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Highly conducting lamellar diffraction gratings

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Abstract. We outline an improved root-finding algorithm necessary for the solution of the eigenvalue equation associated with the diffraction formalism for lossy lamellar gratings. A numerical example is presented, demonstrating the adequacy of this technique for a highly-conducting aluminium grating.

In the previous paper [1], we developed a new technique for solving the problem of the diffraction of a plane wave by a lossy lamellar grating. One of the essential steps in the method was to determine numerically a sufficient number of solutions (β) of the transcendental equation

$$\begin{aligned} f(\beta) &= \cos\beta c\cos\gamma g - \frac{1}{2}\left(q\frac{\beta}{\gamma} + \frac{1}{q}\frac{\gamma}{\beta}\right)\sin\beta c\sin\gamma g - \cos\alpha d \\ &= 0 \end{aligned} \tag{1}$$

where $\gamma^2 = \beta^2 + \zeta^2$ and

$$q = \begin{cases} 1 & \text{for } P \text{ polarization} \\ \dfrac{r_2^2}{r_1^2} & \text{for } S \text{ polarization.} \end{cases}$$

In the above β, γ, ζ and q are complex quantities, and α, c, g and d are real (their physical significance is dealt with in [1]).

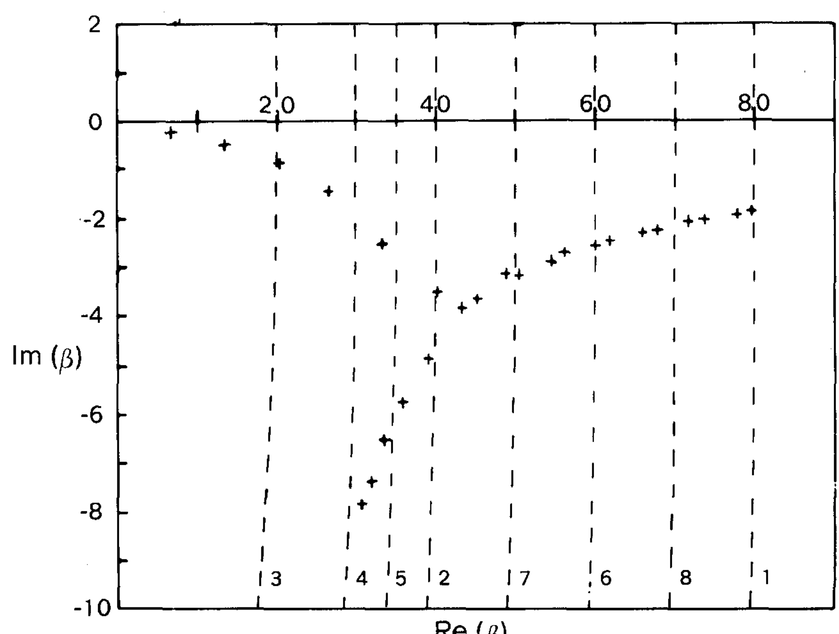
The numerical technique described in [1] for the solution of (1) was based on a generalization [2] to complex functions of the *regula falsi* rule. This method suffered from two limitations, namely an excessive usage of computer time and more importantly an unreliability in the determination of all required roots, particularly in the case of medium to high refractive indices. Given the widespread usage of metallic gratings, which in the visible and infrared regions have refractive indices of large modulus, this numerical limitations detracted seriously from the usefulness of the formalism [1]. In this paper, we give a brief discussion of a powerful complex root-finding technique which removes both of the above limitations.

The method relies on the argument principle of complex variable theory:

$$\frac{1}{2\pi i}\int_C \beta^p \frac{f'(\beta)}{f(\beta)}\,d\beta = \sum_{i=1}^{n} \beta_i^p, \tag{2}$$

where C denotes a closed contour in the complex β plane containing the n zeros $\{\beta_i\}$ of the analytic function $f(\beta)$. Our technique is a refinement of the method of Delves and Lyness [3]. Equation (2) may be used to determine the $\{\beta_i\}$ for a given contour C in the following manner. Firstly, the integral in (2) is evaluated with $p=0$ to determine the number of roots, n. Subsequently, the above integral is evaluated with $p=1,\ldots,n$ and the resulting sums are used with Newton's formulae [4] to form a polynomial of degree n (with leading coefficient 1) having the same roots (within the contour C) as $f(\beta)$. This polynomial equation is then solved by a standard technique such as Muller's method (see, for example, [5]) to give numerical estimates $\{\beta_i'\}$ of the actual set of zeros $\{\beta_i\}$. The differences $\{\beta_i-\beta_i'\}$ are due predominantly to quadrature errors. The estimates $\{\beta_i'\}$ are then refined by a further application of Muller's method, this time to the original function $f(\beta)$. The numerical accuracy and stability of Muller's method in the determination of the estimates $\{\beta_i'\}$ can be assured provided that the degree of the polynomial n is kept small (say $n\leqslant 5$).

For the lossy lamellar grating problem we need at least 20 zeros, β_i, of (1) and frequently as many as 60 zeros. Thus it is necessary to sub-divide the area enclosed by the contour C into sub-regions containing no more than five roots. Whereas Delves and Lyness [3] used a division into a family of overlapping circles, we have found it more efficient to apply a search algorithm based on a division of the region



A plot of the zeros $\{\beta_i\}$ (within the semicircle $|\beta|<80$, $\mathrm{Re}(\beta)\geqslant 0$) of the P polarization eigenvalue equation (1) corresponding to a copper grating with parameters: $d=1{\cdot}0$, $c=0{\cdot}4$, $g=0{\cdot}6$, $\lambda=0{\cdot}55$, $\phi=5°$, $r_1=1{\cdot}0$, $r_2=0{\cdot}756+i2{\cdot}462$. The sequence of the subdivision of the annular rings is shown adjacent to the appropriate circular arc. Note that the radius is successively halved until the number of zeros within a circle (in this case circle 3) is less than or equal to 4 (in this case 2 zeros). These roots are then extracted. Note that more than four roots lie in the annular region between circles 2 and 3, and so this region is then bisected by circle 4. The roots between circles 3 and 4 are then calculated (since there are no more than 4 (in this case 2 zeros)) and the bisections continue until all roots within the semicircle have been found. The units of d, c and g are μm.

into non-overlapping annular regions and, if necessary, the sub-division of the annuli into sectors. We illustrate the method of sub-division of a contour for a typical problem in the figure.

We have found this method to be both robust and computationally efficient. Its use has reduced the ratio of the computation times for root finding and the solution of the diffraction problem from approximately 100 : 1 to 1 : 1. A fuller description of the root finding algorithm will appear elsewhere [6].

Reciprocity results.

Grating parameters: $d=1{\cdot}0$, $c=0{\cdot}9$, $h=0{\cdot}1$,
$r_1=1{\cdot}0$, $r_2=1{\cdot}8+i\,7{\cdot}12$, $r_3=1{\cdot}0$.
Wavelength: $\lambda=0{\cdot}75$.
Incidence parameters: Problem 1, $\phi=5{\cdot}0°$,
Problem 2, $\phi=-56{\cdot}84098°$,
Problem 3, $\phi=41{\cdot}51715°$.
Method parameters: Number of modes = 57,
Number of Rayleigh orders = 25.

Problem	Quantity	*P* polarization	*S* polarization	A.D.†
1	Φ^R_{-1}*	($5{\cdot}0188\times10^{-2}$, $-144{\cdot}3009°$)	($1{\cdot}1805\times10^{-2}$, $-57{\cdot}6700°$)	$-41{\cdot}517°$
	Φ^T_{-1}*	($6{\cdot}9461\times10^{-2}$, $-130{\cdot}3894°$)	($3{\cdot}5350\times10^{-3}$, $140{\cdot}7344°$)	
	Φ^R_0	($3{\cdot}7312\times10^{-2}$, $-123{\cdot}9594°$)	($1{\cdot}1674\times10^{-2}$, $-31{\cdot}7228°$)	$5{\cdot}000°$
	Φ^T_0	($6{\cdot}3190\times10^{-1}$, $40{\cdot}0338°$)	($9{\cdot}4823\times10^{-1}$, $52{\cdot}4268°$)	
	Φ^R_1**	($7{\cdot}6169\times10^{-2}$, $-112{\cdot}8329°$)	($7{\cdot}7967\times10^{-3}$, $-27{\cdot}1172°$)	$56{\cdot}841°$
	Φ^T_1**	($9{\cdot}5205\times10^{-2}$, $-102{\cdot}6638°$)	($3{\cdot}3386\times10^{-3}$, $170{\cdot}6148°$)	
	E.R.	0·16367	0·03128	
	E.T.	0·79654	0·95510	
	E.D.	0·03977	0·01362	
	Q	0·03978	0·01361	
2	Φ^R_{-1}**	($7{\cdot}6168\times10^{-2}$, $-112{\cdot}8330°$)	($7{\cdot}8063\times10^{-3}$, $-27{\cdot}1092°$)	$-5{\cdot}000°$
	Φ^T_{-1}**	($9{\cdot}5205\times10^{-2}$, $-102{\cdot}6630°$)	($3{\cdot}3384\times10^{-3}$, $170{\cdot}6217°$)	
	E.R.	0·33591	0·03464	
	E.T.	0·59326	0·94331	
	E.D.	0·07082	0·02205	
	Q	0·07084	0·02205	
3	Φ^R_1*	($5{\cdot}0187\times10^{-2}$, $-144{\cdot}3010°$)	($1{\cdot}1813\times10^{-2}$, $-57{\cdot}6655°$)	$-5{\cdot}000°$
	Φ^T_1*	($6{\cdot}9460\times10^{-2}$, $-130{\cdot}3895°$)	($3{\cdot}5353\times10^{-3}$, $140{\cdot}7375°$)	
	E.R.	0·21722	0·04037	
	E.T.	0·72537	0·94184	
	E.D.	0·05741	0·01779	
	Q	0·05743	0·01778	

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

In the table we present a numerical example of the use of the formalism for an aluminium grating operated in the near infrared. The results shown are in excellent accord with the criteria of conservation of energy and reciprocity, and confirm the applicability of the method of [1], even in the extreme case of highly-conducting gratings.

On présente un algorithme amélioré pour recherche de racines nécessaire pour résoudre l'équation de valeur propre associée au formalisme de diffraction pour des réseaux lamellaires. Un exemple est présenté, montrant que cette technique convient pour un réseau très conducteur en aluminium.

Wir beschreiben einen verbesserten Lösungsalgorithmus zur Eigenwertgleichung für die Beugung an verlustbehafteten Lamellengittern. Ein numerisches Beispiel zeigt die Eignung dieses Verfahrens für ein hochleitendes Aluminiumgitter.

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