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Pseudospectral Modal Method for Conical Diffraction of Gratings

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For lamellar gratings and other layered periodic structures, the modal methods (including both analytic and numerical ones) are often the most efficient, since they avoid the discretization of one spatial variable. The pseudospectral modal method (PSMM) previously developed for in-plane diffraction problems of one-dimensional gratings achieves high accuracy for a small number of discretization points, and it outperforms most other modal methods. In this paper, an extension of the PSMM to conical diffraction problems is presented and implemented. Numerical examples are used to demonstrate the high accuracy and excellent convergence property of this method for both dielectric and metallic gratings.

Keywords: diffraction gratings; numerical methods; modal method; pseudospectral method.

1. Introduction

Diffraction gratings and other periodic structures play important roles in photonics [1, 2]. For design and optimization of grating structures, efficient numerical methods are needed. Although general numerical methods such as the finite-difference time-domain method [3] and the finite element method [4], are widely available, it is possible to develop more efficient numerical methods by taking advantage of the geometric features of the grating structure. Modal methods are highly suitable for lamellar gratings and other layered periodic structures, where the field can be expanded in eigenmodes in each layer. Modal methods include the analytic modal method [5–7] and different kinds of numerical modal methods. For some problems, the analytic modal method may be difficult to use, since it requires a systematic method for root-finding in the complex plane. The Fourier modal method (FMM) [8–14] calculates the eigenmodes using expansions in

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Fourier series, and is extremely popular due to its simplicity. Over the years, other numerical modal methods have also been developed, for example, based on the finite difference method [15–17], piecewise polynomial expansions [18, 19], spline functions [20], etc. The pseudospectral modal method (PSMM) [21–24] is relatively easy to implement and it outperforms most other numerical modal methods. PSMM shares some principle with the polynomial expansion modal methods, but it works on the wave field in physical space directly (instead of expansion coefficients), and is applicable to gratings with arbitrary piecewise smooth (instead of piecewise constant) refractive index profiles. It is interesting to note that the most accurate implementation of the PSMM [23] uses numerically calculated modes even in the homogeneous media above and below the grating layers.

So far, the PSMM has only been implemented for in-plane diffraction problems of one-dimension (1D) gratings. For these problems, the structure and the electromagnetic field are independent of one spatial variable (z in this paper), and the Maxwell's equations are reduced to scalar Helmholtz equations for two different polarizations. In this paper, we implement the PSMM for conical diffraction of 1D gratings. In that case, the field depends on z as $\exp(i\gamma_0 z)$ for a given γ_0, and four field components are needed to solve the problem. Conical diffractions are important for practical applications. Although some other modal methods (analytic, Fourier, finite difference, etc) are already available for conical diffraction problems, it is worthwhile to extend the PSMM, since it achieves high accuracy for in-plane diffraction problems. Numerical results indicate that PSMM indeed outperforms the FMM and a high order finite difference modal method (FDMM) for conical diffraction problems.

2. Formulation and modal method

We consider a two-dimensional non-magnetic periodic structure described by a dielectric function $\varepsilon(x, y)$. The structure is z invariant, as $\varepsilon(x, y)$ is independent of z, and it is periodic in x with period L. We also assume that the structure consists of a finite number of layers separated by $0 = y_0 < y_1 < \cdots < y_J = D$, such that $\varepsilon = \varepsilon^{(j)}(x)$ is y-independent for $y_{j-1} < y < y_j$, i.e., in the jth layer. In addition, we assume $\varepsilon = \varepsilon^{(*)}$ for $y > D$ and $\varepsilon = \varepsilon^{(0)}$ for $y < 0$, where $\varepsilon^{(*)}$ and $\varepsilon^{(0)}$ are constants. Notice that the periodic structure is actually restricted to $0 < y < D$, and the media above ($y > D$) and below ($y < 0$) the periodic structure are homogeneous. Here, we consider x and y as the axes in the horizontal and vertical directions, respectively.

Let $\boldsymbol{H}$ be the magnetic field multiplied by the free space impedance, the frequency domain

Maxwell's equations for the time dependence $\exp(-i\omega t)$ are

$$\nabla \times \boldsymbol{E} = ik_0\boldsymbol{H}, \quad \nabla \times \boldsymbol{H} = -ik_0\varepsilon\boldsymbol{E}, \tag{1}$$

where $\boldsymbol{E}$ is the electric field and k_0 is the free space wavenumber. For conical diffraction, the electromagnetic field is assumed to have a simple z dependence $\exp(i\gamma_0 z)$, where γ_0 is a given constant. To study conical diffraction problems, we need the four components E_x, H_x, E_z and H_z. On the horizontal interfaces between different layers, i.e, at $y = y_j$ for $0 \le j \le J$, we need to enforce the continuity of these four components.

For a given plane incident wave in the top region ($y > D$), our objective is to calculate the reflected and transmitted waves in the top and bottom ($y < 0$) regions. Let the wave vector of the incident wave be $(\alpha_0, -\beta_0^{(*)}, \gamma_0)$, where $\beta_0^{(*)} > 0$ and $\alpha_0^2 + [\beta_0^{(*)}]^2 + \gamma_0^2 = k_0^2\varepsilon^{(*)}$, the reflected and transmitted waves can be expanded in plane waves with wave vectors $(\alpha_l, \beta_l^{(*)}, \gamma_0)$ and $(\alpha_l, -\beta_l^{(0)}, \gamma_0)$ respectively, where

$$\alpha_l = \alpha_0 + 2\pi l/L, \quad \beta_l^{(*)} = [k_0^2\varepsilon^{(*)} - \alpha_l^2 - \gamma_0^2]^{1/2}, \quad \beta_l^{(0)} = [k_0^2\varepsilon^{(0)} - \alpha_l^2 - \gamma_0^2]^{1/2}, \tag{2}$$

and l is any integer.

Since the structure consists of a few layers, where each layer is y independent, it is natural to use the modal method. To simplify the presentation, we follow our previous work [16] and skip the derivations. In the jth layer where $\varepsilon = \varepsilon^{(j)}(x)$, we need to solve two eigenvalue problems. The first problem is for eigenfunction ϕ and eigenvalue δ^2:

$$\varepsilon\frac{d}{dx}\left(\frac{1}{\varepsilon}\frac{d\phi}{dx}\right) + (k_0^2\varepsilon - \gamma_0^2)\phi = \delta^2\phi, \qquad 0 < x < L, \tag{3}$$

$$\phi(L) = \rho\phi(0), \tag{4}$$

$$\frac{1}{\varepsilon(L^-)}\frac{d\phi}{dx}(L^-) = \frac{\rho}{\varepsilon(0^+)}\frac{d\phi}{dx}(0^+), \tag{5}$$

where $\rho = e^{i\alpha_0 L}$. The second eigenvalue problem is for ψ and ν^2:

$$\frac{d^2\psi}{dx^2} + (k_0^2\varepsilon - \gamma_0^2)\psi = \nu^2\psi, \qquad 0 < x < L, \tag{6}$$

$$\psi(L) = \rho\psi(0), \tag{7}$$

$$\frac{d\psi}{dx}(L) = \rho\frac{d\psi}{dx}(0). \tag{8}$$

Each of these eigenvalue problems gives rise to an infinite sequence of eigenpairs. We denote the eigenpairs by $\{\phi_m, \delta_m^2\}$ and $\{\psi_m, \nu_m^2\}$ for $m = 1, 2, 3, \cdots$, then the x and z components of the electromagnetic field are given by

$$E_x(x,y) = \sum_{m=1}^{\infty} \frac{\gamma_0^2+\delta_m^2}{\varepsilon(x)} \phi_m(x) \left[a_m e^{i\delta_m(y-y_{j-1})} + b_m e^{-i\delta_m(y-y_j)}\right], \tag{9}$$

$$H_x(x,y) = \sum_{m=1}^{\infty} (\gamma_0^2+\nu_m^2)\psi_m(x) \left[c_m e^{i\nu_m(y-y_{j-1})} + d_m e^{-i\nu_m(y-y_j)}\right], \tag{10}$$

$$E_z(x,y) = \sum_{m=1}^{\infty} \frac{i\gamma_0}{\varepsilon(x)} \frac{d\phi_m(x)}{dx} \left[a_m e^{i\delta_m(y-y_{j-1})} + b_m e^{-i\delta_m(y-y_j)}\right] \tag{11}$$
$$+ \sum_{m=1}^{\infty} k_0\nu_m\psi_m(x) \left[c_m e^{i\nu_m(y-y_{j-1})} - d_m e^{-i\nu_m(y-y_j)}\right],$$

$$H_z(x,y) = \sum_{m=1}^{\infty} -k_0\delta_m\phi_m(x) \left[a_m e^{i\delta_m(y-y_{j-1})} - b_m e^{-i\delta_m(y-y_j)}\right] \tag{12}$$
$$+ \sum_{m=1}^{\infty} i\gamma_0 \frac{d\psi_m(x)}{dx} \left[c_m e^{i\nu_m(y-y_{j-1})} + d_m e^{-i\nu_m(y-y_j)}\right].$$

For simplicity, we have removed the z dependence $e^{i\gamma_0 z}$ in the above expansions. Notice that the eigenfunctions, eigenvalues and coefficients are specific to the jth layer. To be more precise, we should add a subpscript (j) to these quantities, that is, $\phi_m^{(j)}$, $\delta_m^{(j)}$, $\psi_m^{(j)}$, $\nu_m^{(j)}$, $a_m^{(j)}$, $b_m^{(j)}$, $c_m^{(j)}$ and $d_m^{(j)}$.

In the top and bottom regions, the field components are expanded in plane waves which are related to the eigenfunctions. For the top region, the eigenvalue problems (3-5) and (6-8) have the trivial solutions:

$$\phi_l = \psi_l = e^{i\alpha_l x},$$
$$\delta_l^2 = \nu_l^2 = k_0^2\varepsilon^{(*)} - \gamma_0^2 - \alpha_l^2,$$

where l is any integer. The case for the bottom region is similar.

3. Pseudospectral modal method

To solve the eigenvalue problems (3-5) and (6-8), we use the Chebyshev pseudospectral method [25]. A detailed description of the method is given in [22]. In the following, we briefly summarize the main steps for problem (3-5).

First, we need to identify the discontinuities of ε along the x axis. The grating structure has a few layers, and the dielectric function ε is assumed to be piecewise smooth in each layer. If the discontinuities are located at $x_0, x_1, \cdots, x_P$ satisfying $0 = x_0 < x_1 < \cdots < x_P = L$, then we discretize the pth segment $x_{p-1} < x < x_p$ by

$$\xi_{p,k} = x_{p-1} + \frac{x_p - x_{p-1}}{2}\left[1 - \cos\left(\frac{k\pi}{q_p}\right)\right], \quad 0 \le k \le q_p, \tag{13}$$

where q_p is a positive integer, $\xi_{p,0} = x_{p-1}$ and $\xi_{p,q_p} = x_p$. The Chebyshev pseudospectral method gives us a matrix $\boldsymbol{C}_p$, such that

$$\begin{bmatrix} \phi'(x_{p-1}^+) \\ \boldsymbol{\phi}_p' \\ \phi'(x_p^-) \end{bmatrix} \approx \boldsymbol{C}_p \begin{bmatrix} \phi(x_{p-1}) \\ \boldsymbol{\phi}_p \\ \phi(x_p) \end{bmatrix}, \tag{14}$$

where $\boldsymbol{\phi}_p$ is a column vector for ϕ at the interior points $\{\xi_{p,k} \ : \ 1 \le k \le q_p - 1\}$, and $\phi' = d\phi/dx$.

We can use $\boldsymbol{C}_p$, $1 \le p \le P$, to evaluate one-side limits of ϕ' at all discontinuity points, set up a system of equations based on the continuity of $\frac{1}{\varepsilon}\phi'$ and the quasi-periodic conditions (4-5), and obtain a matrix $\boldsymbol{A}_0$ such that

$$\begin{bmatrix} \phi(x_0) \\ \phi(x_1) \\ \vdots \\ \phi(x_P) \end{bmatrix} \approx \boldsymbol{A}_0 \begin{bmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \\ \vdots \\ \boldsymbol{\phi}_P \end{bmatrix}. \tag{15}$$

The above equation relates the eigenfunction at the discontinuity points to the eigenfunction at all interior points $\{\xi_{p,k} \ : \ 1 \le k \le q_p - 1, \ 1 \le p \le P\}$. The total number of interior points is $N = (q_1 - 1) + (q_2 - 1) + \cdots = \sum_{p=1}^{P} q_p - P$. When the governing equation (3) is discretized at all N interior points based on the differentiation matrices $\boldsymbol{C}_p$, $1 \le p \le P$, we obtain the following matrix eigenvalue problem

$$\boldsymbol{A} \begin{bmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \\ \vdots \\ \boldsymbol{\phi}_P \end{bmatrix} = \delta^2 \begin{bmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \\ \vdots \\ \boldsymbol{\phi}_P \end{bmatrix}. \tag{16}$$

The discretization process involves ϕ at the discontinuity points, but they have been eliminated using Eq. (15). When the matrix eigenvalue problem (16) is solved, we can use Eq. (15) again to find the eigenfunction at the discontinuity points and use Eq. (14) to find the derivative of the eigenfunctions. In the top and bottom homogeneous regions, although the eigenvalue problems have simple analytic solutions, we also calculate numerical eigenfunctions and eigenvalues based on the same discretization points and the same Chebyshev pseudospectral method.

After the numerical eigenmodes for each layer are found, we can evaluate E_x, H_x, E_z and H_z at the N interior points on both sides of the horizontal interfaces, i.e. at $y = y_j^\pm$ for $0 \le j \le J$. Of course, these vector representations involve the four sets of unknown coefficients $\{a_m^{(j)}, b_m^{(j)}, c_m^{(j)}, d_m^{(j)} : 1 \le m \le N\}$ for each layer (i.e. $1 \le j \le J$), as well as the unknown reflection and transmission amplitudes in the top and bottom regions. The continuity of these four components gives rise to a linear system for all $4(J+1)N$ unknowns. From the reflection and transmission amplitudes, we can find the diffraction efficiencies. The method requires $O(JN^3)$ operations for computing the eigenmodes in different layers and for solving the final linear system. Typically, the required CPU time is dominated by the computation of the eigenmodes. The memory requirement is $O(JN^2)$.

4. Numerical examples

In this section, we present a few numerical examples to validate and illustrate the accuracy of our conical PSMM. The first example is shown in Fig. 1(a). It is a metallic lamellar grating with

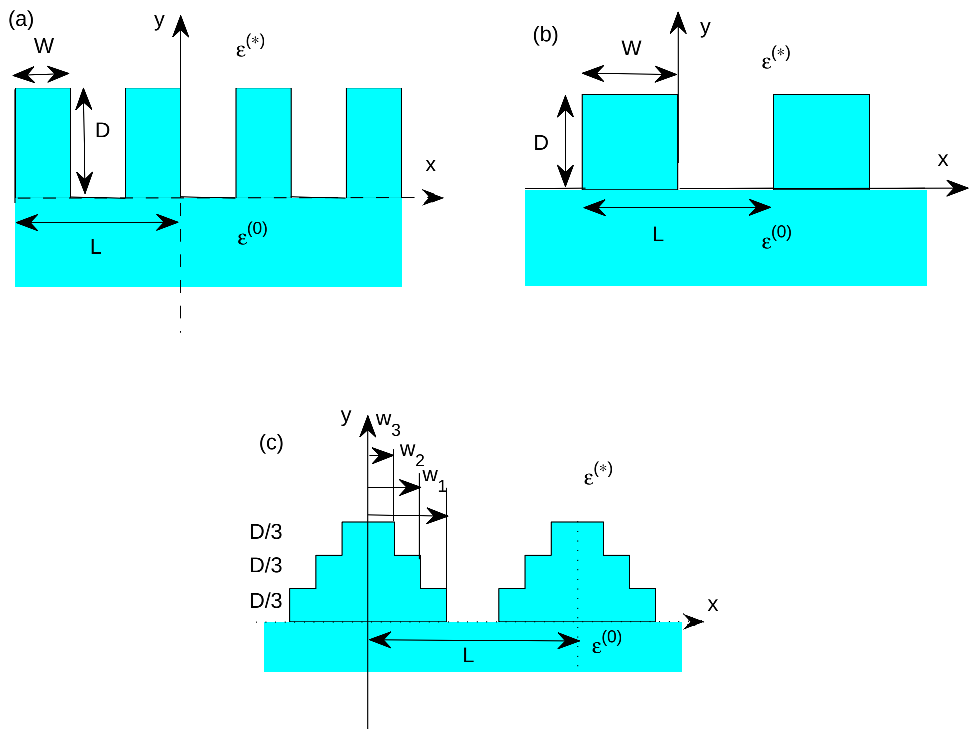

Figure 1. (a) A metallic lamellar grating. (b) A dielectric lamellar grating. (c) A metallic grating with three layers.

$L = D = 1\,\mu$m and $W = 0.5\,\mu$m, where L is the period, D is the depth of the grooves, and W is the width of the ridges. For this structure, we consider a plane incident wave with a free space wavelength $\lambda = 0.5\,\mu$m and an incident wave vector $(\alpha_0, -\beta_0^{(*)}, \gamma_0) = k_0(\sqrt{2}/4, -\sqrt{3}/2, \sqrt{2}/4)$, where $k_0 = 2\pi/\lambda = 4\pi\,(\mu\text{m})^{-1}$. The electric field of the incident wave is given by

$$\boldsymbol{E}^{(i)}(x,y,z) = \begin{bmatrix} \sqrt{3}/4 - 1/2 \\ \sqrt{2}/4 \\ \sqrt{3}/4 + 1/2 \end{bmatrix} \exp\{i[\alpha_0 x - \beta_0^{(*)}(y-D) + \gamma_0 z]\}.$$

The magnetic field of the incident wave can be easily obtained using the Maxwell's equations. We assume that the dielectric constant of the metal is $\varepsilon^{(0)} = (0.1+5.0i)^2$ and the medium above the grating is air (thus $\varepsilon^{(*)} = 1$). This problem has been previously analyzed by an analytic modal method [7] and a boundary integral equation (BIE) method [27]. For this incident wave, the grating has four propagating diffraction orders in the reflected wave. In Table 1 we compare

Table 1. Metallic lamellar grating: diffraction efficiency of the zeroth reflected order computed by the FMM, FDMM and PSMM.

N	FMM	FDMM	PSMM
96	0.441907	0.44083	0.44157307
192	0.441605	0.44133	0.44158363
300	0.441572	0.44144	0.44158516
384	0.441566	0.44148	0.44158551
492	0.441567	0.44151	0.44158569
600	0.441570	0.44153	0.44158578
768	0.441573	0.44156	0.44158584

the diffraction efficiency of the zeroth reflected order obtained by the FMM, a high order FDMM [16] and our conical PSMM. For FDMM and PSMM, the integer N is the number of points for discretizing one period in x. For FMM, N is the total number of retained terms in the Fourier series. For all three methods, N is also the size of the matrices in the resulting matrix eigenvalue problems. Since all three methods require $O(JN^3)$ operations for solving the eigenvalue problems and the final linear systems, it is fair to compare the methods for the same N. For $N \geq 384$, all PSMM results round to the same six digits $R_0 = 0.441586$. Notice that for $N = 192$, we get $R_0 = 0.441584$ and it is already very accurate. In contrast, both FMM and FDMM can only reach the first four correct digits when $N = 768$. These results agree with the previous result given in [27].

The second example is the dielectric lamellar grating shown in Fig. 1(b). The dielectric constant of the medium is $\varepsilon^{(0)} = 2.25^2$, and the medium above the grating is air (i.e. $\varepsilon^{(*)} = 1$). The geometric parameters are $L = 1\,\mu$m and $D = W = 0.5\,\mu$m. For this structure, we specify a plane incident wave with the electric field

$$\boldsymbol{E}^{(i)}(x,y,z) = \begin{bmatrix} 1/2 + i/\sqrt{2} \\ 1/\sqrt{2} \\ 1/2 - i/\sqrt{2} \end{bmatrix} \exp\{i[\alpha_0 x - i\beta_0^{(*)}(y-D) + \gamma_0 z]\},$$

where $(\alpha_0, -\beta_0^{(*)}, \gamma_0) = k_0(1/2, -1/\sqrt{2}, 1/2)$ and $k_0 = 4\pi\,(\mu\text{m})^{-1}$, i.e. the free space wavelength is $\lambda = 0.5\,\mu$m. This problem has been analyzed before by the analytic modal method [7] and the BIE methods [26, 28]. For the above incident wave, there are five propagating diffraction orders in the transmitted wave. In Table 2 we list the diffraction efficiencies of the first and zeroth

Table 2. Dielectric lamellar grating: diffraction efficiencies of the first and zeroth transmitted orders computed by the PSMM.

N	T_1	T_0
60	0.378262173	0.1419188289
100	0.378266145	0.1419195190
200	0.378267520	0.1419195448
300	0.378267708	0.1419195324
400	0.378267761	0.1419195273
500	0.378267782	0.1419195249
600	0.378267792	0.1419195237
700	0.378267798	0.1419195230
800	0.378267801	0.1419195225
900	0.378267803	0.1419195223
1000	0.378267805	0.1419195221

transmitted orders computed by the PSMM with different values of N. It can be seen that when $N = 200$, we obtain a solution with six correct digits $T_1 \approx 0.378268$, and when $N = 400$, we get a solution with seven correct digits $T_1 \approx 0.3782678$. This agrees with the previous results $T_1 = 0.37826780866$ given in [28], $T_1 = 0.37827$ given in [7], and $T_1 = 0.3783$ given in [26].

Finally, we consider the three-layer metallic grating shown in Fig. 1(c). This structure has been studied before by Zolla *et al.* [29]. It is assumed that the dielectric constant of the metal is $\varepsilon^{(0)} = (1 + 10i)^2$, the medium above the grating is air (i.e., $\varepsilon^{(*)} = 1$), the period of the grating is $L = 2\pi\,\mu$m, the total height of the grating is D, the height of each layer is $D/3$, the widths of the metal in the layers are $w_1 = 3\pi/4\,\mu$m, $w_2 = \pi/2\,\mu$m, and $w_3 = \pi/4\,\mu$m, respectively. We specify a plane incident wave with the electric field given by

$$\boldsymbol{E}^{(i)}(x, y, z) = \begin{bmatrix} 1/2 + \sqrt{2}/4 \\ 1/2 \\ 1/2 - \sqrt{2}/4 \end{bmatrix} \exp\{i[\alpha_0 x - \beta_0^{(*)}(y - D) + \gamma_0 z]\}$$

where $(\alpha_0, -\beta_0^{(*)}, \gamma_0) = k_0(1/2, -\sqrt{2}/2, 1/2)$. In Fig. 2, we show the zeroth, minus first and

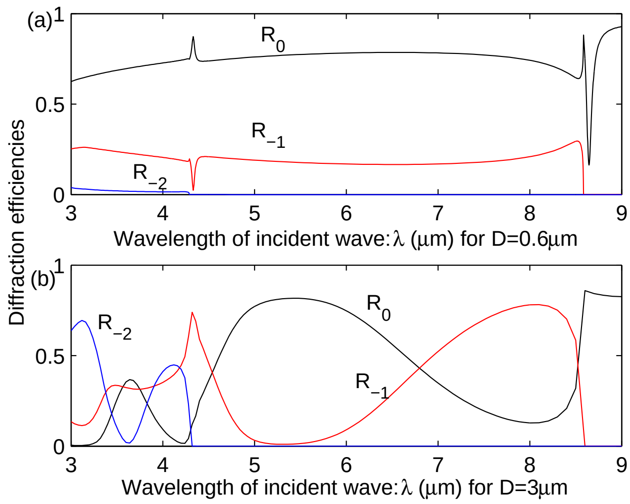

Figure 2. Dependence of reflected diffraction efficiencies R_0, R_{-1} and R_{-2} on free space wavelength λ for (a) $D = 0.6\,\mu$m, and (b) $D = 3\,\mu$m.

minus second reflected diffraction efficiencies R_0, R_{-1} and R_{-2} as functions of the free space wavelength λ for $D = 0.6\,\mu$m and $D = 3\,\mu$m. Our results show a good agreement with those reported in [29]. Notice that the number of propagating reflected diffraction orders changes in the wavelength range shown in the figures, thus R_{-1} and R_{-2} cease to exist when the wavelength is too large. To check the convergence of our method, we fix $D = 0.6\,\mu$m and $\lambda = 6\,\mu$m, and compare numerical solutions for different values of N. The results for R_0 and R_{-1} are listed in Table 3. It appears that a solution for R_0 with six correct digits, i.e., $R_0 \approx 0.782458$, can be obtained with $N = 234$.

5. Conclusion

In the previous sections, we presented a PSMM for analyzing conical diffraction of gratings. The method is an extension of the PSMM [21–24] developed for in-plane diffraction problems. Following the approach of Granet [23], we use numerical eigenmodes even in the homogeneous media above and below the grating layer, and match the field on horizontal interfaces at all

Table 3. Metallic lamellar grating in a conical mounting: diffraction efficiency of zeroth and minus-first reflected order.

N	R_0	R_{-1}
54	0.78244768	0.16936466
84	0.78246492	0.16934320
144	0.78245970	0.16933706
174	0.78245889	0.16933624
234	0.78245809	0.16933565
294	0.78245779	0.16933540
354	0.78245766	0.16933527
414	0.78245758	0.16933520
474	0.78245754	0.16933516
534	0.78245752	0.16933513

discretization points. The method is suitable for gratings with one or a few layers where each layer is invariant in the vertical direction perpendicular to the grating layer. It delivers high accuracy for relatively small number of discretization points and shows good convergence for both dielectric and metallic gratings. The method clearly outperforms the standard FMM and our own high order FDMM [16], and it is easy to implement.

This version of the PSMM becomes less competitive if the grating has many layers and the dielectric function has many different vertical discontinuities, since the discretization points are identical for all layers and must cluster around each discontinuous point. In that case, it may be more efficient to use different discretization points for different layers and matching the Fourier coefficients of the field on horizontal interfaces [22]. Alternatively, we may use the PSMM for each layer separately to calculate the scattering matrix of the layer, then use the scattering matrix method to find the final solution. Like most modal methods, the PSMM is not suitable if the dielectric function has general (not just vertical and horizontal) discontinuity curves. In that case, other methods, such as the BIE method, are more appropriate.

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