl)}$) located in the plane $x=0$ is equal to

$$\mathbf{E}(\mathbf{r}) = \frac{j}{2bc\varepsilon_0}\sum_{s,l} [\mathbf{k}_{s,l}^{\mathrm{sgn}(x)} \times [\mathbf{k}_{s,l}^{\mathrm{sgn}(x)} \times \mathbf{p}]]\frac{e^{-j(\mathbf{k}_{s,l}^{\mathrm{sgn}(x)}\cdot\mathbf{R})}}{k_{s,l}^x}, \quad (36)$$

where $\mathbf{k}_{s,l}^{\pm}=(\pm k_{s,l}^x, k_s^y, k_l^z)^T$, $k_s^y=q_y+(2\pi s/b)$, $k_l^z=q_z+(2\pi l/c)$, $k_{s,l}^x=\sqrt{k^2-(k_s^y)^2-(k_l^z)^2}$, and $k$ is the wave number of free space. One should choose the square root in the expression for $k_{s,l}$ so that $\mathrm{Im}(\sqrt{\cdot})<0$. The sign $\pm$ corresponds to half spaces $x>0$ and $x<0$, respectively.

The formula (36) defines an expansion of the field produced by a single grid of dipoles in terms of plane waves and it can be obtained using a double Poisson summation formula to the series of fields produced by single scatterers in free space. These plane waves have wave vectors $\mathbf{k}_{s,l}^{\pm}$. They are also called Floquet harmonics and represent a spatial spectrum of the field [compare with (14)]. Floquet harmonics are widely used in the analysis of phased array antennas.[28]

Using (36) we get the following expression for $\beta_n$ ($n \neq 0$):

$$\beta_n = \sum_{s,l} \gamma_{s,l}^{-\mathrm{sgn}(n)} e^{-jk_{s,l}^x a|n|}, \quad (37)$$

where $\gamma_{s,l}^{\pm}=[k^2-(\mathbf{k}_{s,l}^{\pm}\cdot\mathbf{d})^2]/(2jbc\varepsilon_0 k_{s,l}^x)$. After the substitution of (37) into (35), changing the order of summation and using the formula for the sum of the geometrical progression we obtain the dispersion equation in the following form:

$$\alpha^{-1} = \beta_0 + \sum_{s,l}\left[\frac{\gamma_{s,l}^-}{e^{j(k_{s,l}^x+q_x)a}-1} + \frac{\gamma_{s,l}^+}{e^{j(k_{s,l}^x-q_x)a}-1}\right]. \quad (38)$$

This is a transcendental equation expressed by a rapidly convergent series. Dispersion properties of the crystal under consideration can be studied with the help of the numerical solution of the latter equation. The case of dipoles oriented along one of the crystal axes of the orthorhombic crystal has been considered in, Ref. 11; the dispersion equation was solved and typical dispersion curves and isofrequency contours for resonant scatterers were presented.

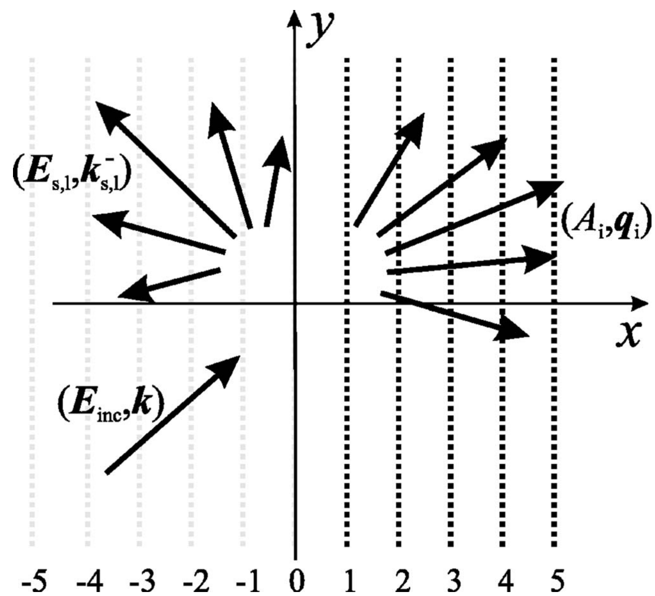


FIG. 6. Geometry of a semi-infinite electromagnetic crystal formed by uniaxial dipolar scatterers.

### C. Semi-infinite crystal

Now let us consider a semi-infinite electromagnetic crystal, the half-space $x \geqslant a$ filled by the crystal formed by point dipoles (see Fig. 6). The structure is excited by a plane electromagnetic wave with the wave vector $\mathbf{k}=(k_x,k_y,k_z)^T$ and the intensity of the electric field $\mathbf{E}_{\mathrm{inc}}$. Let us denote the component of the incident electric field along the direction of dipoles as $E_{\mathrm{inc}}=(\mathbf{E}_{\mathrm{inc}}\cdot\mathbf{d})$. The axis $x$ is assumed to be normal to the interface. The tangential (with respect to the interface) distribution of dipole moments in excited semi-infinite crystal is determined by the tangential component of the incident wave vector. It means that $p_{n,s,l}=p_n e^{-j(k_y bs+k_z cl)}$, where the polarizations of zero-numbered scatterers from planes with the index $n$ (parallel to the interface) are denoted as $p_n = p_{n,0,0}$. The plane-to-plane distribution $\{p_n\}$ is unknown and it has to be found. Using the local field approach one can write the infinite linear system of equations for this distribution as

$$p_m = \alpha\left(E_{\mathrm{inc}}e^{-jk_x am} + \sum_{n=1}^{+\infty}\beta_{n-m}p_n\right), \quad \forall\, m \geqslant 1. \quad (39)$$

The distribution $\{p_n\}$ of polarization in the excited semi-infinite crystal can be determined solving the system of Eqs. (39). The known distribution of polarization allows us to determine the scattered field in the half-space $x<a$ with the help of the expansion by Floquet harmonics (36)

$$\mathbf{E} = \sum_{s,l} \mathbf{E}_{s,l}e^{-j(\mathbf{k}_{s,l}^-\cdot\mathbf{R})}, \quad (40)$$

where the amplitudes of Floquet harmonics are the following:

$$\mathbf{E}_{s,l} = \frac{j}{2ab\varepsilon_0 k_{s,l}^x}[\mathbf{k}_{s,l}^- \times [\mathbf{k}_{s,l}^- \times \mathbf{d}]]\sum_{n=1}^{+\infty} p_n e^{-jk_{s,l}^x an}. \quad (41)$$

If the crystal supports propagating modes, it is quite difficult to find a solution of (39) numerically. Simple methods such as a system truncating (considering a slab with finite thickness instead of half-space like in Ref. 29) results in nonconvergent oscillating solutions which have nothing to do with actual solution of (39).

### D. Expansion by eigenmodes

In order to solve (39) accurately one has to use an expansion of the polarization by eigenmodes (Ref. 10)

$$p_n = \sum_i A_i e^{-jq_x^{(i)}an}, \tag{42}$$

where $A_i$ are amplitudes of eigenmodes and $q_x^{(i)}$ are the $x$ components of their wave vectors. Every eigenmode is assumed to be a solution of the dispersion equation (38) with the wave vector $\mathbf{q}_i=(q_x^{(i)},k_y,k_z)^T$. In formula (42) the summation is taken by eigenmodes which either transfer energy into half-space $x\geqslant a$ $[dq_x^{(i)}/d\omega>0]$ or decay along the $x$ axis $[\mathrm{Im}(q_x^{(i)})<0]$.

Let us assume that the dispersion equation (38) is solved (for example numerically) and the necessary set of eigenmodes $\{q_x^{(i)}\}$ is found. Then the substitution of (42) into (39) will replace the set of unknown polarizations of planes by a set of unknown amplitudes of eigenmodes

$$\alpha^{-1}\sum_i A_i e^{-jq_x^{(i)}am} = E_{\mathrm{inc}}e^{-jk_xam} + \sum_{n=1}^{+\infty}\beta_{n-m}\sum_i A_i e^{-jq_x^{(i)}an}. \tag{43}$$

Applying the auxiliary relation evidently following from (38):

$$\alpha^{-1}e^{-jq_x^{(i)}am} - \sum_{n=-\infty}^{0}\beta_{n-m}e^{-jq_x^{(i)}an} = \sum_{n=1}^{+\infty}\beta_{n-m}e^{-jq_x^{(i)}an}, \tag{44}$$

the Eq. (43) can be transformed as follows:

$$\sum_i A_i\left(\sum_{n=-\infty}^{0}\beta_{n-m}e^{-jq_x^{(i)}an}\right) = E_{\mathrm{inc}}e^{-jk_xam}. \tag{45}$$

It should be noted that using the definition of Mahan and Obermair for the polarization of fictitious planes ($p_n=\Sigma_i A_i e^{-jq_x^{(i)}an}, \forall n\leqslant 0$) one can rewrite (45) as

$$\sum_{n=-\infty}^{0}\beta_{n-m}p_n = E_{\mathrm{inc}}e^{-jk_xam}. \tag{46}$$

It is evident that the assumption of Mahan and Obermair, requiring all polarizations of fictitious planes to be zeros, contradicts with (46). This fact proves that the nearest-neighbor approximation made in Ref. 10 is not accurate.

The system of equations (45) can be truncated and solved numerically quite easily in contrast to (39). As a result, the amplitudes of eigenmodes $\{A_i\}$ can be found and the polarization distribution can be restored using formula (42). The amplitudes of scattered Floquet harmonics (41) can also be expressed in terms of excited eigenmode amplitudes by means of substitution of (42) into (41), changing the order of summation and evaluating sums of geometrical progressions. The final expression for the amplitudes of scattered Floquet harmonics is the following [compare with (28)]:

$$\mathbf{E}_{s,l} = \frac{[\mathbf{k}_{s,l}^{-}\times[\mathbf{k}_{s,l}^{-}\times\mathbf{d}]]}{2jab\varepsilon_0 k_{s,l}^x}\sum_i A_i\frac{1}{1-e^{j(q_x^{(i)}+k_{s,l}^x)a}}. \tag{47}$$

One can stop at this stage and claim that the problem of the semi-infinite electromagnetic crystal excitation is solved. However, in this case the solution would require long numerical calculations, such as solving the system (45) and substituting the obtained solution into (47). The possibility of making all described operations analytically in the closed form is shown below.

### E. Analytical solution

Substituting the expansion (37) into (45) we obtain:

$$\sum_i A_i\left(\sum_{n=-\infty}^{0}\left[\sum_{s,l}\gamma_{s,l}^{+}e^{-jk_{s,l}^x a|n-m|}\right]e^{-jq_x^{(i)}an}\right) = E_{\mathrm{inc}}e^{-jk_xam}. \tag{48}$$

Changing the order of summations in (48), taking into account that $n-m<0$, and using the formula for the sum of geometrical progression, we obtain

$$\sum_{s,l}\gamma_{s,l}^{+}\left(\sum_i A_i\frac{1}{1-e^{j(q_x^{(i)}-k_{s,l}^x)a}}\right)e^{-jk_{s,l}^x am} = E_{\mathrm{inc}}e^{-jk_xam}. \tag{49}$$

This is a system of linear equations where unknowns are given by expressions in brackets. It has a unique solution because the determinant of the system has finite nonzero value. Note that $k_{s,l}^x=k_x$ only if $(s,l)=(0,0)$. Thus, the solution of (49) has the following form:

$$\sum_i A_i\frac{1}{1-e^{j(q_x^{(i)}-k_{s,l}^x)a}} = \begin{cases} E_{\mathrm{inc}}/\gamma_{0,0}^{+} & \text{if } (s,l)=(0,0) \\ 0 & \text{if } (s,l)\neq(0,0). \end{cases} \tag{50}$$

This equation could be directly obtained from the general expression (26) by substitution of a delta function instead of the polarization density of eigenmodes, but as we already mentioned above we intentionally re-deduced it since we suppose that it can help us to understand the background for the deduction of (26) for general case. The values at the right side of (50) are the normalized amplitudes of incident Floquet harmonics, and the series at the left side are the normalized amplitudes of Floquet harmonics produced by the whole semi-infinite crystal polarization which cancel the incident harmonics. Thus, Eq. (50) represents the generalization of the Ewald-Oseen extinction principle already formulated above for the general case of semi-infinite crystals: The polarization in a semi-infinite electromagnetic crystal excited by a plane wave is distributed in such a way that it cancels the incident wave together with all high-order spatial harmonics associated with periodicity of the boundary.

Note that the formula for the amplitudes of scattered Floquet harmonics (47) contains series that have the same form as (50), but another sign in front of $k^x_{s,l}$.

The amplitudes of the excited modes $A_i$ can be found numerically from the infinite set of Eqs. (50) and substitution of $A_i$ into (47) will give us amplitudes of scattered Floquet harmonics. However, it is possible to obtain a closed-form analytical solution of (50).

In order to solve the set of Eqs. (50) one should consider a characteristic function $f(x)$ (see also Ref. 21) of the form

$$f(u) = u\sum_i A_i \frac{1}{u - e^{jq_x^{(i)}a}}. \quad (51)$$

Comparing (47) and (50) with (51) one can see that the function $f(u)$ has the following properties:

(a) It has poles at $u = e^{jq_x^{(i)}a}$.

(b) It has roots at $u = e^{jk^x_{s,l}a}$, $(s,l) \neq (0,0)$, and $u=0$.

(c) It has a known value $E_{\text{inc}}/\gamma^+_{0,0}$ at $u=e^{jk_xa}$.

(d) Its values at $u=e^{-jk^x_{s,l}a}$ are equal to the normalized amplitudes of scattered Floquet harmonics.

(e) Its residues at $u = e^{jq_x^{(i)}a}$ are equal to the normalized amplitudes of excited eigenmodes.

It is possible to restore the function $f(u)$ using the known values of its poles, roots, and a value at one point,

$$f(u) = \frac{E_{\text{inc}} u}{\gamma^+_{0,0} e^{jk_xa}} \prod_{(s,l)\neq(0,0)} \frac{u - e^{jk^x_{s,l}a}}{e^{jk_xa} - e^{jk^x_{s,l}a}} \prod_i \frac{e^{jk_xa} - e^{jq_x^{(i)}a}}{u - e^{jq_x^{(i)}a}}. \quad (52)$$

The knowledge of the characteristic function $f(u)$ provides us with the complete solution of our diffraction problem. The amplitudes of excited eigenmodes with indices $n$ are equal to residues of $f(u)$ at $u = e^{jq_x^{(n)}a}$

$$A_n = \operatorname{Res} f(u)|_{u=e^{jq_x^{(i)}a}} = \frac{E_{\text{inc}}(1 - e^{j(q_x^{(n)} - k_x)a})}{\gamma^+_{0,0}} \prod_{(s,l)\neq(0,0)} \frac{e^{jq_x^{(n)}a} - e^{jk^x_{s,l}a}}{e^{jk_xa} - e^{jk^x_{s,l}a}} \prod_{i\neq n} \frac{e^{jk_xa} - e^{jq_x^{(i)}a}}{e^{jq_x^{(n)}a} - e^{jq_x^{(i)}a}}, \quad (53)$$

and the amplitudes of scattered Floquet harmonics with indices $(r,t)$ can be expressed through values of $f(u)$ at $u = e^{-jk^x_{r,t}a}$,

$$\mathbf{E}_{r,t} = \frac{E_{\text{inc}} e^{-jk^x_{r,t}a}[\mathbf{k}^-_{r,t} \times [\mathbf{k}^-_{r,t} \times \mathbf{d}]]}{2jab\varepsilon_0 k^x_{r,t} \gamma^+_{0,0} e^{jk_xa}} \times \prod_{(s,l)\neq(0,0)} \frac{e^{-jk^x_{r,t}a} - e^{jk^x_{s,l}a}}{e^{jk_xa} - e^{jk^x_{s,l}a}} \prod_i \frac{e^{jk_xa} - e^{jq_x^{(i)}a}}{e^{-jk^x_{r,t}a} - e^{jq_x^{(i)}a}}. \quad (54)$$

The products in the formulas (53) and (54) have very rapid convergence. It is enough to take a few terms in order to reach excellent accuracy. The main requirement for truncation of these infinite products is to take into account all terms corresponding to propagating $\text{Re}(k^x_{s,l})=0$ and slowly decaying $\text{Im}(k^x_{s,l}) \ll 2\pi/a$ Floquet harmonics as well as propagating $\text{Re}(q_x^{(i)})=0$ and slowly decaying $\text{Im}(q_x^{(i)}) \ll 2\pi/a$ eigenmodes.

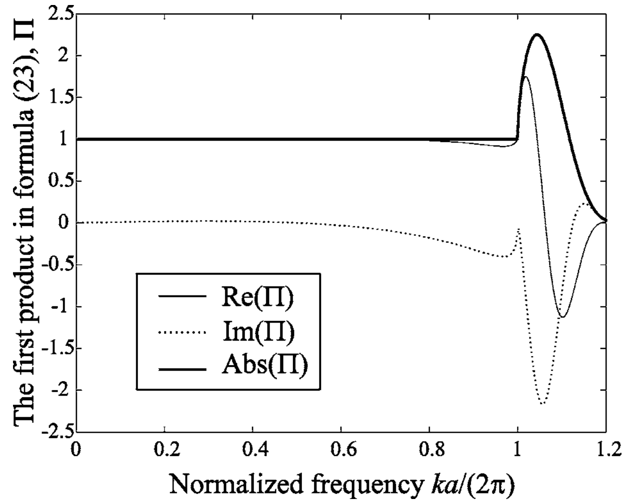


FIG. 7. Dependence of Π vs normalized frequency $ka/(2\pi)$.

### F. Comparison with other theories

Let us consider the case from Ref. 10 when $\mathbf{d}=\mathbf{y}_0$, and $a=b=c$. In this case the formula (54) for the fundamental Floquet harmonic $(r=t=0)$ can be rewritten in terms of the reflection coefficient

$$R = -e^{-2jk_xa} \prod_{(s,l)\neq(0,0)} \frac{e^{-jk_xa} - e^{jk^x_{s,l}a}}{e^{jk_xa} - e^{jk^x_{s,l}a}} \prod_i \frac{e^{jk_xa} - e^{jq_x^{(i)}a}}{e^{-jk_xa} - e^{jq_x^{(i)}a}}. \quad (55)$$

Comparing that result with the final result of the (Ref. 10) [the next formula after (C7) on page 841] one can see that the first product in our formula (55)

$$\Pi = \prod_{(s,l)\neq(0,0)} \frac{e^{-jk_xa} - e^{jk^x_{s,l}a}}{e^{jk_xa} - e^{jk^x_{s,l}a}} \quad (56)$$

is absent in the result of Mahan and Obermair. This difference is a consequence of the fact that in our study we considered interaction between crystal planes accurately taking into account all Floquet harmonics for any distance between planes in contrast to the nearest-neighbor approximation used in the approach of Mahan and Obermair.

The dependence of the product Π vs normalized frequency is plotted in Fig. 7 for the case of normal incidence $k_y=k_z=0$ and $k_x=k$. One can see that the value of the product is nearly equal to the unity for $ka<1.6\pi$, but for $ka>2\pi$ the value of the product significantly differs from the unity. Thus we conclude that the theory of Mahan and Obermair is valid in the low frequency range when periods of the lattice are small compared to the wavelength. Our theory does not have such a restriction (within the frame of the dipole model of electromagnetic crystal).

The comparison with the results of Ref. 21 shows that (55) is equivalent to formula (46) from (Ref. 21) with Π

$=\exp(\Gamma)$ where $\Gamma$ is given by the contour integral (47) from Ref. 21. The calculation of $\Pi$ using (56) requires taking into account only a few terms in the infinite products, because they are very rapidly convergent. This is a significant advantage of our approach as compared to Ref. 21 which requires a complicated numerical calculation of the contour integral.

In the long-wavelength limit, the series in Eq. (34) for the cubic lattice can be replaced by the integral taken over the whole space except unit cell $V$ and we obtain

$$\alpha^{-1} = \left[ \left( \int_{R^3/V} \bar{\bar{G}}(\mathbf{R}) e^{-j(\mathbf{q}\cdot\mathbf{R})} d\mathbf{R} \right) \mathbf{d} \right] \cdot \mathbf{d}. \tag{57}$$

The integral in the right-hand side of Eq. (57) can be evaluated by means of the same technique that was used while deducing the Ewald-Oseen extinction principle in Ref. 9. The result is the following:

$$\alpha^{-1} = \left[ \frac{1}{3} + \frac{(\mathbf{q}\cdot\mathbf{d})^2 - |\mathbf{q}|^2}{K^2 - |\mathbf{q}|^2} \right] \frac{V}{\varepsilon_0}. \tag{58}$$

The obtained dispersion equation (58) can be transformed in the common form

$$\tilde{\varepsilon}(k^2 - q_d^2) = \varepsilon_0(|\mathbf{q}|^2 - q_d^2), \tag{59}$$

where

$$\tilde{\varepsilon} = \varepsilon_0 \left( 1 + \frac{\alpha/(\varepsilon_0 V)}{1 - \alpha/(3\varepsilon_0 V)} \right), \tag{60}$$

and $q_d = (\mathbf{q}\cdot\mathbf{d})$ is the component of the wave vector $\mathbf{q}$ along the anisotropy axis.

The formula (59) is a classical form of the dispersion equation for uniaxial dielectrics[9] with permittivity $\tilde{\varepsilon}$ along the anisotropy axis and $\varepsilon$ in the transverse plane. The expression (60) is the Clausius-Mossotti formula for the effective permittivity of cubic lattices of scatterers.

In the long-wavelength limit the formula (54) for the amplitude of reflected wave simplifies as follows:

$$\mathbf{E}_R = -\frac{(\mathbf{E}_{\mathrm{inc}}\cdot\mathbf{d})[\mathbf{k}^- \times [\mathbf{k}^- \times \mathbf{d}]]}{[k^2 - (\mathbf{k}\cdot\mathbf{d})^2]} \frac{k_x - q_x}{k_x + q_x}, \tag{61}$$

where $\mathbf{k}^- = (-k_x, k_y, k_z)^T$ is the wave vector of the reflected wave. The formula (61) represents a compact form of an expression for the electric field amplitude of a wave reflected from an interface between an isotropic dielectric and an uniaxial dielectric [see, e.g., Ref. 30]. Note that in our case the situation is simplified as compared to the general case, because the incident wave comes from isotropic dielectric with permittivity $\varepsilon$ which is equal to the permittivity of uniaxial dielectric in the transverse plane. It means that an incident wave with normal polarization with respect to the anisotropy axis transforms at the interface in a refracted ordinary wave without reflection.

Let us consider the reflection problem at the special case when $\mathbf{d} = \mathbf{y}_0$, $k_y = 0$ and $\mathbf{E}_{\mathrm{inc}} \| \mathbf{y}_0$. The nonzero components of the wave vector for the incident wave can be expressed in terms of the incident angle $\theta_i$ as $k_z = k \sin\theta_i$ and $k_x = k\cos\theta_i$. From (59) we obtain that in this case the transmitted wave has an $x$ component of the wave vector equal to $q_x = \sqrt{\tilde{\varepsilon}k^2/\varepsilon_0 - k_z^2} = \sqrt{\tilde{\varepsilon}/\varepsilon_0}\, k\cos\theta_t$, where $\theta_t$ in angle or refraction. With the result (61) we get the reflection coefficient in the form

$$R = \frac{k_x - q_x}{k_x + q_x} = \frac{n_1\cos\theta_i - n_2\cos\theta_t}{n_1\cos\theta_i + n_2\cos\theta_t}, \tag{62}$$

where $n_1 = \sqrt{\varepsilon_0\mu_0}$ and $n_2 = \sqrt{\tilde{\varepsilon}\mu_0}$ are indices of refraction of the materials. The formula (62) coincide with the classical Fresnel equation.[9] This fact can be treated as an additional verification of the presented theory.

## IV. LATTICE OF SPLIT-RING RESONATORS

In this section we apply the theory presented in the preceding sections for the study of the reflection from a semi-infinite cubic lattice of split-ring resonators.

The general dispersion equation (6) of the integral form in the case of point electric scatterers transforms into a transcendental equation (38). In the case when $\mathbf{d} = \mathbf{y}_0$ the dispersion equation (38) can be rewritten in the following closed form convenient for numerical calculations (see Ref. 11 for details):

$$\varepsilon_0 \alpha^{-1}(\omega) = C(k, \mathbf{q}, a, b, c), \tag{63}$$

where $C(k,\mathbf{q},a,b,c)$ is a dynamic interaction constant of the form

$$\begin{aligned} C(k,\mathbf{q},a,b,c) = &-\sum_{l=1}^{+\infty} \sum_{\mathrm{Re}(p_s)\neq 0} \frac{p_s^2}{\pi b} K_0(p_s c l)\cos(q_z c n) + \sum_{s=-\infty}^{+\infty}\sum_{l=-\infty}^{+\infty} \frac{p_s^2}{2jbck_{s,l}^x} \frac{e^{-jk_{s,l}^x a} - \cos q_x a}{\cos k_{s,l}^x a - \cos q_x a} \\ &- \sum_{\mathrm{Re}(p_s)=0} \frac{p_s^2}{2bc} \left\{ \frac{1}{jk_{s,0}^x} + \sum_{l=1}^{+\infty} \left[ \frac{1}{jk_{s,l}^x} + \frac{1}{jk_{s,-l}^x} - \frac{c}{\pi l} - \frac{r_s c^3}{8\pi^3 l^3} \right] + 1.202 \frac{r_s c^3}{8\pi^3} + \frac{c}{\pi}\left( \log\frac{c|p_s|}{4\pi} + \gamma \right) + j\frac{c}{2} \right\} \\ &+ \frac{1}{4\pi b^3} \left[ 4\sum_{s=1}^{+\infty} \frac{(2jkb+3)s+2}{s^3(s+1)(s+2)} e^{-jkbs}\cos(q_y bs) - (jkb+1)[t_+^2 \log t^+ + t_-^2 \log t^- + 2e^{jkb}\cos(q_y b)] \right. \\ &\left. - 2jkb(t_+ \log t^+ + t_- \log t^-) + (7jkb+3) \right], \end{aligned} \tag{64}$$

and the following notations are used:

$$p_s = \sqrt{(k_s^y)^2 - k^2}, \quad r_s = 2q_z^2 - p_s^2,$$

$$t^+ = 1 - e^{-j(k+q_z)c}, \quad t^- = 1 - e^{-j(k-q_z)c},$$

$$t_+ = 1 - e^{j(k+q_z)c}, \quad t_- = 1 - e^{j(k-q_z)c}.$$

The calculations using (64) can be restricted to the real part of the dynamic interaction constant $C(k,\mathbf{q},a,b,c)$ only because its imaginary part is given by a much simpler expression [see Ref. 11 for details]

$$\mathrm{Im}\{C(k,\mathbf{q},a,b,c)\} = \frac{k^3}{6\pi}. \quad (65)$$

The series in (64) have excellent convergence that ensure very rapid numerical calculations.

The case of magnetic scatterers can be considered using the duality principle. The expression (55) can be used for a calculation of the reflection coefficient by magnetic field (originally, this equation represented reflection coefficient by electric field). The dispersion equation (63) has to be rewritten for the case of magnetic point scatterers in the following form:

$$\mu_0 \alpha_m^{-1}(\omega) = C(k,\mathbf{q},a,b,c), \quad (66)$$

where $\alpha_m(\omega)$ is the magnetic polarizability of the scatterers. The analytical expressions for the magnetic polarizability $\alpha(\omega)$ of split-ring resonators with geometry plotted in Fig. 4 were derived and validated in Ref. 31. The final result reads as follows:[11]

$$\alpha(\omega) = \frac{A\omega^2}{\omega_0^2 - \omega^2 + j\omega\Gamma}, \quad (67)$$

where $A$ is the amplitude, $\omega_0$ is the resonant frequency, and $\Gamma = A\omega k^3/(6\pi\mu_0)$ is the radiation reaction factor. The expressions for amplitude $A$ and resonant frequency $\omega_0$ in terms of dimensions of split-ring resonators are available in Refs. 11 and 31. In the present paper we will use the typical parameters $A = 0.1\mu_0 a^3$ and $\omega_0 = 1/(a\sqrt{\varepsilon_0\mu_0})$.

The dispersion properties of the cubic lattice of split-ring resonators with such parameters have been extensively studied in Ref. 11. Using the theory of the present paper we will study reflection properties of such metamaterial. Let us consider the case of the cubic lattice ($a=b=c$), normal incidence ($k_y=k_z=0$), and the magnetic field of the incident wave along the direction of the magnetic dipoles $\mathbf{d}=\mathbf{y}_0$. The numerical solution of dispersion equation (66) with $q_y=k_y=0$ and $q_z=k_z=0$ allows one to get a set of wave vectors of excited eigenmodes $\{q_i^x\}$. These wave vectors are plotted at the top of Fig. 8 as functions of normalized frequency $ka$. The point $ka=1$ corresponds to the resonant frequency $\omega_0$ as split-ring resonators. One can see that the propagating modes [$\mathrm{Im}(q_x)=0$] exist only for $ka \leqslant 0.978$ and $ka \geqslant 1.044$. It means that a partial resonant band gap is observed for $ka \in [0.978, 1.044]$. At the frequencies inside of the band gap

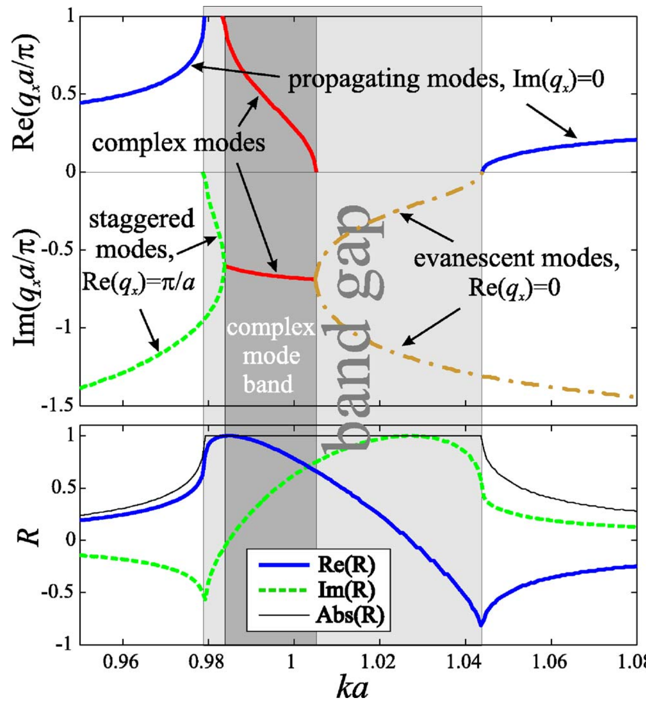


FIG. 8. (Color online) Dependencies of the normalized wave vectors $q_x a/\pi$ of excited eigenmodes (imaginary and real parts) and the reflection coefficient $R$ calculated using (55) on normalized frequency $ka$ for a semi-infinite cubic lattice of split-ring resonators with $A=0.1\mu_0 a^3$ and $\omega_0 = 1/(a\sqrt{\varepsilon_0\mu_0})$.

all the eigenmodes decay with distance. Note, that such decaying modes exist at all frequencies, not only inside of the band gap. The Fig. 8 shows only the eigenmodes with slowest decay $|\mathrm{Im}(q_x)| < 1.5\pi/a$. There is an infinite number of other decaying modes which decay with distance more rapidly. The contribution of such modes into the reflection coefficient is negligible as it was shown above. The decaying modes can be separated into the following three classes.

(i) Evanescent modes, the modes which have $\mathrm{Re}(q_x)=0$; they decay exponentially from one crystal plane to the other one.

(ii) Staggered modes, the modes which have $\mathrm{Re}(q_x) = \pi/a$; they exponentially decay from one crystal plane to the other one by absolute value, but the dipoles in the neighboring plane are excited in out of phase; and

(iii) Complex modes, the most general case of the decaying modes which have $\mathrm{Re}(q_x) \neq 0$; they experience both exponential decay and phase variation from one crystal plane to the other.

The evanescent modes are the most common type of decaying modes. They can be observed in dielectrics with negative permittivity, for example. The staggered modes are limiting the case of the complex modes and can be widely observed in periodical structures in the vicinity of the band gap edges; see, for example, Refs. 32 and 33. The complex modes of the general kind are quite exotic for common materials.

In the system under consideration we are able to observe all three kinds of mentioned decaying modes. The presence of staggered and complex modes are evidence of spatial dispersion in this material reported in Ref. 11. The staggered modes exist for $ka \geqslant 0.984$, evanescent modes for $ka \geqslant 1.015$, and complex modes for $ka \in [0.984, 1.015]$ (see Fig. 8). One can see that for a fixed frequency from the range $ka \in [0.978, 0.984]$ there are two staggered modes and in the range $ka \in [1.015, 1.044]$ there are two evanescent modes. Actually, in the range $ka \in [0.984, 1.015]$ there are also two complex modes which have the same imaginary parts but differ by a sign of the real part. Thus, we conclude that for every frequency from the range $ka \in [0.95, 1.08]$ that we consider the incident wave will excite in the crystal a pair of modes with $|\mathrm{Im}(q_x)| < 1.5\pi/a$ (propagating and staggered, two staggered, two complex, two evanescent or propagating, and evanescent). Using the usual approach one has to introduce an additional boundary condition to solve this problem since the usual condition of tangential component continuity is not enough in the case of excitation of two modes.

Using the theory introduced in the previous section it is enough to substitute obtained wave vectors of eigenmodes into (55) when the reflection coefficient is calculated. The reflection coefficient is plotted at the bottom of Fig. 8. One can see that at the frequencies in the vicinity of the bottom and top edges of the band gap the semi-infinite crystal operate nearly as the electric and magnetic walls, respectively, as was predicted in Ref. 32. At the frequency $ka = 0.984$ the reflection coefficient is equal to +1 (electric wall), and at $ka = 1.044$ it is $-0.8 + 0.6j$ (nearly magnetic wall). Note that the frequency corresponding to the electric wall effect is not equal to the bottom edge of the band gap and there is no frequency exactly corresponding to the magnetic wall effect. By using the usual formulas for the reflection coefficient from the magnetic and Clausius-Mossotti formulas, which do not take into account the effects of spatial dispersion, one could get the idea that magnetic and magnetic wall effects have to happen at the edges of the band gap. Our study demonstrates that if the spatial dispersion is taken into account accurately then it is not so.

Thus, we have demonstrated how the proposed theory can be used for modeling the reflection from semi-infinite crystals with spatial dispersion. Our theory can be treated as a generalization of the results of Mahan and Obermair,[10] which have been widely applied for modeling of various kinds of reflection problems. We hope that the present generalization can find many more applications in the modeling of the reflection from spatially dispersive materials since it has no restriction on the period of the lattice to be smaller than the wavelength and allows us to consider electromagnetic crystals of the general kind.

## V. CONCLUSION

In this paper an approach for solving problems of plane-wave diffraction on semi-infinite electromagnetic crystals is proposed. The boundary conditions for the interface between isotropic dielectric and electromagnetic crystal of the general kind are deduced in the form of an infinite system of equations relating amplitudes of incident wave, excited eigenmodes, and scattered spatial harmonics. This system of equations represents mathematical content of the generalized Ewald-Oseen extinction principle which is formulated in this paper; the polarization of the semicrystal excited by the plane wave is distributed in such a way that it cancels the incident wave together with all high-order spatial harmonics associated with the periodicity of the boundary. In our opinion, the proof of the generalized Ewald-Oseen extinction principle presented in this paper is an important theoretical fact which helps us to understand the interrelation between reflection and dispersion properties of electromagnetic crystals. If the eigenmodes of the infinite crystal are known then the system can be solved numerically, which provides a numerical method for solving the diffraction problem under consideration. We believe in the quite good prospects for the application of the described method in further studies of dielectric and even metallic electromagnetic crystals at both microwave and optical ranges.

For the special case when the crystal is formed by small scatterers which can be effectively replaced by dipoles with fixed orientation, the deduced system of equations is solved analytically using a method of the characteristic function. The closed form expressions for the amplitudes of excited eigenmodes and scattered spatial harmonics are provided in terms of rapidly convergent products. These expressions can be treated as a generalization of the classical result of Mahan and Obermair[10] for the case when the period of the lattice can be large as compared to the wavelength. The proposed method is applied for the calculation of the reflection coefficient from semi-infinite crystal formed by resonant magnetic scatterers (split-ring resonators) at the frequencies corresponding to the strong spatial dispersion.

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