Optical response of three-dimensional photonic lattices: Solutions of inhomogeneous Maxwell's equations and their applications

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We have formulated a Green's function method for the radiation field in an arbitrary three-dimensional photonic lattice to deal with the source term of an extrinsic polarization field $\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)$. It is shown that the induced field is expressed as a superposition of $\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)$ itself and the photonic-band eigenmodes of a nonzero frequency. The longitudinal eigenmodes of zero frequency, which are important for the closure relation of photonic bands, is shown to contribute nothing to the propagating electric field. We have applied this method to the treatments of sum frequency generation, dipole radiation, and free induction decay. [S0163-1829(96)01532-9]

I. INTRODUCTION

In recent years, materials that have a spatially periodic dielectric constant, which are called photonic crystals or photonic lattices, have attracted much interest.[1–22] The main reason of the intense investigations is the possibility of the realization of photonic-band gaps, that is, the frequency ranges where no electromagnetic mode exists.[1–3] The photonic-band gaps, especially those in the optical region, are expected to bring about quite peculiar physical phenomena, such as the inhibition of spontaneous emission[4] and energy transfer,[5] localized *donor* and *acceptor* modes,[6,7] stable solitary waves,[8,9] and nonexponential decay of spontaneous emission near a band edge,[10,11] etc. Several technological applications such as single-mode light emitting diodes with improved coherence, low noise, and high efficiency are also expected.[2] However, most of the experimental investigations reported so far are concerned with the microwave region because of the difficulty of sample preparation.

Quite recently, one of the authors and his co-workers have reported the fabrication of two-dimensional triangular lattices with lattice constants of about 1 μm and the observation of near-infrared band gaps.[12,13] In addition, the numerical analysis of the optical transmittance of them and similar two-dimensional lattices revealed the presence of two kinds of opaque frequency ranges, one due to the band gaps and the other due to uncoupled modes.[14–16] The presence of the modes inactive to external plane-wave lights was first pointed out by Robertson *et al.*[17,18] A group theoretical analysis based on the symmetry of the two-dimensional lattices showed that those uncoupled modes found by the numerical calculation of the optical transmittance exactly belong to this category.[19] As is clearly shown in this example, the nature of the wave function of the eigenmodes substantially affects the optical properties of the photonic lattices.

The same holds for the optical response occurring in photonic lattices. For example, the intensity of the radiation from an oscillating point dipole embedded in a photonic lattice may change according to where it is located, because the amplitude of the electric field of the eigenmodes, and hence, the coupling strength between the dipole and the radiation field is different from site to site. Therefore, a theory for the optical response that incorporates not only the photonic density of states but also the whole information on the eigenfunctions is quite necessary for photonic lattices.

In a previous paper,[20] we formulated a Green's function method to calculate the nonlinear optical response of an arbitrary two-dimensional photonic lattice and applied it to the sum frequency generation in a square lattice composed of circular air-rods formed in a $LiNbO_3$. We could obtain the intensity of the induced nonlinear field based on the numerical calculation of the dispersion relation and the wave functions. We also derived a generalized phase matching condition and selection rules, and showed the enhancement of the nonlinear optical processes due to the extraordinarily low group velocity at the band edges. Because the Green's function includes the complete information concerned with the eigenfrequencies and the eigenfunctions, the extension of this method to the three-dimensional case provides us with the desired method mentioned above.

The present paper is organized as follows. In Sec. II, we will formulate the Green's function method and solve the general inhomogeneous Maxwell's equation with an extrinsic polarization field as an inhomogeneous term. This method will then be applied in subsequent sections to three subjects; sum frequency generation in a cubic lattice (Sec. III), radiation from an oscillating dipole moment (Sec. IV), and free induction decay from two-level atoms (Sec. V). Several properties of the eigenmodes of the photonic lattice will be discussed in Appendix A. Their representation in the **k** space in several gauges will be examined in Appendix B.

II. GENERAL FORMULA

Now, we start from the following Maxwell's equations:

$$\nabla\cdot\{\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r},t)+4\pi\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)\}=0, \tag{1}$$

$$\nabla\cdot\mathbf{H}(\mathbf{r},t)=0, \tag{2}$$

$$\nabla\times\mathbf{E}(\mathbf{r},t)=-\frac{1}{c}\frac{\partial}{\partial t}\mathbf{H}(\mathbf{r},t), \tag{3}$$

$$\nabla\times\mathbf{H}(\mathbf{r},t)=\frac{1}{c}\frac{\partial}{\partial t}\{\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r},t)+4\pi\mathbf{P}_{\rm ex}(\mathbf{r},t)\}. \tag{4}$$

Here, $\epsilon(\mathbf{r})$, which is assumed to be positive and independent of frequency, and c are the position-dependent dielectric constant of the photonic lattice and the light velocity in vacuum, respectively. $\mathbf{P}_{\rm ex}(\mathbf{r},t)$ is an extrinsic polarization field that is not described by $\epsilon(\mathbf{r})$. The nonlinear polarization of the lattice and the dipole moments of impurity atoms induced by external fields are the examples of such a polarization field. The magnetic permeability was put to unity.

When we eliminate the magnetic field $\mathbf{H}(\mathbf{r},t)$ in Eqs. (3) and (4), we obtain the inhomogeneous wave equation for the electric field $\mathbf{E}(\mathbf{r},t)$:

$$-\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}+\mathcal{H}\right)\mathbf{Q}(\mathbf{r},t)=\frac{4\pi}{c^2\sqrt{\epsilon(\mathbf{r})}}\frac{\partial^2}{\partial t^2}\mathbf{P}_{\rm ex}(\mathbf{r},t), \tag{5}$$

where the differential operator $\mathcal{H}$ and the wave function $\mathbf{Q}(\mathbf{r},t)$ are defined as follows:

$$\mathcal{H}\mathbf{Q}(\mathbf{r},t)=\frac{1}{\sqrt{\epsilon(\mathbf{r})}}\nabla\times\left\{\nabla\times\frac{1}{\sqrt{\epsilon(\mathbf{r})}}\mathbf{Q}(\mathbf{r},t)\right\}, \tag{6}$$

$$\mathbf{Q}(\mathbf{r},t)=\sqrt{\epsilon(\mathbf{r})}\mathbf{E}(\mathbf{r},t). \tag{7}$$

We can easily verify that $\mathcal{H}$ is a Hermitian operator. Therefore, its eigenfunctions form an orthogonal complete set. In Appendix A, we will show that these eigenfunctions are classified into transverse-wave solutions $\mathbf{Q}^{(T)}_{\mathbf{k}n}(\mathbf{r})$ and longitudinal-wave solutions $\mathbf{Q}^{(L)}_{\mathbf{k}n}(\mathbf{r})$ with the following properties. (Here, $\mathbf{k}$ is a wave vector in the first Brillouin zone of the photonic lattice and n is a band index.) For the transverse mode,

$$\mathcal{H}\mathbf{Q}^{(T)}_{\mathbf{k}n}(\mathbf{r})=\frac{\omega^{(T)2}_{\mathbf{k}n}}{c^2}\mathbf{Q}^{(T)}_{\mathbf{k}n}(\mathbf{r}) \tag{8}$$

and

$$\nabla\cdot\{\sqrt{\epsilon(\mathbf{r})}\mathbf{Q}^{(T)}_{\mathbf{k}n}(\mathbf{r})\}=\mathbf{0}, \tag{9}$$

where $\omega^{(T)}_{\mathbf{k}n}$ is the eigenangular frequency of the transverse mode. On the other hand, the eigenangular frequency of the longitudinal mode $\omega^{(L)}_{\mathbf{k}n}$ is zero and its wave function is characterized by the following relation:

$$\nabla\times\left\{\frac{1}{\sqrt{\epsilon(\mathbf{r})}}\mathbf{Q}^{(L)}_{\mathbf{k}n}(\mathbf{r})\right\}=0. \tag{10}$$

Note that $\mathbf{Q}^{(T)}_{\mathbf{k}n}$ or $\mathbf{Q}^{(L)}_{\mathbf{k}n}$ alone is *not* purely transverse nor longitudinal, because of the spatial variation of $\epsilon(\mathbf{r})$, but the terms ''transverse'' and ''longitudinal'' are adopted here to emphasize that Eqs. (9) and (10) reduce, when $\epsilon(\mathbf{r})$ is a constant, to the usual relations defining transverse and longitudinal waves, respectively.

Now, we normalize these wave functions as follows:

$$\int_V d\mathbf{r}\mathbf{Q}^{(\alpha)*}_{\mathbf{k}n}(\mathbf{r})\cdot\mathbf{Q}^{(\beta)}_{\mathbf{k}'n'}(\mathbf{r})=V\delta_{\alpha\beta}\delta_{\mathbf{k}\mathbf{k}'}\delta_{nn'}, \tag{11}$$

with α, $\beta=T$ or L, and V the volume of the photonic lattice on which the periodic boundary condition is imposed. Note that $\mathbf{Q}^{(\alpha)}_{\mathbf{k}n}(\mathbf{r})$ and $\mathbf{E}^{(\alpha)}_{\mathbf{k}n}(\mathbf{r})$ $[\equiv\sqrt{\epsilon(\mathbf{r})}\mathbf{Q}^{(\alpha)}_{\mathbf{k}n}(\mathbf{r})]$ are dimensionless by definition. The completeness of the eigenfunctions leads to

$$\sum_{\mathbf{k}n}\mathbf{Q}^{(T)}_{\mathbf{k}n}(\mathbf{r})\otimes\mathbf{Q}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')+\sum_{\mathbf{k}n}\mathbf{Q}^{(L)}_{\mathbf{k}n}(\mathbf{r})\otimes\mathbf{Q}^{(L)*}_{\mathbf{k}n}(\mathbf{r}')=V\overleftrightarrow{E}\delta(\mathbf{r}-\mathbf{r}'), \tag{12}$$

where $\otimes$ denotes a tensor, the elements of which are given by the product of the elements of two vectors, i.e., $(\mathbf{A}\otimes\mathbf{B})_{ij}=A_iB_j$ and $\overleftrightarrow{E}$ is the unit tensor.

Because of these orthonormality and completeness relations, the eigenvectors $\mathbf{Q}^{(T)}_{\mathbf{k}n}$ and $\mathbf{Q}^{(L)}_{\mathbf{k}n}$ may be used as the convenient basis vectors to express various quantities of a photonic crystal. For example, an analysis may be carried out to find out the normal modes of the vector and scalar potentials in various gauges, which will be helpful in considering the response of a photonic crystal to an external transverse or longitudinal probe, to an incoming charged particle, for example. For fear of interrupting the mainstream of the present paper, we give it in Appendix B. What we are persuing in what follows also belongs in its essence to the same category.

We now return to Eq. (5). We define a retarded Green's (tensor) function $\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t)$, such that

$$-\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}+\mathcal{H}\right)\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t-t')=\overleftrightarrow{E}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'), \tag{13}$$

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t-t')=0\quad\text{for } t<t'. \tag{14}$$

Then, we can obtain the solution of Eq. (5) by the convolution integral of the Green's function and the inhomogeneous term:

$$\begin{aligned}\mathbf{E}(\mathbf{r},t)&\equiv\frac{1}{\sqrt{\epsilon(\mathbf{r})}}\mathbf{Q}(\mathbf{r},t)\\&=\frac{1}{\sqrt{\epsilon(\mathbf{r})}}\int d\mathbf{r}'\int_{-\infty}^{\infty}dt'\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t-t')\\&\quad\times\frac{4\pi}{c^2\sqrt{\epsilon(\mathbf{r}')}}\frac{\partial^2}{\partial t'^2}\mathbf{P}_{\rm ex}(\mathbf{r}',t').\end{aligned} \tag{15}$$

Now, the Fourier transform of $\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t)$, which will be denoted by $\overleftrightarrow{\mathcal{G}}(\mathbf{r},\mathbf{r}',\omega)$, is given by

$$\overleftrightarrow{\mathcal{G}}(\mathbf{r},\mathbf{r}',\omega)\equiv\int_{-\infty}^{\infty}dt\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t)e^{i\omega t}$$
$$=\frac{c^2}{V}\sum_{\mathbf{k}n}\frac{\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(T)*}(\mathbf{r}')}{(\omega-\omega_{\mathbf{k}n}^{(T)}+i\delta)(\omega+\omega_{\mathbf{k}n}^{(T)}+i\delta)}+\frac{c^2}{V}\sum_{\mathbf{k}n}\frac{\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(L)*}(\mathbf{r}')}{(\omega+i\delta)^2}. \tag{16}$$

Here, δ is a positive infinitesimal that assures the causality of the solution of Eq. (5). That Eq. (16) indeed satisfies Eq. (13) or its Fourier transform,

$$\left(\frac{\omega^2}{c^2}-\mathcal{H}\right)\overleftrightarrow{\mathcal{G}}(\mathbf{r},\mathbf{r}',\omega)=\overleftrightarrow{E}\delta(\mathbf{r}-\mathbf{r}') \tag{17}$$

is seen from Eq. (12). The inverse transform of Eq. (16) then leads to

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',t)=\frac{c^2}{2\pi V}\sum_{\mathbf{k}n}\frac{\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(T)*}(\mathbf{r}')}{2\omega_{\mathbf{k}n}^{(T)}}\int_C\left(\frac{1}{\omega-\omega_{\mathbf{k}n}^{(T)}+i\delta}-\frac{1}{\omega+\omega_{\mathbf{k}n}^{(T)}+i\delta}\right)e^{-i\omega t}d\omega$$
$$+\frac{c^2}{2\pi V}\sum_{\mathbf{k}n}\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(L)*}(\mathbf{r}')\int_C\frac{e^{-i\omega t}}{(\omega+i\delta)^2}d\omega$$
$$=\begin{cases}-\dfrac{c^2}{V}\sum_{\mathbf{k}n}\left\{\dfrac{\sin\omega_{\mathbf{k}n}^{(T)}t}{\omega_{\mathbf{k}n}^{(T)}}\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(T)*}(\mathbf{r}')+t\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})\otimes\mathbf{Q}_{\mathbf{k}n}^{(L)*}(\mathbf{r}')\right\} & (t\geqslant 0)\\ 0 & (t<0),\end{cases} \tag{18}$$

where the contour C is depicted in Fig. 1. For the expression for $t\geqslant 0$, we closed the path of integration in the lower half of the complex ω plane, while that for $t<0$ is obtained by the contour enclosing the analytic upper plane.

Finally, from Eqs. (15), (18), and (12), we obtain

$$\mathbf{E}(\mathbf{r},t)+\frac{4\pi\mathbf{P}_{\rm ex}(\mathbf{r},t)}{\epsilon(\mathbf{r})}=\frac{4\pi}{V}\sum_{\mathbf{k}n}\frac{\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\int d\mathbf{r}'\int_{-\infty}^{t}dt'\times\frac{\mathbf{Q}_{\mathbf{k}n}^{(T)*}(\mathbf{r}')\cdot\mathbf{P}_{\rm ex}(\mathbf{r}',t')}{\sqrt{\epsilon(\mathbf{r}')}}\times\omega_{\mathbf{k}n}^{(T)}\sin\omega_{\mathbf{k}n}^{(T)}(t-t'). \tag{19}$$

In deriving Eq. (19), we assumed that the extrinsic polarization $\mathbf{P}_{\rm ex}(\mathbf{r},t)$ was introduced adiabatically, i.e., $\mathbf{P}_{\rm ex}(\mathbf{r},-\infty)=0$, and carried out the integration by parts twice for t'. What matters in the above derivation is that (a) the role of the longitudinal modes is only to reconstruct the extrinsic dipolar field and they do not contribute to the propagating radiation field, i.e., to the right-hand side of Eq. (19), and that (b) Eq. (1) holds, as it should, because of Eq. (9).

III. SUM FREQUENCY GENERATION

In this section, we assume that the photonic lattice is composed of a material with the second order nonlinearity. So, we introduce a position-dependent second order susceptibility tensor $\overleftrightarrow{\chi}^{(2)}(\mathbf{r})$ that is periodic under the translation by an elementary lattice vector. We also assume for simplicity the lattice to be simple cubic with a lattice constant a. So, $V=N_xN_yN_za^3$, where N_x, N_y, N_z are positive integers that denote the number of unit cells in each direction. In order to clarify the phase matching condition, we further assume that $\overleftrightarrow{\chi}^{(2)}(\mathbf{r})$ is nonzero only at $0\leqslant z\leqslant an_z$, where n_z is a positive integer. The nonlinear polarization $\mathbf{P}_{\rm NL}(\mathbf{r},t)$ induced by two electric fields, $\mathbf{E}_{\mathbf{k}_1n_1}^{(T)}(\mathbf{r})$ and $\mathbf{E}_{\mathbf{k}_2n_2}^{(T)}(\mathbf{r})$, which are both transverse eigenmodes and assumed to be excited by appropriate incident waves from outside the photonic lattice, yields the nonlinear radiation field.

A comment is in order for the excitation of Bloch waves, because the excitation involves the local field correction. In general, an incident light of frequency ω excites within a photonic crystal a linear combination of Bloch waves of that frequency. The excited amplitude of a particular Bloch wave, the coefficient of the linear combination, is determined by the boundary condition at the entrance surface of the photonic crystal.[23] In the paper by one of the authors,[24] it is quantitatively shown that for a ω matching well with a peak of

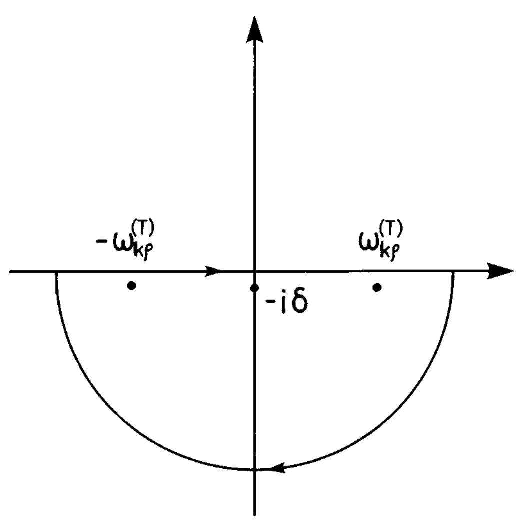

FIG. 1. The contour of the integration in Eq. (18) for $t\geqslant 0$. For $t<0$, the contour should enclose the upper half plane.

the density of states of an optically active photonic band, the field intensity is highly enhanced near the surface of arrayed dielectrics, even by a factor of 10^2 in a good situation of a large dielectric constant causing an appreciable electromagnetic confinement effect. Let us denote the amplitude of the excited Bloch waves simply as A, which involves already this enhancement correction. Then, the nonlinear polarization is given by

$$\mathbf{P}_{\mathrm{NL}}(\mathbf{r},t)=\frac{1}{2}A^2\overleftrightarrow{\chi}^{(2)}(\mathbf{r}):\mathbf{E}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r})\mathbf{E}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r})\times\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})t\},\tag{20}$$

with the symbol ":" denoting the product of $\overleftrightarrow{\chi}^{(2)}(\mathbf{r})$ with $\mathbf{E}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r})$ and $\mathbf{E}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r})$ as a tensor. Note that we wrote down the positive frequency part of the polarization field. The actual real field is given by the sum of the above field and its complex conjugate. The same holds for the electric field derived below.

Substituting $\mathbf{P}_{\mathrm{NL}}(\mathbf{r},t)$ for $\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)$ in the general solution Eq. (19), we get the sum frequency component of the electric field $\mathbf{E}_{\mathrm{NL}}(\mathbf{r},t)$.

$$\begin{aligned}\mathbf{E}_{\mathrm{NL}}(\mathbf{r},t)+\frac{4\pi\mathbf{P}_{\mathrm{NL}}(\mathbf{r},t)}{\epsilon(\mathbf{r})}=&\frac{2\pi A^2}{V}\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})t\}\\&\times\sum_{\mathbf{k}n}\omega^{(T)}_{\mathbf{k}n}\mathbf{E}^{(T)}_{\mathbf{k}n}(\mathbf{r})\int_0^\infty dt'\sin\omega^{(T)}_{\mathbf{k}n}t'\\&\times\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-i\delta)t'\}\\&\times\int_V d\mathbf{r}'\,\mathbf{E}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')\cdot\overleftrightarrow{\chi}^{(2)}(\mathbf{r}):\mathbf{E}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r}')\mathbf{E}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r}').\end{aligned}\tag{21}$$

We have introduced $-i\delta$ in the exponent of the integrand of Eq. (21) in order to assure the adiabatic switching of the nonlinear polarization field. From the Bloch's theorem, the eigenfunction $\mathbf{E}^{(T)}_{\mathbf{k}n}(\mathbf{r})$ can be expressed as follows:

$$\mathbf{E}^{(T)}_{\mathbf{k}n}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{u}^{(T)}_{\mathbf{k}n}(\mathbf{r}),\tag{22}$$

where $\mathbf{u}^{(T)}_{\mathbf{k}n}(\mathbf{r})$ is a periodic (vector) function, invariant by the lattice translation. Then, the spatial integral in Eq. (21) is calculated as

$$\begin{aligned}&\int_V d\mathbf{r}'\,\mathbf{E}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')\cdot\overleftrightarrow{\chi}^{(2)}(\mathbf{r}):\mathbf{E}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r}')\mathbf{E}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r}')\\&=\sum_{l_1=0}^{N_x-1}\sum_{l_2=0}^{N_y-1}\sum_{l_3=0}^{n_z-1}\int_{V_0}d\mathbf{r}'\,\mathbf{u}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')\cdot\overleftrightarrow{\chi}^{(2)}(\mathbf{r}'):\mathbf{u}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r}')\mathbf{u}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r}')\exp\{i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k})\cdot(\mathbf{r}'+a\mathbf{l})\}\\&=V_0N_xN_y\delta_{k_x,k_{1x}+k_{2x}-(2p\pi/a)}\delta_{k_y,k_{1y}+k_{2y}-(2q\pi/a)}\frac{\sin(an_z\Delta k_z/2)}{\sin(a\Delta k_z/2)}e^{ia(n_z-1)\Delta k_z/2}F(\mathbf{k}n,\mathbf{k}_1n_1,\mathbf{k}_2n_2),\end{aligned}\tag{23}$$

where $\mathbf{l}=(l_1,l_2,l_3)$, V_0 the volume of the unit cell and

$$\Delta k_z=k_{1z}+k_{2z}-k_z.\tag{24}$$

The quantity F is given by

$$\begin{aligned}F(\mathbf{k}n,\mathbf{k}_1n_1,\mathbf{k}_2n_2)&=\frac{1}{V_0}\int_{V_0}d\mathbf{r}'\,\mathbf{u}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')\cdot\overleftrightarrow{\chi}^{(2)}(\mathbf{r}'):\mathbf{u}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r}')\mathbf{u}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r}')\\&\times\exp\left\{\frac{2\pi i(px'+qy')}{a}\right\}\exp(i\Delta k_zz'),\end{aligned}\tag{25}$$

which may be regarded as an effective nonlinear susceptibility with respect to the initial and the final states. The two integers p and q were introduced to make allowance for the umklapp processes. Namely, because of the periodicity of $\mathbf{u}^{(T)*}_{\mathbf{k}n}(\mathbf{r}')\cdot\overleftrightarrow{\chi}^{(2)}(\mathbf{r}'):\mathbf{u}^{(T)}_{\mathbf{k}_1n_1}(\mathbf{r}')\mathbf{u}^{(T)}_{\mathbf{k}_2n_2}(\mathbf{r}')$ and the periodic boundary condition, the integration over x' and y' in Eq. (23) is nonzero only when $k_{1x}+k_{2x}-k_x$ and $k_{1y}+k_{2y}-k_y$ are multiples of $2\pi/a$. Actually, p and q are equal to -1, 0, or 1, because $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}$ are the vectors within the first Brillouin zone. On the other hand, the temporal integral in Eq. (21) is obtained as

$$\int_0^\infty dt'\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-i\delta)t'\}\sin\omega^{(T)}_{\mathbf{k}n}t'\simeq-\frac{1}{2(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-\omega^{(T)}_{\mathbf{k}n}+i\delta)}.\tag{26}$$

When we convert the summation on k_z into integration in Eq. (21), we get

$$\mathbf{E}_{\mathrm{NL}}(\mathbf{r},t)+\frac{4\pi\mathbf{P}_{\mathrm{NL}}(\mathbf{r},t)}{\epsilon(\mathbf{r})}\simeq-\frac{A^2}{2}\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})t\}\sum_n\int dk_z\frac{\omega^{(T)}_{\overline{\mathbf{k}}n}\mathbf{E}^{(T)}_{\overline{\mathbf{k}}n}(\mathbf{r})F(\overline{\mathbf{k}}n,\mathbf{k}_1n_1,\mathbf{k}_2n_2)}{\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-\omega^{(T)}_{\overline{\mathbf{k}}n}+i\delta}\times\frac{\sin(an_z\Delta k_z/2)}{\sin(a\Delta k_z/2)}\exp\{ia(n_z-1)\Delta k_z/2\}. \tag{27}$$

In Eq. (27),

$$\overline{\mathbf{k}}=\left(k_{1x}+k_{2x}-\frac{2p\pi}{a},k_{1y}+k_{2y}-\frac{2q\pi}{a},k_z\right). \tag{28}$$

Now, we denote the ''group velocity'' of the nth band in the z direction by $v_g(\omega,n)$:

$$v_g(\omega,n)=\left(\frac{\partial\omega^{(T)}_{\overline{\mathbf{k}}n}}{\partial k_z}\right)_{k_x=\overline{k_x},k_y=\overline{k_y},\omega^{(T)}_{\overline{\mathbf{k}}n}=\omega}. \tag{29}$$

Then, converting the integration on k_z into the integration on $\omega^{(T)}_{\overline{\mathbf{k}}n}$ and using the following approximation,[20]

$$\frac{1}{\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-\omega^{(T)}_{\overline{\mathbf{k}}n}+i\delta}\simeq-\pi i\delta(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2}-\omega^{(T)}_{\overline{\mathbf{k}}n}), \tag{30}$$

we finally obtain

$$\mathbf{E}_{\mathrm{NL}}(\mathbf{r},t)+\frac{4\pi\mathbf{P}_{\mathrm{NL}}(\mathbf{r},t)}{\epsilon(\mathbf{r})}\simeq\frac{aA^2i\pi(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})}{2}\exp\{-i(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})t\}\sum_{\{n\}'}\frac{\mathbf{E}^{(T)}_{\overline{\mathbf{K}}_nn}(\mathbf{r})F(\overline{\mathbf{K}}_nn,\mathbf{k}_1n_1,\mathbf{k}_2n_2)}{v_g(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2},n)}\times\frac{\sin(an_z\overline{\Delta k_z}/2)}{\sin(a\overline{\Delta k_z}/2)}\exp\{ia(n_z-1)\overline{\Delta k_z}/2\}, \tag{31}$$

where

$$\overline{K_{nx}}=\overline{k_x},\quad \overline{K_{ny}}=\overline{k_y}, \tag{32}$$

$$\omega^{(T)}_{\overline{\mathbf{K}}_nn}=\omega_{\mathbf{k}_1n_1}+\omega_{\mathbf{k}_2n_2}, \tag{33}$$

and $\overline{\Delta k_z}=k_{1z}+k_{2z}-\overline{K_{nz}}$. The summation on n in Eq. (31) is over bands which include $\omega_{\mathbf{k}_1n_1}+\omega_{\mathbf{k}_2n_2}$ as an eigenfrequency. If there is only one such band that is denoted by ν, the field intensity at $z\geqslant an_z$ is

$$|\mathbf{E}_{\mathrm{NL}}(\mathbf{r},t)|^2\simeq\frac{a^2A^2\pi^2(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2})^2|\mathbf{E}^{(T)}_{\overline{\mathbf{K}}_\nu\nu}(\mathbf{r})|^2}{4v_g^2(\omega^{(T)}_{\mathbf{k}_1n_1}+\omega^{(T)}_{\mathbf{k}_2n_2},\nu)}\times\frac{\sin^2(an_z\overline{\Delta k_z}/2)}{\sin^2(a\overline{\Delta k_z}/2)}|F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}_1n_1,\mathbf{k}_2n_2)|^2. \tag{34}$$

Here, we should note that (1) the field intensity is proportional to v_g^{-2} and we can expect its enhancement at the photonic-band edge where v_g tends to zero; (2) the phase matching condition is fulfilled when $\overline{\Delta k_z}=0$, i.e., when the crystalline momentum is conserved; and (3) the effective nonlinear susceptibility $F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}_1n_1,\mathbf{k}_2n_2)$ may vanish for particular combinations of $\mathbf{k}_1n_1$ and $\mathbf{k}_2n_2$ in a highly symmetric photonic lattice, because of the symmetry of the relevant wave functions, and this fact gives an additional selection rule besides that due to the crystallographic symmetry of the host crystal. These three features were pointed out for two-dimensional photonic lattices in the previous paper.[20] The results of this section is their natural extension to the three-dimensional lattice. We should also note that these three features are common to other nonlinear optical processes in the photonic lattice for which the phase matching condition is imposed by the momentum conservation law.

IV. RADIATION FROM AN OSCILLATING DIPOLE MOMENT

In this section, we treat the field irradiated from an oscillating dipole moment. Suppose that there is an oscillating dipole moment of frequency ω at the position $\mathbf{r}_0$ in the photonic lattice and let $\mathbf{P}_d(\mathbf{r},t)$ be the external polarization $\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)$ of this problem:

$$\mathbf{P}_d(\mathbf{r},t)=\boldsymbol{\mu}\delta(\mathbf{r}-\mathbf{r}_0)e^{-i\omega t}. \tag{35}$$

Here, $\boldsymbol{\mu}$ is the dipole moment with a fixed magnitude. By substituting $\mathbf{P}_d(\mathbf{r},t)$ for $\mathbf{P}_{\rm ex}(\mathbf{r},t)$ in Eq. (15), we obtain

$$\mathbf{E}_d(\mathbf{r},t)+\frac{4\pi\mathbf{P}_d(\mathbf{r},t)}{\epsilon(\mathbf{r})}=\frac{2\pi}{V}e^{-i\omega t}\sum_{\mathbf{k}n}\omega_{\mathbf{k}n}^{(T)}\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})\times\{\mathbf{E}_{\mathbf{k}n}^{(T)*}(\mathbf{r}_0)\cdot\boldsymbol{\mu}\}\times\left(\frac{1}{\omega+\omega_{\mathbf{k}n}^{(T)}+i\delta}-\frac{1}{\omega-\omega_{\mathbf{k}n}^{(T)}+i\delta}\right). \tag{36}$$

Now, the time-averaged Poynting's vector $\langle\mathbf{S}(\mathbf{r},t)\rangle$ is given by

$$\langle\mathbf{S}(\mathbf{r},t)\rangle=\frac{c}{8\pi}\mathrm{Re}[\mathbf{E}_d(\mathbf{r},t)\times\mathbf{H}_d^*(\mathbf{r},t)], \tag{37}$$

where the magnetic field $\mathbf{H}_d(\mathbf{r},t)$ is given by

$$\mathbf{H}_d(\mathbf{r},t)=\frac{c}{i\omega}\nabla\times\mathbf{E}_d(\mathbf{r},t). \tag{38}$$

From Eqs. (4), (38), and (36), we get

$$\nabla\cdot\langle\mathbf{S}(\mathbf{r},t)\rangle=\frac{i\omega}{4}\{\mathbf{E}_d^*(\mathbf{r},t)\cdot\mathbf{P}_d(\mathbf{r},t)-\mathbf{E}_d(\mathbf{r},t)\cdot\mathbf{P}_d^*(\mathbf{r},t)\}=\frac{\pi^2\omega^2}{V}\delta(\mathbf{r}-\mathbf{r}_0)\sum_{\mathbf{k}n}|\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r}_0)|^2\delta(\omega-\omega_{\mathbf{k}n}^{(T)}). \tag{39}$$

When we denote a small volume which includes $\mathbf{r}_0$ by V_1 and its surface by S_1, the radiation energy U emitted per unit time by the oscillating dipole is given by the surface integral of the normal component of the Poynting's vector, which can be transformed to a volume integral by means of the Gauss's theorem:

$$U=\int_{S_1}dS\langle S_n(\mathbf{r},t)\rangle=\int_{V_1}d\mathbf{r}\nabla\cdot\langle\mathbf{S}(\mathbf{r},t)\rangle=\frac{\pi^2\omega^2}{V}\sum_{\mathbf{k}n}|\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r}_0)|^2\delta(\omega-\omega_{\mathbf{k}n}^{(T)}). \tag{40}$$

This expression coincides with the result by quantum mechanical calculation under the dipole approximation for an excited atom with a transition dipole moment $\boldsymbol{\mu}$. The quantization of the radiation field in the photonic lattice and the quantum mechanical treatment will be presented elsewhere.

V. FREE INDUCTION DECAY

In this section, we will treat free induction decay (FID) as an example of the coherent optical processes in the photonic lattice. We assume that impurity atoms with two electronic levels, which will be denoted by e (excited state) and g (ground state), are uniformly distributed in the lattice with the density n. Their transition dipole moment is denoted by $\boldsymbol{\mu}$. Now, we introduce their position- and time-dependent density matrix $\rho(\mathbf{r},t)$. Then, the polarization due to these impurity atoms, which is denoted by $\mathbf{P}_{\rm FID}$, is proportional to the trace of the dipole operator times the density matrix:

$$\mathbf{P}_{\rm FID}(\mathbf{r},t)=n\boldsymbol{\mu}\{\rho_{ge}(\mathbf{r},t)+\rho_{eg}(\mathbf{r},t)\}. \tag{41}$$

Here, we assume that the system was driven by an external field $\mathbf{E}_{\rm ex}(\mathbf{r},t)$ for $t\leqslant t_0$, which is an excited photonic-band mode:

$$\mathbf{E}_{\rm ex}(\mathbf{r},t)=\frac{A}{2}\{\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})\exp(-i\omega_{\mathbf{k}n}^{(T)}t)+\mathbf{E}_{\mathbf{k}n}^{(T)*}(\mathbf{r})\exp(i\omega_{\mathbf{k}n}^{(T)}t)\}. \tag{42}$$

The factor A has the same meaning as discussed in Eq. (20). Then, the equation of motion for the density matrix leads to

$$\frac{\partial}{\partial t}\rho_{ee}(\mathbf{r},t)=\frac{i}{\hbar}\boldsymbol{\mu}\cdot\mathbf{E}_{\rm ex}(\mathbf{r},t)\{\rho_{eg}^*(\mathbf{r},t)-\rho_{eg}(\mathbf{r},t)\}-\frac{\rho_{ee}(\mathbf{r},t)}{T_1}, \tag{43}$$

$$\frac{\partial}{\partial t}\rho_{eg}(\mathbf{r},t)=-i\Omega_{eg}\rho_{eg}(\mathbf{r},t)-\frac{\rho_{eg}(\mathbf{r},t)}{T_2}-\boldsymbol{\mu}\cdot\mathbf{E}_{\rm ex}(\mathbf{r},t)\{2\rho_{ee}(\mathbf{r},t)-1\}, \tag{44}$$

where we have introduced the longitudinal relaxation time T_1 and the transverse relaxation time T_2 in order to describe the population and phase relaxation processes, respectively. In Eq. (44),

$$\Omega_{eg}=\frac{1}{\hbar}(E_e-E_g), \tag{45}$$

where E_e (E_g) is the energy of the excited (ground) state. Under the assumption of a weak excitation and rotating wave approximation, we obtain

$$\rho_{eg}(\mathbf{r},t_0)\simeq\frac{A}{2\left(\frac{1}{T_2}-i\Delta\omega\right)}\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})\exp(-i\omega_{\mathbf{k}n}^{(T)}t_0). \tag{46}$$

For $t>t_0$, the external field is switched off, and so,

$$\frac{\partial}{\partial t}\rho_{eg}(\mathbf{r},t)=-i\Omega_{eg}\rho_{eg}(\mathbf{r},t)-\frac{\rho_{eg}(\mathbf{r},t)}{T_2}. \tag{47}$$

Then, we get

$$\rho_{eg}(\mathbf{r},t)=\exp\left\{-\left(i\Omega_{eg}+\frac{1}{T_2}\right)(t-t_0)\right\}\rho_{eg}(\mathbf{r},t_0)\simeq\frac{A\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})}{2\left(\frac{1}{T_2}-i\Delta\omega\right)}\exp\left\{-\left(i\Omega_{eg}+\frac{1}{T_2}\right)t\right\}\times\exp\left\{-\left(i\Delta\omega-\frac{1}{T_2}\right)t_0\right\}, \tag{48}$$

where $\Delta\omega=\omega_{\mathbf{k}n}^{(T)}-\Omega_{eg}$. Therefore, from Eq. (41),

$$\mathbf{P}_{\mathrm{FID}}(\mathbf{r},t)=\frac{An\boldsymbol{\mu}\{\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})\}}{2\left(\frac{1}{T_2}-i\Delta\omega\right)}\exp\left\{-\left(i\Omega_{eg}+\frac{1}{T_2}\right)t\right\}\times\exp\left\{-\left(i\Delta\omega-\frac{1}{T_2}\right)t_0\right\}+\mathrm{c.c.} \tag{49}$$

Substituting Eq. (49) for $\mathbf{P}_{\mathrm{ex}}(\mathbf{r},t)$ in Eq. (15), we obtain the electric field for FID, $\mathbf{E}_{\mathrm{FID}}(\mathbf{r},t)$, which oscillates with the atomic angular frequency Ω_{eg}:

$$\mathbf{E}_{\mathrm{FID}}(\mathbf{r},t)+\frac{4\pi\mathbf{P}_{FID}(\mathbf{r},t)}{\epsilon(\mathbf{r})}\simeq\frac{An\pi\omega_{\mathbf{k}n}^{(T)}\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r})}{iV\left(\frac{1}{T_2}-i\Delta\omega\right)^2}\times\langle|\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r}')|^2\rangle\times\exp\left\{-\left(i\Omega_{eg}+\frac{1}{T_2}\right)(t-t_0)\right\}\times\exp(-i\omega_{\mathbf{k}n}^{(T)}t_0), \tag{50}$$

where

$$\langle|\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r}')|^2\rangle=\frac{1}{V}\int_V d\mathbf{r}'\,|\boldsymbol{\mu}\cdot\mathbf{E}_{\mathbf{k}n}^{(T)}(\mathbf{r}')|^2. \tag{51}$$

VI. CONCLUSION

In this paper, we have derived the general solution of the inhomogeneous wave equation in an arbitrary photonic lattice by means of the Green's function method. We have shown that the electric field induced by the external polarization field is expressed by the superposition of the transverse eigenmodes of the photonic lattice and the polarization field itself, and therefore, the longitudinal eigenmodes do not contribute to the propagating electromagnetic field.

The present method is applicable to various kinds of optical processes in the photonic lattice. We have presented three examples: (1) sum frequency generation in a cubic lattice, (2) radiation from an oscillating dipole moment, and (3) free induction decay. For the first example, we have derived the generalized phase matching condition, and have shown that the field intensity of the sum frequency component is proportional to its (group velocity)$^{-2}$, and therefore, an enhancement is expected at photonic-band edges where the group velocity tends to zero. We have also pointed out the presence of the selection rule due to the spatial symmetry of the photonic lattice. For the second example, we have calculated the Poynting's vector of the radiated electromagnetic field and we have obtained a formula that represents the emitted energy per unit time. The last example is one of typical coherent optical processes. We have shown that we can treat this case within the present formulation by describing the coherent polarization field with the density matrix.

We would like to conclude this paper by pointing out an important aspect of the present formulation. Namely, the present method is quite suitable to numerical evaluation of various optical processes in the photonic lattice, because the Green's function of the lattice is composed of the eigenfrequencies and eigenfunctions of the lattice that can be accurately calculated by the plane-wave expansion method,[21,22] the vector KKR method,[25] or others.

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APPENDIX A

We will show below that the operator $\mathcal{H}$ in Eq. (6) is Hermitian, and we will derive several properties of $\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})$ and $\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})$. Now, the inner product of two periodic complex (vector) functions $\mathbf{Q}_1(\mathbf{r})$ and $\mathbf{Q}_2(\mathbf{r})$ is defined by

$$\langle\mathbf{Q}_1,\mathbf{Q}_2\rangle\equiv\int_V d\mathbf{r}\,\mathbf{Q}_1^*(\mathbf{r})\cdot\mathbf{Q}_2(\mathbf{r}), \tag{A1}$$

where V is the volume on which the periodic boundary condition is imposed. As a vector identity, the next equation holds.

$$\nabla\cdot(\mathbf{A}\times\mathbf{B})=(\nabla\times\mathbf{A})\cdot\mathbf{B}-\mathbf{A}\cdot(\nabla\times\mathbf{B}). \tag{A2}$$

Using this identity, we obtain

$$\begin{aligned}\langle\mathcal{H}\mathbf{Q}_1,\mathbf{Q}_2\rangle&\equiv\int_V d\mathbf{r}\left[\nabla\times\left\{\nabla\times\frac{\mathbf{Q}_1^*(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\right]\cdot\frac{\mathbf{Q}_2(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\\&=\int_S dS\left[\left\{\nabla\times\frac{\mathbf{Q}_1^*(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\times\frac{\mathbf{Q}_2(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right]_n\\&\quad+\int_V d\mathbf{r}\left\{\nabla\times\frac{\mathbf{Q}_1^*(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\cdot\left\{\nabla\times\frac{\mathbf{Q}_2(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\},\end{aligned} \tag{A3}$$

where S denotes the surface of V and the first integral on the right-hand side is the surface integral of the normal component of the integrand. This surface integral is equal to zero because of the periodic boundary condition. Then, applying the identity Eq. (A2) again,

$$\begin{aligned}\langle\mathcal{H}\mathbf{Q}_1,\mathbf{Q}_2\rangle&=\int_S dS\left[\frac{\mathbf{Q}_1^*(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\times\left\{\nabla\times\frac{\mathbf{Q}_2(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\right]_n\\&\quad+\int_V d\mathbf{r}\frac{\mathbf{Q}_1^*(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\cdot\left[\nabla\times\left\{\nabla\times\frac{\mathbf{Q}_2(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\right]\\&=\langle\mathbf{Q}_1,\mathcal{H}\mathbf{Q}_2\rangle,\end{aligned} \tag{A4}$$

where we have again used the fact that the surface integral is equal to zero. Therefore, $\mathcal{H}$ is a Hermitian operator.

Next, we can easily show that $\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})$ given by

$$\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})=C\sqrt{\epsilon(\mathbf{r})}\frac{\mathbf{k}+\mathbf{G}_n}{|\mathbf{k}+\mathbf{G}_n|}\exp\{i(\mathbf{k}+\mathbf{G}_n)\cdot\mathbf{r}\}, \quad (A5)$$

where $\mathbf{G}_n$ is a reciprocal lattice vector and C is a normalization constant, satisfies Eq. (10). Then,

$$\mathcal{H}\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})=0. \quad (A6)$$

Therefore, the eigenangular frequency of this solution is zero. There exists one such solution for each $\mathbf{k}$ and n. In general,

$$\nabla\cdot\{\epsilon(\mathbf{r})\mathbf{E}_{\mathbf{k}n}^{(L)}(\mathbf{r})\}\equiv\nabla\cdot\{\sqrt{\epsilon(\mathbf{r})}\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})\}\neq 0. \quad (A7)$$

Therefore, we call $\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})$ a longitudinal-wave solution. Strictly speaking, $\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})$'s defined by Eq. (A5) are not orthogonal to each other. But their orthogonalization can be readily accomplished by Schmidt's method. We denote the orthogonalized longitudinal-wave solutions by the same symbols.

On the other hand, there exist transverse-wave solutions that correspond to the transverse plane waves in a uniform lattice. The eigenangular frequency defined in Eq. (8) is generally nonzero. From Eq. (8),

$$\nabla\cdot\{\sqrt{\epsilon(\mathbf{r})}\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})\}=\frac{c^2}{\omega_{\mathbf{k}n}^{(T)2}}\nabla\cdot\left[\nabla\times\left\{\nabla\times\frac{\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})}{\sqrt{\epsilon(\mathbf{r})}}\right\}\right]\equiv 0, \quad (A8)$$

i.e., Eq. (9) holds.

APPENDIX B

In the treatment of the electromagnetic normal modes of a photonic crystal, it is more familiar to work in the Fourier space than in the $\mathbf{r}$ space. So that we begin by relating the eigenvectors $\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})$ and $\mathbf{Q}_{\mathbf{k}n}^{(L)}(\mathbf{r})$ in the text to the familiar eigenvectors of the $\mathbf{k}$-space treatment.

The periodic dielectric function $\epsilon(\mathbf{r})$ of a photonic crystal is Fourier expanded as

$$\epsilon(\mathbf{r})=\sum_{\mathbf{G}}\epsilon(\mathbf{G})\exp(i\mathbf{G}\cdot\mathbf{r}), \quad (B1)$$

with

$$\epsilon(\mathbf{G})=\frac{1}{V_0}\int d\mathbf{r}\,\epsilon(\mathbf{r})\exp(-i\mathbf{G}\cdot\mathbf{r}), \quad (B2)$$

$\mathbf{G}$ being a reciprocal lattice vector and V_0 the volume of the unit cell. Here, we have denoted the Fourier component of $\epsilon(\mathbf{r})$ by the same character, because it does not seem confusing. In the same way as $\epsilon(\mathbf{G})$, we may define the Fourier components $\epsilon^{-1}(\mathbf{G})$, $\epsilon^{1/2}(\mathbf{G})$ and $\epsilon^{-1/2}(\mathbf{G})$ by the Fourier components of the periodic functions $1/\epsilon(\mathbf{r})$, $\sqrt{\epsilon(\mathbf{r})}$ and $1/\sqrt{\epsilon(\mathbf{r})}$, respectively. Note that $\epsilon^{-1}(\mathbf{G})$, for example, is not the inverse of $\epsilon(\mathbf{G})$. Let $\underline{\epsilon}$ be the matrix, the $\mathbf{GG}'$ matrix element of which is defined by

$$\underline{\epsilon}(\mathbf{GG}')=\epsilon(\mathbf{G}-\mathbf{G}'). \quad (B3)$$

For the inverse matrix $\underline{\epsilon}^{-1}$, it holds that

$$\underline{\epsilon}^{-1}(\mathbf{GG}')=\epsilon^{-1}(\mathbf{G}-\mathbf{G}'), \quad (B4)$$

and for the square-root matrix $\underline{\epsilon}^{1/2}$, which is defined by

$$\underline{\epsilon}(\mathbf{GG}')=\sum_{\mathbf{G}_1}\underline{\epsilon}^{1/2}(\mathbf{GG}_1)\underline{\epsilon}^{1/2}(\mathbf{G}_1\mathbf{G}'), \quad (B5)$$

it holds that

$$\underline{\epsilon}^{1/2}(\mathbf{GG}')=\epsilon^{1/2}(\mathbf{G}-\mathbf{G}'). \quad (B6)$$

Equations (B4) and (B6) assert that the Fourier components of the periodic function $\epsilon(\mathbf{r})^{-1}$ and $\epsilon(\mathbf{r})^{1/2}$ define $\underline{\epsilon}^{-1}$ and $\underline{\epsilon}^{1/2}$, respectively. In the same way it holds that the matrix $\underline{\epsilon}^{-1/2}$, the inverse of $\underline{\epsilon}^{1/2}$, is given by the Fourier transform of $\epsilon^{-1/2}(\mathbf{r})$. The proof of these relations is based upon the unitarity of the Fourier transform, i.e.,

$$\sum_{\mathbf{G}}\langle\mathbf{r}|\mathbf{G}\rangle\langle\mathbf{G}|\mathbf{r}'\rangle=\delta(\mathbf{r}-\mathbf{r}'), \quad (B7)$$

for $\mathbf{r}$ and $\mathbf{r}'$ within a unit cell and

$$\int_{\text{cell}}d\mathbf{r}\langle\mathbf{G}|\mathbf{r}\rangle\langle\mathbf{r}|\mathbf{G}'\rangle=\delta_{\mathbf{GG}'} \quad (B8)$$

for the integral over the unit cell with

$$\langle\mathbf{r}|\mathbf{G}\rangle=\frac{1}{\sqrt{V_0}}\exp(i\mathbf{G}\cdot\mathbf{r}). \quad (B9)$$

In view of Eqs.(B4) and (B6), there will be no confusion if we write the matrix elements simply as $\epsilon^{-1}(\mathbf{GG}')$, $\epsilon^{1/2}(\mathbf{GG}')$, and $\epsilon^{-1/2}(\mathbf{GG}')$, without using the underbar.

For the plane-wave expansion of the Bloch electric field of wave vector $\mathbf{k}$ (dropping the suffix $\mathbf{k}$ everywhere for brevity)

$$\mathbf{E}(\mathbf{r})=\frac{1}{\sqrt{V_0}}\sum_{\mathbf{G}}\mathbf{e}(\mathbf{G})\exp(i\mathbf{k}_{\mathbf{G}}\cdot\mathbf{r}), \quad (B10)$$

with

$$\mathbf{k}_{\mathbf{G}}=\mathbf{k}+\mathbf{G}, \quad (B11)$$

the amplitude $\mathbf{e}(\mathbf{G})$ is determined by

$$\sum_{\mathbf{G}}\sum_{j}\left\{[|\mathbf{k}_{\mathbf{G}}|^2\delta_{ij}-(\mathbf{k}_{\mathbf{G}})_i(\mathbf{k}_{\mathbf{G}})_j]\delta_{\mathbf{GG}'}-\frac{\omega^2}{c^2}\epsilon(\mathbf{GG}')\delta_{ij}\right\}\mathbf{e}(\mathbf{G}')_j=0, \quad (B12)$$

with i and j denoting the three Cartesian components. The eigenvector $\mathbf{e}(\mathbf{G})$ of the nth photonic band with frequency $\omega_{\mathbf{k}n}$ is denoted as $\mathbf{e}_n^{(T)}(\mathbf{G})$ and that of the longitudinal modes with zero frequency as $\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})$, the latter being taken to be a unit vector parallel to $\mathbf{k}_{\mathbf{G}}$:

$$\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G}')=\delta_{\mathbf{GG}'}\frac{\mathbf{k}_{\mathbf{G}}}{|\mathbf{k}_{\mathbf{G}}|}. \quad (B13)$$

Note that the suffix $\mathbf{G}$ labels the longitudinal modes. The notations $\mathbf{e}_n^{(T)}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$ will be used for the column vectors constructed by aligning $\mathbf{e}_n^{(T)}(\mathbf{G})_j$ and $\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})_j$, respectively, in order of $\mathbf{G}$ and j.

The matrix $\epsilon^{1/2}(\mathbf{GG}')$ induces a linear transformation of $\mathbf{e}_n^{(T)}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$:

$$\tilde{\mathbf{e}}_n^{(T)}(\mathbf{G})_j = \sum_{\mathbf{G}'} \epsilon^{1/2}(\mathbf{GG}')\mathbf{e}_n^{(T)}(\mathbf{G}')_j ,$$

$$\tilde{\mathbf{e}}_{\mathbf{G}'}^{(L)}(\mathbf{G})_j = \epsilon^{1/2}(\mathbf{GG}')\mathbf{e}_{\mathbf{G}'}^{(L)}(\mathbf{G}')_j . \tag{B14}$$

Equation (B6) used on the right-hand side then shows that the Fourier amplitudes $\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{G})$ and $\mathbf{Q}_{\mathbf{kG}}^{(L)}(\mathbf{G})$ of $\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})$ and $\mathbf{Q}_{\mathbf{kG}}^{(L)}(\mathbf{r})$, defined by Eq. (7), are nothing but these transformed vectors apart from the normalization constant:

$$\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{G})_j = \tilde{\mathbf{e}}_n^{(T)}(\mathbf{G})_j ,$$

$$\mathbf{Q}_{\mathbf{kG}}^{(L)}(\mathbf{G}')_j = \tilde{\mathbf{e}}_{\mathbf{G}}^{(L)}(\mathbf{G}')_j . \tag{B15}$$

Strictly speaking, before arriving at $\mathbf{Q}_{\mathbf{kG}}^{(L)}$ which forms by definition an orthonormal set, an additional transformation is necessary within the space spanned by the vectors $\tilde{\mathbf{e}}_{\mathbf{G}}^{(L)}$ which are not necessarily mutually orthogonal.

For real and positive $\epsilon(\mathbf{r})$, the matrix $\epsilon^{1/2}(\mathbf{GG}')$ is positive definite, meaning that the closure relation Eq. (12) setup among $\mathbf{Q}_{\mathbf{k}n}^{(T)}(\mathbf{r})$ and $\mathbf{Q}_{\mathbf{kG}}^{(L)}(\mathbf{r})$ is transferred directly to the linear independence of the eigenvectors $\mathbf{e}_n^{(T)}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$ of the secular equation of Eq. (B12). The conclusion is thus that any vectors in the $\mathbf{k}$ space may be expressed as a superposition of $\{\mathbf{e}_n^{(T)}\}$ (over n) and $\{\mathbf{e}_{\mathbf{G}}^{(L)}\}$ (over $\mathbf{G}$).

With these preparations, we now proceed to determining the eigenmodes for the vector and scalar potentials, $\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$, which are connected with $\mathbf{E}(\mathbf{r})$ through

$$\mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r}) + i\frac{\omega}{c}\mathbf{A}(\mathbf{r}). \tag{B16}$$

Let $v(\mathbf{G})$ and $\mathbf{a}(\mathbf{G})$ be their Fourier components.

(I) In the gauge of $V(\mathbf{r})=0$.

This is a trivial case since Eq. (B16) shows the eigenvectors for $\mathbf{a}(\mathbf{G})$ to be $-ic/\omega$ times that of the electric field. Specifying the normal mode of the vector potential by the index n, we find

$$\mathbf{a}_n^{(T)}(\mathbf{G}) = -\frac{ic}{\omega_{\mathbf{k}n}}\mathbf{e}_n^{(T)}(\mathbf{G}) \tag{B17}$$

for the photonic-band state $\mathbf{k}n$. Note that for the longitudinal eigenmodes $\mathbf{e}_{\mathbf{G}}^{(L)}$ a finite $\mathbf{a}_{\mathbf{G}}^{(L)}$ is not determined, because of the divergent prefactor $(-ic/\omega)$ with $\omega=0$.

(II) In the Coulomb gauge of $\nabla\cdot\mathbf{A}(\mathbf{r})=0$.

In terms of $v(\mathbf{G})$ and $\mathbf{a}(\mathbf{G})$, Maxwell's equations reduce to

$$\sum_{\mathbf{G}}\sum_{j}\left\{[|\mathbf{k}_{\mathbf{G}}|^2\delta_{ij}-(\mathbf{k}_{\mathbf{G}})_i(\mathbf{k}_{\mathbf{G}})_j]\delta_{\mathbf{GG}'} - \frac{\omega^2}{c^2}\epsilon(\mathbf{GG}')\delta_{ij}\right\}\mathbf{a}(\mathbf{G}')_j = -\frac{\omega}{c}\sum_{\mathbf{G}'}\epsilon(\mathbf{GG}')(\mathbf{k}_{\mathbf{G}'})_i v(\mathbf{G}'). \tag{B18}$$

In solving this eigenvalue equation, it is important to note that the electric field constructed by $\mathbf{a}(\mathbf{G})$ and $v(\mathbf{G})$, satisfying Eq. (B18) and the gauge condition, automatically satisfies the full set of Maxwell's equations. To obtain the eigenvalue ω and the eigenvector for $\mathbf{a}(\mathbf{G})$ and $v(\mathbf{G})$, let us expand the vector potential as follows:

$$\mathbf{a}(\mathbf{G}) = \sum_n \alpha_n\mathbf{e}_n^{(T)}(\mathbf{G}) + \beta_{\mathbf{G}}\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G}), \tag{B19}$$

with α_n and $\beta_{\mathbf{G}}$ as expansion coefficients. The gauge condition $[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{a}(\mathbf{G})]=0$, or $[\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})\cdot\mathbf{a}(\mathbf{G})]=0$ from Eq. (B13), eliminates the coefficient $\beta_{\mathbf{G}}$, leading to

$$\mathbf{a}(\mathbf{G}) = \sum_n \alpha_n\left\{\mathbf{e}_n^{(T)}(\mathbf{G}) - \frac{1}{|\mathbf{k}_{\mathbf{G}}|}[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})]\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})\right\}. \tag{B20}$$

Inserting this into Eq. (B18) and remembering that $\mathbf{e}_n^{(T)}$ is a solution of Eq. (B18) for the eigenvalue $\omega=\omega_{\mathbf{k}n}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$ for $\omega=0$, we obtain

$$\sum_n (\omega_{\mathbf{k}n}^2-\omega^2)\alpha_n\mathbf{e}_n^{(T)}(\mathbf{G}) - \omega^2\beta_{\mathbf{G}}\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G}) = -c\,\omega\mathbf{k}_{\mathbf{G}}v(\mathbf{G}). \tag{B21}$$

Equating the coefficients of the vector $\mathbf{e}_n^{(T)}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$ on both sides, with $\mathbf{k}_{\mathbf{G}}=|\mathbf{k}_{\mathbf{G}}|\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})$ on the right-hand side, then leads to

$$\omega=\omega_{\mathbf{k}n}, \tag{B22}$$

with

$$\alpha_n\neq 0, \quad v(\mathbf{G}) = -\frac{\omega_{\mathbf{k}n}}{c|\mathbf{k}_{\mathbf{G}}|^2}[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})]\alpha_n . \tag{B23}$$

This is a nth photonic-band solution. For the solution of $\omega=0$, we find that $\alpha_n=0$ for all n and $v(\mathbf{G})$ is arbitrary. The electric field obtained from Eq. (B16) is confirmed to reproduce properly the transverse and longitudinal eigenmodes given by the eigenvector $\mathbf{e}_n^{(T)}$ and $\mathbf{e}_{\mathbf{G}}^{(L)}$, respectively. From Eq. (B20), we conclude that only the photonic bands that are not genuinely transverse carry the nonzero scalar potential. These bands will then couple strongly with a longitudinal external probe, an impinging charged particle, for example.

(III) In the Lorentz gauge of $\nabla\cdot\mathbf{A}(\mathbf{r})-i(\omega/c)V(\mathbf{r})=0$.

Expanding the vector potential as in Eq. (B19), the gauge condition now reads

$$\sum_n \alpha_n[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})] + \beta_{\mathbf{G}}[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})] - \frac{\omega}{c}v(\mathbf{G}) = 0. \tag{B24}$$

Eliminating the scalar potential in Eq. (B18) leads to

$$\sum_n (\omega_{\mathbf{k}n}^2-\omega^2)\alpha_n\mathbf{e}_n^{(T)}(\mathbf{G}) - \omega^2\beta_{\mathbf{G}}\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G}) = -c^2\mathbf{k}_{\mathbf{G}}\left\{\sum_n \alpha_n[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})] + \beta_{\mathbf{G}}[\mathbf{k}_{\mathbf{G}}\cdot\mathbf{e}_{\mathbf{G}}^{(L)}(\mathbf{G})]\right\}. \tag{B25}$$

As in the Coulomb gauge, it then follows that

$$(\omega_{\mathbf{k}n}^2-\omega^2)\alpha_n=0,$$

$$(\omega^2-c^2|\mathbf{k_G}|^2)\beta_\mathbf{G}=\sum_n \alpha_n c^2|\mathbf{k_G}|[\mathbf{k_G}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})]. \tag{B26}$$

We have two cases from the first equation:
(a) $\omega=\omega_{\mathbf{k}n}$ with $\alpha_n\neq 0$,
(b) $\alpha_n=0$ for all n.

In the case (a) the second of Eq. (B26) leads to

$$\beta_\mathbf{G}=\frac{c^2|\mathbf{k_G}|}{\omega_{\mathbf{k}n}^2-c^2|\mathbf{k_G}|^2}[\mathbf{k_G}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})]\alpha_n. \tag{B27}$$

From Eq. (B24), the scalar potential is obtained as

$$v(\mathbf{G})=\frac{c\,\omega_{\mathbf{k}n}}{\omega_{\mathbf{k}n}^2-c^2|\mathbf{k_G}|^2}[\mathbf{k_G}\cdot\mathbf{e}_n^{(T)}(\mathbf{G})]\alpha_n. \tag{B28}$$

Again, the electric field is then seen from Eq. (B16) to be proportional to $\mathbf{e}_n^{(T)}$ as it should be.

In the case (b), we obtain from the second of Eq. (B26)

$$(\omega^2-c^2|\mathbf{k_G}|^2)\beta_\mathbf{G}=0, \tag{B29}$$

from which we have an interesting solution,

$$\omega=c|\mathbf{k_G}|, \tag{B30}$$

with $\beta_\mathbf{G}\neq 0$, $v(\mathbf{G})=\beta_\mathbf{G}$, and $\mathbf{a}(\mathbf{G})=\beta_\mathbf{G}\mathbf{e}_\mathbf{G}^{(L)}(\mathbf{G})$. This is an eigenmode of a purely longitudinal vector potential, with a different eigenvalue. However, Eq. (B16) leads then to $\mathbf{e}(\mathbf{G})=\mathbf{0}$, implying that the solution is a kind of ghost solution. The eigenmode with $\omega=0$, excluded from the cases (a) and (b), is identical to that of the Coulomb gauge, because the gauge condition reduces in this case to $\nabla\cdot\mathbf{A}(\mathbf{r})=\mathbf{0}$.

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