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The finitely conducting lamellar diffraction grating

L. C. BOTTEN and M. S. CRAIG
School of Mathematical Sciences,
The New South Wales Institute of Technology,
P.O. Box 123, Broadway, N.S.W. 2007, Australia

R. C. McPHEDRAN
Department of Theoretical Physics, The University of Sydney,
N.S.W. 2006, Australia

J. L. ADAMS and J. R. ANDREWARTHA
Department of Physics, The University of Tasmania,
G.P.O. Box 252C, Hobart, Tasmania 7001, Australia

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Abstract. A rigorous modal theory describing the diffraction properties of a finitely conducting lamellar grating is presented. The method used is the generalization to lossy structures of an earlier formalism for the dielectric lamellar grating. Sample results of the method are given, demonstrating its accuracy and its ability to deal with problems intractable by the widely used integral- equation formalisms of diffraction grating theory.

1. Introduction

In a previous paper [1], we presented a new modal formalism for the diffraction properties of the dielectric lamellar diffraction grating. The lossless nature of the structure led to an expression of the diffraction problem in a self-adjoint form—i.e. there existed a complete set of orthogonal modes. In this paper, we shall generalize the modal formalism to encompass the presence of loss (or energy dissipation) in the grating material, even though the introduction of loss into the diffraction problem renders it non-self-adjoint. To our knowledge, this is the first rigorous modal formulation for diffraction by a lossy structure.

We present a concise exposition of the generalized theory, relying, for the sake of brevity, upon the material presented in [1]. We emphasize the differences which arise when the refractive index of the grating material is made complex. We show the validity of our theory using numerical results satisfying physical criteria such as reciprocity and the conservation of energy. We give results indicating the adequacy of the formalism for dealing with extreme grating profiles, e.g. those having depths as large as several hundred times their period.

2. The formalism

2.1. *Notation and method*

We consider the diffraction of an S-polarized plane wave of free space wavelength λ incident at some angle ϕ upon the structure shown in figure 1. The various parameters of the grating are defined here exactly as in [1], except that here we admit the possibility that the refractive indices r_i of the regions D_i for $i=1, 2, 3$ are complex.

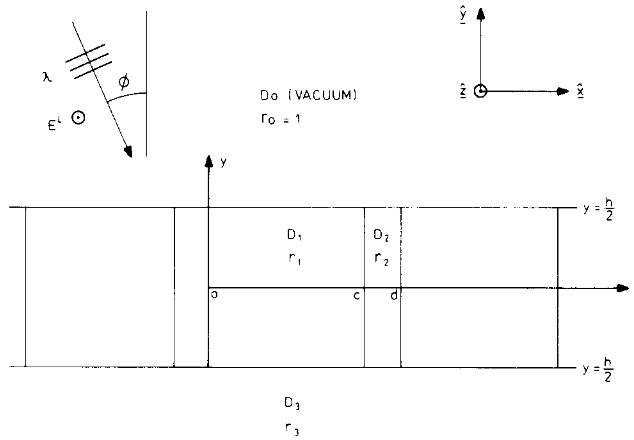

Figure 1. The geometry of the diffraction problem. In the P polarization case shown, the z component of the total electric field must be continuous and have a continuous normal derivative at any boundary. This function and its normal derivative must also be pseudo-periodic, as in (31) and (32) of [1].

For the case of S polarization, the incident magnetic field is aligned with the z axis and the total magnetic field and its normal derivative divided by the square of the refractive index (of the medium in question) are continuous at all boundaries. These quantities must also be pseudo-periodic.

The spatial part of the total magnetic field $\mathbf{H}$ has only a single non-zero component along the z-axis (i.e. $\mathbf{H} = H\hat{\mathbf{z}}$) and in regions D_0, D_3 obeys the Helmholtz equations

$$\left.\begin{aligned}(\nabla^2 + k_0^2)H = 0 \quad \text{in} \quad D_0 \\ (\nabla^2 + k_3^2)H = 0 \quad \text{in} \quad D_3\end{aligned}\right\} \tag{1}$$

where $k_0 = 2\pi/\lambda$ and $k_3 = k_0 r_3$.

In D_0, we express H in terms of the plane-wave or Rayleigh series

$$H(x, y) = \sum_{p=-\infty}^{\infty} [\exp(-i\chi_0(y - h/2))\delta_{p,0} + R_p \exp(i\chi_p(y - h/2))]e_p(x), \tag{2}$$

where

$$e_p(x) = \exp(i\alpha_p x)/\sqrt{d}, \tag{3}$$

$$\alpha_p = \alpha_0 + 2\pi p/d, \tag{4}$$

$$\left.\begin{aligned}\alpha_0 = k_0 \sin\phi \\ \chi_0 = k_0 \cos\phi\end{aligned}\right\} \tag{5}$$

$$\chi_p = \begin{cases} \sqrt{(k_0^2 - \alpha_p^2)} & \text{for} \quad |\alpha_p| \le k_0 \\ i\sqrt{(\alpha_p^2 - k_0^2)} & \text{for} \quad |\alpha_p| > k_0 \end{cases} \tag{6}$$

and $\delta_{p,0}$ is the Kronecker delta symbol. Similarly, in region D_3,

$$H(x, y) = \sum_{p=-\infty}^{\infty} T_p \exp(-i\eta_p(y + h/2))e_p(x), \tag{7}$$

where

$$\eta_p = \sqrt{(k_3^2 - \alpha_p^2)}, \tag{8}$$

the imaginary part of η_p, $\mathrm{Im}(\eta_p)$, being chosen to be non-negative. The sets $\{R_p, T_p | p = 0, \pm 1, \pm 2, \ldots\}$ are the sets of reflection and transmission (absorption) plane wave coefficients.

In the grating $(D_1 \cup D_2)$ we expand the field in an eigenfunction series, each term of which obeys the appropriate wave equation and the necessary continuity and pseudo-periodicity conditions stated in the caption of figure 1.

2.2. *The eigenvalue problem*

We proceed in the manner of § 2.4 of [1] to solve the wave equation within the grating region:

$$\frac{\partial}{\partial x}\left[\frac{1}{k^2}\frac{\partial H}{\partial x}\right] + \frac{\partial}{\partial y}\left[\frac{1}{k^2}\frac{\partial H}{\partial y}\right] + H = 0, \tag{9}$$

where

$$k = k_0 r(x), \tag{10}$$

and $r(x)$ is a periodic function defined on its period $[0, d]$ by

$$r(x) = \begin{cases} r_1 & \text{for} \quad 0 < x < c \\ r_2 & \text{for} \quad c < x < d. \end{cases} \tag{11}$$

The solution is written in the separable form

$$H(x, y) = u(x) v(y), \tag{12}$$

and we derive

$$k^2\left[\frac{1}{k^2} u'\right]' + \zeta^2 S(x - c) u = -\beta^2 u, \tag{13}$$

$$v'' + \mu^2 v = 0, \tag{14}$$

where the prime denotes differentiation,

$$\mu^2 = k_1^2 - \beta^2, \tag{15}$$

$$\zeta^2 = k_2^2 - k_1^2, \tag{16}$$

$$\left.\begin{aligned} k_1 &= k_0 r_1, \\ k_2 &= k_0 r_2, \end{aligned}\right\} \tag{17}$$

and

$$S(x - c) = \begin{cases} 0 & \text{for} \quad x < c \\ 1 & \text{for} \quad x > c. \end{cases} \tag{18}$$

The solution of the eigenvalue equation (13) subject to the boundary conditions (31) and (32) of [1] is of the form

$$u(x) = \theta(x) + \omega \psi(x), \tag{19}$$

where $\theta(x)$ and $\psi(x)$ are two linearly independent solutions of (13), given in equations (33) and (34) of [1], and

$$\omega = \frac{\tau - \theta(d^-)}{\psi(d^-)}, \tag{20}$$

subject to the non-linear eigenvalue equation

$$\cos(\beta c)\cos(\gamma g) - \frac{1}{2}\left(\frac{r_2^2 \beta}{r_1^2 \gamma} + \frac{r_1^2 \gamma}{r_2^2 \beta}\right)\sin(\beta c)\sin(\gamma g) = \cos(\alpha_0 d), \tag{21}$$

in which

$$\gamma^2 = \beta^2 + \zeta^2. \tag{22}$$

In (20), τ is a period phase-shift associated with the incident wave:

$$\tau = \exp(i\alpha_0 d). \tag{23}$$

2.3. *The adjoint problem*

Equation (13) may be rewritten in the form

$$Lu = -\beta^2 u, \tag{24}$$

where the differential operator L is given by

$$L = k^2 \frac{d}{dx}\left(\frac{1}{k^2}\frac{d}{dx}\right) + \zeta^2 S(x-c). \tag{25}$$

The refractive indices r_1 and r_2 being complex, ζ^2 is now complex, and so the operator L loses the self-adjoint property demonstrated in [1]. Consequently, its eigenfunctions $\{u\}$ no longer form an orthogonal set. However, in order for the solution of the field equations to proceed by the method of moments as in [1], it is essential to have a set of functions, say $\{u^+\}$, orthogonal to the $\{u\}$. To obtain the $\{u^+\}$ we introduce the operator

$$L^+ = \bar{k}^2 \frac{d}{dx}\left(\frac{1}{\bar{k}^2}\frac{d}{dx}\right) + \bar{\zeta}^2 S(x-c) \tag{26}$$

(where the bars denote complex conjugation). We then consider the eigenvalue problem

$$L^+ u^+ = -(\beta^+)^2 u^+, \tag{27}$$

subject to the constraint that u^+ and $\left(\dfrac{du^+}{dx}\right)/\bar{k}^2$ are continuous at $x=c$, d and pseudo-periodic between $x=0$ and $x=d$.

We will now show that L^+ is the adjoint of L, with respect to the inner product of two functions $f(x)$ and $g(x)$,

$$\langle f, g\rangle = \int_0^d \frac{1}{k^2(x)} \bar{f}(x) g(x)\, dx. \tag{28}$$

The choice of the weight function $(1/k^2(x))$ in (28) is a natural consequence of the forms (25) and (26) of the differential operators L and L^+.

Consider the quantity

$$Q_1 = \langle u^+, Lu\rangle - \langle L^+u^+, u\rangle$$
$$= \int_0^d \frac{1}{k^2}\left\{\bar{u}^+\left[k^2\left(\frac{1}{k^2}u'\right)' + \zeta^2 S(x-c)u\right] - u\left[k^2\left(\frac{1}{k^2}\bar{u}^{+\prime}\right)' + \zeta^2 S(x-c)\bar{u}^+\right]\right\} dx.$$

This simplifies to

$$Q_1 = \int_0^d \left[\bar{u}^+\left(\frac{1}{k^2}u'\right) - u\left(\frac{1}{k^2}\bar{u}^{+\prime}\right)\right]' dx,$$

i.e.

$$Q_1 = 0$$

because of the pseudo-periodicity conditions satisfied by u and u^+. As asserted, L^+ is the adjoint of L:

$$\langle u^+, Lu\rangle = \langle L^+u^+, u\rangle. \tag{29}$$

2.4. *The relation between the eigenvalue problem and the adjoint problem*

In a manner similar to that outlined in § 2.2, and in § 2.4 of [1], we proceed to solve equation (27). We write

$$u^+(x) = \theta^+(x) + \omega^+\psi^+(x), \tag{30}$$

where $\theta^+(x)$ and $\psi^+(x)$ are two linearly independent solutions of (27) obeying the boundary conditions at $x=c$ specified in § 2.3 and the initial conditions

$$\left.\begin{array}{ll} \theta^+(0)=1, & \theta^{+\prime}(0)=0 \\ \psi^+(0)=0, & \psi^{+\prime}(0)=1. \end{array}\right\} \tag{31}$$

The explicit forms of these functions are

$$\theta^+(x) = \begin{cases} \cos(\beta^+ x), \quad 0<x<c, \\ \cos(\beta^+ c)\cos(\gamma^+(x-c)) - \left(\dfrac{\bar{r}_2}{\bar{r}_1}\right)^2 \dfrac{\beta^+}{\gamma^+}\sin(\beta^+ c)\sin(\gamma^+(x-c)) \quad c<x<d; \end{cases} \tag{32}$$

$$\psi^+(x) = \begin{cases} \dfrac{1}{\beta^+}\sin(\beta^+ x), \quad 0<x<c, \\ \dfrac{1}{\beta^+}\left[\sin(\beta^+ c)\cos(\gamma^+(x-c)) + \left(\dfrac{\bar{r}_2}{\bar{r}_1}\right)^2 \dfrac{\beta^+}{\gamma^+} \right. \\ \left. \times\cos(\beta^+ c)\sin(\gamma^+(x-c))\right], \quad c<x<d, \end{cases} \tag{33}$$

where

$$(\gamma^+)^2 = (\beta^+)^2 + (\bar{\zeta})^2. \tag{34}$$

The constant ω^+ in (29) is determined by the pseudo-periodicity constraints and is

$$\omega^+ = \frac{\tau - \theta^+(d^-)}{\psi^+(d^-)}. \tag{35}$$

The same constraints also yield the non-linear eigenvalue equation for the adjoint problem:

$$\cos(\bar{\beta}^{+}c)\cos(\bar{\gamma}^{+}g)-\frac{1}{2}\left(\frac{r_2^2}{r_1^2}\frac{\bar{\beta}^{+}}{\bar{\gamma}^{+}}+\frac{r_1^2}{r_2^2}\frac{\bar{\gamma}^{+}}{\bar{\beta}^{+}}\right)\sin(\bar{\beta}^{+}c)\sin(\bar{\gamma}^{+}g)=\cos(\alpha_0 d), \quad (36)$$

with

$$(\bar{\gamma}^{+})^2=(\bar{\beta}^{+})^2+(\zeta)^2. \quad (37)$$

Comparison of (36) and (37) with (21) and (22) reveals that

$$\beta^{+}=\bar{\beta}, \quad (38)$$

$$\gamma^{+}=\bar{\gamma}, \quad (39)$$

$$\theta^{+}(x)=\bar{\theta}(x) \quad (40)$$

and

$$\psi^{+}(x)=\bar{\psi}(x). \quad (41)$$

2.5. *Orthogonality and completeness*

We saw in [1] that for the lossless lamellar grating, there exists a countably infinite set of solutions $\beta_n^2 (n=1,2,3,\dots)$ of the eigenvalue equations (21) and (22). It may be shown that, as the imaginary part of a refractive index $r_i (i=1,2)$ is increased from zero, the eigenvalues β_n^2 move continuously away from their positions on the real axis into the complex plane (see figure 2), and that all the complex eigenvalues may be found by following the paths illustrated, starting from real eigenvalues. As the real part of the eigenvalues β_n^2 approaches infinity (that is, as $n\to\infty$) the complex eigenvalues approach the real eigenvalues of the simpler problem, consisting of the differential equation (13), with $\zeta^2=0$, and the boundary conditions (31) and (32) of [1]. Further, the eigenfunctions $\{u_n\}$ approach the eigenfunctions of this simpler problem.

Let us now consider the question of orthogonality of the eigenfunctions $\{u_n\}$ with their adjoint functions $\{u_n^+\}$. Let u_n be an eigenfunction of L corresponding to an eigenvalue β_n^2, as in (24), and let u_m^+ be an eigenfunction of L^+ corresponding to an eigenvalue $(\beta_m^+)^2$, as in (27). From (29), we see that

$$\langle L^+u_m^+, u_n\rangle=\langle u_m^+, Lu_n\rangle$$

or

$$-\bar{\beta}_m^{+\,2}\langle u_m^+, u_n\rangle=-\beta_n^2\langle u_m^+, u_n\rangle,$$

which (using (38)) implies that

$$(\beta_m^2-\beta_n^2)\langle u_m^+, u_n\rangle=0. \quad (42)$$

In other words, the sets of eigenfunctions $\{u_n^+\}$ and $\{u_n\}$ are orthogonal with respect to the inner product defined in (28), and may be normalized by setting

$$\langle u_n^+, u_n\rangle=1.$$

It may be shown, using arguments similar to those in [2, Chap. 12], that the eigenfunctions $\{u_n\}$ are complete in the sense that any continuous and piecewise

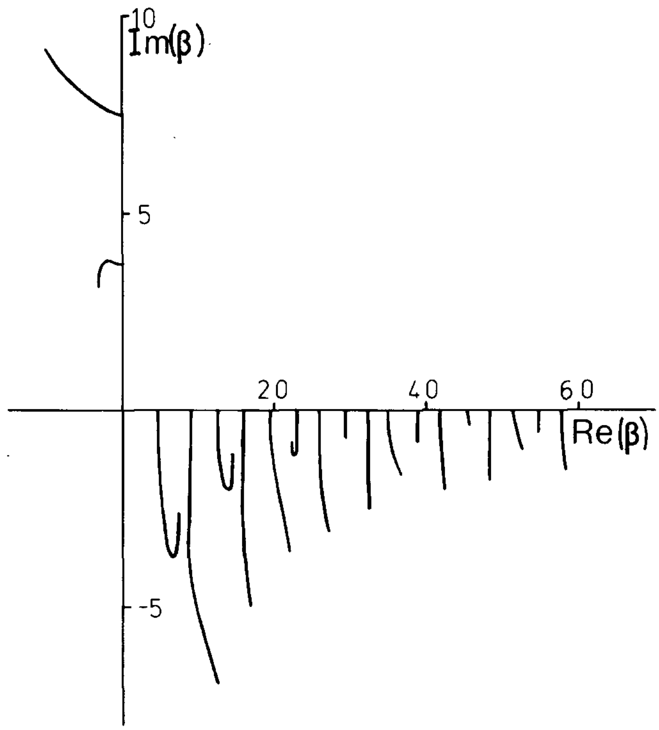

Figure 2. Evolution of the first 20 complex eigenvalues β_p with increasing imaginary part of r_2 from 0·0 to 1·0, for the S polarization diffraction problem of table 1.

differentiable function $f(x)$, satisfying the boundary conditions (31) and (32) of [1], may be expanded as

$$f(x)=\sum_{n=0}^{\infty} a_n u_n(x),$$

where

$$a_n=\langle u_n^+, f\rangle.$$

Thus it follows that the general solution for the total magnetic field H can be expressed in the form

$$H(x,y)=\sum_n (a_n \sin(\mu_n y)+b_n \cos(\mu_n y))u_n(x) \qquad (43)$$

which will now be matched to the plane wave solution at $y=\pm h/2$.

2.6. *Method of moments*

With the form of the fields now prescribed for all regions, we can proceed to solve the diffraction problem using the method of moments. The continuity of the magnetic field across the interface $y=h/2$ is given by

$$\sum_p (R_p+\delta_{p0})e_p(x)=\sum_m (a_m^*+b_m^*)u_m(x) \quad \text{for} \quad 0\le x\le d, \qquad (44)$$

where

$$a_m^* = a_m \sin(\mu_m h/2),$$

$$b_m^* = b_m \cos(\mu_m h/2).$$

We multiply the left- and right-hand sides of (44) by

$$\bar{u}_n^+(x)/k^2(x),$$

and integrate with respect to x over a period, to obtain

$$a_n^* + b_n^* = \sum_p (R_p + \delta_{p0})\bar{K}_{pn} \quad \text{for} \quad n = 1, 2, \ldots, \tag{45}$$

where

$$K_{pn} = \int_0^d \frac{1}{\bar{k}^2(x)} \bar{e}_p(x) u_n^+(x)\, dx. \tag{46}$$

The system of equations (45) may be more concisely written as

$$a^* + b^* = K^{\mathscr{H}}(R + F), \tag{47}$$

where $a^* = [a_n^*]$, $b^* = [b_n^*]$, $K = [K_{pn}]$, $R = [R_p]$, F is a vector whose entries are $F_p = \delta_{p0}$, and the superscript $\mathscr{H}$ is used to denote the hermitian conjugate of a matrix. Similarly, the continuity of H at $y = -h/2$ gives

$$-a^* + b^* = K^{\mathscr{H}} T, \tag{48}$$

where $T = [T_p]$.

Next, consider the boundary condition

$$\frac{1}{k^2(x)} \frac{\partial H}{\partial y}\bigg|_{y = h/2-} = \frac{1}{k_0^2} \frac{\partial H}{\partial y}\bigg|_{y = h/2+}. \tag{49}$$

This is

$$\frac{1}{k_0^2} \sum_p i\chi_p (R_p - \delta_{p0}) e_p(x) = \sum_m (D_{1m} a_m^* + D_{2m} b_m^*) \frac{u_m(x)}{k^2(x)} \quad \text{for} \quad 0 \le x \le d, \tag{50}$$

where

$$\left.\begin{aligned} D_{1m} &= \mu_m \cot(\mu_m h/2) \\ D_{2m} &= -\mu_m \tan(\mu_m h/2). \end{aligned}\right\} \tag{51}$$

We multiply both sides of (50) by $\bar{e}_q(x)$ (for some integer value q) and integrate over a period to obtain

$$i\chi_q (R_q - \delta_{q0}) = k_0^2 \sum_m (D_{1m} a_m^* + D_{2m} b_m^*) J_{qm} \quad \text{for} \quad q = 0, \pm 1, \pm 2, \ldots, \tag{52}$$

where

$$J_{qm} = \int_0^d \frac{1}{k^2(x)} \bar{e}_q(x) u_m(x)\, dx. \tag{53}$$

Equations (52) are, in matrix form,

$$R = F - i\chi^{-1} J(D_1 a^* + D_2 b^*), \tag{54}$$

where

$$\chi = \operatorname{diag}(\chi_p/k_0^2),$$
$$D_1 = \operatorname{diag}(D_{1m}),$$
$$D_2 = \operatorname{diag}(D_{2m}).$$

Similarly, at the interface $y = -h/2$ we find that

$$T = i\eta^{-1} J(D_1 a^* - D_2 b^*) \tag{55}$$

where $\eta = \operatorname{diag}(\eta_p/k_3^2)$.

We now substitute (54) and (55) into (47) and (48) and arrive at a coupled pair of linear equations in the a_m^* and the b_m^*:

$$\begin{bmatrix} I + iK^{\#}\chi^{-1}JD_1 & I + iK^{\#}\chi^{-1}JD_2 \\ -(I + iK^{\#}\eta^{-1}JD_1) & I + iK^{\#}\eta^{-1}JD_2 \end{bmatrix} \begin{bmatrix} a^* \\ b^* \end{bmatrix} = 2\begin{bmatrix} K^{\#}F \\ 0 \end{bmatrix} \tag{56}$$

where I denotes the identity matrix of appropriate dimension. The infinite system of equations (56) is truncated and solved numerically by a standard elimination technique. The form of (56) gives rise to a matrix which is numerically stable under inversion. Once the a^* and b^* are known from (56), they can be substituted into (54) and (55) to yield the reflection and transmission coefficients $\{R_p, T_p | p = 0, \pm 1, \pm 2, \ldots\}$.

2.7. *The energy balance*

As stated (without proof) in [1], the criterion of energy conservation is not available as a test on the accuracy of numerical results for the dielectric lamellar grating, since it is analytically satisfied (independently of truncation errors) by the modal formalism. We will now show that this criterion can furnish information concerning truncation errors in calculations for the lossy lamellar grating. In considering this question we must look at both the absorption of energy within various regions and the flux of energy across various surfaces.

The component of the flux of energy perpendicular to the surface of the grating is the y component S_y of the Poynting vector, where

$$S_y = \frac{1}{2\omega\varepsilon_0} \operatorname{Im}\left(\bar{H} \frac{1}{\nu^2} \frac{\partial H}{\partial y} \right), \tag{57}$$

ν denoting the complex refractive index of the medium in question:

$$\nu(x, y) = \begin{cases} 1 & \text{for} \quad y > h/2 \\ r(x) & \text{for} \quad -h/2 < y < h/2 \\ r_3 & \text{for} \quad y < -h/2, \end{cases}$$

for all values of x. We are thus led to consider the following integral quantity for various ranges of y:

$$P(y) = \int_0^d \left(\bar{H} \frac{1}{\nu^2} \frac{\partial H}{\partial y} - H \frac{1}{\bar{\nu}^2} \frac{\partial \bar{H}}{\partial y} \right) dx. \tag{58}$$

In free space ($y>h/2$), $P(y)$ is independent of y and has the value

$$P(y)=2i[\sum_p \mathrm{Re}(\chi_p)|R_p|^2-\chi_0]. \tag{59}$$

Note that $\mathrm{Re}(\chi_p)$ is non-zero only for a finite set of integer values of p (the propagating orders in free space).

In the dissipative grating region ($-h/2<y<h/2$), $P(y)$ ceases to be independent of y, and so we consider

$$\Delta P=P[(h/2)^-]-P[(-h/2)^+] \tag{60}$$

and

$$Q_2=\iint_{D_1\cup D_2}\mathrm{div}\left[\bar{H}\frac{1}{r^2(x)}\,\mathrm{grad}\,H-H\frac{1}{\bar{r}^2(x)}\,\mathrm{grad}\,\bar{H}\right]dA, \tag{61}$$

the area integral being over the grating region $0\le x\le d$, $-h/2\le y\le h/2$. ΔP and Q_2 are identical physically, as is shown by a simple application of Green's theorem in conjunction with the definition (59) of P. However, as we shall now show, they are also analytically identical, their equality not being affected by the errors which arise in fields when the infinite modal series (9) is truncated to a finite sum.

Let us now consider the ohmic loss Q_2 within the grating. Using (9) in (61), we obtain

$$\begin{aligned}Q_2&=\iint_{D_1\cup D_2}\left[\frac{1}{r^2(x)}-\frac{1}{\bar{r}^2(x)}\right]\mathrm{grad}\,H\cdot\mathrm{grad}\,\bar{H}\,dA\\
&=\sum_{mn}\left\{\int_{-h/2}^{h/2}(\bar{a}_m\sin\bar{\mu}_m y+\bar{b}_m\cos\bar{\mu}_m y)(a_n\sin\mu_n y+b_n\cos\mu_n y)\,dy\right.\\
&\qquad\times\int_0^d \bar{u}_m'(x)u_n'(x)\left[\frac{1}{r^2(x)}-\frac{1}{\bar{r}^2(x)}\right]dx\\
&\quad+\bar{\mu}_m\mu_n\int_{-h/2}^{h/2}(\bar{a}_m\cos\bar{\mu}_m y-\bar{b}_m\sin\bar{\mu}_m y)(a_n\cos\mu_n y-b_n\sin\mu_n y)\,dy\\
&\qquad\left.\times\int_0^d \bar{u}_m(x)u_n(x)\left[\frac{1}{r^2(x)}-\frac{1}{\bar{r}^2(x)}\right]dx.\right\}\end{aligned} \tag{62}$$

The first x integral occurring in (62) may be simplified using integration by parts. We consider

$$\begin{aligned}\int_0^d\frac{u_n'(x)}{r^2(x)}\bar{u}_m'(x)\,dx&=-\int_0^d\bar{u}_m(x)\left[\frac{u_n'(x)}{r^2(x)}\right]'dx\quad\text{(by pseudo-periodicity)}\\
&=\int_0^d\bar{u}_m(x)u_n(x)\left[k_0^2-\frac{\mu_n^2}{r^2(x)}\right]dx\quad\text{(from 13).}\end{aligned}$$

Hence,

$$\int_0^d\bar{u}_m'(x)u_n'(x)\left[\frac{1}{r^2(x)}-\frac{1}{\bar{r}^2(x)}\right]dx=\int_0^d\bar{u}_m(x)u_n(x)\left[\frac{\bar{\mu}_m^2}{\bar{r}^2(x)}-\frac{\mu_n^2}{r^2(x)}\right]dx \tag{63}$$

On substituting (63) into (62) and performing the y integrations, we arrive at

$$Q_2=2\sum_{mn}\left[(D_{1n}\bar{a}_m^*a_n^*+D_{2n}\bar{b}_m^*b_n^*)\int_0^d\frac{1}{r^2(x)}\bar{u}_m(x)u_n(x)\,dx - (\bar{D}_{1m}\bar{a}_m^*a_n^*+\bar{D}_{2m}\bar{b}_m^*b_n^*)\int_0^d\frac{1}{\bar{r}^2(x)}\bar{u}_m(x)u_n(x)\,dx\right]. \tag{64}$$

We now turn to expression (60). Using

$$H(x,y=\pm h/2)=\sum_m(\pm a_m^*+b_m^*)u_m(x)$$

and

$$\frac{\partial H}{\partial y}(x,y=\pm h/2)=\sum_n(D_{1n}a_n^*\pm D_{2n}b_n^*)u_n(x),$$

elementary manipulations enable us to derive

$$\Delta P=Q_2. \tag{65}$$

At no stage during this demonstration has it been necessary to specify the range of the summation indices m and n. In other words, (65) holds whether the quantities ΔP and Q_2 are evaluated for the physical fields or their truncated representations.

The situation is different when we compare the quantity $P(y)$ for $y=h/2^+$ and for $y=h/2^-$. Equation (59) can be written in the form

$$P(h/2^+)=2i\,\mathrm{Im}\,[\sum_p i\chi_p(R_p-\delta_{p0})(\bar{R}_p+\delta_{p0})]. \tag{66}$$

In (66) and in what follows, all summations without explicit indication to the contrary will run over the truncated set of values occurring in any computer implementation of the theory. Now, from (52)

$$P(h/2^+)=2i\,\mathrm{Im}\,[k_0^2\sum_n(D_{1n}a_n^*+D_2b_n^*)\sum_p(\bar{R}_p+\delta_{p0})J_{pn}]. \tag{67}$$

Similarly, using (45),

$$P(h/2^-)=2i\,\mathrm{Im}\left[\sum_n k_0^2(D_{1n}a_n^*+D_{2n}b_n^*)\sum_m(\bar{a}_m^*+\bar{b}_m^*)\int_0^d\frac{1}{k^2(x)}\bar{u}_m(x)u_n(x)\,dx\right]$$

$$=2i\,\mathrm{Im}\left[\sum_n k_0^2(D_{1n}a_n^*+D_{2n}b_n^*)\sum_{mp}(\bar{R}_p+\delta_{p0})K_{pm}\int_0^d\frac{1}{k^2(x)}\bar{u}_m(x)u_n(x)\,dx\right] \tag{68}$$

For (67) and (68) to be identical we require that

$$J_{pn}=\sum_m K_{pm}\int_0^d\frac{1}{k^2(x)}\,\bar{u}_m(x)u_n(x)\,dx. \tag{69}$$

Consider the series expansion

$$e_p(x)=\sum_{m=1}^{\infty}c_m u_m(x), \tag{70}$$

which is valid as the $\{u_m(x)|m=1,2,\ldots\}$ form a complete set on $[0, d]$. Of course, any subset of the full set of the $\{u_m\}$ is not complete and so a truncated sum in (70) would lead to numerical errors. On multiplying throughout (70) by $\bar{u}_l^+(x)/k^2(x)$ and integrating over $[0, d]$, we obtain

$$c_l = \bar{K}_{pl}$$

from the previously elaborated orthonormality properties. Thus

$$J_{pn} = \int_0^d \frac{1}{k^2(x)} \bar{e}_p(x) u_n(x)\, dx = \sum_{m=1}^{\infty} K_{pl} \int_0^d \frac{1}{k^2(x)} \bar{u}_m(x) u_n(x)\, dx. \tag{71}$$

Comparing (69) and (71) we deduce that the quantity $[P(h/2^+) - P(h/2^-)]$ can be used in the estimation of truncation errors in numerical calculations. The same remark, of course, applies at the lower grating surface $y = -h/2$.

2.8. *The P polarization diffraction problem*

In this section we shall briefly discuss the relevant differences in the form of the P polarization problem (brought about by the different forms taken by the boundary conditions). Here we concentrate our attention mainly on the eigenvalue problem, drawing on the material in § 2.2 of this paper and § 2.2 of [1] for the sake of brevity.

In the region $D_1 \cup D_2$ we must solve the Helmoltz equation

$$\frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + k^2(x)E = 0,$$

where both E and $\partial E/\partial x$ are continuous at $x = c$ and pseudo-periodic between $x = 0$ and $x = d$.

By writing E in separable form as

$$E(x, y) = u(x)v(y),$$

we arrive at the operator equation derived in [1],

$$Lu = -\beta^2 u, \tag{72}$$

where

$$L = \frac{d^2}{dx^2} + \zeta^2 S(x - c). \tag{73}$$

The solution of equation (72), obeying the above boundary conditions, has the form

$$u(x) = \theta(x) + \omega\psi(x)$$

where

$$\omega = \frac{\tau - \theta(d)}{\psi(d)}$$

and $\theta(x)$ and $\psi(x)$ are defined in equations (12)–(13) of [1]. The eigenvalues $(-\beta^2)$ obey the non-linear equation (18) of [1],

$$\cos(\beta c)\cos(\gamma g) \frac{1}{2}\left(\frac{\beta}{\gamma} + \frac{\gamma}{\beta}\right) \sin(\beta c)\sin(\gamma g) = \cos(\alpha_0 d), \tag{74}$$

where γ and β are linked by equation (22).

Following the discussion of § 2.3 we introduce the operator equation

$$L^{+}u^{+}=-(\beta^{+})^{2}u^{+} \tag{75}$$

with

$$L^{+}=\frac{d^{2}}{dx^{2}}+\bar{\zeta}^{2}S(x-c)$$

subject to the constraints that u^{+} and its normal derivative are continuous at $x=c$ and pseudo-periodic between $x=0$ and $x=d$. Some simple manipulation reveals that L^{+} is the adjoint of L with respect to the inner product

$$\langle f,g\rangle=\int_{0}^{d}\bar{f}(x)g(x)\,dx. \tag{76}$$

In a manner analogous to that used in § 2.4, we may demonstrate that the eigenfunctions $\{u^{+}(x)\}$ of equation (75) obey the relation

$$\bar{u}^{+}(x)=\theta(x)+\bar{\omega}^{+}\psi(x),$$

where

$$\bar{\omega}^{+}=\frac{\bar{\tau}-\theta(d)}{\psi(d)}.$$

Here we note that $\beta^{+}=\bar{\beta}$ and $\gamma^{+}=\bar{\gamma}$.

The orthogonality of the set $\{u\}$ with the set $\{u^{+}\}$ with respect to the inner product (76) may also be easily verified. The completeness of the set of eigenfunctions $\{u_{n}(x)\}$ may be established along the same lines as the discussion in sections § 2·5 and § 2.2.2 (iii) of [1], and thus we may expand E in $D_{1}\cup D_{2}$ in the eigenfunction series

$$E(x,y)=\sum_{n}[a_{n}\sin(\mu_{n}y)+b_{n}\cos(\mu_{n}y)]u_{n}(x), \tag{77}$$

where

$$\mu^{2}=k_{1}^{2}-\beta^{2}=k_{2}^{2}-\gamma^{2}.$$

For later convenience, we choose to make the $\{u_{n}\}$ and $\{u_{n}^{+}\}$ orthonormal bases with respect to (76).

The solution of the diffraction problem proceeds according to the analysis of § 2.6 with the following modifications:

$$\chi=\mathrm{diag}\,(\chi_{p})$$

$$\eta=\mathrm{diag}\,(\eta_{p})$$

$$J_{qm}=\int_{0}^{d}\bar{e}_{p}(x)u_{m}(x)\,dx$$

and

$$K_{pn}=\int_{0}^{d}\bar{e}_{q}(x)u_{n}^{+}(x)\,dx.$$

Similar conclusions concerning the energy balance criterion (§ 2.7) can be drawn for this polarization.

2.9. *Numerical solution of the eigenvalue equation*

Any numerical implementation of the above formalism must involve the solution of the complex, non-linear equations (21) and (74) for the two fundamental polarization cases. The problem of solving such equations poses substantial numerical difficulties, as it is essential to find a complete set of roots with modulus smaller than a specified tolerance. The use of an incomplete set of eigenvalues and modes leads to intolerable numerical errors.

The numerical method used here is based on a generalization [3] to complex numbers of the standard numerical *regula falsi* technique [4]. It has proved adequate in the case where the modulus of the complex refractive index is not too large. However, when this modulus does become large, the computation times become excessive and in some cases the algorithm does not find a complete set of eigenvalues. Evidently an alternative algorithm will have to be devised in this case. Investigations into this problem are in progress.

3. Numerical verification of the formalism

The formalism has been implemented numerically and the program results have been tested using various criteria. Firstly, the numerical results for lossless structures have been shown to agree with those of the formalism presented in [1]. Note that the lossless structure encompasses both the case where refractive indices are purely imaginary as well as purely real. Secondly, we have used the criteria of conservation of energy and the reciprocity theorem to confirm the numerical results. A typical result of such a verification is given in table 1, in which the following notations are adopted for brevity:

$$\Phi_p^R = (\rho_p^R, \arg(R_p)), \tag{78}$$

where ρ_p^R is the efficiency [1] of the pth reflected order, and $\arg(R_p)$ is the phase of the pth reflected order; E.R. is the total reflected energy, E.T. the total transmitted energy, and E.D. $= 1 -$ E.R. $-$ E.T.

From table 1 it can be seen that the numerical results are in excellent accord with the reciprocity theorem, whether the returned order be reflected or transmitted. The agreement is slightly less satisfactory for the S polarization results than for the P polarization results. This feature is also evident in the criterion of conservation of energy (as can be seen by comparing E.D. with Q for each problem). It is a general situation in diffraction grating theory that in corresponding S and P polarization calculations, the results of numerical errors are more evident for the former than for the latter.

One characteristic of the present formalism is that the convergence of the modal expansions it employs grows more rapid as the ratio of groove depth to period becomes large. This characteristic has been exploited previously in discussions of inductive grids [5, 6], and is well exemplified by the modal amplitudes given (for a relatively extreme case) in table 2. The formalism is here shown to provide results of good accuracy for a grating with a ratio of groove depth to period of two hundred. When a similar calculation was attempted with the most powerful existing integral equation formalism [7], adequate accuracy was achievable only for values of this ratio substantially smaller than five.

Note that the good accuracy of the numerical results in table 2 is obtained with a very small number of modes used in the calculations. In fact, the accuracy of these

Table 1. Reciprocity results.

Grating parameters: $d = 1{\cdot}0000\,\mu m$, $c = 0{\cdot}4001\,\mu m$, $h = 0{\cdot}1000\,\mu m$,
$r_1 = 1{\cdot}0$, $r_2 = 1{\cdot}5 + i\,1{\cdot}0$, $r_3 = 1{\cdot}0$.
Wavelength: $\lambda = 0{\cdot}80\,\mu m$,
Incidence parameters: Problem 1, $\phi = 11{\cdot}50°$,
Problem 2, $\phi = 36{\cdot}91518°$,
Problem 3, $\phi = -87{\cdot}96276°$.
Method parameters: Number of modes = 20,
Number of Rayleigh orders = 51.

Problem	Quantity	P polarization	S polarization	A.D.†
1	Φ^R_{-1}*	$(2{\cdot}8529 \times 10^{-2}, 92{\cdot}7502°)$	$(1{\cdot}6772 \times 10^{-2}, -78{\cdot}6682°)$	$-36{\cdot}915°$
	Φ^T_{-1}*	$(3{\cdot}8574 \times 10^{-2}, 96{\cdot}3899°)$	$(2{\cdot}1372 \times 10^{-2}, 117{\cdot}5688°)$	
	Φ^R_0	$(6{\cdot}2128 \times 10^{-2}, -139{\cdot}1595°)$	$(9{\cdot}5755 \times 10^{-2}, 32{\cdot}6897°)$	$11{\cdot}500°$
	Φ^T_0	$(4{\cdot}6913 \times 10^{-1}, 44{\cdot}8301°)$	$(3{\cdot}9939 \times 10^{-1}, 50{\cdot}8365°)$	
	Φ^R_1**	$(4{\cdot}6011 \times 10^{-3}, -61{\cdot}1899°)$	$(1{\cdot}2779 \times 10^{-3}, 120{\cdot}5751°)$	$87{\cdot}963°$
	Φ^T_1**	$(5{\cdot}4894 \times 10^{-3}, -59{\cdot}6281°)$	$(3{\cdot}6226 \times 10^{-3}, -46{\cdot}2306°)$	
	E.R.	0·09526	0·11381	
	E.T.	0·51319	0·42438	
	E.D.	0·39155	0·46181	
	Q_2	0·39156	0·46047	
2	Φ^R_{-1}*	$(2{\cdot}8529 \times 10^{-2}, 92{\cdot}7501°)$	$(1{\cdot}6772 \times 10^{-2}, -78{\cdot}6671°)$	$-11{\cdot}500°$
	Φ^T_{-1}*	$(3{\cdot}8574 \times 10^{-2}, 96{\cdot}3899°)$	$(2{\cdot}1372 \times 10^{-2}, 117{\cdot}5694°)$	
	E.R.	0·16745	0·06755	
	E.T.	0·37027	0·43902	
	E.D.	0·46229	0·49343	
	Q_2	0·46229	0·49184	
3	Φ^R_1**	$(4{\cdot}6012 \times 10^{-3}, -61{\cdot}1899°)$	$(1{\cdot}2800 \times 10^{-3}, 120{\cdot}5788°)$	$-11{\cdot}500°$
	Φ^T_1**	$(5{\cdot}4894 \times 10^{-3}, -59{\cdot}6281°)$	$(3{\cdot}6223 \times 10^{-3}, -46{\cdot}2321°)$	
	E.R.	0·89431	0·82541	
	E.T.	0·00993	0·02269	
	E.D.	0·09575	0·15190	
	Q_2	0·09575	0·15151	

† The angle of diffraction in air of the order in question.
Quantities equal according to the reciprocity theorem are identified by * and **.

results has been seen to be not significantly reduced if only the first mode is used in field expansions inside the grating groove region.

4. Conclusions

We have presented a modal formalism describing the diffraction properties of the finitely conducting lamellar grating. The finite conductivity of the structure makes it necessary to consider not only the boundary value problem associated with the physical structure, but also that associated with the adjoint structure. Despite this complicating factor, the resultant formalism lacks none of the elegance of our previous formalism for the lossless lamellar grating.

The numerical implementation of the formalism has been well verified in the case of gratings whose complex refractive index is not too large. Further work on

Table 2. Results for a grating with large h/d.
Grating parameters: $d = 0{\cdot}0040\,\mu$m, $c = 0{\cdot}0024\,\mu$m, $h = 0{\cdot}8000\,\mu$m, $h/d = 200$, $r_1 = 1{\cdot}0$, $r_2 = 2{\cdot}7 + i\,0{\cdot}5$, $r_3 = 2{\cdot}7 + i\,0{\cdot}5$.
Incidence parameters: $\lambda = 0{\cdot}80\,\mu$m, $\phi = 0°$.
Method parameters: Number of modes = 3,
Number of Rayleigh orders = 31.

Quantity	P polarization	S polarization
$\lvert a_1^*\rvert$	$3{\cdot}1734 \times 10^{-1}$	$6{\cdot}5833 \times 10^{-1}$
$\lvert b_1^*\rvert$	$3{\cdot}7891 \times 10^{-1}$	$6{\cdot}4689 \times 10^{-1}$
$\lvert a_2^*\rvert$	$1{\cdot}1223 \times 10^{-5}$	$3{\cdot}5221 \times 10^{-9}$
$\lvert b_2^*\rvert$	$1{\cdot}3451 \times 10^{-5}$	$4{\cdot}2734 \times 10^{-9}$
$\lvert a_3^*\rvert$	$5{\cdot}0528 \times 10^{-9}$	$1{\cdot}0174 \times 10^{-3}$
$\lvert b_3^*\rvert$	$6{\cdot}0571 \times 10^{-9}$	$1{\cdot}0678 \times 10^{-3}$
E.R.	0·10043	0·04284
E.T.	0·02295	0·71290
E.D.	0·87663	0·24426
Q_2	0·87663	0·24416

alternative techniques for the location of eigenvalues in the complex plane should enable this restriction to be removed.

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Une théorie modale rigoureuse décrivant les propriétés de diffraction d'un réseau lamellaire à conductivité finie est présentée. La méthode utilisée est la généralisation aux structures à pertes d'un formalisme précédent pour un réseau lamellaire diélectrique. On donne des exemples de résultats de la méthode démontrant sa précision et son aptitude à résoudre des problèmes difficiles à traiter par les formalismes largement utilisés d'équations intégrales de la théorie des réseaux de diffraction.

Es wird eine streng modale Theorie zur Beschreibung der Beugungseigenschaften eines endlich leitenden Lamellengitters präsentiert. Das benutzte Verfahren ist die Verallgemeinerung eines früher für das dielektrische Lamellengitter benutzten Formalismus auf verlustbehaftete Strukturen. Probeweise Ergebnisse des Verfahrens demonstrieren seine Genauigkeit und seine Fähigkeit, Probleme zu behandeln, die mit dem vielbenutzten Integralgleichungsformalismus der Beugungsgittertheorie nicht handhabbar sind.

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