Macroscopic optical response and photonic bands

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Abstract. We develop a formalism for the calculation of the macroscopic dielectric response of composite systems made of particles of one material embedded periodically within a matrix of another material, each of which is characterized by a well-defined dielectric function. The nature of these dielectric functions is arbitrary, and could correspond to dielectric or conducting, transparent or opaque, absorptive and dispersive materials. The geometry of the particles and the Bravais lattice of the composite are also arbitrary. Our formalism goes beyond the long-wavelength approximation as it fully incorporates retardation effects. We test our formalism through the study of the propagation of electromagnetic waves in two-dimensional photonic crystals made of periodic arrays of cylindrical holes in a dispersionless dielectric host. Our macroscopic theory yields a spatially dispersive macroscopic response which allows the calculation of the full photonic band structure of the system, as well as the characterization of its normal modes, upon substitution into the macroscopic field equations. We can also account approximately for the spatial dispersion through a local magnetic permeability and analyze the resulting dispersion relation, obtaining a region of left handedness.
1. Introduction

The propagation of light within homogeneous materials is completely characterized by using their electromagnetic response. In the optical regime, magnetic effects are typically negligible so that knowledge of the dielectric response is sufficient for the study of wave propagation [1]. However, when the system has spatial inhomogeneities, the behavior of light is not trivial and this has captured the attention of many researchers [2–11]. As an example, plasmon–polariton spectra of quasiperiodic superlattices have been investigated [12, 13] and have been shown to have a fractal character. Novel effects have been obtained, for example, negative refraction, inverse Doppler effect, optical invisibility cloaking and optical magnetism, etc [14–17].

Effective medium theories [18–26] have been proposed for describing inhomogeneous systems, such as diluted colloidal suspensions in the quasistatic or long-wavelength limit, in terms of a homogeneous macroscopic response. Further developments on homogenization of composites have been proposed [27–35] and their limits of validity have been discussed [2, 36, 37].

In this paper, we obtain the macroscopic optical response using a computationally efficient reformulation of a procedure [5, 6] originally developed for accounting for the local field effect of systems with spatial fluctuations. Our main result is that for any system, the macroscopic response to an external excitation is simply the average projection of the corresponding microscopic response. We apply this general result to Maxwell equations in order to obtain an explicit expression for the macroscopic dielectric response of binary composites. We illustrate its use with numerical results for a two-dimensional (2D) periodic photonic crystal. As the wavelength of the electromagnetic field becomes comparable with the characteristic microscopic spatial lengthscale of the system, retardation effects become important, yielding a non-local [38, 39] macroscopic response, with a strong dependence on the wavevector besides its usual dependence on frequency. When the full spatial dispersion is taken into account, the photonic band structure of the system can be obtained and analyzed from its macroscopic response.

This paper is organized as follows. In section 2, we formulate a general theory for the macroscopic dielectric response of composite systems. In section 3, we adapt our formulation to periodic systems made of two alternating materials, each characterized by well-defined dielectric functions. In section 4, we develop an efficient computational scheme which allows

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4 See the special section on negative refraction and metamaterials for optical science and engineering in [17].
the numerical calculation of the macroscopic response without recourse to explicit operations between large matrices. In section 5, we obtain the non-local macroscopic dielectric tensor and use it to calculate macroscopically the full band structure of a 2D photonic crystal made up of non-dispersive dielectric components; we compare it with exact results as well as with results within a local approximation that partially accounts for spatial dispersion through an effective magnetic permeability. Finally, in section 6, we present the conclusions.

2. General theory

Consider a non-magnetic inhomogeneous system characterized by its dielectric response \( \hat{\epsilon} \), defined through the constitutive equation \( \mathbf{D} = \hat{\epsilon} \mathbf{E} \), where \( \mathbf{D} \) and \( \mathbf{E} \) are the microscopic displacement and electric fields, respectively. We designate these fields as microscopic as they have spatial fluctuations due to the inhomogeneities of the material. They are not microscopic in the atomic scale, but rather on the scale of the spatial inhomogeneities of the system. We use a caret (\( \hat{\ } \)) over a symbol to denote its operator nature and leave implicit the dependence of the dielectric response on position as well as on frequency. Our purpose is to obtain the macroscopic dielectric response of the system, relating the macroscopic displacement and electric fields, from which the fluctuations have been removed.

We start from Maxwell equations for monochromatic microscopic fields. We follow the usual procedure [40] to decouple the magnetic field from the electric field to obtain the second-order wave equation

\[
\hat{\mathbf{W}}\mathbf{E} = \frac{4\pi c}{i q} \mathbf{J}.
\]

(1)

where

\[
\hat{\mathbf{W}} = \hat{\epsilon} - \frac{1}{q^2} \nabla \times \nabla \times = \hat{\epsilon} + \frac{1}{q^2} \nabla^2 \hat{\mathbf{P}}^T
\]

(2)

is the wave operator, \( q = \omega/c \) is the wavenumber of light in vacuum, \( \omega \) is the frequency, \( c \) is the speed of light in vacuum and \( \mathbf{J} \) is the external electric current density. Here we introduced the transverse projector \( \hat{\mathbf{P}}^T \) such that the transverse projection of a field \( \mathbf{F} \) is \( \mathbf{F}^T = \hat{\mathbf{P}}^T \mathbf{F} \). For completeness, we also introduce the longitudinal projector \( \hat{\mathbf{P}}^L \) such that \( \hat{\mathbf{P}}^L + \hat{\mathbf{P}}^T = \hat{1} \), with \( \hat{1} \) the identity operator. Note that equation (1) contains both a longitudinal and a transverse part, so it describes not only transverse waves, but also allows for the possible excitation of longitudinal waves such as plasmons [41].

We solve equation (1) formally for \( \mathbf{E} \) to obtain

\[
\mathbf{E} = \frac{4\pi c}{i q} \hat{\mathbf{W}}^{-1} \mathbf{J}.
\]

(3)

As we are interested on the macroscopic response of the system, we introduce the average \( \hat{\mathbf{P}}_a \) and fluctuation \( \hat{\mathbf{P}}_f \) projectors, such that an arbitrary field \( \mathbf{F} \) can be written as \( \mathbf{F} = \mathbf{F}_a + \mathbf{F}_f \) with \( \mathbf{F}_a = \hat{\mathbf{P}}_a \mathbf{F} \) its average and \( \mathbf{F}_f = \hat{\mathbf{P}}_f \mathbf{F} \) its fluctuating part, and we identify the average field with the macroscopic field \( \mathbf{F}_a \equiv \mathbf{F}_M \). Later, we will provide appropriate explicit definitions for \( \hat{\mathbf{P}}_a \) and \( \hat{\mathbf{P}}_f \); here we remark that they must be idempotent \( \hat{\mathbf{P}}_a^2 = \hat{\mathbf{P}}_a, \hat{\mathbf{P}}_f^2 = \hat{\mathbf{P}}_f \), i.e. the average of the average is the average, and the fluctuations of the fluctuations are the fluctuations [5]. Furthermore, \( \hat{\mathbf{P}}_a \hat{\mathbf{P}}_f = \hat{\mathbf{P}}_f \hat{\mathbf{P}}_a = 0 \) and \( \hat{\mathbf{P}}_a + \hat{\mathbf{P}}_f = \hat{1} \).

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As the macroscopic response would be useless unless the **external excitations are devoid of microscopic spatial fluctuations**, we assume that the external current has no fluctuations, so \( \mathbf{J}_f = 0 \) and \( \mathbf{J} = \mathbf{J}_M = \hat{P}_a \mathbf{J}_M \), where we used the idempotency of \( \hat{P}_a \). Thus, acting on both sides of equation (3) with \( \hat{P}_a \) we obtain

\[
\mathbf{E}_M = \frac{4\pi c}{iq} \mathbf{W}^{-1}_a \mathbf{J}_M .
\]

Here we define \( \hat{O}_{\alpha\beta} \equiv \hat{P}_\alpha \hat{O} \hat{P}_\beta \), with \( \alpha, \beta = a,f \) for any operator \( \hat{O} \). As equation (4) relates the macroscopic external electric current to the macroscopic electric field, we may identify the macroscopic inverse wave operator \( \mathbf{W}^{-1}_M \),

\[
\mathbf{E}_M = \frac{4\pi c}{iq} \mathbf{W}^{-1}_M \mathbf{J}_M ,
\]

where

\[
\mathbf{W}^{-1}_M = \mathbf{W}^{-1}_a .
\]

We summarize this result stating that the macroscopic inverse wave operator is simply the average of the microscopic inverse wave operator. This is a particular case of a more general result: the macroscopic response to an external excitation is simply the average of the corresponding microscopic response.

From the macroscopic Maxwell equations, we may further relate the macroscopic wave operator in equations (5) and (6) to the macroscopic dielectric response of the system \( \hat{\epsilon}^M \) through

\[
\mathbf{W}^M = \hat{\epsilon}^M + \frac{1}{q^2} \nabla^2 \hat{P}_a \hat{P}_T
\]

in analogy to equation (2). Thus, we have to invert the wave operator, average it and invert it again to finally identify the macroscopic dielectric response. Note that we have made no approximation whatsoever. We remark that as \( \hat{\epsilon} \) relates to two fields, \( \mathbf{E} \) and \( \mathbf{D} \), that have spatial fluctuations, we may not simply average \( \hat{\epsilon} \) to obtain its macroscopic counterpart, i.e. \( \hat{\epsilon}^M \neq \hat{\epsilon}_a \).

The difference constitutes the **local field effect** [5].

Our result may easily be generalized to other situations and other response functions. The procedure consists of first identifying the response (in our case \( \mathbf{W}^{-1} \)) to the **external perturbation** (i.e. \( \mathbf{J} \)) and then averaging it to yield the corresponding macroscopic response (i.e. \( \mathbf{W}^{-1}_M = \mathbf{W}^{-1}_a \)), which may further be related to the **desired** macroscopic response operator (i.e. \( \hat{\epsilon}^M \)).

### 3. Periodic binary systems

In this section, we use equation (6) to obtain the optical properties of an artificial binary crystal made of two materials \( A \) and \( B \) with dielectric functions \( \epsilon_A \) and \( \epsilon_B \). We assume that both media are local and isotropic so that \( \epsilon_A \) and \( \epsilon_B \) are simply complex functions of the frequency. For convenience, we will further assume that \( \epsilon_A \) is real, although this assumption is easily relaxed [42].

We introduce the characteristic function \( B(\mathbf{r}) \) of the inclusions, such that \( B(\mathbf{r}) \equiv 1 \) whenever \( \mathbf{r} \) is on the region \( B \) occupied by the inclusions, and \( B(\mathbf{r}) \equiv 0 \) otherwise. Thus, we may write the microscopic dielectric response as

\[
\epsilon(\mathbf{r}) = \frac{\epsilon_A}{u} (u - B(\mathbf{r})) ,
\]

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where we defined the spectral variable \( u \equiv 1/(1 - \epsilon_B/\epsilon_A) \) \[19\]. The microscopic wave operator of equation (2) may be written as

\[
\hat{\mathcal{W}} = \frac{\epsilon_A}{u}(u\hat{g}^{-1} - \hat{B}),
\]

where the characteristic operator \( \hat{B} \) corresponds to multiplication by \( B(\mathbf{r}) \) in real space, and we defined

\[
\hat{g} = \left( \frac{\nabla^2 \hat{P}_T}{q^2 \epsilon_A} \right)^{-1},
\]

which, as shown below, plays the role of a metric.

Using equation (9) we write equation (6) as

\[
\hat{\mathcal{W}}_M^{-1} = \frac{u}{\epsilon_A} \hat{g}_{aa}(u - \hat{B}\hat{g})_{aa}^{-1},
\]

where we have taken advantage of the fact that \( \hat{g} \) is unrelated to the texture of the crystal, so that it does not couple the average to fluctuating fields.

Using Bloch’s theorem \[43\], we consider an electric field of the form \[21\]

\[
\mathbf{E}_k(\mathbf{r}) = \sum \mathbf{E}_G e^{i((k+G)\cdot \mathbf{r})},
\]

where \( k \) is a given wavevector, \( \{G\} \) is the reciprocal lattice of our crystal and the coefficients \( \mathbf{E}_G \) represent the field in reciprocal space. In this representation, all operators may be written as matrices with vector index pairs \( G, G' \), besides other possible indices, such as Cartesian ones. Thus, we represent the longitudinal projector as the matrix

\[
\mathcal{P}^{L}_{GG'} = \delta_{GG'} \frac{(k + G)(k + G')}{|k + G| |k + G'|}
\]

with \( \delta_{GG'} \) the Kronecker’s delta, so the transverse projector becomes \( \mathcal{P}^{T}_{GG'} = \mathbf{I} \delta_{GG'} - \mathcal{P}^{L}_{GG'} \) with \( \mathbf{I} \) the Cartesian identity matrix. The Laplacian operator in reciprocal space is represented by

\[
\nabla^2 \rightarrow -(k + G)^2 \delta_{GG'}
\]

and we can define the average projector as a cutoff in the reciprocal space \[6\]

\[
(\mathcal{P}_a)_{GG'} = \delta_{G0} \delta_{G'0},
\]

so that average fields simply keep the contributions with vector \( k \) while all other wavevectors are filtered out.

As shown by equation (11), we only require

\[
(u - \hat{B}\hat{g})_{aa}^{-1} = (u - \hat{B}\hat{g})_{00}^{-1}
\]

to obtain the macroscopic inverse wave operator, where the subindices \( 0 \) denote the projection onto the subspace with \( G = 0 \).
4. Recursive method

The calculation of equation (16) is analogous to that of a projected Green’s function [44, 45]
\[ G_{aa}(\varepsilon) = \langle a|\hat{G}(\varepsilon)|a \rangle \] (17)
on to a given state \(|a\rangle\), where
\[ \hat{G}(\varepsilon) = (\varepsilon - \hat{H})^{-1} \] (18)
is the Green’s operator corresponding to some Hermitian Hamiltonian \(\hat{H}\) and \(\varepsilon\) is a complex energy. In [28] a similar result was obtained, where the Hamiltonian \(\hat{H}\) was identified with the longitudinal projection of the characteristic function \(\hat{B}^{LL}\), the energy \(\varepsilon\) with the spectral variable \(u\), and \(|a\rangle\) with a slowly varying longitudinal wave, and it was shown that the corresponding projected Green’s function was proportional to the inverse of the longitudinal macroscopic dielectric function. Haydock’s method may be applied to obtain the projected Green’s function (17) in a very efficient way [46, 47], and it has been adapted previously [28] to the calculation of the optical response of nanostructured systems in the long-wavelength local limit. In this section, we generalize the approach of [28] to arbitrary frequencies and wavevectors.

Equations (17) and (18) are similar to equation (16), although the operator product \(\hat{H} = \hat{B}\hat{g}\) that plays the role of a Hamiltonian does not correspond to a symmetric matrix. Nevertheless, it would correspond to a Hermitian operator if we use \(\hat{g}\) as a metric, that is, if we use \(\langle \psi|\hat{g}|\phi \rangle\) instead of \(\langle \psi|\phi \rangle\) as the scalar product of two arbitrary states \(|\psi\rangle\) and \(|\phi\rangle\). Then, it is easy to verify the Hermiticity condition \([\langle \psi|\hat{g}(\hat{H}|\phi\rangle)]^* = \langle \phi|\hat{g}(\hat{H}|\psi\rangle\). Note, however, that \(\hat{g}\) is not positive definite.

According to equation (11), we need the average \((u - \hat{B}\hat{g})^{-1}_{aa} \rightarrow \langle a|(u - \hat{B}\hat{g})^{-1}|a \rangle\), where we projected onto an average state \(|a\rangle = b_0|0\rangle\) consisting of a plane wave with a given wavevector \(k\), frequency \(\omega\) and polarization \(e\). Here, \(|0\rangle\) is normalized according to the metric \(\hat{g}\), i.e. \(\langle 0|\hat{g}|0 \rangle = g_0 = \pm 1\), and the coefficient \(b_0\) is a real positive number chosen to guarantee that \(|a\rangle\) is normalized in the usual sense \((a|a\rangle) = 1\). Now, we define \(|-1\rangle \equiv 0\) and we obtain new states by means of the recursion relation
\[ |n + 1\rangle \equiv \hat{B}\hat{g}|n\rangle = b_{n+1}|n + 1\rangle + a_n|n\rangle + g_{n-1}b_n|n - 1\rangle, \] (19)
where all the states \(|n\rangle\) are orthonormalized according to the metric \(\hat{g}\), that is,
\[ \langle n|\hat{g}|m \rangle = g_n\delta_{nm} \] (20)
with \(g_n = \pm 1\) and \(\delta_{nm}\) the Kronecker’s delta function. The requirement of orthonormality yields the generalized Haydock coefficients \(a_n\), \(b_{n+1}\) and \(g_{n+1}\) given the previous coefficients \(b_n\), \(g_n\) and \(g_{n-1}\). Thus, \(a_n\) are obtained from
\[ \langle n|\hat{g}|n + 1\rangle = a_ng_n \] (21)
and \(b_{n+1}\) from
\[ \langle n + 1|\hat{g}|n + 1\rangle = g_{n+1}b_{n+1}^2 + g_n a_n^2 + g_{n-1}b_n^2, \] (22)
where we choose the sign $g_{n+1} = \pm 1$ so that $b_{n+1}^2$ is positive and we may choose $b_{n+1}$ as a real positive number. In the basis $|n\rangle$, $\hat{B}_g$ is represented by a tridiagonal matrix with $a_n$ along the main diagonal, $b_n$ along the subdiagonal and $g_{n-1} g_n b_n$ along the supradiagonal, so that

$$u - \hat{B}_g \rightarrow \begin{pmatrix} u - a_0 & -b_1 g_1 g_0 & 0 & 0 & \cdots \\ -b_1 & u - a_1 & -b_2 g_2 g_1 & 0 & \cdots \\ 0 & -b_2 & u - a_2 & -b_3 g_3 g_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$  \hspace{1cm} (23)

Note that we may represent the states $|n\rangle$ through the corresponding Cartesian field components for each reciprocal vector $G$ or for each position $r$ within a unit cell. Thus, the action of $\hat{g}$ is a trivial multiplication in reciprocal space, while that of $\hat{B}$ is a trivial multiplication in real space, and we may repeatedly compute $\hat{B}_g |n\rangle$ and Haydock’s coefficients without performing any large matrix multiplication, by alternatingly fast-Fourier transforming our representation between real and reciprocal space. More explicitly, we represent a state $|n\rangle$ through its components $n_{G,i} = \langle G, i | n\rangle$, where $| G, i \rangle$ corresponds to a normalized plane wave with wavevector $k + G$ and polarization $i$ along the $i$th Cartesian direction. Then, $\hat{g} |n\rangle$ is represented by $\phi_{G,i} = \langle G, i | \hat{g} | n\rangle = g_{ij}(G) n_{G,j}$, where, according to equation (10),

$$g_{ij}(G) = \frac{\epsilon_s q^2 \delta_{ij} - (k_i + G_i) (k_j + G_j)}{\epsilon_s q^2 - (k + G)^2}$$ \hspace{1cm} (24)

is a small Cartesian matrix for each $G$. Performing a fast Fourier transform, we obtain $\langle r, i | \phi \rangle = \phi_{r,i}$ in real space, which we then multiply by $B(|r\rangle)$ to obtain $|n+1\rangle$, represented in real space by $(n+1)_{r,i} = B(|r\rangle) \phi_{r,i}$. Fourier transforming back into reciprocal space and orthonormalizing, we obtain Haydock coefficients $a_n$, $b_{n+1}$ and $g_{n+1}$, and the new state $|n+1\rangle$ represented by $(n+1)_{G,i} = \langle G | n+1 \rangle$. As discussed above, we iterate this procedure to obtain enough coefficients to converge the continued fraction (25).

According to equation (11), we do not require the full inverse of the matrix (23), but only the element in the first row and the first column. Following [28], we obtain that element as a continued fraction, which when substituted into equation (11) yields

$$\hat{W}_M^{-1} \rightarrow \sum_{ij} e_i (W_M^{-1})_{ij} e_j = \frac{u}{\epsilon_A u - a_0 - \frac{g_0 b_0^2}{u - a_1 - \frac{g_1 b_1^2}{u - a_2 - \frac{\epsilon_s q^2}{\epsilon_s q^2 - (k + G)^2}}}}.$$ \hspace{1cm} (25)

The right-hand side of equation (25) denotes the macroscopic response projected onto a state with the given wavevector $k$, frequency $\omega$ and polarization $e$. Due to the translational invariance of the homogenized system, the inverse wave operator for a given $k$ corresponds simply to a tensor with Cartesian components $(W_M^{-1})_{ij}$. Thus, so far we have calculated its inner products with $e$, as shown by the second term of equation (25). We may repeat the calculation above for different orientations of the (possibly complex) unit polarization vector $e$ and solve the resulting equations for all the individual Cartesian components $(W_M^{-1})_{ij}$. Finally, we perform a matrix inversion of this macroscopic tensor and we use equations (6) and (7) to compute the macroscopic dielectric tensor

$$\epsilon_{ij}^M(\omega, k) = \frac{1}{q^2} (k^2 \delta_{ij} - k_i k_j) + \chi_{ij}^M(\omega, k).$$ \hspace{1cm} (26)
Figure 1. Longitudinal macroscopic dielectric function $\epsilon_M^L(\omega)$ of a 2D system (inset) made up of a square array with lattice parameter $a$ of empty cylindrical holes ($\epsilon_B = 1$) of circular cross section with radius $\rho = 0.45a$ within a dielectric medium with permittivity $\epsilon_A = 12$. We show the results of using the Maxwell–Garnett (MG) formula, of a non-retarded (NR) calculation, of a numerically exact matrix calculation (diamonds) and of our theory (solid lines) for two different lattice parameters $a = 40$ and 120 nm.

Equations (25) and (26) constitute the main result of our formalism. Note that, in general, this dielectric tensor would depend on both $\omega$ and $k$, that is, it is a temporal and spatially dispersive response function.

5. Results

To test our formalism, we first calculate the local limit of the longitudinal macroscopic dielectric function $\epsilon_M^L(\omega) \equiv \epsilon_M^L(\omega, k \to 0\hat{x})$ of a 2D system made up of a square array of empty cylindrical holes ($\epsilon_B = 1$) placed with lattice parameter $a$ within a dielectric medium with permittivity $\epsilon_A = 12$. The holes are of circular cross section with radius $\rho = 0.45a$. We assume that the axes of the cylinders are parallel to the $z$-axis. This system has been frequently been used as a testground for calculations of photonic crystal properties [48]. In this calculation, we took the limit $k \to 0$ along the $x$-direction, and we introduced the Cartesian unit vectors $\hat{x}$, $\hat{y}$ and $\hat{z}$. We remark that it is important to assign a direction to $k$ even in this limit, as the transverse T and longitudinal L projection of $\chi_M^d$ differ, although, for this system, the resulting $\epsilon_M^L(\omega) = \epsilon_M^L(\omega, k \to 0\hat{x})$ is isotropic within the $xy$-plane.

In figure 1, we show $\epsilon_M^L(\omega)$ calculated for two different lattice parameters $a = 40$ and 120 nm. Our calculations were performed using the Perl Data Language [49]. The figure shows that our formalism yields the same results as a full straightforward matricial calculation [32] that solves Maxwell equations in a plane wave basis. Nevertheless, our calculation is much more economical in memory usage, as we do not have to store the full matrices that represent the dynamics of the system, and is at least four orders of magnitude faster as we do not perform any matrix manipulation with our scheme. For example, to obtain a 1% accuracy, we used an $N \times N$ reciprocal lattice and an $N \times N$ pixel image of the system in real space, where $N \approx 10^2$;

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Figure 2. Out-of-plane macroscopic dielectric function $\epsilon^M_T(\omega, k_\Delta)$ of the same system as in figure 1 for a given wavevector $k_\Delta$ along the $\Delta$ line of the first BZ (solid lines). The line $(k_\Delta/q)^2$ (long dashes) intersects (circles) $\epsilon^M_T(\omega, k_\Delta)$ at the frequencies $\omega_{\alpha}(k_\Delta)$ of the TE normal modes, with $\alpha = I, II, IV$ and $V$. The intersections (diamonds) of $\epsilon^M_T(\omega, k_{\Delta}')$ (short dashes) with $(k_{\Delta}')^2$ (long dashes) corresponding to a shifted wavevector $k_{\Delta}' = k_\Delta + (2\pi/\alpha)y$ yield the modes $\alpha = III$ and IV (see the text).

we have verified that the accuracy of our calculation scales with $1/N$. An in-plane field is described by two coordinates for each reciprocal vector. Thus, to represent a state requires $2N^2$ numbers. The matrix calculation of [32] would require calculating, storing, multiplying and solving equations with $2N^2 \times 2N^2$ matrices that have $\approx 4 \times 10^8$ elements, while our calculation only manipulates vectors with $\approx 2 \times 10^4$ elements. Thus, each point in figure 1 requires several hours when parallelized and run in a cluster with 40 cores, while it took a few seconds in one CPU of a laptop.

To illustrate the effects of retardation, in the figure we also show the result of using the non-retarded (NR) calculation of [28], together with those of the well-known 2D MG effective medium formula [21]. As the dielectric functions of the components are independent of the frequency, since the constituents were taken to be non-dispersive, in this case the frequency dependence of the result arises solely from the finite ratio of the free space wavelength to the lengthscale of the system, namely, the lattice parameter $a$. Thus, in the $\omega \to 0$ limit our results approach those of the NR calculation. The difference between the NR and MG calculations is due to the high filling fraction $f \approx 0.64$ of the cylinders, which interact non-dipolarly with their nearest neighbors which they almost touch, while MG contains only dipolar interactions. Naturally, retardation effects become stronger as $a$ increases. Furthermore, $\epsilon^M_T(\omega, k)$ depends only on the products $qa$ and $ka$ so that the two curves shown in figure 1 could be collapsed into one curve if appropriately plotted. We use this in figure 2, which shows the transverse response $\epsilon^M_T(\omega, k_\Delta) = \epsilon^M_Z(\omega, k_\Delta)$ corresponding to out-of-plane or transverse electric (TE) polarization as a function of the normalized frequency $qa/2\pi$. Here, we have chosen a finite in-plane wavevector $k_\Delta = (\pi/2a, 0, 0)$, corresponding to the midpoint of the $\Delta$ line between $\Gamma$ and $X$ in the first Brillouin zone (BZ) [43]. This figure covers a larger frequency range than figure 1 and therefore it displays a series of poles related to resonant multiple coherent reflections at the interfaces between the $A$ and $B$ regions.
Figure 3. Photonic bands of the TE modes of the same system as in figure 1 obtained by solving equation (27) (circles). For comparison, we also show the photonic bands obtained from the solution of the corresponding eigenvalue problem, equation (28), as described in the text (solid lines). We also show the modes obtained by shifting the wavevector \( k \rightarrow k' = k + (2\pi/a)y \) (diamonds).

The dispersion relation of transverse waves with TE polarization propagating along the \( xy \)-plane can be simply written as [50]

\[
\varepsilon_T^M(\omega, k) = \frac{k^2}{q^2}.
\] (27)

Therefore, in figure 2 we also plotted the curve \((k_\Delta/q)^2\). Those points where it intersects the curves for \( \varepsilon_T^M \) correspond to normal TE modes of the system with frequencies \( \omega_\alpha(k = k_\Delta) \), \( \alpha = I, II, \ldots \). Here, we use roman numerals to number the modes in increasing frequency order.

In figure 3, we show the photonic bands (circles) of the TE modes of our system obtained by solving the dispersion relation (27) as \( k \) travels along the line \( \Gamma - \Delta - X - Z - M - \Sigma - \Gamma \) within the first BZ. In order to test our theory, we also plot the TE modes obtained by solving the eigenvalue equation [51]

\[
\left( \frac{1}{\sqrt{\varepsilon(r)}} \nabla^2 \frac{1}{\sqrt{\varepsilon(r)}} \right) \left( \sqrt{\varepsilon(r)} E_z(r) \right) = -\frac{\omega^2}{c^2} \left( \sqrt{\varepsilon(r)} E_z(r) \right)
\] (28)

through an implicitly restarted Arnoldi iteration [52], applying \( 1/\sqrt{\varepsilon(r)} \) in real space and \( \nabla \rightarrow i(k + G) \) in reciprocal space [42]. We further verified our results by recalculating them with the freely available MIT Photonic-Bands Package (MPB) [53] and comparing it with previous results [48] for the same system. The agreement between these calculations shows that it is feasible to use the macroscopic dielectric response of the system to obtain its photonic band structure. However, to succeed, we have to account fully for the spatial dispersion of \( \varepsilon_T^M(\omega, k) \).

We remark that although we obtained the correct photonic bands even for large wavevectors, going all the way around the first BZ, there are some regions where we failed to obtain all of the normal modes. For example, our procedure did not produce the third band (labeled III in the figure) along the \( \Delta \) line, nor the fourth band (IV) along the \( \Sigma \) line, between \( M \) and \( \Gamma \). Furthermore, it did not yield the second band (II), which is almost degenerate with the third band (III) along \( \Sigma \). It is easily shown that the microscopic field corresponding to the missing band along \( \Delta \) is antisymmetric with respect to the reflection \( G_y \leftrightarrow -G_y \) about the \( \Delta \)
line. Similarly, the missing bands along the region $\Sigma$ are antisymmetric with respect to the reflection $G_y \leftrightarrow G_x$ about the $\Sigma$ line. Thus, the reciprocal vector $0$ does not contribute to the electric field for those bands [54], i.e. the missing modes have no macroscopic field components and thus, apparently, they may not be obtained from the roots of the macroscopic dispersion relation (27).

Nevertheless, within our formalism, the wavevector $k$ is actually not restricted to lie within the first BZ. Thus, we may calculate the macroscopic dielectric function for wavevectors beyond the first BZ, and obtain the modes in the extended scheme. In figure 2, we show part of the macroscopic dielectric function $\varepsilon^M_\perp(\omega, k_\perp)$ with a wavevector that has been shifted out of the first BZ from $k_\perp$ along the $y$-direction by the reciprocal vector $(2\pi/a)y$, i.e. $k_\perp' = k_\perp + (2\pi/a)y$. We remark that $\varepsilon^M(\omega, k)$ is not a periodic function of $k$, as it corresponds to a specific plane wave, not to a microscopic Bloch’s wave. The intersection of the curve $(k_\perp'/q)^2$ with $\varepsilon^M_\perp(\omega, k_\perp')$ yields the corresponding macroscopic modes. For example, the diamonds in figure 2 illustrate two of the normal modes that could be obtained using this shifting procedure. One of these modes is identical to the mode labeled IV that was obtained previously using the unshifted response $\varepsilon^I_\perp(\omega, k_\perp)$. Nevertheless, another mode, labeled III, appears just below $qa/2\pi = 0.4$ and corresponds to one of the previously missing modes. We may shift it back into the first BZ in order to display it in the reduced zone scheme. Proceeding in this fashion, we have obtained all of the previously missing bands, shown by diamonds in figure 3. Thus, we have shown that we can calculate the full photonic band structure for the TE modes from the macroscopic non-local dielectric function of the composite system. The converse, obtaining the non-local response from the dispersion relation [38], can also be attempted, although the results would not be uniquely defined and are not expected to be valid for wavevectors and frequencies that do not lie in the dispersion relation. Our procedure has no such limitation.

A similar procedure to that discussed above can be employed also for the transverse magnetic (TM) modes (with an out of plane magnetic field) of the system, with the electric field within the $xy$-plane. In figure 4, we show the in-plane macroscopic dielectric function $\varepsilon_{xx}^M(\omega, k_\perp)$ and $\varepsilon_{yy}^M(\omega, k_\perp)$ of the system for the same wavevector $k_\perp$, as in figure 2. This wavevector and the system are symmetric under $y \leftrightarrow -y$ reflections. Therefore, $\varepsilon_{xy}^M = 0$ and we may identify the transverse and longitudinal responses as $\varepsilon^M_\perp(\omega, k_\perp) = \varepsilon_{yy}^M(\omega, k_\perp)$ and $\varepsilon^M_L(\omega, k_\perp) = \varepsilon_{xx}^M(\omega, k_\perp)$, respectively. The normal modes are then obtained from the transverse dispersion relation (27) and the longitudinal dispersion relation [50]

\[
\varepsilon^M_L(\omega, k) = 0.
\]

These are identified with circles and diamonds in the figure.

In figure 5, we perform a similar calculation but along the $\Sigma$ line, for the wavevector $k_\Sigma = (\pi/2a, \pi/2a)$. Along this line, the wavevector and the system are symmetric under the reflection $x \leftrightarrow y$, and thus $\varepsilon_{xx}^M(\omega, k_\Sigma) = \varepsilon_{yy}^M(\omega, k_\Sigma)$. We may now identify the transverse and longitudinal responses as $\varepsilon^M_\perp(\omega, k_\Sigma) = \varepsilon_{xx}^M(\omega, k_\Sigma) - \varepsilon_{yy}^M(\omega, k_\Sigma)$ and $\varepsilon^M_L(\omega, k_\Sigma) = \varepsilon_{xx}^M(\omega, k_\Sigma) + \varepsilon_{yy}^M(\omega, k_\Sigma)$, respectively. In figure 5(a), we show $\varepsilon^M(\omega, k_\Sigma)$, $(k_\Sigma/q)^2$ and their intersections (circles) which yield the transverse modes, while in figure 5(b), we display $\varepsilon^M_L(\omega, k_\Sigma)$ and its zero (diamond) which correspond to a longitudinal mode.

Along the $Z$ line, from $X$ to $M$, there is no crystal symmetry operation that leaves the wavevector invariant, and thus transverse and longitudinal fields mix among themselves, i.e. there are no longitudinal or transverse modes. Nevertheless, we may obtain the frequencies of
Figure 4. (a) In-plane macroscopic dielectric functions $\epsilon^M_T(\omega, k)\Delta_1$ and (b) $\epsilon^M_L(\omega, k)\Delta_1$ of the same system as in figure 1 for the same wavevector $k\Delta_1$ as in figure 2. The line $(k\Delta/q)^2$ (dashes) intersects (circles) $\epsilon^M_T(\omega, k)\Delta_1$ at the frequencies $\omega_\alpha(k\Delta)$ of the TM transverse normal modes, with $\alpha = I$, II and IV. The zeros (diamonds) of $\epsilon^M_L(\omega, k)\Delta_1$ yields the longitudinal mode III (see the text).

the mixed modes through the singularities of the wave operator matrix

$$\det [\mathcal{W}^M(\omega, k)] = 0$$

as illustrated in figure 6 for a wavevector $k_Z = (\pi/a, \pi/2a)$ along the Z line.

From calculations such as those illustrated by figures 4–6, or more generally, from the zeros of $\det [\mathcal{W}^M(\omega, k)]$ for arbitrary wavevectors $k$, we can obtain the full TM photonic band structure, as shown by figure 7. In order to test our theory, we also plot the TM modes obtained by solving the eigenvalue equation [51]

$$\nabla \cdot \frac{1}{\epsilon(r)} \nabla B_z(r) = -\frac{\omega^2}{c^2} B_z(r)$$

using similar methods [42, 52] as for the TE case and comparing them successfully with previous results [48] for the same system. The agreement between these calculations shows that it is also feasible to use the macroscopic dielectric response of the system for obtaining its photonic band structure in the TM case.

An approximate band structure could be obtained for transverse waves in the region of small wavevectors $k \to 0$ by expanding the lhs of equation (27) up to second order in $k$ and
Figure 5. (a) In-plane macroscopic dielectric functions $\epsilon^M_T(\omega, k_\Sigma)$ and (b) $\epsilon^M_L(\omega, k_\Sigma)$ of the same system as in figure 1 for a given wavevector $k_\Sigma$ along the $\Sigma$ line. The line $(k_\Sigma/q)^2$ (dashes) intersects (circles) $\epsilon^M_T(\omega, k_\Sigma)$ at the frequencies $\omega_\alpha(k_\Sigma)$ of the TM transverse normal modes, with $\alpha = I$, II and IV. The zeros (diamonds) of $\epsilon^M_L(\omega, k_\Sigma)$ yield the longitudinal mode III (see the text).

Figure 6. Determinant of the macroscopic wave operator matrix $\mathcal{W}^M(\omega, k_Z)$ for a given wavevector $k_Z$ along the $Z$ line. The normal modes of the system $\omega_\alpha(k_Z)$, $\alpha = I$–IV, correspond to its zeros (squares).
The modes between $\Gamma$ and $X$ and between $M$ and $\Gamma$ may be obtained by solving equation (27) for the transverse (T) modes (circles) and equation (29) for the longitudinal (L) modes (diamonds) or equation (30) for both of them. The modes from $X \rightarrow M$ are obtained from equation (30) and have a mixed polarization (squares). For comparison, we also show the photonic bands obtained from the solution of the corresponding eigenvalue problem, equation (31), as described in the text (solid lines).

Solving for $k^2$. The result is a local dispersion relation

$$k^2 = q^2 \epsilon^M(\omega)\mu(\omega), \quad (32)$$

where the non-locality of $\epsilon^M(\omega, \mathbf{k})$ is partially accounted for through an effective magnetic permeability [25],

$$\mu(\omega) = \left. \frac{1}{1 - \frac{q^2}{2} \frac{\partial^2}{\partial k^2} \epsilon^M(\omega, k\mathbf{x})} \right|_{k=0}. \quad (33)$$

In figure 8(a), we show the resulting approximate bands for the TE case. We can see that the acoustic band within the local approximation is indistinguishable from the exact result for small wavevectors. This local acoustic band extends up to the frequency $qa/2\pi \approx 0.2$ for which $\mu$ has a pole, see figure 8(c). The local approximation also reproduces the upper band of the exact calculation (labeled V in figure 3), but only in the immediate vicinity of $\Gamma$, close to the zero $qa/2\pi \approx 0.43$ of $\epsilon^M(\omega)$. For larger wavevectors it acquires a larger positive dispersion. As discussed above, the band labeled III in figure 3 does not couple to macroscopic fields for $\mathbf{k}$ along the $\Delta$ line, while the band labeled IV does not couple along the $\Sigma$ line. Thus, neither band couples to macroscopic fields at $\Gamma$, and as a consequence, these bands are not reproduced at all by the local approximation (32).

In the region $qa/2\pi \approx 0.36$–0.40, the local approximation predicts a curious band that displays backbending. Its lower part begins at the pole of $\epsilon^M(\omega)$, which corresponds to a double zero of $\mu(\omega)$ [42]. This part of the local dispersion relation is spurious, as the second-order Taylor expansion of the dielectric function that yields equations (33) and (32) starting from equation (27) would be meaningless at a pole. Consequently, this part of the local band does not correspond to any band within the exact calculation. On the other hand, the upper part of the backbending band starts at a simple zero of $\mu$, which arises from a different kind of singular
Figure 8. (a) Local dispersion relation for the same system as in figure 1 for the TE case (solid line), obtained from equation (32). (b) Local dielectric function $\epsilon^M(\omega)$. (c) Local magnetic permeability $\mu(\omega)$ (solid line) and $10^4 \mu(\omega)$ (dash-dotted line). For comparison purposes, we also show the exact dispersion relation of (a) (dashed line).

behavior, consisting of a pole in $\epsilon^M_T(\omega, k)$ at $qa/2\pi \approx 0.40$, which is suppressed at $k = 0$ as its weight is approximately proportional to $k^2$. This part of the local dispersion relation agrees with band II of figure 3 at $\Gamma$ and displays a negative dispersion as does band II. Furthermore, for this band, both $\epsilon^M$ and $\mu$ are negative. Thus, our photonic crystal, made up of holes within a dispersionless dielectric, behaves for some frequencies like a left-handed metamaterial [55, 56]. Nevertheless, caution should be exercised when using equations (33) and (32) close to singularities of $\epsilon^M_T(\omega, k)$.

6. Conclusions

We have shown that the macroscopic inverse wave operator of composite systems with arbitrary spatial fluctuations is simply given by the average projection of the corresponding microscopic operator. These operators may be related to the macroscopic and microscopic dielectric functions respectively, thus yielding a general procedure for incorporating the effects of spatial fluctuations into the calculation of all the components of the macroscopic dielectric tensor of the system. We have extended Haydock’s recursive scheme in order to calculate very efficiently the response of periodic two-component systems in terms of a continued fraction whose coefficients may be obtained without recourse to operations with the large matrices that characterize the microscopic response and the field equations. We illustrated and tested our results through the calculation of the wavevector and frequency-dependent macroscopic dielectric tensor of a 2D dielectric system with non-dispersive non-dissipative components. We identified the transverse and longitudinal components of the response for wavevectors along symmetry lines and obtained all the components of the tensorial response for the case of reduced symmetry. The macroscopic response has a series of poles, related to resonant multiple coherent reflections, and by accounting for its spatial dispersion we obtained the full photonic band structure of the system from the dispersion relations corresponding to the homogenized material. Besides yielding the correct bands from a macroscopic approach, our
scheme allowed us to classify the polarization of each mode as either transverse, longitudinal or mixed. Even though the macroscopic approach might fail to yield some modes, namely, those which have no coupling to the macroscopic field due to symmetry, they may be recovered by extending the notion of macroscopic state, allowing its wavevector to lie beyond the first BZ. The non-locality of the dielectric response may be partially accounted for through a magnetic permeability which can then be employed in the calculation of the optical properties of the system. We compared the band structure obtained through this local approximation to the exact results and we obtained partial agreement close to $\Gamma$ for those bands that do couple to long wavelength fields. In particular, we showed that this approach can yield a negative dispersion in frequency regions where both the permittivity and permeability are negative. Nevertheless, we discussed some shortcomings of the local approach. Although here we presented results for dispersionless transparent dielectrics, our calculation does not require that the materials that make up the system be non-dispersive or non-dissipative, so that calculations for real dielectrics and metals may be performed with the same low computational costs.

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**References**

[1] Brédov M, Rumiantsev V and Toptiguin L 1985 *Classical Electrodynamics* (Moscow: Mir)
[2] Notomi M 2000 Theory of light propagation in strongly modulated photonic crystals: refraction-like behavior in the vicinity of the photonic band gap *Phys. Rev.* B **62** 10696–705
[3] Barrera R G, Reyes-Coronado A and García-Valenzuela A 2007 Nonlocal nature of the electrodynamic response of colloidal systems *Phys. Rev.* B **75** 184202
[4] Yeh P, Yariv A and Hong C-S 1977 Electromagnetic propagation in periodic stratified media: I. General theory *J. Opt. Soc. Am.* **67** 423–38
[5] Luis Mochán W and Barrera R G 1985 Electromagnetic response of systems with spatial fluctuations: I. General formalism *Phys. Rev.* B **32** 4984–8
[6] Luis Mochán W and Barrera R G 1985 Electromagnetic response of systems with spatial fluctuations: II. Applications *Phys. Rev.* B **32** 4989–5001
[7] Kosaka H, Kawashima T, Tomita A, Notomi M, Tamamura T, Sato T and Kawakami S 1998 Superprism phenomena in photonic crystals *Phys. Rev.* B **58** R10096–9
[8] Stroud D and Pan F P 1978 Self-consistent approach to electromagnetic wave propagation in composite media: application to model granular metals *Phys. Rev.* B **17** 1602–10
[9] Ortiz G P and Mochán W L 2003 Scaling of light scattered from fractal aggregates at resonance *Phys. Rev.* B **67** 184204
[10] Ortiz G P and Mochán W L 2003 Scaling condition for multiple scattering in fractal aggregates *Physica* B **338** 54
[11] Hilke M 2009 Seeing Anderson localization *Phys. Rev.* A **80** 063820
[12] Vasconcelos M S and Albuquerque E L 1993 Plasmon–polariton fractal spectra in quasiperiodic multilayers *Phys. Rev.* B **57** 2826–33
[13] Albuquerque E L and Cottam M G 1993 Superlattice plasmon–polaritons *Phys. Rep.* **233** 67–135

*New Journal of Physics* **15** (2013) 043037 (http://www.njp.org/)
[14] Chen J et al 2011 Observation of the inverse doppler effect in negative-index materials at optical frequencies Nature Photon. 5 239–45
[15] Zhang B, Luo Y, Liu X and Barbastathis G 2011 Macroscopic invisibility cloak for visible light Phys. Rev. Lett. 106 033901
[16] Lezec H J, Dionne J A and Atwater H A 2007 Negative refraction at visible frequencies Science 316 430–2
[17] Urzhumov Y A and Shvets G 2008 Optical magnetism and negative refraction in plasmonic metamaterials Solid State Commun. 146 208–20
[18] Milton G W, McPhedran R C and McKenzie D R 1981 Transport properties of arrays of intersecting cylinders Appl. Phys. A 25 23–30
[19] Bergman D J and Dunn K-J 1992 Bulk effective dielectric constant of a composite with a periodic microgeometry Phys. Rev. B 45 13262–71
[20] Tao R, Chen Z and Sheng P 1990 First-principles Fourier approach for the calculation of the effective dielectric constant of periodic composites Phys. Rev. B 41 2417–20
[21] Datta S, Chan C T, Ho K M and Soukoulis C M 1993 Effective dielectric constant of periodic composite structures Phys. Rev. B 48 14936–43
[22] Alexopoulos A 2010 Effective-medium theory of surfaces and metasurfaces containing two-dimensional binary inclusions Phys. Rev. E 81 046607
[23] Doyle W T 1989 Optical properties of a suspension of metal spheres Phys. Rev. B 39 9852–8
[24] Ludwig A and Webb K J 2010 Accuracy of effective medium parameter extraction procedures for optical metamaterials Phys. Rev. B 81 113103
[25] Costa J T, Silveirinha M G and Maslovski S I 2009 Finite-difference frequency-domain method for the extraction of effective parameters of metamaterials Phys. Rev. B 80 235124
[26] Ortiz G P, L´opez-Bastidas C, Maytorena J A and Moch´an W L 2003 Bulk response of composite from finite samples Physica B 338 103
[27] Silveirinha M G 2006 Nonlocal homogenization model for a periodic array of epsilon-negative rods Phys. Rev. E 73 046612
[28] Mochan L W, Ortiz G P and Mendoza B S 2010 Efficient homogenization procedure for the calculation of optical properties of 3D nanostructured composites Opt. Express 18 22119–27
[29] Myroshnychenko V and Brosseau C 2010 Analysis of the effective permittivity in percolative composites using finite element calculations Proc. 8th Int. Conf. on Electrical Transport and Optical Properties of Inhomogeneous Media, ETOPIM-8; Physica B 405 3046–9
[30] Guenneau S, Zolla F and Nicolet A 2007 Homogenization of 3D finite photonic crystals with heterogeneous permittivity and permeability Waves Random Media 17 653–97
[31] C˘abuz A I, Nicolet A, Zolla F, Felbacq D and Bouchit´e G 2011 Homogenization of nonlocal wire metamaterial via a renormalization approach J. Opt. Soc. Am. B 28 1275–82
[32] Ortiz G P, Mart´ınez-Z´erega B E, Mendoza B S and Moch´an L W 2009 Effective optical response of metamaterials Phys. Rev. B 79 245132
[33] Raghunathan S B and Budko N V 2010 Effective permittivity of finite inhomogeneous objects Phys. Rev. B 81 054206
[34] Halevi P, Krokhin A A and Arriaga J 1999 Photonic crystal optics and homogenization of 2D periodic composites Phys. Rev. Lett. 82 719–22
[35] Reyes-Arenda˜no J A et al 2011 From photonic crystals to metamaterials: the bianisotropic response New J. Phys. 13 073041
[36] Simovski C R 2011 On electromagnetic characterization and homogenization of nanostructured metamaterials J. Opt. 13 013001
[37] Menzel C, Paul T, Rockstuhl C, Pertsch T, Tretyakov S and Lederer F 2010 Validity of effective material parameters for optical fishnet metamaterials Phys. Rev. B 81 035320
[38] Elser J, Podolskiy V A, Salakhutdinov I and Avrutsky I 2007 Nonlocal effects in effective-medium response of nanolayered metamaterials Appl. Phys. Lett. 90 191109

New Journal of Physics 15 (2013) 043037 (http://www.njp.org/)
[39] Barrera R G, Reyes-Coronado A and García-Valenzuela A 2005 Nonlocal effective medium for the electromagnetic response of colloidal systems: a t-matrix approach Progress in Electromagnetic Research Symp. (Hangzhou, China, 2005) pp 646–9
[40] Jackson J D 1998 Classical Electrodynamics (New York: Wiley)
[41] Mochán L W 2005 Plasmons Encyclopedia of Condensed Matter Physics ed G Bassani, G Liedl and P Wyder p 310–17
[42] Pérez-Huerta J S, Mendoza B S, Ortiz G and Luis Mochán W in preparation
[43] Sakoda K 2004 Optical Properties of Photonic Crystals (Springer Series in Optical Sciences) (Berlin: Springer)
[44] Sutton A P 2004 Electronic Structure of Materials (Oxford: Oxford University Press)
[45] Datta S 1997 Electronic Transport in Mesoscopic Systems (Cambridge Studies in Semiconductor Physics and Microelectronic Engineering) (Cambridge: Cambridge University Press)
[46] Haydock R, Heine V and Kelly M J 1972 Electronic structure based on the local atomic environment for tight-binding bands J. Phys. C: Solid State Phys. 5 2845
[47] Haydock R, Heine V and Kelly M J 1975 Electronic structure based on the local atomic environment for tight-binding bands: II J. Phys. C: Solid State Phys. 8 2591
[48] Busch K, von Freymann G, Linden S, Mingaleev S F, Tkeshelashvili L and Wegener M 2007 Periodic nanostructures for photonics Phys. Rep. 444 101–202
[49] Glazebrook K and Economou F 1997 PDL: the Perl data language Dr. Dobb’s J. 9719 45
[50] Landau L D and Lifshits E M 1984 Electrodynamics of continuous media Course of Theoretical Physics (Oxford: Pergamon)
[51] Joannopoulos J D, Johnson S G, Winn J N and Meade R D 2008 Photonic Crystals: Molding the Flow of Light 2nd edn (Princeton, NJ: Princeton University Press)
[52] Saad Y 2011 Numerical Methods for Large Eigenvalues Problems (Philadelphia: SIAM)
[53] Johnson S G and Joannopoulos J D 2001 Block-iterative frequency-domain methods for Maxwell’s equations in a plane-wave basis Opt. Express 8 173–90
[54] Robertson W M and Arjavalingam G 1992 Measurement of photonic band structure in a two-dimensional periodic dielectric array Phys. Rev. Lett. 68 2023
[55] Peng L, Ran L, Chen H, Zhang H, Kong J A and Grzegorczyk T M 2007 Experimental observation of left-handed behavior in an array of standard dielectric resonators Phys. Rev. Lett. 98 157403
[56] Vynck K, Felbacq D, Centeno E, Cábuz A I, Cassagne D and Guizal B 2009 All-dielectric rod-type metamaterials at optical frequencies Phys. Rev. Lett. 102 133901