

## Multiple light diffraction theory in volume gratings using perturbative integral expansion method

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Light wave diffraction from multiple superposed volume gratings is investigated using a perturbative iteration method of the integral equation of Maxwell's wave equation. The host material and index gratings are anisotropic and non-coplanar multiple volume gratings are considered. In this method, the paraxial approximation and lack of backward scattering in conventional coupled mode theory are not assumed. Systematic analysis of anisotropic wave diffraction due to multiple non-coplanar volume index gratings is performed in increasing level of diffraction orders corresponding to successive iterations.

### I. INTRODUCTION

Light diffraction from superposed volume index gratings has been investigated extensively theoretically and experimentally[1-5]. Various applications of the theory were considered in understanding and designing new optical devices using volume gratings. Holographic optical devices utilizing volume gratings are among the most important applications[6-11]. Usually the analysis concentrated on the diffraction efficiency of a single volume grating and cross-talk caused by simultaneous interaction of light and multiple gratings. Theoretical study was largely based on two methods. The first one is the coupled mode analysis[1-3]. Perturbative expansion of the integral representation of the Maxwell's wave equation is the second method[4,5]. Rigorous coupled mode theory has been applied to the case of a small number of superposed gratings, typically two, due to the complicated procedure of solving coupled algebraic equations. However, the number of gratings increases rapidly when holographic data storage and volume holographic interconnections are considered. In this case, rigorous coupled mode theory is not adequate to study the cross-talk arising from interactions of light with millions of volume gratings.

Recently, a technique using an iteration method of the integral equation of Maxwell's wave equation was introduced to study the cross-talk effects in the case of a large number of gratings[4,5]. In this technique it is not necessary to solve the complicated algebraic equations. The final results are described as a product of simple analytical expressions. It has been shown that the technique is simple and systematic enough to handle a large number of gratings. However, this analysis has the following limitations. The analysis

was limited to the case of isotropic host materials and transverse optical polarization. Furthermore, the wave vectors of the incident light and volume index gratings were assumed to be in the same plane. These two assumptions eliminated the possibility of polarization mixing, and *graddivE* term in the Maxwell's wave equation automatically disappeared. In a real situation, incident light waves propagate in many different directions. Volume index gratings also have different wave vectors and they are not in the same plane. Therefore, polarization mixing of the light waves should be considered to obtain correct results on cross-talk effects.

In this paper, we use a rigorous method of perturbative integral expansion to study light diffraction from superposed volume gratings. This method can be applied to an arbitrary interaction geometry of optical waves and volume index gratings. It also accounts for backward as well as forward diffraction simultaneously. In section II, a general formula of perturbative integral expansion is introduced. In section III, the meaning of the Fourier decomposition of the Green's function in solving the integral equation of the Maxwell's wave equations is explained. The formulae for first and second level diffraction are derived in section IV. The general formula for high level diffraction is presented in section V. Finally, conclusions are described.

### II. PERTURBATIVE INTEGRAL EXPANSION

The interaction geometry between light waves and volume gratings is shown in Fig. 1. It consists of an infinite slab bounded by  $z = 0$  and  $z = d$ . To simplify the analysis, we eliminate complicated boundary reflection at  $z = 0$  and  $z = d$  by assuming that

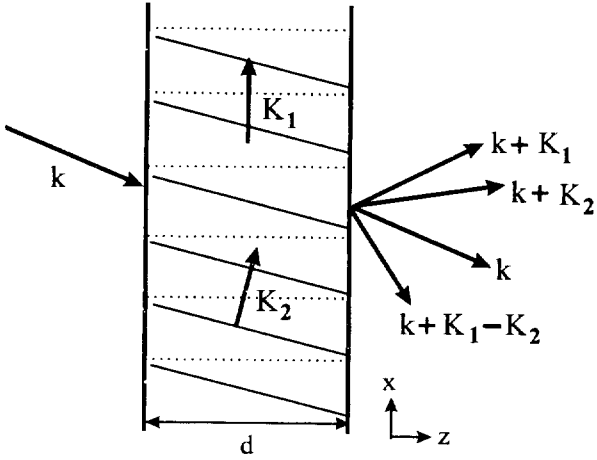


FIG. 1. Interaction geometry of a volume grating. Various diffraction orders are shown.

the average value of the slab permittivity is equal to the exterior permittivity. Anisotropic host materials and anisotropic volume index gratings are considered in general. The assumption about boundary effects is valid if anti-reflection coatings are used at  $z = 0$  and  $z = d$ . The macroscopic polarization is given by

$$\mathbf{P}(\mathbf{r}, t) = \varepsilon_0 \chi \mathbf{E}(\mathbf{r}, t) + \varepsilon_0 \gamma(\mathbf{r}) \mathbf{E}(\mathbf{r}, t), \quad (2.1)$$

where  $\varepsilon_0$  is the permittivity of the vacuum,  $\chi$  is the susceptibility tensor of the anisotropic host material.  $\gamma(\mathbf{r})$  is a second rank tensor describing the perturbation caused by anisotropic volume gratings and thus it is zero outside the slab. Maxwell's wave equation for monochromatic light waves with frequency  $\omega$  in MKS units reads

$$(\nabla^2 - \text{grad div} + k_0^2 \varepsilon) \mathbf{E} = -k_0^2 \gamma \mathbf{E}, \quad (2.2)$$

where  $\varepsilon = 1 + \chi$  and  $k_0 = \omega/c$ . We assumed that the material is non magnetic and there is no free charge. In Eq.(2.2), the left side describes free waves with frequency  $\omega$  in an anisotropic host material having dielectric tensor  $\varepsilon$ . Defining a Green's function for Eq.(2.2) as

$$(\nabla^2 - \text{grad div} + k_0^2 \varepsilon) g(\mathbf{r}, \mathbf{r}') = -\mathbf{I} \delta(\mathbf{r} - \mathbf{r}'), \quad (2.3)$$

where  $\mathbf{I}$  is a unit matrix and  $g$  is a second rank tensor. Then, the integral representation of Eq.(2.2) is given by [4]

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 \exp[i\mathbf{k} \cdot \mathbf{r}] + k_0^2 \int d\mathbf{r}' g(\mathbf{r}, \mathbf{r}') \gamma(\mathbf{r}') \mathbf{E}(\mathbf{r}'), \quad (2.4)$$

where  $\mathbf{r}'$  denotes the secondary source position vector which ranges over all the points inside the slab. The homogeneous solution is taken as a plane incident wave

$$\mathbf{E}_{\text{inc}}(\mathbf{r}, t) = \mathbf{E}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)], \quad (2.5)$$

Fourier integral representation  $G(\mathbf{q})$  of the Green's function in Eq.(2.3) is defined by

$$g(\mathbf{r}, \mathbf{r}') = -\left(\frac{1}{2\pi}\right)^3 \int d\mathbf{q} G(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')]. \quad (2.6)$$

Fourier integral form of  $\delta(\mathbf{r} - \mathbf{r}')$  is given by

$$\delta(\mathbf{r} - \mathbf{r}') = -\left(\frac{1}{2\pi}\right)^3 \int d\mathbf{q} \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')]. \quad (2.7)$$

Then,  $G(\mathbf{q})$  can be described as a matrix form that satisfies

$$\sum_{j=1}^3 (q_i q_j - |\mathbf{q}|^2 \delta_{ij} + k_0^2 \varepsilon_{ij}) G_{jk}(\mathbf{q}) = \delta_{ik}. \quad (2.8)$$

The solution of Eq.(2.8) is represented by

$$G_{ij}(\mathbf{q}) = A d_{ij}(\mathbf{q}) / D(\mathbf{q}), \quad (2.9)$$

where  $D(\mathbf{q})$  and  $A d_{ij}(\mathbf{q})$  are determinant and adjoint matrix respectively. In Cartesian coordinates, each of the nine components in the  $A d_{ij}(\mathbf{q})$  is a polynomial in  $q_x, q_y$  and  $q_z$ . Because of the exponential term under the integral sign of Eq.(2.6), the  $q_x, q_y$  and  $q_z$  which appear in the polynomials can be conveniently replaced by differential operators  $-i\partial/\partial x, -i\partial/\partial y$  and  $-i\partial/\partial z$  respectively, when the adjoint matrix is taken out from the integral. Hence, Eq.(2.6) can be rewritten in the following form

$$g(\mathbf{r}, \mathbf{r}') = -\frac{\mathbf{M}'}{(2\pi)^3} \left\{ \int d\mathbf{q} \frac{\exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')] }{D(\mathbf{q})} \right\}. \quad (2.10)$$

The operator  $\mathbf{M}'$  operates on  $\mathbf{r}$ . If we iterate Eq.(2.4), we obtain the perturbative integral expansion

$$\mathbf{E}(\mathbf{r}) = \sum_{n=0}^{\infty} \mathbf{E}^{(n)}(\mathbf{r}), \quad (2.11)$$

where  $\mathbf{E}^{(0)}$  is the incident plane wave, and the  $n$ -th level amplitude becomes

$$\mathbf{E}^{(n)}(\mathbf{r}) = k_0^{2n} \int d\mathbf{r}_n g(\mathbf{r}, \mathbf{r}_n) \gamma(\mathbf{r}_n) \cdots \int d\mathbf{r}_1 g(\mathbf{r}_2, \mathbf{r}_1) \gamma(\mathbf{r}_1) \mathbf{E}_0 \exp[i\mathbf{k} \cdot \mathbf{r}_1]. \quad (2.12)$$

The diffracted light amplitude is obtained in increasing level of iterations by calculating Eq.(2.12).

### III. POLES IN THE GREEN'S FUNCTION

It is well known that the equation  $D(\mathbf{q}) = 0$  describes two wave normal surface[12]. For a given propagation direction  $\mathbf{s}$ , it provides two indices of refraction and the corresponding eigenmode polarization. However,

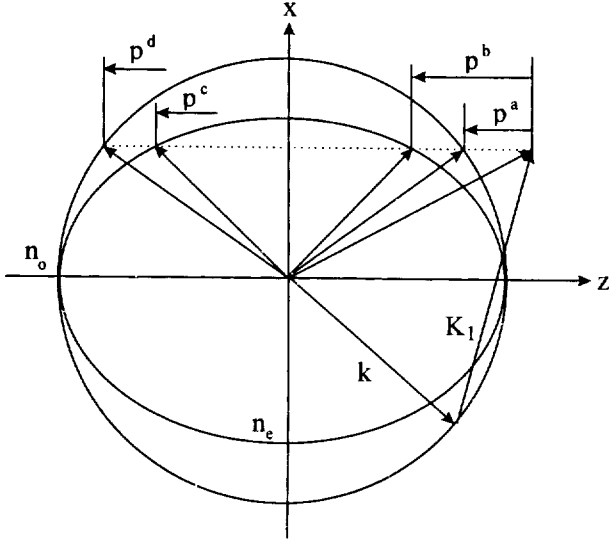


FIG. 2. Wave normal surfaces in the  $x - z$  plane of a uniaxial crystal and phase mismatch of the diffracted wave due to grating  $K_1$ .

as will be shown in the following sections, in our theory  $q_x$  and  $q_y$  are real independent parameters which can have any values. What we need in the following is factorization of  $D(\mathbf{q})$  with respect to  $q_z$  for given values of  $q_x$  and  $q_y$ . It is well known that  $D(\mathbf{q})$  is a polynomial of order four in  $q_z$  for real symmetric dielectric tensor  $\epsilon$ . Thus,  $D(\mathbf{q})$  can be factorized fully into a product of four linear terms.

To illustrate the physical meaning of the poles of  $G(\mathbf{q})$ , we consider a uniaxial crystal with its optic axis coincident with the  $z$ -axis. In the uniaxial crystal, physical properties are the same as the crystal rotates around the optic axis. The wave normal surfaces in the  $x$ - $z$  plane are shown in Fig. 2. Now,  $D(\mathbf{q})$  and  $Ad_{ij}(\mathbf{q})$  in the coordinate system where  $\epsilon$  is diagonalized are given by

$$D(\mathbf{q}) = k_0^2[q_z^2 + (q_x^2 + q_y^2) - k_0^2\epsilon_{xx}] \\ [\epsilon_{zz}q_z^2 + \epsilon_{xx}(q_x^2 + q_y^2) - k_0^2\epsilon_{xx}\epsilon_{zz}], \quad (3.1)$$

$$Ad_{11} = q_z^2(q_x^2 - k_0^2\epsilon_{zz}) + (q_x^2 + q_y^2 - k_0^2\epsilon_{zz})(q_x^2 - k_0^2\epsilon_{xx}), \\ Ad_{12} = q_x q_y (q_z^2 + q_x^2 + q_y^2 - k_0^2\epsilon_{zz}), \\ Ad_{13} = q_x q_z (q_z^2 + q_x^2 + q_y^2 - k_0^2\epsilon_{xx}), \\ Ad_{22} = q_z^2(q_y^2 - k_0^2\epsilon_{zz}) + (q_x^2 + q_y^2 - k_0^2\epsilon_{zz})(q_y^2 - k_0^2\epsilon_{xx}), \\ Ad_{23} = q_y q_z (q_z^2 + q_x^2 + q_y^2 - k_0^2\epsilon_{xx}), \\ Ad_{33} = (q_z^2 - k_0^2\epsilon_{xx})(q_z^2 + q_x^2 + q_y^2 - k_0^2\epsilon_{xx}), \quad (3.2)$$

where  $Ad$  is symmetric. We see that the poles of Eq.(2.9) with respect to the variable are given by four zeros of Eq.(3.1). For a positive uniaxial crystal, i.e.,  $\epsilon_{zz} > \epsilon_{xx}$ , the four zeros are all pure imaginary if  $(q_x^2 + q_y^2)$  is larger than  $k_0^2\epsilon_{zz}$ , and they represent non-propagating eigenmodes. If  $(q_x^2 + q_y^2)$  is larger than

$k_0^2\epsilon_{xx}$  and smaller than, or equal to  $k_0^2\epsilon_{xx}$ , two zeros are pure imaginary and two zeros are real. The two real zeros represent extraordinary waves propagating in the positive and negative  $z$ -direction. Finally, if  $(q_x^2 + q_y^2)$  is smaller than or equal to  $k_0^2\epsilon_{xx}$ , the four zeros are all real and they represent forward and backward ordinary and extraordinary waves. The four poles of Eq.(2.9) for the uniaxial crystal represent ordinary and extraordinary waves if they are real, and the two poles are in the upper complex plane and the other two poles are in the lower part of the complex plane. The poles having positive real values are located in the upper complex plane and those having negative real values are located in the lower complex plane in the usual way. The four poles of  $D(\mathbf{q})$  given by Eq.(3.1) become real when  $\mathbf{q}$  is on the wave normal surface. In particular, two of them are positive describing eigenmodes propagating in the positive  $z$ -direction. The other two are negative and they represent eigenmodes propagating in the negative  $z$ -direction. Otherwise, the poles are complex. The two poles in the upper complex plane are denoted as  $u^a$  and  $u^b$ , and the other two in the lower complex plane are denoted as  $u^c$  and  $u^d$ .

#### IV. MULTIPLE GRATING FORMULATION

In the case of multiplexed volume gratings, the perturbation  $\gamma(\mathbf{r})$  consists of a sum of sinusoidal refractive index gratings. Consider  $N$  such gratings having wave vectors  $\mathbf{K}_i$ ,  $i = 1, 2, \dots, N$ . Then,  $\gamma(\mathbf{r})$  may be written as

$$\gamma(\mathbf{r}) = \sum_{i=1}^{2N} \alpha_i \exp[i\mathbf{k}_i \cdot \mathbf{r}] = \sum_{i=1}^{2N} \gamma_i(\mathbf{r}), \quad (4.1)$$

where  $\alpha_i$  is a second rank tensor that represents the volume grating magnitude.  $\alpha_{2n} = \alpha_{2n-1}$  and  $\mathbf{K}_{2n} = -\mathbf{K}_{2n-1}$ ,  $n = 1, 2, \dots, N$ . The  $n$ -th level diffraction light amplitude due to perturbation of Eq.(4.1) is a sum of  $(2N)^n$  terms of  $n$ -tuple integrals represented by a sequence of  $2N$  wave vectors  $\mathbf{K}_i$  and  $-\mathbf{K}_i$ . To illustrate how to calculate such integrals for various levels, integration of single and double integrals is carried out in the following section.

##### IV. A. Single integral

The integral we have to calculate is of the form

$$\mathbf{E}^{(1)}(\mathbf{r}) = k_0^2 \int d\mathbf{r}_1 g(\mathbf{r}, \mathbf{r}_1) \gamma_1(\mathbf{r}_1) \mathbf{E}_0 \exp[i\mathbf{k} \cdot \mathbf{r}_1], \quad (4.2)$$

where we considered one term represented by  $\gamma_1$  and  $\mathbf{K}_1$  in Eq.(4.1) for the first-level amplitude. If we use Eq.(2.10) with  $D(\mathbf{q})$  given in section III and Eq.(4.1) for  $\gamma_1$ , the integral in Eq.(4.2) becomes

$$\begin{aligned}
\mathbf{E}^{(1)}(\mathbf{r}) &= -\frac{k_0^2}{(2\pi)^3} \int d\mathbf{r}_1 \left[ \mathbf{M}' \left\{ \int d\mathbf{q} \frac{e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_1)}}{D(\mathbf{q})} \right\} \right] \alpha_1 e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} \mathbf{E}_0 e^{i\mathbf{k}_1 \cdot \mathbf{r}} \\
&= -\frac{k_0^2}{(2\pi)^3} \int d\mathbf{r}_1 \mathbf{M} \left\{ \int d\mathbf{q} \frac{\mathbf{E}_0 e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_1)} \cdot e^{i(\mathbf{k} + \mathbf{k}_1) \cdot \mathbf{r}_1}}{D(\mathbf{q})} \right\} \\
&= -\frac{k_0^2}{(2\pi)^3} \mathbf{M} \iint d\mathbf{q} d\mathbf{r}_1 \left\{ \frac{\mathbf{E}_0 e^{i(\mathbf{q} - \mathbf{k}_1) \cdot (\mathbf{r} - \mathbf{r}_1)}}{D(\mathbf{q})} \right\} \quad (4.3)
\end{aligned}$$

Here, operator  $\mathbf{M}$  is defined by  $Ad(\mathbf{q})\alpha_1$  and similarly for the operator  $\mathbf{M}'$ . If we define  $\mathbf{k}_1 = \mathbf{k} + \mathbf{K}_1$  and change the integral variable to  $\mathbf{r}' = \mathbf{r} - \mathbf{r}_1$  and replace  $D(\mathbf{q})$  with Eq.(3.1), then

$$\begin{aligned}
\mathbf{E}^{(1)}(\mathbf{r}) &= \frac{\mathbf{M}}{(2\pi)^3 \varepsilon_{zz}} \left\{ e^{i\mathbf{k}_1 \cdot \mathbf{r}} \iint d\mathbf{q} dx' dy' dz' \right. \\
&\quad \left. \frac{\mathbf{E}_0 e^{i(q_x - k_{1x})x'} e^{i(q_y - k_{1y})y'} e^{i(q_z - k_{1z})z'}}{\prod_{\beta=a}^d (q_z - u^\beta(q_x, q_y))} \right\}. \quad (4.4)
\end{aligned}$$

As for the infinite slab material, the integral ranges are  $-\infty \leq x' \leq +\infty$ ,  $-\infty \leq y' \leq +\infty$  and  $z - d \leq z' \leq z$ . Then the integral with respect to  $x'$  and  $y'$  yield delta functions  $2\pi\delta(q_x - k_{1x})$  and  $2\pi\delta(q_y - k_{1y})$ . Hence, Eq.(4.4) leads to

$$\begin{aligned}
\mathbf{E}^{(1)}(\mathbf{r}) &= \frac{\mathbf{M}}{(2\pi)\varepsilon_{zz}} \left\{ e^{i\mathbf{k}_1 \cdot \mathbf{r}} \int_{-\infty}^{+\infty} dq_z \int_{z-d}^z dz' \frac{\mathbf{E}_0 e^{i(q_z - k_{1z}) \cdot z'}}{\prod_{\beta=a}^d (q_z - u_1^\beta)} \right\} \\
&= \frac{\mathbf{M}}{(2\pi i)\varepsilon_{zz}} \left\{ e^{i\mathbf{k}_1 \cdot \mathbf{r}} \int_{-\infty}^{+\infty} dq_z \frac{\mathbf{E}_0}{\prod_{\beta=a}^d (q_z - u_1^\beta)} \left[ \frac{e^{i(q_z - k_{1z})z} - 1}{q_z - k_{1z}} \right. \right. \\
&\quad \left. \left. + \frac{1 - e^{i(q_z - k_{1z})(z-d)} - 1}{q_z - k_{1z}} \right] \right\} \quad (4.5)
\end{aligned}$$

where  $u_1^\beta = u^\beta(k_{1x}, k_{1y})$ . There are four poles  $u_1^\beta$  effective in calculating the complex contour integral of Eq.(4.5). However, the diffracted light wave is in the region  $z > d$ . This implies that the counter should include the upper half part of the complex plane and only two poles  $u_1^a$  and  $u_1^b$  are effective. This yields for the first level diffracted light wave amplitude by Cauchy's integral theorem as below

$$\begin{aligned}
\mathbf{E}^{(1)}(\mathbf{r}) &= -\frac{\mathbf{M}}{\varepsilon_{zz}} \left\{ e^{i\mathbf{k}_1^a \cdot \mathbf{r}} \cdot \frac{\mathbf{E}_0}{\prod_1^a} \cdot \frac{1 - e^{-ip_1^a d}}{p_1^a} \right. \\
&\quad \left. + e^{i\mathbf{k}_1^b \cdot \mathbf{r}} \cdot \frac{\mathbf{E}_0}{\prod_1^b} \cdot \frac{1 - e^{-ip_1^b d}}{p_1^b} \right\}. \quad (4.6)
\end{aligned}$$

Now the operator  $\mathbf{M}$  operates on the exponential term, so that Eq.(4.6) can be written as

$$\begin{aligned}
\mathbf{E}^{(1)}(\mathbf{r}) &= \frac{1}{\varepsilon_{zz}} \left[ \frac{\mathbf{A}(\mathbf{k}_1^a) 1 - e^{-ip_1^a d}}{\prod_1^a p_1^a} \mathbf{E}_0 \exp(i\mathbf{k}_1^a \cdot \mathbf{r}) \right. \\
&\quad \left. + \frac{\mathbf{A}(\mathbf{k}_1^b) 1 - e^{-ip_1^b d}}{\prod_1^b p_1^b} \mathbf{E}_0 \exp(i\mathbf{k}_1^b \cdot \mathbf{r}) \right], \quad (4.7)
\end{aligned}$$

where

$$\mathbf{k}_1^{a,b} = k_{1x}\hat{x} + k_{1y}\hat{y} + u_1^{a,b}\hat{z}, \quad (4.8)$$

$$p_1^{a,b} = u_1^{a,b} - k_{1z}, \quad (4.9)$$

$$\prod_1^{a,b} = \prod_{\beta \neq a,b}^d (u_1^{a,b} - u_1^\beta), \quad (4.10)$$

$$\mathbf{A}(\mathbf{k}_1^{a,b}) = Ad(k_{1x}, k_{1y}, u_1^{a,b})\alpha_1, \quad (4.11)$$

Eq.(4.7) shows that the first-level diffracted light waves consists of two plane waves. In the following we discuss the two waves. For the wave vector  $\mathbf{k}_1$ , which is called a first-level diffraction vector, we have two types of propagation vectors having the same x and y components,  $k_{1x}$  and  $k_{1y}$ , as shown in eqs.(4.7) and (4.8). One is the forward propagation vector  $\mathbf{k}_1^a$  representing an eigenmode, a. The other is forward propagation vector  $\mathbf{k}_1^b$  describing another eigenmode, b. Both  $\mathbf{k}_1^a$  and  $\mathbf{k}_1^b$  satisfy  $D(\mathbf{k}_1^{a,b}) = 0$  implying that they represent homogeneous solutions of the wave equation. In general, a diffraction wave vector  $\mathbf{k}_1$  does not represent a homogeneous solution, because  $\mathbf{k}_1$  does not satisfy  $D(\mathbf{k}_1^{a,b}) = 0$ . The propagation vector derived from a diffraction vector may be classified into free propagation vector and evanescent propagation vector. In the first case, the z-component of the propagation vector is real. This implies that the wave propagates freely in the material. In the second case, the z-component of the propagation vector has an imaginary part. In this case, the amplitude of the wave decreases exponentially and it represent an evanescent wave. In our case, the thickness of the slab is large and thus evanescent wave are ignored. We may call  $p_1^{a,b}$  phase-matching functions because  $[1 - \exp(-ip_1^{a,b}d)]/p_1^{a,b}$  represent *sinc* functions with respect to the variables  $p_1^{a,b}$ . They have maximum absolute values  $d$  when  $p_1^{a,b} = 0$ . This implies that  $p_1^{a,b}$  are the same as the phase-matching functions in the conventional coupled mode theory[1].

#### IV. B. Double integral

The double integral described by  $\gamma_1, \mathbf{K}_1$  and  $\gamma_2, \mathbf{K}_2$ , and represented by a sequence  $[\mathbf{K}_1, \mathbf{K}_1]$ , is

$$\begin{aligned}
\mathbf{E}^{(2)}(\mathbf{r}) &= k_0^4 \int d\mathbf{r}_2 g(\mathbf{r}, \mathbf{r}_2) \gamma_2(\mathbf{r}_2) \\
&\quad \int d\mathbf{r}_1 g(\mathbf{r}_2, \mathbf{r}_1) \gamma_1(\mathbf{r}_1) \mathbf{E}_0 \exp[i\mathbf{k} \cdot \mathbf{r}_1] \quad (4.12)
\end{aligned}$$

Following the same procedure used for the single integral, the integral over  $\mathbf{r}_1$  is the same as Eq.(4.7) except for replacing  $\mathbf{r}$  with  $\mathbf{r}_2$ . However,  $z_1$  in Eq.(4.12) is in the interval  $0 < z_1 < d$ . This implies that  $z_1$  is positive and  $(z_1 - d)$  is negative. Thus, the contour for

$$\mathbf{E}^{(1)}(\mathbf{r}) = -\frac{1}{\varepsilon_{zz}} \sum_{\beta=a}^b \left[ \frac{\mathbf{A}(\mathbf{k}_1^\beta) - \mathbf{A}(\mathbf{k}_1) e^{-ip_1^\beta z}}{\prod_1^\beta p_1^\beta} \right] \mathbf{E}_0 e^{i\mathbf{k}_1^\beta \cdot \mathbf{r}} - \frac{1}{\varepsilon_{zz}} \sum_{\beta=c}^d \left[ e^{ip_1^\beta d} \frac{\mathbf{A}(\mathbf{k}_1^\beta) - \mathbf{A}(\mathbf{k}_1^\beta - p_1^\beta z) e^{-ip_1^\beta z}}{\prod_1^\beta p_1^\beta} \right] \mathbf{E}_0 e^{i\mathbf{k}_1^\beta \cdot \mathbf{r}}. \quad (4.13)$$

The double integral Eq.(4.12) can be obtained by using Eq.(4.13), and following the same procedure utilized in

$$\mathbf{E}^{(2)}(\mathbf{r}) = \frac{1}{(\varepsilon_{zz})^2} \sum_{\beta_2=a}^b \sum_{\beta_1=a}^d \left[ -\frac{\mathbf{A}(\mathbf{k}_2^{\beta_2}) \mathbf{A}(\mathbf{k}_1)}{\prod_2^{\beta_2} \prod_1^{\beta_1}} \cdot \frac{1 - \exp(-ip_2^{\beta_2} d)}{p_2^{\beta_2} p_1^{\beta_1}} - \frac{\mathbf{A}(\mathbf{k}_2^{\beta_2}) \mathbf{A}(\mathbf{k}_1^{\beta_1})}{\prod_2^{\beta_2} \prod_1^{\beta_1}} \cdot f_1(\beta_1) \cdot \frac{1 - \exp\{-i(p_2^{\beta_2} - p_1^{\beta_1})d\}}{p_1^{\beta_1} (p_1^{\beta_1} - p_2^{\beta_2})} \right] \cdot \mathbf{E}_0 \exp(i\mathbf{k}_2^{\beta_2} \cdot \mathbf{r}), \quad (4.14)$$

$$\text{where } \begin{cases} f_1(\beta_1) = 1 & \text{for } \beta_1 = a, b \\ f_1(\beta_1) = \exp(-ip_1^{\beta_1} d) & \text{for } \beta_1 = c, d \end{cases} \quad (4.15)$$

$$p_2^{\beta_2} = u_2^{\beta_2} - k_{2z}, \quad (4.16)$$

$$\mathbf{k}_2^{\beta_2} = k_{2x} \hat{x} + k_{2y} \hat{y} + u_2^{\beta_2} \hat{z}, \quad (4.17)$$

$$\mathbf{k}_2 = \mathbf{k} + \mathbf{K}_1 + \mathbf{K}_2. \quad (4.18)$$

The general expression for the n-tuple integral represented by a diffraction sequence  $[\mathbf{K}_n, \dots, \mathbf{K}_2, \mathbf{K}_1]$  will be presented in the next section.

## V. GENERAL FORMULA FOR HIGHER DIFFRACTION LEVELS

In this section we present a general formula for higher-level diffraction. As in Eq.(4.1), we assume  $N$  sinusoidal perturbations described by wave vectors  $\mathbf{K}_i, i = 1, 2, \dots, N$ . Consider n-th level diffracted light consisting of  $(2N)^n$  n-tuple integrals. Each n-tuple integral is uniquely represented by a  $2N$  dimensional sequence of wave vectors whose component can be selected from any one of  $2N$  wave vectors:  $\mathbf{K}_1, -\mathbf{K}_1, \mathbf{K}_2, -\mathbf{K}_2, \dots, \mathbf{K}_N, -\mathbf{K}_N$ . In the following, we adopt the notation that describes the above  $2N$  wave vectors as  $1, -1, 2, -2, \dots, N, -N$ . Then the sequence of wave vectors representing perturbations above is called a diffraction sequence and we use bracket [...] to denote it. Consider an n-tuple integral represented by a sequence  $[\mathbf{K}_n, \mathbf{K}_{n-1}, \dots, \mathbf{K}_2, \mathbf{K}_1]$ . The results in section IV on the single and double integrals can be extended easily by induction to n-tuple integral.

the first term in Eq.(4.5) should enclose the upper half plane, and the two poles  $u_1^{a,b}$  are effective. On the other hand, for the second term in Eq.(4.5), the lower half plane should be used and the poles  $u_1^{c,d}$  are effective. Thus, the integral over  $\mathbf{r}_1$  in Eq.(4.5) becomes

obtaining the first-level diffracted light waves.

The various parameters in the above section are generalized in a straightforward way. Then, the n-tuple integral is given by[6]

$$\mathbf{E}^{(n)}(\mathbf{r}) = \sum_{\beta_n=a}^d S_n^{\beta_n} \Phi_n^{\beta_n} \mathbf{E}_0 \exp(i\mathbf{k}_n^{\beta_n} \cdot \mathbf{r}), \quad (5.1)$$

$$\text{where } S_n^{\beta_n} = \frac{1}{(\varepsilon_{zz})^n} s(\beta_n) \sum_{\beta_{n-1}=a}^d \sum_{\beta_{n-2}=a}^d \dots \sum_{\beta_1=a}^d \frac{1}{\prod_n^{\beta_n} \prod_{n-1}^{\beta_{n-1}} \dots \prod_1^{\beta_1}},$$

$$\begin{cases} s(\beta_n) = 1 & \text{for } \beta_n = a, b \\ s(\beta_n) = -1 & \text{for } \beta_n = c, d \end{cases} \quad (5.2)$$

and the phase correlation function  $\Phi$  is defined as

$$\begin{aligned} & \Phi_n^{\beta_n} \\ &= -\mathbf{A}(\mathbf{k}_n^{\beta_n}) \prod_{q=n-1}^1 \mathbf{A}(\mathbf{k}_q) \cdot \frac{1 - \exp(-ip_n^{\beta_n} d)}{p_n^{\beta_n} \prod_{q=1}^{n-1} p_q^{\beta_q}} \\ &+ (-1)^{n-1} \sum_{q=1}^{n-1} \mathbf{A}(\mathbf{k}_n^{\beta_n}) \prod_{h=n-1}^q \mathbf{A}(\mathbf{k}_h + p_q^{\beta_q} \hat{z}) \cdot \\ & f_q(\beta_q) \cdot \frac{1 - \exp\{i(p_n^{\beta_n} - p_q^{\beta_q})d\}}{p_q^{\beta_q} (p_q^{\beta_q} - p_n^{\beta_n}) \prod_{h=1, h \neq q}^{n-1} (p_q^{\beta_q} - p_h^{\beta_h})}. \end{aligned} \quad (5.3)$$

$f_q(\beta_q)$  for  $q > 1$  in Eq.(5.3) is obtained by using the following formulas:

$$f_q(\beta_q) = (-1)^{q-1} \frac{\prod_{h=q-1}^1 \mathbf{A}(\mathbf{k}_h) (p_q^{\beta_q} - p_h^{\beta_h})}{\prod_{h=1}^{q-1} p_h^{\beta_h}} - \sum_{t=1}^{q-1} \left[ \frac{p_q^{\beta_q} \prod_{h=q-1}^t (\mathbf{A}(\mathbf{k}_h) - p_t^{\beta_t} \hat{z}) \prod_{h=1}^{q-1} (p_q^{\beta_q} - p_h^{\beta_h})}{p_t^{\beta_t} \prod_{h=1, h \neq t}^q (p_t^{\beta_t} - p_h^{\beta_h})} \cdot f_t(\beta_t) \right] \quad \text{for } \beta_q = a, b, \quad (5.4)$$

$$f_q(\beta_q) = \left[ (-1)^{q-1} \frac{\prod_{h=1}^{q-1} \mathbf{A}(\mathbf{k}_h)(p_q^{\beta_q} - p_h^{\beta_h})}{\prod_{h=1}^{q-1} p_h^{\beta_h}} - \sum_{t=1}^{q-1} \frac{p_q^{\beta_q} \prod_{h=1}^{t-1} \mathbf{A}(\mathbf{k}_h - p_t^{\beta_t} \hat{z}) \prod_{h=1}^{q-1} (p_q^{\beta_q} - p_h^{\beta_h})}{p_t^{\beta_t} \prod_{h=1, h \neq t}^q (p_t^{\beta_t} - p_h^{\beta_h})} \cdot g_t(\beta_t) \right] \cdot e^{-ip_q^{\beta_q} d}$$

for  $\beta_q = c, d$ , (5.5)

where  $g_q(\beta_q) = f_q(\beta_q) \exp(ik_q^{\beta_q} d)$  for all  $q$  (5.6)

$$\begin{cases} f_1(\beta_1) = 1 & \text{for } \beta_1 = a, b \\ f_1(\beta_1) = \exp(-ip_1^{\beta_1}) & \text{for } \beta_1 = c, d \end{cases} \quad (5.7)$$

$$\prod_j^{\beta_j} = \prod_{\beta_t = a, \beta_t \neq \beta_j}^d (u_j^{\beta_j} - u_t^{\beta_t}), \quad (5.8)$$

$$p_j^{\beta_j} = u_j^{\beta_j} - \mathbf{k}_{jz} = u_j^{\beta_j} - (k_z + \sum_{t=1}^j \mathbf{K}_{tz}), \quad (5.9)$$

$$\mathbf{k}_j^{\beta_j} = k_{jx} \hat{x} + k_{jy} \hat{y} + u_j^{\beta_j} \hat{z}. \quad (5.10)$$

Eqs.(5.1)-(5.10) are a generalization of the results described in section IV. It shows that the diffracted light waves are sum of four eigenmodes. Two of them propagate in the positive z-direction and represented by the poles  $u^a$  and  $u^b$ . The other two propagate in the negative z-direction and are represented by the poles  $u^c$  and  $u^d$ . The amplitude of each eigenmode is a sum of  $4^{n-1}$  terms. Each term is characterized by  $n-1$  intermediate diffraction process. At each intermediate step, input waves interact with a perturbation grating and they generate four plane waves which interact with the next grating. Four plane waves are generated at an intermediate step because forward and backward diffraction stemming from the poles in the upper and lower complex plane are allowed. For the case of single and double integrals, it was shown that the wave vectors of the integrals depend only on the overall diffraction vectors. Eq.(5.1) shows that this is true for arbitrary  $n$ -tuple integrals. The overall diffraction vector is uniquely determined by a diffraction sequence. However, different sequences may have the same overall diffraction vectors. The overall diffraction vectors can be always represented by

$$\mathbf{k} + \sum_{j=1}^N n_j \mathbf{K}_j, \quad (5.11)$$

This implies that any overall diffraction vector is uniquely represented by an  $N$ -dimensional integer vector  $(n_1, n_2, \dots, n_N)$ , where  $n_j, j = 1, 2, \dots, N$ , are integers. We call this vector a diffraction order, and use parenthesis to denote it. Therefore, light amplitude having a specific diffraction order can be obtained to any prescribed accuracy by summing the appropriate diffraction-level terms using the above equations.

## VI. CONCLUSIONS

The integral expansion method of Maxwell's equation was applied to light diffraction from volume index gratings in anisotropic host materials. The method has been shown to be powerful in handling a large number of volume gratings in a systematic and natural way. The general formula at each iteration level of the integral equation has been derived. In the appendix, we verify that the derived general formula should become the eigenmode that satisfies Maxwell's wave equations. Applications and numerical results based on the general formula such as cross-talk effects arising from superposed volume gratings for arbitrary light polarization, interaction geometry, and anisotropy of the host material will be presented in the next paper.

## APPENDIX A: EIGENMODE IDENTIFICATION

It is important to recognize that the  $n$ -tuple diffracted wave described in Eq.(5.1) should become the eigenmode that satisfies the Maxwell wave equations. Hence, we verify that the diffraction of the electric field vector of  $n$ -tuple diffracted wave  $\mathbf{E}^{(n)}$  in Eq.(5.1) is equal to the direction of the electric field eigenvector, which is determined by the wave vector  $\mathbf{k}_n^{\beta_n}$ . From Eq.(2.2)

$$(\nabla^2 - \nabla \nabla \cdot + k_0^2 \epsilon) \mathbf{E}^{(n)} = 0, \quad (A1)$$

$$\begin{pmatrix} k_0^2 \epsilon_x - k_y^2 - k_z^2 & k_x k_y & k_x k_z \\ k_x k_y & k_0^2 \epsilon_y - k_x^2 - k_z^2 & k_y k_z \\ k_x k_z & k_y k_z & k_0^2 \epsilon_z - k_x^2 - k_y^2 \end{pmatrix} \times \begin{pmatrix} E_{nx} \\ E_{ny} \\ E_{nz} \end{pmatrix} = 0, \quad (A2)$$

For nontrivial solutions to exist, the determinant of the matrix in Eq.(A.2) must vanish. This leads to a relation

$$\frac{k_x^2}{k^2 - k_0^2 \epsilon_x} + \frac{k_y^2}{k^2 - k_0^2 \epsilon_y} + \frac{k_z^2}{k^2 - k_0^2 \epsilon_z} = 1, \quad (A3)$$

The direction of the electric field eigenvector can also be obtained from Eq.(A.2)

$$\begin{pmatrix} \frac{k_x^2}{k^2 - k_0^2 \varepsilon_x} \\ \frac{k_y^2}{k^2 - k_0^2 \varepsilon_y} \\ \frac{k_z^2}{k^2 - k_0^2 \varepsilon_z} \end{pmatrix}. \quad (\text{A4})$$

Using Eq.(5.1), the n-tuple diffracted wave is given by

$$\mathbf{E}^{(n)} \propto \mathbf{A}(\mathbf{k}_n^{\beta n}) \mathbf{B} \mathbf{E}_0 \exp(i\mathbf{k}_n^{\beta n} \cdot \mathbf{r}), \quad (\text{A5})$$

where  $\mathbf{B}$  is a 3 x 3 matrix and  $\mathbf{A}(\mathbf{k}_n^{\beta n}) = Ad(\mathbf{k}_n^{\beta n})\alpha_n$ . Then

$$\mathbf{E}^{(n)} \propto \mathbf{E}_n \exp(i\mathbf{k}_n^{\beta n} \cdot \mathbf{r}), \quad (\text{A6})$$

$$\text{where } \mathbf{E}_n = Ad(\mathbf{k}_n^{\beta n}) \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}. \quad (\text{A7})$$

$Ad(\mathbf{k}_n^{\beta n})$  can be obtained from Eq.(3.2) and Eq.(5.10). Thus,

$$\begin{pmatrix} ZY \left\{ \left( 1 - \frac{(u_n^{\beta n})^2}{Z} - \frac{k_{ny}^2}{Y} \right) \alpha + \frac{k_{nx}k_{ny}}{Y} \beta + \frac{k_{nx}u_n^{\beta n}}{Z} \gamma \right\} \\ ZX \left\{ \frac{k_{nx}k_{ny}}{X} \alpha + \left( 1 - \frac{(u_n^{\beta n})^2}{Z} - \frac{k_{nx}^2}{X} \right) \beta + \frac{k_{ny}u_n^{\beta n}}{Z} \gamma \right\} \\ XY \left\{ \frac{k_{nx}u_n^{\beta n}}{X} \alpha + \frac{k_{ny}u_n^{\beta n}}{Y} \beta + \left( 1 - \frac{k_{nx}^2}{X} - \frac{k_{ny}^2}{Y} \right) \gamma \right\} \end{pmatrix}, \quad (\text{A8})$$

$$\text{where } X = (k_n^{\beta n})^2 - k_0^2 \varepsilon_x, \quad Y = (k_n^{\beta n})^2 - k_0^2 \varepsilon_y, \\ Z = (k_n^{\beta n})^2 - k_0^2 \varepsilon_z.$$

Using Eq.(A.3) and Eq.(A8), the direction of the electric field vector is given by

$$\mathbf{E}_n = \left( \frac{k_{nx}}{X} \alpha + \frac{k_{ny}}{Y} \beta + \frac{u_n^{\beta n}}{Z} \gamma \right) \begin{pmatrix} \frac{k_{nx}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_x} \\ \frac{k_{ny}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_y} \\ \frac{u_n^{\beta n}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_z} \end{pmatrix}. \quad (\text{A9})$$

Using Eq.(A.4), the direction of the electric field eigenvector determined by the wave vector  $\mathbf{k}_n^{\beta n} (= k_{nx}\hat{x} + k_{ny}\hat{y} + k_{nz}\hat{z})$  is given by:

$$\begin{pmatrix} \frac{k_{nx}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_x} \\ \frac{k_{ny}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_y} \\ \frac{u_n^{\beta n}}{(k_n^{\beta n})^2 - k_0^2 \varepsilon_z} \end{pmatrix}. \quad (\text{A10})$$

Consequently, the direction of  $\mathbf{E}^{(n)}$  the electric field vector of is the same as the direction of the electric field eigenvector determined by the wave vector  $\mathbf{k}_n^{\beta n}$ .

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