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LETTER TO THE EDITOR

$k \cdot p$ theory of photonic band structures in periodic dielectrics

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Abstract. A $k \cdot p$ band-structure formalism is presented to describe photonic dispersion relations in periodic dielectric structures, within the scalar wave approximation. A reciprocal effective dielectric tensor is defined and an expression analogous to the f-sum rule for semiconductors is derived. Application of the present formalism is discussed using a two-band model. The generalization to vector waves is outlined.

Wave propagation in multi-component composites has generated much interest recently [1]. Particular attention has focussed on the propagation of electromagnetic (EM) waves in a periodic dielectric structure such as a regular array of dielectric spheres embedded in a host medium with a different dielectric constant [2, 3]. It has been observed experimentally that there exist ranges of frequencies in which propagation of EM waves is not allowed [4]. These frequency ranges are termed 'photonic band gaps' in analogy with the electronic band gaps in solids. Many optical and microwave devices are now being designed based on the existence of such photonic band gaps [5].

Photonic band structures have been calculated for different systems in 1, 2 and 3 dimensions using various traditional electronic band structure techniques including a plane wave expansion and a Green function (KKR) method [6–13]. However, these techniques are highly computationally intensive. The $k \cdot p$ theory [14–16] has been proven to be a simple and highly successful method for describing various electronic properties in ordered and disordered semiconductors, *without* the need for full-scale numerical calculations. The technique leads to the f-sum rule relating the effective mass of a band to the coupling between energy bands and the energy separation between bands. This method, although simple, has not been applied to describe photonic properties. This Letter provides a formal development of this technique to describe photonic dispersion relations in periodic dielectrics. In particular: (i) we present a $k \cdot p$ formulation for the photon band structure problem. (ii) An effective dielectric tensor is defined and an expression analogous to the f-sum rule is derived. (iii) Applications of the present formalism are discussed within a two-band model. In particular, application of the method to determine the imaginary band structure within the photonic gap is discussed.

For simplicity, the present paper gives results for scalar waves. The generalization of the formalism to the vector EM problem is straightforward and will be discussed at the end. The extent to which the scalar theory represents a good approximation to vector EM theory has been discussed many times in the literature [17] and will not be dealt with here. We note that the scalar wave equation *exactly* describes the vector photon problem for a 1-dimensional periodic dielectric [18] and for the TM (transverse magnetic) mode in a 2-dimensional periodic dielectric [19]. In addition, the present scalar formalism has a general application; it *exactly* describes any type of disturbance satisfying the scalar wave equation

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in a medium with a periodic inhomogeneity in 1, 2 or 3 dimensions. An equally important application of the present scalar theory would therefore be to acoustic waves.

Consider the problem of propagation of scalar waves in a periodic dielectric (or, for general scalar waves, composite) structure. The scalar wave equation is [20–21]

$$\left(\nabla^2 + \frac{\omega^2}{c^2}\epsilon(\boldsymbol{r})\right)\langle \boldsymbol{r}|\Psi\rangle = 0 \tag{1}$$

where $\langle \boldsymbol{r}|\Psi\rangle$ is the scalar field and $\epsilon(\boldsymbol{r})$ is a periodic function of $\boldsymbol{r}$ satisfying

$$\epsilon(\boldsymbol{r}) = \epsilon(\boldsymbol{r} + \boldsymbol{R}) \tag{2}$$

with $\boldsymbol{R}$ being any lattice vector of the periodic structure. Since $\epsilon(\boldsymbol{r})$ is periodic, Bloch's theorem holds [22]. The eigenstates of equation (1) are Bloch functions $\langle \boldsymbol{r}|n\boldsymbol{k}\rangle$ of the form:

$$\langle \boldsymbol{r}|n\boldsymbol{k}\rangle = \frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_n(\boldsymbol{k}, \boldsymbol{r}) \tag{3}$$

where n is a band index and $\boldsymbol{k}$ lies within the first Brillouin zone (BZ). The function $u_n(\boldsymbol{k}, \boldsymbol{r})$ is periodic in $\boldsymbol{r}$ with the same periodicity as $\epsilon(\boldsymbol{r})$, and Ω is the volume of the crystal. The corresponding eigenvalues of these Bloch functions are $\omega_{n\boldsymbol{k}}^2$, yielding the band structure or the dispersion relation. The Bloch functions $\langle \boldsymbol{r}|n\boldsymbol{k}\rangle$ form a complete set for all n and $\boldsymbol{k}$, and they form the basis set for the crystal momentum representation (CMR). The completeness relation is given by [23]

$$\epsilon(\boldsymbol{r}') \sum_{n\boldsymbol{k}} \langle \boldsymbol{r}|n\boldsymbol{k}\rangle\langle n\boldsymbol{k}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{4}$$

The orthogonality relation is given by [23]

$$\langle n'\boldsymbol{k}'||n\boldsymbol{k}\rangle \equiv \int \langle n'\boldsymbol{k}'|\boldsymbol{r}\rangle\epsilon(\boldsymbol{r})\langle \boldsymbol{r}|n\boldsymbol{k}\rangle d\boldsymbol{r} = \delta_{nn'}\delta_{\boldsymbol{k}\boldsymbol{k}'} \tag{5}$$

where the integral is over the whole volume Ω. Throughout this paper, the inner product $\langle||\rangle$ will denote integration with $\epsilon(\boldsymbol{r})$ acting as a weighting function, as shown explicitly in equation (5).

The Kohn–Luttinger functions $\langle \boldsymbol{r}|n\boldsymbol{k}\rangle$ are defined as [22, 24]

$$\langle \boldsymbol{r}|n\boldsymbol{k}\rangle = \frac{1}{\sqrt{\Omega}} u_n(\boldsymbol{k}_0, \boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = e^{i(\boldsymbol{k}-\boldsymbol{k}_0)\cdot\boldsymbol{r}} \langle \boldsymbol{r}|n\boldsymbol{k}_0\rangle \tag{6}$$

where $\boldsymbol{k}_0$ is some fixed $\boldsymbol{k}$ vector within the first BZ. The orthogonality relation, with $\epsilon(\boldsymbol{r})$ as the weighting function, is

$$\langle n'\boldsymbol{k}'||n\boldsymbol{k}\rangle = \delta_{nn'}\delta_{\boldsymbol{k}\boldsymbol{k}'}. \tag{7}$$

The Kohn–Luttinger functions form a complete set for all n and $\boldsymbol{k}$. They form the basis set for the effective mass representation (EMR). The completeness relation is given by

$$\epsilon(\boldsymbol{r}') \sum_{n\boldsymbol{k}} \langle \boldsymbol{r}|n\boldsymbol{k}\rangle(n\boldsymbol{k}|\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{8}$$

To set up a $k \cdot p$ approach for the scalar wave band structure problem, we solve for the eigenstates in equation (1) by expanding the Bloch functions in terms of the Kohn–Luttinger functions,

$$\langle r|nk\rangle = \sum_j A_{nj}(k)\langle r|jk\rangle \tag{9}$$

where the coefficient $A_{nj}(k) = (jk||nk\rangle$ is the wavefunction in the EMR. If we substitute equation (9) into the scalar wave equation (equation (1)) for the periodic dielectric structure, multiply by $u_\ell^*(k_0, r)$ and integrate over a unit cell, we obtain the following equation for the coefficients:

$$\sum_j \left[\frac{1}{c^2}(\omega_{nk}^2 - \omega_{jk_0}^2)\delta_{j\ell} + P_{\ell j}(k)\right] A_{nj}(k) = 0 \tag{10}$$

where

$$P_{\ell j}(k) \equiv (k - k_0) \cdot p_{\ell j} + (k_0^2 - k^2)q_{\ell j}. \tag{11}$$

Let v_c be the volume of a unit cell. The vector $p_{\ell j}$ is defined as

$$p_{\ell j} = \frac{2i}{v_c}\int_{v_c} u_\ell^*(k_0, r)\nabla u_j(k_0, r)\mathrm{d}r \tag{12}$$

and the scalar $q_{\ell j}$ is given by

$$q_{\ell j} = \frac{1}{v_c}\int_{v_c} u_\ell^*(k_0, r)u_j(k_0, r)\mathrm{d}r. \tag{13}$$

Note that p and q satisfy the properties $p_{\ell j}^* = p_{j\ell}$ and $q_{\ell j}^* = q_{j\ell}$. Writing $s = k - k_0$, we can express $P_{\ell j}(k)$ as

$$P_{\ell j}(k) = s \cdot (p_{\ell j} - 2k_0 q_{\ell j}) - s^2 q_{\ell j}. \tag{14}$$

Note that $P_{\ell j}(k)$ is the term analogous to the $k \cdot p$ term in the effective mass representation of the electronic problem for semiconductor band structures [8]. The scalar $q_{\ell j}$ involves the integral of two u functions and is in general non-vanishing due to the presence of the factor $\epsilon(r)$ in the orthogonality relation (equation (5)). Recall that our aim is to solve for the eigenvalue ω_{nk}. There is one equation for each value of the band index ℓ. For each ℓ, equation (10) gives an equation for all the coefficients A_{nj}, with j running over all the bands. Thus, the index n on A_{nj} refers to the nth solution of the set of equations. Thus solving the band structure ω_{nk}^2 amounts to finding the eigenvalues of a matrix H with elements $H_{\ell j}$ given by

$$H_{\ell j} = \frac{1}{c^2}\omega_{jk_0}^2\delta_{j\ell} - P_{\ell j}(k). \tag{15}$$

We note that the formalism is *exact* up to this point. The method attracted particular attention in semiconductor physics because one can regard the momentum matrix element $\sim \int u_\ell^* \nabla u_j \mathrm{d}r$ as a parameter fitted to the best band structure calculation or to measured physical parameters. Thus, the band structure around some particular point in k-space for

some important group of bands (usually the lowest conduction and the highest valence bands in semiconductors) can be reproduced accurately. In the case of photonic band structures, one could take the integrals $p_{\ell j}$ and $q_{\ell j}$ as parameters obtained by fitting to the many highly accurate band structures obtained so far using computationally intensive schemes, and thereby reproduce the band structure around some interesting region in the BZ accurately. Such a formalism should be useful in that it is computationally simple to obtain the dispersion relation about some particular point in k-space provided that the eigenfrequencies at that point are known.

We are often interested in the dispersion relation around some point k_0 in the BZ. In this case, $k \approx k_0$ and thus $s = |s|$ is small. For example, the particular point of interest may correspond to the band extremum. Using ordinary second order perturbating theory, we obtain the dispersion relation of the nth band as

$$\frac{\omega_{nk}^2}{c^2} = \frac{\omega_{nk_0}^2}{c^2} - P_{nn}(k) + \sum_{j(\neq n)} \frac{c^2 P_{nj} P_{jn}}{(\omega_{nk_0}^2 - P_{nn}(k)) - (\omega_{jk_0}^2 - P_{jj}(k))}. \tag{16}$$

Keeping terms only to second order of s and using equation (11), we have

$$\frac{\omega_{nk}^2}{c^2} = \frac{\omega_{nk_0}^2}{c^2} - s \cdot \pi_{nn} + s^2 q_{nn} + \sum_{j(\neq n)} \frac{c^2 (s \cdot \pi_{nj})(s \cdot \pi_{jn})}{(\omega_{nk_0}^2 - \omega_{jk_0}^2)} \tag{17}$$

where

$$\pi_{nj} = p_{nj} - 2k_0 q_{nj}. \tag{18}$$

If k_0 is the point corresponding to a band extremum, then the term linear in s vanishes, i.e. $\pi_{nn} = 0$, and the dispersion relation around k_0 is given by

$$\frac{\omega_{nk}^2}{c^2} = \frac{\omega_{nk_0}^2}{c^2} + s^2 q_{nn} + \sum_{j(\neq n)} \frac{c^2 (s \cdot \pi_{nj})(s \cdot \pi_{jn})}{\omega_{nk_0}^2 - \omega_{jk_0}^2}. \tag{19}$$

Motivated by the form of dispersion relation in a uniform dielectric medium $\omega^2 = c^2 k^2 / \epsilon$, we define a reciprocal effective dielectric tensor as

$$\left(\frac{1}{\epsilon_n^{\text{eff}}}\right)_{\alpha\beta} = \frac{1}{2c^2} \frac{\partial^2(\omega_{nk}^2)}{\partial k_\alpha \partial k_\beta} \tag{20}$$

where α, β correspond to the Cartesian components relative to some chosen axis. Using equation (19), the effective dielectric tensor is given by

$$\left(\frac{1}{\epsilon_n^{\text{eff}}}\right)_{\alpha\beta} = q_{nn}\delta_{\alpha\beta} + \frac{1}{2} \sum_{j(\neq n)} \frac{c^2 (\pi_{nj}^\beta \pi_{jn}^\alpha + \pi_{nj}^\alpha \pi_{jn}^\beta)}{(\omega_{nk_0}^2 - \omega_{jk_0}^2)}. \tag{21}$$

If principal axes are chosen, the tensor is diagonal and its elements are given by

$$\left(\frac{1}{\epsilon_n^{\text{eff}}}\right)_{\alpha\alpha} = q_{nn} + \sum_{j(\neq n)} \frac{c^2 |\pi_{nj}^\alpha|^2}{\omega_{nk_0}^2 - \omega_{jk_0}^2}. \tag{22}$$

Equations (21) and (22) relate the effective dielectric constant of the nth band to the interaction between the nth band and the other bands. The coupling is characterized by π_{nj}. The denominator is the separation in frequency at k_0 and thus corresponds to the gap frequency. These equations are thus analogous to the f-sum rule in dealing with the electronic properties of solids.

To illustrate the usefulness of the $k \cdot p$ formalism, we consider a two-band model in which only two bands are considered as relevant, the others being neglected or subsequently incorporated using perturbation theory. Let 1(2) denote the lower (upper) band. The dispersion relation around k_0 in the BZ can be obtained by diagonalizing the following 2×2 hamiltonian

$$H(k) = \begin{pmatrix} \omega_{2k_0}^2/c^2 - s \cdot \pi_{22} + s^2 q_{22} & -s \cdot \pi_{21} + s^2 q_{21} \\ -s \cdot \pi_{12} + s^2 q_{12} & \omega_{1k_0}^2/c^2 - s \cdot \pi_{11} + s^2 q_{11} \end{pmatrix}. \tag{23}$$

If k_0 corresponds to band extrema for both bands 1 and 2, then $\pi_{11} = \pi_{22} = 0$ and $H(k)$ becomes

$$H(k) = \begin{pmatrix} \omega_{2k_0}^2/c^2 + s^2 q_{22} & -s \cdot \pi_{21} + s^2 q_{21} \\ -s \cdot \pi_{12} + s^2 q_{12} & \omega_{1k_0}^2/c^2 + s^2 q_{11} \end{pmatrix}. \tag{24}$$

Note that π_{nj} has a term related to k_0 and equation (24) corresponds to the general case of band extrema at some point k_0 within the Brillouin zone. If the band extrema correspond to the zone centre, then equation (24) can be further simplified. In general, the eigenfrequencies within a two-band model near the band extrema are obtained by solving the equation

$$(\omega_{2k_0}^2 + c^2 s^2 q_{22} - \omega^2)(\omega_{1k_0}^2 + c^2 s^2 q_{11} - \omega^2) - c^2 (s \cdot \pi_{21} - s^2 q_{21})(s \cdot \pi_{12} - s^2 q_{12}) = 0. \tag{25}$$

Equation (25) can also be used to estimate the imaginary wavevector corresponding to frequencies within the gap. The magnitude of this imaginary wavevector is related to the wave attenuation at frequencies within the gap. This is an important piece of information for optoelectronic device design.

The generalization of the present formalism to describe vector EM waves is straightforward since the vector wave equation is also a generalized Hermitian eigenvalue problem. The vector wave equation describing the electric field E is given by

$$\nabla \times \nabla \times E - \frac{\omega^2}{c^2} \epsilon(r) E = 0 \tag{26}$$

and resembles the form of equation (1). The orthogonality relation for the electric field Bloch functions has the same form as that given above for the scalar field, except that it now involves the dot product of two vector fields together with the weighting function $\epsilon(r)$. The general structure of the corresponding $k \cdot p$ equations and the f-sum rule is the same as for the scalar case considered here [25].

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