Maxwell equations in Fourier space: fast-converging formulation for diffraction by arbitrary shaped, periodic, anisotropic media

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We establish the most general differential equations that are satisfied by the Fourier components of the electromagnetic field diffracted by an arbitrary periodic anisotropic medium. The equations are derived by use of the recently published fast-Fourier-factorization (FFF) method, which ensures fast convergence of the Fourier series of the field. The diffraction by classic isotropic gratings arises as a particular case of the derived equations; the case of anisotropic classic gratings was published elsewhere. The equations can be resolved either through classic differential theory or through the modal method for particular groove profiles. The new equations improve both methods in the same way. Crossed gratings, among which are grids and two-dimensional arbitrarily shaped periodic surfaces, appear as particular cases of the theory, as do three-dimensional photonic crystals. The method can be extended to nonperiodic media through the use of a Fourier transform. © 2001 Optical Society of America

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1. INTRODUCTION

For many years the classic differential theory[1] of diffraction gratings has been limited in its range of applicability. For deep gratings made from highly reflecting metal the Fourier series of the field showed poor convergence in TM polarization, so the corresponding numerical results often turned out to be unreliable; this problem did not occur in TE polarization. Recently Li[2] pointed out that the problem derives from the way in which the Fourier components of the product of two periodic discontinuous functions are calculated and distinguished among three types of products. Laurent's rule of factorization[2] applies to functions with no concurrent discontinuities, whereas the inverse rule[2] applies to functions with complementary jump discontinuities. Laurent's rule is well known to any theoretician. It states that the Fourier components h_n of the product $h(x)$ of two arbitrary functions $f(x)$ and $g(x)$ are simply given by

$$h_n = \sum_{m=-\infty}^{+\infty} f_{n-m} g_m . \quad (1)$$

Although it is easy to establish the result for infinite series, this result is not obvious for truncated series. If $2N + 1$ Fourier components (from $-N$ to $+N$) of $g(x)$ are known, what is the best way to obtain $2N + 1$ Fourier components h_n of $h(x)$? When $h_n^{(N)}$ denotes the Fourier components obtained through a truncation at order N, Laurent's rule assumes that

$$h_n^{(N)} = \sum_{m=-N}^{+N} f_{n-m} g_m .$$

A justification of this rule is given in Appendix A.

To further simplify the calculations we introduce matrix notation. We denote by $[g]$ the column vector constructed with the $2N + 1$ Fourier components g_m and by $[\![f]\!]$ the $(2N + 1) \times (2N + 1)$ Toeplitz matrix whose (n, m) entry is f_{n-m}. The preceding equation is simply rewritten as:

$$[h] = [\![f]\!][g]. \quad (2)$$

We recall that, if f and g have pairwise complementary jump discontinuities, $h_n^{(N)}$ must be calculated through the inverse rule[2]:

$$[h] = [\![1/f]\!]^{-1}[g]. \quad (3)$$

Using Eqs. (2) and (3), Li was able to explain the spectacular improvement in the convergence of Fourier series obtained by the modal method for lamellar gratings.[3,4] However, these rules were not directly applicable to arbitrary groove shapes, for which the classic differential theory requires finding the Fourier components of products of periodic functions that have concurrent, but not complementary, jump discontinuities and for which no known rule applies. A recent breakthrough was described in Ref. 5, which explained how to overcome the difficulty. By introducing, in the entire cross-section plane, a suitable continuation of the tangential and normal components of the field, components that are defined on the grating profile, we were able to factorize the products mentioned above by using Laurent's rule and the inverse rule. We called that technique the fast-Fourier-factorization (FFF) method. A variant of the method has been proposed[6] for studying anisotropic gratings. In the present paper we use the FFF method to establish the dif-

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ferential equations that are satisfied by the Fourier components of the field for the most general situation. The diffracting device is allowed to be one-, two-, or three-dimensionally periodic. The material is isotropic or anisotropic. In the latter case, both electric and magnetic permittivity are tensors. The material is transparent or lossy, even in case of anisotropy. Special cases are derived from the general equations, and the particular way of dealing with them is pointed out.

2. GENERAL, FAST-CONVERGING PROPAGATION EQUATIONS IN FOURIER SPACE

We consider a periodic surface described by its Cartesian equation $f(x, y, z) = 0$. This surface is assumed to have a normal vector $\mathbf{N}$ everywhere and separates two media characterized by their tensors $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$, which degenerate into scalars for isotropic media. Harmonic Maxwell equations

$$\operatorname{curl}\mathbf{E} = i\omega\mathbf{B}, \tag{4}$$

$$\operatorname{curl}\mathbf{H} = -i\omega\mathbf{D} \tag{5}$$

lead to partial-derivative equations for the Cartesian coordinates of $\mathbf{E}$ or $\mathbf{H}$. As these components are discontinuous through the $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$ discontinuity surface, we make use of continuous components in Fourier analysis. In the plane tangent to the periodic surface at any point M, we introduce two orthogonal unit vectors $\mathbf{T}_1$ and $\mathbf{T}_2$ such that $\mathbf{T_2} \times \mathbf{T_1} = \mathbf{N}$, where $\mathbf{T}_1$ is arbitrary but is conveniently chosen to be parallel to the xOy plane. The tangential components of the electrical field are thus given by

$$E_{T_1} = \mathbf{T}_1 \bullet \mathbf{E}, \tag{6}$$

$$E_{T_2} = \mathbf{T}_2 \bullet \mathbf{E}. \tag{7}$$

Here the dot product is the well-known scalar product of two vectors, but we use special notation (large dots) to introduce the more-general dot product between matrices that represent tensors and vectors of different ranks. The generalized dot product means contraction of one of the indices, i.e., a summation with respect to one of the indices. With that notation, the normal component of $\mathbf{D}$ is given in the form

$$D_N = \mathbf{N} \bullet \mathbf{D} = \mathbf{N} \bullet \bar{\bar{\epsilon}} \bullet \mathbf{E}. \tag{8}$$

From the laws of electromagnetism, vector $\mathbf{F}_\epsilon = (E_{T_1}, D_n, E_{T_2})$ is continuous through the periodic surface. The first step is to relate it to $\mathbf{E}$ to link the Fourier components of $\mathbf{D}$ with those of $\mathbf{E}$.

A. Relationship between [D] and [E]

In as much as $[g]$ denotes a vector constructed with the Fourier components of $g(x)$, $[\mathbf{D}]$ will denote a vector made with the three blocks $[D_x]$, $[D_y]$, and $[D_z]$. Each of these blocks will have $2N + 1$ Fourier components for a one-dimensional periodic medium, $(2N + 1)^2$ components for a bidimensional medium that has two periods of the same order of magnitude, etc.

Expressing Eqs. (6)–(8) leads to

$$E_{Ti} = T_{ix}E_x + T_{iy}E_y + T_{iz}E_z, \qquad i = 1, 2, \tag{9}$$

$$\begin{aligned} D_N = {} & N_x(\epsilon_{xx}E_x + \epsilon_{xy}E_y + \epsilon_{xz}E_z) \\ & + N_y(\epsilon_{yx}E_x + \epsilon_{yy}E_y + \epsilon_{yz}E_z) \\ & + N_z(\epsilon_{zx}E_x + \epsilon_{zy}E_y + \epsilon_{zz}E_z). \end{aligned} \tag{10}$$

If we introduce a matrix A_ϵ, defined by

$$\mathbf{F}_\epsilon = A_\epsilon \bullet \mathbf{E} \equiv A_\epsilon\mathbf{E}, \tag{11}$$

Eqs. (9) and (10) immediately show that

$$A_\epsilon = \begin{bmatrix} T_{1x} & T_{1y} & T_{1z} \\ N_x\epsilon_{xx} + N_y\epsilon_{yx} + N_z\epsilon_{zx} & N_x\epsilon_{xy} + N_y\epsilon_{yy} + N_z\epsilon_{zy} & N_x\epsilon_{xz} + N_y\epsilon_{yz} + N_z\epsilon_{zz} \\ T_{2x} & T_{2y} & T_{2z} \end{bmatrix}.$$

Because E_{Ti} and D_N are defined only on the surface of discontinuity of $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$, Eqs. (9)–(11) are valid only on this surface, defined by the equation $f(x, y, z) = 0$. However, as was previously done,[5] we extend the validity of Eqs. (9)–(11), $\forall x, y, z$, through a suitable continuation of $\mathbf{T}_i$ and $\mathbf{N}$ outside the surface. The continuation must ensure that these vectors are continuous on the surface; they may be discontinuous at points where $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$ are continuous.

Let us thus introduce a vector denoted $(\mathbf{N} \bullet \bar{\bar{\epsilon}})$, where the dot product stands for a summation over one of the indices of $\bar{\bar{\epsilon}}$, as has already been discussed above. Then $D_N = (\mathbf{N} \bullet \bar{\bar{\epsilon}}) \bullet \mathbf{E}$, and matrix A_ϵ can be expressed simply as

$$A_\epsilon = \begin{bmatrix} T_{1x} & T_{1y} & T_{1z} \\ (\mathbf{N} \bullet \bar{\bar{\epsilon}})_x & (\mathbf{N} \bullet \bar{\bar{\epsilon}})_y & (\mathbf{N} \bullet \bar{\bar{\epsilon}})_z \\ T_{2x} & T_{2y} & T_{2z} \end{bmatrix}. \tag{12}$$

Because $\bar{\bar{\epsilon}}$ never vanishes, the determinant of A_ϵ is of a quadratic positive or negative form; thus A_ϵ has an inverse C_ϵ, so $\mathbf{E} = C_\epsilon\mathbf{F}_\epsilon$. As a result, the equation $\mathbf{D} = \bar{\bar{\epsilon}} \bullet \mathbf{E}$ can be written as $\mathbf{D} = \bar{\bar{\epsilon}} \bullet C_\epsilon\mathbf{F}_\epsilon = \bar{\bar{\epsilon}} \bullet C_\epsilon A_\epsilon\mathbf{E}$. In this way, $\mathbf{D}$ is represented as the product of a discontinuous quantity $\bar{\bar{\epsilon}} \bullet \mathbf{C}_\epsilon$ and a continuous quantity $\mathbf{F}_\epsilon$ (or $A_\epsilon\mathbf{E}$). Its Fourier components can then be obtained through Laurent's rule: $[\mathbf{D}] = [\![\bar{\bar{\epsilon}} \bullet C_\epsilon]\!][\mathbf{F}_\epsilon]$. Of course, because both $[\mathbf{D}]$ and $[\mathbf{F}_\epsilon]$ are vectors formed by blocks, the Toeplitz matrix that relates them will be made from blocks that are the Toeplitz matrices of the various elements of matrix $\bar{\bar{\epsilon}} \bullet \mathbf{C}_\epsilon$. Using the inverse rule to find the Fourier components of the continuous product $A_\epsilon\mathbf{E}$, we obtain

$$[\mathbf{D}] = [\![\bar{\bar{\epsilon}} \bullet C_\epsilon]\!][\![C_\epsilon]\!]^{-1}[\mathbf{E}]. \tag{13}$$

This is a key point of the theory. Tedious, but elementary, calculations show that the inverse of A_ϵ is given by

$$C_\epsilon = \frac{1}{\xi_\epsilon}\begin{bmatrix} [(N \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_2]_x & N_x & -[(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_1]_x \\ [(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_2]_y & N_y & -[(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_1]_y \\ [(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_2]_z & N_z & -[(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_1]_z \end{bmatrix}, \tag{14}$$

where ξ_ϵ is the determinant of A_ϵ and is equal to $\mathbf{N} \bullet \bar{\bar{\epsilon}} \bullet \mathbf{N}$. Thus Eq. (13) can be written in compact form:

$$[\mathbf{D}] = Q_\epsilon[\mathbf{E}], \tag{15}$$

where $Q_\epsilon = [\![\bar{\bar{\epsilon}} \bullet C_\epsilon]\!][\![C_\epsilon]\!]^{-1}$ is a known matrix.

B. Relationship between [B] and [H]

For the most general problem, the relationships between [**B**] and [**H**] and between [**D**] and [**E**] are completely symmetric. We thus introduce a vector $\mathbf{F}_\mu$, given by $\mathbf{F}_\mu = (H_{T1}, B_N, H_{T2})$, and a matrix A_μ, defined by $\mathbf{F}_\mu = A_\mu \mathbf{H}$. We derive the expressions for A_μ and its inverse C_μ, respectively, from Eqs. (12) and (14) by replacing $\bar{\bar{\epsilon}}$ with $\bar{\bar{\mu}}$. As a result, we obtain

$$[\mathbf{B}] = Q_\mu[\mathbf{H}], \tag{16}$$

where $Q_\mu = [\![\bar{\bar{\mu}} \bullet C_\mu]\!][\![C_\mu]\!]^{-1}$.

C. Set of Differential Equations in Fourier Space

After they are projected on the coordinate axis, Maxwell equations (4) and (5) can be written as

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = i\omega B_x, \tag{17}$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = i\omega B_y, \tag{18}$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = i\omega B_z, \tag{19}$$

$$\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = -i\omega D_x, \tag{20}$$

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = -i\omega D_y, \tag{21}$$

$$\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = -i\omega D_z. \tag{22}$$

The resolution of these equations will now depend on the problem, in the sense that, depending on the kind of periodicity and invariance of the device, some derivative will vanish. For example, for a single grating with the direction of its rulings parallel to the Oz axis and illuminated in the cross-section plane, $\partial/\partial z = 0$; moreover, if the grating is periodic with respect to the x direction, the derivatives with respect to x will be expressed explicitly. We then obtain the equations published in Ref. 6 for an anisotropic material and those in Ref. 5 for an isotropic material. For a three-dimensional periodic photonic crystal, the periodicity along the three dimensions of space eliminates all derivatives, and the problem is reduced to an eigenvalue problem. However, in most cases of periodicity in one or two directions only, the modulated region is limited inside a y interval, let us say from 0 to a, where a is the groove depth, whereas the x or z periodicity or both, or invariance, will permit simple expressions of the x or z derivatives or both. Only the y derivative remains in the set of Eqs. (17)–(22). After one- or two-dimensional Fourier analysis, the Fourier components of the field will depend only on y and will be solutions of the following equations:

$$\frac{\partial[E_z]}{\partial y} - \frac{\partial[E_y]}{\partial z} = i\omega[B_x], \tag{17$'$}$$

$$\frac{\partial[E_x]}{\partial z} - \frac{\partial[E_z]}{\partial x} = i\omega[B_y], \tag{18$'$}$$

$$\frac{\partial[E_y]}{\partial x} - \frac{\partial[E_x]}{\partial y} = i\omega[B_z], \tag{19$'$}$$

$$\frac{\partial[H_z]}{\partial y} - \frac{\partial[H_y]}{\partial z} = -i\omega[D_x], \tag{20$'$}$$

$$\frac{\partial[H_x]}{\partial z} - \frac{\partial[H_z]}{\partial x} = -i\omega[D_y], \tag{21$'$}$$

$$\frac{\partial[H_y]}{\partial x} - \frac{\partial[H_x]}{\partial y} = -i\omega[D_z], \tag{22$'$}$$

where $[D_j]$ and $[B_j]$, with $j = x, y, z$, have to be expressed through Eqs. (15) and (16); in these equations it is understood that, for a device that is periodic with period d_j along the j axis, $\partial/\partial j$ must be replaced with multiplication by $i\alpha_j$, where α_j is a diagonal matrix with elements $\alpha_{j,nm} = (\alpha_{j,0} + n2\pi/d_j)\delta_{nm}$ and $\alpha_{j,0}$ is the j component of the wave vector of the incident wave and δ_{nm} is the Krönecker symbol. We can deal with the particular case of a j-invariant device by taking $d_j \to \infty$, so $\alpha_{j,nm} = \alpha_{j,0}\delta_{nm}$. If, moreover, the incident wave vector is perpendicular to the j axis, then $\alpha_{j,nm} = 0$, which leads to invariance with respect to the j coordinate, $\partial/\partial j = 0$.

The resolution of the set (17′)–(22′), which is now indeed a set of first-order classic differential equations with respect to y only, is conducted in the following way: We keep as unknown functions only the vectors $[E_x]$, $[E_z]$, $[H_x]$, and $[H_z]$, which are, respectively, solutions of Eqs. (19′), (17′), (22′), and (20′). To that end, we eliminate $[E_y]$ and $[H_y]$ in the following way: Eq. (15) leads to

$$[D_y] = Q_{\epsilon,yx}[E_x] + Q_{\epsilon,yy}[E_y] + Q_{\epsilon,yz}[E_z],$$

from which we get

$$[E_y] = Q_{\epsilon,yy}{}^{-1}([D_y] - Q_{\epsilon,yx}[E_x] - Q_{\epsilon,yz}[E_z]).$$

In this equation $[D_y]$ is expressed in terms of $[H_x]$ and $[H_z]$ only, as the result of Eq. (21′). We then get

$$[E_y] = Q_{\epsilon,yy}{}^{-1}\left\{\frac{i}{\omega}\left(\frac{\partial}{\partial z}[H_x] - \frac{\partial}{\partial x}[H_z]\right) - Q_{\epsilon,yx}[E_x] - Q_{\epsilon,yz}[E_z]\right\}. \tag{23}$$

Similarly, for H_y,

$$[H_y] = Q_{\mu,yy}{}^{-1}\left\{ -\frac{i}{\omega}\left(\frac{\partial}{\partial z}[E_x] - \frac{\partial}{\partial x}[E_z]\right) - Q_{\mu,yx}[H_x] - Q_{\mu,yz}[H_z]\right\}. \tag{24}$$

Of course, the convention concerning the interpretation of the x and z partial derivative as stated above still applies. We thus obtain a set of first-order differential equations of the form

$$\frac{\mathrm{d}}{\mathrm{d}y}\begin{pmatrix}[E_x]\\ [E_z]\\ [H_x]\\ [H_z]\end{pmatrix} = M\begin{pmatrix}[E_x]\\ [E_z]\\ [H_x]\\ [H_z]\end{pmatrix}, \tag{25}$$

where M is a known matrix with elements given by

$$M_{11} = -i\alpha_x Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx} - iQ_{\mu,zy}Q_{\mu,yy}{}^{-1}\alpha_z\,,$$

$$M_{12} = -i\alpha_x Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yz} + iQ_{\mu,zy}Q_{\mu,yy}{}^{-1}\alpha_x\,,$$

$$M_{13} = i\omega Q_{\mu,zy}Q_{\mu,yy}{}^{-1}Q_{\mu,yx} - i\frac{\alpha_x}{\omega}Q_{e,yy}{}^{-1}\alpha_z - i\omega Q_{\mu,zx}\,,$$

$$M_{14} = i\omega Q_{\mu,zy}Q_{\mu,yy}{}^{-1}Q_{\mu,yz} + i\frac{\alpha_x}{\omega}Q_{\epsilon,yy}{}^{-1}\alpha_x - i\omega Q_{\mu,zz}\,,$$

$$M_{21} = -i\alpha_z Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx} + iQ_{\mu,xy}Q_{\mu,yy}{}^{-1}\alpha_z\,,$$

$$M_{22} = -i\alpha_z Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yz} - iQ_{\mu,xy}Q_{\mu,yy}{}^{-1}\alpha_x\,,$$

$$M_{23} = -i\omega Q_{\mu,xy}Q_{\mu,yy}{}^{-1}Q_{\mu,yx} - i\frac{\alpha_z}{\omega}Q_{\epsilon,yy}{}^{-1}\alpha_z + i\omega Q_{\mu,xx}\,,$$

$$M_{24} = -i\omega Q_{\mu,xy}Q_{\mu,yy}{}^{-1}Q_{\mu,yz} + i\frac{\alpha_z}{\omega}Q_{\epsilon,yy}{}^{-1}\alpha_x + i\omega Q_{\mu,xz}\,,$$

$$M_{31} = -i\omega Q_{\epsilon,zy}Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx} + i\frac{\alpha_x}{\omega}Q_{\mu,yy}{}^{-1}\alpha_z + i\omega Q_{\epsilon,zx}\,,$$

$$M_{32} = -i\omega Q_{\epsilon,zy}Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yz} - i\frac{\alpha_x}{\omega}Q_{\mu,yy}{}^{-1}\alpha_x + i\omega Q_{\epsilon,zz}\,,$$

$$M_{33} = -i\alpha_x Q_{\mu,yy}{}^{-1}Q_{\mu,yx} - iQ_{\epsilon,zy}Q_{\epsilon,yy}{}^{-1}\alpha_z\,,$$

$$M_{34} = -i\alpha_x Q_{\mu,yy}{}^{-1}Q_{\mu,yz} + iQ_{\epsilon,zy}Q_{\epsilon,yy}{}^{-1}\alpha_x\,,$$

$$M_{41} = i\omega Q_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx} + i\frac{\alpha_z}{\omega}Q_{\mu,yy}{}^{-1}\alpha_z - i\omega Q_{\epsilon,xx}\,,$$

$$M_{42} = i\omega Q_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yz} - i\frac{\alpha_z}{\omega}Q_{\mu,yy}{}^{-1}\alpha_x - i\omega Q_{\epsilon,xz}\,,$$

$$M_{43} = -i\alpha_z Q_{\mu,yy}{}^{-1}Q_{\mu,yx} + iQ_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1}\alpha_z\,,$$

$$M_{44} = -i\alpha_z Q_{\mu,yy}{}^{-1}Q_{\mu,yz} - iQ_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1}\alpha_x\,. \tag{25$'$}$$

At the boundaries of the modulated region, the field can be expressed by Rayleigh expansions. Thus the most general diffraction problem is reduced to the numerical integration of a set of differential equations, with the boundary conditions taken into account. This boundary-value problem is turned into an initial-value problem by use of the classic shooting method.[7] The numerical integration is then done with the help of a suitable algorithm.[1] Numerical problems may arise, however, if the integration process is conducted over a long interval, i.e., if groove depth a is large enough. This kind of problem is well known in other domains of science, among which are meteorology and the theory of deterministic chaos. It comes from the extreme sensitivity of the searched-for solution to the initial values. In as much as computers work with finite accuracy, an error of 10^{-16} at the beginning of the integration will introduce a small amount of undesirable growing exponential functions associated with evanescent orders during the integration process. Because the arguments of these exponential functions increase with the permittivity of the material, the more conducting the metal, the sooner the contamination will appear. The best way to avoid contamination is to use the so-called S-matrix propagation algorithm,[8] which was specially adapted[9] to be coupled to the differential theory.

The conclusion is that Eqs. (25) and (25′) constitute a new, fast-converging formulation of the Maxwell equations in Fourier space that has to be used to produce numerical results (with truncated series) for diffraction by periodic objects.

3. SOME PARTICULAR SITUATIONS

As it is well known that the most-general theory is not always the best suited for analyzing much simpler situations, we consider here some particular cases of interest.

A. Classic Gratings Made from Isotropic, Nonmagnetic Materials

The diffractive device considered here is periodic with period d along the x direction and is illuminated by an incident plane wave propagating in the cross-section plane ($\alpha_{z,0} = 0$). The grating material is isotropic, so $\epsilon_{ij} = \epsilon(x, y)\delta_{ij}$; we assume that $\mu_{ij} = \mu_0\delta_{ij}$, where μ_0 is the vacuum magnetic permittivity. Because the direction of the rulings is the z axis, we choose in the tangential plane $\mathbf{T}_2 = \hat{z}$, where $\hat{z}$ is the unit vector of the z axis. The normal vector is given by $\mathbf{N} = (N_x, N_y, 0)$, and its components are proportional to $\overrightarrow{\mathrm{grad}}\, f(x, y)$, where $f(x, y) = 0$ is the equation for the groove profile. From the equation $\mathbf{T}_2 \times \mathbf{T}_1 = \mathbf{N}$ or $\mathbf{T}_1 = \mathbf{N} \times \mathbf{T}_2$, we obtain $\mathbf{T}_1 = (N_y, -N_x, 0)$. Determination of matrix C_ϵ requires the calculation of $\mathbf{N} \bullet \bar{\bar{\epsilon}} \bullet \mathbf{N}$, $(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_2$, and $(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_1$. At first, $\mathbf{N} \bullet \bar{\bar{\epsilon}} \bullet \mathbf{N} = \epsilon(x, y)\mathbf{N} \bullet 1I \bullet \mathbf{N}$, where $1I$ is the unit square matrix. Thus $\mathbf{N} \bullet \bar{\bar{\epsilon}} \bullet \mathbf{N} = \epsilon(x, y)$; next, $(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_2 = \epsilon(x, y)(N_y, -N_x, 0)$ and $(\mathbf{N} \bullet \bar{\bar{\epsilon}}) \times \mathbf{T}_1 = \epsilon(x, y)(0, 0, -1)$.

Thus matrix C_ϵ reads as

$$C_\epsilon = \begin{bmatrix} N_y & N_x/\epsilon & 0\\ -N_x & N_y/\epsilon & 0\\ 0 & 0 & 1\end{bmatrix}, \qquad \epsilon C_\epsilon = \begin{bmatrix} \epsilon N_y & N_x & 0\\ -\epsilon N_x & N_y & 0\\ 0 & 0 & \epsilon\end{bmatrix}.$$

Because N_x and N_y will be defined outside the grating surface in a continuous way, as was previously explained in Ref. 5, the corresponding Toeplitz matrices are

$$[\![C_\epsilon]\!] = \begin{bmatrix} [\![N_y]\!] & [\![1/\epsilon]\!][\![N_x]\!] & 0 \\ [\![-N_x]\!] & [\![1/\epsilon]\!][\![N_y]\!] & 0 \\ 0 & 0 & 1I \end{bmatrix}, \tag{26}$$

$$[\![\epsilon C_\epsilon]\!] = \begin{bmatrix} [\![\epsilon]\!][\![N_y]\!] & [\![N_x]\!] & 0 \\ -[\![\epsilon]\!][\![N_x]\!] & [\![N_y]\!] & 0 \\ 0 & 0 & [\![\epsilon]\!] \end{bmatrix}. \tag{27}$$

Inverting matrix $[\![C_\epsilon]\!]$ of Eq. (26) gives

$$[\![C_\epsilon]\!]^{-1} = \begin{bmatrix} [\![N_y]\!] & -[\![N_x]\!] & 0 \\ [\![1/\epsilon]\!]^{-1}[\![N_x]\!] & [\![1/\epsilon]\!]^{-1}[\![N_y]\!] & 0 \\ 0 & 0 & 1I \end{bmatrix},$$

so

$$Q_\epsilon = [\![\epsilon C_\epsilon]\!] \bullet [\![C_\epsilon]\!]^{-1} = \begin{bmatrix} [\![\epsilon]\!][\![N_y^2]\!] + [\![1/\epsilon]\!]^{-1}[\![N_x^2]\!] & -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_y]\!] & 0 \\ -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_y]\!] & [\![\epsilon]\!][\![N_x^2]\!] + [\![1/\epsilon]\!]^{-1}[\![N_y]\!]^2 & 0 \\ 0 & 0 & [\![\epsilon]\!] \end{bmatrix}.$$

The derivation of this equation has assumed the commutativity of some Toeplitz matrices, as will be justified in Appendix B.

Because $\mu = \mu_0$ everywhere, matrix Q_μ reduces to a scalar μ_0. With the grating illuminated in the cross-section plane ($\alpha_{z,0} = 0$) and the null elements of Q_ϵ taken into account, most of the elements of matrix M given by Eq. (25′) vanish:

$$M = \begin{bmatrix} -i\alpha_x Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx} & 0 & 0 & -i\omega\mu_0 + \dfrac{i\alpha_x^2}{\omega}Q_{\epsilon,yy}{}^{-1} \\ 0 & 0 & i\omega\mu_0 & 0 \\ 0 & i\omega Q_{\epsilon,zz} - \dfrac{i\alpha_x^2}{\omega\mu_0} & 0 & 0 \\ -i\omega(Q_{\epsilon,xx} - Q_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1}Q_{\epsilon,yx}) & 0 & 0 & -i\alpha_x Q_{\epsilon,xy}Q_{\epsilon,yy}{}^{-1} \end{bmatrix},$$

which leads to the basic propagation equations for classic gratings with in-plane illumination for both TE and TM polarization. However, in this simple case there is a simpler way to derive the equations, which is presented below.

For TE polarization, $E_x = E_y = 0 = H_z$. Because $\mu = \mu_0$ everywhere, Eq. (17′) leads to $\mathrm{d}[E_z]/\mathrm{d}y = i\omega\mu_0[H_x]$; Eqs. (22′) and (15) give $\mathrm{d}[H_x]/\mathrm{d}y = i\omega Q_{\epsilon,zz}[E_z] + i\alpha_x[H_y]$, where $[H_y]$ is given by Eq. (24), which reduces to $[H_y] = -(\alpha_x/\omega\mu_0)[E_z]$. We thus obtain

$$\begin{aligned}\frac{\mathrm{d}^2[E_z]}{\mathrm{d}y^2} &= i\omega\mu_0\left\{i\omega[\![\epsilon]\!][E_z] - \frac{i\alpha_x^2}{\omega\mu_0}[E_z]\right\} \\ &= -\mu_0\omega^2[\![\epsilon]\!][E_z] + \alpha_x^2[E_z].\end{aligned} \tag{28}$$

This is the original propagation equation that was used in Ref. 1.

For TM polarization, $H_x = H_y = 0 = E_z$. Equations (20′) and (15) lead to

$$\frac{\mathrm{d}[H_z]}{\mathrm{d}y} = -i\omega\{Q_{\epsilon,xx}[E_x] + Q_{\epsilon,xy}[E_y]\}, \tag{29}$$

in which $[E_y]$ is derived from Eq. (23):

$$[E_y] = Q_{\epsilon,yy}{}^{-1}\left\{\frac{\alpha_x}{\omega}[H_z] - Q_{\epsilon,yx}[E_x]\right\}. \tag{30}$$

Equation (19′), however, leads to

$$\frac{\mathrm{d}[E_x]}{\mathrm{d}y} = -i\omega\mu_0[H_z] + i\alpha_x[E_y]. \tag{31}$$

Substituting the expression for $[E_y]$ given by Eq. (30) into Eqs. (29) and (31) leads, after some algebraic calculations, to Eqs. (19) and (20) of Ref. 5. Thus our general equations reduce to the basic equations, which lead to the fast convergence that has already been derived for isotropic gratings.

B. Anisotropic Gratings

Anisotropic gratings are of great interest for information processing. Thus a special study has been devoted to them and will be published elsewhere.[6] The research submitted for publication in Ref. 6 concerns both types of electric and magnetic anisotropy and includes the case of lossy materials. It concerns in-plane diffraction, i.e., it assumes that the incident wave vector is in the cross-section plane of the grating. We have verified that the present method leads to the same equations in that particular case. However, it also includes conical diffraction, i.e., an incident wave vector outside the cross-section plane; moreover, it is able to deal with crossed anisotropic gratings with surfaces periodic in both the x and the z directions, whereas both $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$ tensors exhibit arbitrarily valued components.

C. Special Groove Geometry: Modal Theory

It is well known that for some special geometries the numerical integration of Eq. (25) can be avoided. This occurs, for example, for lamellar gratings, for which, inside the grooves, the Fourier components of ϵ and μ (and also of $\mathbf{N}$) do not depend on ordinate y. The result is that, in Eq. (25), matrix M has constant elements, and the solution can be expressed in terms of eigenvalues and eigenvectors. This method of solving the problem is known as the modal method[10] or the rigorous coupled-wave theory.[11] The convergence rate of the Fourier series of the field was recently much improved by the heuristic changes in the propagation equations suggested in Refs. 3 and 4. The present theory includes those equations, which are valid in the particular case of lamellar gratings, because it includes Eqs. (19) and (20) of Ref. 5 which have proved to include the basic equations of Refs. 3 and 4. The situation is somehow different for slanted lamellar gratings. In that situation, ϵ depends on y through a phase factor only. Although the modal method is not directly applicable, an adaptation by the use of suitable coordinates can be made.[12] A separate paper[13] will explain how the idea developed in Ref. 5 and in the present paper has been used to improve the modal method in both classic and conical diffraction and will show the fast converging results obtained with deep, slanted gold lamellar gratings.

D. Crossed Gratings

Crossed gratings have x and z directions of periodicity. They can be made from isotropic or anisotropic materials. In the isotropic situation, grids have interesting polarizing properties. Grids are crossed gratings made with periodic holes inside a film of dielectric or metal, such that the groove profile does not depend on the y coordinate, and their diffracting capabilities may be analyzed through the modal method. A recent paper[14] brought experimental evidence of extraordinary transmission. Although much theoretical effort was made to explain the unexpected effect, all authors worked on unidimensional models and thus were unable to produce the correct explanation, which turns out to be specific to two-dimensional periodic arrays. Using the ideas presented here, we developed a computer code that is able to analyze a grid made with highly conducting metal such as gold, based on the modal theory.[15] We were thus able to show that the two-dimensional structure of the device introduces a new channel for light transmission, which does not exist for one-dimensional grids. The success of these computations, which were impossible to perform with any other existing grating theory, illustrates the capabilities of the present method.

For two-dimensional modulated surfaces, which require numerical integration along the y coordinate in the groove region, the present theory reduces to a formalism that is similar to the one developed in Subsection 3.A for classic gratings, except that matrix α_z is not zero. The main difference lies in the fact that the Fourier components of the field components are $(2N + 1) \times (2N + 1)$ matrices, but they may be turned into vectors with $(2N + 1)^2$ components through a suitable subroutine. Also, in that case the diffraction problem does not reduce to TE and TM cases, so four coupled differential equations on $[E_x]$, $[E_z]$, $[H_x]$, and $[H_z]$ have to be integrated simultaneously, as stated in Eq. (25). But the boundary-value problem is not more difficult to handle than for the classic grating used in conical diffraction, which has been analyzed with success[13] with the the eigenvalue technique.

If the grating is made from isotropic materials, the form of matrices C_ϵ and ϵC_ϵ is similar to those of classic gratings, Eqs. (26) and (27); however, the normal vector has three nonnull components, so inverting $[\![C_\epsilon]\!]$ analytically by blocks is more difficult to do. Fortunately, in the isotropic case, one can use a more straightforward approach to find matrix Q_ϵ, which is described in Appendix B. The result is written in the form

$$Q_\epsilon = \begin{bmatrix} [\![\epsilon]\!] - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_x^2]\!] & -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_y]\!] & -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_z]\!] \\ -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_y]\!] & [\![\epsilon]\!] - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_y^2]\!] & -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_yN_z]\!] \\ -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_xN_z]\!] & -([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_yN_z]\!] & [\![\epsilon]\!] - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![N_z^2]\!] \end{bmatrix},$$

which differs from the classic grating case (Subsection 3.A) because of the three components of $\mathbf{N}$, which are, in general, nonnull. These components depend on the profile. For example, a double-sinusoidal profile is defined by the equation

$$y = (H/2)\sin(K_x x)\sin(K_z z),$$

i.e.,

$$f(x, y, z) \equiv (H/2)\sin(K_x x)\sin(K_z z) - y = 0.$$

Here H is the total groove depth and K_x and K_y are linked with the grating periods d_x and d_y in the x and z directions: $K_x = 2\pi/\mathrm{d}_x$ and $K_z = 2\pi/\mathrm{d}_z$. Then it is possible to define $\mathbf{N}$ *independently of ordinate* y, so the Fourier transform of its components is made once before numerical integration along y. $\mathbf{N}$ is proportional to $\overrightarrow{\mathrm{grad}}\, f(x, y, z)$:

$$\mathbf{N} = \frac{1}{|\overrightarrow{\mathrm{grad}}\, f|}\left[\frac{HK_x}{2}\cos(K_x x)\sin(K_z z), \quad -1, \right.$$
$$\left. \frac{HK_z}{2}\sin(K_x x)\cos(K_z z)\right],$$

with

$$|\overrightarrow{\mathrm{grad}} f| = \left[1 + \left(\frac{HK_x}{2}\right)^2 \cos^2(K_x x)\sin^2(K_z z) + \left(\frac{HK_z}{2}\right)^2 \sin^2(K_x x)\cos^2(K_z z)\right]^{1/2}.$$

E. Three-Dimensional Photonic Crystals

Three-dimensional photonic crystals are made with an arbitrary object periodically repeated in the three Cartesian coordinate directions. In that case, in addition to the x and z periodicities that are found in crossed gratings, the additional y periodicity allows the d/dy derivatives to be expressed analytically. The result is that the differential set [Eq. (25)] reduces to an eigenvalue–eigenvector problem, which can be resolved by means of standards subroutines. In another paper,[16] both theory and numerical results obtained in this particular case for isotropic materials will be presented.

4. CONCLUSION

Although Maxwell equations have been known for more than a century, the best way to write them in Fourier space was not clear until now. The beautiful research of Li warned the community of grating theoreticians of the convergence problem linked to the usual way of factorizing Fourier series, so we were able to propose a fast-Fourier-factorization (FFF) method[5] that surmounted the difficulties encountered in analyzing metallic gratings in TM polarization. Here we have enlarged the FFF method to the most general case of a diffraction problem. The important point appears in Eq. (13), which relates the Fourier components of [**E**] and [**D**], namely,

$$[\mathbf{D}] = [\![\bar{\bar{\epsilon}} \bullet C_\epsilon]\!][\![C_\epsilon]\!]^{-1}[\mathbf{E}], \tag{32}$$

and which does not reduce to

$$[\mathbf{D}] = [\![\bar{\bar{\epsilon}}]\!][\mathbf{E}]. \tag{33}$$

A similar equation is valid for [**H**] and [**B**]. Figure 1 presents a comparison of the convergence rates when the two factorization rules, Eqs. (32) and (33), are used for a slanted lamellar gold grating used in TM polarization. The improvement of the convergence is spectacular.

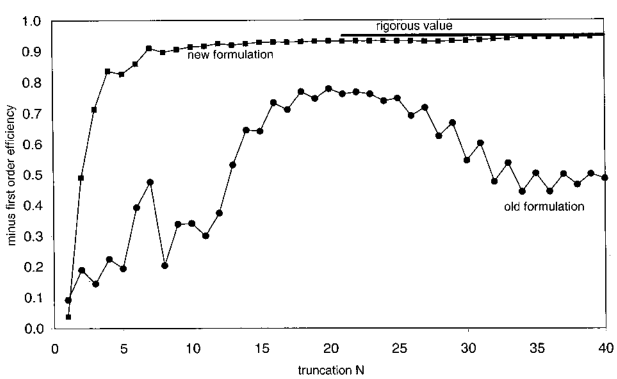

Fig. 1. Convergence rates for two rules of factorization, Eq. (32), represented by squares, and Eq. (33), represented by circles. The −1st diffracted order efficiency as a function of truncation parameter N for a gold grating (refractive index, $0.2 + i6.71$) consisting of lamellae slanted at 45° with filling ratio 0.5, period 1 μm, and height 0.5 μm, is shown as used in TM polarization at 0.8-μm wavelength and 30° incidence. The rigorous value was calculated with the integral formalism found in Ref. 17.

Here we give in compact form the elements of the matrices C_ϵ and $\bar{\bar{\epsilon}} C_\epsilon$ for any kind of geometry and material and explain how to reduce the diffraction problem to a simple boundary-value problem. It can then be analyzed through differential or modal theory when some special geometries are involved. Several numerical results for particular cases have already been obtained through this method of solving the convergence problem. Although the method was derived with periodic diffracting devices in mind, one can analyze nonperiodic elements by replacing Fourier series by Fourier transforms. For isolated two- or three-dimensional objects, the 2π periodicity with respect to the angular cylindrical or spherical coordinates can be used, so the present theory is applicable to objects without evident periodicity.

APPENDIX A: LAURENT'S RULE OF FACTORIZATION OF FOURIER SERIES

Let us denote by f_c and f_d, respectively, two periodic functions of the variable x, with period d_x, that are, respectively, continuous and discontinuous. If we consider the corresponding infinite Fourier series, Laurent's rule states that one can obtain the Fourier series of the product $f_d f_c$ by factorizing the Fourier series of f_d and f_c through the convolution product, known as "Laurent's rule":

$$(f_d f_c)_n = \sum_{m=-\infty}^{+\infty} f_{d,n-m} f_{c,m},$$

$$[f_d f_c] = [\![f_d]\!][f_c] = [\![f_c]\!][f_d]. \tag{A1}$$

The question now is: What is the best way to calculate the truncated Fourier series of $f_d f_c$, limited to $2N + 1$ terms (from $-N$ to $+N$). The truncation implies that this product, as well as f_d, is correctly approximated by the sum of its $2N + 1$ components on the Fourier basis $\exp(inKx)$, with $K = 2\pi/\mathrm{d}_x$. The very concept of factorizing Fourier series states that $[f_d f_c]$ will be an appropriate product of two operators, F_1 and F_2:

$$[f_1 f_2] = F_1(f_1) F_2(f_2), \tag{A2}$$

where $\partial F_1/\partial f_2 = 0 = \partial F_2/\partial f_1$; we want to establish what kinds of operators and products have to be used. In the truncated Fourier basis of $\exp(inKx)$ functions, these operators will be represented by matrices. To obtain a vector after we find their product, we represent $F_1(f_1)$ by a $(2N + 1) \times (2N + 1)$ square matrix, denoted $\overleftrightarrow{F}_1(f_1)$, whereas $F_2(f_2)$ will be represented by a vector, denoted $\mathbf{F}_2(f_2)$, with $2N + 1$ components. Thus Eq. (A2) will read as

$$[f_1 f_2] = \overleftrightarrow{F}_1(f_1) \bullet \mathbf{F}_2(f_2). \tag{A3}$$

In a first step, we choose for f_2 one of the $2N + 1$ functions of the Fourier basis: $f_2 = \exp(inKx)$, with $n \in (-N, +N)$. We obviously have $\forall n$, $\mathbf{F}_2(f_2) = I_n$, where I_n is a vector with $2N$ elements equal to zero and the nth element equal to 1. The mth Fourier component of $f_1 \exp(inKx)$ is

$$[f_1 \exp(inKx)]_m = [f_1]_{m-n}. \tag{A4}$$

However, because $\mathbf{F}_2(f_2) = I_n$, Eq. (A3) leads to

$$[f_1 \exp(inKx)]_m = [\vec{\vec{F}}(f_1) I_n]_m = [\vec{\vec{F}}_1(f_1)]_{m,n}. \tag{A5}$$

Equations (A4) and (A5) show that $[\vec{\vec{F}}_1(f_1)]_{m,n} = [\![f_1]\!]_{m,n}$, i.e.,

$$\vec{\vec{F}}_1(f_1) = [\![f_1]\!]. \tag{A6}$$

As $\partial F_1/\partial f_2 = 0$, Eq. (A6) is established, whatever the choice of f_2 may be.

As a second step, we choose $f_1 = \exp(imKx)$, with $m \in [-N, +N]$, for which $[\![f_1]\!]_{n,p} = [f_1]_{n-p} = \delta_{n-p,m}$ (Krönecker symbol).

In the same way as above, $[\exp(imKx) f_2]_n = [f_2]_{n-m}$, whereas, Eqs. (A3) and (A6) lead to $[\exp(imKx) f_2]_n = \{[\![f_1]\!]\mathbf{F}_2(f_2)\}_n = \Sigma_p\, \delta_{m,n-p}[\mathbf{F}_2(f_2)]_p\, [\mathbf{F}_2(f_2)]_{n-m}$. The result is that $\mathbf{F}_2(f_2) = [f_2]$. With Eq. (A6) taken into account, Eq. (A3) reads as $[f_1 f_2] = [\![f_1]\!][f_2]$, which establishes the validity of Laurent's rule for truncated series.

If one of the two functions, e.g., f_1, is discontinuous at x, provided that it is piecewise continuous, piecewise smooth, and bounded, its Fourier series converges at x to $\{f_1(x+0) + f_1(x-0)\}/2$. With that point kept in mind, it is then easy to establish that Laurent's rule applied to the product $f_d f_c$ will yield Fourier components with the corresponding Fourier series converging to $\{f_d(x+0) + f_d(x-0)\} f_c(x)/2$. Thus Laurent's rule,

$$[f_d f_c] = [\![f_d]\!][f_c], \tag{A7}$$

is the best way to factorize the product $f_d f_c$.

However, if f_2 is also discontinuous at x, Laurent's rule will give Fourier coefficients that do not lead to a convergence toward the correct value of the functions at x: $\{f_1(x+0) f_2(x+0) + f_1(x-0) f_2(x-0)\}/2$. Instead, it will converge to $\{f_1(x+0) + f_1(x-0)\}\{f_2(x+0) + f_2(x-0)\}/4$. However, if the two discontinuous functions f_1 and f_2 have complementary jump discontinuities, i.e., if $f_1 f_2$ is continuous at x, the Fourier components of the product can be correctly computed by means of the inverse rule, which can immediately be derived from Eq. (A7). Let us state that $f_c = f_1 f_2 \Rightarrow f_2 = (1/f_1) f_c$, where $1/f_1$ is discontinuous and f_c is continuous. Applying Laurent's rule, we get

$$[f_2] = [\![1/f_1]\!][f_c],$$

from which we derive

$$[f_c] = [\![1/f_1]\!]^{-1}[f_2] \quad \text{or} \quad [f_1 f_2] = [\![1/f_1]\!]^{-1}[f_2].$$

This is the inverse rule.

APPENDIX B: ISOTROPIC MATERIALS

In the case of isotropic materials it is possible to obtain matrix Q_ϵ in a simple way because $\bar{\bar{\epsilon}}$ reduces to a scalar, ϵ.

Starting from $[\mathbf{D}] = [\epsilon \mathbf{E}] = [\epsilon \mathbf{E}_T + \epsilon \mathbf{E}_N]$, where $\mathbf{E}_N = \mathbf{N}(\mathbf{N} \bullet \mathbf{E})$ and $\mathbf{E}_T = \mathbf{E} - \mathbf{E}_N$, we first remark that $\epsilon \mathbf{E}_T$ is discontinuous, whereas $\epsilon \mathbf{E}_N$ is continuous. We thus obtain

$$\begin{aligned}[\mathbf{D}] &= [\![\epsilon]\!][\mathbf{E}_T] + [\![1/\epsilon]\!]^{-1}[\mathbf{E}_N] \\ &= [\![\epsilon]\!][\mathbf{E} - \mathbf{N}(\mathbf{N} \bullet \mathbf{E})] + [\![1/\epsilon]\!]^{-1}[\mathbf{N}(\mathbf{N} \bullet \mathbf{E})].\end{aligned}$$

We introduce a square matrix denoted $(\mathbf{NN})$ whose elements are given by $(\mathbf{NN})_{i,j} = N_i N_j$; the previous equation leads to

$$[\mathbf{D}] = [\![\epsilon]\!][\mathbf{E}] - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![\mathbf{NN}]\!][\mathbf{E}],$$

where we recognize a matrix Δ that is equal to

$$[\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1},$$

which we introduced previously.[5] Thus

$$Q_\epsilon = [\![\epsilon]\!] - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})[\![\mathbf{NN}]\!].$$

This equation has to be interpreted in a block form as

$$(Q_\epsilon)_{mn,ij} = [\![\epsilon]\!]_{mn}\delta_{ij} - ([\![\epsilon]\!] - [\![1/\epsilon]\!]^{-1})_{mn}[\![\mathbf{N}_i \mathbf{N}_j]\!],$$

$$i, j = x, y, z, \quad m, n = -N{:}N,$$

which leads to the expression given in the core of this paper and justifies the assumed commutativity of the truncated Toeplitz matrices.

Another way to arrive at the same conclusion is to follow the same procedure as outlined on p. 1776 of our previous paper,[5] i.e., to change the orders of the various terms in the product before taking the Fourier components.

Let us demonstrate the method on the first element of Q_ϵ, for example; for a classic isotropic grating for which $N_z = 0$, we have

$$\begin{aligned}Q_{\epsilon,xx} &= [\![(\epsilon C_\epsilon)_{xx}(C_\epsilon^{-1})_{xx} + (\epsilon C_\epsilon)_{xy}(C_\epsilon^{-1})_{yx} \\ &\quad + (\epsilon C_\epsilon)_{xz}(C_\epsilon^{-1})_{zx}]\!] \\ &= [\![\epsilon N_y N_y + N_x (1/\epsilon)^{-1} N_x]\!] \\ &= [\![\epsilon N_y^2 + (1/\epsilon)^{-1} N_x^2]\!] = [\![\epsilon]\!][\![N_y^2]\!] + [\![1/\epsilon]\!]^{-1}[\![N_x^2]\!],\end{aligned}$$

which we obtained by assuming the commutativity of the various matrices.

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REFERENCES

1. M. Nevière, P. Vincent, and R. Petit, "Sur la théorie du réseau conducteur et ses applications à l'optique," Nouv. Rev. Opt. **5**, 65–77 (1974).
2. L. Li, "Use of Fourier series in the analysis of discontinuous periodic structures," J. Opt. Soc. Am. A **13**, 1870–1876 (1996).
3. P. Lalanne and G. M. Morris, "Highly improved convergence of the coupled-wave method for TM polarization," J. Opt. Soc. Am. A **13**, 779–784 (1996).
4. G. Granet and B. Guizal, "Efficient implementation of the coupled-wave method for metallic gratings in TM polarization," J. Opt. Soc. Am. A **13**, 1019–1023 (1996).
5. E. Popov and M. Nevière, "Grating theory: new equations in Fourier space leading to fast converging results for TM polarization," J. Opt. Soc. Am. A **17**, 1773–1784 (2000).
6. K. Watanabe, R. Petit, and M. Nevière, "Differential theory of gratings made of anisotropic materials," J. Opt. Soc. Am. A (to be published).
7. P. Vincent, "Differential methods," in *Electromagnetic Theory of Gratings*, Vol. 22 of Springer Topics in Current

Physics, R. Petit, ed. (Springer-Verlag, Berlin, 1980), pp. 101–121.

8. L. Li, "Formulation and comparison of two recursive matrix algorithms for modelling layered diffraction gratings," J. Opt. Soc. Am. A **13**, 1024–1035 (1996).
9. F. Montiel, M. Nevière, and P. Peyrot, "Waveguide confinement of Cerenkov second-harmonic generation through a graded-index grating coupler: electromagnetic optimization," J. Mod. Opt. **45**, 2169–2186 (1988).
10. L. Li, "A modal analysis of lamellar diffraction gratings in conical mountings," J. Mod. Opt. **40**, 553–573 (1993).
11. M. G. Moharam and T. K. Gaylord, "Diffraction analysis of dielectric surface-relief gratings," J. Opt. Soc. Am. **72**, 1385–1392 (1982).
12. E. Glytsis and T. Gaylord, "Three-dimensional (vector) rigorous coupled-wave analysis of anisotropic grating diffraction," J. Opt. Soc. Am. A **7**, 1399–1419 (1990).
13. B. Chernov, M. Nevière, and E. Popov, "Fast Fourier factorization method applied to modal analysis of slanted lamellar diffraction gratings in conical mountings," submitted to Opt. Commun.
14. T. W. Ebbesen, H. J. Lezec, H. F. Ghaemi, T. Thio, and P. A. Wolff, "Extraordinary optical transmission through sub-wavelength hole arrays," Nature **391**, 667–669 (1998).
15. E. Popov, M. Nevière, S. Enoch, and R. Reinisch, "Theory of light transmission through sub-wavelength periodic hole arrays," Phys. Rev. B **63**, 16,000–16,008 (2000).
16. S. Enoch, E. Popov, and M. Nevière, "Electromagnetic theory of 3-dimensional photonic crystals," Proc. SPIE (to be published).
17. D. Maystre "Integral Method," in *Electromagnetic Theory of Gratings*, R. Petit, ed. (Springer-Verlag, Berlin, 1980), Chap. 3.