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Abstract

In a previous paper we established that solutions to problems of diffraction of light in a periodic structure behave analytically with respect to variations of the interface. Here we present an algorithm based on this observation for the numerical solution of the problem. The principal component of the algorithm is a simple recursive formula for the derivatives of the efficiencies with respect to the height of the grating. A conformal mapping mechanism is introduced to enhance the convergence of the series. This permits us to deal with the types of profiles and wavelengths usually considered in practice. To illustrate our method we give numerical results for sinusoidal and echelette gratings.

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1 Introduction

In a previous paper [1] we established that solutions to problems of diffraction of light in a periodic structure behave analytically with respect to variations of the interface. One motivation for such investigation, whose subject had been the cause of some controversy ([17], p. 411, [8] p. 789, [6]), was the recognition that the property of analyticity of the solution could be made the basis of a method for its numerical evaluation. Several other applications of these ideas to theoretical and numerical problems of partial differential equations suggest themselves, but will not be dealt with here. The purpose of this paper is to present an algorithm, based on variation of the boundaries, for the solution of diffraction problems.

Because of its theoretical interest and its industrial and scientific applications [5], the problem of diffraction of electromagnetic waves by a periodic interface between two materials has received considerable attention in the last few decades. To review this problem, consider a plane wave incident on an interface between two dielectrics or a dielectric and a perfect conductor. If the interface is a plane, the wave is diffracted according to Snell's law. If the interface is not a plane but a periodic surface, a more complicated diffraction phenomenon occurs, leading to an infinite number of diffracted waves. However, only a finite number of waves can propagate away from the interface, the remaining ones being exponentially decaying with the distance to the surface. This fundamental observation due to Rayleigh [15], is a consequence of a simple Fourier series argument leading to the so-called Rayleigh expansions.

A quick look at the literature reveals a variety of methods that have been employed, e.g., Rayleigh expansions, differential methods and methods of integral equations (see the set of review articles edited by R. Petit [13] and the references therein). All of these numerical methods are devices which produce the amplitudes of the diffracted waves given the geometry and the incident wave. The simplest one of them consists of finding the amplitudes in such a way that the functions defined by the Rayleigh series verify the boundary conditions at the interface. It is well known now, however, that such a simple procedure is not, in general, a correct one. In fact Petit and Cadilhac [14] showed that for a sinusoidal interface

$$y = \frac{h}{2}\sin(2\pi x/d) \tag{1}$$

the Rayleigh series does not converge up to the interface if $h/d > 0.142$. Later, Millar [7] established the complementary result: if $h/d < 0.142$ then the convergence up to the boundary is guaranteed. In any case, the Rayleigh series describes the physics in the region of interest, but for $h/d > 0.142$ its coefficients cannot be found by evaluating it at the interface.

The method we propose is not unrelated to Millar's observation. We have shown [1] that for any periodic analytic function $f(x)$, the solution $u = u(x, y, \delta)$ to a diffraction problem with profile

$$y = \delta f(x) \tag{2}$$

is an analytic function of the three variables x, y and δ. More precisely, we generalized Millar's result by showing that given such an analytic profile and the incoming wave, there is a domain $W = \{(x, y) : y \geq y_0\}$, $y_0 < 0$, with the property that the function $u(x, y, \delta)$ can be extended to an analytic function of x and y for $(x, y) \in W$ and all small δ. In addition to this, we showed that this extended function u is also an analytic function of δ for δ small enough. Finally, we showed that for *any* real value of δ and for y large enough, u is again an analytic function of all three variables.

Because the function u is analytic in the domain W for δ small enough, it is permissible to evaluate u at the profile, thus obtaining the known boundary values, and differentiate a number of times this equality with respect to δ at $\delta = 0$. It turns out that this procedure yields a simple recursive formula for the subsequent derivatives of u with respect to δ at $\delta = 0$. Since u is analytic in δ for all real δ provided y is large, it follows that the Rayleigh coefficients $B_n = B_n(\delta)$ are analytic *for all real values of* δ, and therefore, they are determined once their derivatives at $\delta = 0$ are known.

To proceed to evaluate $B_n(\delta)$ at a given value of δ, the first idea that comes to mind is to sum its Taylor series. It turns out that this series converges for values of δ corresponding to relatively shallow gratings. Thus, we introduce a mechanism, based on conformal transformations, to enhance the convergence of the series. With this addition our algorithm is capable of solving diffraction problems for the types of profiles and wavelengths usually considered in practice.

Our numerical results are in agreement with those presented by other authors (e.g. [11,12,10,18,3]), and the algorithm is very easy to implement. The evaluation of the derivatives of the coefficients B_n by the algorithm in its present form is more computationally expensive than the corresponding cost of evaluating the B_n's for a given height by other methods, e.g. the integral method. This disadvantage is compensated, however, by the fact that once the derivatives are calculated, the efficiencies can be obtained for any number of different groove depths at virtually no cost. To illustrate this point we present, in addition to other numerical results, a table (see appendix A) containing the coefficients of six polynomials of degree 24 which approximate the real and imaginary parts of the coefficients B_n, $n = 0, 1, 2$, for a diffraction problem for the sinusoidal profile (1) with wavelength-to-period ratio

$\lambda/d = 0.4368$. This approximate formula gives the efficiencies with an accuracy (according to the energy balance criterion) of order 10^{-4} for all gratings with $h/d \leq 0.30$. Much higher accuracy can be obtained, and deeper gratings can be dealt with by using a higher number of derivatives, as we will see below.

The method we present for the calculation of the derivatives of the coefficients B_n is perhaps the most natural one, but it is not, by any means, the only possible one. We feel that there is room for substantial improvement in this direction. We expect that further elaboration of the ideas mentioned above will prove fruitful in this and other problems of mathematical physics.

2 Preliminaries

2.1 The Helmholtz equation

We consider the problem of diffraction of electromagnetic waves across a periodic structure. More precisely, we consider two regions, Ω^+ and Ω^-, which are either filled with materials of dielectric constants ϵ^+ and ϵ^- or with a dielectric with dielectric constant ϵ^+ and a perfect conductor. The two regions are separated by a surface

$$y = f(x)$$

where f is a periodic function of period d. The permeability of the dielectrics is assumed to be equal to μ_0, the permeability of vacuum.

When the grating is illuminated by a plane wave

$$\vec{E}^i = \vec{A} e^{i\alpha x - i\beta y} e^{(-i\omega t)}$$

$$\vec{H}^i = \vec{B} e^{i\alpha x - i\beta y} e^{(-i\omega t)}.$$

this incident wave will be diffracted by the grating into the regions above the interface (i.e. Ω^+) and below it (Ω^-).

In the case of a grating between a dielectric and a perfect conductor, the total field in Ω^+ is given by

$$\vec{E}^{up} = \vec{E}^i + \vec{E}^{refl}$$
$$\vec{H}^{up} = \vec{H}^i + \vec{H}^{refl}. \tag{3}$$

while it vanishes in Ω^-. Dropping the factor $e^{-i\omega t}$, the incident, reflected and total fields satisfy the time harmonic Maxwell equations

$$\nabla \times \vec{E} = i\omega\mu_0 \vec{H} \ , \ \nabla \cdot \vec{E} = 0 \ ,$$
$$\nabla \times \vec{H} = -i\omega\epsilon^+ \vec{H} \ , \ \nabla \cdot \vec{H} = 0 \ , \tag{4}$$

in the region Ω^+. Furthermore, at the interface the *total* field satisfies

$$n \times \vec{E}^{up} = 0 \ , \ n \times \vec{H}^{up} = 0 \ \text{on} \ y = f(x) \ , \tag{5}$$

where n is the unit normal vector to the interface. In the case that the regions Ω^+ and Ω^- are filled by two dielectrics the total field in Ω^- also satisfies an equation of the form (4) and the transmission conditions:

$$n \times (\vec{E}^{up} - \vec{E}^{down}) = 0 \ , \ n \times (\vec{H}^{up} - \vec{H}^{down}) = 0 \ \text{on} \ y = f(x). \tag{6}$$

Finally, the periodicity of the geometry is reflected in the fields in that they must be quasiperiodic: if v is one of the fields $\vec{E}$ or $\vec{H}$, we have

$$v(x+d,y) = e^{i\alpha d} v(x,y). \tag{7}$$

It is well known that in the situation described above, the fields $\vec{E}$ and $\vec{H}$ are independent of z and the system of equations (4),(5) (or (4),(6)) can be reduced to pairs of equations for a single unknown [4]. Indeed, the function $u(x,y)$ equal to either one of the transverse components E_z (Field Transverse Electric, TE) or H_z (Field Transverse Magnetic, TM), is easily seen to satisfy, in either case, the Helmholtz equation

$$\Delta u + (k^{\pm})^2 u = 0 \ , \ \text{in}\, \Omega^{\pm} \, , \tag{8}$$

where $k^{\pm} = \omega\sqrt{\mu_0 \epsilon^{\pm}}$. The boundary conditions (5), (6) can be translated into Dirichlet, Neumann or transmission conditions for the unknown u. In sum, the solution of the diffraction problems mentioned above is given by an α-quasiperiodic function u which satisfies Helmholtz equation together with one of the following boundary conditions:

(i) *Dielectric-Perfect Conductor interface: TE mode.*

Here we let $u = E_z^{refl}$ and the boundary conditions become

$$u = -e^{i\alpha x - i\beta f(x)} \ , \ \text{on} \ \ y = f(x). \tag{9}$$

(ii) *Dielectric-Perfect Conductor interface: TM mode.*

In this case $u = H_z^{refl}$ and the condition is

$$\frac{\partial u}{\partial n} = -\frac{\partial}{\partial n}(e^{i\alpha x - i\beta y}) \ , \ \text{on} \ \ y = f(x). \tag{10}$$

(iii) *Interface between two dielectrics: TE mode.*

We let $u^+ = E_z^{refl}$, $u^- = E_z^{refr}$ and the conditions at the interface become

$$\begin{aligned} u^+ - u^- &= -e^{i\alpha x - i\beta f(x)} \ , \ \text{on} \ \ y = f(x) \, , \\ \frac{\partial u^+}{\partial n} - \frac{\partial u^-}{\partial n} &= -\frac{\partial}{\partial n}(e^{i\alpha x - i\beta y}) \ , \ \text{on} \ \ y = f(x). \end{aligned} \tag{11}$$

(iv) *Interface between two dielectrics: TM mode.*

Here u^+ and u^- are defined as in (iii) and the transmission conditions take the form

$$u^+ - u^- = -e^{i\alpha x - i\beta f(x)} \quad , \quad \text{on } y = f(x) \, ,$$
$$\frac{\partial u^+}{\partial n} - \frac{1}{\nu_0^2}\frac{\partial u^-}{\partial n} = -\frac{\partial}{\partial n}(e^{i\alpha x - i\beta y}) \quad , \quad \text{on } y = f(x) \, , \tag{12}$$

where

$$\nu_0^2 = \frac{\epsilon^-}{\epsilon^+} = \left(\frac{k^-}{k^+}\right)^2 . \tag{13}$$

2.2 Rayleigh Expansion, Radiation Conditions and Energy Balance

Let us recall that certain condition of radiation at infinity must be added to equation (8) in order to determine the physical solution u: the fields should remain bounded at infinity and the solution should consist of outgoing waves. Here we briefly discuss this and other related issues for future reference and in order to fix our notation.

Set

$$K = \frac{2\pi}{d} \quad , \quad \alpha_n = \alpha + nK \quad , \quad \alpha_n^2 + (\beta_n^\pm)^2 = (k^\pm)^2 \, , \tag{14}$$

where $\beta_n^\pm$ is determined by $Im\beta_n^\pm > 0$ or $\beta_n^\pm \geq 0$. We shall assume that

$$k^+ \neq \pm(\alpha + nK) \quad , \quad k^- \neq \pm(\alpha + nK) \tag{15}$$

for all integers n. The case in which $k^\pm = \pm(\alpha + nK)$ for some n is related to an interesting phenomenon known as "Wood anomalies", first observed by R. W. Wood [19] and accounted for mathematically by Lord Rayleigh [16] (see also [2,9]). This phenomenon will not be discussed here at any length, however, and relation (15) will always be assumed to hold.

Under this assumption, *any* α-quasiperiodic solution to the Helmholtz equation in the region Ω^+ is given, for $y > y_M = \max f$, by the Rayleigh expansion

$$u^+ = \sum_{n=-\infty}^{\infty} A_n^+ e^{i\alpha_n x - i\beta_n^+ y} + \sum_{n=-\infty}^{\infty} B_n^+ e^{i\alpha_n x + i\beta_n^+ y}. \tag{16}$$

Analogously, any solution u^- to the Helmholtz equation in Ω^- is given, for $y < y_m = \min f$, by

$$u^- = \sum_{n=-\infty}^{\infty} A_n^- e^{i\alpha_n x - i\beta_n^- y} + \sum_{n=-\infty}^{\infty} B_n^- e^{i\alpha_n x + i\beta_n^- y}. \tag{17}$$

A solution u (the diffracted field) of (8) in $\Omega^\pm$ verifies the radiation condition at infinity mentioned above if

$$A_n^+ = 0 \text{ and } B_n^- = 0 \text{ for all } n. \tag{18}$$

Let us finally recall that the principle of conservation of energy yields a relation between the Rayleigh coefficients of u which is commonly used as a convergence test for the numerical solution of diffraction problems [4]. For example, in the case in which Ω^- is filled with a perfect conductor and k^+ is real, this "energy balance criterion" is given by

$$\sum_{n \in U^+} \beta_n^+ |B_n^+|^2 = \beta_0^+ \tag{19}$$

where U^+ is the finite set

$$U^+ \equiv \{n : \beta_n^+ > 0\}. \tag{20}$$

Equivalently

$$\sum_{n \in U^+} e_n = 1 \tag{21}$$

where $e_n = \beta_n^+ |B_n^+|^2 / \beta_0^+$. The coefficient e_n is called the *n-th order efficiency.*

3 The Algorithm

In this section we derive an algorithm, based on variation of the boundary, for the evaluation of the Rayleigh coefficients $B_n = B_n(\delta)$ of the solution $u(x, y, \delta)$. The basic idea is that differentiation of the boundary (or transmission) conditions with respect to δ yields a recursive formula for the coefficients in the power series expansion (about $\delta = 0$, i.e. flat interface) of the B_n's. The theoretical foundations that allow us to predict the convergence of the power series were given in [1].

We consider the diffraction problem for a d-periodic grating $f(x)$ which we assume, for simplicity, can be represented as a finite Fourier series

$$f(x) = \sum_{r=-F}^{F} C_{1,r} e^{iKrx} \, , \; K = \frac{2\pi}{d}. \tag{22}$$

Let us first consider the case of TE polarization when Ω^- is filled by a perfect conductor, i.e. problem (8),(9), in which case the reflected field u satisfies Helmholtz' equation in Ω^+ as well as Dirichlet boundary conditions. Set

$$f_\delta(x) = \delta f(x) \, ,$$

and let $u(x, y, \delta)$, $y > f_\delta(x)$, denote the field reflected by the grating $f_\delta(x)$. Then, from (9) we have

$$u(x, \delta f(x), \delta) = -u_i(x, \delta f(x)) = -e^{i\alpha x - i\beta\delta f(x)}. \tag{23}$$

In order to obtain a power series in δ

$$B_n(\delta) = \sum_{l=0}^{\infty} d_{l,n} \delta^l \tag{24}$$

for the Rayleigh coefficients of u, we shall compute the successive *total* δ-derivatives of the equation (23) and recursively find the *partial* δ-derivatives of u at $y = 0$, $\delta = 0$.

Differentiation of the Rayleigh series gives

$$\frac{1}{l!}\frac{\partial^l u}{\partial \delta^l}(x,0,0) = \sum_r d_{l,r} e^{i\alpha_r x} \tag{25}$$

and since

$$\frac{\partial^l u}{\partial \delta^l}(x,y,0)$$

is a solution of Helmholtz equation in $\{y > 0\}$ (consisting of outgoing waves) we conclude that

$$\frac{1}{l!}\frac{\partial^l u}{\partial \delta^l}(x,y,0) = \sum_r d_{l,r} e^{i\alpha_r x + i\beta_r y}. \tag{26}$$

Upon differentiating (23) n times with respect to δ we obtain

$$\frac{1}{n!}\frac{\partial^n u}{\partial \delta^n}(x,0,0) = -\frac{(-i\beta)^n}{n!} f(x)^n e^{i\alpha x} - \sum_{k=0}^{n-1} \frac{f(x)^{n-k}}{(n-k)!}\frac{\partial^{n-k}}{\partial y^{n-k}}\left(\frac{1}{k!}\frac{\partial^k u}{\partial \delta^k}\right)(x,0,0). \tag{27}$$

Now, from relations (22), (23) and (27), it is readily seen that the r-th Fourier coefficient of $\frac{\partial^n u}{\partial \delta^n}(x,0,0)$ vanishes if $|r| > nF$, that is, the summation in (25) (and therefore in (26)) is restricted to

$$-nF \le r \le nF.$$

Clearly, the same is true for the Fourier coefficients of f^n, so that we can write

$$f(x)^n = \sum_{r=-nF}^{nF} C_{n,r} e^{iKrx}. \tag{28}$$

Hence, we can rewrite (27) in the form

$$\frac{1}{n!}\frac{\partial^n u}{\partial \delta^n}(x,0,0) = -\frac{(-i\beta)^n}{n!}\left(\sum_{r=-nF}^{nF} C_{n,r} e^{iKrx}\right) e^{i\alpha x}$$

$$-\sum_{k=0}^{n-1}\frac{1}{(n-k)!}\left(\sum_{r=-(n-k)F}^{(n-k)F} C_{n-k,r} \quad e^{iKrx}\right)\frac{\partial^{n-k}}{\partial y^{n-k}}\left(\sum_{r=-kF}^{kF} d_{k,r} e^{i\alpha_r x + i\beta_r y}\right)\Bigg|_{y=0},$$

or, equivalently,

$$\frac{1}{n!}\frac{\partial^n u}{\partial \delta^n}(x,0,0) = \sum_{r=-nF}^{nF} e^{i\alpha_r x}\Big\{-\frac{(-i\beta)^n}{n!}C_{n,r}$$

$$-\sum_{k=0}^{n-1}\sum_{p+q=r} \tfrac{C_{n-k,p}}{(n-k)!} \quad (i\beta_q)^{n-k} d_{k,q}\Big\}.$$

Therefore, the recursive formula takes the form

$$d_{n,r} = -\frac{(-i\beta)^n}{n!}C_{n,r} - \sum_{k=0}^{n-1}\sum_{q=\max(-kF,r-(n-k)F)}^{\min(kF,r+(n-k)F)} \frac{C_{n-k,r-q}}{(n-k)!}(i\beta_q)^{n-k} d_{k,q}\,, \tag{29}$$

where $-nF \le r \le nF$.

For the case of a perfect conductor in TM mode (Neumann boundary conditions) a similar argument to the one just described yields the following relation for the Fourier coefficients of the successive δ-derivatives:

$$d_{n,r} = -\frac{i}{\beta_r}\frac{(-i\beta)^{n-1}}{n!}C_{n,r}\left(\beta^2 - \alpha r K\right)$$

$$-\frac{i}{\beta_r}\sum_{k=0}^{n-1}\sum_{q=\max(-kF,r-(n-k)F)}^{\min(kF,r+(n-k)F)} \tfrac{C_{n-k,r-q}}{(n-k)!} \quad (i\beta_q)^{n-k-1}\left((\beta_q)^2 - \alpha_q(r-q)K\right) d_{k,q}\,. \tag{30}$$

The case of two dielectrics (transmission conditions) can be handled in an analogous way.

Let us take, for example, the case of the grating

$$f(x) = 2\cos(Kx) = e^{iKx} + e^{-iKx}, \tag{31}$$

for which $F=1$, $C_{n,k}=0$ if $n-k$ is odd and $C_{n,k} = \binom{n}{\frac{n-k}{2}}$ if $n-k$ is even. Then, it is easy to see from (29) or (30) that the non–zero coefficients $d_{n,r}$ are

$$\begin{array}{ccccccccc} & & & & d_{0,0}=-1 & & & & \\ & & & d_{1,-1} & & d_{1,1} & & & \\ & & d_{2,-2} & & d_{2,0} & & d_{2,2} & & \\ & d_{3,-3} & & d_{3,-1} & & d_{3,1} & & d_{3,3} & \\ d_{4,-4} & & d_{4,-2} & & d_{4,0} & & d_{4,2} & & d_{4,4} \\ & & & & etc. & & & & \end{array}$$

If an N-th order approximation to the Taylor series in (24) is to be computed, it is clearly unnecessary to produce *all* of the coefficients $d_{n,r}$ for $n \leq N$. In fact, to compute B_0 with $N = 4$ we need only generate

$$\begin{array}{ccccc} & & d_{0,0}=-1 & & \\ & d_{1,-1} & & d_{1,1} & \\ d_{2,-2} & & d_{2,0} & & d_{2,2} \\ & d_{3,-1} & & d_{3,1} & \\ & & d_{4,0} & & \end{array} \tag{32}$$

Of course, in general we wish to calculate not only B_0 but a number w of amplitudes (corresponding to the non–evanescent modes), and the array (32) must be augmented accordingly. Similar considerations apply to profiles given by an arbitrary finite Fourier series.

In practice, and in order to reduce the number of operations, one can choose to truncate the inner sum in equations (29) and (30) by setting $d_{k,q} = 0$ for $|q| > q_0$. The parameter q_0 has to be chosen judiciously. Our experiments indicate that in the case of the sinusoidal profile (31), no truncation is permissible (e.g. in (32) one cannot take $q_0 < 2$). On the other hand, for the grating given by

$$f(x) = 2\cos(Kx) + \frac{1}{5}\cos(3Kx) \tag{33}$$

the effect of the higher order harmonics generated by the second summand can be truncated. In other words, even though the actual formulae (29), (30) for this profile involve frequencies roughly as high as $\frac{3}{2}N + w$, one can take $q_0 = \frac{N}{2} + w$ with errors comparable to the roundoff errors. This is related to the fact that the height-to-period ratio h/d of the first term in (33) is larger than the one for the second term. Thus, in the general case of a function as in (22), q_0 should be chosen so that no truncation would occur if all but the principal term in (22) (i.e. the one with the largest h/d) were neglected. Naturally, as the height-to-period ratio of a secondary term approaches the one for the principal term, the value of q_0 should be increased. The ultimate choice of q_0 must be made by consideration of the actual errors as measured by the energy balance criterion.

There still remains the question about the radius of convergence of the series (24). From [1] we know that the functions $B_l(\delta)$ are analytic in a common neighborhood of the real axis and therefore, the series in (24) certainly has a positive radius of convergence. It turns out that this series only allows us to calculate the Rayleigh coefficients for some shallow to relatively deep gratings, since it diverges for larger values of δ; see Tables 1.a and 1.b. We therefore need a mechanism to improve the convergence of the series.

4 Enhanced Convergence and Numerical Results

Even though the Taylor series of an analytic function at a point determines the function completely, it is not an easy matter to use the information contained in the power series to evaluate the function outside its circle of convergence. (For example, one may wish to evaluate numerically the function $q(z) = (z^2 + 1)^{-1}$ at $z = 2$).

The theory of *Padé approximants* has been devised to serve this approximating purpose. However, due to the large number of derivatives we will be dealing with (roughly between 30 and 100) we have shied away from Padé approximation.

Instead, we shall follow a different approach based on conformal mappings.

Suppose that a function $g(\omega)$ is analytic in a wedge

$$\{\,|\arg(\omega)| < \frac{\pi}{2\alpha}\,\}, \tag{34}$$

for some $\alpha > 1$, and let $\mathcal{D}_1$ denote the circle of convergence about $\omega = 1$ (see Figure 1). Then, if P is the leftmost point of intersection of $\partial\mathcal{D}_1$ with the real line, the segment $\overline{0P}$ lies outside $\mathcal{D}_1$ and therefore the values of g at these points cannot be directly computed using the Taylor series about $\omega = 1$. However, the simple procedure of mapping the wedge onto the right half-plane by

$$\xi = w^{\alpha} \tag{35}$$

and considering the power series expansion of

$$g(\omega(\xi)) = g(\xi^{1/\alpha})$$

about $\xi = 1$ allows one to compute directly the values of g on $\overline{0P}$, since this segment is now included in the circle of convergence $\mathcal{D}_2$ (Figure 1).

To implement this idea of "enhanced convergence" for the computation of the coefficients $B_r(\delta)$, we will use a preliminary conformal mapping to approach a situation like the one described above. In Figure 2, the set labeled $\mathcal{C}$ represents the neighborhood of the real line in the complex δ-plane where $B_r(\delta)$ is analytic. We have also drawn the circle $\mathcal{D}$ of convergence about $\delta = 0$. Our objective is to compute $B_r(\delta_0)$ where δ_0 is as in the figure: it lies outside of $\mathcal{D}$. For this purpose we consider an elongated region consisting of the intersection of two discs ($\mathcal{L}$ in Figure 1) which we map onto a wedge in the ω-plane via

$$\omega = \frac{A-\delta}{A+\delta}. \tag{36}$$

Clearly the image ω_0 of δ_0 lies between 0 and 1. The parameter σ controls the angle of the wedge which is of the form (34) with

$$\alpha = \arctan[2A\sigma/(A^2 - \sigma^2)].$$

Finally, the transformation (35) has the effect of "opening" the domain of convergence, thereby allowing us to use the expansion about $\xi = 1$ (or, equivalently, about $\delta = 0$) to calculate $B_r(\delta_0)$.

In Tables 1.a and 1.b we compare the convergence of the power series for $e_1(\delta) = B_1(\delta)\beta_1/\beta_0$ about $\delta = 0$ ("Direct") with that of $e_1(\xi) = B_1(\xi)\beta_1/\beta_0$ about $\xi = 1$ ("Enhanced"), with increasing number n of terms. The error in the energy relation (21) is denoted by

$$\epsilon = 1 - \sum_{n \in U^+} e_n.$$

We have taken the example of a sinusoidal grating in TE mode. The incoming wave was taken to be normally incident with wavelength-to-period ratio $\lambda/d = 0.4368$, so that there are five propagating modes: $U^+ = \{0, \pm 1, \pm 2\}$. The parameters of the conformal map were set to $\sigma = 0.13$ and $A = 9.0$. Tables 1.a and 1.b correspond to height-to-period ratios h/d of 0.3 and 0.4, respectively. We observe that even in the case $h/d = 0.3$, in which the direct series converges, the convergence is substantially enhanced by the conformal mapping. In case $h/d = 0.4$ the direct method does not converge.

From the ideas discussed above it is clear that the actual programming of both the algorithm for the calculation of derivatives (as described in section 3) and the one for convergence enhancement is fairly straightforward. The latter algorithm does not introduce any further truncation, and once it has been applied the calculation of the efficiencies for a given value of the height only involves evaluation of a polynomial.

It is therefore easily checked that the additional computational cost introduced by the conformal mapping mechanism is negligible.

To conclude we present the results of some numerical experiments. Tables 2 and 3 give the values of the efficiencies for sinusoidal and echelette gratings and for various values of the height-to-period ratio. Normal incidence and $\lambda/d = 0.4368$ was again assumed, and enhanced convergence with double precision arithmetic was used in all cases.

Tables 2.a and 2.b correspond to the grating

$$y = \frac{h}{2}\cos(2\pi x/d),$$

that is to say the grating (31) with $\delta = h/4$, in the cases of TE and TM polarization, respectively. In the TM mode, the slower convergence of the power series prevented us from considering gratings as deep as those in table 2.a.

Tables 3 correspond, respectively, to the TE and TM modes for the grating

$$y = \frac{h}{2}g(2\pi x/d)$$

where g is the echelette profile

$$g(x) = \begin{cases} -\frac{2x}{\pi} - 2 & \text{if } -\pi \leq x \leq -\frac{\pi}{2} \\ \frac{2x}{\pi} & \text{if } -\frac{\pi}{2} \leq x \leq \frac{\pi}{2} \\ -\frac{2x}{\pi} + 2 & \text{if } \frac{\pi}{2} \leq x \leq \pi. \end{cases} \tag{37}$$

The echelette profile (37) was approximated by its truncated Fourier series

$$\sum_{r=-F}^{F} C_{1,r} e^{iKrx}$$

with $F = 10$. Slower convergence in the TM mode is again observed.

In order to distinguish the roundoff errors from the errors of truncation of the series in a study of convergence, we generated table 4 using quadruple precision arithmetic. This table corresponds to the case of TE polarization for the sinusoidal profile as considered in table 2.a. One hundred terms in the Taylor expansion of the B_r's were used. Due to the larger number of terms, we obtain a substantial improvement in the accuracy with respect to table 2.a.

A Appendix

Here we present approximate formulae for the Rayleigh coefficients $B_r(\delta)$ corresponding to a sinusoidal grating in TE polarization as in the previous section. These formulae consist of six polynomials of degree 24 in the variable ξ of section 4 (cf. (35), (36)), whose coefficients are given in table 5. More precisely, the approximate formulae read

$$B_r = B_r(\delta) = \sum_{n=0}^{24} B_r^n(\xi - 1)^n, \quad \xi = \xi(\delta), \quad r = 0, \pm 1, \pm 2 \tag{38}$$

with B_r^n as in table 5. These formulae give the efficiencies

$$e_r(\delta) = B_r(\delta)\frac{\beta_r}{\beta_0}$$

of the propagating modes with an accuracy of order at least 10^{-4} for $h/d = \delta/(4d) \leq 0.30$.

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Captions for tables

Table 1: Comparison between direct and enhanced convergence. First order efficiency for a sinusoidal grating in TE polarization. Table 1.a: h/d=0.3, Table 1.b: h/d = 0.4

Table 2.a: Efficiencies for $f(x) = \frac{h}{2}\sin(2\pi x/d)$ in TE polarization with $A = 9$, $\sigma = 0.13$ and 60 terms of the Taylor expansion.

Table 2.b: Efficiencies for $f(x) = \frac{h}{2}\sin(2\pi x/d)$ in TM polarization with $A = 9$, $\sigma = 0.13$ and 60 terms of the Taylor expansion.

Table 3.a: Efficiencies for $f(x) = \frac{h}{2}g(2\pi x/d)$ in TE polarization with $A = 9$, $\sigma = 0.20$, $F = 10$ and 30 terms of the Taylor expansion.

Table 3.b: Efficiencies for $f(x) = \frac{h}{2}g(2\pi x/d)$ in TM polarization with $A = 9$, $\sigma = 0.20$, $F = 10$ and 40 terms of the Taylor expansion.

Table 4: Efficiencies for $f(x) = \frac{h}{2}\sin(2\pi x/d)$ in TE polarization with $A = 9$, $\sigma = 0.13$ and 100 terms of the Taylor expansion. Quadruple precision arithmetic.

Table 5: Coefficients in equations (38) in the case of normal incidence on a sinusoidal grating with $\lambda/d = 0.4368$, $A = 9$ and $\sigma = 0.20$.

Table 1.a

	Direct		Enhanced	
n	e_1	ϵ	e_1	ϵ
10	0.5034545E–02	1.5E–01	0.1735547E–01	8.3E–02
15	0.1073396E–01	5.3E–02	0.1204894E–01	1.3E–05
20	0.1045474E–01	4.0E–03	0.1157684E–01	5.1E–04
25	0.1140532E–01	3.2E–03	0.1163189E–01	3.1E–05
30	0.1161950E–01	2.2E–04	0.1163870E–01	–8.4E–06
35	0.1165000E–01	1.1E–05	0.1163798E–01	–7.3E–07
40	0.1162548E–01	–3.2E–05	0.1163793E–01	–4.4E–08
45	0.1163059E–01	5.1E–05	0.1163793E–01	2.2E–08
50	0.1164204E–01	1.2E–05	0.1163793E–01	2.0E–09
55	0.1164090E–01	–1.7E–05	0.1163793E–01	–3.7E–11
60	0.1163616E–01	–4.0E–06	0.1163793E–01	–4.5E–11

Table 1.b

	Direct		Enhanced	
n	e_1	ϵ	e_1	ϵ
10	0.3897061E+00	−7.2E−01	0.4018525E+00	−4.5E−01
15	0.4713435E+01	−1.4E+01	0.1649737E+00	−7.3E−02
20	0.3635994E+01	−1.5E+01	0.1568326E+00	3.1E−02
25	0.3848452E+01	−1.2E+01	0.1687898E+00	4.8E−03
30	0.3357765E+00	−5.5E+00	0.1698172E+00	3.0E−04
35	0.1276039E+01	−2.4E+01	0.1701259E+00	−4.0E−04
40	0.4143993E+02	−2.2E+02	0.1700261E+00	−1.3E−04
45	0.1665033E+03	−1.6E+03	0.1699795E+00	1.3E−05
50	0.1406855E+04	−8.2E+03	0.1699760E+00	1.1E−05
55	0.7075471E+04	−6.9E+04	0.1699781E+00	2.5E−06
60	0.7847034E+05	−4.1E+05	0.1699792E+00	−4.8E−07

Table 2.a

h/d	e_0	e_1	e_2	ϵ
0.05	0.786	0.105	0.002	–1.6E–15
0.10	0.337	0.310	0.021	–4.2E–15
0.15	0.030	0.403	0.082	–1.2E–14
0.20	0.051	0.299	0.176	–3.7E–14
0.25	0.266	0.110	0.257	–1.2E–13
0.30	0.423	0.012	0.277	–4.5E–11
0.35	0.415	0.062	0.230	–9.5E–09
0.40	0.337	0.170	0.162	–4.8E–07
0.45	0.317	0.211	0.131	–3.4E–06
0.50	0.355	0.161	0.161	2.1E–04

Table 2.b

h/d	e_0	e_1	e_2	ϵ
0.05	0.743	0.125	0.004	1.3E–14
0.10	0.263	0.319	0.050	3.0E–14
0.15	0.012	0.313	0.180	3.3E–15
0.20	0.031	0.126	0.359	–5.0E–14
0.25	0.050	0.001	0.474	7.7E–10
0.30	0.000	0.071	0.429	1.1E–06
0.35	0.194	0.164	0.239	2.6E–04

Table 3.a

h/d	e_0	e_1	e_2	ϵ
0.05	0.856	0.071	0.001	–3.8E–15
0.10	0.515	0.230	0.012	–1.2E–14
0.15	0.180	0.358	0.052	–2.1E–11
0.20	0.012	0.366	0.128	–1.1E–08
0.25	0.029	0.261	0.224	–6.6E–07
0.30	0.136	0.125	0.307	–9.9E–06
0.35	0.230	0.043	0.342	–5.6E–05
0.40	0.287	0.041	0.315	–3.4E–04
0.45	0.363	0.078	0.242	–3.7E–03

Table 3.b

h/d	e_0	e_1	e_2	ϵ
0.05	0.826	0.085	0.003	6.4E–15
0.10	0.447	0.241	0.035	1.8E–14
0.15	0.134	0.296	0.137	–5.6E–12
0.20	0.011	0.195	0.299	–1.2E–08
0.25	0.001	0.049	0.451	–1.5E–06
0.30	0.001	0.002	0.497	6.7E–05
0.35	0.071	0.068	0.394	5.1E–03

Table 4

h/d	e_0	e_1	e_2	ϵ
0.05	0.786186	0.105346	0.001561	–6.7E–16
0.10	0.337470	0.310013	0.021252	–6.7E–16
0.15	0.029851	0.403106	0.081969	–4.4E–16
0.20	0.050728	0.298916	0.175721	–2.2E–16
0.25	0.266100	0.110307	0.256643	1.1E–16
0.30	0.422850	0.011638	0.276937	1.2E–15
0.35	0.415025	0.062114	0.230374	1.6E–14
0.40	0.336781	0.169979	0.161630	3.2E–12
0.45	0.316566	0.211003	0.130714	–6.9E–09
0.50	0.354656	0.161227	0.161446	–1.8E–06
0.55	0.355306	0.100680	0.221733	–1.3E–04
0.60	0.291421	0.100459	0.255925	–4.2E–03

Table 5

n	$\Re(B_0^n)$	$\Im(B_0^n)$	$\Re(B_1^n)$	$\Im(B_1^n)$	$\Re(B_2^n)$	$\Im(B_2^n)$
0	−.100000E1	0.000000E0	0.000000E0	0.000000E0	0.000000E0	0.000000E0
1	0.000000E0	0.000000E0	0.000000E0	−.366240E1	0.000000E0	0.000000E0
2	0.120659E2	0.000000E0	0.000000E0	0.183120E1	0.603297E1	0.000000E0
3	−.120659E2	0.000000E0	0.000000E0	0.174845E2	−.603297E1	0.000000E0
4	−.216846E2	0.000000E0	0.000000E0	−.271423E2	−.111752E2	−.380572E1
5	0.554351E2	0.000000E0	0.339145E1	−.175230E1	0.283834E2	0.761144E1
6	−.396319E2	0.510032E1	−.847861E1	0.499232E2	−.232030E2	−.588873E1
7	−.257249E2	−.153010E2	0.831214E1	−.712169E2	−.436600E1	−.136243E1
8	0.942712E2	0.250151E2	0.582640E0	0.425568E2	0.332829E2	0.165146E2
9	−.119643E3	−.286560E2	−.230162E2	0.248016E2	−.425071E2	−.419404E2
10	0.710781E2	0.127133E2	0.644671E2	−.102437E3	0.225744E2	0.604651E2
11	0.665820E2	0.442465E2	−.111613E3	0.140317E3	0.244029E2	−.353669E2
12	−.241697E3	−.153574E3	0.122598E3	−.645790E2	−.698274E2	−.539671E2
13	0.284629E3	0.298528E3	−.376349E2	−.146219E3	0.437083E2	0.176385E3
14	−.116718E2	−.397621E3	−.200220E3	0.345609E3	0.116423E3	−.240966E3
15	−.515904E3	0.249303E3	0.570540E3	−.247040E3	−.352775E3	0.116678E3
16	0.848156E3	0.382847E3	−.825457E3	−.313696E3	0.432458E3	0.279684E3
17	−.388622E3	−.138528E4	0.471224E3	0.106433E4	−.722920E2	−.786617E3
18	−.102513E4	0.190230E4	0.796900E3	−.125021E4	−.773232E3	0.863182E3
19	0.256792E4	−.680245E3	−.234218E4	0.657669E2	0.161550E4	0.100792E3
20	−.243376E4	−.253639E4	0.239538E4	0.246262E4	−.141090E4	−.194779E4
21	−.104509E4	0.554980E4	0.692025E3	−.459416E4	−.779761E3	0.312092E4
22	0.716020E4	−.409791E4	−.611648E4	0.309440E4	0.435766E4	−.137439E4
23	−.109858E5	−.477287E4	0.921189E4	0.428027E4	−.604872E4	−.396214E4
24	0.490457E4	0.176833E5	−.341893E4	−.146534E5	0.125694E4	0.977718E4

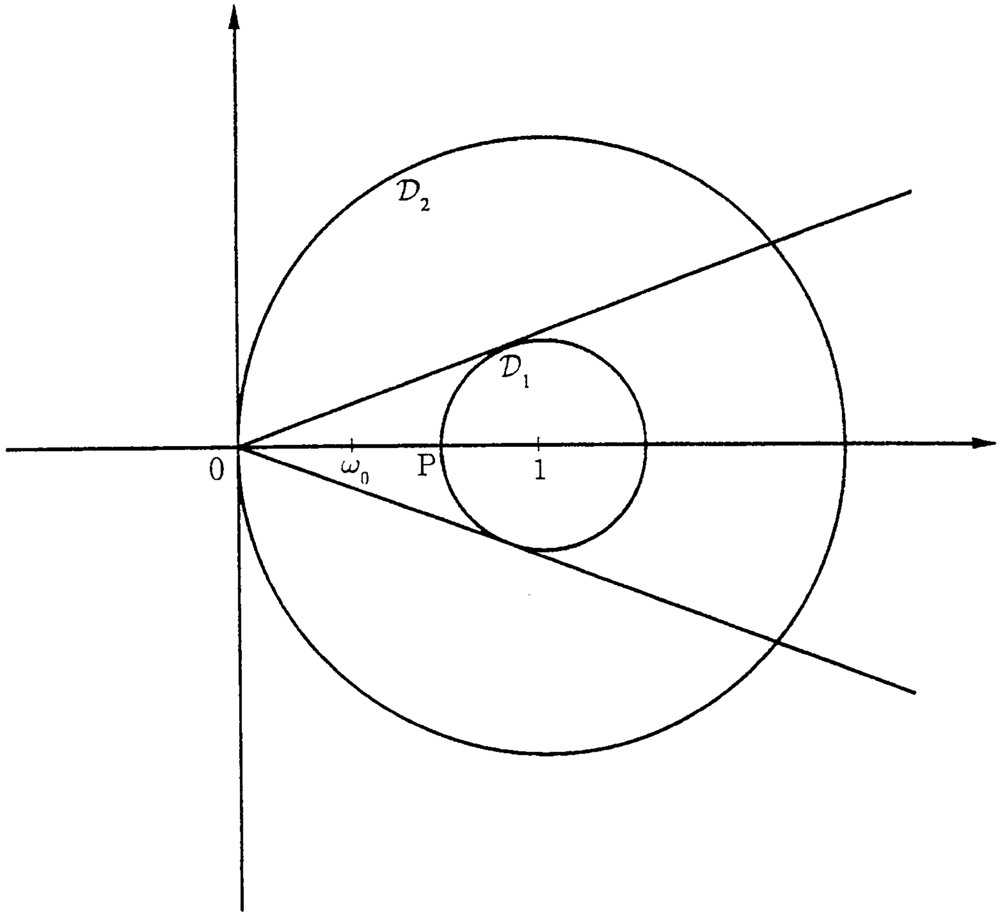

Figure 1

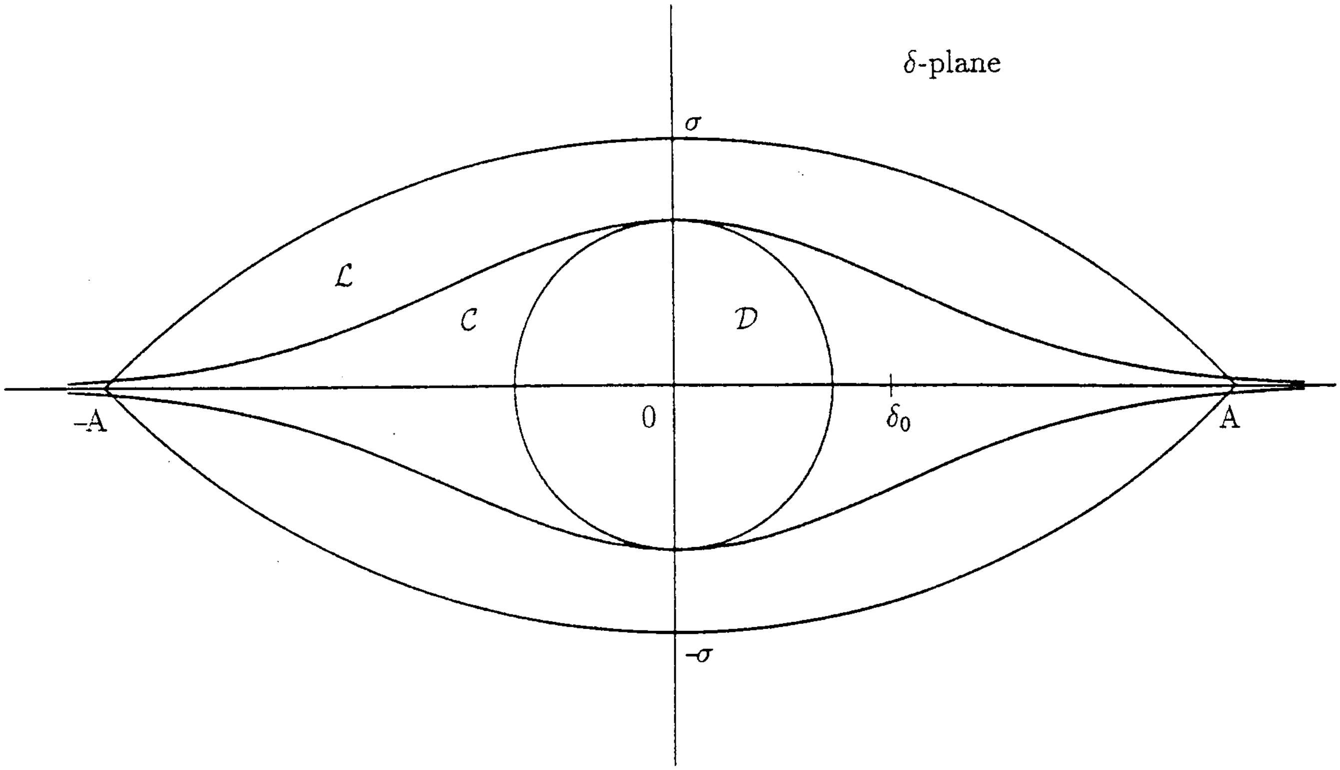

Figure 2

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