Comment on "Theory of Photon Bands in Three-Dimensional Periodic Dielectric Structures"

In a recent Letter, Satpathy, Zhang, and Salehpour[1] (SZS) computed the photon band structure for periodic dielectric spheres in the scalar-wave approximation. This problem has recently received attention from both theory[2] and experiment.[3]

Since electromagnetic (EM) waves are vector in nature, the key question is as follows: How good is the scalar-wave approximation? In particular, we would like to see how well does the scalar wave predict the onset of the photonic band gap, and the position and size of the gap. Figure 4(b) of SZS (Ref. 1) gave an impression that the scalar wave offers a good prediction of the onset of the band gap. This is due to the misplacement of the experimental point. The experiment is done[3] with $\epsilon=12.25$ ($n=3.5$) but Ref. 1 marked the experimental point at $\epsilon=3.5$. At $n=3.5$, the scalar-wave equation gives a gap for a filling fraction (f) at about 0.6, while the experiment with EM waves shows a gap for much higher values of $f>0.74$. This is expected since one important difference between scalar and EM waves is the absence of an s-wave resonance due to the transverse nature of the EM wave. As for the position and size of the gap, we note that experiment[3] (fcc with $a=12.7$ mm) obtained a gap of width 1 GHz, centered at 15 GHz. Our calculations[4] for the scalar-wave "representation of the experiment" give a gap of about 2.2 GHz, centered at 12.5 GHz. The scalar-wave approximation, hence, gives too large a gap at too low a frequency. Economou and Soukoulis[5] have recently suggested that the photon band gap obtained for the periodic structure is, in fact, the remnant of a Mie resonance obtained for a single sphere. The frequency of the first two Mie resonances of an isolated sphere for the scalar case are 4.74 and 9.47 GHz; while for the EM case are 12.04 and 15.40 GHz, which are much closer to the experimental value.[5] However, band-structure calculations for the EM case are surely needed to clarify the remaining issues.

In their paper,[1] SZS reduced the wave equation to a determinantal equation which was solved by a root-search scheme. The problem can be reformulated slightly so that the computationally faster matrix diagonalization scheme can be applied.

In the scalar-wave approximation, the electric field E is given by

$$\nabla^2 E+(\omega^2/c^2)\epsilon(\mathbf{r})E=0\,,$$

where $\epsilon(\mathbf{r})$ determines the periodic structure of the dielectrics.

Expanding in plane waves,

$$E=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{G}}\psi_{\mathbf{G}}e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

(Ω denotes the normalization volume). The wave equation can be expressed as a matrix equation:

$$[-T+(\omega^2/c^2)\epsilon]\psi=0\,,$$

where

$$T_{GG'}=|\mathbf{k}+\mathbf{G}|^2\delta_{GG'},\quad \epsilon_{GG'}=\frac{1}{\Omega}\int e^{-i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}}\epsilon(\mathbf{r})dr^3\,.$$

Now for nonzero k, T is positive definite and we can rewrite the equation as

$$(T^{-1/2}\epsilon T^{-1/2})\psi'=(c^2/\omega^2)\psi',\quad \psi'=T^{1/2}\psi\,.$$

The problem is transformed to an eigenvalue problem;[6] the eigenvalues of the matrix $T^{-1/2}\epsilon T^{-1/2}$ will give the allowed photon modes at that wave vector. We note that the method, with a slight modification, can be applied to the solution of the vector-wave equation.

Since the initial submission of this Comment, an erratum was published by SZS,[7] the vector-wave problem has been solved,[8-10] and we have found photonic gaps in diamondlike structures.[10]

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