SINGLE IMPURITY IN A PHOTONIC CRYSTAL

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Abstract. Formulae for the density of states (DOS) and integrated DOS (IDOS) are discussed for the case when the dielectric constant ε is a general function of frequency.

PACS numbers: 42.70.Qs - Photonic bandgap materials
PACS numbers: 61.72.-y - Defects and impurities in crystals
PACS numbers: 71.55.-i - Impurity and defect levels

Introduction.- Photonic crystals are characterized by a periodically modulated dielectric constant ε. Some of such structures occur in nature, for instance, opals and nanostructured colour wings of butterflies [1]. There is a common belief that in the near future photonic crystals will give us the same control over photons as ordinary crystals do over electrons [2]. At the same time, photonic structures are of great promise to become a laboratory for testing fundamental processes involving interactions of radiation with matter in novel conditions.

Similar to the case of electrons moving in a periodic potential, photons can propagate in a given direction inside a photonic crystal only if their frequency falls within an allowed band. In the presence of impurities, localized photon modes can appear with frequencies within the forbidden bands (gaps), which separate the allowed bands (see Fig. 1). These localized modes can serve as resonance cavities with a very high quality factor [3]. In a finite crystal these modes are responsible for sharp transmission peaks at frequencies within a frequency gap of a parent system. Numerous applications involving impurities,

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for instance, efficient bandpass filters, channel drop filters, and waveguide crossing without cross-talk have been suggested thus far.

In the Schrödinger case, for an electron moving in a potential V, the density of states (DOS) $n(E)$ and the integrated DOS (IDOS) $N(E)$ are defined as

$$n(E) = \int n(E, \mathbf{x})\, d\mathbf{x}, \qquad N(E) = \int_{-\infty}^{\omega} n(t)\, dt, \tag{1}$$

where $n(E, \mathbf{x})$ is the local DOS (LDOS),

$$n(E, \mathbf{x}) = -\frac{1}{\pi}\, \mathrm{Im}\, G(E; \mathbf{x}, \mathbf{x}). \tag{2}$$

$G(E; \mathbf{x}, \mathbf{x})$ here is the Green function, defined as the limit

$$G(E; \mathbf{x}, \mathbf{x}) = \lim_{s \to +0} \left\langle \mathbf{x} \,\middle|\, [E + is - H]^{-1} \,\middle|\, \mathbf{x} \right\rangle, \tag{3}$$

where H is the Hamiltonian. According to its definition, $N(E)$ describes the number of modes with $E' \leq E$ and $dN(E) = n(E)\, dE$. Formally,

$$n(E) = -\frac{1}{\pi}\, \mathrm{Im}\ \mathrm{Tr}\, G(E), \tag{4}$$

$$N(E) = \frac{1}{\pi}\, \mathrm{Im}\ \mathrm{Tr}\, \ln G(E). \tag{5}$$

One can show that $\mathrm{Im}\, G(E; \mathbf{x}, \mathbf{x}) \leq 0$ for any self-adjoint operator H. Hence, as expected, both $n(E)$ and $N(E)$ are positively defined.

The above formulae are derived under the assumption that the potential V is energy independent. However, for the Maxwell equations, the analogue of a potential V is

$$V = -\omega^2(\varepsilon - 1)/c^2, \tag{6}$$

where ω is frequency, c is the speed of light in vacuum (set to one in the following), and the analogue of energy is $E = \omega^2/c^2$. Moreover, in all realistic cases the dielectric constant ε is a complicated function of frequency. Thus the potential in the Maxwell case is both explicitly and implicitly frequency dependent. Therefore a question arises what is the analogue of the formulae (4) and (5) in the Maxwell case. Note that previous discussions of a single impurity in a photonic crystal [4, 5, 6] dealt with the idealistic case of a nondispersive ε.

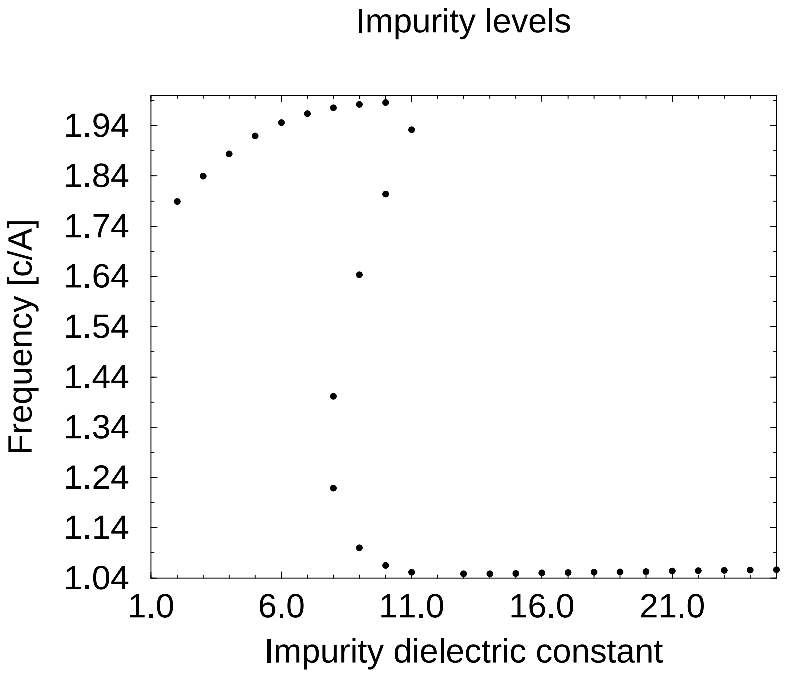

Figure 1: Substitutional impurity levels within the first forbidden band of a parent structure composed of alternating dielectric layers with $\varepsilon_1 = 1$ and $\varepsilon_2 = 12$. A is the length of a unit cell. The width of impurity layer is d_2 ($d_2/A = 0.4$), the same as of the layers with the dielectric constant ε_2.

Dispersive impurity.- It has been surprising to find out that in the dispersive Maxwell's case the formula (5) for the IDOS is still valid. Consequently, the change in the IDOS of a parent system induced by an impurity is given by

$$\Delta N(E) = -\frac{1}{\pi}\,\mathrm{Im}\ \mathrm{Tr}\ \ln[1 - G(E)W] \tag{7}$$

where $G(E)$ is the Green function of unperturbed system and W is the difference of potentials with and without the impurity. However, the DOS of a parent system and the change in the DOS induced by an impurity are given by

$$n(E) = -\frac{1}{\pi}\,\mathrm{Im}\ \mathrm{Tr}\ [G(E)(1 - dV/dE)]\,, \qquad \Delta n(E) = -\frac{1}{\pi}\,\mathrm{Im}\ \mathrm{Tr}\ [G(E)(1 - dW/dE)]\,. \tag{8}$$

Note that in the nondispersive case, the first formula in (8) reduces to

$$n(E) = -\frac{1}{\pi}\,\mathrm{Im}\ \mathrm{Tr}\ \left\{G(E)\,\frac{d}{d\omega^2}\,[\omega^2\varepsilon(\omega)]\right\} = -\frac{1}{\pi}\,\mathrm{Im}\ \mathrm{Tr}\ [G(E)\,\varepsilon]\,, \tag{9}$$

which has been used, for example, in [7].

As shown in [8], combining formulae (8) with the photonic analogue of the KKR method [9] allows one to treat efficiently the problem of dispersive impurities in a photonic crystal. Indeed, the impurity spectrum calculations using the plane-wave method are quite time consuming. The number of plane waves used to achieve convergence within 1% is typically 5×10^2, 2.5×10^4, and 7.5×10^5 in one, two, and three dimensions, respectively, [4]. On the other hand, using the photonic analogue of the KKR method [9], the impurity spectrum calculation in one dimension involves only matrices of the size 2×2. Even in three dimensions, the size of matrices involved do not exceed 300×300 [8].

I should like to thank Dr. A. Tip for careful reading of the manuscript and discussions. This work is part of the research programme of the Stichting voor Fundamenteel Onderzoek der Materie (Foundation for Fundamental Research on Matter) which was made possible by financial support from the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Netherlands Organization for Scientific Research).

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