Sum-frequency generation in a two-dimensional photonic lattice

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We have formulated the Green's-function method for describing nonlinear optical processes in an arbitrary two-dimensional photonic lattice with particular regard to sum-frequency generation. In addition to the derivation of the generalized phase-matching condition, we have shown that the field intensity and the average Poynting's vector of the sum-frequency component are proportional to its (group velocity)$^{-2}$ and (group velocity)$^{-1}$, respectively. Therefore, an enhancement is expected for both of them at photonic band edges, where the group velocity tends to zero. This method was applied to a square lattice composed of circular air-rods formed in a $LiNbO_3$ crystal, and the average intensity of the electric field of the second harmonic and the effective nonlinear susceptibility were numerically calculated. [S0163-1829(96)07832-0]

I. INTRODUCTION

Periodic dielectric structures called photonic crystals or photonic lattices have attracted much interest.[1–16] The main reason for the recent intensive investigations lies in the fact that a photonic band gap, in which the existence of electromagnetic modes is forbidden, can be realized by means of the proper choice of the lattice structure and the dielectric constants.[1–3] Many peculiar physical phenomena due to the photonic band gap, such as the suppression of spontaneous emission[4] and energy transfer,[5] localized donor and acceptor modes,[6,7] and stable solitary waves,[8,9] have been predicted, and some of them were confirmed experimentally. The symmetry of the wave functions of the eigenmodes was also analyzed, and the existence of uncoupled modes that cannot be excited by an external plane wave was shown.[10–14] Moreover, it is expected that the photonic band gaps in luminescent semiconductors, for example, realize several technological applications such as single-mode light-emitting diodes.[2]

In addition to these phenomena, which originate purely from the zero-state density in the photonic band gaps, the divergent state density at the band edges also yield possibilities. For example, John and Quang discussed spontaneous emission near a band edge, and showed its nonexponential decay, etc.[15,16] On the other hand, the divergent state density at an edge of any branch of the photonic bands brings about an enhancement of nonlinear optical processes.

Let us consider a situation where both the frequency and the wave vector of the final state of a nonlinear optical process are located near a photonic band edge by the constraint due to energy and momentum conservations. Then the probability of the nonlinear process is enhanced compared with that in a uniform material due to the divergent state density at the band edge. In addition, the phase-matching condition can be fulfilled by an appropriate use of the band dispersion. In this paper, we will demonstrate this enhancement, and the modified phase-matching condition for the case of sum-frequency generation. First we will formulate the Green's-function method for describing sum-frequency generation in an arbitrary two-dimensional (2D) photonic lattice with the second-order optical nonlinearity and derive the phase-matching condition by taking into account the umklapp process. We will also show some results of numerical calculations on the effective nonlinear susceptibility, and the intensity of the induced nonlinear field.

The analytical formula and the phase-matching condition will be given in Sec. II. In Sec. III, the intensity of the induced second-harmonic field in a 2D square lattice will be numerically calculated based on the dispersion relation and the eigenfunctions given by the plane-wave expansion method. The selection rule due to the symmetry of the eigenfunctions of the fundamental and harmonic waves will be also discussed. The reduction of our formula to the case of a uniform crystal will be examined in Appendix A. An efficient method to calculate the group velocity in 2D lattices will be given in Appendix B.

II. THEORY

In this section, we will derive an expression for sum-frequency generation in an arbitrary 2D photonic lattice. An example of a 2D lattice is shown in Fig. 1, which is the top view of a square lattice composed of identical cylinders with a radius R, where the dielectric constants of the cylinder and the background are denoted by ϵ_1 and ϵ_2, respectively. In this case, the 2D elementary lattice vectors are $(a,0)$ and $(0,a)$ where a is the lattice constant. In a general case, we take these vectors as $(a,0)$ and (b_x,b_y), and there is no restriction on the position-dependent dielectric constant $\epsilon(\mathbf{x})$ except the periodicity under the translation by an elementary lattice vector. Here $\mathbf{x}$ is the 2D position vector (x,y). The elementary reciprocal-lattice vectors in the general case are $(2\pi/a,-2\pi b_x/ab_y)$ and $(0,2\pi/b_y)$. The z axis is taken as to be perpendicular to the 2D plane.

Now we assume that the 2D lattice is composed of a material with second-order nonlinearity. Thus, we introduce a position-dependent second-order susceptibility $\chi^{(2)}(\mathbf{x})$ that is also a periodic function of $\mathbf{x}$. We assume that the wave

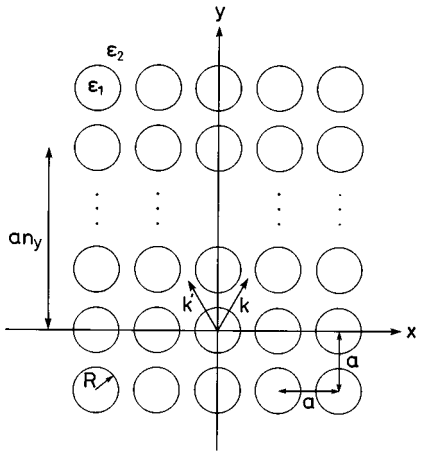

FIG. 1. An example of a 2D lattice. This figure is the top view of a square lattice with a lattice constant a composed of identical cylinders with a radius R. The dielectric constants of the cylinder and the background are denoted by ϵ_1 and ϵ_2, respectively. The position-dependent second-order susceptibility $\chi^{(2)}(\mathbf{x})$ is assumed to be nonzero at $0 \leqslant y \leqslant a n_y$ in this example. Two incident eigenmodes of E polarization with wave vectors $\mathbf{k}$ and $\mathbf{k}'$, and angular frequencies $\omega_{\mathbf{k}\mu}$ and $\omega_{\mathbf{k}'\mu'}$ generate the sum-frequency component.

vectors of two incident waves, which are eigenmodes of the 2D photonic lattice, lie in the (x,y) plane. Then the vector Maxwell's equations are reduced to two independent scalar equations.[17] The eigenmodes of these scalar equations are called the E polarization, for which the electric field is parallel to the z axis, and the H polarization, for which the magnetic field is parallel to the z axis. In this paper, we will consider the case of E polarization.

The z component of the electric displacement vector D_z is given by

$$D_z(\mathbf{x},t) = \epsilon(\mathbf{x}) E_z(\mathbf{x},t) + 4\pi \chi^{(2)}(\mathbf{x}) E_z^2(\mathbf{x},t). \tag{1}$$

We assume that D_x and D_y are zero. This situation can be realized if we use, for example, a nonlinear crystal of $3m$-C_{3v} symmetry such as $LiNbO_3$, with its crystalline c axis parallel to the z axis. Then the E polarization corresponds to the extraordinary wave in the above uniaxial crystal. We will omit the suffix z hereafter. In order to clarify the phase-matching condition, we further assume that $\chi^{(2)}(\mathbf{x})$ is nonzero only at $0 \leqslant y \leqslant n_y b_y$, where n_y is a positive integer.

The second-order nonlinear polarization produced by $\chi^{(2)}(\mathbf{x})$ yields the sum-frequency component whose wave function $E(\omega_{\mathbf{k}\mu} + \omega_{\mathbf{k}'\mu'}:\mathbf{x},t)$ satisfies the following equation, which can be easily derived from Maxwell's equations with an assumption that the amplitude of the sum-frequency component is much smaller than those of the fundamental waves:

$$\mathcal{L}\left[i\frac{\partial}{\partial t} \right] E(\omega_{\mathbf{k}\mu} + \omega_{\mathbf{k}'\mu'}:\mathbf{x},t) \equiv \left[-\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \frac{1}{\epsilon(\mathbf{x})}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] E(\omega_{\mathbf{k}\mu} + \omega_{\mathbf{k}'\mu'}:\mathbf{x},t)$$
$$= -\frac{4\pi \chi^{(2)}(\mathbf{x})(\omega_{\mathbf{k}\mu} + \omega_{\mathbf{k}'\mu'})^2 A^2}{c^2 \epsilon(\mathbf{x})} E_{\mathbf{k}\mu}(\mathbf{x}) e^{-i\omega_{\mathbf{k}\mu} t} E_{\mathbf{k}'\mu'}(\mathbf{x}) e^{-i\omega_{\mathbf{k}'\mu'} t}, \tag{2}$$

where $E_{\mathbf{k}\mu}(\mathbf{x})\exp(-i\omega_{\mathbf{k}\mu}t)$ and $E_{\mathbf{k}'\mu'}(\mathbf{x})\exp(-i\omega_{\mathbf{k}'\mu'}t)$ are the wave functions of the two incident eigenmodes with the wave vectors of $\mathbf{k}$ and $\mathbf{k}'$ and the eigenangular frequencies of $\omega_{\mathbf{k}\mu}$ and $\omega_{\mathbf{k}'\mu'}$, A is their amplitude, μ and μ' are the indices for specifying the band, c is the light velocity in vacuum, and the magnetic permeability was taken to be unity. Then $E_{\mathbf{K}\nu}(\mathbf{x})$ satisfies the following equation:[17]

$$\mathcal{L}[\omega_{\mathbf{K}\nu}] E_{\mathbf{K}\nu}(\mathbf{x}) \equiv \left[\frac{\omega_{\mathbf{K}\nu}^2}{c^2} + \frac{1}{\epsilon(\mathbf{x})}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] E_{\mathbf{K}\nu}(\mathbf{x}) = 0. \tag{3}$$

According to Bloch's theorem, the eigenfunction of the photonic lattice can be expressed as

$$E_{\mathbf{k}\mu}(\mathbf{x}) = \exp(i\mathbf{k}\cdot\mathbf{x}) u_{\mathbf{k}\mu}(\mathbf{x}), \tag{4}$$

where $u_{\mathbf{k}\mu}(\mathbf{x})$ is a periodic function under the translation by an elementary lattice vector.

In order to calculate the wave function of the sum-frequency component in Eq. (2), we have to solve an inhomogeneous equation of the following type:

$$\mathcal{L}\left[i\frac{\partial}{\partial t} \right] E(\mathbf{x},t) = f(\mathbf{x}) e^{-i\omega t}. \tag{5}$$

This can be accomplished by the Green's-function method as follows. First, we define differential operators $\mathcal{L}_2$ and $\mathcal{H}$ such that

$$\mathcal{L}_2\left[i\frac{\partial}{\partial t} \right] \equiv -\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \mathcal{H},$$
$$\mathcal{H} \equiv -\frac{1}{\sqrt{\epsilon(\mathbf{x})}}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \frac{1}{\sqrt{\epsilon(\mathbf{x})}}. \tag{6}$$

Then the eigenequation Eq. (3) is equivalent to the following equation:

$$\mathcal{H} Q_{\mathbf{K}\nu}(\mathbf{x}) = \frac{\omega_{\mathbf{K}\nu}^2}{c^2} Q_{\mathbf{K}\nu}(\mathbf{x}), \tag{7}$$

where

$$Q_{\mathbf{K}\nu}(\mathbf{x}) = \sqrt{\epsilon(\mathbf{x})} E_{\mathbf{K}\nu}(\mathbf{x}). \tag{8}$$

Because $\mathcal{H}$ is a Hermitian operator, its eigenfunctions $\{Q_{\mathbf{K}\nu}\}$ form a complete orthonormal set.

We assume, without a loss of generality, the periodic boundary condition for $Q_{\mathbf{k}\mu}(\mathbf{x})$ over a 2D volume V that is spanned by $N_1(a,0)$ and $N_2(b_x,b_y)$, and that $Q_{\mathbf{k}\mu}(\mathbf{x})$ is normalized in a unit volume. Here N_1 and N_2 are positive integers. Then the orthogonality condition is

$$\int_V d\mathbf{x}\, Q_{\mathbf{K}\nu}(\mathbf{x}) Q^*_{\mathbf{K}'\nu'}(\mathbf{x}) = V\delta_{\mathbf{K}\mathbf{K}'}\delta_{\nu\nu'}, \tag{9}$$

where $\delta_{\mathbf{K}\mathbf{K}'}$ and $\delta_{\nu\nu'}$ are the Kronecker δ's. In addition, the completeness of the eigenfunctions leads to

$$\sum_{\mathbf{K}} \sum_{\nu} Q_{\mathbf{K}\nu}(\mathbf{x}) Q^*_{\mathbf{K}\nu}(\mathbf{x}') = V\delta(\mathbf{x}-\mathbf{x}'), \tag{10}$$

where $\delta(\mathbf{x})$ is the Dirac δ function.

Now, Eq. (5) is modified to

$$\mathcal{L}_2\left[i\frac{\partial}{\partial t}\right]\sqrt{\epsilon(\mathbf{x})}E(\mathbf{x},t) = \sqrt{\epsilon(\mathbf{x})}f(\mathbf{x})e^{-i\omega t}. \tag{11}$$

We define the retarded Green's function of Eq. (11) by

$$\mathcal{L}_2\left[i\frac{\partial}{\partial t}\right]G(\mathbf{x},\mathbf{x}',t-t') = \delta(\mathbf{x}-\mathbf{x}')\,\delta(t-t'),$$

$$G(\mathbf{x},\mathbf{x}',t-t') = 0 \quad \text{for} \quad t<t'. \tag{12}$$

Then, $\sqrt{\epsilon(\mathbf{x})}E(\mathbf{x},t)$ is, as usual, given by

$$\begin{aligned}\sqrt{\epsilon(\mathbf{x})}E(\mathbf{x},t) &= \int_V d\mathbf{x}' \int_{-\infty}^{\infty} dt'\, G(\mathbf{x},\mathbf{x}',t-t') \\ &\quad\times \sqrt{\epsilon(\mathbf{x}')}f(\mathbf{x}')e^{-i\omega t'} \\ &= e^{-i\omega t}\int_V d\mathbf{x}'\, \mathcal{G}(\mathbf{x},\mathbf{x}',\omega)\sqrt{\epsilon(\mathbf{x}')}f(\mathbf{x}'),\end{aligned} \tag{13}$$

where $\mathcal{G}(\mathbf{x},\mathbf{x}',\omega)$, which is the Fourier transform of $G(\mathbf{x},\mathbf{x}',t)$, is given by

$$\begin{aligned}\mathcal{G}(\mathbf{x},\mathbf{x}',\omega) &\equiv \int_{-\infty}^{\infty} dt\, G(\mathbf{x},\mathbf{x}',t)e^{i\omega t} \\ &= \frac{c^2}{V}\sum_{\mathbf{K}}\sum_{\nu}\frac{Q_{\mathbf{K}\nu}(\mathbf{x})Q^*_{\mathbf{K}\nu}(\mathbf{x}')}{(\omega-\omega_{\mathbf{K}\nu}+i\delta)(\omega+\omega_{\mathbf{K}\nu}+i\delta)},\end{aligned} \tag{14}$$

where δ is a positive infinitesimal. The last equality in Eq. (14) is derived from Eqs. (7) and (10), and the following relation:

$$\mathcal{L}_2[\omega]\mathcal{G}(\mathbf{x},\mathbf{x}',\omega) = \delta(\mathbf{x}-\mathbf{x}'). \tag{15}$$

Inclusion of $i\delta$ in the denominator in Eq. (14) assures the retarded solution of Eq. (11).

Then, from Eq. (13),

$$\begin{aligned}E(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}:\mathbf{x},t) &= -\frac{4\pi(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})^2A^2}{V}\exp[-i(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})t] \\ &\quad\times\sum_{\mathbf{K}}\sum_{\nu}\frac{E_{\mathbf{K}\nu}(\mathbf{x})}{(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}-\omega_{\mathbf{K}\nu}+i\delta)(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}+\omega_{\mathbf{K}\nu}+i\delta)} \\ &\quad\times\int_V d\mathbf{x}'\,\chi^{(2)}(\mathbf{x}')E^*_{\mathbf{K}\nu}(\mathbf{x}')E_{\mathbf{k}\mu}(\mathbf{x}')E_{\mathbf{k}'\mu'}(\mathbf{x}'),\end{aligned} \tag{16}$$

where the summation with respect to $\mathbf{K}$ is over the first Brillouin zone. Substituting Eq. (4), the integral in Eq. (16) is calculated as

$$\begin{aligned}\int_V d\mathbf{x}'\,\chi^{(2)}(\mathbf{x}')E^*_{\mathbf{K}\nu}(\mathbf{x}')E_{\mathbf{k}\mu}(\mathbf{x}')E_{\mathbf{k}'\mu'}(\mathbf{x}') &= \delta_{K_x,k_x+k'_x-(2n\pi/a)}\int_V d\mathbf{x}'\,\chi^{(2)}(\mathbf{x}')u^*_{\mathbf{K}\nu}(\mathbf{x}')u_{\mathbf{k}\mu}(\mathbf{x}')u_{\mathbf{k}'\mu'}(\mathbf{x}')\exp\left(\frac{2n\pi i x'}{a}\right) \\ &\quad\times\exp[i(k_y+k'_y-K_y)y'],\end{aligned} \tag{17}$$

where $\delta_{K_x,k_x+k'_x-2n\pi/a}$ is the Kronecker δ, and n is an integer that was introduced to make allowance for an umklapp process. Because of the periodicity of $\chi^{(2)}(\mathbf{x})u^*_{\mathbf{K}\nu}(\mathbf{x})u_{\mathbf{k}\mu}(\mathbf{x})u_{\mathbf{k}'\mu'}(\mathbf{x})$ and the periodic boundary condition, the integration over x' in Eq. (17) is nonzero only when the difference $k_x+k'_x-K_x$ is a multiple of $2\pi/a$. Actually, n is equal to -1, 0, or 1 because $\mathbf{K}$, $\mathbf{k}$, and $\mathbf{k}'$ all belong to the first Brillouin zone. Now we define $\bar{K}_x$ as $\bar{K}_x = k_x+k'_x-2n\pi/a$. Then, Eq. (17) equals

$$\begin{aligned}&\delta_{K_x,\bar{K}_x}\sum_{j=0}^{N_1-1}\sum_{l=0}^{n_y-1}\int_{V_0}d\mathbf{x}'\,\chi^{(2)}(\mathbf{x}')u^*_{\mathbf{K}\nu}(\mathbf{x}')u_{\mathbf{k}\mu}(\mathbf{x}')u_{\mathbf{k}'\mu'}(\mathbf{x}')\exp\left[\frac{2n\pi i}{a}(x'+ja+lb_x)\right]\exp[i(k_y+k'_y-K_y)(y'+lb_y)] \\ &= N_1V_0\delta_{K_x,\bar{K}_x}F(\mathbf{K}\nu,\mathbf{k}\mu,\mathbf{k}'\mu')\frac{1-\exp[i\{(k_y+k'_y-K_y)b_y+2n\pi b_x/a\}n_y]}{1-\exp[i\{(k_y+k'_y-K_y)b_y+2n\pi b_x/a\}]},\end{aligned} \tag{18}$$

where

$$F(\mathbf{K}\nu,\mathbf{k}\mu,\mathbf{k}'\mu')=\frac{1}{V_0}\int_{V_0}d\mathbf{x}'\chi^{(2)}(\mathbf{x}')u^{*}_{\mathbf{K}\nu}(\mathbf{x}')u_{\mathbf{k}\mu}(\mathbf{x}')u_{\mathbf{k}'\mu'}(\mathbf{x}')\exp\left(\frac{2n\pi ix'}{a}\right)\exp[i(k_y+k_y'-K_y)y'], \tag{19}$$

which may be regarded as an effective nonlinear susceptibility with respect to the initial and final states, and V_0 denotes the volume of the unit cell.

Next, we denote the ''group velocity'' of the νth band to the y direction by $v_g(\omega,\nu)$:

$$v_g(\omega,\nu)=\left(\frac{\partial\omega_{\mathbf{K}\nu}}{\partial K_y}\right)_{K_x=\overline{K}_x,\omega_{\mathbf{K}\nu}=\omega}. \tag{20}$$

Then, converting summation over K_y into an integration over $\omega_{\overline{K}_x K_y\nu}$ in Eq. (16), we obtain

$$\begin{aligned}E(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}:\mathbf{x},t)=&-2(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})^2A^2b_y\exp[-i(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})t]\\&\times\sum_{\nu}\int d\omega_{\overline{K}_x K_y\nu}\frac{E_{\overline{K}_x K_y\nu}(\mathbf{x})F(\overline{K}_x K_y\nu,\mathbf{k}\mu,\mathbf{k}'\mu')}{v_g(\omega_{\overline{K}_x K_y\nu},\nu)(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}-\omega_{\overline{K}_x K_y\nu}+i\delta)(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}+\omega_{\overline{K}_x K_y\nu}+i\delta)}\\&\times\frac{1-\exp[i\{(k_y+k_y'-K_y)b_y+2n\pi b_x/a\}n_y]}{1-\exp[i\{(k_y+k_y'-K_y)b_y+2n\pi b_x/a\}]}.\end{aligned} \tag{21}$$

Here we define the wave vector $\overline{\mathbf{K}}_\nu$ such that

$$\overline{K}_{\nu x}=\overline{K}_x \quad\text{and}\quad \omega_{\overline{\mathbf{K}}\nu}=\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}. \tag{22}$$

The last term on the right-hand side of Eq. (21), which leads to the phase-matching condition, as we will show below, substantially restricts the region of integration on $\omega_{\overline{K}_x K_y\nu}$ when n_y is sufficiently large, because it consists of a sharp peak. Then the rest of the integrand may be regarded as slowly varying around this peak, except for the next term,

$$\frac{1}{\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}-\omega_{\overline{K}_x K_y\nu}+i\delta}=\frac{\mathcal{P}}{\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}-\omega_{\overline{K}_x K_y\nu}}-\pi i\delta(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}-\omega_{\overline{K}_x K_y\nu}), \tag{23}$$

where $\mathcal{P}$ denotes Cauchy's principal value. The phase matching is realized when the peak of the last term of Eq. (21) coincides with the pole of Eq. (23). Then the second term on the right-hand side of Eq. (23) makes the dominant contribution, and we neglect the first term. We also neglect the contribution from those bands which do not include $\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}$ as an eigenfrequency. In Appendix A, we will discuss the relation between this approximation and the rigorous calculation for the case of a *uniform lattice*. In a general case, analytical evaluation of the integral is not possible, and the above approximation leads to

$$\begin{aligned}E(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}:\mathbf{x},t)\simeq&\pi i(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})A^2b_y\exp[-i(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'})t]\sum_{\{\nu\}'}\frac{E_{\overline{\mathbf{K}}_\nu\nu}(\mathbf{x})F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}\mu,\mathbf{k}'\mu')}{v_g(\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'},\nu)}\\&\times\frac{1-\exp[i\{(k_y+k_y'-\overline{K}_{\nu y})b_y+2n\pi b_x/a\}n_y]}{1-\exp[i\{(k_y+k_y'-\overline{K}_{\nu y})b_y+2n\pi b_x/a\}]},\end{aligned} \tag{24}$$

where the summation is over bands which include $\omega_{\mathbf{k}\mu}+\omega_{\mathbf{k}'\mu'}$ as an eigenfrequency.

Apart from the weak dependence of $F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}\mu,\mathbf{k}'\mu')$ on $\overline{\mathbf{K}}_\nu$, $\mathbf{k}$, and $\mathbf{k}'$, Eq. (24) leads to the phase-matching condition

$$\overline{K}_{\nu y}=k_y+k_y'+\frac{2n\pi b_x}{ab_y}-\frac{2m\pi}{b_y}, \tag{25}$$

where m is -1, 0, or 1. Together with the momentum conservation in the x direction,

$$\overline{\mathbf{K}}_\nu=\mathbf{k}+\mathbf{k}'-n\left(\frac{2\pi}{a},-\frac{2\pi b_x}{ab_y}\right)-m\left(0,\frac{2\pi}{b_y}\right). \tag{26}$$

Equation (26) means that the conservation of the crystalline momentum assures the phase matching. In addition, we have to note that $F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}\mu,\mathbf{k}'\mu')$, which is regarded as an effective nonlinear susceptibility with respect to the initial and final states, may vanish for particular combinations of $\mathbf{k}\mu$ and $\mathbf{k}'\mu'$ in highly symmetric photonic lattices because of the symmetry of the relevant wave functions. This gives a kind of selection rules. We will discuss this point for a particular case of a square lattice in Sec. III.

We should also note that the field intensity is proportional to $|c/v_g|^2$, and we can expect a large enhancement at the photonic band edge where v_g tends to zero. On the other hand, the average velocity of energy flow is equal to v_g,[19] and so the average Poynting's vector is proportional to $|c/v_g|$.

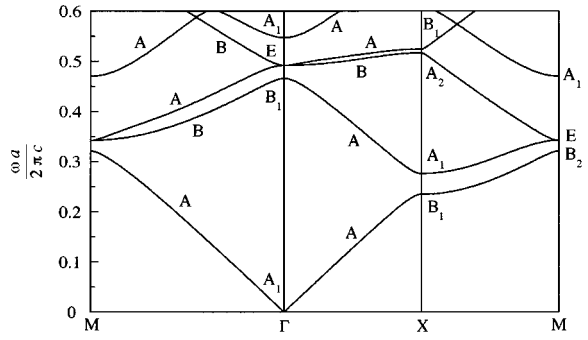

FIG. 2. The dispersion relation of the square lattice of circular air rods formed in a $LiNbO_3$ crystal. The ordinate is the normalized angular frequency. The following values were assumed: $R/a=0.3$, $\epsilon_1=1.0$, and $\epsilon_2=4.9912$, which is the dielectric constant of $LiNbO_3$ at 532 nm. The symmetry of the eigenfunctions are also shown.

We would like to conclude this section by making two remarks. First, as is apparent from the above derivation, the enhancement of the induced electric field and the Poynting's vector due to a small v_g, or, in other words, to a divergent state density at a photonic band edge, which was shown here for sum-frequency generation, is a universal feature of nonlinear optical processes in photonic lattices. Second, the extension of the present calculation to three-dimensional (3D) lattices is straightforward if we take into consideration the 3D variation of the position-dependent dielectric constant and the vector nature of the eigenfunctions.

III. NUMERICAL CALCULATION AND DISCUSSION

In this section, we apply our method to second-harmonic generation (SHG) in a square lattice of circular air rods formed in a $LiNbO_3$ crystal. We assume that the crystalline c axis of this uniaxial crystal of $3m$-C_{3v} symmetry is aligned along the z axis. Then the incident fundamental waves of the E polarization yield only the z component of the harmonic electric displacement vector, and, therefore, the method given in Sec. II is applicable. Similar situations can be realized for crystals of 4-C_4, $4mm$-C_{4v}, 3-C_3, 6-C_6, and $6mm$-C_{6v} symmetry as well.

Figure 2 shows the photonic band structure of the square lattice, where we assumed that $R/a=0.3$, $\epsilon_1=1.0$, and $\epsilon_2=4.9912$, which is the dielectric constant of $LiNbO_3$ at 532 nm. The calculation was performed by the plane-wave expansion method according to Plihal and Maradudin.[17] The number of basis plane waves was 289, and the accuracy was estimated as better than 1%. The Brillouin zone of the 2D square lattice has two highly symmetric points beside the Γ point. They are the X point $(0,\pi/a)$ and the M point $(\pi/a,\pi/a)$. Figure 2 is drawn for these points. The symmetry of the eigenfunctions are also shown in Fig. 2.[13]

Now, we assume for simplicity that $\mathbf{k}=(k_x,k_y)$ and $\mathbf{k}'=(-k_x,k_y)$ $(k_y>0)$. Then, the phase-matching condition is fulfilled when

$$\overline{K_x}=0 \quad \text{and} \quad \overline{K_{\nu y}}=2k_y-\frac{2m\pi}{a} \quad (m=0,1). \tag{27}$$

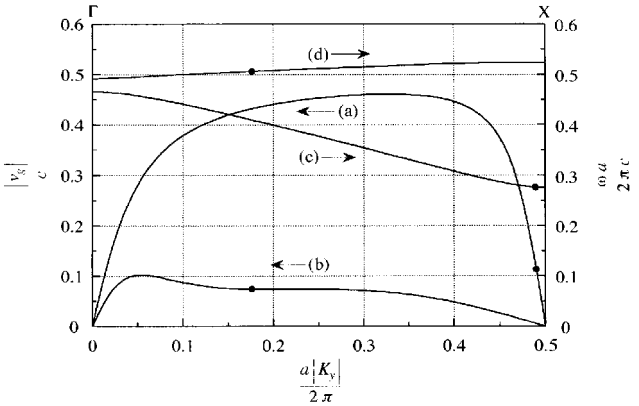

FIG. 3. The group velocity of (curve a) the second branch and (curve b) the fourth branch on segment $\overline{\Gamma X}$. Curves (c) and (d) are their dispersion relations. The same parameters as for Fig. 2 were assumed. The data points corresponding to cases 1 and 2 are denoted by solid circles (see text).

Here we consider two examples. In case 1, two incident waves in the lowest branch induce the second harmonic in the second lowest branch on segment $\overline{\Gamma X}$, $\omega a/2\pi c\simeq 0.14$ for the fundamental wave, and $m=0$. In case 2, the second harmonic in the fourth branch on segment $\overline{\Gamma X}$ with negative K_y is induced by similar incident waves. $\omega a/2\pi c\simeq 0.25$ and $m=1$ for this case. The effective nonlinear susceptibility $F(\mathbf{K}_\nu\nu,\mathbf{k}1,\mathbf{k}'1)$ ($\nu=2$ or 4) is nonzero for both cases. On the other hand, the third branch does not contribute to SHG since $F(\overline{\mathbf{K}_3}3,\mathbf{k}1,\mathbf{k}'1)=0$. This is because the wave function of the third branch on segment $\overline{\Gamma X}$ is antisymmetric under the mirror reflection at the yz plane, whereas the induced electric displacement of the second harmonic is symmetric. As seen in this example, $F(\mathbf{K}\nu,\mathbf{k}\mu,\mathbf{k}'\mu')$ vanishes for particular combinations of the initial and final states in a highly symmetric lattice, and this gives selection rules that are not relevant to the crystallographic symmetry of the host crystal.

Figure 3 shows the group velocity of the second and fourth branches on segment $\overline{\Gamma X}$ together with their dispersion curves. The former was calculated by means of Hellmann-Feynman theorem. The detail is described in Appendix B. As is understood from this figure, the group velocity of both bands tends to zero at the Γ and X points. In addition, the group velocity of the fourth band is small over the whole branch due to the flatness of its dispersion curve.

Now we take the angular frequency of the fundamental wave ω such that $\omega a/2\pi c=0.138$ for case 1 and $\omega a/2\pi c=0.253$ for case 2. Then $|v_g|/c$ at 2ω is 0.114 and 0.0740, respectively. The corresponding data points are denoted by solid circles in Fig. 3, where we have to note that $K_y<0$ for case 2. Figure 4 shows two contours of the lowest branch for both cases where the dielectric constant of the host crystal ϵ_2 is assumed to be 4.6483, which is that of $LiNbO_3$ at 1064 nm. In order to use this value consistently with the assumed angular frequency of the fundamental waves, the lattice constant a should be about 0.15 μm for case 1 and 0.27 μm for case 2. From the dispersion relations of the second and fourth bands, we find that the phase-matching condition is fulfilled when $ak_y/2\pi=0.245$ for case 1 and $ak_y/2\pi=0.413$ for case 2, respectively. Note that

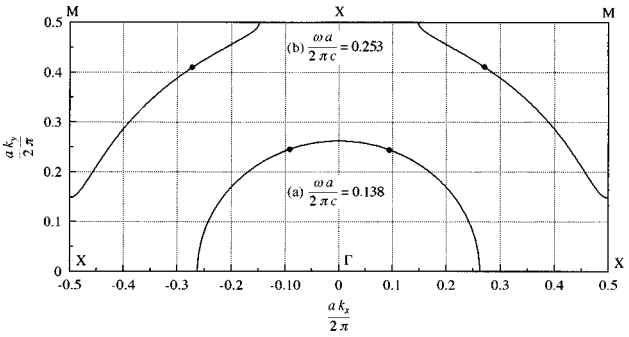

FIG. 4. Contours of the lowest branch for (a) case 1: $\omega a/2\pi c=0.138$; and (b) case 2: $\omega a/2\pi c=0.253$. The same parameters as for Fig. 2 were assumed except that $\epsilon_2=4.6483$, which is the dielectric constant of $LiNbO_3$ at 1064 nm. The data points for which the phase-matching condition for SHG is fulfilled are denoted by solid circles.

phase matching is impossible for E polarization in a uniform $LiNbO_3$ crystal because the dielectric constant at 2ω is larger than that at ω.

The average intensity of the electric field of the second harmonic, $\overline{|E(2\omega:\mathbf{x},t)|^2}$, is given by

$$\overline{|E(2\omega:\mathbf{x},t)|^2}=16\pi^4A^4\left(\frac{\omega a}{2\pi c}\right)^2\left(\frac{c}{v_g}\right)^2\overline{|E_{\mathbf{K}_\nu\nu}(\mathbf{x})|^2}\times|F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}1,\mathbf{k}'1)|^2\left|\frac{\sin(\Delta k n_y a/2)}{\sin(\Delta k a/2)}\right|^2, \tag{28}$$

where

$$\Delta k=2k_y-\overline{K}_{\nu y}-\frac{2m\pi}{a}. \tag{29}$$

The results of the numerical calculation are shown in Fig. 5, where n_y was assumed to be 100 and $\chi^{(2)}$ of $LiNbO_3$ was taken as 1.94×10^{-7} (esu).[18] The abscissa is the angle of incidence of the fundamental waves, and the angular dependence of $|F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}1,\mathbf{k}'1)|$ is also shown. In this figure, we find the sharp peaks of $\overline{|E(2\omega:\mathbf{x},t)|^2}$ at the phase-matched angles, which are 20.9° for case 1 [Fig. 5(a)] and 33.1° for case 2 [Fig. 5(b)]. We also find the fairly weak angular variation of the effective nonlinear susceptibility around the peak, which was assumed when we derived the phase-matching condition in Sec. II. The sharpness of the peak depends on n_y. For a very small n_y, the peak becomes broad, and the angular variation of $|F(\overline{\mathbf{K}}_\nu\nu,\mathbf{k}\mu,\mathbf{k}'\mu')|$ may somewhat affect the peak position. On the other hand, the height of the peak is proportional to n_y^2. Therefore, the peak height increases quadratically with the sample thickness an_y. It was assumed to be about 15 or 27 μm for the present cases.

IV. CONCLUSION

We have formulated the Green's-function method for sum-frequency generation in an arbitrary 2D photonic lattice. In addition, we have derived the generalized phase-matching condition by taking into account the umklapp process, and shown that the conservation of the crystalline momentum assures the phase matching. We have also shown that the effective nonlinear susceptibility vanishes for particular combinations of the fundamental and second-harmonic waves in highly symmetric photonic lattices, and this fact gives a kind of selection rules beside those derived from the crystallographic symmetry of the host crystal.

We have applied our method to a 2D square lattice composed of circular air rods formed in a $LiNbO_3$ crystal, and numerically calculated the angular dependence of the effective nonlinear susceptibility and the average intensity of the second harmonic. Because of the weak angular dependence of the former, the peak position of the latter is almost rigorously determined by the generalized phase-matching condition.

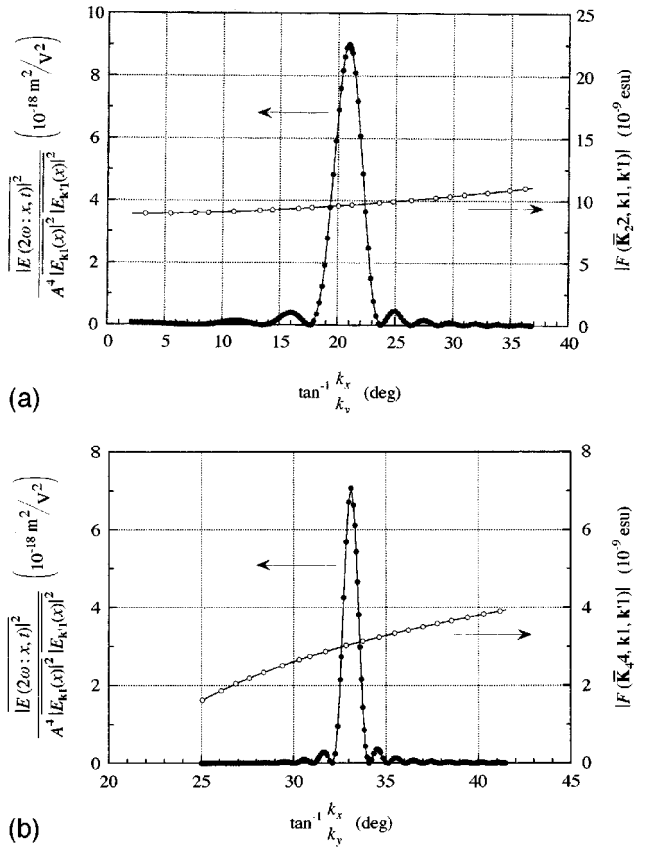

FIG. 5. The angular dependence of the average intensity of the electric field of the second harmonic (solid circles) and the effective nonlinear susceptibility (open circles) for (a) case 1 and (b) case 2. n_y is assumed to be 100, and therefore, the sample thickness an_y is 15 or 27 μm, respectively. The abscissa is the angle of incidence of the fundamental waves.

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APPENDIX A

Now we examine the result of the approximation given in Eq. (23) for the case of a uniform lattice. We take $\epsilon(\mathbf{x})$ and $\chi^{(2)}(\mathbf{x})$ as to be independent of $\mathbf{x}$. We further assume that $\mathbf{k}=\mathbf{k}'$ for simplicity, and we take the y axis as to be parallel to $\mathbf{k}$, i.e., $\mathbf{k}=(0,k)$ $(k>0)$.

Since the eigenfunction is a plane wave in a uniform lattice,

$$u_{\mathbf{k}}(\mathbf{x})=\frac{1}{\sqrt{\epsilon_\omega}},\quad u_{\mathbf{K}}(\mathbf{x})=\frac{1}{\sqrt{\epsilon_{2\omega}}},\quad v_g(2\omega)=\frac{c}{\sqrt{\epsilon_{2\omega}}}, \tag{A1}$$

where ϵ_ω and $\epsilon_{2\omega}$ are the dielectric constants at ω and 2ω, respectively. In Eq. (A1), we took the extended zone scheme, and the suffix to distinguish the band was omitted. Because the umklapp process is absent in a uniform lattice, Eq. (19) is reduced to

$$\begin{aligned}F(\mathbf{K},\mathbf{k},\mathbf{k})&=\frac{\chi^{(2)}}{V_0\epsilon_\omega\sqrt{\epsilon_{2\omega}}}\int_{V_0}d\mathbf{x}'\exp[i(2k-K_y)y']\\&=\frac{\chi^{(2)}\{\exp[i(2k-K_y)b_y]-1\}}{ib_y\epsilon_\omega\sqrt{\epsilon_{2\omega}}(2k-K_y)}.\end{aligned} \tag{A2}$$

Then Eq. (21) is

$$\begin{aligned}E(2\omega:\mathbf{x},t)=&-\frac{8\omega^2\chi^{(2)}A^2L}{c\epsilon_\omega\sqrt{\epsilon_{2\omega}}}\exp(-2i\omega t)\left\{-\int_\infty^0 d\Omega\,\frac{\exp(iK_y^{(-)}y)}{(2\omega-\Omega+i\delta)(2\omega+\Omega+i\delta)}\,\frac{\exp[i(2k-K_y^{(-)})L]-1}{i(2k-K_y^{(-)})L}\right.\\&\left.+\int_0^\infty d\Omega\,\frac{\exp(iK_y^{(+)}y)}{(2\omega-\Omega+i\delta)(2\omega+\Omega+i\delta)}\,\frac{\exp[i(2k-K_y^{(+)})L]-1}{i(2k-K_y^{(+)})L}\right\},\end{aligned} \tag{A3}$$

where

$$L=n_yb_y\quad\text{and}\quad K_y^{(\pm)}=\pm\frac{\sqrt{\epsilon_{2\omega}}}{c}\Omega. \tag{A4}$$

The approximation of Eq. (23) leads to

$$\begin{aligned}E(2\omega:\mathbf{x},t)\simeq&\frac{2\pi i\omega\chi^{(2)}A^2L}{c\epsilon_\omega\sqrt{\epsilon_{2\omega}}}\exp[i(K_{2\omega}y-2\omega t)]\\&\times\exp(i\Delta kL/2)\,\frac{\sin(\Delta kL/2)}{\Delta kL/2},\end{aligned} \tag{A5}$$

where

$$K_{2\omega}=\frac{2\omega\sqrt{\epsilon_{2\omega}}}{c}\quad\text{and}\quad\Delta k=2k-K_{2\omega}, \tag{A6}$$

and the contribution from the first integral in Eq. (A3) was neglected because it does not give a phase-matched solution.

On the other hand, for the case of a uniform lattice, the integrals in Eq. (A3) can be evaluated rigorously. Actually, when we change the sign of the variable in the first integral of Eq. (A3), modify the path of the integration to enclose the upper half of the complex Ω plane, and apply the residue theorem, for $y\geqslant L$ we obtain

$$\begin{aligned}E(2\omega:\mathbf{x},t)=&-\frac{8\omega^2\chi^{(2)}A^2L}{c\epsilon_\omega\sqrt{\epsilon_{2\omega}}}\exp(-2i\omega t)\int_{-\infty}^\infty d\Omega\,\frac{\exp(iK_y^{(+)}y)}{(2\omega-\Omega+i\delta)(2\omega+\Omega+i\delta)}\,\frac{\exp[i(2k-K_y^{(+)})L]-1}{i(2k-K_y^{(+)})L}\\=&\frac{4\pi i\omega\chi^{(2)}A^2L}{c\epsilon_\omega\sqrt{\epsilon_{2\omega}}}\exp[i(K_{2\omega}y-2\omega t)]\exp(i\Delta kL/2)\,\frac{\sin(\Delta kL/2)}{\Delta kL/2}.\end{aligned} \tag{A7}$$

Therefore, the rigorous expression is twice as large as the approximate one. The difference stemmed from the neglected principal value integrated on the whole real axis. For the case of general photonic lattices, a rigorous evaluation is not possible, since the path of the integration is not the whole real axis, and the analyticity of the eigenfunctions is unknown.

APPENDIX B

The group velocity of 2D photonic bands can be readily calculated by means of Hellmann-Feynman theorem. We show the method below.

The dispersion relation for E polarization is given by the eigenequation[17]

$$\mathrm{M}(\mathbf{k})\mathbf{A}_{\mu}(\mathbf{k})=\frac{\omega_{\mathbf{k}\mu}^{2}}{c^{2}}\mathbf{A}_{\mu}(\mathbf{k}). \tag{B1}$$

Here $\mathrm{M}(\mathbf{k})$ is a $\mathbf{k}$-dependent matrix whose $(\mathbf{G},\mathbf{G}')$ component is defined by the following equation:

$$\mathrm{M}(\mathbf{k}:\mathbf{G},\mathbf{G}')=|\mathbf{k}+\mathbf{G}||\mathbf{k}+\mathbf{G}'|\kappa(\mathbf{G}-\mathbf{G}'), \tag{B2}$$

where $\mathbf{G}$ and $\mathbf{G}'$ are the reciprocal-lattice vectors of the 2D photonic lattice, and $\kappa(\mathbf{G})$ is the Fourier transform of $1/\epsilon(\mathbf{x})$. The $\mathbf{k}$-dependent vector $\mathbf{A}_{\mu}(\mathbf{k})$ gives the eigenfunction $E_{\mathbf{k}\mu}(\mathbf{x})$ as

$$E_{\mathbf{k}\mu}(\mathbf{x})=h\sum_{\mathbf{G}}\frac{A_{\mu}(\mathbf{k}:\mathbf{G})}{|\mathbf{k}+\mathbf{G}|}\exp[i(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}], \tag{B3}$$

and it is normalized to unity, i.e., $|\mathbf{A}_{\mu}(\mathbf{k})|=1$. In Eq. (B3), h is a constant required to normalize $\sqrt{\epsilon(\mathbf{x})}E_{\mathbf{k}\mu}(\mathbf{x})$ in a unit volume.

Here we assume that $\epsilon(\mathbf{x})$ is real. Then $\kappa(-\mathbf{G})=\kappa^{*}(\mathbf{G})$, and $\mathrm{M}(\mathbf{k})$ is an Hermitian matrix. Therefore, we can apply the Hellmann-Feynman theorem to the present problem, and we obtain

$$\mathbf{A}_{\mu}^{t*}(\mathbf{k})\frac{\partial\mathrm{M}(\mathbf{k})}{\partial k_{y}}\mathbf{A}_{\mu}(\mathbf{k})=\frac{\partial}{\partial k_{y}}\left(\frac{\omega_{\mathbf{k}\mu}^{2}}{c^{2}}\right)=\frac{2\omega_{\mathbf{k}\mu}}{c^{2}}v_{g}(\omega_{\mathbf{k}\mu},\mu), \tag{B4}$$

where t denotes the transposed matrix, and

$$\frac{\partial\mathrm{M}(\mathbf{k}:\mathbf{G},\mathbf{G}')}{\partial k_{y}}=\left[\frac{|\mathbf{k}+\mathbf{G}'|}{|\mathbf{k}+\mathbf{G}|}(k_{y}+G_{y})+\frac{|\mathbf{k}+\mathbf{G}|}{|\mathbf{k}+\mathbf{G}'|}(k_{y}+G_{y}')\right]\times\kappa(\mathbf{G}-\mathbf{G}'). \tag{B5}$$

Therefore, the group velocity $v_{g}(\omega,\mu)$ can be readily evaluated once the eigenvector $\mathbf{A}_{\mu}(\mathbf{k})$ and the eigenvalue $\omega_{\mathbf{k}\mu}^{2}/c^{2}$ are obtained by the band calculation based on the plane-wave expansion method.

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