Electromagnetic Wave Propagation in Periodic Structures: Bloch Wave Solution of Maxwell's Equations

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We examine the propagation of electromagnetic waves in periodic dielectric structures by solving the vector Maxwell equations with the plane-wave method. Contrary to experimental reports as well as results of scalar-wave calculations, we do not find a true gap extending throughout the Brillouin zone in the fcc structure. However, there is a depletion in the photon density of states, seemingly a remnant of the Mie resonance, giving rise to a pseudogap in the spectrum which is quite strong for dielectric-sphere packing fraction $\beta \sim 0.3-0.4$. An effect analogous to the Borrman effect in x-ray diffraction is predicted where certain photon modes will propagate an anomalously long distance before getting absorbed.

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The propagation of electromagnetic (EM) waves in a medium with a collection of scatterers is an old problem\textsuperscript{1,2} having to do with such diverse subjects such as x-ray diffraction in crystals, the blue color of the sky, the theory of rainbows, light scattering from interstellar dusts, rainfall measurement using radar, etc. In the last four examples the scatterers are randomly distributed in the medium. Recently, there has been growing interest in EM wave propagation in man-made structures with a periodic array of scatterers of macroscopic dimensions. New stimulus for this has been provided by the experiments of Yablonovitch and Gmitter,\textsuperscript{3} where the existence of photon bands in the fcc crystal of dielectric spheres has been demonstrated and the possibility of the existence of a band gap in the “photonic band structure” has been raised.

In the frequency range of the photonic gap the EM wave would not propagate through the medium but rather would decay exponentially. Such a structure could exhibit potentially new physical phenomena such as inhibition of electron-hole radiative recombination if the corresponding photon frequency falls in the gap region.\textsuperscript{4} For an atom or molecule left in such a medium, John and Wang have recently suggested that the single-photon spontaneous emission is inhibited and a qualitatively new quantum electrodynamical bound state of the photon in the vicinity of the atom is formed.\textsuperscript{5} Kurizki and Genack\textsuperscript{6} have earlier shown that the dipole-dipole interaction between two atoms is also suppressed in such a situation. Another interesting phenomenon is the possibility of Anderson localization for the EM waves.\textsuperscript{7–10}

So far, the photon bands in periodic structures have been examined theoretically only in the scalar-wave approximation where the vector nature of the EM field is neglected. This has been studied by several authors using the plane-wave (PW),\textsuperscript{11,12} the Korringa–Kohn–Rostoker (KKR),\textsuperscript{13} or the augmented-plane-wave (APW) method with the general result that for the face-centered-cubic structure a gap appears in the entire Brillouin zone (BZ) if the dielectric-constant ratio between the spheres and the background exceeds a critical value of $\sim 3$ or so. However, the vector nature of the EM waves as shown here has important consequences.

Scattering of vector EM waves from a single sphere has been studied in great detail since the pioneering work of Mie.\textsuperscript{15} We consider here the wave equation for the electric displacement vector $D$ in a periodic structure with a space-dependent real dielectric constant $\varepsilon(r)$ and with the magnetic permeability $\mu$ being uniform throughout. The dielectric constant $\varepsilon(r)$ is periodic with the value $\varepsilon_o$ inside the spheres and $\varepsilon_b$ in the background. The corresponding refractive indices are denoted by $n_o$ and $n_b$, respectively. From Maxwell’s equations, we have the wave equation for $D$:

$$- \nabla^2 D = (\omega^2/c^2) D + \nabla \times \nabla \times [V(r) D],$$

where the “potential” $V(r)$ is given by

$$V(r) = 1 - 1/\varepsilon(r)$$

and $c$ is the vacuum speed of light. It is sufficient to solve Eq. (1) for the displacement field $D$, since once it is known, the other EM field vectors, viz., $E$, $H$, and $B$, are uniquely determined. For a periodic dielectric structure $V(r)$ can be expanded in terms of its Fourier components $V(G)$, $G$ being a reciprocal-lattice vector. The electric displacement $D$ which satisfies Bloch’s theorem can be expanded in terms of the plane waves:

$$D = \sum_G d_G e^{i(k+G) \cdot r},$$

where $k$ is the Bloch momentum. The zero divergence condition for $D$, $\nabla \cdot D = 0$, applied to Eq. (3), implies that each component in the plane-wave expansion is orthogonal to the wave vector of the corresponding plane wave:

$$d_G \cdot (k + G) = 0.$$  

Substituting Eq. (3) into Eq. (1) one obtains the equation for the expansion coefficients $d_G$:

$$H_G d_G + \sum_G V(G - G') \{(k + G) \cdot d_G (k + G)$$

$$- |k + G|^2 d_G\} = 0,$$

where

$$H_G = |k + G|^2 - \omega^2/c^2.$$

In fact, this equation is familiar from the dynamical theory of x-ray diffraction\textsuperscript{1,16} in crystals, where it is used.
to describe the Bragg scattering of x rays using two plane waves. Here we solve for the electric displacement field \( \mathbf{D} \) using many plane waves in the expansion (3) to study the eigenmodes of the EM waves in the periodic dielectric structure. Expressing \( \mathbf{d}_0 \) in terms of its Cartesian components, it follows from Eq. (5) that the following determinant must vanish:

\[
\det[H_G \delta_{G,G'} \delta_{i,j} + \nu(G'-G)[(k+G'),(k+G')]
- \omega^2 \mathbf{k}\mathbf{k}/\nu = 0, \tag{7}
\]

where \( i = x, y, \) or \( z. \) If we retain \( N \) plane waves in the expansion (3), then Eq. (7) is a \( 3N \times 3N \) determinant the solution of which provides us with \( 3N \) eigenmodes. However, since EM waves are transverse waves with two distinct helicity modes for each plane wave, we should have in total only \( 2N \) modes. This apparent discrepancy in the number of eigenmodes is explained by taking the dot product of Eq. (5) with the vector \( \mathbf{k} + \mathbf{G} \) and observing that the orthogonality condition, Eq. (4), is satisfied only for those solutions \( \omega \) for which \( H_G \mathbf{k} = \mathbf{k} + \mathbf{G} \) and \( \omega^2 \mathbf{k} = 0. \) Thus the orthogonality condition must be explicitly checked in the solution of Eq. (7) to discard the \( N \) unphysical solutions, one per plane wave in the expansion. The remaining \( 2N \) solutions are the true eigenmodes.

Our numerical calculations were performed for the fcc lattice with the dielectric constants varied between \( \sim 1 \) and 36 and for a number of sphere packing fractions \( \beta = \Omega_{\text{sphere}}/\Omega_{\text{cell}}. \) The value of \( \beta = 0.74 \) corresponds to close packing of spheres beyond which they overlap. \( \Omega_{\text{cell}} \) is the unit-cell volume and \( \Omega_{\text{sphere}} = (4\pi/3)R_s^3 \) when the spheres of radius \( R_s \) are not overlapping. We examined the cases of both “air atoms” \( (\varepsilon_a = 1 \) with \( \varepsilon_b \) varied) and dielectric spheres \( (\varepsilon_b = 1 \) with \( \varepsilon_a \) varied). We retained typically \( \sim 300 \) plane waves in the expansion which results in an accuracy better than \( \leq 3\% \) or so in the lower-lying eigenmodes.

A typical photon band structure for the vector waves is shown in Fig. 1. The parameters correspond to the case where a true gap was reported experimentally. In striking contrast with the experiment, we do not find a true gap existing throughout the BZ. However, the calculated effective refractive index \( n_{\text{eff}} \) shown in Fig. 2 agrees reasonably well with the measured value. This was calculated from the average value of the frequencies of the first four modes at the \( X \) point to directly compare with the experimentally reported values. As in the experiment we found \( n_{\text{eff}} \) calculated this way to be extremely close to that calculated using the long-wavelength limit, viz.,

\[
n_{\text{eff}} = \lim_{k \to 0} \frac{1}{c} \frac{d\omega}{dk}.
\]

The calculated width of the forbidden gap at the \( X \) and \( L \) points (Fig. 3) does not agree very well with the experimental data, indicating a necessity for repeating the experiments with improved accuracy. The calculated widths tend to zero in the limit \( \beta \to 0 \) or 1 as they should since these limits correspond to a uniform medium without scatterers.

For the entire range of \( \varepsilon_a \) and \( \varepsilon_b \) we did not find a true gap of significant magnitude in the fcc structure. This is in marked contrast to the scalar-wave result where for ratios of the two dielectric constants exceeding a critical value of \( \sim 3 \) a true gap was found.

Even though a gap is absent throughout the BZ, in
certain situations there is a strong pseudogap present in
the density of states for the photon modes. The density
of states ρ(ω) is defined such that ρ(ω)dω is the number
of photon modes including both helicities between the
frequency ω and ω+dω. It may be calculated by in-
tegrating over the irreducible BZ in a standard man-
er. The density of states was calculated using the
tetrahedron integration scheme with 120 k points in
the irreducible BZ and ~100 plane waves.

First, we note that for a homogeneous medium, the
linear dispersion relation is linear, ω = ̃c(k, gives rise to an
ω² dependence of the density of states (DOS):

$$\rho(\bar{\omega}) = 2\pi \bar{\omega}^2,$$

where the dimensionless quantity ̃ω is defined as
̃ω ≡ (2π/ω)⁻¹ω/c, where ̃c is the speed of light, ̃c ≡ c/nc.
Since the linear dispersion relation is followed in the
long-wavelength limit, for sufficiently small values of ω
the density of states has a similar ω² dependence.

Figure 4 shows the gradual evolution of a pseudogap
in the DOS as the strength of the scatterers is varied by
changing the sphere packing fraction β. Even though
there is no true gap extending throughout the BZ we find
that the depletion of the DOS can be very large. Unlike
the corresponding scalar case where the magnitude of
the gap is optimized for a packing fraction β of ~10%–
15%, we find in the vector case that the magnitude of
the pseudogap is optimized generally for β ~ 30%–40%.
A true gap in the entire BZ, although absent for the fcc
structure, could conceivably exist in other periodic struc-
tures.

The photon bands are the result of interplay between
the coherent scattering due to the periodic structure and
the scattering due to the individual spheres, the latter ex-
hibiting characteristic Mie resonances for certain in-
cident wavelengths. A relevant question, therefore, is
how much of the Mie resonance effect is retained in the
photon bands. Clearly, if the spheres are too large,
single-sphere scattering is expected to be a poor approxi-
mation for the periodic structures; on the other hand, for
small spheres the scattering strength, which scales as
πR³, is small enough that any Mie resonance effect is
likely to be blurred by the lattice effects. In fact, by
definition, in the limit β = 0 or 1, the Mie resonance
effects would obviously be absent since in those limits we
do not have any scatterers. For the case β ~ 0.3 shown
in Fig. 4, the first three Mie resonances occur at ̃ω ~ 0.91,
1.19, and 1.33 and the scattering coefficient is
significantly large in the entire range of ̃ω between
~0.87 and 1.35. The position and width of the pseudogap
comparatively well with the single-sphere Mie resonances
as indicated in Fig. 4. This suggests that the pseudogap
is a remnant of the single-sphere Mie resonances.

An interesting phenomenon associated with x-ray
diffraction is the Borrman absorption. It occurs when
the Bragg condition is nearly satisfied, with one of the
doubly refracted rays avoiding the region of the atoms
where photoelectric absorption takes place. Absorption
is thereby minimized for this ray while the other ray
behaves in just the opposite way. Thus, the first ray
propagates an anomalously longer distance than except-
ed while the second one is absorbed anomalously faster.

A similar phenomenon is expected to occur for the
periodic dielectric structures as well. This is illustrated
in Fig. 5 where we plot the electric displacement vector
D on the x-y plane for the modes belonging to the lowest
two branches at the X point. Each branch consists of
two helicity modes with nearly identical frequencies. For
the lower two modes the magnitude of D inside the
the BZ for the fcc structure when the vector nature of the EM waves is taken into account. However, even though a true gap is absent, we find that for moderate values of the dielectric constants a pseudogap develops in the photon spectrum, the optimal value for which is in the range of $\beta \sim 30\%$-$40\%$. We have also illustrated the existence of the Borrman effect in the periodic dielectric structure.

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