MODAL EXPANSION THEORIES FOR
SINGLY - PERIODIC DIFFRACTION GRATINGS

by

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A thesis submitted in fulfilment
of the requirements for the degree
of Doctor of Philosophy.

UNIVERSITY OF TASMANIA
HOBART

August, 1981
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John R. Andrewartha
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APPENDIX 1: EFFICIENCY SPECTRA FOR THE INFINITELY-CONDUCTING LAMELLAR GRATING

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APPENDIX 4: EFFICIENCY SPECTRA FOR THE SEMI-CIRCULAR GROOVE GRATING
This thesis reports on the analysis and development of rigorous modal expansion techniques for determining the scattering properties of singly-periodic diffraction gratings. Both reflection and transmission gratings are considered, and although emphasis is given to a theoretical study of the formalisms, many numerical results obtained with the latter are also presented. Most of the formalisms pertain to gratings having specific groove geometries and infinitely-conducting surfaces. However, in two cases one or other of these constraints is removed.

Several of the established formalisms, based on a variety of non-modal techniques, are reviewed, and the essence of their method described. The advantages that modal treatments have over these methods are explained, and previous applications of the former are summarised.

Initial theoretical investigations concern the rectangular-groove grating. Intensive studies reveal an alternative approach to the concept of diffraction resonance anomalies. They also provide new insight into the understanding of this grating's overall behaviour, including its blazing and passing-off properties in the first-order Littrow mounting. These ideas are usefully extended throughout the thesis to encompass the behaviour of all gratings.

The theoretical treatment for the rectangular-groove grating is adapted to account for the diffraction properties of three unusual profiles which also possess a rectangular geometry. Two of these structures consist of a transmission grating on a reflecting element, and are shown to exhibit a pronounced resonance action. Tuning of the various grating parameters governs the behaviour of the resonances and indicates the potential use of these devices as a type of reflecting Fabry-Perot interferometer. The third structure is a stepped reflection
grating which proves capable of accurately modelling the performance of general profile gratings including those with sinusoidal and triangular profiles.

Single and bi-modal expansions are shown to provide useful field approximations for not only the conventional rectangular-groove grating, but also for two of the three related structures. These approximations aid in the examination of resonances and other spectral phenomena. Their regions of accuracy and validity are determined.

The assumption of perfect conductivity is relaxed in a formalism which is described for dielectric and lossy metallic surfaces. The method is tailored specifically to the rectangular-groove profile and is one of the few modal expansion techniques appropriate to non-perfectly conducting gratings.

The thesis concludes with the presentation of two formalisms which employ an impedance-related condition to completely specify a set of modal functions. The first formalism prescribes a solution for a grating whose grooves are semi-circular in cross-section. Eigenfunctions for a circular waveguide constitute the modal functions. The second formalism accommodates reflection profiles of general groove cross-section, and utilizes a superposition of the rectangular-waveguide eigenfunctions. The first formalism is employed to evaluate in detail the spectral performance of the semi-circular groove grating, while the second is applied, not only to this grating, but also to the triangular and sinusoidal groove gratings.
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Chapter 1

INTRODUCTION

Since high-speed computers were introduced in the early 1960's, rigorous electromagnetic theories have been developed to the stage where they can successfully account for the diffraction properties of virtually any kind of grating. This includes gratings of arbitrary profile and conductivity, as well as multi-layered and doubly-periodic structures. Hence there is little need for new formalisms if it is desired only to perform numerical calculations with, for example, the aim of optimizing profile parameters. However, it is worthwhile to develop additional theories if by so doing we can improve our general understanding of the spectral behaviour of gratings. This has been the basic motivation behind the work presented in this thesis, which is concerned with the efficiency and energy distribution of plane singly-periodic reflection and transmission gratings. We are not concerned with their spectroscopic properties. The underlying theme therefore, is the rigorous application of Maxwell's equations, in conjunction with the appropriate boundary conditions, to model the classical diffraction process.

The majority of currently available diffraction theories are based on methods in which the mechanism of this process is lost in a complexity of mathematics. The methods employed in this thesis help to remove this deficiency by being less intricate and easier to implement numerically. They also provide the theorist with a clearer picture of the dynamics of the physical problem. Termed modal expansion methods, they reduce the problem to one of field matching between regions where the electromagnetic field is everywhere describable by known series expansions.
One objective of this thesis has been the development of a modal expansion formalism which is capable of dealing with gratings of arbitrary profile. Although this goal has not been completely achieved, it is felt that substantial progress has been made. Also, in the course of investigations leading towards this goal, significant contributions have been made to the general understanding of grating phenomena.

In serving as an introduction to the field of grating theory, this chapter is confined to a brief description, since many comprehensive reviews of what has developed into a rich speciality are now available [1.1-1.4]. Section 1.1 discusses the nature of the diffraction problem and explains many of the concepts and terms which are used at various stages throughout the thesis. Some of the early attempts at solving the problem are also mentioned and this is followed in Section 1.2 by a review of the more important theories that have led to those in use today. These are predominantly integral and differential methods and it is hoped that sufficient detail is given to enable the reader to perform a comparison between those methods and the modal expansion methods used in this thesis.

The only modal technique not to be discussed in detail in Chapters 2 to 7 is that of Jovicevic and Sesnic [1.5], and so to form a complete coverage of this type of approach for singly-periodic structures, the essence of their method is described in Section 1.3. The final section of this chapter summarises the contents of the remainder of the thesis and puts the methods used in perspective with those described in Section 1.2.

It should be noted, that throughout the thesis, emphasis is on the theoretical aspect of gratings. Information with greater relevance to the manufacture and experimental use of gratings may be obtained from, for example, references [1.1, 1.4, 1.6, 1.7].
1.1 INTRODUCTION TO GRATING THEORY AND DEFINITION OF TERMS

1.1.1 The Grating Equation and Diffraction Problem

For the purposes of this thesis, a grating is assumed to be a plane structure which extends "infinitely" in both directions in its plane, and which has a profile function periodic in one direction. The convention adopted here is that the grating lies in the xz-plane with the grooves parallel to the z-direction. The profile function is then given by \( y = f(x) = f(x+d) \), where \( d \) is the grating period.

Although gratings had been known for some thirty years earlier, the origin of systematic grating studies is associated with the work of Fraunhofer, who in 1821 described the dispersive action of gratings by the now well-known classical "grating equation",

\[
\sin \theta_p = \sin \theta + \frac{p \lambda}{d} \quad p = 0, \pm 1, \pm 2 \ldots \quad \ldots (1.1)
\]

where \( \lambda \) is the wavelength of the incident radiation, \( \theta \) is the angle of incidence and \( \theta_p \) is the angle of propagation of the \( p^{th} \) diffracted order. In the form taken by equation (1.1), \( \theta \) is positive if measured in an anti-clockwise sense from the grating normal and \( \theta_p \) is positive if measured in a clockwise direction from the same line.

The term "diffraction problem" refers to the problem of determining the distribution of incident wave energy into the various directions defined by equation (1.1). This distribution is a function of \( \lambda, \theta, \) the function \( f(x) \), and the grating material.

In this thesis consideration is only given to gratings in a classical mounting configuration. This is the mounting most commonly used in practice, and is defined as one in which the wave-vector of an incident plane wave lies in the plane orthogonal to the direction of the grooves.
The alternative to this type of mounting is the conical diffraction mounting in which the wave-vector lies out of this plane and the diffracted-order wave-vectors lie on the surface of a cone.

For the classical configuration described above it is meaningful to speak of two orthogonal cases of polarization. These are termed (i) **P** polarization \((\mathbf{E} = E_z \hat{z})\) where the electric field vector of the incident wave is aligned parallel to the grooves, and (ii) **S** polarization \((\mathbf{H} = H_z \hat{z})\) where it is the magnetic field whose sole non-zero component is parallel to the grooves. In the literature these are often referred to as **E//** and **H//**, or less commonly, TE and TM polarizations respectively. By framing the diffraction problem in either one of these two polarizations, it is necessary only to consider the \(z\)-component of the field, which must then satisfy three basic conditions. These are the two-dimensional Helmholtz equation, the boundary conditions which must be satisfied on the grating surface and the outgoing-wave condition (Sommerfield Radiation condition [1.8]).

(For a perfectly-conducting surface, S and P polarizations are referred to as the fundamental polarizations since the solution to the conical diffraction problem can be recovered from the S and P solutions [1.4].)

For the majority of cases discussed in this thesis the grating surface is assumed to be perfectly conducting. It then supports a surface current \(j_s\) where \(\mathbf{n} \times \mathbf{H} = j_s\), \(\mathbf{n}\) being a unit vector normal to the grating surface. The condition specifying continuity of \(\mathbf{n} \times \mathbf{E}\) reduces in the case of P polarization to a Dirichlet boundary condition, \(E_z = 0\) on the grating surface. For S polarization it reduces to a Neumann boundary condition, \(\partial H_z / \partial n = 0\). For the case of finite conductivity (a surface of complex refractive index) or lossless dielectrics (a surface of real
refractive index) the boundary conditions require that both \( \mathbf{n} \times \mathbf{E} \) and \( \mathbf{n} \times \mathbf{H} \) be continuous across the surface, since no surface charge or currents reside there.

The outgoing-wave condition requires that at infinity the scattered field be bounded and consist only of terms relating to outgoing waves. Coupled with the boundary conditions this specifies a unique solution to the incident field and hence a unique solution to the diffraction problem. (A discussion of the mathematics associated with the uniqueness of such a solution can be found in Chapter 2 of reference [1.4].)

Consider then a plane wave \( \mathbf{E}^i(x,y) \) to be incident on the grating at an angle \( \theta \). Suppressing the temporal dependent term \( \exp(-i\omega t) \), this wave can be expressed in the form

\[
\mathbf{E}^i(x,y) = \exp[i(\alpha_0 x - \chi_0 y)],
\]

where \( \alpha_0 = \frac{2\pi}{\lambda} \sin \theta \) and \( \chi_0 = \frac{2\pi}{\lambda} \cos \theta \). The function \( \mathbf{E}^i(x,y) \) is said to be "pseudo-periodic" in the sense that it obeys the relation

\[
\mathbf{E}^i(x+d,y) = \mathbf{E}^i(x,y) \exp(i\alpha_0 x).
\]

If \( \mathbf{E}(x,y) \) represents the total field, then by defining \( \mathbf{E}^d(x,y) = \mathbf{E}(x,y) - \mathbf{E}^i(x,y) \) it can be shown as a consequence of uniqueness that \( \mathbf{E}^d(x,y) \exp(-i\alpha_0 x) \) is a periodic function of \( x \). That is, it also obeys the pseudo-periodicity relation

\[
\mathbf{E}^d(x+d,y) = \mathbf{E}^d(x,y) \exp(-i\alpha_0 x),
\]

where the grating is assumed infinite in extent.

By expressing \( \mathbf{E}^d(x,y) \) as an expansion of plane-wave terms of the form

\[
\mathbf{E}^d(x,y) = \sum_{p=-\infty}^{\infty} R_p \exp[i(\alpha_p x + \chi_p y)],
\]
where $\alpha_p = \frac{2\pi}{\lambda} \sin \theta_p$,

$$\chi_p = \begin{cases} 
\left(\frac{2\pi}{\lambda}\right)^2 - \alpha_p^2)^{\frac{1}{2}}, & \frac{2\pi}{\lambda} > |\alpha_p| \\
\alpha_p^2 - \left(\frac{2\pi}{\lambda}\right)^2)^{\frac{1}{2}}, & |\alpha_p| > \frac{2\pi}{\lambda}
\end{cases} \quad \text{(i)}$$

and $R_p$ are constant amplitudes,

then equation (1.3) reduces to

$$\alpha_p = \alpha_0 + \frac{2\pi p}{d},$$

which is simply another form of the grating equation given by equation (1.1). This derivation can be found in more detail in reference [1.4], but the first use of expansion (1.4) is attributed to Lord Rayleigh [1.9] and so it is termed the Rayleigh expansion. It represents the diffracted field away from the region of modulation of the grating and plays a key role in all formalisms presented in this thesis.

Condition (1.5), if $\chi_p$ is real-valued, corresponds to a real or propagating order of diffraction, while if $\chi_p$ is positive imaginary, it corresponds to an evanescent wave travelling parallel to the top of the grating (the x-axis). The positive sign given to $\chi_p$ ensures that the evanescent wave is damped exponentially away from the grating surface.

Only the real orders carry energy and the term "efficiency" in a particular order is defined as the energy propagating normal to the grating surface relative to the incident energy. For a lossless surface, energy conservation is therefore represented by the equation

$$\sum_p E(p) = 1, \quad (p: \chi_p \text{ real}) \quad \text{...(1.6)}$$

where $E(p)$ denotes efficiency in the $p^{th}$ order.

At this point it is also useful to define the frequently used terms "passing off" and "Rayleigh wavelength". Equation (1.1) shows that at
certain wavelengths, \( \sin \theta_p = \pm 1 \). Under these conditions the \( p^{th} \) order is grazing the grating surface during the transition from a propagating state to an evanescent state. The order is then said to be passing off and the wavelength is labelled a Rayleigh wavelength, \( \lambda_R \).

1.1.2 Scalar Theories

Dating back to the late 19th Century [1.10], the earliest theories devoted to solving the diffraction problem were based on Kirchoff's scalar theory. These scalar theories clearly pre-dated the computing age. Nevertheless, they maintained viability by formulating efficiency predictions in a closed form. However, this advantage was offset by the general deficiency of scalar theories, which is their failure to take account of the polarization of the incident wave. That is, they yield identical results for both S and P polarizations, whereas it has been known from early experimental evidence that gratings are capable of quite pronounced polarizing properties.

This inability to distinguish between the fundamental polarizations is sometimes not deleterious. This is true for coarsely-ruled gratings where the normalised wavelength \( \lambda/d \) is less than 0.1. For the visible region this upper limit may be raised to 0.4 if the groove depth is sufficiently small. Most experimental usage of gratings requires however, normalised wavelengths in excess of the above values, thus curtailing the usefulness of the scalar theories.

More recently, attempts have been made to improve their performance [1.11, 1.12], including an attempt in the latter reference to include polarization effects. Nevertheless these theories remain non-rigorous and the need for "exact" vectorial theories is clearly evident. This is especially so in regard to the prediction of diffraction anomalies,
phenomena which comprise a rapid fluctuation in the spectral energy
distribution. In the past these phenomena have served as a "litmus test" for
the accuracy of a theory.

A detailed discussion of anomalies is given in Chapter 3, while an
outline of the modern vectorial theories is given in Section 1.2.

1.1.3 Properties of the Field Amplitudes

Clearly with any new theoretical formalism there exists the need to
verify its validity and also the accuracy of its numerical predictions.
These may often be checked through the comparison of results with those
furnished by alternative formalisms, and by experiment, for example in the
region of anomalies. However, neither of these avenues guarantees complete
confirmation of validity and so one desires tests which are more rigorous.

Two such tests exist which are very powerful and which have become
fundamental to the validation of new grating theories. The more obvious of
these is the Law of Conservation of Energy while the other is termed the
Theorem of Reciprocity.

Conservation of Energy was instrumental in revealing the faults which
existed with the early scalar theories. This law has been discussed in
several papers, including references [1.13-1.15]. The first of these by
Petit describes the form it takes for perfectly-conducting gratings and
which is used throughout the thesis.

The Theorem of Reciprocity is an extremely useful tool for the grating
theorist and is discussed in the case of infinite conductivity by Petit
[1.14], Uretsky [1.15], Maystre and Petit [1.16] and Fox [1.17]. The
Theorem has been extended to deal with finite conductivity by Maystre and
McPhedran [1.18] and to deal with transmission gratings by Neviere and
Vincent [1.19]. The ramifications of the Theorem are as follows.
Assume a plane wave is incident on a grating at an angle $\theta$ such that it gives rise to a $p^{th}$ diffracted order at an angle $\theta_p$ and with efficiency $E(p)$. Then if another wave is returned with angle of incidence $-\theta_p$, its $p^{th}$ order emerges at an angle equal to $\theta$ and it also has efficiency equal to $E(p)$. A corollary of the Theorem states that the efficiency of the $0^{th}$ reflected order is invariant with respect to a $180^\circ$ rotation of the grating in its own plane, irrespective of any asymmetry in the grating profile. For dielectric transmission gratings, such as those discussed in Chapter 5, a returned transmitted order must maintain the same wavelength in the dielectric, and of course this will differ from that of the original incident radiation.

Many examples of the numerical application of the above two criteria are given throughout the thesis. In particular, they are used as crucial tests for new formalisms in Chapters 4, 5, 6 and 7. They also confirm the accuracy of calculations provided by a known formalism in Chapter 2.

A third type of test is also available to be used in conjunction with reciprocity and conservation of energy. Termed "symmetry properties" [1.20], these criteria are not as widely applicable as the previous constraints since they only pertain to lossless structures which possess some geometric symmetry in their groove profile. Their use is in being able to inter-relate the phases and moduli of both real and evanescent field amplitudes. A comprehensive description of these properties is deferred to Chapter 2.

1.1.4 The Littrow Mounting

The Littrow mounting is a classical mounting configuration used widely by spectroscopists and is also adopted extensively throughout this thesis to illustrate properties and performances of various gratings. The Littrow mounting in order $n$ is defined as one in which the $n^{th}$ order (the order of
interest) is diffracted with wave-vector equal and opposite to that of the incident wave. (For reasons of practicality, near-Littrow mountings are often used with a small angular deviation between these two directions [1.21], however this variation is not considered here.) Equation (1.1) implies that the angle of incidence for such a mounting is given by

$$\sin \theta = -\frac{n\lambda}{2d} \quad \cdots (1.7)$$

while the angles of diffraction are

$$\sin \theta_p = \frac{\lambda}{d} (p- \frac{n}{2}). \quad \cdots (1.8)$$

Littrow spectra thus consist of a coupled variation in wavelength and angle of incidence. It is noted that $n$ must necessarily denote a "negative" order, if $\theta$ is to be positive.

From the above equations it is seen that the sines of the two angles of incidence involved in the Reciprocity Theorem for a particular order, are symmetrical about the sine of the Littrow angle for that order, i.e. $-\frac{n\lambda}{2d}$. The implication is that the efficiency in a particular order, as a function of $\sin \theta$, is symmetrical about $-\frac{n\lambda}{2d}$.

The main reason behind the extensive use of the Littrow mounting is its optimal blazing capability. It is normally used in the wavelength region where only two orders are propagating. In a more pronounced fashion than the other classical mountings, it has the ability to preferentially distribute energy into the single diffracted order. This is especially true for $S$ polarization. The application of the Marechal-Stroke [1.22] and Reciprocity Theorems, to the right-angled triangular-groove grating, shows in fact that 100% blazing is attained for two wavelengths for a perfectly-conducting surface. These are termed blaze wavelengths, $\lambda_B$. References [1.23-1.26] demonstrate that a similar phenomenon exists for holographic, general triangular and rectangular-groove gratings, even though these are not subject to the Marechal-Stroke Theorem.
The studies of Chapters 3 and 4 demonstrate the interesting qualities of the Littrow mounting, both from a theoretical point of view and because it gives rise to prominent resonance anomalies. These qualities stem from the symmetrical nature of the mounting, i.e. the fact that two orders pass off simultaneously. (This is seen from equation (1.8) for \( p = q \) and \( p = -q - 1, q = 0, 1, 2, \ldots \).) This symmetry also enables the scattering matrices as well as other series terms in the modal formalisms to be greatly simplified.

1.2 MODERN GRATING THEORIES

1.2.1 The Rayleigh Method

This section is concerned with the first class of formalisms to be based on a series expansion approach to the diffraction problem. This was the earliest vectorial treatment to be devised, being introduced by Lord Rayleigh in 1907 [1.9]. His "dynamical theory of gratings" was founded on the premise that a plane-wave expansion (the Rayleigh expansion of equation (1.4)), which satisfies the Helmholtz equation and the outgoing-wave equation, could be used to represent the field in the entire free-space region up to and including the grating surface. Rayleigh experienced some success with the method by providing reasonable agreement with experimental results, especially with regard to anomalies.

Subsequent theories based on the Rayleigh assumption were derived by numerous authors including Meecham [1.27], Stroke [1.28], Bousquet [1.29], and Petit [1.30]. By implementing numerical techniques such as Point-Matching (P.M.M.) and Fourier Series Methods (F.S.M.) they were able to satisfy the necessary boundary conditions and hence solve for the field amplitudes from a truncated set of linear equations.
The above theories were developed in spite of objections to the methods by Lippmann [1.31]. He proclaimed as invalid, the assumption that the groove-region field could be expressed in terms of outgoing-wave contributions only. His arguments were not rigorous however, since it was known the Rayleigh expansion was entirely valid for the right-angled echelette grating in the Marechal-Stroke configuration [1.22].

It was soon found that unacceptable results were produced by the Rayleigh method for gratings with deep grooves. Petit and Cadilhac [1.32] showed that the method is not valid for sinusoidal profiles if the groove depth $h$ exceeds 0.14$d$. In accord with this result, Millar [1.33] showed the Rayleigh hypothesis is valid if $h < 0.14$d. Nevertheless, confusion still reigned on the general validity of the Rayleigh method. This question has now been put on a firm footing however, and is summarised in papers by Millar [1.34] and Van den Berg and Fokkema [1.35].

Consider $y = f(x)$ to represent the groove profile and let the solution to the appropriate boundary value problem be expressed in terms of a convergent series of plane waves. Then if $f(x)$ is an analytic function, allowing the possibility of analytically continuing the solution down to $y = \min f(x)$, the expansion will converge to the actual field for $y > f(x)$. The condition is however, that no singularities in the analytic continuation of the solution can exist in the region $y > \min f(x)$. Thus the validity or otherwise of the hypothesis depends on the location of these singularities. Studies in this direction have been conducted by Millar [1.36] and Neviere and Cadilhac [1.37].

Van den Berg and Fokkema [1.35] developed a method for testing the validity of the Rayleigh hypothesis for gratings with analytic profile, functions. Their conclusions confirm the earlier results of Petit and Cadilhac [1.32] and Millar [1.33] with regard to the sinusoidal profile and they show that the hypothesis is never valid for strict triangular profiles (unless of course the Marechal-Stroke condition applies) or the
rectangular profile. In fact, it never holds for gratings with "corners".

One concludes then, that although the earlier objections to Rayleigh's assumption have proven to be realistic, they were not founded on the correct reasons. That is, it is not always mandatory for downgoing waves to be included in the groove region.

Despite the above controversy, it is to be noted that a method has emerged which is a variation on Rayleigh's method and which is potentially viable. It utilizes the least-squares technique. The earlier attempts at solving the boundary value problem used P.M.M. and F.S.M. methods and these are now known to be unacceptable if the Rayleigh assumption is invalid. Millar [1.34] has shown however, that if the boundary values are satisfied in a least-squares sense, then a linear combination of plane-wave terms is able to converge uniformly to the exact field for $y > f(x)$ and to also satisfy the boundary conditions. Whereas this expansion agrees with the Rayleigh expansion when the Rayleigh hypothesis is valid, it differs from it when the latter is not valid. The success of the method relies on the completeness of the expansion functions in a least-squares sense on the grating surface.

Although Meecham [1.27] and Ikuno and Yasuura [1.38] have implemented least-squares techniques for echelette and sinusoidal gratings, it appears that these series approaches remain inferior to the methods described in following sections and so their use today is uncommon.

1.2.2 Integral Theories

Coinciding with the growing criticism of the Rayleigh method, a new type of approach based on an integral equation was developed. This was to lead to the first rigorous and general solution of the grating diffraction problem. Unlike the Rayleigh expansion, the integral representation for the field is valid for all points $y > f(x)$. The integral equation is
obtained by applying Green's Theorem to the solution via an appropriate Green's function. This function can either take the form of the free-space Green's function with integration on an infinite interval, or a periodic Green's function can be used directly, thus restricting integration to a single period.

The method was initiated by Petit and Cadilhac [1.39] and Petit [1.40], and was concerned with perfectly-conducting gratings for P polarization. They formulated the boundary value problem as a Fredholm integral equation of the first kind, where the unknown function was related to the surface current density. The integral equation was solved using a Fourier series technique, which proved to be numerically unwieldy except for profiles consisting of linear facets. The method did provide the first reliable results for deep triangular profiles. Other authors to work with the integral approach at about the same time were Wirgin [1.41] and Uretsly [1.15].

Petit [1.42] established a corresponding technique for S polarization. However its validity was in some doubt, and so it was the papers of Pavageau et al. [1.43] and Pavageau and Bousquet [1.44] which contained the first numerically successful formulation for S polarization. Involving the same unknown function of the previous theories, the latter method required the solution of a Fredholm equation of the second kind. An iterative method was chosen for the numerical solution and it had the advantage over the F.S.M. of being more readily applied to arbitrary profiles. Since then, the P.M.M. has been found superior to either the F.S.M. or the iterative technique [1.6, 1.45].

Extension to the case of conical diffraction requires a pair of integral equations and was performed by Maystre and Petit [1.46] and Van den Berg [1.47].
A major advance was the extension of the integral method to treat finitely-conducting surfaces. This step was very significant in the light of evidence that the infinite-conductivity model breaks down in the visible region [1.48]. Early work was carried out by Neureuther and Zaki [1.49] and Van den Berg [1.50], who formulated the problem in terms of two coupled integral equations involving two unknown functions, namely the field and its normal derivative at the surface. This method had the disadvantage of requiring substantial computing resources. A second and more elegant approach needing far less computing time was developed by Maystre and Vincent [1.51], initially for diffraction by a finitely-conducting or dielectric cylinder and then for metallic gratings [1.52-1.54]. In this method the previous two integrals are replaced with a single integral equation (involving double integrals) in one suitably-chosen unknown function analogous to the surface current density of the infinite-conductivity case. Able to account for gratings of arbitrary profile, with and without corners, and for low and high conductivity, this technique is clearly preferable to any other.

The versatility of the integral method has more recently been demonstrated by solving the diffraction from dielectric coated gratings [1.55, 1.56] and bimetallic gratings [1.57]. It is to be realized, that at this stage the grating formalism has reached a point of high complexity and sophistication, far removed from simple physical concepts.
1.2.3 Differential Theories

The Rayleigh method is differential in nature since it is based on a solution of a second order partial differential equation (the Helmholtz equation). However, the term "differential theory" is normally only applied to that class of rigorous formalisms which were established around ten years ago, at about the same time as the integral theories. By contrast with the latter, the differential method was initially applied to the case of a non-infinitely conducting surface.

Having been originally suggested by Petit [1.58], the technique was first implemented by Cerutti-Maori et al. [1.59] and later improved by Nevière et al. [1.60]. Although good results were obtained for dielectric materials, numerical difficulties were experienced for highly-conducting gratings in S polarization. Further application included the study of dielectric-coated metallic gratings [1.61].

The differential method used by the above authors is based on the direct application of the Helmholtz equation to the diffracting region. After expressing the field as a Fourier series, projection of this equation onto the plane-wave basis functions leads to an infinite system of coupled differential equations. These must be solved subject to the appropriate boundary conditions. This solution demands very cautious numerical integration. The method also requires the use of a Fourier series to represent the variation of refractive index across the region of modulation and it is the convergence of this series which has posed certain numerical problems.

It was only in the early 'seventies that differential formalisms were adapted to deal with perfectly-conducting gratings. Developed by Nevière et al. [1.62] for arbitrary profiles, the technique employs a conformal transformation of the profile to more easily accommodate the boundary conditions. (This transformation is necessary since a Fourier series can no longer cope with infinite changes in permittivity of the metal.)
Iteration techniques have been used to establish the appropriate transformations for various profiles [1.63, 1.64]. A disadvantage of the method is the resultant complication of the wave equation. Just as in the finite-conductivity case, a system of second-order differential equations is integrated numerically to give the final solution.

Through implementation of the conformal transformation method, Nevière et al. [1.65] were able to provide the first predictions of the effect of a dielectric overlay on a grating. The differential method is perhaps more versatile than the integral method, having been applied to a wide range of structures, for example grating couplers [1.66]. While simpler, both theoretically and numerically than the integral approach, the differential method has nevertheless suffered from the numerical instabilities for high conductivity. The new integral theory of Maystre [1.56] has also removed much of the superiority it once enjoyed.

1.2.4 Modal Expansion Methods

Semi-analytic techniques based on modal expansions are also differential in nature. They are similar to the Rayleigh method in that the field is everywhere characterised by a series expansion of known functions with unknown coefficients. The difference is that different expansions are used for different regions. In the free-space region away from the grating, the outgoing plane-wave field is still represented by the Rayleigh expansion, but in the groove region the field is expanded in terms of mode functions which are closely related to the functions associated with waveguide theory. They therefore account for both outgoing and ingoing waves within the grooves. Matching the modal and plane-wave expansions at the appropriate interfaces leads to an infinite set of linear equations. These define what is termed the scattering matrix for the problem. After truncation, the unknown expansion coefficients are readily recovered from the inversion of this matrix.
The mode functions are solutions to the Helmholtz equation and we usually rely on orthogonality and separability properties of that equation to secure their analytic form. Thus, successful application of the method has been, to this date, limited to grooves of specific geometries for which the profile is parallel to a co-ordinate axis. In such cases the boundary conditions can be satisfied analytically, and if the mode functions are orthogonal on the interface, the Method of Moments [1.67] can be implemented in the field-matching process, i.e. the continuity of the field and its normal derivative can be projected onto the set of plane-wave functions or mode functions, whichever is appropriate.

The first grating profile for which a modal expansion technique yielded rigorous results was the rectangular or square-wave profile [1.68]. Using a Green's function approach, Wirgin [1.69] has presented a complete theory for infinite conductivity and both polarizations. A detailed discussion of subsequent analysis of this grating is given in Chapters 2 and 3. The treatment of non-infinitely conducting rectangular profiles has been carried out by Knop [1.70] and Botten et al. [1.71], the latter method being the subject of Chapter 5.

The second profile for which a modal method was implemented belongs to the triangular-groove or echelette grating. In 1972, Jovicevic and Sesnic [1.5] adopted an approach in which the mode functions were wedge solutions of the Helmholtz equation expressed in polar co-ordinates. Section 1.3 contains an outline of their method and includes a discussion of the controversy which has surrounded its validity for asymmetric triangular profiles.

The general problem of scattering by perfectly-conducting reflection gratings has been investigated by Fox [1.17]. He stipulates four desired properties of the mode functions, namely that they should (i) be real-valued, (ii) form a complete set of eigensolutions of the Helmholtz
equation on the groove region, (iii) form an orthogonal set on the groove aperture, and (iv) satisfy an impedance-type constraint on the groove aperture. Fox showed that accordance with these conditions assures unitarity of the scattering matrix and that the reciprocity condition is satisfied. His condition (iv) is closely related to a similar condition imposed on the mode functions in the formalisms of Chapters 6 and 7.

A grating for which a modal-related technique has been recently devised by Beunen [1.72], is the circular-wire transmission grating. This method is capable of handling both the lossless and lossy situations. It utilizes a least-squares approach [1.34, 1.73] to satisfy the boundary conditions at the interfaces between discrete regions, thus incorporating Millar's adaption of the Rayleigh method [1.34] into a modal treatment. When boundary conditions are not analytically satisfied, a least-squares treatment is often to be preferred to the P.M.M. or F.S.M. methods, and Beunen illustrated the success of the former method by showing that the discrepancies in the boundary values diminish as more expansion terms are included.

Although not of direct concern to this thesis, modal methods have been found ideally suited to doubly-periodic structures where they facilitate simpler numerical solutions than do alternative methods. Motivated by the possibility of using such structures as solar selective surfaces, Chen [1.74], McPhedran and Maystre [1.75] and Bliek et al. [1.76] have considered the diffraction by inductive grids with either square or round holes. Adams et al. [1.77] have also extended the two-dimensional rectangular-profile theory to account for a three-dimensional structure consisting of two spatially-separated rectangular-wire transmission gratings.
1.2.5 Miscellaneous Theories

There have been of course many diffraction theories proposed which do not fit into the above categories and it would be a formidable task to mention them all. Most are specialist approaches which are not widely applicable, for example the formalism of Itoh and Mittra [1.78] which is a waveguide-type approach that has only been applied to right-angled echelette gratings.

One treatment of the problem which has made a significant impact on the field, and which deserves mention, is the formalism of Hessel and Oliner [1.79]. Their method is not a practical one in the sense that one is unable to use it to make physical efficiency predictions. It has however, made important contributions to the study of the anomalous behaviour of gratings, and these are discussed in Chapter 3. The basis of their method is that the grating is replaced by a plane which is characterised by a periodic surface reactance. Above this plane the field can be readily expressed in terms of the Rayleigh expansion. The appropriate reactance values can, however, only be deduced from a complete knowledge of the tangential electric and magnetic fields along the top of the real grating. Neviere et al. [1.80] demonstrated that even estimates of the surface impedance are insufficiently accurate for most problems and so the method appears doomed from a practical viewpoint.

A very recent formalism which is generally applicable, has been published by Chandezon et al. [1.81]. Although differential in nature, this approach contains fundamental differences from the formalisms described in Section 1.2.3. Using a transformed co-ordinate system to map the grating profile onto a plane, and expressing Maxwell's equations in covariant form, they obtained a system of linear partial differential equations with constant coefficients. The numerical problem is reduced to one of solving an eigenvalue problem of a matrix whose elements are known
in closed form. To date only the results for perfectly-conducting gratings have been given and these are in good agreement with those of the integral method.

1.3 THE METHOD OF JOVICEVIC AND SESNIC

Since this thesis attempts to present a complete picture of modal formalisms for singly-periodic gratings, it is appropriate to include here an outline of the method employed by Jovicevic and Sesnic [1.71] for the echelette grating.

The grating they consider is assumed to be perfectly conducting and to have a triangular profile. Both rectangular and polar co-ordinate systems are used, as shown in Figure 1.1. Treating the case for \( P \) polarization first, the total field above the grating \( E_R(x,y) \) is equal to the sum of the incident wave \( E^I(x,y) \) and a series of outgoing plane-waves \( E^d(x,y) \) represented by the Rayleigh expansion (see equations (1.2) and (1.4)).

Within the groove region, where the boundary conditions specify that the field must vanish for \( \theta = \alpha \) and \( \theta = \beta + \alpha \), the field derives its angular dependence from the functions

\[
\sin\left(\frac{m\pi}{\beta} \left( \theta - \alpha \right) \right) \quad m = 1, 2, \ldots \quad \ldots (1.9)
\]

Substitution into the Helmholtz equation then secures for the total electric field a modal expansion in terms of Bessel functions of the first kind, namely

\[
E^M(r,\theta) = \sum_{m=1}^{\infty} a_m u_m(r,\theta) = \sum_{m=1}^{\infty} a_m J_\nu(kr)\sin(\nu(\theta - \alpha)) \quad \ldots (1.10)
\]

where \( \nu = \frac{m\pi}{\beta} \) and the \( a_m \) are the unknown amplitudes of the mode functions \( u_m(r,\theta) \).
Figure 1.1 The geometry of the diffraction problem considered by Jovicevic and Sesnic [1.5].
These amplitudes are determined by invoking the conditions of continuity of the electric and magnetic fields along \( y = 0 \) for \(-c < x < d-c\), where the latter condition is tantamount to the continuity of the \( y \)-derivative of \( E \). The former continuity condition is resolved by projecting it onto the plane-wave functions \( \{\exp(i\alpha x)\} \), which form an orthogonal set on the interval \(-c < x < d-c\). Because the Bessel function has no useful orthogonality properties, the Method of Moments is not applicable. Jovicevic and Sesnic chose to enforce the continuity of the field derivatives by expressing the equation in rectangular coordinate form and multiplying both sides by \( J_{\mu}[k(x^2+h^2)^{\frac{3}{2}}] \) where \( \mu = \frac{2\pi}{\beta} \), \( \lambda = 1,2,... \). The result is then integrated over the groove aperture.

The above choice of sampling function is claimed to yield a higher rate of convergence of the resulting inner-product terms than do alternative functions. The final solution is obtained by combining the above two equations to produce an infinite set of linear equations. Truncation and inversion of this system yields the modal amplitudes \( a_m \), from which the order amplitudes and hence efficiencies can be recovered.

For \( S \) polarization the analysis is similar, with the groove region field being given by

\[
H^M(r,\theta) = \sum_{m=0}^{\infty} b_m J_\nu(kr) \cos[\nu(\theta-\alpha)]. \tag{1.11}
\]

Jovicevic and Sesnic complement their theoretical presentation with a set of calculated efficiency curves for both polarizations. The majority of their results are for right-angled echelettes, since \( \beta = \pi/2 \) implies the Bessel functions are of integral order, thus ensuring easier numerical computation.

They subjected their calculations to two numerical tests. These are energy conservation and the agreement of the positions of anomalies with the Rayleigh wavelengths. The latter is certainly not a rigorous test and
no mention is made of the Reciprocity Theorem which is more powerful. As it happens, their results do not precisely satisfy energy conservation and this they attribute to insufficient terms in the expansions.

As regards reciprocity, they have presented a curve (figure 9 of their paper) which is not in agreement with the corollary of the Theorem as discussed in Section 1.1.3. These discrepancies prompted some authors, including Petit [1.3], to question the validity of the method in the case of profiles asymmetric about the y-axis. Petit suggested that the method, when applied to such profiles, placed undue constraints on the field outside the groove region. Maintaining support for their method, Jovicevic and Sesnic stated in a subsequent paper [1.82] that their original calculations contained an error in integration limits. Having verified that reciprocity should be satisfied by modal methods, Fox [1.17] also judges numerical errors to be at fault. He disputed Petit's argument, pointing out that although the modal expansion converges outside the groove region, it is not bound to agree with the field there. The method does conform with the conditions stated by Lewis [1.83], that both field representations are valid and complete at the common boundary.

1.4 CONTENTS OF THE THESIS

One aim of this thesis is to demonstrate that modal expansion methods are attractive in providing a complete knowledge of field behaviour in the groove region. Unfortunately, this advantage is countered by their lack of versatility when compared with the methods described in Section 1.2. Thus, to a large extent, the work presented here has also been motivated by the desire to generalise the modal technique to account for diffraction by arbitrary profile gratings. With these two goals in mind, investigations have been carried out into the properties of existing formalisms, while some new specialized ones have also been developed. This thesis concludes
with a description of studies into a new formalism for general profile reflection gratings.

In the investigations, much emphasis is placed on the study of the anomalous behaviour of gratings, since this is one area in which modal methods are proving to be superior to the alternative methods of Section 1.2. The analyticity they provide for the field representations facilitates a better understanding of the causes of anomalies. With regard to the class of anomalies referred to as resonance anomalies, the concept followed throughout this thesis is that these phenomena originate from singularities in the modal amplitudes. These in turn produce singularities in the diffracted order amplitudes. A detailed knowledge of the fields in the groove region is therefore required and this is where integral and related theories furnish little information.

Chapter 2 introduces the reader to the rectangular-profile or lamellar grating and describes what has evolved to be the most efficient formalism for that grating in the case of perfect conductivity. The formalisms are based on the Method of Moments, and are given for both reflection and transmission gratings and for both fundamental polarizations. A set of symmetry properties relating field amplitudes and phases is derived as these prove useful for checking not only the lamellar grating results, but also those of the formalisms described in subsequent chapters. Efficiency results are presented and conditions given for when these may be accurately calculated using modal expansions containing only one or two terms. This search for simplified models stems from similar motives to those of such authors as Ulrich [1.84] who have investigated the potential of equivalent circuit models.

The treatment used in Chapter 2 is exploited in Chapter 3 to analyse in detail the dynamical behaviour of the lamellar grating. The work on resonance anomalies was done in collaboration with J.R. Fox and I.J. Wilson
and culminated in the publication of two papers [1.85, 1.86]. The properties of the structure are discussed in terms of the individual modal amplitudes, which possess singularities at complex wavelengths. It is proposed that these singularities are dynamical entities, fundamental to determining the spectral characteristics of the grating. Furthermore, it is suggested that since all gratings exhibit essentially similar behaviour, they too should be thought of in terms of mode resonances. Evidence to support this is given in the form of some complex resonance pole positions found for a few alternative profiles.

In Chapter 4, the author takes advantage of the simple lamellar theory to study the behaviour of slightly more complex singly-periodic structures which have rectangular geometries. The first of these has been called the bottle grating as a result of its unusual groove profile. Its interesting properties, similar to those of a Fabry-Perot interferometer, have been recently reported by the author [1.87]. The second device appears not to have been studied previously and so this was briefly investigated to enable a comparison of its performance with the bottle grating. It consists simply of a lamellar transmission grating placed close to a perfectly-reflecting mirror. The third structure is again a reflection grating but this time consisting of an arbitrary number of right-angled steps of almost arbitrary dimension. Through an appropriate choice of steps, surprisingly not very great in number, it is shown that such a grating is quite capable of modelling the behaviour of many of the conventional gratings.

The afore-mentioned chapters have all dealt with the case of perfect conductivity and this constraint is relaxed in Chapter 5. Working in collaboration with L.C. Botten, M.S. Craig, R.C. McPhedran and J.L. Adams [1.70, 1.88] a model formalism has been developed which rigorously accounts for the diffraction of both lossless dielectric and lossy metallic lamellar gratings. The mode functions are related to those of the infinite-
conductivity case and are solutions of the differential equation gained from the wave-equation subject to the necessary boundary and pseudo-periodicity conditions. For the dielectric case the self-adjoint nature of the problem leads to an orthogonal set of modes, while for metallic gratings the problem is simply adjoint and the modes obey a bi-orthogonal relationship. The numerical implementation involves the solution of a transcendental eigenvalue equation followed by the determination of the amplitudes from an infinite set of linear equations.

In Chapter 6 attention is directed away from the rectangular geometries, and towards a reflection grating whose grooves are semi-circular in cross-section. The aim of the study was twofold - firstly, to investigate the blazing properties of this uncommon profile, and secondly, to test the viability of a new impedance eigenvalue condition through its inclusion in a modal approach. The mode functions are established from the eigenfunctions for a circular waveguide, i.e. in terms of Bessel functions of the first kind. The numerical calculation involves the solution of a straightforward eigenvalue problem and the subsequent solution of a system of linear equations. The efficiency results are quite interesting, showing very high blaze performances for $S_p$ polarization. Their excellent agreement with numerical tests and the results of an integral formalism indicate that the impedance condition is a suitable means of specifying the modal field.

Chapter 7 deals with the use of the same impedance condition in the establishment of a modal expansion appropriate to perfectly-conducting gratings with grooves of arbitrary cross-section. In this case however, the mode functions are based on the eigenfunctions of the rectangular waveguide and the resulting eigenvalue problem proves to be numerically unstable, especially for deep grooves. The formalism does, however, provide acceptable results for gratings of shallow to moderate groove depth, depending on the profile concerned.
The work of both Chapters 6 and 7 was carried out in collaboration with R.C. McPhedran and G.H. Derrick and has been reported in two recent papers [1.89, 1.90].
REFERENCES


Chapter 2
THE INFINITELY-CONDUCTING LAMELLAR GRATING

2.1 INTRODUCTION

Having the simplest and most straightforward profile for which a modal expansion technique can be implemented, the lamellar (rectangular-groove) grating presents itself as the obvious starting-point for an investigation into the general application of modal methods to singly-periodic diffraction gratings. This chapter is the first of two which deal with an extensive study of various aspects concerning both the lossless lamellar reflection and lossless lamellar transmission gratings, whose structures are depicted in Figures 2.1 and 2.2 respectively. These aspects include symmetry properties and resonance phenomena associated with the field amplitudes as well as general efficiency behaviour and blazing characteristics. It is suggested that the many interesting features revealed from the analysis of the theory and performance for this particular profile indicate directions to follow in the development of modal representations applicable to other grating profiles.

One of the first theoretical treatments given to the lamellar grating was that of Deriugin [2.1, 2.2]. However his method is not valid when the grating period is an integral multiple of the groove width. The problem was put on a rigorous basis when Wirgin [2.3-2.6] used a Green's function method to justify the modal expansion which has since become widely accepted by authors as the means to explicitly represent the field in the rectangular-groove region.

In 1971-72, De Santo [2.7, 2.8] presented a solution to the problem for a special type of lamellar profile and for the two cases of P and S polarization. The structure he considered has a surface which consists of an infinite number of infinitesimally thin vertical plates of finite depth, i.e. it is a lamellar surface where the groove width (c) is equal
to the period (d). Following the matching of the standing-wave field in the apertures to the outgoing plane-wave field above the surface, De Santo employed a residue calculus technique to solve the resulting equations for the amplitudes, which become residues of a meromorphic function. The method is clearly more complex than that which is described in the following section and which has been confirmed to yield similar results if c is allowed to equal d.

(Note that in reference [2.9], Heath and Jull state that their modal formulation gives results appropriate to a flat plate for c = d, i.e. all mode amplitudes falling to zero. They had been restricted to setting c = 0.9999d for the thin-comb problem. This restriction has been found not to exist with the formulation presented in Section 2.2, where as expected, the modes do not vanish for c = d but reproduce De Santo's results precisely.)

Maystre and Petit [2.10] have introduced a slightly different formulation to that of Wirgin and this has been subsequently further improved [2.11, 2.12] by eliminating the need to use a relatively slowly converging Fourier series to match the modal field to the plane-wave field. What in fact has been used is a direct application of the Method of Moments and this forms the basis of the formalisms outlined in Section 2.2. Similar techniques have been implemented by Hessel et al. [2.13] and Heath and Jull [2.9].

One of the earliest reports containing quantitative efficiency measurements for the lamellar grating, is that of Palmer et al. [2.14] who used this particular profile to study diffraction anomalies. The results they obtained were also used by Wirgin [2.4] to compare with his theoretical predictions for S polarization. Although the measurements were taken in the millimetre-wave region, where the use of a perfectly-conducting model is justified, agreement with the theory was in some
instances quite poor. A probable explanation for this became apparent following the experiments of Deleuil [2.15] who took measurements for S and P polarizations, also in the millimetre-wave region. By slightly altering the groove parameters in the theoretical calculations based on Wirgin's formalism, he was able to significantly reduce the discrepancies between theory and experiment and hence gain encouraging results. This indicates the sensitivity that the spectra are able to show towards small deviations in profile shape.

In 1969, Wirgin and Deleuil [2.16] carried out further tests on the lamellar grating both theoretically and experimentally and obtained excellent conformity between the two sets of results, concluding that profile tolerances should be better than $\lambda/200$ to produce acceptable agreement between measurements and theoretical calculations. Their work was also able to reveal the very interesting spectral properties of the lamellar grating, including its high blazing performance compared with echelette gratings and its remarkable polarizing ability.

An area which has seen extensive practical use of a lamellar-type structure is far infra-red Fourier transform spectroscopy. In this long wavelength portion of the spectrum, say $1/\lambda < 50 \text{ cm}^{-1}$, the lamellar grating interferometer [2.17-2.20] has been found to yield superior performances when compared to the Michelson interferometer. An advantage it has over the latter is that it does not require a separate beam splitter, since both this task and the interferometric modulation are achieved with the interleaving facets which make up the grating and which control the groove depth. It also has the benefit of requiring less incident flux, and this is useful for wave numbers $< 30 \text{ cm}^{-1}$ where radiant energy from conventional sources is very weak. During early use of the lamellar interferometer, calculations were based on a simple scalar theory from which the fundamental action of the interferometer is derived. That is, the zero order intensity
varies with groove depth according to $\cos^2(kh)$ where $k = \frac{2\pi}{\lambda}$ is the wave number. Subsequently, Wirgin [2.21] has utilized the rigorous electromagnetic theory for the lamellar profile to examine more closely the behaviour of the interferometer and hence assess more accurately its regions of usefulness and its limitations. His findings revealed that the scalar theory is not a good approximation for wavelengths exceeding $d/10$ and that in many cases experimenters are using the lamellar interferometer for ratios of $c/\lambda$ which are far too small.

On the basis of the polarizing ability of the rectangular profile, Roumiguieres [2.22] has suggested a possible application of the symmetrical lamellar grating ($c/d = 0.5$) as a reflection polarizer in the infra-red region. Using a groove depth of $h/d = 0.275$ he has demonstrated theoretically that when unpolarized light strikes such a surface at an angle of incidence of $50^\circ$, with its wave vector orthogonal to the grooves and wavelength in the range $1.1 < \frac{\lambda}{d} < 1.7$, over 75% of the $P$ polarized light is reflected in the zero order. For $S$ polarized light it is less than 4%. In his report it was also shown that for this example, the groove dimensions are not critical, nor is the angle of incidence, for the above performance to be maintained. Tolerances up to 10% are acceptable and present technology is quite capable of producing such devices within these limits.

In fact, using photoresist techniques, Knop [2.23] has been able to reproduce the lamellar profile and fully confirm experimentally the predictions of Roumiguieres. To operate in the infra-red region, the metallic reflection gratings were made with a period $d = 7.72 \mu m$ and groove parameters within 2% of those mentioned above were achieved. More recently, Josse and Kendall [2.24] have also fabricated high quality lamellar gratings for use in the infra-red and visible wavelength regions. Their technique was photolithography and the anisotropic etching of single-crystal silicon. By taking advantage of the angles inherent in the silicon
crystal structure they have been able to obtain grooves with very flat faces and of consistent shape. With improvements in the manufacture of gratings by such methods as these occurring more frequently, it is anticipated that further experimental verification of the behaviour of lamellar gratings at short wavelengths will become increasingly possible.

An application of the lamellar transmission grating is also found in the field of photolithography, where contact masks which are approximately this shape are used in the production of integrated circuits. For large groove spacing, geometrical optics is all that is required to predict the masking action of the grating onto the photoresist underneath. However, in the fabrication of micro-circuits, where the groove parameters are of the same order as the wavelength, rigorous diffraction theory should be used. Such a problem formed the basis of a study by Roumiguieres et al. [2.25], who employed the theory of Maystre and Petit [2.10] to predict that theoretical difficulties with the mask duplication are encountered as soon as the grating period is less than 1 μ. Finite conductivity is an aspect which must also be considered at these wavelengths and this reduces the usefulness of the modal theories at their present level of development.

The sampling of high-powered laser beams has provided another avenue of application for the rectangular-groove profile. It is often necessary to be able to monitor the wavefront and phase of the beam and since most available beam splitters are unable to withstand the intensity, low efficiency gratings which diffract only a minute percentage of the incident energy, present themselves as an alternative. Using a model consisting of a lamellar grating of very low modulation and coated with gold (virtually a perfect conductor at gas-laser wavelengths) Loewen et al. [2.26] sought the optimum groove parameters and angle of incidence which would produce the desired properties of (i) an efficiency of about 1% in the -1 order, and (ii) minimal polarization dependence.
These factors are controlled in the following way. For low normalised groove depths \((h/d)\) efficiency is proportional to \(h^2/d^2\), while both efficiency and polarization are governed by the normalised groove width \((c/d)\). The conclusion of the above investigation was that normalised depths of about 0.01 are required for a \(\lambda/d\) ratio near 0.8 and an angle of incidence near 45°. Acceptable polarization independence was only found for a \(c/d\) ratio near 0.9, which is not altogether suitable in practical terms.

Elson [2.27] has also proposed a theory for low-efficiency gratings which involves a perturbation solution of Maxwell's equations. This method is only correct to a first order in \(h/\lambda\) and provides no change in polarization ratio when either \(h\) or \(c\) is varied. This is in disagreement with the work of Loewen et al. Elson adapted his method for the beam-sampling problem to the case of a shallow lamellar grating with dielectric overlays with the hope of simultaneously minimising energy absorption and polarization effects. The ability of such layers to withstand the intensity of the laser beam is, however, not well known.

A considerable amount of time has been spent over recent years investigating the blazing characteristics of the lamellar reflection grating from a computational point of view. The primary aim has been to endeavour to obtain simultaneous blazing for both polarizations, hence rendering the device useful for spectroscopic purposes. It should be noted that although the 90° echelette grating is one which cannot provide simultaneous blazing [2.42], the property is not confined solely to the lamellar profile.

Hessel et al. [2.13] conjectured that the Bragg condition (or Littrow condition, \(\lambda = 2d \sin \theta\)) is a necessary condition for blazing (attainment of 100% efficiency) in the -1 order in the case of perfect conductivity. In support of their proposal they have presented the results of a numerical survey in which, for constant groove widths, they have varied \(h\) for different angles of incidence until 100% efficiency is realized in the
-1 order. By plotting such a set of curves for both polarizations, simultaneous blazing is achieved for the groove parameters and angle of incidence specifying the intersection points. Roumiguieres et al. [2.28] repeated their experiment but produced more curves in the case of S polarization. They also plotted several efficiency curves corresponding to the specifications for dual blazing, and by utilizing integral formalisms were able to show that in the visible and UV regions of the spectrum, the lossy nature of real metals severely curtails the blazing properties. However, the overall results, which pertain to gratings with fairly large grooves (h/d > 0.6, c/d > 0.5) have indicated the possible application of such gratings in areas of filtering, mirrors for tunable lasers etc.

In the microwave region, the above blazing properties have been confirmed experimentally by Jull et al. [2.29], who proposed that a lamellar-type corrugation on the exterior of buildings would help eliminate unwanted specular reflections in the radio region of the spectrum. Heath and Jull [2.9] extended the examination of blazing phenomena by including both slot (small c/d) and comb (large c/d) gratings in the range of parameters they considered. In the former case blazing is not possible at all for P polarization while in the latter case dual blazing is theoretically possible at large angles of incidence, but the depths involved are large and the bandwidth is reduced. Close tolerances are also required on the groove dimensions.

The Littrow mounting again receives attention in a paper by Loewen et al. [2.30] in which is derived an asymptotic formalism for diffraction in the case of infinite conductivity. Valid only at short wavelengths and for gratings of shallow depth, their formulation assumes the field above the grating surface to be everywhere describable by a Rayleigh expansion of plane waves. They thus secure a simple analytic expression for the unknown amplitudes. Along with other groove shapes, this formula was applied to
the lamellar profile to calculate efficiencies in the -1 order. By forming comparisons with rigorous calculations they concluded that the asymptotic formalism yields good results up to a depth of h/d = 0.1. The simplified theory was also found to predict maximum efficiencies for groove widths equal to half a period.

This latter result was also the conclusion reached by Loewen et al. [2.31] when they used the rigorous electromagnetic theory to evaluate spectra for moderate groove depths. However, in this non-scalar situation the asymptotic formalism is only appropriate for S polarization efficiency, for which a blazing action superior to sinusoidal gratings could be attained. The P polarization blaze peak was shown to be narrower and hence inferior to those of other profiles. Their report concluded with a description of the effect on efficiency of finite conductivity and non-zero angular deviation - both of which detract from the performance.

Because the efficiency of the lamellar reflection grating compares unfavourably with blazed ruled and holographic gratings when used in unpolarized light, it is not likely to replace them for normal spectroscopic purposes. However, as mentioned above it has obvious specialist applications and is becoming easier to fabricate with higher groove densities and to within finer tolerances as technology improves.

The remainder of this chapter contains an outline of the modal expansion theory which has been employed to solve the scalar-wave diffraction problem for both the lamellar reflection and transmission gratings of infinite conductivity. Both of the two fundamental polarizations are considered. Section 2.3 details some symmetry properties pertaining to both types of grating as well as those with alternative profiles which also contain one or more axes of symmetry. These properties are later found useful both for checking the formalism and computer codes and for assisting in an analysis of the dynamics of the gratings.
Aspects of the theoretical implementation, such as numerical convergence, are given in Section 2.4. The subsequent section concerns a property relating the reflection grating to a transmission grating of similar aperture width and period, but twice the depth. A description of the efficiency characteristics of the two kinds of grating is presented in Section 2.6 and the chapter is concluded with an examination of the conditions under which the predictions of the full modal expansion can be suitably approximated by just one or two modes.

2.2 THEORETICAL FORMALISMS

2.2.1 The Reflection Grating

The method described here has been implemented successfully in our laboratory and is closely allied to that of Maystre and Petit [2.10]. The major difference between the treatments lies in the procedure by which a second equation relating the field amplitudes is established. Both formulations make use of the orthogonality properties of the plane-wave basis functions when first matching the fields across the free-space-aperture interface. It is only the method described below which takes advantage of the orthogonality properties of the mode basis functions in securing a second matching. In place of doing this, Maystre and Petit chose to define a function $F(x,y)$ to be equal to the field multiplied by a step function $C(x)$ - the latter being represented by a slowly-converging Fourier series. $F(x,y)$ was then projected onto the set of plane-wave functions to yield the required second equation.

The treatment detailed here circumvents the necessity of making the above definitions and hence eliminates much calculation including that of Fourier coefficients. It also results in less matrix manipulation and hence results in shorter computation times and improved numerical convergence.
Consider then an infinitely-conducting lamellar grating of period $d$ and having grooves of depth $h$ and width $c$. The geometrical configuration for the problem is depicted in Figure 2.1 and is chosen so that the $z$-axis is parallel to the generating axis of the grooves and the $y$-axis is normal to the grating surface. The origin of the coordinate system is placed at the top-centre of a groove in order that relations of symmetry are more readily detected in the phases of the mode and plane-wave amplitudes.

2.2.1.1 $P$ Polarization

A plane wave of unit amplitude and wavelength $\lambda$ is assumed to be incident upon the structure shown in Figure 2.1 at an angle $\theta$ and with its electric vector aligned in the $z$-direction. Since the resultant diffracted field is similarly polarized, the representation of the total electric field in the region above the grating surface includes a Rayleigh expansion. With the deletion of the temporal dependent term, $\exp(-i\omega t)$, it may therefore be expressed by

$$E(x,y) = \exp \left[i(\alpha_0 x - \chi_0 y)\right] + \sum_{p=-\infty}^{\infty} A_p \exp \left[i(\alpha_p x + \chi_p y)\right], \quad y > 0 \quad \text{(2.1)}$$

where $\alpha_0 = \frac{2\pi}{\lambda} \sin \theta$, $\chi_0 = \frac{2\pi}{\lambda} \cos \theta$,

$$\alpha_p = \frac{2\pi}{\lambda} \sin \theta_p = \frac{2\pi}{\lambda} \left(\sin \theta + \frac{p\lambda}{d}\right)$$

and $\chi_p = \frac{2\pi}{\lambda} \cos \theta_p$ and is chosen to be positive real or positive imaginary depending on whether $\sin \theta_p \leq 1$ or $\sin \theta_p > 1$. $A_p$ is the constant amplitude of the $p^{th}$ diffracted order and since the incident beam has unit amplitude, efficiency is expressed by

$$E(p) = \sum_{p} |A_p|^2 \frac{\chi_p}{\chi_0} \quad \text{(2.2)}$$

and must be conserved according to equation (1.6).
Figure 2.1 The geometry of the diffraction arrangement for the perfectly-conducting lamellar reflection grating.

Figure 2.2 The geometry of the diffraction arrangement for the perfectly-conducting lamellar transmission grating.
Due to the simplicity of the grating profile, the electric field in the groove region may be explicitly represented by a discrete expansion of waveguide-type modes written in the form

\[ E_{II}(x,y) = \sum_{m=1}^{\infty} a_m \phi_m(x,y), \quad -h < y < 0 \]

\[ \frac{-c}{2} < x < \frac{c}{2} \]

where the \( a_m \) are the mode amplitudes and the \( \phi_m(x,y) \) are functions which must satisfy both the Helmholtz equation and the boundary conditions. The latter specify that the field should vanish on all metal surfaces, and so remembering the work of Wirgin [2.3] it is easily shown that the appropriate separable solution of the wave equation is

\[ \phi_m(x,y) = \sin\left(\frac{m\pi}{c}(x + \frac{c}{2})\right) \sin\left(\frac{\mu_m(y+h)}{\mu} \right) \]

... (2.4)

where \( \mu_m = \left\{ \begin{array}{ll}
\frac{\pi}{\lambda_c^2} - \frac{m^2}{\lambda_c^2} \mu, & \lambda < \frac{2c}{m} \\
\frac{i\pi}{\lambda_c^2} - \frac{4}{\lambda_c^2} \mu, & \lambda > \frac{2c}{m}
\end{array} \right. \)

... (2.5)

The functions \( \phi_m(x,o) \) are seen to form an orthogonal set on the interval \( -\frac{c}{2} < x < \frac{c}{2} \).

Solutions for the unknown field amplitudes are now obtained by invoking the Method of Moments [2.32]. Continuity of the electric field across the interface separating free-space and the grating asserts that

\[ E_{II}(x,o), \quad \frac{-c}{2} < x < \frac{c}{2} \]

\[ E_{I}(x,o) = 0, \quad \frac{c}{2} < x < \frac{d-c}{2}. \]

... (2.6)

Projection of this equality onto the set of functions \( \{ \exp(i\alpha x) \} \), orthogonal on \( -\frac{c}{2} < x < \frac{d-c}{2} \), yields the equation

\[ \delta_{\alpha,\mu} + A_{\mu} = \frac{1}{d} \sum_{m=1}^{\infty} a_m \sin(\mu_m h) I_{mp} \]

... (2.7)

where \( \delta_{\alpha,\mu} \) is the Kronecker delta function, and \( I_{mp} \) is an inner-product.
defined by

\[ I_{mp} = \frac{c}{2} \int_{-c/2}^{c/2} \sin \left( \frac{\eta m}{c} (x + \frac{c}{2}) \right) \exp \left(-i\alpha_{p} x\right) dx \]

\[ = -\frac{\alpha_{p}}{2c} \left[ \text{sinc} \left( \frac{\eta m}{c} - \alpha_{p} \right) \frac{c}{2} - (-1)^{m} \text{sinc} \left( \frac{\eta m}{c} + \alpha_{p} \right) \frac{c}{2} \right], \quad \alpha_{p} = \pm \frac{\eta m}{c} \]

\[ = (\pm i)^{m-1} \frac{c}{2}, \quad \alpha_{p} = \pm \frac{\eta m}{c} \]

[sinc \( x \) is used to denote \( \frac{\sin x}{x} \)].

Continuity of the tangential component of the magnetic field across the groove aperture leads to the equality,

\[ \frac{\partial E^{I}(x, 0)}{\partial y} = \frac{\partial E^{II}(x, 0)}{\partial y}, \quad -\frac{c}{2} < x < \frac{c}{2} \]

\[ \text{or} \]

\[ \frac{\partial E^{I}(x, 0)}{\partial y} = \frac{\partial E^{II}(x, 0)}{\partial y}, \quad -\frac{c}{2} < x < \frac{c}{2} \]

which when expanded and projected onto the orthogonal set of functions \( \{\phi_{m}(x, 0)\} \), provides the equation

\[ -i\eta_{0} T_{m0} + \sum_{p=-\infty}^{\infty} i\eta_{p} A_{p} T_{mp} = a_{m} V_{m} \cos \left( \frac{\mu_{m} h}{2} \right) \]

Elimination of the \( A_{p} \) by inserting equation (2.7) into equation (2.10) results in an infinite set of linear equations in the unknown mode amplitudes \( a_{m} \), namely

\[ \sum_{m=1}^{\infty} a_{m} \left[ \sin(\eta_{m} h) \frac{1}{d} \sum_{p=-\infty}^{\infty} (i\eta_{p} T_{mp} T_{np}) - \delta_{n,m} \nu_{n} \cos \left( \frac{\mu_{n} h}{2} \right) \right] = 2i\eta_{0} T_{n0} \]

Following suitable truncation of the two infinite sums involved, this system is solved numerically using a standard Gauss-Jordan reduction method.

This enables the plane-wave amplitudes \( A_{p} \) to be reconstructed from equation (2.7) and hence the efficiencies may be obtained from equation (2.2).
It has often been of interest to investigate profiles for which \( h \) is very large, say up to two periods. Under these circumstances equation (2.11) has been found to present numerical problems in its implementation on the available computer, a Burroughs B6700. These problems are due to numbers involved in the calculation of \( \sin (\mu_m h) \) or \( \cos (\mu_m h) \) exceeding the machine's capability when \( m \) is high and \( \mu_m h \) is large and imaginary. To overcome these difficulties it has been found beneficial to define

\[
a_m^* = a_m \sin (\mu_m h)
\]  

(2.12)

where upon equation (2.11) becomes

\[
\sum_{m=1}^{\infty} a_m^* \left( \frac{1}{\sqrt{p}} \sum_{p=-\infty}^{\infty} (ix_{pl}m^p) - \delta_{m,n} \mu_n \cot (\mu_n h/2) \right) = 2i\chi_0 I_{n0}
\]  

(2.13)

For \( \mu_m \) imaginary and large values for \( h \), \( \cot (\mu_m h) \) can now be equated to \(-i\) when \( \mu_m h \) is sufficiently large so as to prevent the incurring of any significant error. In equation (2.7), \( a_m \sin (\mu_m h) \) is replaced by \( a_m^* \) and similarly the evaluation of the \( A_p \) is rendered safer for large \( h \). It should be noted however, that isolated wavelengths for which \( \sin (\mu_m h) = 0 \) are not permitted by this numerical treatment. Another advantage obtained from the redefining of the mode amplitude according to equation (2.12), is that the modified mode function of equation (2.3) becomes

\[
\phi_m^* (x,y) = \sin \left[ \frac{\mu m}{C} (x+C) \right] \frac{\sin \left[ \mu m (y+h) \right]}{\sin (\mu_m h)}
\]  

(2.14)

which is always real-valued. The usefulness of this property is demonstrated in a following section on conservation relations.
2.2.1.2 S Polarization

The formulation in this case is similar to that for the previous polarization - the essential difference being due to the boundary conditions which now stipulate that it is the normal derivative of the magnetic field which should equal zero on the grating surfaces. The magnetic field component is parallel to the long axis of the grooves and so the problem is completely specified in terms of $H^I_z(x,y)$ and $H^{II}_z(x,y)$, where the $z$-subscript is henceforth omitted.

Equations (2.1) to (2.3) remain unchanged except for a change in notation to label the $p$th order amplitude by $B_p$ and the $m$th mode amplitude by $b_m$. In equation (2.4) the change in boundary conditions forces the sines to be replaced by cosines and hence the appropriate form of the waveguide function is given by

$$\phi_m(x,y) = \cos\left[\frac{\pi m}{d}(x+C_y)\right]\cos\left[\mu_m(y+h)\right] \quad \ldots(2.15)$$

where an $m = 0$ term is now included in all modal expansions.

By applying conditions of continuity of the field along $y = 0$ for $-\frac{C_y}{2} < x < \frac{C_y}{2}$ and continuity of the $y$-derivative for $-\frac{C_y}{2} < c < d - \frac{C_y}{2}$, the orthogonality properties of the basis functions $\{\cos\left[\frac{\pi m}{d}(x+C_y)\right]\}$ and $\{\exp(i\alpha_x x)\}$ are implemented respectively to furnish the equations

$$J_{m0} + \sum_{p=-\infty}^{\infty} B_p J_{mp} = b_m \cos(\mu_m h) \frac{\partial}{\partial x} \quad \ldots(2.16)$$

and

$$-\delta_{\alpha_x} + B_p = \frac{i}{d} \sum_{m=0}^{\infty} b_m \mu_m \sin(\mu_m h) J_{mp} \frac{\partial}{\partial x} \quad \ldots(2.17)$$
where \( J_{mp} \) is given by

\[
J_{mp} = \frac{c}{2} \cos \left[ \frac{m\pi}{c} \left( x - \frac{c}{2} \right) \right] \exp \left( -i\alpha_p x \right) dx
\]

and

\[
\alpha_p = \pm \frac{m\pi}{c} \neq 0
\]

and

\[ \tilde{e}_m = \begin{cases} 
1, & m = 0 \\
\tilde{e}_m, & m > 1.
\end{cases} \quad ...(2.19) \]

Substitution of \( B_p \) from equation (2.17) into equation (2.16) leads to the set of equations

\[
\sum_{m=0}^{\infty} b_m \left[ \mu_m \sin (\mu_m h) \frac{1}{d} \sum_{p=-\infty}^{\infty} \frac{iJ_{mp}}{x_p} \right] \delta_{m,n} \tilde{e}_n c \cos (\mu_n h) = -2J_{n0} \quad ...(2.20)
\]

This infinite linear system in the \( b_m \) is dealt with numerically as for the previous polarization - followed by evaluation of the \( B_p \) from equation (2.17).

By defining \( b^*_m = b_m \cos (\mu_m h) \), to allow a wider range of groove profiles to be numerically handled as before, equation (2.20) reduces to

\[
\sum_{m=0}^{\infty} b^*_m \left[ \mu_m \tan (\mu_m h) \frac{1}{d} \sum_{p=-\infty}^{\infty} \frac{iJ_{mp}}{x_p} \right] \delta_{m,n} \tilde{e}_n c = -2J_{n0} \quad ...(2.21)
\]

As is evident from this equation and also equation (2.13), shallow profiles secure more stable calculations due to the diagonal dominance of the matrices involved.
2.2.2 The Transmission Grating

The extension of the treatment in the previous section to the perfectly-conducting rectangular-wire grating illustrated in Figure 2.2 is straightforward. There are, however, twice as many unknown sets of coefficients to determine. For ease of verification of symmetry properties described in Section 2.3, the origin of the coordinate system is chosen to lie in the centre of the groove aperture. This also enables the solution of the problem to be decoupled into equations for y-symmetric and y-antisymmetric modes.

2.2.2.1 P Polarisation

Using the notation prescribed in the previous sections, the electric field in each of the three regions designated in Figure 2.2 is represented by

\[ E^I(x, y) = \exp[i(\alpha_0 x + \chi_0 y)] + \sum_{p=\pm\infty}^\infty A_p \exp[i(\alpha_p x + \chi_p y)], \quad y > \frac{h}{2} \]  \hspace{1cm} \ldots(2.22)

\[ E^{II}(x, y) = \sum_{m=1}^\infty [a_m \sin(\mu_my) + b_m \cos(\mu_my)] \sin\left[\frac{\mu_m}{c}(x+c)\right] \]

for \(-\frac{h}{2} < y < \frac{h}{2}\), \(-\frac{c}{2} < x < \frac{c}{2}\)

\[ = 0 \quad \text{for} \quad \frac{h}{2} < y < \frac{h}{2}, \quad \frac{c}{2} < x < d-\frac{c}{2} \]  \hspace{1cm} \ldots(2.23)

\[ E^{III}(x, y) = \sum_{p=\pm\infty}^\infty \hat{A}_p \exp[i(\alpha_p x + \chi_p y)], \quad y < \frac{h}{2} \]  \hspace{1cm} \ldots(2.24)

\[ A_p \text{ and } \hat{A}_p \text{ are the } p^{th} \text{ order amplitudes of the upward-going and the downward-going plane waves respectively, and } a_m \text{ and } b_m \text{ are amplitudes of } y\text{-antisymmetric and } y\text{-symmetric mode terms respectively.} \]
Consider the functions $E^+_R(x,y)$ and $E^-_R(x,y)$ defined on the interval $\frac{-C}{2} < x < \frac{d-C}{2}$ by

$$E^+_R(x,y) = E^I(x,y) + E^III(x, -y)$$

$$E^-_R(x,y) = E^I(x,y) - E^III(x, -y) \quad \ldots \text{(2.25)}$$

Setting $y = \frac{h}{2}$ in these definitions and then inserting equations (2.22) and (2.24) gives

$$E^+_R(x, \frac{h}{2}) = \sum_{p=-\infty}^{\infty} \left[ S_p + \delta_0 p \exp\left(-i\frac{h}{2}^2\right) \right] \exp(i\alpha_p x) \quad \ldots \text{(2.26)}$$

$$E^-_R(x, \frac{h}{2}) = \sum_{p=-\infty}^{\infty} \left[ D_p + \delta_0 p \exp\left(-i\frac{h}{2}^2\right) \right] \exp(i\alpha_p x) \quad \ldots \text{(2.27)}$$

where

$$S_p = (A_p + \hat{A}_p) \exp\left(i\frac{h}{p^2}\right)$$

$$D_p = (A_p - \hat{A}_p) \exp\left(i\frac{h}{p^2}\right).$$

Similar definitions are secured for the modal field and lead to the following decoupling of the mode coefficients:

$$E^+_M(x, \frac{h}{2}) = E^II(x, \frac{h}{2}) + E^II(x, -\frac{h}{2})$$

$$= 2 \sum_{m=1}^{\infty} b_m \cos\left(\mu_m \frac{h}{2}\right) \sin[\frac{m\pi}{C} (x + \frac{C}{2})], \quad \frac{C}{2} < x < \frac{C}{2} \quad \ldots \text{(2.28)}$$

$$= 0, \quad \frac{C}{2} < x < d-\frac{C}{2}$$

$$E^-_M(x, \frac{h}{2}) = E^II(x, \frac{h}{2}) - E^II(x, -\frac{h}{2})$$

$$= 2 \sum_{m=1}^{\infty} a_m \sin\left(\mu_m \frac{h}{2}\right) \sin[\frac{m\pi}{C} (x + \frac{C}{2})], \quad \frac{C}{2} < x < \frac{C}{2} \quad \ldots \text{(2.29)}$$

$$= 0, \quad \frac{C}{2} < x < d-\frac{C}{2}$$

The continuity of the tangential component of $\mathbf{E}$ across the planes given by $y = \pm\frac{h}{2}$, requires that
These conditions are expanded and the Method of Moments applied by multiplying both sides by $\exp(-ia_p x)$ and integrating over one period. The resulting equations are

$$S_p = \frac{2}{d} \sum_{m=1}^{\infty} b_m \cos \left( \mu_m \frac{h}{2} \right) I_{mp} - \delta_0, p \exp \left( -i \chi_0 \frac{h}{2} \right) \quad \ldots(2.30)$$

$$D_p = \frac{2}{d} \sum_{m=1}^{\infty} a_m \sin \left( \mu_m \frac{h}{2} \right) I_{mp} - \delta_0, p \exp \left( -i \chi_0 \frac{h}{2} \right) \quad \ldots(2.31)$$

where $I_{mp}$ is the identical inner-product to that for the reflection grating and given by equation (2.8).

Requirements for the continuity of the normal derivative of $E$ are expressed as

$$\frac{\partial E^+_R(x, \frac{h}{2})}{\partial y} = \frac{\partial E^+_M(x, \frac{h}{2})}{\partial y} \quad , \quad -\frac{c}{2} < x < \frac{c}{2}$$

Expanding these constraints and employing the orthogonality properties of the functions $\{\sin[\mu_m (x+\frac{c}{2})]\}$ on the required interval, yields the two equations,

$$i \sum_{p=-\infty}^{\infty} X_p \left[ D_p - \delta_0, p \exp \left( -i \chi_0 \frac{h}{2} \right) \right] T_{mp} = 2\mu_m a_m \cos \left( \mu_m \frac{h}{2} \right) \frac{c}{2} \quad \ldots(2.32)$$

$$i \sum_{p=-\infty}^{\infty} X_p \left[ S_p - \delta_0, p \exp \left( -i \chi_0 \frac{h}{2} \right) \right] T_{mp} = -2\mu_m b_m \sin \left( \mu_m \frac{h}{2} \right) \frac{c}{2} \quad \ldots(2.33)$$

It is now a straightforward matter to substitute equation (2.31) into (2.32) and equation (2.30) into (2.33) to resolve two sets of linear equations in the mode amplitudes $a_m$ and $b_m$. With the redefinition of these amplitudes as
\[ a^*_m = a_m \sin \left( \mu_m \frac{h}{2} \right) \]
\[ b^*_m = b_m \cos \left( \mu_m \frac{h}{2} \right) \]

the two final linear systems are written in the form

\[ \sum_{m=1}^{\infty} a^*_m \left( \frac{1}{d} \sum_{p=-\infty}^{\infty} (i\chi_p i m p T_{mp}) - \delta_{m,n} \mu_n \cot \left( \mu_n \frac{h}{2} \right) \right) = i\chi_0 T_{mn} \exp \left( -i\chi_0 \frac{h}{2} \right) \quad \ldots (2.35) \]

and

\[ \sum_{m=1}^{\infty} b^*_m \left( \frac{1}{d} \sum_{p=-\infty}^{\infty} (i\chi_p i m p T_{mp}) + \delta_{m,n} \mu_n \tan \left( \mu_n \frac{h}{2} \right) \right) = i\chi_0 T_{mn} \exp \left( -i\chi_0 \frac{h}{2} \right) \quad \ldots (2.36) \]

It is noted that for small h, the former of these two sets of equations has the more diagonally dominant matrix. This matrix is the same as that expressed in equation (2.13) which pertains to the reflection grating of half the depth for the case of P polarization. The fact that the trigonometric terms in equations (2.35) and (2.36) contain h/2 as opposed to h for the reflection case, also means that transmission gratings of much greater groove depth can be dealt with numerically before problems are encountered with the computations when the definitions of equation (2.34) are not implemented.

Following the numerical solution of equations (2.35) and (2.36) for the \( a^*_m \) and \( b^*_m \), the quantities \( S_p \) and \( D_p \) are calculated from equations (2.30) and (2.31) and then the plane-wave amplitudes \( A_p \) and \( \hat{A}_p \) are reconstructed [see equations (2.27)] from the relations

\[ A_p = \frac{S_p + D_p}{2 \exp \left( i\chi_p \frac{h}{2} \right)} \quad \ldots (2.37) \]
\[ \hat{A}_p = \frac{S_p - D_p}{2 \exp \left( i\chi_p \frac{h}{2} \right)} \]
2.2.2.2 S Polarization

For this polarization, the following changes are made to equations (2.22) - (2.24): $E$ is replaced by $H$, $A_p$ and $\hat{A}_p$ are replaced by $B_p$ and $\hat{B}_p$ while in equation (2.23) $\sin \left( \frac{\pi t}{C} (x + \frac{C}{2}) \right)$ becomes $\cos \left( \frac{\pi t}{C} (x + \frac{C}{2}) \right)$.

Following a similar treatment to that described in the previous section and using the appropriate boundary conditions and continuity conditions detailed in Section 2.2.1.2, the following decoupled sets of linear equations are finally established for the $y$-symmetric and $y$-antisymmetric mode amplitudes:

\[
\sum_{m=0}^{\infty} a^* \left( \mu_m \cot \left( \mu_m \frac{h}{2} \right) \frac{1}{d} \sum_{p=-\infty}^{\infty} \left( \frac{i J_{mp}}{X_p} \right) \right) + \delta_{m,n} c \tilde{v}_n
\]
\[
= \exp \left( -i \chi_0 \frac{h}{2} \right) J_{n0} \quad \ldots (2.38)
\]

\[
\sum_{m=0}^{\infty} b^* \left( \mu_m \tan \left( \mu_m \frac{h}{2} \right) \frac{1}{d} \sum_{p=-\infty}^{\infty} \left( \frac{i J_{mp}}{X_p} \right) - \delta_{m,n} c \tilde{v}_n \right)
\]
\[
= -\exp \left( -i \chi_0 \frac{h}{2} \right) J_{n0} \quad \ldots (2.39)
\]

The same notation has been maintained throughout and so $J_{mp}$ and $\tilde{v}_n$ are given by equations (2.18) and (2.19) respectively. As expected, the left-hand side of equation (2.39) is identical to the analogous result for the reflection grating of half the depth - as given by equation (2.21).

Replacing $A_p$, $\hat{A}_p$ by $B_p$, $\hat{B}_p$, these order amplitudes are evaluated from equation (2.37) where in this case $S_p$ and $D_p$ are given by the relations

\[
S_p = \frac{2i}{d} \sum_{m=0}^{\infty} b^* \mu_m \tan \left( \mu_m \frac{h}{2} \right) \frac{J_{mp}}{X_p} + \delta_{0,p} \exp \left( -i \chi_0 \frac{h}{2} \right) \quad \ldots (2.40)
\]

\[
D_p = \frac{-2i}{d} \sum_{m=0}^{\infty} a^* \mu_m \cot \left( \mu_m \frac{h}{2} \right) \frac{J_{mp}}{X_p} + \delta_{0,p} \exp \left( -i \chi_0 \frac{h}{2} \right) \quad \ldots (2.41)
\]
2.3 SYMMETRY PROPERTIES

Before proceeding with an account of the numerical considerations involved in solving the linear systems of Section 2.2 for their respective mode amplitudes, it is appropriate that a description be given here of certain symmetry properties which pertain to, not only the lamellar grating results, but also to the results obtained for the majority of the structures investigated in this thesis. These properties require that the grating under consideration be infinitely-conducting and they are based on work previously described by McPhedran and Maystre [2.33], Botten [2.34] and Botten et al. [2.35].

Once a grating formalism has been developed there are at the theorist's disposal a number of analytic tests to which the numerical results may be subjected in order that both the formalism itself and the computer code be validated. Two such tests which have been discussed earlier are those of energy conservation and reciprocity. Both of these can be applied to all structures irrespective of the groove geometry or conductivity of the grating material. Energy conservation represents a crucial test of convergence for integral and differential theories, but it is shown by Amitay and Galindo [2.36] to be of limited use in the case of modal scattering from infinite phased-arrays. This is because energy balance is automatically satisfied independently of truncation limits imposed on the infinite field expansions. However, it still offers an indication of whether the computer code has been programmed correctly. On the other hand, the Reciprocity Theorem [2.37] remains a valuable criterion for checking results from all modal-based theories as well as the integral and differential formalisms.

A third check on calculations is secured by the application of a series of conservation relations which stem from the symmetry as well as
the lossless nature of the structure. Some of these relations have been described in one form or another for reflection and transmission gratings in references [2.11, 2.34] and for grid structures in reference [2.33]. A more comprehensive study has been presented by Botten et al. [2.35] in the case of perfectly-conducting transmission (wire) gratings. A requirement for these arrays is that the groove apertures possess symmetry in either a left-right (LR) sense and/or an up-down (UD) sense. For the symmetry properties to be readily observed the coordinate axes should coincide with these axes of symmetry. This explains the choice of origin in the geometry used for the lamellar grating.

Although some properties connecting the real order amplitudes were derived using a straight-forward Green's Theorem integral method, more powerful relations have been derived by the above authors by applying the concept of time-reversibility to the two most useful cases of

(a) a long-wavelength mounting ($\lambda > d(\sin \theta + 1)$)
(b) a -1 Littrow mounting ($\sin \theta = \lambda/2d$) where only the -1 and 0 orders are propagating.

This principle simply states that the electromagnetic field remains unchanged if all wavevectors have their directions reversed and all complex amplitudes are conjugated. The principle has been shown to duplicate the predictions of the integral treatment as well as providing additional relations concerning the evanescent orders and also the mode amplitudes.

A necessary condition in the case of the mode amplitudes is that the separable $x$ and $y$ components of the modal field be real and so this provides as extra motive for redefining the mode amplitudes in the manner described in the previous section. There, the redefinition caused the $y$-dependent functions to become always real-valued, as can be seen in relation (2.14) for the reflection grating and $P$ polarization.
Reference [2.35] deals only with transmission gratings and a summary of those relevant results is given after a brief derivation of the useful relations which are applicable to reflection gratings and which evolve from a similar treatment. The two cases of the long-wavelength mounting and the -1 Littrow mounting are considered separately.

2.3.1 Long-Wavelength Relations

Let $F(x,y)$ be the function describing the total scalar-field (either electric for $P$ polarization or magnetic for $S$ polarization) in the vicinity of a lossless, symmetrical-profile reflection grating placed in a coordinate system similar to that of Figure 2.1, such that the axis of groove symmetry coincides with the $y$-axis. Also, let $R_p$ be the $p$th order amplitude of the Rayleigh field above the grating and let $a_m$ be the amplitude of the $m$th mode describing the field within the groove region.

Consider an incident beam of unit amplitude, with wavelength $\lambda > d(\sin \theta + 1)$ and with wavevector in the $xy$ plane, striking the surface at an arbitrary angle. This gives rise to only one order—the specularly reflected zeroth order with amplitude $R_0$. By returning a second incident wave of amplitude $R_0$ in the reverse direction, time-reversibility gives

$$F(x,y) = R_0 F(-x,y)$$  ...(2.42)

Substituting into this equation a plane-wave expansion for $F$, and equating like terms yields

(i) $|R_0|^2 = 1$

(ii) $R_p = R_0 R_p$  ...(2.43)

from which it is easily shown that
The left-right symmetry of the grooves makes it possible to separate
the modes into $x$-symmetric $[E_m(x)]$ and $x$-antisymmetric $[O_m(x)]$ components
which are defined by

\[ E_m(x) = E_m(-x), \quad O_m(x) = -O_m(-x) \]  

Inserting a modal expansion for $F(x,y)$ of the form

\[ F(x,y) = \sum_m [a_e^m E_m(x) + a_o^m O_m(x)] \phi_m(y) \]

into equation (2.42) leads to the relations

\[
\begin{align*}
(i) \quad \arg(a_e^m) &= \frac{1}{2} \arg(R_o) (\pm \pi) \\
(ii) \quad \arg(a_o^m) &= \frac{1}{2} \arg(R_o) + \pi/2 (\pm \pi)
\end{align*}
\]

where the mode functions have been assumed real-valued and to be independent
of one another. ($\pm \pi$ denotes a possible additive factor of $\pm \pi$.)

Now consider a transmission grating in identical circumstances to
those described above. The orders of transmission are labelled by $T_p$.
If the structure is assumed to possess up-down (as well as left-right)
symmetry about the $x$-axis then there exist separable solutions to the
$y$-component of the modal field and this introduces two more coefficients
labelled $b_e^m$ and $b_o^m$. The general expression for $F(x,y)$ in the groove
region is then of the form

\[ F(x,y) = \sum_m [a_e^m E_m(x) + a_o^m O_m(x)] \phi_m(y) \]

\[ \quad + [b_e^m E_m(x) + b_o^m O_m(x)] E_m(y) \]

Using time-reversal, the relevant results from reference [2.35],
which are analogous to equations (2.43), (2.44) and (2.47) are
\begin{align*}
(i) & \quad |R_0|^2 + |T_0|^2 = 1 \\
(ii) & \quad \text{Re}(R_0 T_0) = 0 \\
(iii) & \quad \bar{T}_p = \bar{R}_o T_p + \bar{T}_o R_p \\
(iv) & \quad \bar{R}_p = \bar{R}_o R_p + \bar{T}_o T_p \\
(i) & \quad \arg(P_p) = \frac{1}{2} \arg(P_0) (+\pi) \\
(ii) & \quad \arg(M_p) = \frac{1}{2} \arg(M_0) (+\pi) \quad p \neq 0 \\
(i) & \quad \arg(a^e_m) = \frac{1}{2} \arg(M_0) (+\pi) \\
(ii) & \quad \arg(a^o_m) = \frac{1}{2} \arg(M_0) + \pi/2 (+\pi) \\
(iii) & \quad \arg(b^e_m) = \frac{1}{2} \arg(P_0) (+\pi) \\
(iv) & \quad \arg(b^o_m) = \frac{1}{2} \arg(P_0) + \pi/2 (+\pi) \\
\end{align*}

where $P_p = R_p + T_p$

and $M_p = R_p - T_p$.

From equation (2.49(ii)) it is easily derived that the phases of the reflected and transmitted real orders are linked by

$$\arg(T_0) - \arg(R_0) = \pi/2 (+\pi) \quad \ldots (2.52)$$

This result was first reported by McPhedran and Maystre [2.33] for grids which have orthogonal periodicity. A combination of the conservation of energy relation (2.49(i)) with equations (2.52) and (2.51(i) & (iii)) leads to the relations

$$\cos^2[\arg(a^e_m) - \arg(b^e_m)] = |R_0|^2 \quad \ldots (2.53)$$

and

$$\arg(a^e_m) + \arg(b^e_m) = \arg(R_0) \quad \ldots (2.54)$$

These constraints serve as a useful numerical check connecting the phases of the $y$-symmetric and $y$-antisymmetric mode amplitudes, to the efficiency of the propagating orders. They also reveal that the real diffracted field
can be completely reconstructed from a knowledge of the phases of, for example, the fundamental mode.

2.3.2 Littrow Relations

The situation is now considered wherein the incident beam strikes the same reflection grating as described earlier, but at an angle \( \sin^{-1}(\lambda/2d) \) and with wavelength given by \( 2/3 \, d < \lambda < 2d \). Thus, only two propagating orders exist. Using the treatment of the previous section, returning the two waves \( \bar{R}_0 \) and \( \bar{R}_{-1} \) gives

\[
F(x,y) = \bar{R}_0 \, F(-x,y) + \bar{R}_{-1} \, F(x,y) \quad \ldots \quad (2.55)
\]

Expanding this equation using a Rayleigh series and collecting like terms furnishes, for the real orders,

(i) \( |R_0|^2 + |R_{-1}|^2 = 1 \)

(ii) \( \Re (R_0 \bar{R}_{-1}) = 0 \),

while for the evanescent orders one obtains

\[
\bar{R}_p = \bar{R}_0 R_p + \bar{R}_{-1} R_{-p-1} \quad \ldots \quad (2.57)
\]

From this latter equation, phases of the amplitudes are found to be related by

(i) \( \arg (R_p + R_{-p-1}) = \frac{1}{2} \arg (R_0 + R_{-1}) \, (+\pi) \) \( \quad \text{for} \quad p \neq 0 \)

(ii) \( \arg (R_p - R_{-p-1}) = \frac{1}{2} \arg (R_0 - R_{-1}) \, (+\pi) \)

By inserting the modal expansion form for \( F(x,y) \) from equation (2.46) into equation (2.55), the following constraints are derived for the mode amplitudes:

(i) \( \arg (a_{m}^0) = \frac{1}{2} \arg (R_{-1} + R_0) \, (+\pi) \)

(ii) \( \arg (a_{m}^1) = \frac{1}{2} \arg (R_{-1} - R_0) \, (+\pi) \)

It is a simple matter to secure from equation (2.56(ii)), an interesting property connecting the phases of the two real orders. This has been previously noted in references [2.11, 2.34] and is written here
in the form
\[ \arg(R_{-1}) - \arg(R_0) = \pi/2 \quad (+\pi) \quad \ldots (2.60) \]

This expression is analogous to equation (2.52), which applies to the case of only two real orders for a transmission grating. As a consequence, a similar procedure to the derivation of equation (2.53) may be adopted to yield a corresponding result for the reflection grating in -1 Littrow.

With the aid of equations (2.56(i)), (2.60) and (2.59) one obtains the constraints,
\[ \cos^2 [\arg(a_m^e) - \arg(a_m^o)] = |R_{-1}|^2 \quad \ldots (2.61) \]
\[ \arg(a_m^e) + \arg(a_m^o) = \arg(R_{-1}) \quad \ldots (2.62) \]

from which one is again able to calculate the diffracted energy given the phases of, say, the first two mode amplitudes. (Different modes are usually referred to by different values of m. Successive values of m usually correspond to modes of opposite x-symmetry if a single series expansion is used.)

Returning now to the case of a single layer transmission grating with both left-right and up-down symmetry, consider it placed in the first-order Littrow mounting where a total of four real orders are in evidence. The appropriate expression provided by time-reversibility (see reference [2.35]), is
\[ F(x,y) = R_{-1}F(x,y) + R_0F(-x,y) + T_{-1}F(x,-y) + T_0F(-x,-y) \quad \ldots (2.63) \]

Employing a plane-wave expansion for \( F(x,y) \), and equating like terms for the real orders, leads to the equations
\[
\begin{align*}
(\text{i}) & \quad |R_0|^2 + |R_{-1}|^2 + |T_0|^2 + |T_{-1}|^2 = 1 \\
(\text{ii}) & \quad \Re(R_0R_{-1}^* + T_0T_{-1}^*) = 0 \\
(\text{iii}) & \quad \Re(R_0T_{-1}^* + R_{-1}T_0^*) = 0 \\
(\text{iv}) & \quad \Re(R_0T_0^* + R_{-1}T_{-1}^*) = 0
\end{align*}
\]

Similar expressions for the evanescent orders are presented in reference [2.35]. Together with equations (2.64) they furnish the relations:
By substituting equation (2.48) for $F(x,y)$ into equation (2.63) the following conservation relations are derived:

\[
\begin{align*}
(i) \quad & \arg (P_p + P_{p-1}) = \frac{1}{2} \arg (P_0 + P_{-1}) (+\pi) \\
(ii) \quad & \arg (M_p + M_{p-1}) = \frac{1}{2} \arg (M_0 + M_{-1}) (+\pi) \\
(iii) \quad & \arg (P_p - P_{p-1}) = \frac{1}{2} \arg (P_0 - P_{-1}) (+\pi) \\
(iv) \quad & \arg (M_p - M_{p-1}) = \frac{1}{2} \arg (M_0 - M_{-1}) (+\pi)
\end{align*}
\]

...(2.65)

The relation which is analagous to equations (2.53) and (2.61) and which does not appear to have been reported previously, is now derived for the case of four real orders in the Littrow mounting and whose directions are therefore mirror images about the $x$ and $y$ axes. (In each of the previous two cases there were only two real orders whose directions were symmetric about the $y$-axis in one case and the $x$-axis in the other.)

Let $A = R_{-1} + R_0$

and $B = T_{-1} + T_0$.

From equations (2.64(i) and (ii)) one can write

\[
\begin{align*}
A &= \cos \delta \exp \left[ i \arg (A) \right] \\
B &= \sin \delta \exp \left[ i \arg (B) \right]
\end{align*}
\]

...(2.66)

Adding equations (2.64(iii)) and (2.64(iv)) gives

\[
\Re (AB) = 0,
\]

which when expanded shows that

\[
\arg (A) - \arg (B) = \pi/2 (+\pi)
\]

...(2.67)

Equations (2.66(i) and (iii)) may now be manipulated to give

\[
\begin{align*}
\arg (a^e_m) &= \frac{1}{2} \arg (A-B) = \frac{1}{2} [\arg (A) + \delta] \\
\arg (b^e_m) &= \frac{1}{2} \arg (A+B) = \frac{1}{2} [\arg (A) - \delta]
\end{align*}
\]
and hence one obtains the relation

$$\cos^2 [\arg (a_m^e) - \arg (b_m^e)] = \cos^2 \delta = |R_0 + R_{-1}|^2 \quad \ldots(2.69)$$

By defining $C = R_{-1} - R_0$ and $D = T_{-1} - T_0$ and subtracting equation (2.64(ii)) from (2.64(iii)), a similar treatment to that from equation (2.67) through to (2.69) yields for the $x$-antisymmetric modes,

$$\cos^2[\arg (a_0^0) - \arg (b_0^0)] = |R_{-1} - R_0|^2 \quad \ldots(2.70)$$

Adding this relation to equation (2.69) gives

$$\frac{1}{2} \left[ \cos^2[\arg (a_m^e) - \arg (b_m^e)] + \cos^2[\arg (a_m^0) - \arg (b_m^0)] \right] = |R_0|^2 + |R_{-1}|^2 \quad \ldots(2.71)$$

which is the required result, i.e. an expression linking the modal phases to the total reflected efficiency.

### 2.3.3 Normal Incidence

This section is concluded with a property pertaining to the modal field present in a structure of left-right symmetry when operated in a normal incidence mounting at an arbitrary wavelength.

As given by equations (2.45) and (2.46) the appropriate form of the field, when the origin is taken to be on the axis of symmetry, is represented in separable form as

$$F(x,y) = \sum_m [a_m^e E_m(x) + a_m^0 O_m(x)] \phi_m(y)$$

For the mounting type being considered, the field everywhere must be symmetric about $x = 0$ and we can therefore write

$$F(x,y) = F(-x,y).$$

Substituting the above expression in this equality gives

$$\sum_m a_m^0 O_m(x) \phi_m(y) = 0$$
from which the orthogonality of the mode functions gives the result,

\[ a_m^0 = 0 \quad \text{for all } m. \]

That is, all x-antisymmetric modes have zero amplitude in the case of normal incidence.

2.4 NUMERICAL CONSIDERATIONS

Before a numerical solution of equations (2.13), (2.21), (2.35), (2.36), (2.38) and (2.39) can proceed, it is clear that the infinite series involved must be truncated to finite limits. There are two independent truncations to be made - one governing the number of orders of diffraction and the other the number of groove modes. By allowing the index \( p \) to vary from \(-P\) to \(+P\), the total number of orders is \( 2P+1 \), while if the indices \( m \) and \( n \) are varied from 1 to \( M \) for \( P \) polarization and 0 to \( M-1 \) for \( S \) polarization, then a total of \( M \) modes are included.

Initial convergence studies consisted of increasing \( P \) and \( M \) while observing the change in diffracted energy in a particular order. The results of these tests showed that convergence of efficiency is usually better than 0.5% when \( P = 7 \) and \( M = 8 \) and better than 0.1% when \( P = 10 \) and \( M = 20 \). These figures also apply to regions of anomalies where efficiency is undergoing rapid change. The figures also compare more than favourably with those of Maystre and Petit [2.10] who used corresponding values of \( P = 7 \) and \( M = 15 \). Figure 2.3 traces the results of some convergence tests carried out on the theory for both polarizations and both types of grating for the normal incidence and -1 Littrow mounting configurations. It is interesting, that in each case the convergence for \( S \) polarization is superior to that for \( P \) polarization.

As mentioned in the previous section, energy conservation fails as an analytic test of the numerical accuracy of the results because it is always satisfied irrespective of the truncation limits.
Figure 2.3 Convergence of lamellar grating efficiency results as a function of the number of modes included in the field expansions. For the curves, P=11 for the reflection grating and P=9 for the transmission grating. The points correspond to P=7, M=8. In each case d=1.0.

(a) Refln. grating: $\theta=0^\circ, \lambda=0.4, c=0.6, h=0.9$
(b) Trans. grating: $\theta=0^\circ, \lambda=0.4, c=0.6, h=0.9$
(c) Refln. grating: $\theta=24.68^\circ, \lambda=0.835, c=0.43, h=0.7$
(d) Trans. grating: $\theta=24.68^\circ, \lambda=0.835, c=0.43, h=0.7$
[Equation (1.6) is found to always be satisfied by the computations to at least 10 decimal places.] This therefore leaves the Reciprocity Theorem and the conservation relations discussed in Section 2.3 as the next most suitable means of verifying the accuracy of the formalisms.

Table 2.1 displays the results of a reciprocity test for both the reflection and transmission gratings with a fairly large groove depth of \( h = 0.9 \) periods. These calculations were made with \( P = 10 \) and \( M = 20 \) for the former grating and \( P = 9 \) and \( M = 20 \) for the latter. Excellent results were achieved with compliance being better than 0.06% and 0.02% respectively. When the series limits were reduced to \( P = 7 \) and \( M = 8 \) these figures were found to worsen only slightly to become 0.3% and 0.25% respectively. The reason for the transmission grating having the superior results is due to the fact that \( h/2 \) rather than \( h \) is the determining factor in the calculations.

Numerical results conforming with the long-wavelength symmetry relations given in Section 2.3.1 are detailed in Table 2.2 while those which correspond to the \(-1\) Littrow relations of Section 2.3.2 are presented in Table 2.3. The moduli and phases of the mode amplitudes given in these tables are calculated from the "starred" quantities of Section 2.2 in order that the mode functions be real-valued, as required by the symmetry relations. That is, the appropriate modal functions for equations (2.46) are of the form:

\[
P \text{ polarization: } \phi_m(y) = \sin \left[ \mu_m(y+h) \right]/\sin \left( \mu_m h \right)
\]

\[
E_m(x) = (-1)^{(m-1)/2} \cos \left( \frac{m \pi x}{c} \right) \quad m = 1, 3, \ldots 
\]

\[
0_m(x) = (-1)^{m/2} \sin \left( \frac{m \pi x}{c} \right) \quad m = 2, 4, \ldots
\]
### TABLE 2.1

**Reciprocity Results for the Infinitely-Conducting Lamellar Grating**

Efficiency and phase calculations are presented to confirm agreement with the Reciprocity Theorem. The mounting configurations are defined by:

- **Problem 1:**
  - (a) $\theta = 0^\circ$, $\lambda = 0.4$
  - (b) $\theta = 0^\circ$, $\lambda = 0.41$

- **Problem 2:**
  - (a) $\theta = 23.5782^\circ$, $\lambda = 0.4$
  - (b) $\theta = 24.2048^\circ$, $\lambda = 0.41$

- **Problem 3:**
  - (a) $\theta = 53.1301^\circ$, $\lambda = 0.4$
  - (b) $\theta = 55.0847^\circ$, $\lambda = 0.41$

Groove parameters: $d = 1.0$, $c = 0.6$, $h = 0.9$

Number of Expansion Terms: $M = 20$ (a) $P = 10$ (b) $P = 9$

<table>
<thead>
<tr>
<th></th>
<th>P Polarization</th>
<th>S Polarization</th>
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<tbody>
<tr>
<td>(a) Reflection Grating</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Problem 1</td>
<td>$</td>
<td>R_0</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>R_{\pm 1}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>R_{\pm 2}</td>
</tr>
<tr>
<td>Problem 2</td>
<td>$</td>
<td>R_{-1}</td>
</tr>
<tr>
<td>Problem 3</td>
<td>$</td>
<td>R_{-2}</td>
</tr>
<tr>
<td>(b) Transmission Grating</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Problem 1</td>
<td>$</td>
<td>R_0</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>T_0</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>R_{\pm 1}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>T_{\pm 1}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>R_{\pm 2}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>T_{\pm 2}</td>
</tr>
<tr>
<td>Problem 2</td>
<td>$</td>
<td>R_{-1}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>T_{-1}</td>
</tr>
<tr>
<td>Problem 3</td>
<td>$</td>
<td>R_{-2}</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>T_{-2}</td>
</tr>
</tbody>
</table>
TABLE 2.2

Long-Wavelength Symmetry Properties for the
Infinitely-Conducting Lamellar Grating

Phase values for the plane-wave and modal amplitudes are tabulated and
confirm agreement with the symmetry relations of Section 2.3. The
equation number of the appropriate relation is given in the right-hand
column.

Groove Parameters:  \( d = 1.0, \ c = 0.6, \ h = 0.9 \)
Mounting Parameters:  \( \lambda = 1.3, \ \theta = 10^\circ \)
Number of Expansion Terms:  \( P = 7, \ M = 8 \)

<table>
<thead>
<tr>
<th></th>
<th>P Polarization</th>
<th>S Polarization</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Reflection Grating</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \arg(R_0) )</td>
<td>-121.0725</td>
<td>-170.6107</td>
<td></td>
</tr>
<tr>
<td>( \frac{1}{2}\arg(R_0) )</td>
<td>-60.5363</td>
<td>-85.3054</td>
<td></td>
</tr>
<tr>
<td>( \frac{1}{2}\arg(R_0) + \pi/2 )</td>
<td>29.4637</td>
<td>4.6946</td>
<td></td>
</tr>
<tr>
<td>( \arg(R_{1+}) )</td>
<td>-60.5363</td>
<td>94.6946</td>
<td>2.44</td>
</tr>
<tr>
<td>( \arg(R_{1-}) )</td>
<td>-60.5363</td>
<td>-85.3054</td>
<td>2.44</td>
</tr>
<tr>
<td>( m,\arg(a^*_m) )</td>
<td>1,-60.5363</td>
<td>0,94.6946</td>
<td>2.47(i)</td>
</tr>
<tr>
<td></td>
<td>3,-60.5363</td>
<td>2,-85.3054</td>
<td>2.47(i)</td>
</tr>
<tr>
<td></td>
<td>5,-60.5363</td>
<td>4,-85.3054</td>
<td>2.47(i)</td>
</tr>
<tr>
<td>( m,\arg(a^*_m) )</td>
<td>2,29.4637</td>
<td>1,4.6946</td>
<td>2.47(\text{i})</td>
</tr>
<tr>
<td></td>
<td>4,29.4637</td>
<td>3,4.6946</td>
<td>2.47(\text{i})</td>
</tr>
<tr>
<td>(b) Transmission Grating</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(</td>
<td>R_0</td>
<td>^2,\arg(R_0) )</td>
<td>.9822,-5.5939</td>
</tr>
<tr>
<td>(</td>
<td>T_0</td>
<td>^2,\arg(T_0) )</td>
<td>.0178,84.4061</td>
</tr>
<tr>
<td>( \arg(R_{1+}),\arg(R_{1-}) )</td>
<td>177.6512,177.6860</td>
<td>-28.3427,-38.4508</td>
<td></td>
</tr>
<tr>
<td>( \arg(T_{1+}),\arg(T_{1-}) )</td>
<td>-152.9450,-154.7621</td>
<td>57.2898,60.5514</td>
<td></td>
</tr>
<tr>
<td>( \frac{1}{2}\arg(R_{0+T_0}) )</td>
<td>1.0361</td>
<td>28.7943</td>
<td>2.50(i)</td>
</tr>
<tr>
<td>( \frac{1}{2}\arg(R_{0-T_0}) )</td>
<td>-6.6300</td>
<td>87.9129</td>
<td>2.50(\text{ii})</td>
</tr>
<tr>
<td>( \arg(R_{1+T_1})+\pi )</td>
<td>1.0359</td>
<td>28.7926</td>
<td>2.50(\text{i})</td>
</tr>
<tr>
<td>( \arg(R_{1-T_1})+\pi )</td>
<td>1.0360</td>
<td>28.7928</td>
<td>2.50(\text{i})</td>
</tr>
<tr>
<td>( \arg(R_{1+T_{1-}})+\pi )</td>
<td>-6.6296</td>
<td>-92.0853</td>
<td>2.50(\text{ii})</td>
</tr>
<tr>
<td>( \arg(R_{1-T_{1-}})+\pi )</td>
<td>-6.6299</td>
<td>-92.0861</td>
<td>2.50(\text{ii})</td>
</tr>
<tr>
<td>( m,\arg(a^*_m) )</td>
<td>1,-6.6300</td>
<td>0,-92.0872</td>
<td>2.51(\text{i})</td>
</tr>
<tr>
<td></td>
<td>2,83.3700</td>
<td>1,-2.0872</td>
<td>2.51(\text{ii})</td>
</tr>
<tr>
<td>( m,\arg(b^*_m) )</td>
<td>1,1.0361</td>
<td>0,28.7943</td>
<td>2.51(\text{ii})</td>
</tr>
<tr>
<td></td>
<td>2,91.0361</td>
<td>1,118.7943</td>
<td>2.51(\text{ii})</td>
</tr>
<tr>
<td>( \arg(T_0)-\arg(R_0) )</td>
<td>90.0000</td>
<td>-90.0000</td>
<td>2.52</td>
</tr>
<tr>
<td>( \cos^2[\arg(a^<em>_m)-\arg(b^</em>_m)] )</td>
<td>.9822</td>
<td>.2634</td>
<td>2.53</td>
</tr>
<tr>
<td>( \arg(a^<em>_m)+\arg(b^</em>_m) )</td>
<td>-5.5939</td>
<td>-63.2929</td>
<td>2.54</td>
</tr>
</tbody>
</table>
TABLE 2.3  
Littrow Symmetry Properties for the Infinitely-Conducting Lamellar Grating

Intensity and phase values of the field amplitudes are presented and are shown to conform with the symmetry relations of Section 2.3.

Groove Parameters:  
d = 1.0, c = 0.6, h = 0.9

Mounting Parameters:  
λ = 1.1, θ = 33.3670°

Number of Expansion Terms:  
P = 7, M = 8.

(a) Reflection Grating

<table>
<thead>
<tr>
<th>Equation Number</th>
<th>S Polarization</th>
</tr>
</thead>
<tbody>
<tr>
<td>B₀</td>
<td>.3615, -77.3082</td>
</tr>
<tr>
<td>B₁</td>
<td>.6385, -167.3082</td>
</tr>
<tr>
<td>B₂</td>
<td>.0485, 147.4426</td>
</tr>
<tr>
<td>B₃</td>
<td>.0141, 28.1295</td>
</tr>
<tr>
<td>arg(B₀+B₁)</td>
<td>-65.1738</td>
</tr>
<tr>
<td>arg(B₀-B₁)</td>
<td>-12.1344</td>
</tr>
<tr>
<td>arg(B₁+B₂)</td>
<td>-65.1713</td>
</tr>
<tr>
<td>arg(B₁-B₂)</td>
<td>-12.1355</td>
</tr>
<tr>
<td>arg(bᵣ), m=0, 2</td>
<td>-65.1738, -65.1738</td>
</tr>
<tr>
<td>arg(bᵣ), m=1</td>
<td>-102.1344</td>
</tr>
<tr>
<td>cos²[arg(bᵣ)-arg(bᵣ)]</td>
<td>.6385</td>
</tr>
<tr>
<td>arg(bᵣ)+arg(bᵣ)</td>
<td>-167.3082</td>
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</table>

(b) Transmission Grating

<table>
<thead>
<tr>
<th>Equation Number</th>
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</thead>
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<tr>
<td>A₀</td>
<td>0.866, -50.9159</td>
</tr>
<tr>
<td>A₁</td>
<td>-158.5673</td>
</tr>
<tr>
<td>A₂</td>
<td>.4980, 118.7812</td>
</tr>
<tr>
<td>A₃</td>
<td>-158.5662</td>
</tr>
<tr>
<td>arg(P₀+P₁)</td>
<td>88.4170</td>
</tr>
<tr>
<td>arg(P₀-P₁)</td>
<td>-29.0821</td>
</tr>
<tr>
<td>arg(P₁+P₂)</td>
<td>23.0163</td>
</tr>
<tr>
<td>arg(P₁-P₂)</td>
<td>-29.0839</td>
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<tr>
<td>arg(M₀+M₁)</td>
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<tr>
<td>arg(M₀-M₁)</td>
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<tr>
<td>arg(aᵣ)</td>
<td>88.4166</td>
</tr>
<tr>
<td>arg(aᵣ)</td>
<td>23.0163</td>
</tr>
<tr>
<td>arg(bᵣ)</td>
<td>60.9151</td>
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<td>arg(bᵣ)</td>
<td>88.4170</td>
</tr>
<tr>
<td>arg(bᵣ)</td>
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<tr>
<td>L.H.S. of eq.(2.71)</td>
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</tr>
<tr>
<td></td>
<td>0.5866</td>
</tr>
</tbody>
</table>
S polarization:  \( \phi_m(y) = \cos(\mu_m(y+h))/\cos(\mu_m h) \)

\[
E_m(x) = (-1)^{m/2} \cos(\frac{\mu_m x}{c}) \quad m = 0, 2, ...
\]

\[
O_m(x) = (-1)^{(m+1)/2} \sin(\frac{\mu_m x}{c}) \quad m = 1, 3, ...
\]

while those appropriate to equation (2.48) for the transmission grating are:

\[
E_m(y) = \cos(\mu_m y)/\cos(\mu_m h/2)
\]

\[
O_m(y) = \sin(\mu_m y)/\sin(\mu_m h/2)
\]

\[
E_m(x), O_m(x) \text{ as above.}
\]

Some of the phases in Tables 2.2 and 2.3 have been adjusted by a factor of \( \pi \), as allowed for by the phase relations, in order that direct comparisons may be made more readily. The overall result of these tests is that conformity with all the conservation relations of Section 2.3 is excellent - the maximum discrepancy being 0.002° where the values for M and P are 8 and 7 respectively.

A further check on the computer programs in the case of the transmission grating, was to evaluate the energy flux of each mode in the aperture in a negative \( y \)-direction. (There is no coupling between the individual modes which are orthogonal.) The sum of this energy over all modes can then be compared with the total energy appearing in the transmitted real orders. By using the Poynting vector, the total down-going energy flux for each polarization is expressed by

\[
P \text{ polarization } S_y = \frac{1}{2\omega \mu} \int_{-c/2}^{d-c/2} \text{Im} \left[ E_z \frac{\partial E_z}{\partial y} \right] dx
\]

\[
S_y = \frac{-1}{2\omega e} \int_{-c/2}^{d-c/2} \text{Im} \left[ H_z \frac{\partial H_z}{\partial y} \right] dx
\]
By inserting the appropriate modal expansions for $E_z$ and $H_z$ into these equations, and then repeating the procedure for the incident wave, the normalised energy flux for the $m^{th}$ mode is derived to be

$$
P \text{ polarization } \quad E.F._m = \frac{c}{2\chi_0 d} \text{ Im} (b_m \overline{\nu_m a_m}) \quad m = 1, 2, \ldots$$

$$
S \text{ polarization } \quad E.F._m = \frac{c e_m}{\chi_0 d} \text{ Im} (b_m \overline{\nu_m a_m}) \quad m = 0, 1, \ldots \quad \text{(2.75)}$$

Calculations made with these formulae were found to conform with maximum possible precision to the transmitted energy sum, irrespective of the number of modes being used. This is the result expected since this test should be analytically satisfied as is total energy conservation.

A final analysis of the numerical calculations was to study the effect on the boundary values of increasing the size of $M$. These values are of course analytically constrained by the formalisms on the vertical metal walls but it is of interest to determine the accuracy obtained in the matching of modal fields with plane-wave fields. To do this, the values of the $y$-derivatives of the respective fields were calculated along $y = 0$ for the reflection grating in the case of $S$ polarization. Table 2.4 shows the match of the real component of the magnetic field derivative, as a function of $x$, for values of $M$ ranging from 3 to 20. The value of $c$ is 0.6d and as expected the mismatch is worst near the metal-free space discontinuity at $x = \pm 0.3d$. As was not expected however, the overall matching does not improve as $M$ is increased. In fact the reverse is true. The reason for this is not clear, however it is assumed to have have no adverse effect on the accuracy or otherwise of the formalisms. This information is useful to remember during the analysis of boundary value calculations for alternative formalisms, as described in later chapters.
TABLE 2.4
S Polarization Field Matching for the Lamellar Reflection Grating

The real part of the mismatch between the free-space and groove region magnetic field derivatives along the top grating surface, is given as a function of the number of terms included in the field expansions.

Groove Parameters: \( d = 1.0, \ c = 0.6, \ h = 0.9 \)
Mounting Parameters: \( \lambda = 0.4, \ \theta = 0^\circ \)

| \( x \) co-ordinate | Field Mismatch \( P_{,M} \) |
|---------------------|--|--|--|--|--|
|                    | 10.3 | 10.5 | 7.8 | 10.8 | 10.20 |
| 0.500              | 0.15  | 0.26  | -0.62 | 0.35  | 0.74  |
| 0.429              | -0.12 | -0.04 | 0.66  | -0.06 | 0.08  |
| 0.357              | -0.30 | -0.51 | -0.81 | -0.69 | -1.39 |
| 0.286              | -0.77 | -1.30 | -2.10 | -1.73 | -5.10 |
| 0.214              | -0.09 | -0.15 | 0.40  |       | -2.04 |
| 0.142              | 0.10  | 0.18  | -0.14 | 0.24  | -0.53 |
| 0.071              | 0.02  | 0.03  | 0.06  |       | 0.53  |
| 0.0                | -0.08 | -0.14 | -0.03 | -0.19 | 0.90  |
The conclusion to be drawn from the material presented in this section is that it forms positive evidence of the accuracy and validity of the theoretical formulations described in Section 2.2. The truncation limits on the infinite series of \( P = 7 \) and \( M = 8 \) have proved to be more than adequate for the tests that were imposed. As a result, these values for \( P \) and \( M \) have been used for the majority of the numerical work presented hereafter. The final section in this chapter demonstrates that smaller values of \( M \) are adequate in certain circumstances.

2.5 A PROPERTY RELATING THE REFLECTION AND TRANSMISSION GRATING AMPLITUDES

As observed in Section 2.2, basic similarities exist between the scattering matrices for the reflection and transmission gratings. In fact, reference to equations (2.13) and (2.35) for the case of \( P \) polarization shows that, allowing for a phase difference of \( \chi_0 h \) (due to the origin shift), the \( y \)-antisymmetric mode amplitudes \( a^* \) for a transmission grating of depth \( 2h \) are equal to one-half of those for a reflection grating of the same width but of groove depth \( h \). A similar result is apparent in the case of \( S \) polarized radiation but in that case it is the \( y \)-symmetric amplitudes \( b^* \) which exhibit the same relationship.

This property is explained as follows for the general case when a transmission grating with up-down groove symmetry is compared with a reflection grating whose grooves consist of only the top-half of those of the former.

Consider the case for \( P \) polarization. Using the conventional \( xyz \) coordinate system, let a separable modal field in the aperture of the transmission grating be represented by

\[
E^T(x,y) = \sum_m [a^T_m \phi_m(y) + b^T_m \phi_m(y)] \phi_m(x) \quad ...(2.76)
\]
where the origin has been chosen to lie half-way between the upper and lower surfaces such that \( O_m(y) = -O_m(-y) \) and \( E_m(y) = E_m(-y) \). The field for the corresponding reflection grating, whose origin lies on the groove bottom, can therefore be expressed by

\[
E^R(x, y) = \sum_m a_m^R O_m(y) \phi_m(x) \tag{2.77}
\]

For the field to vanish on the groove bottom \((y = 0)\), as required by the appropriate boundary condition, we must have \( O_m(0) = 0 \).

Now consider a function \( D(x, y) \) defined by \( D(x, y) = E^T(x, y) - E^T(x, -y) \) and which reduces to

\[
D(x, y) = 2 \sum_m a_m^T O_m(y) \phi_m(x) \tag{2.78}
\]

This function represents the difference of the fields which would be present in the aperture of the transmission grating if two incident beams symmetrically placed about the x-axis were to strike that grating. As is evident from equation (2.78), \( D(x, y) \) vanishes along the line \( y = 0 \) and so satisfies the same boundary conditions as does \( E^R(x, y) \). These two representations are therefore equivalent in describing the same problem and one can therefore equate their respective expansion coefficients to give

\[
a_m^R = 2a_m^T \quad \text{for all } m. \tag{2.79}
\]

This property indicates that the phases of the reflection grating mode amplitudes are equal to those of the y-antisymmetric mode amplitudes belonging to a transmission grating of twice the depth when operated in an identical mounting configuration. The moduli of the former are also twice those of the latter. These relationships have been found to be accurately met by the numerical results provided by the formalisms of Section 2.2 (see Table 2.5).
Phases and moduli of the modal amplitudes are tabulated for confirmation of the properties discussed in Section 2.5.

Groove Parameters: \( d = 1.0, c = 0.6, h = 0.45 \) (Ref. Grating) 
\( h = 0.90 \) (Trans. Grating)

Mounting Parameters: \( \lambda = 1.3, \theta = 30^\circ \)

Number of Expansion Terms: \( P = 7, M = 8 \)

<table>
<thead>
<tr>
<th>P Polarization</th>
<th>S Polarization</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>(</td>
</tr>
<tr>
<td>Reflection Grating</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.9616</td>
</tr>
<tr>
<td>2</td>
<td>0.1972</td>
</tr>
<tr>
<td>3</td>
<td>0.1608</td>
</tr>
</tbody>
</table>

| 2 | 0.1972 | 69.5109 | 1 | 1.3138 | 165.4773 |
| 3 | 0.1608 | -165.0309 | 2 | 0.0979 | -55.3459 |

(Note: Due to the different positions of the origin, a phase factor of \( \chi_0 h \) has been subtracted from the reflection grating results.)
In the case of S polarization, a corresponding analysis to the above establishes that the y-symmetric mode amplitudes obey the relation
\[ b_m^R = 2b_m^T \text{ for all } m. \] ...\((2.80)\)

Although these properties are probably of little use in comparing overall efficiency performance between the two types of grating, they are demonstrated in the following chapter to aid in the prediction of the occurrence of resonance anomalies in the transmission grating spectra, given their presence in the spectra for the reflection grating.

2.6 SPECTRAL PROPERTIES

Preliminary examination of the diffraction behaviour of the lamellar profile involved the computation of various efficiency spectra as functions of both the groove width c and the groove depth h. Since the grating surfaces being dealt with are perfectly conducting, the actual physical values of the input variables are not significant but rather the values of these quantities relative to the grating period \( d \). Therefore, if not specified here (or in subsequent chapters), all grating parameters and the wavelengths \( \lambda \), are assumed to be normalised to the value of \( d \).

As explained in Section 1.1.4, one of the most important mounting configurations is the Littrow mounting and so this is adopted as the configuration for a detailed study of the behaviour of the reflection grating. For the transmission profile a normal incidence mounting is chosen since possible uses for this device are with filter applications. In both cases the primary regions of interest are those wavelength bands where only two diffraction orders are propagating. In the former case this is the interval \( 2/3 < \lambda < 2.0 \), while in the latter case it is defined by \( \lambda > 1.0 \).
2.44

Figure 2.4 illustrates an example of the efficiency spectra obtained for both profile types while in Appendix 1 a more comprehensive set of curves is to be found for a range of groove dimensions.

2.6.1 Reflection Grating Spectra

The spectra for the reflection grating are discussed first. A most notable feature observed is the marked polarizing property of the profile. In general, and in line with the results for alternative profiles used in this mounting, S polarization exhibits the superior performance in being able to furnish high efficiency in the -1 order over large bandwidths. On the other hand, the energy diffracted into this order for P polarization is relatively poor, especially for intermediate groove widths and depths where the bandwidths are much narrower.

This polarizing action prompted Roumiguieres [2.22] to suggest a possible application of the lamellar reflection grating as an infra-red polarizer when he predicted similar behaviour for a constant angle of incidence mounting.

A definite feature of all the Littrow spectra is the different manner in which the -1 order efficiency for the two fundamental polarizations approaches zero just before the 0 and -1 orders "pass off", i.e. at \( \lambda = 2.0 \). For S polarization the efficiency usually drops quite abruptly just prior to grazing incidence, while for P polarization it decreases far more gradually. An explanation of this phenomenon is discussed in the next chapter, motivated by the fact that it could lead to further information concerning modal expansions for alternative profiles which exhibits similar behaviour.

For narrow groove widths, of say \( c < 0.3 \), and irrespective of groove depth, the P polarization efficiency curves show very little energy being channelled into the -1 order. This is expected because the surface current flows parallel with the grooves and if the surface is predominantly "land"
Figure 2.4 Efficiency spectra for the perfectly-conducting lamellar grating ($P=7, M=8$).

(- - - -) $P$ polarization (--- - -) $S$ polarization

(a) Refl. Grating: $d=1.0, c=0.5, h=0.25, -1$ Littrow
(b) Refl. Grating: $d=1.0, c=0.5, h=0.40, -1$ Littrow
(c) Trans. Grating: $d=1.0, c=0.8, h=0.20, \theta=0^\circ$.
then the majority of the radiation will be reflected. For S polarization the current flows across the grooves and hence overall behaviour is less predictable.

For larger groove widths, the general action for P polarization can be described as a series of broad blaze peaks which move to longer wavelengths with increasing groove depth. Figure 2.4(a) shows the first of these peaks just emerging from the Rayleigh wavelength at $\lambda_R = 2/3$. The subsequent peaks which emerge from this wavelength are similar in shape and are separated by zeros in efficiency - a subject which is discussed further below. The larger the value of $c$, the wider are the spectral maxima and so the best performance for P polarization is achieved for $c$ approaching $d$ (i.e. a "comb" grating) and for a moderate value of $h$ in order that only one maximum occurs in $\lambda > \lambda_R$.

The efficiency behaviour for S polarization is not as uniform as the above, but in general distinctive features move to longer wavelengths with increasing groove depth. The most obvious characteristic of the curves for S polarization, which is not so evident for P polarization, is the existence of anomalous behaviour, i.e. very dramatic changes in efficiency. Figure 2.4(a) indicates the presence of a resonance anomaly near $\lambda = 0.8$. This presence is more obvious in Figure 2.4(b) where it has moved to $\lambda = 0.9$ with the increase in groove depth. Also to be seen in this spectrum is a Wood anomaly at a wavelength very near $\lambda_R = 2/3$ and this is attributed to a redistribution of energy as the -2,+1 orders pass off.

The existence of these two types of anomalies complicates any overall acceptable prediction of S polarization efficiency behaviour with variation of groove parameters. This must be replaced by numerical investigations.
An outstanding feature of the S polarization resonances is their extreme sharpness when compared with those produced by more conventional gratings such as sinusoidal, holographic or ruled gratings. It is not uncommon to find resonance peaks in some of the spectra to have normalised bandwidths less than 0.01, where it must be remembered that the wavelength is of the order of the period of the grating. In these situations one needs to be very careful not to overlook resonances altogether when computing efficiency curves. It is therefore useful to be able to predict their position and movement. Efforts towards this end are reported in a detailed analysis of resonance anomalies in Chapter 3.

Because the efficiency of the lamellar grating is dependent on two groove parameters compared with only one for the sinusoidal or right-angled echelette gratings, determination of the profile giving optimum performance for a particular mounting would be an enormous task, especially for unpolarized radiation. Experience has shown however, that for S polarization the best results for the -1 Littrow mounting are obtained for relatively shallow groove depths and intermediate groove widths. Figure 2.4(a) presents such an example and shows that an efficiency of above 90% is maintained over a normalised bandwidth of 1.09. The parameters used here are \( c = 0.50 \) and \( h = 0.25 \), and are found to be close to the optimum for this polarization and this mounting type -- a conclusion which was also reached by Loewen et al. [2.31]. For comparison, the optimum right-angled echelette and sinusoidal profiles for S polarization are deduced from the results of McPhedran [2.38] to be those with approximate normalised depths of 0.433 and 0.3 respectively. Both of these gratings have bandwidths for the 90% efficiency level of about 1.1.

As the depth of the lamellar grating grooves is increased beyond low values, resonance anomalies move from shorter wavelengths and tend to curtail the blaze, as can be seen in Figure 2.4(b).
Since $P$ polarization exhibits its best performance for $c$ approaching unity and for medium groove depths, the best results for unpolarized radiation occur for groove dimensions slightly larger than those given above for $S$ polarization. As an example, a groove profile of $h = 0.3$ and $c = 0.8$ (see Appendix 1) yields an unpolarized radiation efficiency of 50% for a bandwidth of approximately 1.1 periods.

The $-1$ Littrow condition, often referred to as the Bragg condition for gratings (defined by $\lambda = 2d \sin \theta$), has been proposed as a necessary condition for a blaze of 100% efficiency in the $-1$ order [2.13]. Subsequent to this proposal, work has been carried out with this mounting to locate conditions for simultaneous blazing for $S$ and $P$ polarizations for the lamellar reflection grating [2.28, 2.29, 2.9]. This work has been purely of a numerical nature, in that for each polarization the groove depth was varied and the corresponding angle of incidence which produces 100% blazing was found by computing efficiency values. In Chapter 3 the lamellar theory is analysed in an attempt to predict blaze wavelengths for the $-1$ Littrow mount. However, at this juncture a brief discussion is given of the nulls in the $-1$ order efficiency, i.e. the anti-blaze wavelengths.

Consider the case for $S$ polarization. It has been observed that wavelengths for which the general $-1$ order efficiency is low (excluding resonance behaviour), are those wavelengths predicted by the relation

$$\mu_0 h = \mu \pi, \quad \lambda = 1, 2, 3, \ldots \quad (2.81a)$$

Since $\mu_0 = k = 2\pi/\lambda$, these are the wavelengths,

$$\lambda = 2h/\mu. \quad (2.81b)$$

Reference to Figure 2.4(b) shows such a minimum in efficiency near $\lambda = 0.82$. It is probably the influence of the nearby resonance which has displaced
this from a null at \( \lambda = 0.8 \), the wavelength predicted by the above equation with \( \lambda = 1 \).

The physical explanation for the above phenomenon is that at these wavelengths, along the line \( y = 0 \), the \( m = 0 \) mode function \( \phi_0(x,y) \) satisfies the condition \( \partial \phi_0 / \partial y = 0 \), which is the appropriate boundary condition for an infinitely conducting surface. That is, as far as the \( m = 0 \) mode is concerned, the groove behaves like a closed resonant cavity. If this mode is the dominant mode of the groove field (a subject to be discussed in the next section) then it is representative of the total field, and overall the grating behaves very close to that of a mirror with all energy being specularly reflected. An exception to this behaviour will occur if one of the other modes is either dominant or resonating (usually the \( m = 1 \) mode), thus allowing energy to leak into the \(-1\) order.

It is interesting to note that equation (2.81b) may be deduced from the Marechal-Stroke Theorem [2.39] when the latter (which is only valid for \( S \) polarization) is applied to the lamellar reflection grating in a normal incidence mounting. Under these conditions the theorem states that all energy is reflected back in the direction of the incident beam if the groove depth is an integral number of half-wavelengths, i.e. equation (2.81b). The deduction is therefore, that this equation becomes rigorous for predicting minima in diffracted efficiency when the angle of incidence is zero.

In the case of \( P \) polarization the situation is slightly different, since in the wavelength range of interest it is quite often no longer possible to distinguish between resonant and non-resonant contributions from the modes. This is because both are usually due to the same mode which is the lowest and dominant \( m = 1 \) mode. The zeros in the \(-1\) order efficiency now occur at wavelengths such that
\[ \mu_1 h = \lambda \pi, \lambda = 1,2,\ldots \]

\[ \text{i.e. } \lambda = \frac{2ch}{\sqrt{\lambda^2 c^2 + h^2}} \quad \ldots(2.82) \]

At these points, \( \phi_1(x,y) = 0 \) along the groove-top interface and this is equivalent to a mirror-like surface being there in so far as the \( m = 1 \) mode is concerned. In Figure 2.4(b) a null in efficiency is observed at a wavelength very close to 0.62, which is the value predicted by equation (2.82) with \( \lambda = 1 \).

Though the \( m = 1 \) mode is the dominant one for \( P \) polarization, it is not clear why the efficiency should become precisely zero at the aforementioned wavelengths. The efficiency would only be expected to be low since the higher order modes which do not vanish along \( y = 0 \) would be expected to play a minor role. It does appear, however, that the efficiency becomes zero at these points only if the groove width \( c \) is small enough so that modes of order higher than the first are evanescent. This conforms with conclusions drawn earlier, that the best performance for \( P \) polarization efficiency is obtained for large values of \( c \).

The above considerations suggest that in the development of a modal expansion technique applicable to an arbitrary profile, one could glean some information from the efficiency curves for that profile. That is, the zeros in the \(-1\) order efficiency could provide some knowledge of the nature of the dominant modes within the groove field.

Some further work has been carried out with the insertion of a dielectric plug into the grooves of the reflection grating. However, this is observed to have a detrimental effect on the blaze action because the resonance anomalies move to larger wavelengths with the increase in refractive index in the groove region. It appears that the efficiency curves retain their original shape and are simply displaced along the wavelength axis.
In conclusion then, we can say that following an extensive survey of the efficiency spectra for the lamellar reflection grating, the latter behaves not unlike the sinusoidal and other gratings [2.38] and that although very spectacular blaze action can be attained for S polarization, the efficiency for unpolarized radiation is curtailed due to the generally poor performance for P polarization and also the unfavourable effect of resonance anomalies. (The fact that these phenomena appear to be more pronounced for the rectangular profile as compared with say the sinusoidal profile, is the topic of a later discussion.) The overall similarity seen between the efficiency curves with those of alternative profiles is understandable in the light of work by Breidne and Maystre [2.40], who developed an equivalence rule which states that profiles which have the same fundamental in their Fourier series representation will possess essentially the same efficiency characteristics if only two orders are propagating in a constant deviation mounting. Because this rule is valid only for profiles which can be expressed as a Fourier sine series, it only applies to the symmetrical lamellar profile. This does not significantly limit its usefulness however, since the latter is found to be near to the optimum for spectroscopic purposes.

When all the criteria discussed in this section are considered along with the relative difficulty of manufacturing the rectangular-profile grating and the fine tolerances which must be adhered to in forming its groove dimensions, then this does detract to some degree from the overall suitability of the grating as a standard spectroscopic tool.

2.6.2 Transmission Grating Spectra

A discussion is now given of the efficiency spectra, evaluated for the transmission grating and shown in Figure 2.4(c) as well as in Appendix 1. These are predominantly for a normal incidence mounting although some work has been undertaken with constant wavelength and
Littrow mounting configurations. Very few results concerning the rectangular-wire grating have previously been published.

It is known that as the wavelength-to-period ratio becomes much greater than unity, any array will become increasingly reflecting for P polarized radiation while on the other hand allowing greater amounts of incident energy to be transmitted in the case of S polarization. This extreme polarizing ability of the grating at long wavelengths is clearly seen in Figure 2.4(c) and may be understood in terms of the theory of Section 2.2 as follows.

Assuming zero angle of incidence for simplicity, \( \chi_0 = 2\pi/\lambda \) is seen to tend to zero as \( \lambda \) increases. Using this fact in equations (2.35) and (2.36) for P polarization, analysis shows that the mode amplitudes \( a^* \) and \( b^* \) decline in magnitude and so with a vanishing field in the apertures, the grating behaves more like a mirror allowing less energy to pass through. For S polarization the situation is different. As \( \chi_0 \) tends towards zero, all modes disappear with the exception of the \( m = 0 \) mode. By considering only contributions for this value of \( m \), only the first term on the left-hand side of equation (2.38) is significant and \( a^*_0 \) behaves as \( d/[i c \cot(\mu_0 h/2)] \). With equation (2.39) it is the second term which is significant and \( b^*_0 \) tends towards +1. Substitution of these values into equation (2.75) for the transmitted energy flux asserts that in the limit of \( \chi_0 = 0 \), the \( m = 0 \) mode carries 100% of the incident energy through the aperture to be coupled to the zeroth diffracted order.

The efficiency curves indicate that maximum transmission is attained for P polarization for aperture widths \( c \) as large as possible. For widths less than half a period virtually all energy is reflected when operating in the long-wavelength region above \( \lambda/d = 1.0 \). Between the Rayleigh wavelengths of \( \lambda_R = 0.5d \) and \( \lambda_R = 1.0d \), total transmitted efficiency is relatively constant at a level which rises roughly proportional with \( c \).
as this quantity is increased. For large groove widths this level attains a value of 100% at $\lambda/d = 1.0$ where the ±1 orders pass off, before falling away towards zero in the long-wavelength region. The effect of increasing groove depth is to heighten the rate at which this efficiency falls away. That is, the larger the depth, the sharper is the filtering action. For $c = 0.8$ and $\lambda/d = 3.0$, $E^T(0) = 30\%$ for $h = 0.02$, whereas if $h$ is increased to 0.5, $E^T(0)$ drops to 1%.

For $S$ polarization, the transmitted efficiency is strongly influenced by the presence of resonance anomalies which are most prominent just above $\lambda/d = 1.0$. This is especially the case for narrow apertures, where it is quite remarkable that on a negligible background efficiency, sharp peaks reaching 100% transmitted efficiency are achieved. These phenomena are analysed in Chapter 3. As groove depth is increased they are observed to move towards longer wavelengths and broaden in half-width. For large groove apertures, very little evidence is seen of the anomalies and practically all incident energy is transmitted in the zero order over the entire long-wavelength region (see Figure 2.4(c)). This behaviour is essentially unaffected by variations in groove depth. Between $\lambda_R = 0.5d$ and $\lambda_R = 1.0d$, the total transmitted efficiency for $S$ polarization behaves very similarly to that for $P$ polarization in that it remains fairly constant over the interval and increases with widening of the groove aperture. Little evidence is seen of anomalous fluctuations in this region.

Mention was made in the discussion on the reflection grating spectra, of predictions concerning the wavelengths at which nulls occur in the diffracted order efficiency. This behaviour is not appropriate to the transmission grating because each mode function consists of a $y$-symmetric and a $y$-antisymmetric component for which it is impossible to choose a wavelength such that they simultaneously vanish along the groove top.
2.7 LIMITED MODE APPROXIMATIONS

2.7.1 Introductory Remarks

During discussions presented in the previous section, the term "dominant mode" often arose. This is because in certain situations, observation has shown that only one or possibly two modes (usually including the fundamental mode) play a significant role in characterizing the field within the groove region. This is especially so in the case of \( P \) polarized radiation if the groove aperture is not too large. The same comment is applicable for the orthogonal polarization if higher order resonances are not prominent. It therefore seems valuable to be able to decide under what circumstances approximations can justifiably be made to the modal expansions with the benefit that the calculations can be performed simply on a small calculator rather than a computer. Herein lies another advantage of a modal expansion technique over the integral methods for which such approximations cannot easily be made.

Previous work with monomodal models has been carried out by Chen [2.41] and McPhedran and Maystre [2.33], who took advantage of such a field truncation while studying inductive grids. The latter authors found that their model yielded greater accuracy for small apertures and large depths. This is in concordance with results given below for both the reflection and transmission gratings.

2.7.2 Theory and Discussion of Results

2.7.2.1 The Reflection Grating

Consider first the case of the reflection grating and initially assume it to be illuminated by \( P \) polarized radiation. The dominant mode is usually the \( m = 1 \) or lowest-order mode. By truncating the modal expansion of equation (2.3) to a single term, the first mode amplitude \( a_1 \) is given immediately from equation (2.13) to be
The p\textsuperscript{th} order amplitude is now expressed via equation (2.7) in the simple form,

\[ A_p = \frac{1}{d} a_1^* I_{1p} - \delta_{0,p} \] \tag{2.85}

A similar procedure to the above may be followed for S polarization. Using only \( m = 0 \) contributions, one obtains from equation (2.21),

\[ b_0^* = \frac{2dJ_{\infty}}{cd - \mu_0 \tan (\mu_0 h) K_{S0}^S} \] \tag{2.87}

where \( K_{mn}^S = \sum_{p=-\infty}^{\infty} i x_p J_{mp} J_{np} \) \tag{2.87}

The plane-wave coefficients \( B_p \) are given in terms of the single mode amplitude by the expression

\[ B_p = \frac{1}{d} b_0^* \mu_a \tan (\mu_a h) J_{sp} \] \tag{2.88}

Equations (2.85) and (2.88) provide means for a very rapid determination of the order amplitudes for the reflection grating once the summations framed by equations (2.84) and (2.87) have been evaluated.

Investigations to be reported later in this section reveal that adequate field representation in the regions of resonance anomalies and "passing-off" is only achieved for S polarization if at least two modes are included in the expansions. For this reason, the slightly more complicated bimodal expressions are now detailed for that polarization.

By allowing the indices \( m, n \) to only take on the values 0,1 in equation (2.21), one derives expressions for \( b_0^* \) and \( b_1^* \) which, when inserted
into equation (2.17), finally yield for the order amplitudes,

$$B_p = \frac{1}{d \chi_p} \frac{N_p}{D} + \delta_0, \ldots \text{(2.89)}$$

where

$$N_p = \frac{2}{d} \left( t_0 \cdot t_1 \left\{ J_{10}^0 J_{01} S^0 - J_{00}^0 J_{10} S^0 - J_{00}^0 J_{01} S^0 \right\} + c t_0 J_{00}^0 J_{01} p + 2 c t_1 J_{00}^0 J_{10} p \right) + \ldots \text{ (2.90)}$$

and

$$D = \frac{t_0 t_1}{d^2} \left( K_{00}^S K_{11}^S - K_{01}^S K_{11}^S \right) - \frac{c t_0}{2d} K_{00}^S - \frac{c t_1}{d} K_{11}^S + \frac{c^2}{2} \ldots \text{ (2.91)}$$

and $t_0 = \mu_0 \tan (\mu_0 h)$, $t_1 = \mu_1 \tan (\mu_1 h)$.

Calculation of the amplitudes in this case is clearly more tedious since four of the summations embodied by equation (2.87) must now be evaluated.

The spectral regions for which the above formulae produce acceptable results are now examined. Concentration is given to the -1 Littrow mounting although some other mounting types have been studied. A sample of the results of the investigation is contained in Figures 2.5 and 2.6 where the efficiencies provided by the limited-mode models are compared with those based on expansions containing at least eight modes.

One of the most important factors governing the accuracy of the approximations is the groove width $c$. As this parameter is increased, more modes are gradually required to adequately represent the field. In fact, it is clear that all the "real" modes as opposed to "evanescent" modes must necessarily be included in the expansions.

[The terms "real" and "evanescent" refer to the real or imaginary nature respectively of the $\mu_m$ which are the modal-field equivalent of the wave direction-cosines $\chi_p$. From equation (2.5) it can be seen that for $\lambda < \frac{2c}{m}$ the $m^{th}$ mode function is real-valued while for $\lambda > \frac{2c}{m}$ it is purely imaginary. The wavelengths $\frac{2c}{m}$, $m = 0, 1, \ldots$ will often be referred to as the mode thresholds as they are analogous to the Rayleigh wavelengths or order thresholds for the plane waves.]
Figure 2.5  Efficiency curves illustrating the accuracy of the limited-mode models for the lamellar reflection grating in a -1 Littrow mounting. (d=1.0)

(a) c=0.15, h=0.3     (b) c=0.5, h=0.1     (c) c=0.5, h=0.25
Figure 2.5 (Contd.)
(d) c=0.5, h=0.7  (e) c=0.8, h=0.3
(---) 8 modes  (-----) 2 modes  (----) 1 mode
Figure 2.6  Efficiency curves illustrating the accuracy of the limited-mode models for the lamellar reflection grating. \((d=1.0)\)

\[\text{(a) Constant wavelength mounting: } c=0.5, h=0.3, \lambda=0.8\]

\[\text{(b) Normal incidence mounting : } c=0.8, h=0.48\]
The \( m = 0 \) mode is always real since its threshold is at infinity while the \( m = 1 \) mode is real for \( \lambda < 2c \). In this light, let us consider the results displayed in Figure 2.5 in some detail.

The smallest groove width represented by the curves is \( c = 0.15 \) - the width used for Figure 2.5(a). Only the spectra for \( S \) polarization are depicted here because for such narrow apertures (less than about 0.3) an insignificant amount of energy is diffracted into the -1 order for \( P \) polarization. [Note that in all results presented here, the period \( d \) of the grating is taken to be unity.] These curves demonstrate that the monomodal model works well for \( S \) polarization in the case of very narrow grooves. The maximum discrepancy in this particular example is about 5\%, occurring just before the -1,0 orders pass off. The reason for the excellent modelling is due to the fact that the \( m = 1 \) mode threshold is at \( \lambda = 0.3 \), which is so far below the range of concern that the single real \( m = 0 \) mode is capable of reliably representing the field.

Figures 2.5(b) and (c) correspond to \( c = 0.5 \) and groove depths of \( h = 0.1 \) and \( h = 0.25 \) respectively. From them it can be seen that a single-mode model gives an excellent approximation for \( P \) polarization while for \( S \) polarization it fails to account for the anomalies present just above \( \lambda_R = 2/3 \) and also the blaze-peak just before the -1,0 orders pass off at \( \lambda_R = 2.0 \). A bimodal model is necessary to predict these features and in fact gives excellent agreement with the full-expansion - the maximum difference being about 4\% at the Wood anomaly near \( \lambda_R = 2/3 \).

The reason for the first of the failures of the monomodal model is that the resonance anomalies are due to the \( m = 1 \) mode, while the reason for the second of its failures is explained as follows.

As \( \lambda \) approaches the order threshold of \( \lambda_R = 2.0 \), then for the -1 Littrow mount, \( x_0 = x_{-1} \) are both real-valued and decrease towards zero. The values of \( x_p \) for \( p \neq 0,-1 \) are large and imaginary, so from equation (2.87)
Substituting this condition, along with equation (2.86), into equation (2.88) gives the result,

\[ B_p = \frac{-X_0}{X_p} + \delta_{o,p} \text{ as } X_0, X_{-1} \to 0 \]  

which implies that \( B_{-1} \to -1 \) at the order threshold instead of approaching zero. This behaviour is confirmed numerically and points out the inadequacy of a monomodal approximation for \( S \) polarization for the \(-1\) Littrow mount just below \( \lambda_R = 2.0 \).

Careful examination of equations (2.89) to (2.91) reveals how the bimodal model corrects the above failure at \( \lambda_R = 2.0 \). For \( p = -1 \), \( N_{-1} \) is independent of \( X_0 \) while \( D \) behaves as \( 1/X_0 \) as \( X_0, X_{-1} \to 0 \), the result being that \( B_{-1} \to 0 \). For \( p = 0 \), \( N_0 \) behaves as \( 1/X_0 \) and consequently \( N_0/D = 2iX_0d \) whereupon \( B_0 \) now tends towards \(-1\) at the threshold as required. Numerical observations of amplitude phase have confirmed this.

Calculations made with \( c = 0.5 \) for larger depths than those reported above, show that despite the increased number of fluctuations in the efficiency, the monomodal model remains a very effective approximation for \( P \) polarization – even below the threshold at \( \lambda_R = 2/3 \). In fact a slight improvement in agreement with the full expansion is evident from Figure 2.5(d), where \( h \) has been increased to 0.7. Other studies have also indicated that increased depth marginally improves the accuracy of the model. For \( S \) polarization, the bimodal model appears to cope with the increased depth equally well, although some larger discrepancies do occur, as expected, in the vicinity of the abrupt efficiency changes due to the resonance anomalies.
In Figure 2.5(e) the groove width has been increased to 0.8 whereupon the \( m = 2 \) mode threshold is now contained within the wavelength region of interest. For \( S \) polarization this has had no drastic effect on overall efficiency conformity - except in the vicinity of the sharp anomaly seen for \( h = 0.3 \) at \( \lambda = 0.725 \). This feature has not been duplicated by the bimodal model, due to it being the product of a resonance of the \( m = 2 \) mode. On the other hand, the monomodal efficiency predictions for \( P \) polarization have suffered considerably by the increase in \( c \). Substantial discrepancies (up to 50\%) between these results and the values obtained with the full expansion are observed in Figure 2.5(e).

The behaviour mentioned above is maintained for increases in groove depth while \( c \) remains large. That is, a bimodal model is necessary for both polarizations, allowing for the fact that some sharp resonant features may be overlooked for \( S \) polarization. Two modes are nevertheless sufficient to describe the general efficiency pattern for this polarization. Tests additional to those illustrated in Figure 2.5 have indicated that \( c = 0.6 \) is the approximate maximum groove width for \( P \) polarization for which a monomodal expansion suffices to furnish acceptable efficiencies within a few percent of the correct values in the wavelength interval where only two orders are propagating.

Observations for the -1 Littrow mount seem also to be applicable to a constant wavelength mounting, although less work has been carried out in this area. With parameters \( c = 0.5, h = 0.3 \) and \( \lambda = 0.8 \) a monomodal approximation for \( P \) polarization yields efficiencies to within 4\% of the true values for angles of incidence from 0° to 90° where from two to three orders are propagating (see Figure 2.6(a)). A similar approximation for \( S \) polarization is not appropriate near grazing incidence because as seen for the Littrow mount, \( |B_0|^2 \to 0 \) instead of 1. A bimodal model must therefore be implemented and this provides satisfactory efficiency predictions to within 7\% over the complete spectral range.
For a normal incidence mounting the x-antisymmetric modes are non-existent, as shown in Section 2.3.3, and so where a monomodal expansion is not adequate, then a trimodal expansion must be used. This was found to be the case for a grating specified by \( h = 0.48 \) and a relatively large value of \( c = 0.8 \), when illuminated with \( S \) polarized radiation of wavelength \( \lambda = 0.8 \) (see Figure 2.6(b)). The two prominent features which occur at \( \lambda = 0.55 \) and \( \lambda = 0.75 \) are influences of the \( m = 2 \) mode and since they are fairly broad, all of the first three modes should be included in the expansion to account for these phenomena. With \( P \) polarized radiation a monomodal model was found to produce reasonable results to within 10% of the correct values - except near the Wood anomaly close to \( \lambda_R = 0.5 \). This, however, is an improvement on the accuracy of the model secured for the Littrow mounting with a similarly large value for \( c \).

2.7.2.2 The Transmission Grating

Attention is now directed towards the application of limited mode models to the transmission grating, for which it is found that a single-mode model reproduces efficiencies quite accurately for both polarizations in the long-wavelength region.

Consider first the monomodal model for \( P \) polarization. Truncating equations (2.35) and (2.36) to a single term gives the first-order mode amplitudes as

\[
\begin{align*}
a_1^* &= \frac{i \chi_0 T_{10} E_0}{K_{11}^P - \mu_1 \cot \left( \frac{\hbar}{2} \right) \frac{dc}{2}} \quad \text{(2.94)} \\
b_1^* &= \frac{i \chi_0 T_{10} E_0}{K_{11}^P + \mu_1 \tan \left( \frac{\hbar}{2} \right) \frac{dc}{2}} \quad \text{(2.95)}
\end{align*}
\]

where \( K_{11}^P \) is given by equation (2.84) and

\[
E_p = \exp \left( i \chi_p \frac{\hbar}{2} \right) \quad \text{(2.96)}
\]
The order amplitudes are then simply expressed by the relations

\[
A_p = \frac{I_p}{dE_p} \left[ a_1^* + b_1^* \right] - \delta_{0,p} \exp \left( -i \chi_0 h \right) \quad \ldots (2.97)
\]

and \( \hat{A}_p = \frac{I_p}{dE_p} \left[ b_1^* - a_1^* \right] \quad \ldots (2.98) \)

The corresponding equations for a monomodel approximation for S polarization, based on the \( m = 0 \) mode, are as follows.

\[
a_0^* = \frac{d}{cd + \mu_0 \cot \left( \frac{\mu_0 h}{2} \right) K_{00}^S} \quad \ldots (2.99)
\]

\[
b_0^* = \frac{d}{cd - \mu_0 \tan \left( \frac{\mu_0 h}{2} \right) K_{00}^S} \quad \ldots (2.100)
\]

\[
B_p = \frac{i \mu_0 J_{0p}}{d} \frac{E_p}{\chi_p} \left[ b_0^* \tan \left( \frac{\mu_0 h}{2} \right) - a_0^* \cot \left( \frac{\mu_0 h}{2} \right) \right] + \delta_{0,p} \exp \left( -i \chi_0 h \right) \quad \ldots (2.101)
\]

\[
\hat{B}_p = \frac{i \mu_0 J_{0p}}{d} \frac{E_p}{\chi_p} \left[ b_0^* \tan \left( \frac{\mu_0 h}{2} \right) + a_0^* \cot \left( \frac{\mu_0 h}{2} \right) \right] \quad \ldots (2.102)
\]

It is noted that alternative means to equations (2.98) and (2.102) exist for calculating the efficiency in the zeroth transmitted order when this is the only order propagating. Because the \( m = 1 \) (or \( m = 0 \)) mode is assumed to be the only mode present in the groove aperture, then it must carry all the energy which in turn is transferred in total to the only diffracted order. This energy flux is provided by equations (2.75) which establish that:
P polarization  \[ \text{E.F.} = |A_0|^2 = \frac{c}{X_0d} \frac{\text{Im} \left( \frac{b_i^*}{\sin (\mu_1 h)} \right)}{\sin (\mu_0 h)} \]  \( \ldots (2.103) \)

S polarization  \[ \text{E.F.} = |B_0|^2 = \frac{2c\mu_0}{dX_0 \sin (\mu_0 h)} \frac{\text{Im} (b_i^* a_i^*)}{\sin (\mu_0 h)} \]

A second alternative for determining the transmitted efficiency in the long-wavelength region is provided by the conservation property of equation (2.53). From this constraint we have the very simple relations

P polarization  \[ |A_0|^2 = \sin^2 [\arg (a_i^*) - \arg (b_i^*)] \]  \( \ldots (2.104) \)

S polarization  \[ |B_0|^2 = \sin^2 [\arg (a_i^*) - \arg (b_i^*)] \]

Thus, after evaluating the mode amplitudes from equations (2.94), (2.95), (2.99) and (2.100), the transmitted efficiency of the array may be easily calculated from equations (2.98) and (2.102). If the wavelength exceeds the grating period then equations (2.103) and (2.104) provide the answer also, with the latter equation being by far the easier to use.

Numerical investigation of these models has centred around a normal incidence mounting configuration and computed curves are displayed in Figure 2.7, where again the true values are taken as those calculated with at least eight terms in the modal expansion. An indication as to whether the monomodal model will prove suitable in a particular wavelength region can be gained by studying the energy flux in each mode when the full expansion is implemented. These observations have revealed that for wavelengths above \( \lambda_R = 1.0 \), the vast majority of the energy is carried by the fundamental modes for both polarizations and that therefore a single-mode model is adequate in each case. However, below \( \lambda_R = 1.0 \) care must be exercised because although the lowest order modes might appear to carry the bulk of the energy, in some cases the third mode (the second mode having zero amplitude for normal incidence) does have a significant influence.
Figure 2.7 Efficiency curves showing the accuracy of the limited-mode models for the lamellar transmission grating in a normal incidence mounting. (d=1.0)

(a) c=0.4, h=0.2  (b) c=0.4, h=1.0  (c) c=0.8, h=0.02
on the efficiency. Therefore, the flux carried by each mode is only a guide to its overall necessity.

Figures 2.7(a) and (b) show the effectiveness of the monomodal models for a relatively small aperture width and two different groove depths. These curves clearly indicate the excellent accuracy of the model for both of these examples and for both polarizations over the wavelength range from $\lambda = 0.5$ to $\lambda = \infty$. The only exception occurs just above the threshold for the ±2 orders at $\lambda_R = 0.5$, where for S polarization the single-mode efficiency deviates from the true value and drops towards zero. In Figure 2.7(c) the groove parameters are $c = 0.8$ and $h = 0.02$. From the previous work with the reflection grating, this choice of groove dimension could be expected to secure fairly unacceptable results from the single-mode models. Although this is the case for the transmission grating for wavelengths below $\lambda_R = 1.0$, quite good agreement is obtained in the long wavelength region where the maximum discrepancy is about 6% for P polarization. Further testing with increased groove depth has shown this figure to rapidly improve to about 1% when $h = 0.2$.

Below $\lambda_R = 1.0$, the large groove width again has a detrimental effect on the accuracy of the monomodal model and this occurs for both polarizations. In the case of P polarization, large discrepancies are seen to emerge only near the ±2 order threshold. However, as mentioned above, and in line with findings for the reflection grating, the single-mode model for S polarization breaks down severely, not only at the Rayleigh wavelength $\lambda_R = 0.5$ but also at $\lambda_R = 1.0$. Investigations with more modes in the expansion have shown that a trimodal model will remedy this breakdown.

The explanation of why the monomodal model works so well above $\lambda_R = 1.0$ is probably because in this region the only real modes possible are those for $m = 0$ and $m = 1$. In the case of S polarization the latter mode
is not significant for normal incidence and both background and resonance behaviour are therefore due to the same $m = 0$ mode. This is evident from Figure 2.7(b), where two distinct resonance anomalies are due to this mode and hence adequately accounted for by the single-mode approximation. The situation is similar to that which exists for P polarization and the $-1$ Littrow mounting for the reflection grating.

In conclusion, it has been found that over a wide range of configurations, the use of single and double-mode approximations for the groove field is quite justified. The regions of suitability depend heavily on two main factors - the aperture width and the proximity of Rayleigh wavelengths where one or more orders pass off. The aperture width determines the mode thresholds and hence governs the number of modes which are real. The larger the value of $c$, then the greater is the number of real modes which can exist and undergo resonance. (This phenomenon is placed in perspective in the following chapter.) In the case of S polarization, the monomodal model has been found ineffective near Rayleigh wavelengths, except for profiles of very narrow groove width, because it fails to account for the proper energy redistribution. This is apparent for both grating types in different mounting configurations and has been proven theoretically for the reflection grating and the $-1$ Littrow mount at the Rayleigh wavelength $\lambda_R = 2.0$. 

REFERENCES

3.1 INTRODUCTION

A rigorous mathematical treatment of the lamellar grating, along with a description of its spectral properties, has been presented in Chapter 2. This chapter is concerned with relating those two areas of interest by analysing the theory in some detail and hence ascertaining the origin of many of the diffraction phenomena. The relatively simple lamellar theory makes this possible through the use of monomodal and bimodal approximations. However, it is important to realize that the conclusions which are reached here need not be confined to the lamellar grating, but may be applied to gratings in general. In fact, throughout this chapter many examples are cited which demonstrate the wide applicability of many of the concepts.

Attention is predominantly directed towards a study of resonances, the manifestations of which are clearly reflected in the efficiency curves of Chapter 2. The techniques established within this investigation are found useful in accounting for other major behavioural characteristics of the grating.

In Section 3.2, resonance anomalies are seen to arise when the physical wavelength is in close proximity to the free resonance wavelength of the structure. It is asserted that these complex quantities are fundamental in determining the overall behaviour of a grating. The material presented on this subject is based on work reported in references [3.1] and [3.2].

Section 3.3 provides some simple criteria, which when used in conjunction with the limited-mode approximations for the reflection grating, govern the wavelength positions of efficiency maxima for a -1 Littrow
configuration. These formulae are intimately related to the conditions for resonance maxima described in Section 3.2.

In Section 3.4, an explanation is proposed to account for the manner in which the $S$ and $P$ polarization efficiencies vary just prior to the 0 and -1 orders passing off in a first-order Littrow mounting. Included in the discussion is a further description of some of the poles which are responsible for the resonance phenomena detailed in Section 3.2. This particular group of poles is considered to be the dominant influence on the passing-off behaviour for $S$ polarization.

3.2 RESONANCE ANOMALIES

3.2.1 Introduction

The anomalous behaviour of gratings has received considerable attention from both theorists and experimentalists alike. For the latter, this is so because anomalies may well mask genuine spectral features. From a theoretical viewpoint however, anomalies have been studied for two main reasons - their explanation presents a formidable challenge to the theorist, while their prediction in efficiency spectra constitutes a critical test of new grating formalisms. Despite their first being observed by Wood [3.3] in 1902, an accurate prediction of their position and shape remains a difficult task. However, marked progress has been achieved over the past twenty years.

There exist numerous forms of irregular behaviour in grating spectra, but the majority of these are simply the result of imperfections in the groove shape, or periodic errors in the case of ruled gratings. An ideal grating can, however, still produce anomalous behaviour which is manifested as narrow bright or dark bands in the spectra. These were the phenomena seen by Wood and they have hence been termed Wood anomalies. To the theorist they may be described as rapid fluctuations in the intensity of a
particular diffracted order over a narrow range of wavelengths (or for a constant wavelength, over a narrow range in angles of incidence).

Wood discovered that the anomalies were more pronounced for $S$ polarized radiation and that rubbing the grating surface could make them disappear. This was originally thought to be an edge-effect but is now attributed to a decrease in the groove depth.

In 1907, Rayleigh [3.4] formulated his "dynamical theory" for gratings and was able to predict the salient spectral features observed at that time. In the case of $S$ polarization it contained (as do all present theories) singularities at wavelengths coinciding with Wood anomalies. These wavelengths, which provided the first explanation for anomalies, are the Rayleigh wavelengths defined in Section 1.1.4. Rayleigh's theory was incapable of describing the shapes of anomalies, but because it did not predict any anomalous behaviour for $P$ polarization it correlated with the observations of the time.

Further theoretical work was carried out by authors such as Artmann [3.5], Fano [3.6, 3.7] and Twersky [3.8, 3.9] who attempted to explain more qualitatively the form of anomalies. All of these theories proved inadequate in light of the work by Palmer [3.10, 3.11, 3.12] who demonstrated unequivocally the existence of $P$-anomalies for gratings with deep grooves. Because the then contemporary theories were valid only for shallow grooves, they were not able to explain Palmer's observations.

In 1962, Stewart and Gallaway [3.13] presented an extensive array of experimental data concerning Wood anomalies. By plotting the position of $S$-anomalies on a wavelength versus angle of incidence graph, they showed a correlation between these positions and the lines depicting Rayleigh wavelengths. They also reported a new phenomenon termed "repulsion of anomalies". The explanation of this phenomenon is now attributed to the existence of two different types of anomalies. An account of the "repulsion", using the lamellar grating as an example, is detailed in Section 3.2.2.
The distinction between the two types of anomalies was first clarified by Hessel and Oliner [3.14] (see Section 1.2.5). Although limited in its practical application, their method was the first to demonstrate in a qualitative manner, how the shape of anomalies depends on groove profile and how they can exist for both S and P polarizations. The two types of anomalies they recognized are (i) the Rayleigh wavelength anomalies associated with the passing off or onset of a particular order and attributed to the resultant re-distribution of energy, and (ii) resonance anomalies (previously discussed by Twersky) which occur separately from the former type.

Rayleigh wavelength anomalies correspond to branch point singularities in the S polarization theory and are often quite pronounced. For P polarization they are not nearly so evident since the electric vector is parallel to the grooves and "short-circuits" the field of the appropriate order as it grazes the surface. In this chapter, attention is primarily devoted to the more interesting resonance anomalies.

Hessel and Oliner attributed these phenomena to the stimulation of surface-waves, which are supportable by the grating and which travel parallel to the surface. (Fano [3.7] had also discussed the problem in terms of surface waves.) For large values of λ/d where only the reflected order propagates, any guided-wave excited by the incident plane-wave is a purely bound surface-wave. However, when λ/d is small and spectral orders exist, the grating can support leaky waves of complex wave-number. Should the wavelength of the incident beam be such that one of the diffracted orders has its wave-vector coinciding with that of a leaky-wave, then a resonance can occur. Because the wave-number of the plane-wave is real, then the resonance is not a total one but a forced one, and while the intensities of the order amplitudes cannot become infinite, a redistribution of energy between the orders can take place. The larger the groove modulation, the larger is the imaginary part of the complex resonant
frequency and hence the smaller is the Q-value of the resonance.

From the above explanation, it is noted that the resonant spectral order (the one which couples to the guided wave) is always evanescent and so resonance is expected at wavelengths just above a Rayleigh wavelength. The theory of Hessel and Oliner shows that the conditions for producing the two different types of anomaly are quite similar and are in fact equivalent for infinitely-conducting gratings with zero groove modulation. That is, for $h = 0$ and $\lambda = \lambda_R$ the two types of anomaly superimpose with the resonance anomaly moving to slightly longer wavelengths as $h$ increases. This agrees with experimental observations and also the findings for the lamellar grating discussed in the next section. For a plane surface with a non-zero surface reactance, the anomalies are expected to remain separated.

In explaining the anomalous absorption of radiation by finitely-conducting metallic gratings, several authors [3.15-3.22] have attributed the phenomenon to the interaction of the incident electromagnetic wave with plasma waves near the surface of the grating. The resulting resonances, called surface plasma oscillations (S.P.O.'s), are due to the excitation of the plasma mode of oscillation of the electron gas in the metal. Although difficult to detect for plane surfaces, they are easier to locate for a modulated surface. They only exist in the case of S polarization. A very interesting phenomenon associated with S.P.O.'s is the scattering of stray light out of the plane of incidence. Such scattering is caused by grating imperfections and would not occur for "ideal" gratings.

Many investigations into S.P.O. have been made, initially by Teng and Stern [3.15], and subsequently by other authors [3.16-3.19]. While suggested by Hutley and Bird [3.20] as a reason for discrepancies between infinite conductivity and measurements, later work including finite conductivity effects [3.21] eliminated the discrepancy.
Ever since the work of Palmer [3.10], it has been known that anomalies for metal gratings, especially P-anomalies, are enhanced by overcoating the metal with a dielectric layer. A study of this phenomenon has been reported by Hutley et al. [3.22] who suggested that appropriate coatings may lead to the elimination of anomalies. Their experimental results were able to confirm the theoretical predictions of Nevière et al. [3.23] who found that for coated gratings, the -1 Littrow S-anomaly can split into two narrower anomalies, while for P polarization an anomaly can occur which is similar to the S-type anomaly for uncoated gratings. Although they discovered strong similarities between the "coated" efficiency curves for P polarization and the "uncoated" curves for S polarization, the former cannot be explained in terms of surface plasmons and must be attributed to the excitation of leaky modes in the dielectric layer.

The inability of the integral and differential theories to explain resonances was recognized by Maystre and Petit [3.24], who initiated a new approach to the treatment of anomalous absorption of energy by gratings. Their method is based on the analogy which exists between anomalies and the Brewster phenomenon of dielectric materials.

The Brewster angle for conventional materials is given by

\[ \sin \theta_B = \frac{v}{\sqrt{1 + v^2}} \]  

...(3.1)

where \( v \) is the refractive index. Under this condition the reflection coefficient \( r \) is zero. In the case of metals, for which \( v \) is complex, the above condition implies that \( \theta_B \) is complex and the corresponding incident wave is inhomogeneous. Writing \( \sin \theta_B = \alpha_r + i\alpha_i \) we note that \( \alpha_r > 1 \) and so a physical wave can never reduce \( r \) to a small value for a plane surface having \( v \) fixed (\( v \neq 1 \)).

From the Fresnel formula for the reflection at a plane metal interface, it is found that condition (3.1) represents a pole in both the reflected and transmitted coefficients, but for S polarization only.
That is, it gives rise to a reflected and transmitted field without the occurrence of an incident field. This resonance position in the complex $\theta$ plane is related to a surface plasmon. For the plane surface, the complex zero and pole for $r$ coincide. For infinite conductivity this position would be a Rayleigh wavelength while for finite conductivity it is removed from the Rayleigh wavelength.

To stimulate the plasmon resonance in a real situation requires approaching as close as possible to the pole. This is achieved with an evanescent wave with $\alpha \approx \alpha_r$, since for highly conducting metals $\alpha_r > 1$ and $\alpha_i \approx 0$. By roughening the plane surface, a momentum transfer between plasmon and plane-wave is possible and in the case of a shallow grating the dispersion relation is given by

$$\pm \alpha_r = \sin \theta + \frac{n\lambda}{d} \quad \ldots (3.2)$$

where $\alpha_r$ corresponds to one of the diffracted orders. As required, $\alpha_r$ can now be greater than unity. However, this analysis, which shows that the plasmon resonance must occur on the long wavelength side of the Rayleigh wavelength, is only an approximate one because the plasmon dispersion relation is only applicable to plane surfaces. A rigorous solution for this relation requires a complicated derivation from the complex electromagnetic theory. The removal of this deficiency is one motivation for developing a finitely-conducting modal theory for arbitrary profiles.

Some attempts have been made with first-order perturbations for the grating surface to try and resolve the exact nature of the plasmons, but these have had limited success.

The method of Maystre and Petit [3.24] is an attempt to remove the complexity of the rigorous electromagnetic theory and gain a simple but accurate model of the problem. They modified their finite-conductivity theory to accept complex values for $\sin \theta$ and plotted the trajectories of $\alpha_p$ and $\alpha_z$ (corresponding to the pole and zero for $r$ respectively) in the
complex plane as a function of groove depth for the sinusoidal profile. For \( h = 0 \), \( \alpha_p \) and \( \alpha_z \) coincide. As \( h \) is increased, \( \alpha_p \) moves further into the complex plane while \( \alpha_z \) moves the other way across the real-axis. Thus, for a particular value of \( h \), \( \alpha_z \) is real-valued, and for the corresponding value of \( \theta \) a homogeneous incident wave is completely extinguished. (Note that this treatment only applies for the case of one real order.)

Maystre and Petit concluded that the electromagnetic theory is more powerful than the plasmon theory because it is able to predict exactly the resonance position. It should be remembered though, that the analysis is still based on numerical calculations to determine the value of \( h \) which gives total absorption.

Hutley and Maystre [3.25] verified the above predictions experimentally. Numerical evidence was also provided to demonstrate the accuracy with which the formula,

\[
B_0(\alpha_0, h) = r(\alpha_0) \frac{\alpha_0 - \alpha_z(h)}{\alpha_0 - \alpha_p(h)}
\]

models the amplitude of the reflected order near a resonance. Here \( r(\alpha_0) \) is the plane surface reflection coefficient. The derivation of this formula is contained in reference [3.26].

The above treatment has been extended by Nevière et al. [3.27] to successfully account for the absorption of \( P \) polarized radiation by dielectric-coated gratings. Experimental confirmation of the total absorption obtainable for this polarization has been furnished by Loewen and Nevière [3.28] who used a blazed Al grating coated with MgF\(_2\). Employing the electromagnetic theory to plot trajectories of complex poles and zeros, they showed the position of the anomaly to be given approximately by

\[
\sin \theta + \lambda/d = Re(\alpha_z) \approx Re(\alpha_p)
\]
For a dielectric thickness $e < 0.12$, they found the anomalies were below the cut-off region for guided waves. As the thickness was increased, the pole and zero moved so that $\Re(\alpha_z) > 1$, and finally for $e = 0.15$, $\Im(\alpha_z)$ was found to vanish. While the dielectric constants of the layer have only a small role, it is the complex refractive index of the metal, along with the surface modulation, which results in forming the imaginary components of $\alpha_p$ and $\alpha_z$. Loewen et al., unable to draw on the theory for surface plasmons, provided no physical explanation for the total absorption phenomenon for this polarization.

Shah and Tamir [3.29] are critical of the plasmon explanation in stating that total absorption at resonance is not peculiar to metallic gratings but is a property of a range of structures in various configurations, e.g. in the field of acoustics [3.30]. They reasoned the phenomenon in terms of leaky (surface) wave interactions in the presence of metallic or dielectric losses. For a general plane-layered structure, they derive the reflectivity again in terms of poles and zeros and associate the former with surface waves if real, and with leaky waves if complex. For lossless cases, the reflectivity must be 100% and it is shown that the zero is the complex conjugate of the pole. (This is in accordance with findings described in Section 3.2.2.) As conduction losses are introduced, the pole and zero follow trajectories in the complex wave-number plane, and again a point is reached where the zero lies on the real axis. At this point the incident beam is phase-matched to the "leakage angle". Their treatment, which is applicable for both $S$ and $P$ polarizations, is not confined to plane-layered structures and may be adapted to metallic gratings. There the conduction losses cause the movement of the zero, and the modulation enables a diffraction order to be phase-matched. That is, metallic gratings are considered to be only one example of a broad class of leaky-wave structures and complete suppression of the reflected wave is considered possible provided the grating can support a leaky-wave which satisfies the slow leakage condition.
\[ \alpha_i < \alpha_r. \]  \quad \text{(3.5)}

Other theoretical investigations into resonance anomalies have recently been carried out by Maystre et al. [3.31] who generalized their study of absorption to the case of several spectral orders. Also, Utagawa [3.32] attempted a simplified integral equation technique but was only able to apply it to shallow profiles.

To date, the only treatment of resonances which resembles the approach described in Section 3.2.2, is that of Jovicevic and Sesnic [3.33] who analysed their modal method for triangular profiles. They attributed anomalies to a rapid change in the scattering matrix elements which occurs when the phase change of an incident wave over a groove is either a multiple of \( \pi \) or an odd multiple of \( \pi/2 \). The method is specific to their particular case and provides little insight into the general problem of resonance anomalies.

The treatment described in the following section attributes resonances to poles in individual mode amplitudes. Analytic expressions (involving infinite sums) are presented which determine the location of these poles in the complex wavelength plane. No such expressions are available from the integral theories.

3.2.2 Resonances in the Lamellar Reflection Grating

It is clear from the previous discussion, that to gain accurate predictions of resonance behaviour it is essential that an appropriate rigorous electromagnetic theory be used. To this end, the numerical and theoretical studies presented here are based on the classical theory of Chapter 2. They do not rely on approximations such as those inherent in perturbation or surface plasmon theories.

The modal expansion representation for the field within the grooves is found to be particularly fruitful in that the resonances are seen to stem from the mode amplitudes which resonate individually at the natural
frequencies of the grating structure. This is contrary to the argument of Palmer and Lebrun [3.34] that such an approach would obscure the local origin of resonances.

Figures 3.1, 3.2 and 3.3 contain some efficiency curves for both S and P polarizations for the reflection grating when operated in a -1 Littrow mounting. The wavelength range given is confined to the interval near and above the Rayleigh wavelength, \( \lambda_R = \frac{2}{3} d \). The narrow features corresponding to anomalies are clearly visible. They are manifested in the efficiency as either sharp peaks or notches or a combination of both and are more pronounced than those for the sinusoidal grating [3.35]. In Figure 3.2(a) the depth of \( h/d = 0.7 \) is sufficient to produce two resonance anomalies. The efficiency spikes occurring at \( \lambda/d = 2/3 \) in Figures 3.1(c) and (d) and 3.2(a) are Rayleigh wavelength phenomena and receive little attention since their behaviour is fairly well known.

A comparison of the curves of Figure 3.1 with those of Figure 3.3 reveals the marked difference in performance for the two orthogonal polarizations. The S-plane resonances are sharper and superimposed on a slowly-varying background. This is because resonant and non-resonant contributions are due to different modes, shown later to be those with amplitudes \( b_1 \) and \( b_0 \) respectively. For the case of P polarization, contributions are due to the same mode, namely the lowest and more dominant one \( (a_1) \) and hence the total efficiency curve is a manifestation of resonances belonging to that mode.

3.2.2.1 Amplitude Parameterizations

Some useful parameterizations are now derived for \( A_0 (B_0) \) when only the reflected order is real, and for \( A_0 \) and \( A_{-1} (B_0 \) and \( B_{-1} \) when only two orders are propagating in a -1 Littrow mounting. In deriving these relations, the phase properties described in Chapter 2 are used and so \( R_p (T_p) \) represents either \( A_p \) or \( B_p (\hat{A}_p \) or \( \hat{B}_p \). Where a specific
Figure 3.1  S polarization efficiency spectra for the lamellar reflection grating in a -1 Littrow mounting.

Groove parameters: $d=1.0, c=0.43$ (a) $h=0.1$
(b) $h=0.3$
(c) $h=0.4$
(d) $h=0.5$
Figure 3.2 S polarization amplitude and phase variation, characteristic of resonances in the lamellar reflection grating in a -1 Littrow mounting. Plotted as a function of wavelength are:

(a) efficiency of the -1 order,
(b) intensity of the -2 evanescent order,
(c) phase of the -1 order amplitude and also the parameter $\delta$ introduced in the text, and
(d) phase of the $m=1$ mode.

Groove parameters: $d=1.0, c=0.43, h=0.7$
Figure 3.3  P polarization efficiency spectra and m=1 mode phase variation (ψ₁) for the lamellar reflection grating in a -1 Littrow mounting.

Groove parameters: d=1.0, c=0.43
(a) h=0.4
(b) h=0.6
(c) h=1.0
(d) h=1.4
polarization is referred to, the appropriate notation is used.

For the long-wavelength situation, conservation of energy implies that

\[ R_0 = \exp \left( i\phi_0(\lambda) \right) \] (3.6)

where \( \phi_0(\lambda) \) is a real function of wavelength.

For the -1 Littrow case, equations (2.56) imply that

\[ |R_{1-} + R_0| = 1 \] (3.7)

and hence from equations (2.59) we have

(i) \[ R_{-1} + R_0 = \exp(2i \arg(a_m^e)) \] (3.8)

(ii) \[ R_{-1} - R_0 = \exp((2i \arg(a_m^0)) \]

where \( a_m^e \) (\( a_m^0 \)) is the amplitude of the \( m^{th} \) x-symmetric (x-antisymmetric) mode. This decoupling of the functions \( R_{-1} \pm R_0 \) into terms involving only "even" or "odd" modes, is demonstrated for the lamellar grating by the manipulation of equations (2.7) and (2.17), which yield for the -1 Littrow mounting,

(i) \[ A_0 + A_{-1} = -1 + \frac{2}{d} \sum_{m \text{ odd}} a_m \sin(\mu_m h) I_{m_0} \] (P pol. \( \ldots (3.9) \)

(ii) \[ A_{-1} - A_0 = 1 + \frac{2}{d} \sum_{m \text{ even}} a_m \sin(\mu_m h) I_{m_0} \] \( \ldots \)

(i) \[ B_0 + B_{-1} = 1 + \frac{2i}{\lambda_0 d} \sum_{m \text{ even}} b_m \sin(\mu_m h) J_{m_0} \] (S pol. \( \ldots (3.10) \)

(ii) \[ B_{-1} - B_0 = -1 - \frac{2i}{\lambda_0 d} \sum_{m \text{ odd}} b_m \sin(\mu_m h) J_{m_0} \]

(Note: "even" ("odd") refers to even (odd) x-symmetry and corresponds to \( m \text{ odd} \) (even) for P polarization and \( m \text{ even} \) (odd) for S polarization.)

Equations (2.60), (2.61) and (2.62) may now be combined and the functions \( \phi(\lambda) \) and \( \delta(\lambda) \) introduced to give

(i) \[ R_{-1} = \cos(\delta(\lambda)) \exp[i\phi(\lambda)] \] (3.11)

(ii) \[ R_0 = \sin(\delta(\lambda)) \exp[i(\phi(\lambda) - \pi/2)] \]
where

(i) \( \delta(\lambda) = \arg(a^0_m) - \arg(a^e_m) \) 
(ii) \( \phi(\lambda) = \arg(a^e_m) + \arg(a^0_m) \).

From the latter equation, the modal phases are derived to be

(i) \( \arg(a^e_m) = \frac{1}{2}(\phi(\lambda) - \delta(\lambda)) \)
(ii) \( \arg(a^0_m) = \frac{1}{2}(\phi(\lambda) + \delta(\lambda)) \)

and hence from equations (3.8) the parameterization for \( R_{-1} \pm R_0 \) becomes

\[ R_{-1} \pm R_0 = \exp[i(\phi(\lambda) \mp \delta(\lambda))]. \quad \ldots (3.14) \]

Let the \( m \)th mode amplitude for either polarization have phase denoted by \( \psi_m \). Then for S polarization, a combination of equations (3.8)

(i) \( B_{-1} = \frac{1}{2} \exp(2i\psi_0) + \frac{i}{2} \exp(2i\psi_1) \)
(ii) \( B_0 = \frac{1}{2} \exp(2i\psi_0) - \frac{i}{2} \exp(2i\psi_1) \).

For P polarization the equivalent relations are

(i) \( A_{-1} = \frac{1}{2} \exp(2i\psi_1) + \frac{i}{2} \exp(2i\psi_2) \)
(ii) \( A_0 = \frac{1}{2} \exp(2i\psi_1) - \frac{i}{2} \exp(2i\psi_2) \).

Consider the case for S polarization. In fitting equation (3.14) to computed values, there exists some ambiguity in \( \phi \) and \( \delta \). To resolve this, both functions and their first derivatives are assumed to be continuous functions of \( \lambda \), except perhaps at Rayleigh wavelengths. Figure 3.2(c) shows a plot of \( \delta(\lambda) \) and \( \phi_{-1}(\lambda) \) in the region where two anomalies are present. \( \phi_{-1}(\lambda) \) is taken directly from computations. It equals \( \phi(\lambda) \) below \( \lambda/d = 0.8307 \) but differs from it by \( 180^0 \) above this wavelength, because \( B_{-1} \) passes through zero at this point and experiences an instantaneous phase change of \( 180^0 \). The effects of the two resonances are clearly visible in the phase plots at wavelengths of \( \lambda/d = 0.689 \) and \( 0.831 \), as indicated by the sudden fall in phase of almost \( 180^0 \).

The combination \( B_0 + B_{-1} \) is seen to be a superposition of even mode amplitudes which are not observed to resonate in the wavelength range under
consideration. This observation correlates with the fact that the phase of $B_0 + B_{-1}$, namely $\phi(\lambda) - \delta(\lambda) = 2\psi_0(\lambda)$, is a smooth function exhibiting no rapid changes. On the other hand, the phase of $B_{-1} - B_0$, $\phi(\lambda) + \delta(\lambda) = 2\psi_1(\lambda)$, exhibits changes of $-360^0$ in the vicinity of the wavelengths 0.689 and 0.831 (Figure 3.2(c)). This conforms with a rapid increase in the magnitude of $b_1$, a sudden fall by $180^0$ of $\psi_1$ (Figure 3.2(d)) and sharp peaks in the evanescent order intensities (Figure 3.2(b)). (The reason that $[\phi(\lambda) + \delta(\lambda)]$ falls by $360^0$ at each resonance, rather than $180^0$, is explained later.) The $m = 1$ mode is thus confirmed to be the source of the resonance behaviour for $S$ polarization.

For $P$ polarization, $A_{-1} - A_0$ is found to be very nearly constant ($\psi_2(\lambda)$ varying very little over the wavelength interval of interest) and does not resonate. It is the combination $A_0 + A_{-1}$ which now falls in phase by $360^0$ as the wavelength increases through a resonance. In Figures 3.3(a)-(d) the $-1$ order efficiencies (equal to $\cos^2(\delta)$) and the mode phases $\psi_1$ are plotted for various groove depths. In accordance with $S$ polarization, it is the $m = 1$ mode which exhibits the resonance behaviour in this particular region. Due to the absence of an $m = 0$ mode, this mode has the additional role of determining overall efficiency behaviour.

3.2.2.2 Resonance Poles

Numerous references have been made to the term "resonance" without giving it a well-defined meaning. A resonance is identified with a pole of an amplitude in the complex wavelength plane. If such a pole is close to the real or physical wavelength axis, then its presence will be strongly felt at nearby real wavelengths and hence manifested as an "anomaly" in the efficiency.

A function $F(\lambda)$ having a simple pole at $\lambda_p = \lambda_r + i\lambda_i$ may be expressed in the form
where \( f(\lambda) \) is holomorphic in the neighbourhood of \( \lambda_p \). If \( f(\lambda) \) is a constant with unit modulus, then we can write

\[
F(\lambda) = \frac{f(\lambda)}{\lambda - \lambda_p} \quad \ldots (3.17)
\]

from which it is seen that when \( \lambda = \lambda_r \) (the closest one can physically be to the pole) the magnitude of \( F(\lambda) \) will be a maximum with value \( 1/\lambda_i \). The phase of \( F(\lambda) \), for real \( \lambda \), is then given by

\[
\arg (F(\lambda)) = \delta_f + \arctan \left( \frac{\lambda_i}{\lambda - \lambda_r} \right) \quad \ldots (3.19)
\]

For \( \lambda_i > 0 \) (all poles are observed to lie in the upper half-complex plane) this phase is approximately constant at a value \( \delta_f + \pi \) for wavelengths significantly less than \( \lambda_r \), and again almost constant at a value \( \delta_f \) for wavelengths significantly greater than \( \lambda_r \). In between, the phase drops rapidly, reaching a mean value of \( \delta_f + \pi/2 \) when \( \lambda = \lambda_r \). An example of this behaviour is illustrated in Figure 3.2(d), which displays two such drops in phase \( \psi_1 \), indicating the presence of two poles in the mode amplitude \( b_1 \). The central 90° of the phase change takes place over the interval \( (\lambda_r - \lambda_1, \lambda_r + \lambda_1) \) and this fact may be used to estimate the pole position from the computed phase curve.

It is probable of course, that \( f(\lambda) \) is not a constant but has a slowly-varying background phase \( \delta_b(\lambda) \). The phase of \( F(\lambda) \) is then given by

\[
\arg (F(\lambda)) = \delta_b(\lambda) + \arctan \left( \frac{\lambda_i}{\lambda - \lambda_r} \right) \quad \ldots (3.20)
\]

and an example of this behaviour is typified by the curve for \( \delta(\lambda) \) in Figure 3.2(c). If this background phase changes significantly over the region of the pole, the phase drop may be either more or less than 180°.
Also, if $|f(\lambda)|$ varies near $\lambda = \lambda_p$, the maximum of $|F(\lambda)|$ may be slightly displaced from $\lambda_p$.

If $F(\lambda)$ is a function of modulus unity and has a pole at the complex wavelength $\lambda_p$, then it must take the form

$$F(\lambda) = \exp[2i\delta_b(\lambda)] \left( \frac{\lambda - \lambda_p}{\lambda - \lambda_p} \right)$$

...(3.21)

which may be rewritten as

$$F(\lambda) = \exp[2i(\delta_b(\lambda) + \delta_{res}(\lambda))]$$

...(3.22)

where $\delta_b(\lambda)$ is a background phase and $\delta_{res}(\lambda)$ is the resonance phase defined by

$$\exp[2i\delta_{res}(\lambda)] = \frac{\lambda - \lambda_p}{\lambda - \lambda_p}.$$  

...(3.23)

Notice that $F(\lambda)$ has a zero at the complex conjugate of the pole position and its phase drops by $360^0$ as $\lambda$ traverses the resonance. Thus, by writing $2\delta_{res}(\lambda)$ in the exponents of equations (3.22) and (3.23), $\delta_{res}(\lambda)$ falls through $180^0$.

$F(\lambda)$ is now a function which has the same form as either $R_{-1} \pm R_0$ for the -1 Littrow mount when two orders are propagating, or $R_0$ for the long-wavelength case when one order is propagating. Note however, that of these functions which represent both polarizations, only $(B_{-1} - B_0)$, $(A_{-1} - A_0)$ and $B_0$ are observed to undergo resonance.

For various sets of groove parameters, pole positions have been found by fitting expression (3.20) to computed phase data. In a number of cases it has been confirmed that the appropriate amplitude (or combination thereof) which has unit modulus, has a zero at $\lambda = \overline{\lambda}_p$ if it has a pole at $\lambda = \lambda_p$. (It was of course necessary to modify the computer program to deal with complex wavelengths.)

It is of interest to note for the two mountings concerned, i.e. the -1 Littrow mounting or a long-wavelength mounting, that when the amplitude
is expressed in the form (3.22), the background phase $\delta_b(\lambda)$ is almost constant, except near Rayleigh wavelengths. Consequently, the pole term given by equation (3.23) (or a product of two such terms if two poles are present) is an excellent approximation (apart from a constant phase factor) to the amplitude for a wide range of wavelengths.

Near resonance, the individual amplitudes for S polarization, given by equations (3.6) and (3.15), may now be parameterized by the expressions,

$$B_0(\lambda) = \exp\left(2i\delta_b(\lambda)\right) \left(\frac{\lambda-\lambda_p}{\lambda-\lambda_p}\right), \quad \text{long}-\lambda \quad (3.24)$$

and

$$B_{-1}(\lambda) = \frac{1}{2} \exp\left(2i\psi_0(\lambda)\right) + \frac{1}{2} \exp\left(2i\delta_b(\lambda)\right) \left(\frac{\lambda-\lambda_p}{\lambda-\lambda_p}\right), \quad \text{-1 Littrow \quad (3.25)}$$

where $\psi_0(\lambda)$ and $\delta_b(\lambda)$ are approximately constant.

3.2.2.3 Resonances in Efficiencies

When a resonance occurs in the order amplitudes, it is found to be due to a resonance in a solitary mode amplitude. Through equation (2.7) or (2.17) it occurs in all other order amplitudes. The intensities of the evanescent orders are unconstrained by energy conservation and peak sharply near $\lambda = \lambda_r$ (see Figure 3.2(b)). The propagating order amplitudes must, however, not rise above unity.

From the parameterization (3.11) for $R_{-1},R_0$ for the -1 Littrow mount and $\lambda/d > 2/3$, the -1 order efficiency is given by $\cos^2\left((\delta(\lambda))\right)$. Now from equation (3.12(i)), for say S polarization, $\delta(\lambda) = \psi_1(\lambda) - \psi_0(\lambda)$ follows $\psi_1(\lambda)$, the phase of the resonating mode amplitude $b_1$, in falling through almost 180° in the resonance region. Consequently, the efficiency undergoes rapid fluctuation in that region, the exact shape of the curve being determined by any background phase component of $\delta(\lambda)$ (i.e. $\psi_0(\lambda)$), but it must attain the values of 0 or 1 or both as $\delta(\lambda)$ changes by nearly 180°.

Figures 3.1(a)-(d) and 3.2(a) display a series of efficiency curves for S polarization for different values of groove depth. These curves illustrate a number of different shapes of anomalies superimposed on the
slowly-varying background. In each case the phase falls by $150^\circ-160^\circ$ in the resonance region. This figure is less than the $180^\circ$ expected because (i) a rising background phase component, as seen in Figure 3.2(c), increases by $10^\circ-20^\circ$ across the region, and (ii) the pure resonance phase given by equation (3.19) falls through the first and last few degrees only very slowly with increasing wavelength.

It is of interest to study the ability of equation (3.25) to model efficiency behaviour. For $c/d = 0.43$ and $h/d = 0.7$, a pole in $b_1$ was located at $\lambda_p = 0.83 + 0.0012i$. Choosing a constant value for $\delta_b(\lambda)$, two graphs were plotted of $|B_{-1}|^2$ according to equation (3.25). In the first, $\psi_0(\lambda)$ was fixed, and in the second $\psi_0(\lambda)$ was allowed to assume slowly varying values. The two graphs are contained in Figures 3.4(a) and (b) respectively and they should be compared with the "true" efficiency curve of Figure 3.2(a). Figure 3.4(a) reveals that the chosen values of $\delta_b$ and $\psi_0$ lead to the correct type of anomaly, i.e. a notch followed by a peak. Figure 3.4(b) shows that the true efficiency is accurately modelled by equation (3.25) when the varying phase values of $b_0$ are inserted. Further manipulation of values for $\psi_0$ and $\delta_b$ has revealed how the anomalies can take on other common forms (e.g. see Figures 3.4(c) and (d)).

For similar groove depths, poles in the P polarization amplitudes are much further from the real wavelength axis than those for S polarization so that the resonance features are much broader (see Figures 3.3(a)-(d)). As remarked earlier, the resonances are an inseparable part of the P polarization efficiencies even though they may be scarcely apparent, say for small depths. By contrast with S polarization, a resonant part and a non-resonant part of the amplitudes cannot be identified.

It is shown in the next section that resonances occur at wavelengths below $2c$, the $m = 1$ mode threshold (equal to $0.86d$ in the examples given). At wavelengths greater than this value, the P polarization order amplitudes have magnitudes and phases largely independent of the groove depth.
Figure 3.4 The intensity of the -1 order amplitude for the first-order Littrow mounting and S polarization is plotted as a function of wavelength, as prescribed by equation (3.25). The pole position is $\lambda_p=0.83+0.0012i$.

In (a) $\delta_b=89^\circ$ and $\psi_0(\lambda)$ is fixed at $-40^\circ$.
In (b) $\delta_b=89^\circ$ and $\psi_0(\lambda)$ is slowly varying.
In (c) and (d) $\delta_b=0^\circ$ and $\psi_0(\lambda)$ is as for (a) and (b) respectively.
For example, for $c = 0.43d$ and $\lambda = 1.0d$, a change in depth from $h = 0.4d$ to $1.4d$ alters $|A_{-1}|$ by only 5% and the phase by only $1.4^\circ$.

When several orders are propagating, or when the grating is finitely conducting, the order efficiencies need not, and in general do not behave in the manner so far described. Although an efficiency curve may still exhibit a peak or dip at resonance, and the order phase may change, it is only in the evanescent order intensities, and more importantly in the mode intensities and phases (if available), that the resonance is clearly manifested as before.

It is emphasized that the resonance has its origin in the mode amplitudes and that therefore these amplitudes are the objects particularly deserving attention.

3.2.2.4 A General Method for Locating Pole Positions

Consider expressions (3.15(i)) and (3.25), which concern $B_{-1}$ in the vicinity of a resonance. Over this region $\psi_1(\lambda)$ falls rapidly by nearly $180^\circ$ while $\psi_0(\lambda)$ remains fairly constant. As $\lambda$ traverses real values near the pole position, the Argand plot of $B_{-1}$ follows a circle of radius $\frac{\lambda_2}{2}$ and centre $\frac{\lambda_2}{2} \exp(2i\psi_0)$. The circle in distorted by a slow variation in $\psi_0$ and is incomplete because of the finite range of $\lambda$ considered and the change in $\delta_b$. However, its presence in the plot clearly signals the occurrence of a pole. An example is contained in Figure 3.9(c) where the outer circle is for infinite conductivity.

The movement of $B_{-1}$ around the circle, as wavelength varies, is most rapid when the change in $(\lambda - \lambda_p)/(\lambda - \lambda_p)$ is most rapid, i.e. when $\lambda$ is equal to $\lambda_p$.

For real $\lambda$, $(\lambda - \lambda_p)/(\lambda - \lambda_p)$ has unit modulus and an argument $2\rho$ equal to $\pi - 2\arctan((\lambda - \lambda_p)/\lambda_1)$. We can therefore write

$$\frac{\lambda - \lambda_i}{\lambda_1} = \tan \left( \frac{\pi}{2} - \rho \right) = \cot (\rho) \quad \ldots(3.26)$$
whereupon

\[
\frac{\delta \lambda}{\lambda_i} = - \csc^2 \rho \, d\rho
\]  

...(3.27)

for small variations \(\delta \lambda, \delta \rho\).

When \(\lambda = \lambda_r\) then \(\rho = \pi/2\) and the above becomes

\[
\lambda_i = - \frac{\delta \lambda}{\delta \rho}.
\]  

...(3.28)

The pole position may now be located by first ascertaining the wavelength at which \(\rho\) varies most rapidly, i.e. the wavelength at which the angle subtended at the centre of the Argand plot is varying most rapidly with wavelength. This provides the real part of the pole position, \(\lambda_r\). The imaginary part, \(\lambda_i\), is then given by \(-\delta \lambda/\delta \rho\) evaluated at that real wavelength.

It should be noted that the above method of pole location does not rely on a knowledge of the mode amplitudes, unlike the approximate method given in Section 3.2.2.2 which depends on a plot of the mode phase. Thus, when several real orders are propagating, or for general groove profiles, or for the case of finite conductivity, it is still possible to locate resonance poles by a study of the order amplitudes and phases at real wavelengths. In these more general cases, the parameterization (3.21) is no longer strictly valid, but the order amplitudes behave in a similar manner near resonance though the circles may be distorted and have radius less than \(\lambda_0\). The determination of pole positions from these Argand plots is still possible however, and the technique is widely used in particle physics [3.36].

Consider a finitely-conducting lamellar grating in the -1 Littrow mount, with \(\lambda/d > 2/3\), and assume we can write an expression similar to (3.25) for \(B_{-1}\) near resonance, i.e.

\[
B_{-1}(\lambda) = a(\lambda) + r(\lambda) \frac{\lambda - \lambda_p}{\lambda - \lambda_p^*} 
\]  

...(3.29)

where \(a(\lambda)\) and \(r(\lambda)\) are relatively-slowly varying functions of \(\lambda\) and are such that \(|B_{-1}|^2 < 1\). The above expression is virtually essential in
light of the conservation condition for a function having a pole at 
\( \lambda = \lambda_p \). If the assumption is valid, then one expects to obtain a distorted 
circle, or part thereof, in the Argand plot for \( B_{-1} \) for wavelengths near \( \lambda_p \).

Figure 3.9(c) confirms that this is the case where the numerical data for 
finite conductivity were obtained from a programme based on the integral 
method of Maystre [3.37]. (Notice that because \( \lambda_1 \) is discovered to be 
positive for any pole, the circles are described in a clockwise direction 
as \( \lambda \) increases and hence \( -\delta \lambda/\delta \rho \) is positive.)

Amplitudes may have more than one pole over the wavelength range of 
interest. Their Argand plots show a rapid partial circular movement at 
wavelengths nearby, with usually a slow and aimless course in between.
The pole positions may be located as described earlier.

3.2.2.4 Resonance Pole Trajectories

As previously mentioned, there exists two distinct types of anomalies. 
Rayleigh wavelength anomalies are a "threshold effect" and do not change 
position with a change in groove parameters. Resonance anomalies occur 
very close to Rayleigh wavelengths and move to longer wavelengths as groove 
depth increases. In this section, the trajectories of the resonance poles 
for the lamellar reflection grating are traced in the complex plane as 
functions of groove depth, and an understanding is sought of their origin 
within the theory.

The case of \( S \) polarization is treated first. Consider the re-
arrangement of equation (2.21), which yields for the \( m \)th mode amplitude

\[
    b^*_m = \frac{2dJ_{m\omega} + \sum_{n \neq m} b^*_n \mu_n \tan(\mu_n h)K^S_n}{\varepsilon_{mcd} - \mu_m \tan(\mu_m h)K^S_{nn}} \quad ...(3.30)
\]

where \( K^S_{nm} \) is given by equation (2.87) and is noted to be a function of \( \lambda \), 
\( \sin \theta \) and \( c \), but not of \( h \). It is also infinite with square-root branch 
points at the Rayleigh wavelengths where one or more \( \chi_p \) vanish. (This 
results in the Rayleigh wavelength anomalies.)
The amplitude $b^*_m$ is observed to have other singularities at wavelengths such that

$$K^{S}_{mm} = \epsilon_m c d \frac{\cot(\mu_m h)}{\nu_m}, \quad \ldots (3.31)$$

provided that the other mode amplitudes do not combine to make the numerator of equation (3.30) equal to zero at the same wavelength. (Since the modes are deemed to be essentially independent of one another, this is not expected to occur and experience bears this out.)

For a constant groove width and a constant value of $\sin \theta$, equation (3.31) describes a curve or trajectory in the complex $\lambda$ plane as $h$ is varied.

For real $\lambda$, $K^{S}_{mm}$ is purely real positive when no orders are propagating (all $\chi_p$ are positive imaginary), but it develops a positive imaginary part as orders pass on. Thus when $\lambda$ is real, it is always in the first quadrant of the complex plane with an imaginary part that becomes more significant with an increasing number of real orders.

As $\lambda$ decreases towards a Rayleigh wavelength, $K_{mm}$ is dominated by an increasingly large real positive part which suddenly becomes a large positive imaginary part as the threshold is crossed. This is due to the change in the appropriate $\chi_p$.

At real wavelengths, just above a Rayleigh wavelength, equation (3.31) can be satisfied for small values of $h$ and hence large values of $\cot(\mu_m h)$. In fact, for $h = 0$ and $\lambda = \lambda_R$ it can be satisfied with both sides being infinite. As the wavelength increases from $\lambda_R$, the modulus of $K_{mm}$ decreases and its argument increases from zero. For the equality (3.31) to be maintained, $\epsilon_m c d \cot(\mu_m h)/\nu_m$ must do the same. This can be achieved for complex $\lambda$ by allowing an increase in $h$. The aforementioned quantity then also decreases in magnitude and moves into the first quadrant, thus implying that $\lambda_p(h)$, the pole position, develops a positive imaginary component.
It has thus been established that the trajectory of $\lambda_p(h)$ can begin at a Rayleigh wavelength at zero groove depth, and move out into the complex plane as $h$ increases. It is noted however, that this can only occur if $\varepsilon_m c d \cot(\mu_m h)/\mu_m$ is positive for small $h$. That is, $\mu_m$ must be real-valued which implies that $\lambda$ should be less than the mode threshold $2c/m$.

If $h$ is sufficiently large so that $\mu_m h_\lambda = 2\pi$, $\lambda = 1, 2, 3 \ldots$ then $\cot(\mu_m h_\lambda)$ is again infinite, and for $h$ increasing beyond $h_\lambda$, $\cot(\mu_m h_\lambda)$ falls to positive finite values, just as it does for $h$ increasing from zero. Therefore, second and higher order pole trajectories can begin at $\lambda_R$ and move into the first quadrant as $h$ increases.

Expanding the above condition, the depth for which the $\lambda$th trajectory commences is given by

$$h_\lambda = \lambda (\frac{4}{\lambda_R} - \frac{m^2}{c^2})^{-\frac{1}{2}}, \quad \lambda = 0, 1, 2 \ldots \quad \text{(3.32)}$$

Close analysis of equation (3.31) reveals that these trajectories do not follow the same path, nor do they cross one another.

For a groove width of $c = 0.43d$ and a -1 Littrow mounting with $\lambda_R/d = 2/3$, one finds $h_1 = 0.5277d$. Therefore, one expects only one anomaly to be visible for $h = 0.5d$, but two to be visible for $h = 0.7d$. Figures 3.1(d) and 3.2(a) confirm these predictions.

It is difficult from an analysis of equation (3.31) to determine exactly the path of $\lambda_p(h)$, but away from Rayleigh wavelengths $k_m$ does vary only relatively slowly as a function of $\lambda$, and therefore for $\varepsilon_m c d \cot(\mu_m h)/\mu_m$ to do likewise, $|\mu_m|$ must decrease roughly as $1/h$ as $h$ becomes large. This requires $\lambda_p$ to approach $2c/m$, the point at which $\mu_m = 0$. The general trend of the trajectory is therefore such that $\lambda_r$ moves to longer wavelengths as $h$ increases, while $\lambda_l$ moves to positive values for finite $h$ and then returns to zero as $h \to \infty$, the pole position terminating at $\lambda = 2c/m$. 
Analysing equations (3.31) in more detail, we see that as \( h \rightarrow \infty \), the R.H.S. varies rapidly unless \( \mu_m \rightarrow 0 \) in such a way that this expression remains finite. If \( \mu_m \rightarrow 0 \), this requires \( \mu_m h + \pi/2 \) as \( h \rightarrow \infty \) so that condition (3.31) remains satisfied. It is also deduced that the real \( \lambda \) axis is tangent to the trajectory at its endpoint of \( \lambda = 2c/m \).

Consider now the first trajectory. As \( h \) varies from 0 to \( \infty \), \( |\mu_m h| \) increases monotonically from 0 to \( \pi/2 \). At a particular finite value of \( h \), \( |\mu_m h| \) is finite and the pole position \( \lambda_p(h) \) must be such that \( 0 < |\mu_m(\lambda_p)h| < \pi/2 \). This means that

\[
\lambda_1 < \lambda < \lambda_0
\]

where \( \mu_m(\lambda_1)h = \pi/2 \) and \( \mu_m(\lambda_0)h = 0 \), corresponding to the wavelengths

\[
\lambda_1 = \frac{4ch}{\sqrt{c^2+4m^2h^2}} \quad \ldots (3.34)
\]

and

\[
\lambda_0 = \frac{2c}{m} \quad \ldots (3.35)
\]

The wavelength \( \lambda_1 \) increases with \( h \) and as \( h \rightarrow \infty \), \( \lambda_1 \rightarrow \lambda_0 \). \( \lambda_1 \) supplies a lower bound to the real component of the pole position while \( \lambda_0 \) is the upper bound.

Similarly for a second trajectory, one obtains

\[
\lambda_3 < \lambda < \lambda_2
\]

where \( \mu_m(\lambda_k)h = k\pi/2 \). \ldots (3.37)

The lower and upper bounds of the real part of the pole are now \( \lambda_3 \) and \( \lambda_2 \) respectively and these both tend to the threshold \( 2c/m \) as \( h \rightarrow \infty \).

Thus, it has been deduced that as groove depth increases from zero (or a depth given by equation (3.32)) towards infinity, the complex pole follows a path in the upper-half complex plane, commencing at a Rayleigh wavelength and terminating at the mode threshold. Figure 3.5 illustrates the first two trajectories, found numerically, for the poles in mode amplitude \( b_1 \) for the -1 Littrow mounting and \( \lambda_R = 2d/3 \).
Figure 3.5  S polarization pole trajectories in the complex wavelength plane for a lamellar reflection grating of groove width $c=0.43d$. (a) -1 Littrow mounting (b) Normal incidence mounting.
As a function of frequency, the trajectory lies not in the physical sheet, where all \( X_p \) have positive imaginary parts, but in an adjacent sheet where \( X_0, -1 \) have negative imaginary parts. The trajectory terminates at the mode threshold in that adjacent sheet (see Appendix 2). In certain cases, this point may not be at a physical frequency.

Pole trajectories have been investigated numerically in some detail for the \( m = 0 \) mode for a normal incidence mounting, and for the \( m = 0, 1 \) and 2 modes for a -1 Littrow mounting. (More general mountings are discussed in a later section.) For these mountings, the pole in mode \( \bm \) is observed to move towards its threshold at \( \lambda = 2c/m \) as \( h \to \infty \), but only from the next lower Rayleigh wavelength. In view of the foregoing discussion, poles cannot start at Rayleigh wavelengths greater than \( 2c/m \) and experience suggests that they do not start from other lower Rayleigh wavelengths. For alternative mounting types this statement must be modified slightly because trajectories may commence from the next two Rayleigh wavelengths lower than the mode threshold.

The reason why there are only a limited number of points from which trajectories are seen to begin is not fully understood, but it is probably related to the structure of the Riemann surface of the amplitudes (Appendix 2). It is possible of course, that any poles starting at Rayleigh wavelengths far below the mode threshold may have moved so quickly into the complex \( \lambda \) plane with increasing \( h \), that they have avoided detection for the values of \( h \) used.

The \( m = 0 \) mode has its threshold at \( \lambda = \infty \), and so in a normal incidence mounting the next lowest Rayleigh wavelength is \( \lambda_R = 1.0d \). The results of a numerical search between these two wavelengths for the trajectories of the pole in \( \bm_0 \) are shown in Figure 3.5(b) for three different groove widths. As \( h \) increases from zero, the trajectories are seen to move rapidly from the real-wavelength axis so that they cannot be traced in the real-wavelength data. (For this situation the poles are not
manifested in efficiency variation, but they are evident in the phase variation. The larger the value of $c/d$, the faster is this movement, and for $c/d = 0.53$ little evidence can be seen of the pole for $\lambda/d > 1.01$. Presumably, as $h \to \infty$ these trajectories move back towards the real-wavelength axis at $\lambda = \infty$.

For the above mounting, equation (3.32) reduces to $h_\lambda = k/2$ ($m = 0$ and $\lambda_R = 1.0$). Therefore, the groove depths for which higher order trajectories begin are $h/d = 0.5, 1.0, 1.5 \ldots$.

Consider now the first-order Littrow mounting. The Rayleigh wavelength closest to the $m = 0$ mode threshold is $\lambda_R = 2.0d$. For $\lambda/d > 2.0$, this mounting is unphysical, but the mode and order amplitudes remain perfectly well-defined in this region by equation (2.21), or by analytic continuation from physical values of $\lambda$. Poles in $b_0$ can therefore be expected for this mounting for $\lambda/d > 2.0$. Because all values of $X_p$ are positive imaginary in this wavelength region, $k_{b_0}$ is real for real values of $\lambda$. Equation (3.31) can therefore be satisfied for real wavelengths for non-zero $h$. Thus, the pole trajectory follows the real-wavelength axis towards $\infty$ as $h$ increases.

This behaviour was verified by modifying the computer program to cope with the unphysical mounting. For $c/d = 0.43$ and $h/d = 0.1$, a pole was indeed found near $\lambda/d = 2.05$. Because the pole lies on the real axis, its location is straight-forward, since the phase of $b_0$ changes instantaneously by $\pi$ as $\lambda$ traverses $\lambda_p$. At that point the modulus of $b_0$ is infinite. The actual movement of $\lambda_p$ as a function of $h$ is discussed in Section 3.4.

For a groove width of $c/d = 0.43$, the $m = 1$ mode threshold is at $\lambda/d = 0.86$, while for the $m = 2$ mode it is at $\lambda/d = 0.43$. Figure 3.5(a) exhibits the trajectories of the $b_1$ pole which move from the closest Rayleigh wavelength of $\lambda_R = \frac{2}{3}d$, to $\lambda/d = 0.86$ as $h$ is increased from 0 and also from 0.5277d. A pole trajectory for $b_2$ has been observed to lie
between $\lambda_R = \frac{2}{5} d$ and $\lambda/d = 0.43$. Poles in $b_1$ have not been found to move from $\lambda_R = \frac{2}{5} d$ to $\lambda/d = 0.86$.

If $c/d > 2/3$, then both the $m = 1$ and $m = 2$ mode thresholds lie to the right of the Rayleigh wavelength at $\lambda_R = 2d/3$. Under these conditions, anomalies are expected to occur as a result of poles in both $b_1$ and $b_2$. This does appear to be the case, but an example where both modes produce strong anomalous features is difficult to find. For $c/d = 0.7$ and $h/d = 0.45$, anomalies due to $b_1$ are visible near wavelengths of $0.67d$ and $1.13d$. A $b_2$ anomaly has not been detected but it could be sandwiched between the Rayleigh wavelength and the $b_1$ anomalies. When $c/d$ is increased to $0.9$, the poles in $b_1$ move far into the complex plane and have little effect on the efficiency. Instead, a $b_2$ pole produces a very sharp spike in the -1 order efficiency at $\lambda/d = 0.84$.

Turning now to the case of P polarization, a similar treatment is followed to the above, and from equation (2.13) we obtain

$$a_m^* = \frac{2i\alpha_0 T_m \omega}{\sum_{n\neq m} a_n^* k_{nm}^P} \frac{1}{k_{mm}^P - cd \mu_m \cot(\mu_m h)/2} \ldots (3.38)$$

where $k_{mm}^P$ is given by equation (2.84).

The condition which determines the pole position for $a_m^*$ is

$$k_{mm}^P = \frac{cd}{2} \mu_m \cot(\mu_m h) \ldots (3.39)$$

Analysis of this condition reveals that as $h$ increases from 0 to $\infty$, $\lambda_p(h)$ moves in an adjacent sheet from zero to the mode threshold, with $|\mu_m h| \not\in \pi$ in order that the R.H.S. of equation (3.39) remains finite. For small values of $h$, the pole is far from the real-wavelength axis and so an anomaly is not manifested in the efficiency. This conforms with experimental observations.
Second and higher trajectories also move from zero wavelength to the mode threshold with $|\mu_m h|$ increasing towards $2\pi, 3\pi \ldots$.

One is again able to deduce upper and lower wavelength bounds to the real component of the pole position. For a particular value of $h$,

$$\lambda_r > \lambda_{2k}$$

for the $k^{th}$ trajectory, where $\lambda_k$ is given by equation (3.37). The best upper bound established so far is the inequality

$$\lambda_r (k^{th} \text{ trajectory}) > \lambda_r (k+1^{th} \text{ trajectory})$$

but a more stringent one,

$$\lambda_r (k^{th} \text{ trajectory}) < \lambda_{2k-2}$$

is suggested by the numerical results.

Consideration of the -1 Littrow mounting shows that the resonance poles are interspersed between the zeros in the -1 order efficiency, $\lambda_2$, $\lambda_4$, ... (see Figures 3.3(a)-(d).

A P polarization resonance in the efficiency becomes apparent when $h$ is sufficiently large so that $\lambda_r$ is greater than the Rayleigh wavelength, or when the lower bound ($\lambda_{2k}$) is equal to the Rayleigh wavelength. The depths for which this occurs coincide with those for which the next highest S polarization trajectory starts out from the Rayleigh wavelength, as given by equation (3.32).

Numerical work for P polarization has been confined to the -1 Littrow mount and wavelengths greater than $\frac{2}{3} d$. Groove widths have been chosen so that only $m = 1$ mode resonances are expected. Figures 3.3(a)-(d) display -1 order efficiencies and $m = 1$ mode phases for a number of groove depths where $c/d = 0.43$. For $h/d = 0.4$ the effects of the resonance are just appearing as the pole approaches the real-wavelength axis. The very broad peak in efficiency is indicative of the greater imaginary component of this pole when compared with its counterpart for S polarization. This fact is also illustrated in Figure 3.6, which depicts the first pole trajectory,
Figure 3.6  P polarization pole trajectories in the complex wavelength plane for a lamellar reflection grating, of groove width c=0.43d, in a -1 Littrow mounting. Pole positions for a number of groove depths are indicated.
3.35

and also a second trajectory, the presence of which is signalled in the efficiency when the depth reaches $h/d = 1.0$. When these trajectories are compared with those in Figure 3.5(a) for $S$ polarization, it is found that corresponding $P$-poles lie further from the real axis by a factor greater than 10. It appears likely however, that these $P$ polarization poles are closer to the real axis than their counterparts for a sinusoidal profile. This would explain the observation of Breidne and Maystre [3.38], that the $P$ polarization efficiency peaks are narrower for the lamellar profile.

3.2.2.5 Pole Trajectories in the $(\lambda, \sin \theta)$ Plane

In this section, the investigation is extended to include the entire $(\lambda, \sin \theta)$ plane, where potentially both of these quantities are complex.

It is found advantageous to define the variables $v = 1/\lambda$ and $	au = (\sin \theta)/\lambda$. Part of the real two-dimensional space of these variables is illustrated in Figure 3.7. The sets of sloping dashed lines represent the order thresholds. Those of positive slope correspond to the zero and positive orders and those of negative slope correspond to the negative orders. The $p^{th}$ order is propagating in the region above its corresponding threshold. Below the $0^{th}$ order threshold, no order is real since $|\sin \theta| > 1$ in that region. However, amplitudes there can still be obtained from the theory. Mode thresholds, defined by $\lambda = 2c/m$, are depicted as horizontal lines.

An advantage in choosing the variables $v$ and $\tau$, is the symmetry obtained in their two-dimensional space. Equations (3.31) and (3.39), which determine the resonance pole positions, are invariant under the transformation $\tau \rightarrow p/d - \tau$, where $p$ is an integer. This means that a pole trajectory for fixed $h$, and as a function of $v$ and $\tau$, is symmetrical about the lines $\tau = p/2d$, for all $p$. In Figure 3.7, $p$ equals 1, and so the vertical lines of symmetry at $\tau = \frac{p}{2}$ correspond to the -1 Littrow mounting. Constant angle-of-incidence mountings correspond to lines passing through the origin with slope $\csc \theta$, while constant wavelength mountings correspond to lines parallel to the horizontal axis.
Figure 3.7 S polarization pole trajectories for the lamellar reflection grating. Only the real part of the trajectory is shown as a function of the variables $\nu=1/\lambda$ and $\tau=(\sin\theta)/\lambda$.

(a) $c/d=0.43$  (b) $c/d=0.63$
Numerical work has so far only covered selected areas of the \((\nu, \tau)\) plane, and for \(\tau \neq \frac{1}{2}\) it has been confined to S polarization.

The arguments of the previous section, regarding the movements of poles with increasing \(h\), are equally applicable here. Therefore, for small fixed \(h\), one expects to locate their positions \(v_p\), for variable \(\tau\), just below the Rayleigh wavelength lines. As \(h\) increases, the poles move towards the mode thresholds, and so the fixed-\(h\) plots are expected to straighten out and approach the appropriate horizontal mode threshold. Furthermore, since the Rayleigh wavelength is \(\tau\)-dependent, the value of \(h\) for which a second pole emerges from the order threshold depends on the value of \(\tau\) at the threshold point in question.

The above expectations are confirmed in the numerical results of Figure 3.7. In Figure 3.7(a), the real parts of some trajectory points in the \((\nu, \tau)\) plane are given for \(c/d = 0.43\) and for various fixed \(h\). The following poles are shown:-

(i) The pole in \(b_0\) for \(h = 0.1\), for \(\tau = 0\) and \(v_p \leq 1\). (This is a "normal-incidence" pole with \(\lambda_p \geq 1\).) The complex value of this pole position is shown in Figure 3.5(b).

(ii) The pole in \(b_0\) for \(h = 0.1\), for \(\tau = \frac{1}{2}\) and \(v = 0.49\) (\(\lambda = 2.05\)). This is the "unphysical" -1 Littrow pole mentioned in the previous section. The trajectory of this pole has not been followed on either side of \(\tau = \frac{1}{2}\), but it is expected to lie closely below the thresholds \(X_0 = 0\) and \(X_{-1} = 0\) in a similar manner to those discussed in (iii). For increasing \(h\) it should move towards the \(\mu_0 = 0\) threshold which coincides with the horizontal axis.

(iii) The poles in \(b_1\) for \(h = 0.3\) and \(h = 0.7\) (first and second trajectories). These poles are bounded in the triangle formed by \(X_1 = 0\), \(X_{-2} = 0\) and \(\mu_1 = 0\). For small \(h\), the plot follows the order thresholds closely, while for large \(h\) it becomes straighter as the pole becomes increasingly independent of \(\sin \theta\). The first trajectory emerges "simultaneously" from
the thresholds at $h = 0$. However, $h_1$, the depth at which the second trajectory emerges, depends on $\lambda_R$ at that point, and hence on the value of $\theta$ as mentioned previously.

(iv) The poles in $b_2$ for $h = 0.3$ and $0.7$ in the triangle bounded by $X_2 = 0$, $X_{-3} = 0$ and $\mu_2 = 0$.

Further numerical results have been secured for a smaller value of $c$, namely $0.26$, which confirm that poles occur in $b_1$ in the segment of the $(\nu, \tau)$ plane above the one in example (iii). That is, they have loci bounded by $X_2 = 0$, $X_{-3} = 0$ and the mode threshold at $\nu = 1.92$.

The results contained in Figure 3.7(b) are for a larger groove width of $c = 0.63$. This example is of interest because the next lowest Rayleigh wavelength below $\mu_1 = 0$ can vary. For some angles of incidence it is the lines $X_1 = 0$ and $X_{-2} = 0$, while for others it is $X_{-1} = 0$ and $X_0 = 0$.

For small $h$, the trajectories are found to leave the former pair of thresholds for all values of $\theta$, i.e. not always the closest threshold. Plotted are the trajectories for depths of $0.1$, $0.3$ and $0.8$ (first and second). They pass the $X_{-1} = 0$ and $X_0 = 0$ thresholds towards the sides of the diagram, but because the pole positions have a negative imaginary component in $\nu$, the trajectories pass the threshold and away from physical frequencies. With increasing $h$, the pole moves from $\lambda_R$ to the mode threshold in a sheet adjacent to the physical sheet. This behaviour occurs for $\tau$ values near $0$ or $1$, and consequently the effects are not felt at physical wavelengths. Examination of Figure 3.7(b) shows that $c$ must be greater than $0.5$ for this situation to arise.

The property of symmetry of the trajectories about the lines $\tau = \pi/2d$, allows one to follow them indefinitely to the left and right. For example, the poles in $b_1$ will still exist after the trajectories have passed into the unphysical region below and to the right of $X_0 = 0$. The pole position has a positive imaginary wavelength part in this case.
3.39

by contrast with the pole in \( b_0 \), which occurs at a real wavelength in the unphysical region.

3.2.2.6 Poles in \( \sin \theta \)

Analysis of resonances has to this point concentrated on mountings where \( \lambda \) (or \( \nu \)) is varying. However, resonances may also be observed if \( \lambda \) is held fixed and \( \sin \theta \) is allowed to vary such that a fixed-h locus in the \((\nu, \tau)\) plane is crossed.

Consider a set of curvilinear co-ordinates \((\rho, \sigma)\) defined on the \((\nu, \tau)\) plane such that \( \rho \) is a direction normal to a fixed-h trajectory and \( \sigma \) is parallel to it. The order amplitudes will now possess poles as a function of \( \rho \), but not of \( \sigma \). For example, equation (3.24) can be modified to become

\[
B_0 = \exp(2i\delta_b(\rho, \sigma)) \frac{\rho - \rho_p}{\rho - \rho_p}
\]

where only the zeroth order is propagating.

Locally, both \( \rho \) and \( \sigma \) are linear combinations of \( \nu \) and \( \tau \), the former being given by \( \rho = \nu \sin \beta + \tau \cos \beta \), where \( \beta \) is the angle between the trajectory and the \( \nu \) axis. Therefore, if \( \sin \theta \) is held fixed, equation (3.43) exhibits a pole in \( \lambda \), while if \( \lambda \) is held fixed it contains a pole in \( \sin \theta \). If the fixed-h trajectory lies parallel to the line of constant \( \lambda \) at the point of interest, then \( \rho = \nu \). If \( \lambda \) is fixed, then equation (3.43) has no pole as a function of \( \sin \theta \). This situation arises near the Littrow condition, \( \tau = \rho/2d \), for small depths, and almost everywhere in the \((\lambda, \sin \theta)\) plane for large depths.

For constant \( \lambda \), equation (3.43) becomes

\[
B_0 = \exp(2i\delta_b) \frac{\alpha - \alpha_p}{\alpha - \alpha_p},
\]

where \( \alpha = \sin \theta \), \( \alpha_p = \alpha_p(h) \) and \( \text{Im}(\alpha_p) = \sec(\beta) \). When the trajectory at the point of interest is parallel to lines of constant \( \lambda \), \( \beta = 90^\circ \) and the pole recedes to infinity in the complex \( \sin \theta \) plane and in fact ceases to
be a pole. Equation (3.44) reduces to

$$B_0 = -\exp(2i\delta_b).$$

(3.45)

If the trajectory lies at a grazing angle to the lines of constant $\lambda$, then the resonance anomaly as a function of $\sin \theta$ will be very broad.

By contrast with the above, it appears that poles as a function of $\lambda$ can never disappear because their trajectories appear to lie in the $(v, \tau)$ plane such that $\beta$ is always $> 45^\circ$, the minimum slope for such a mounting.

It is of interest to compare the observations made in the foregoing discussion with the studies of Maystre et al. documented in references [3.24-3.26]. These authors investigated resonance behaviour of a finitely-conducting sinusoidal grating, operated in a constant wavelength mounting at angles near normal where only the reflected order propagates.

Equation (3.3) is the expression they obtained for an approximation to $B_0$ in the vicinity of a resonance. Similarities are seen between this expression and equation (3.44). Differences exist because the Fresnel reflection coefficient $r(\alpha_0)$ in their expression is not unity, owing to the lossy nature of the metal. Also, $\alpha_z(h)$ is not the complex conjugate of $\alpha_p(h)$. However, $\alpha_z(h) - \alpha_z(0)$ and $\alpha_p(h) - \alpha_0(h)$ are approximately conjugates, while $\Im(\alpha_p(h)) > \Im(\alpha_z(h))$ as expected. In their case, $\alpha_z(0) = \alpha_p(0)$ is a complex number (the plasmon position for a lossy plane surface), while for the infinite-conductivity case given here, $\alpha_p(0) = \bar{\alpha_p}(0)$ is a real number corresponding to a Rayleigh wavelength.

Hutley and Maystre [3.25] provide four $(\lambda, \sin \theta)$ resonance positions, which if plotted on the $(v, \tau)$ plane, are found to lie just above and parallel to the Rayleigh wavelength line $\chi_{-1} = 0$. This conforms with earlier observations that poles in $\sin \theta$ should lie near the outer edges of the diagrams of Figure 3.7, and close to a Rayleigh wavelength.

The depth-to-period ratios considered by Hutley and Maystre are extremely small, and so for larger depths than these, the tendency of the
trajectories to become parallel to the lines of constant wavelength (assuming their behaviour is similar to that established here) could detract from the usefulness of their representation (3.3).

Some numerical results, emerging from an extension of the investigation to the case of finite conductivity, are reported in Sections 3.2.2.8 and 5.5.3.

3.2.2.7 Repulsion of Anomalies

The above analysis of resonances furnishes an explanation of the phenomenon first reported by Stewart and Gallaway [3.13], in which anomalies appear to repel each other and exchange identity, rather than cross through each other. The phenomenon occurs when two Rayleigh wavelength lines intersect in the \((\lambda, \sin \theta)\) plane, and so Stewart and Gallaway expected the anomalies to cross over, since they attributed them to Rayleigh wavelengths.

McPhedran and Maystre [3.21] recognized that the "repulsion" effect must concern resonance anomalies but they were unable to reproduce it through either their finite conductivity theory or experimental results.

Evidence is provided here, which duplicates the phenomenon for the lamellar grating and hence points to an explanation.

Consider, for example, a range of values for \(\theta\) near 19.47°, where the -2 and +1 order thresholds are coincident. For \(\theta\) below this figure, a constant \(\theta\) efficiency curve may show two anomalies, the shorter wavelength one near the -2 threshold and the longer wavelength one near the +1 threshold. For \(\theta > 19.47°\), these positions are reversed because the thresholds have crossed without the anomalies doing the same. The latter appear to approach and then repel one another without merging.

Experimental results, such as those presented by Stewart and Gallaway [3.13], indicate that the shorter wavelength anomaly remains fairly close to the Rayleigh wavelength, while the longer wavelength anomaly appears to follow a curve in the \((\lambda, \sin \theta)\) plane. Reference to Figure 3.7 (remembering that a constant \(\theta\) efficiency curve is represented by a sloping
line through the origin) shows that the phenomenon can be attributed to a Rayleigh wavelength anomaly occurring at the shorter wavelength, and a resonance anomaly at the longer one. This is because a sloping line on the $(\nu, \tau)$ plane can intersect a fixed-$h$ pole trajectory before it intersects the two Rayleigh wavelength lines. From the diagrams of Figure 3.7, the longer wavelength anomaly is seen to be farthest from the order thresholds when the latter coincide. The anomalies therefore do not "exchange identity" but retain their identities as the thresholds exchange positions.

Numerical evidence is presented in Figure 3.8 for a grating with $c/d = 0.43$ and $h/d = 0.4$. Three angles of incidence were used, namely $16^\circ$, $19.47^\circ$ and $23^\circ$. Associated with the lower wavelength threshold in each case is a Rayleigh wavelength anomaly, while the resonance anomaly remains in position near $\lambda/d = 0.8$. Each anomaly retains its shape, but not necessarily its strength throughout the change in $\theta$. The reason why the latter anomaly does not move in wavelength can be seen from Figure 3.7, where the fixed-$h$ trajectories are virtually flat in the region of interest. For $h = 0.4d$, the trajectory has been plotted on a larger scale in Figure 3.8. In the efficiency curve for $\theta = 23^\circ$ it is noted that three anomalies are visible. This is because a Rayleigh anomaly occurs at both of the -2 and +1 thresholds.

3.2.2.8 Finite Conductivity

To this point, the discussion of resonance anomalies for the lamellar profile has been confined to the case of infinite conductivity. To maintain significance, the results should carry over into the domain of finite conductivity. It is therefore useful to determine whether the introduction of conduction losses drastically changes the behaviour of the resonances described so far, or in fact whether it introduces new features.

To this end, investigations were carried out on a lamellar grating of $c/d = 0.43$ and $h/d = 0.2$, when in a -1 Littrow mounting.
Figure 3.8  S polarization efficiencies in the -1 order, as a function of wavelength, for the lamellar reflection grating and three fixed angles of incidence. The repulsion of the -2 and +1 Wood anomalies with the resonance anomaly at \( \lambda = 0.8 \) is well illustrated. The trajectory of the pole (real part) in the \((\lambda, \sin \theta)\) plane is also shown.

Groove parameters: \( d = 1.0, c = 0.43, h = 0.4 \).
The infinite-conductivity modal theory predicts a sharp S-plane anomaly at $\lambda/d \approx 0.72$. Using a finite-conductivity theory, based on integral equation techniques [3.37], efficiencies were evaluated for aluminium in the appropriate normalised wavelength region for low, medium and high conductivities. (Note: The modal theory described in Chapter 5 was not available at the time of this investigation.)

To maintain the same $\lambda/d$ ratios for the three regions of conductivity, three different periods were chosen. These were $d = 10 \mu m$ (high conductivity), $d = 2 \mu m$ (medium conductivity) and $d = 1 \mu m$ (low conductivity). The latter case corresponds closely to the visible region of the spectrum. The complex refractive indices for aluminium were obtained from reference [3.39]. For the three cases, they take the approximate values $2.0 + 7.0i$, $2.0 + 13.0i$, and $15.0 + 50i$ respectively.

The numerical results for the total of four different conductivities are displayed in Figure 3.9. In (d) the complex wavelength pole is plotted (having been determined using the method described in Section 3.2.2.4) and this is seen to move uniformly into the complex plane, away from both the real and imaginary wavelength axes, as the conductivity decreases. This behaviour manifests itself in Figures 3.9(a) and (b) as only a gradual change in the efficiency and phase curves for the -1 order. Because the pole moves away from the real axis, the resonance feature in the efficiency slowly broadens. This movement of the pole is not unexpected in light of the results of Maystre et al. [3.24-3.26], which showed that for finite conductivity the poles should lie above the real axis for all groove depths.

Within the range of wavelengths studied, no new resonance features have been observed. This is encouraging, and so it can be concluded that the ideas outlined earlier for infinite conductivity have a much broader area of application.
Figure 3.9  S polarization resonance behaviour for lamellar reflection gratings of different surface conductivity.

(a) Littrow efficiency for infinite conductivity and for finite conductivities corresponding to aluminium.

(b) The phases of the amplitude $B_{-1}$ corresponding to (a).

(c) Argand plots of the amplitude $B_{-1}$.

(d) Pole positions in the complex wavelength plane as a function of conductivity.

Groove parameters: $c/d=0.43, h/d=0.2$. 
(Note: In Chapter 5, use of a finite-conductivity modal theory for lamellar gratings indicates once again that resonance can be attributed to poles in mode amplitudes.)

3.2.3 Resonance Poles for Some Alternative Profiles

Previous observations have established that there is a strong resemblance between the actions of the lamellar profile and alternative profiles, for example the sinusoidal profile. This chapter has shown that resonances in the lamellar grating form an integral part of that grating's overall efficiency behaviour. In this section, the method of Section 3.2.2.4 is employed to locate pole positions for general groove profiles, and this information is correlated with their efficiency spectra. It is noted first, that the lamellar grating produces the sharpest resonance features of any known conventional grating, and hence any poles for other profiles are expected to lie much farther from the real-wavelength axis. (A possible exception to this occurs for the bottle grating discussed in Section 4.2.)

The starting point for the investigation was a symmetrical lamellar profile of depth $h/d = 0.5$. The $-1$ Littrow efficiency curve for this profile contains a strong $S$-anomaly near $\lambda/d = 0.92$. The $b_1$ pole responsible for this resonance occurs at $\lambda_p = 0.925 + 0.0034i$.

An infinite conductivity theory, based on the method of Pavageau and Bousquet [3.40, 3.35], was implemented to calculate efficiencies in $B_{-1}$ for gratings whose groove profiles lie between the rectangular profile and a sinusoidal profile. All profiles were constrained to a normalised groove depth of 0.5. They include a semi-circular profile and some trapezoidal profiles.

The results for the sinusoidal and trapezoidal profiles are displayed in Figure 3.10. The efficiency curves for the latter show a gradual change in behaviour as the groove walls are tilted, with the anomaly moving from
Figure 3.10  Littrow efficiency curves for the lamellar, trapezoidal and sinusoidal profiles. In each case d=1.0 and h=0.5.

(-- -) lamellar profile, c=0.5

(---) aperture width =0.6(top), 0.4(bottom)

(-----) aperture width =0.7(top), 0.3(bottom)

(- - - -) sinusoidal profile
\( \lambda/d = 0.92 \) to wavelengths below \( \lambda/d = 0.8 \). For the sinusoidal profile, the resonance has become very broad and its exact position is not clear. Also, the efficiency no longer varies from 0 to 100%.

Plots of \( B_1 \) in the Argand plane were constructed and the method of Section 3.2.2.4 used to evaluate the pole positions. The results are illustrated in Figure 3.11. They show that the pole for the trapezoidal profiles moves rapidly and uniformly out into the complex plane, with a decreasing real wavelength component, until it terminates at the position corresponding to the sinusoidal profile. The imaginary component of the latter was extremely difficult to locate precisely, but was estimated to lie between .04 and .08.

The pole positions of the semi-circular profile and some lamellar profiles of differing groove widths, have also been plotted. The former is discovered to lie very close to the original trajectory, while the poles for the lamellar profile gain longer real and imaginary wavelength components as the groove width increases. For \( c/d = 0.7 \), the lamellar pole attains an imaginary component as large as that estimated for the sinusoidal profile.

Regarding the latter grating, it is also of interest to estimate the position of the pole trajectory as \( h \) tends to infinity. (For the lamellar grating it terminates at the \( m = 1 \) mode threshold of \( \lambda = 2c \).) As the groove modulation becomes large, the sinusoidal grating assumes a profile similar in shape to a deep lamellar grating of \( c/d = 1.0 \). The latter has its \( m = 1 \) mode threshold at \( \lambda/d = 2.0 \). It is therefore suggested that the pole for the sinusoidal profile approaches the same real wavelength as the groove depth becomes large. Numerical evidence to confirm this has not been obtained.
Figure 3.11  $S$ polarization pole positions in the complex wavelength plane for various infinitely-conducting gratings of equal period and in the -1 Littrow mounting. In each case the normalised groove depth is $h/d=0.5$. Four positions near the dotted line correspond to the four cases of Figure 3.10. The poles for the lamellar profile correspond to $b_1$ mode resonances. (Pole positions with $\text{Im}(\lambda/d)>0.02$ are only approximate).
3.2.4 **Resonances in the Lamellar Transmission Grating**

The similarities which exist between the scattering matrices for the modal amplitudes of the reflection and transmission gratings, have been pointed out in Chapter 2. In fact, it has been shown that for a transmission grating of twice the depth of the reflection grating, one of the modal amplitudes in the former case (either $a_m^*$ or $b_m^*$ depending on the polarization) is equal to one half of its counterpart in the latter case. Therefore, when the reflection grating undergoes a resonance, a similar effect should be visible in the spectrum of the wire grating of twice the depth.

The conditions which determine resonance for the transmission grating are given by equations (3.31) and (3.39), but with the depth dependence modified. They are:

$$K^S_{mm} = \varepsilon_m cd \cot(\nu_m h) / \nu_m \quad ...(3.46)$$

and

$$K^P_{mm} = \frac{cd}{2} \nu_m \cot(\nu_m h). \quad ...(3.47)$$

Resonance behaviour is thus expected to occur in a similar manner to that for the reflection grating, but for larger depths.

Now consider the other $m$th mode amplitude, corresponding to the term of opposite $y$-symmetry, i.e. $a_m^*$ for $S$ polarization and $b_m^*$ for $P$ polarization. Are these amplitudes also capable of resonance? Manipulation of equations (2.38) and (2.36) shows that these amplitudes contain singularities at wavelengths given by

$$K^S_{mm} = -\varepsilon_m cd \tan(\nu_m h) / \nu_m \quad ...(3.48)$$

and

$$K^P_{mm} = -\frac{cd}{2} \nu_m \tan(\nu_m h). \quad ...(3.49)$$

These conditions are the same as the previous two if the transformation $\cot(\nu_m h) \to -\tan(\nu_m h)$ is made. The latter function behaves identically
to the former if its argument is $\pi/2$ greater, therefore resonances in these amplitudes should occur at either larger groove depths, or alternatively shorter wavelengths.

Consider the case for $S$ polarization and a normal incidence mounting. For the reflection grating, some $b^*_0$ pole trajectories are contained in Figure 3.5(b). Because only the zero order is propagating, these poles are not evident in the efficiency curves. However, for the wire grating and $\lambda/d > 1.0$, two orders are propagating and so spectral anomalies are expected. This is confirmed by the $S$ polarization efficiency curves of Figure 2.7(b) and 3.12(a).

The trajectories of Figure 3.5(b) indicate that the smaller the value of $c$, the closer is the pole to the real-wavelength axis, and hence the stronger should be the resonance effect. This has been confirmed numerically for the wire grating and Figure 3.12(a) depicts a transmitted-efficiency curve for $c/d = 0.1$. Three very sharp resonance peaks are visible in the wavelength range $1.0 < \lambda/d < 5.0$, and as a result of the very narrow groove width, very little background energy is transmitted. It is noted that energy transmission reaches 100% at resonance.

The occurrence of the three $m = 0$ resonances, for the depth used above ($h/d = 1.05$) is explained as follows. Equation (3.32) predicts the depths for which pole trajectories start out from Rayleigh wavelengths for the reflection grating. For the wire grating, this equation is modified by replacing $h$ by $h/2$. By then putting $\lambda_R = 1.0d$ and $m = 0$, we obtain

$$h_{\lambda} = \lambda_d, \quad \lambda = 0,1,2...$$

These are the depths for which trajectories in $b^*_0$ commence. In the light of an earlier discussion, trajectories for the amplitudes $a^*_m$ should begin when $u_m h_{\lambda} / 2 = (2\lambda+1)\pi/2$, i.e. when

$$h_{\lambda} = (2\lambda+1)\left(\frac{4}{\lambda_R^2} - \frac{m^2}{c^2}\right)^{-1/2}, \quad \lambda = 0,1,2...$$

For the long-wavelength configuration, this equation reduces to
Figure 3.12 Efficiency spectra which illustrate resonance behaviour in the lamellar transmission grating. (d=1.0)

(a) S polarization, normal incidence: c=0.1, h=1.05
(b) P polarization, normal incidence: c=0.95, h=1.2
(c) S polarization, -1 Littrow: c=0.43, h=0.8
Combining equations (3.50) and (3.52) shows that all resonances emerge from \( \lambda_R = 1.0d \) at depths of \( h/d = 0, 0.5, 1.0, 1.5 \ldots \). Therefore, for the case of \( h/d = 1.05 \), three resonances are evident. Intensities and phases of the mode amplitudes \( a_0^\ast \) and \( b_0^\ast \) confirm that the two outer peaks in Figure 3.12(a) are due to a pole in \( b_0^\ast \), while the central one is due to \( a_0^\ast \).

Thus, due to the fact that two amplitudes may undergo resonance, the wire grating exhibits resonances equal in number to those of the reflection grating of the same depth.

For large groove widths, poles in the mode amplitudes \( a_1^\ast \) and \( b_1^\ast \) should also move out from \( \lambda_R = 1.0d \) with increasing groove depth, but only towards the threshold at \( \lambda = 2c \). These have not been investigated numerically.

For P polarization, poles are possible in \( b_1^\ast \) and \( a_1^\ast \) at wavelengths below the \( \mu_1 = 0 \) threshold. Behaving in a similar manner to those for the reflection grating, their effect is only felt for large depths. For normal incidence, \( c/d \) must be greater than 0.5 for the mode threshold at which the trajectory terminates to be at a wavelength greater than the Rayleigh wavelength of \( \lambda_R = 1.0d \).

Figure 3.12(b) displays the efficiency curve for the grating \( c/d = 0.95, h/d = 1.2 \). The two small peaks at wavelengths \( \lambda/d = 1.2 \) and \( \lambda/d = 1.6 \) are consequences of poles in the amplitudes \( a_1^\ast \) and \( b_1^\ast \) respectively. As expected, the latter pole is the closer of the two to the real-wavelength axis since this one is further advanced towards the mode threshold. In this case, the efficiency fails to reach zero between the resonances, as it does for the Littrow mounting with two real orders. This is because condition (2.82) for total reflection cannot be met by both of the \( m = 1 \) mode amplitudes simultaneously.
The resonance behaviour for P polarization offers a direct explanation of the efficiency behaviour discussed in Section 2.6.2. There it was reported that for wavelengths in excess of \( \lambda/d = 1.0 \), the transmitted efficiency is generally very low, except for a narrow interval between \( \lambda_R = 1.0d \) and a cut-off wavelength where efficiency is high. As \( h \) increases, the cut-off was observed to become steeper. This behaviour is clearly the manifestation of the nearby \( m = 1 \) poles which move towards real values with increasing groove depth. The cut-off wavelength is therefore deduced to be the termination point of the pole trajectories at \( \lambda = 2c \).

The -1 Littrow mounting is of limited practical use for the wire grating, but it is of interest to confirm that resonances occur as predicted, and to determine their influence on efficiency performance when four orders are propagating. To this end, a grating with parameters \( c/d = 0.43 \) and \( h/d = 0.8 \) was investigated for S polarization. Because \( h \) is twice the value used previously for the reflection grating (Figure 3.1(c)), a resonance is expected to occur near \( \lambda/d = 0.8 \). This is confirmed by the sharp anomaly in Figure 3.12(c). The associated pole is in \( b_1^* \), while a second anomaly at \( \lambda/d = 0.69 \) is due to a pole in \( a_1^* \). This latter pole has emerged from the Rayleigh wavelength at a depth (given by equation (3.51)) of \( h/d = 0.5277 \) - the same depth that a second \( b_1 \) pole emerges for the reflection grating.

It is interesting to deduce from the efficiency curves shown in Figure 3.12, that at resonance the energy redistribution favours the -1 transmitted order in preference to the other orders, all of which carry approximately equal amounts of energy at wavelengths away from resonance.
3.3 **BLAZE ACTION OF THE REFLECTION GRATING**

3.3.1 **Introductory Remarks**

In the situation where only two orders are propagating, namely the zeroth order plus one diffracted order, it is possible to find conditions which result in all incident energy being channelled into the diffracted order. The reflection grating concerned is then said to be blazed in that particular order and it is essentially acting as a "non-reflecting" surface. The conditions which permit this phenomenon to occur for a certain wavelength depend on groove profile, polarization and angle of incidence.

Hessel *et al.* [3.41] postulated that a necessary criterion for blazing is given by the Bragg relation (equivalent to the first order Littrow mounting), i.e. that the diffracted order must be "back scattered" in the direction of the incident beam. They also conjectured that any grating may be blazed perfectly (in the case of infinite-conductivity) by the appropriate choice of groove depth, and this they demonstrated for the lamellar grating. They also showed that blazing could be achieved simultaneously in the fundamental polarizations.

For \( S \) polarization, blazing under the Bragg condition has been proven rigorously for the right-angled echelette grating [3.42]. This is a consequence of the Marechal-Stroke Theorem. The simple geometry of that grating shows that the blaze-depth is given by \( h = \lambda \cos \theta/2 \). Application of the above theorem to the lamellar profile shows that in normal incidence all energy is returned in the zero order if the depth equals an integral number of half-wavelengths. No equivalent to the theorem exists for \( P \) polarization.

Based on the criterion of Hessel *et al.* further work has been directed towards the problem of dual-blazing for the lamellar grating [3.43, 3.44, 3.45]. This has been purely of a numerical nature and has consisted of
plotting loci of blazing conditions for each polarization and then finding their intersection points.

Blazing characteristics of various profiles, including the rectangular-profile, have also been the subject of attention in papers by Loewen et al. [3.46] and Breidne and Maystre [3.38], but the conclusions of the former only apply to very shallow profiles (in the case of the lamellar grating, h/d < 0.1). Those of the latter only apply to symmetrical lamellar profiles. However, in the latter case, an equivalence rule (relating the efficiency of different gratings via the fundamental Fourier coefficient of their profile) along with the Marechal-Stroke Theorem, was used to derive simple S polarization formulae which predict blaze depths for angles of incidence near normal and near 90°.

Restricting attention to the -1 Littrow mounting, it is the aim of this section to outline an investigation into the determination of blaze wavelengths by analysing the lamellar modal theory. Such a procedure has already been fruitful in predicting wavelengths of low diffracted efficiency (Section 2.6) and wavelengths of resonance anomalies (Section 3.2).

3.3.2 Blazing Conditions

Consider first the case for P polarization. It has already been established that the m = 1 mode is the dominant one for this polarization and is responsible for both background and resonance behaviour in the -1 order.

Assuming then a monomodal approximation of the theory, substitution of equation (2.83) into (2.85) yields

\[ A_p = \frac{2iX_0 T_{10} I_p}{k_{11} - \mu_1 \cot(\mu_1 h)cd/2} - \delta_{0,p} \quad (3.53) \]

The vanishing of the denominator in this expression corresponds to a resonance pole. Consider now the vanishing of just the real component. For real wavelengths, this is expressed by
\[ Re\left(K_{11}^p\right) - \mu_1 \cot(\mu_1 h) cd/2 = 0. \] \hspace{1cm} ...(3.54)

For -1 Littrow and two real orders we have
\[ K_{11}^p = - \sum_{p \neq 0, -1} |X_p||I_p|^2 + 2iX_0|I_0|^2, \] \hspace{1cm} ...(3.55)

and so insertion of condition (3.54) into (3.53) gives
\[ A_p = \frac{I_p}{I_0} - \delta_{0,p}, \] \hspace{1cm} ...(3.56)

which implies that \(|A_0|^2 = 0\) and \(|A_{-1}|^2 = 1\), where \(I_0 = I_{1,-1}\). Thus, condition (3.54) produces an efficiency of 100% in the -1 diffracted order if the first mode is the dominant one.

Table 3.1 demonstrates the accuracy with which condition (3.54) is satisfied for the example illustrated in Figure 3.3(d) where three blazes occur in the relevant wavelength interval.

For wider apertures, where the \(m = 2\) mode becomes increasingly significant, condition (3.54) gradually becomes less accurate and the exact blaze wavelength is governed by a more complicated condition involving the first two modes. As an example, a grating with \(c/d = 0.6\) and \(h/d = 0.3\) attains 100% efficiency in the -1 order at \(\lambda/d = 0.775\) while condition (3.54) predicts it at \(\lambda/d = 0.8\). This small discrepancy indicates the extent of the influence that modes other than the lowest one are having in determining efficiency behaviour.

In summary, we can say for \(P\) polarization that whenever the single-mode model gives accurate predictions of efficiency, condition (3.54) is a valuable expression for the blaze wavelengths. For cases where one mode is not adequate, it still provides a close approximation.

For \(S\) polarization the situation is slightly more complicated when both the \(m = 0\) and \(m = 1\) modes play a significant role. If a monomodal approximation is assumed, but in the \(m^{th}\) mode, then the \(p^{th}\) order amplitude is given by
TABLE 3.1

Blazing Conditions for the Infinitely-Conducting Lamellar Reflection Grating.

Calculations are presented which demonstrate the accuracy with which equations (3.54), (3.58) and (3.62) predict blazing in the first-order Littrow mounting.

Groove parameters: \(d = 1.0\), \(c = 0.43\), \(h = 1.4\) (P polarization)
\(d = 1.0\), \(c = 0.50\), \(h = 0.25\) (S polarization)

Number of Expansion Terms: \(P = 8\), \(M = 10\).

<table>
<thead>
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<th>(\lambda)</th>
<th>L.H.S. Eq.(3.54)</th>
<th>(E(-1))</th>
<th>(\lambda)</th>
<th>L.H.S. Eq.(3.58)</th>
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\[ B_p = \frac{2iJ_m J_p}{\varepsilon_m c d \cot(\mu_m h) / \mu_m - \kappa_{mm}^S} + \delta_{s,p} \quad \ldots (3.57) \]

Again, the complete disappearance of the denominator leads to a resonance, but for either \( m = 0 \) or \( m = 1 \), the vanishing of only the real part is found to produce 100% efficiency in the -1 order. That is, blaze wavelengths, \( \lambda_B \), occur when

\[ \Re \left( \kappa_{mm}^S \right) - \frac{\varepsilon_m c d \cot(\mu_m h)}{\mu_m} = 0. \quad \ldots (3.58) \]

(At \( \lambda_B \), \( \arg (B_{-1}) = 180^\circ \) and for \( m = 0 \), \( \arg (b_0) = 90^\circ \).)

As mentioned earlier, the efficiency in the vicinity of a mode resonance usually fluctuates rapidly between 0% and 100%. The above condition with \( m = 1 \) corresponds to the "100%" position for a \( b_1 \) mode resonance. For the case \( m = 0 \) however, there is no associated resonance at physical wavelengths and the above condition simply produces a blaze in the background efficiency - but only if this mode is the dominant one.

(The similarity between equations (3.54, 3.58) and the conditions for resonance, seems to be the cause of the efficiency reaching 100% during or near a resonance anomaly, as indicated above for \( m = 1 \). By writing the above equations as \( \Re (\text{Denom}) = 0 \), for complex wavelengths, then \( \text{Denom} = 0 \) corresponds to a pole \( \lambda_R + i\lambda_I \). Two trajectories could be plotted through this pole corresponding to \( \Re (\text{Denom}) = 0 \) and \( \Im (\text{Denom}) = 0 \). It is probable that the former trajectory is roughly parallel to the imaginary wavelength axis and therefore cuts the real wavelength axis at \( \lambda_B \), very close to \( \lambda_R \).

Consider the spectrum in Figure 3.2(a), for \( c/d = 0.43 \) and \( h/d = 0.7 \). For \( m = 1 \), condition (3.58) is satisfied for \( \lambda/d = 0.83 \), while for \( m = 0 \) it is satisfied for \( \lambda/d = 0.97 \). These predictions correlate well with blazes observed at these wavelengths.

Consider the case of \( c/d = 0.5 \) and \( h/d = 0.25 \). The efficiency curve illustrated in Figure 2.5(c) shows the existence of three blazes for
2/3 < \lambda/d < 2.0. These occur near \lambda/d = 0.85, 1.1 and 1.8, the first being close to a \textit{b}_1 resonance. For \( m = 1 \), condition (3.58) is met for \( \lambda/d = 0.83 \), while for \( m = 0 \) it is satisfied for \( \lambda/d = 1.06 \) (see Table 3.1). These values are in reasonable agreement with the observed positions.

Notice however, that (3.58) does not predict the longer wavelength blaze near \( \lambda/d = 1.8 \). This is linked with the fact that this blaze is not due to any particular mode resonance, and that a monomodal model, as shown in Section 2.7, is not a valid approximation in this region just prior to the -1 and 0 orders passing off.

We therefore seek a more accurate constraint than equation (3.58).

Consider the bimodal model contained within equations (2.89) to (2.91). This can be simplified, in the case of two orders propagating in a -1 Littrow mount, to yield

\[
B_0 = \frac{2}{\Omega_0} \left( J_{2,0}^2 \frac{X}{Y} + |J_{1,0}|^2 Y + 1 \right) \quad \cdots (3.59)
\]

where

\[
X = \frac{\kappa_{11}^{S} - \frac{cd \cot(\mu_1 h)}{2\mu_1}}{X_0} \quad \cdots (3.60)
\]

\[
Y = \frac{\kappa_{00}^{S} - \frac{cd \cot(\mu_0 h)}{\omega_0}}{X_0} \quad \cdots (3.61)
\]

and

\[
\kappa_{11}^{S} = \sum_{p \neq 0, -1} \frac{|J_{1p}|^2}{|X_p|^2} + \frac{2i|J_{11}|^2}{X_0}
\]

\[
\kappa_{00}^{S} = \sum_{p \neq 0, -1} \frac{|J_{0p}|^2}{|X_p|^2} + \frac{2iJ_{01}^2}{X_0}.
\]

Vanishing of either \( X \) or \( Y \) corresponds to a pole in the \( m = 1 \) or the \( m = 0 \) modes respectively, while the condition for blazing is now more complicated than simply \( \text{Re} \left( XY \right) = 0 \). Numerical evidence shows it is given by

\[
\text{Re} \left( X \right) \text{Re} \left( Y \right) + \text{Im} \left( X \right) \text{Im} \left( Y \right) = 0, \quad \cdots (3.62)
\]

and this may be verified theoretically as follows. Rewriting equation (3.62) as \( X = iY \frac{\text{Im} \left( X \right)}{\text{Re} \left( Y \right)} \) and substituting this into equation (3.59) gives
Replacing $\text{Im}(Y)$ in this expression by the appropriate term from equation (3.61), and expressing $|J_{10}|^2$ in terms of $\text{Im}(X)$, equation (3.63) simplifies to

$$B_0 = \frac{2}{X_0} \left[ -\frac{J_{10}^2}{\text{Re}(X)} + \left| \frac{J_{10}}{X} \right|^2 \right] + 1 \quad \ldots (3.63)$$

Hence, $|B_{-1}|^2 = 1$ and all energy appears in the -1 order.

Referring back to the previous numerical example, condition (3.62) is satisfied (see Table 3.1) at wavelengths $\lambda/d = .845, 1.10$ and $1.80$. So not only does it accurately define the long-wavelength blaze position, but it also yields more precise values for the other two positions.

For comparison with the above, the simple formulae presented by Breidne and Maystre [3.38] (which only apply for $c/d = 0.5$) predict blazing at $\lambda/d = 0.89$ and $1.79$. The discrepancies between these values and the observed blazed peaks can be attributed to $h/d$ being too large and not being sufficiently close to $0^\circ$ or $90^\circ$. Their empirical formulae cannot of course account for the third blaze peak at the resonance anomaly.

Equation (3.62) is found to be useful in explaining many of the distinctive blazing characteristics which are observed in certain S polarization efficiency spectra. These include the sharp peaks seen in the -1 order efficiency just below $\lambda_R = 2.0d$ when either $h/d$ is very small or $c/d$ is almost unity (in the case of the "comb" grating).

Expansion of equation (3.62) gives

$$\left(\text{Re}(k^S_1) - \frac{cd}{2} \cot(\mu h) \right)\left(\text{Re}(k^S_0) - \frac{cd}{\mu_0} \cot(\mu h) \right) - \frac{4c^2|J_{12}|^2}{X_0} = 0. \quad \ldots (3.64)$$

For $h \to 0$, the "cot" terms tend to infinity, but condition (3.64) can still be satisfied if $X_0 \to 0$, which occurs if $\lambda \to 2.0d$. This conforms with previous observations, including those of Breidne and Maystre, that for shallow profiles blazing is achieved for angles of incidence near grazing.
For $c/d \to 1$, the $m = 1$ mode threshold lies just below $\lambda_R = 2.0d$. Near this point $\mu_1 \approx 0$ and $\cot(\mu_1 h)$ is very large while $X_0 \approx 0$, and so again, equation (3.64) may be satisfied with the result that the $-1$ order efficiency rises to 100%. Similarly, we deduce that for large values of $c$, blazing will occur very near to the mode threshold at $\lambda = 2c$ where both $X_0$ and $\mu_1$ are very small. As $c$ decreases, the value of $X_0$ increases at the mode threshold and so this point separates from the blaze wavelength.

A similar condition to equation (2.62) could, if desired, be derived for a bimodal model for $P$ polarization, and again this would be expected to yield more accurate positions for blaze wavelengths.

3.4 "PASSING OFF" BEHAVIOUR

This section is concerned with a study of the manner in which the efficiency of the $-1$ order for the reflection grating, varies just before that order becomes evanescent. Again, the mounting configuration is assumed to be first-order Littrow. It has long been observed for all gratings, that in this wavelength region, where the angle of incidence approaches $90^\circ$, the efficiencies for $S$ polarization and $P$ polarization always behave in a definite but dissimilar manner. This is exemplified in the efficiency curves of Figure 3.10, which show that just prior to passing off, the $-1$ order efficiency falls abruptly to zero in the case of $S$ polarization, but only gradually to zero for $P$ polarization.

In Section 2.7, it was shown for $S$ polarization, with the aid of the bimodal model, that $|B_{-1}|^2 = 0$ at $\lambda_R = 2.0d$. Similarly, the monomodal model for $P$ polarization may be employed to show that $|A_{-1}|^2 = 0$ at $\lambda_R = 2.0d$. It is the aim here to gain a simple parameterization of these quantities as $\lambda$ approaches 2.0d.

For $P$ polarization the task is straight-forward if one again turns to the monomodal approximation, which from Section 2.7 is known to reproduce very closely the correct efficiency behaviour in the wavelength
region just below 2.0d. From equation (3.53), the first-order amplitude may be expressed by

$$A_{-1} = \frac{2iX_0|I_{10}|^2}{k_{11} - \mu_1 \cot(\mu_1 h) cd/2}.$$  (3.65)

As $\lambda \to 2.0d$, $X_0 \to 0$ and so $A_{-1}$ tends to zero in a smooth fashion. This is because $I_{10}$ is independent of $\lambda$ for the -1 Littrow mount ($I_{m0}$ depends on $\lambda / \sin \theta$ which is a constant) and there are no zeros in the denominator for wavelengths greater than the $m = 1$ mode threshold at 2c. $|A_{-1}|^2$ is thus proportional to $X_0^2$ and in Figure 3.13(a) a sketch illustrates the variation of this quantity as a function of wavelength. The gradual decline to zero at 2.0d conforms well with observed efficiency behaviour and so it is deduced that the relation

$$|A_{-1}|^2 \propto X_0^2$$  (3.66)

is a good representation of the behaviour for P polarization.

A graph has been plotted of $|A_{-1}|^2/X_0^2$ as a function of $h$ for a particular wavelength and groove width. This proved essentially to be a flat line indicating that the constant of proportionality in equation (3.66) is virtually independent of depth. (This fact is in agreement with the observation made in Section 3.2.2.3, that for $\lambda > 2c$ the amplitude $A_{-1}$ changes only fractionally as $h$ is altered.) By contrast, the same graph for a sinusoidal profile is a straight line passing through the origin, thus establishing for that case, that $|A_{-1}|^2 \propto hX_0^2$.

An explanation of the passing-off behaviour for S polarization is more complex. The bimodal model equations, (2.89) to (2.91), may be simplified for the -1 Littrow mounting, to provide an expression for $B_{-1}$ (the complementary equation to (3.59)) which is

$$B_{-1} = \frac{2}{iX_0} \frac{N}{D}.$$  (3.67)

where $N = -J_{00}^2 \cot(\mu_0 h) cd + |J_{10}|^2 \cot(\mu_0 h) cd/\mu_0$  (3.68)
Figure 3.13 Functions which approximate the efficiency of the -1 order near 'passing off' in the -1 Littrow mounting.
(a) P polarization   (b) S polarization

Figure 3.14 Intensity of the -1 order amplitude as a function of wavelength, computed for the lamellar reflection grating in a -1 Littrow mounting and S polarization.
Groove parameters: \(d=1.0, c=0.43, h=0.1\)
and $K_{11}^S$, $K_0^S$ are given after equation (3.61).

In the vicinity of $\lambda/d = 2.0$, where $X_0 = 0$, $K_{11}^S$ and $K_0^S$ behave as $1/X_0$, in which case $N/D$ behaves as $X_0^2$ and so equation (3.67) suggests that again $B_{-1}$ is proportional to $X_0$. However, although there are usually no poles near 2.0 caused by $X$ vanishing, it is known from Section 3.2.2 that poles in the amplitude $b_0$, corresponding to $Y$ vanishing, start out from $\lambda = 2.0d$ at zero groove depth. The proximity of these real-wavelength poles must be considered to affect $B_{-1}$. Analysis of $Y$ reveals that it is an analytic function for $\lambda/d > 2.0$. It decreases monotonically with increasing $\lambda$ and therefore has a simple zero at $\lambda = \lambda_p$. Incorporating this into a parameterization for $B_{-1}$ provides an expression of the type

$$ |B_{-1}| \approx \left| \frac{X_0^2}{(\lambda - \lambda_p)^2} \right| $$

(3.70)

A sketch of this function, given in Figure 3.13(b), is immediately seen to match the abrupt fall in efficiency just prior to $\lambda/d = 2.0$. It also matches the rise in intensity towards $\infty$ in the region of the pole. For comparison, some computed values of $|B_{-1}|^2$ have been plotted in Figure 3.14 for a lamellar profile with $c/d = 0.43$ and $h/d = 0.1$. It should be noted that equation (3.70) is not expected to rigorously predict efficiencies, but to give only a general model of their behaviour. In reality, energy conservation constrains $|B_{-1}|^2$ not to exceed 1 for $\lambda < 2.0d$.

The significance of equation (3.70) is that it does demonstrate how the passing-off behaviour for $S$ polarization differs from that for $P$ polarization through the presence of a nearby pole in the $m = 0$ mode amplitude. It is also encouraging that the curve in Figure 3.13(b) conforms with ideas developed in the previous section on blazing.

It is now of interest to describe theoretically the influence that the position of the $b_0$ pole has on the passing-off behaviour, and to compare these predictions with numerical studies of not only the lamellar profile,
but also two other profiles for which pole positions have been located at real wavelengths in excess of 2.0. Analysis of equation (3.70) reveals that as \( \lambda \) moves away from 2.0 to longer wavelengths, \( \lambda \) (shown in Figure 3.13(b)) moves away also, but to shorter wavelengths. This characteristic agrees well with the data of Table 3.2, which compares positions of efficiency maxima with pole positions for three different profiles. For the lamellar and sinusoidal profiles, this data falls into two sections corresponding to the emergence of two different \( b \) poles from the Rayleigh wavelength, as shown graphically in Figure 3.15. For the lamellar grating, equation (3.32) governs the depths at which these poles appear, namely \( h/d = 0 \) and 1.0. For the sinusoidal grating, the first pole again emerges at zero depth, while it is interesting to find that the second emerges at approximately \( h/d = 1.16 \).

The curves in Figure 3.15, which sweep out to the right, depict pole movements in the first sheet of the Riemann surface \( (X_0, X_{-1} \) positive imaginary). These show that as \( h \rightarrow \infty \) then \( \lambda \rightarrow \infty \) also. The left-hand portions of the right-hand pair of curves represent pole positions on the second sheet \( (X_0, X_{-1} \) negative imaginary). As groove depth increases, the second pole is seen to appear in this sheet at a wavelength greater than 2.0. It then separates with one value moving to longer wavelength in the second sheet and the other moving to shorter wavelengths until it reaches 2.0, where it joins the first sheet and moves back to longer wavelengths.

The shape of these pole trajectories in the case of the lamellar grating may be explained as follows. Consider the pole term \( Y \), in equation (3.69). At \( \lambda/d = 2.0, K^S_{0} \) is real and infinite, as is \( \cot(\mu_{0}h) \) if \( h \) and hence \( \mu_{0}h \) equals zero. This is therefore the starting point of the trajectories. As both \( h \) and \( \lambda \) increase towards infinity, \( Y \) can still equal zero if \( K^S_{0} \) moves on the positive real line towards zero and if \( \cot(\mu_{0}h) \) also remains positive and becomes zero. This is achieved when \( \mu_{0}h = \pi/2 \) which implies \( \lambda/h = 4 \). Therefore, 4 is the limiting value of
TABLE 3.2

For S polarization and a -1 Littrow mounting, real-wavelength pole positions ($\lambda_p$) and blaze wavelengths ($\lambda_B$) are tabulated as a function of groove depth ($h$) for the lamellar, sinusoidal and symmetrical triangular profiles. In each case $d = 1.0$ and for the lamellar profile $c = 0.43$.

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<td>0.4950</td>
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3.67
Figure 3.15  S polarization trajectories of real-wavelength poles, as a function of groove depth for three different profiles in a -1 Littrow mounting. For the lamellar grating the poles are in the modal amplitude $b_0$.  

(-----) Lamellar profile: $c/d=0.43$  
(-----) Sinusoidal profile  
(-----) Triangular profile

Figure 3.16  -1 Littrow efficiency curves for the three profiles of Figure 3.15.
the slope of the first pole trajectory in Figure 3.15. The section of the second pole trajectory on the second sheet corresponds to $\frac{\pi}{2} < \mu_0 h < \pi$ where both $K_{\theta 0}^S$ and cot($\mu_0 h$) are negative. The slope of the outer part of this curve begins at a value of 4. The section of this trajectory on the first sheet, corresponds to $\pi < \mu_0 h < 3\pi/2$ where $K_{\theta 0}^S$ and cot($\mu_0 h$) are positive again. For $\mu_0 h = 3\pi/2$, one deduces $\lambda/h = 4/3$ and this is therefore the limiting slope as both $\lambda$ and $h$ tend to infinity.

A horizontal line in Figure 3.15 at $\lambda_p = 2.11$ would cut the first pole trajectories of the lamellar, sinusoidal and triangular profiles at depths of $h/d = 0.15$, 0.20 and 0.25 respectively. The infinite conductivity efficiency curves for these gratings have been plotted in Figure 3.16 and one is able to see in fact just how close they are to one another - especially in the passing-off region. This suggests a direct relationship between pole position and efficiency behaviour for gratings of arbitrary profile.

Figure 3.17 illustrates the onset and movement of a blaze peak near $\lambda_R = 2.0d$ as the second pole emerges from this wavelength for the lamellar grating of $h/d = 1.0$. When $h/d = 0.9$ the pole is at $\lambda_p = 2.2d$ on the second sheet and is too distant to be "felt", with the result that the efficiency falls to zero in a manner very similar to that for $P$ polarization. For $h/d = 0.99$ a small peak has started to develop at the Rayleigh wavelength and by the time $h/d = 1.0$, this peak has reached 100% efficiency. For further increases in depth, the blaze moves to shorter wavelengths and eventually fails to reach 100% as the pole moves further from 2.0.

In order to gain an understanding of how the groove width affects passing-off behaviour for $S$ polarization, the equation $Y = 0$ was studied numerically. This showed that for small and large values of $c$, the pole lies quite close to $\lambda_R = 2.0d$. For medium values of $c$ it makes a small excursion away from this position. A set of efficiency curves for different groove widths and $h/d = 0.1$, have proved that the movement of the
Figure 3.17  S polarization efficiency curves for a lamellar reflection grating (c/d=0.43) in a -1 Littrow mounting. A peak at λ/d=2.0 is shown to develop for an increasing groove depth near h/d=1.0.

Figure 3.18  Efficiency curves which show the effect of a reduction in surface conductivity for the sinusoidal grating in a -1 Littrow mounting. For P polarization changes are too slight to be shown.

\[ G=\infty : d=1.0, h=0.2 \]

\[ G<\infty : d=0.5\mu m, h/d=0.2 \text{ (aluminium)} \]
3.71 blaze peak conforms with this behaviour. That is, as $c$ increases the peak moves from 2.0 to lower wavelengths and then back to 2.0 again. For example, $c/d = 0.2$, 0.6 and 0.9 correspond to normalised blaze positions of 1.995, 1.96 and 1.99 respectively.

Some finite conductivity calculations have been made to check that the observed behaviour is not confined to infinite conductivity. This is indeed the case, as evidenced by Figure 3.18, which displays a comparison between efficiencies for a perfectly-conducting sinusoidal grating and an aluminium one. The curves show that the blaze peak and passing-off behaviour are essentially unaltered for finite conductivity, except for a reduction in the former due to the losses involved in the metal. One therefore attributes the behaviour, as before, to the nearby presence of a pole.

3.5 CONCLUSION

In Chapter 2, a modal expansion technique has been described which rigorously accounts for the scalar-wave diffraction of plane waves by a perfectly-conducting grating with rectangular grooves. The theory for both the reflection and transmission versions of the grating has been given. The use of symmetry properties and the Reciprocity Theorem have validated the formalisms, which were subsequently implemented to evaluate the spectral properties of the two types of grating. Emphasis throughout this evaluation was given to the -1 Littrow mounting for the reflection grating and a normal incidence mounting for the transmission grating.

In the final section of Chapter 2, it was demonstrated that it is often quite acceptable to replace the full model expansion with one which consists of only one or two terms. For longer wavelengths the first mode is usually sufficient to adequately represent the P-polarization field, while for S polarization two modes are normally required. The validity of the approximations was shown to depend heavily on the aperture width,
a parameter which governs the real or evanescent nature of the modes. As the width is increased, more of the modes become real for a particular wavelength and these should be included in the expansion. For the reflection grating, the monomodal model for P polarization and the bimodal model for S polarization were shown to furnish quite acceptable results for the -1 Littrow mounting for groove widths up to 0.6d and 0.7d respectively. This latter figure corresponds roughly to the emergence of the third mode threshold into the wavelength region where two orders are propagating. The groove depth was observed to have only a minor effect on the accuracy of the models. An increase in depth provided slight improvement.

A useful application of the limited-mode models lies in their ability to assist in an analysis of the modal theory and hence help explain many observed diffraction phenomena. This has been the subject of interest in Chapter 3.

Intensive investigation has been directed towards a study of resonance anomalies in the lamellar grating and an explanation for their existence has been deduced which is unlike most of the earlier explanations, such as those which relate to surface plasmons. The anomalies have been attributed to resonance poles in the modes which characterize the groove field. Coupled with results of Chapter 5, this origin of the anomalies appears to be valid for gratings in general, i.e. those of both infinite and finite conductivity and of arbitrary profile shape.

The trajectories of the resonance poles have been traced in the complex wavelength plane as a function of the groove parameters. Owing to the ambiguity in the complex values of the direction cosines $\chi_p$, the complex wavelength plane has branch cuts which divides it into a multi-sheeted surface. The majority of the poles described in the text, lie in the physical sheet or in the second sheet of this Riemann surface.
Studies in addition to those presented here have been carried out on trajectories which exist on higher-order sheets, but it is thought that the most important results have been detailed here.

The limited-mode approximations were applied to the problem of blazing for the reflection grating, and simple formulae were established which are able to accurately furnish the blaze wavelengths for the -1 Littrow mounting. The formulae for S polarization have provided an explanation of blazing in the -1 order just before it passes off when either the normalised aperture width is large or the normalised depth is very small.

Consistent with the above predictions for S polarization, models have been developed which describe (for both polarizations) the manner in which the -1 order efficiency falls to zero as this order passes off. The difference between this behaviour for the two polarizations is attributed to the presence of an S-resonance pole at wavelengths beyond physical ones for the -1 Littrow mounting.

The major significance of the ideas developed within this chapter, is that they lead to a qualitative explanation of the behaviour of not only the rectangular-groove grating, but of gratings in general. Throughout the work presented here, examples have been given wherever possible which illustrate the wider applicability of the various concepts to other types of gratings. For example, resonance poles were detected for the sinusoidal profile. These poles can be used to explain the observation that not only shallow lamellar and ruled gratings have a blaze peak near grazing incidence for the Littrow mounting, but that the sinusoidal grating does also. This latter observation cannot be predicted from simple geometric rules.
REFERENCES


