

## Variational Method for the Calculation of the Distribution of Energy Reflected from a Periodic Surface. I.\*

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(Received November 28, 1955)

A variational method is presented which is used to calculate the energy appearing in the various diffracted orders set up when a plane wave is incident upon a periodic reflecting surface. Either the first or the second boundary condition can be so treated. A sample problem is worked showing that if the average absolute slope of the reflecting surface is small (segments of surface with large slope may be included) and if the displacement of the surface is not large compared with the wavelength of the incident radiation, the formulation gives results correct to within a few percent. The calculation shows the existence of Wood anomalies; these are discussed in the paper.

### I. INTRODUCTION

THE problem of the reflection of radiation from nonplane surfaces has in the past received the attention of many people employing various approximations in its treatment.<sup>1-5</sup> It is the purpose of this paper to present a variational method for the treatment of such problems, in particular those in which the surface involved has a displacement which is of the order of magnitude of the radiation wavelength and in which the surface may have portions of moderately large slope, though the average absolute slope should be small. This class of problems is one which is not amenable to treatment by the methods at present available.

The method may be described as follows. Following Trefftz,<sup>6</sup> a linear combination of known solutions to the wave equation is chosen to represent the reflected field. The coefficients will be chosen here so that they minimize the square of the error in the boundary condition. (Trefftz chose them so as to minimize the Rayleigh quotient.) This process of minimization is equivalent to orthogonalizing the set of functions formed by evaluating the trial functions on the boundary. Once this set is orthogonalized one can easily construct the estimates of the reflection coefficients for the surface involved.

The class of problems to be considered will now be described. It is desired to find a solution  $\phi$  of the two-dimensional, time-independent wave equation,

$$\left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \right] \phi(x, z) = 0 \quad (1)$$

\* This work was supported in part by the Office of Naval Research. The method described here was presented in a paper before the thirty-eighth Annual Meeting of the Optical Society of America, held October 15, 16, and 17, 1953 in Rochester, New York.

<sup>1</sup> B. B. Baker and E. T. Copson, *The Mathematical Theory of Huygens' Principle* (Oxford University Press, New York, 1950), second edition, Chap. II.

<sup>2</sup> Lord Rayleigh, Proc. Roy. Soc. (London) **A79**, 399 (1907).

<sup>3</sup> V. Twersky, J. Acoust. Soc. Am. **22**, 539 (1950).

<sup>4</sup> C. Eckart, J. Acoust. Soc. Am. **25**, 566 (1953).

<sup>5</sup> L. M. Brekhovskikh, Zhur. Exspi. Teort. Fiz. **23**, 275 (1952). Translated by G. N. Goss, U. S. Navy Electronics Laboratory, San Diego, California.

<sup>6</sup> E. Trefftz, Math. Ann. **100**, 503 (1928).

in a half-space bounded by a periodic surface  $\zeta(x)$  (see Fig. 1). Here  $\zeta$  is assumed to depend only on  $x$ . In Eq. (1)  $k = \omega/c$  when  $\omega$  is the angular frequency of the radiation source and  $c$  is the phase velocity in the homogeneous medium bounded by  $\zeta(x)$ . The solution of the time-dependent wave equation is then given by  $\phi e^{-i\omega t}$ .

Using the method described herein, one may treat either the first or the second boundary value problem.<sup>7</sup> Thus one may require either

$$\phi(x, \zeta(x)) = 0 \quad (2)$$

or,

$$\left. \frac{\partial \phi(x, z)}{\partial n} \right|_{z=\zeta(x)} = 0. \quad (3)$$

Here  $\partial/\partial n$  represents the derivative normal to the surface. It is supposed that the incident radiation consists of a plane wave making an angle  $\theta_i$  with the  $+z$ -direction; then one can write the total field as the sum of two components,

$$\phi = \phi_i + \phi_r \quad (4)$$

where,

$$\phi_i = \exp(ik[x \sin \theta_i + z \cos \theta_i]) \quad (5)$$

with  $\exp(x) = e^x$ .

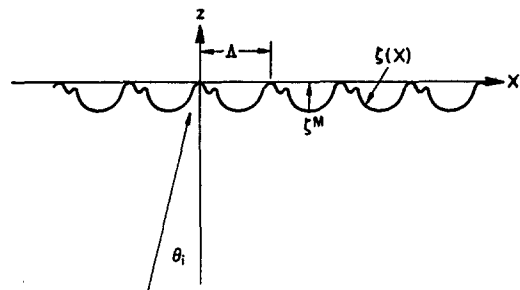


FIG. 1. Sketch showing the definition of the symbols used in the solution of the reflection problem.

<sup>7</sup> One could use the same method to treat problems where the boundary condition is of the form  $[A\phi + B(\partial\phi/\partial n)]_{z=\zeta(x)} = 0$  where  $A$  and  $B$  may be functions of  $x$  or, in fact, the more general problem where one is given two different media separated by a periodic surface and is asked to find the reflected and the transmitted fields.

The boundary conditions given by Eqs. (2) and (3) are frequently encountered in the treatment of problems involving acoustic and electromagnetic radiation. For acoustic problems, the function  $\phi$  may be taken to represent the (time-independent) velocity potential, with  $\phi$  defined by

$$\mathbf{v} = -\nabla\phi \tag{6}$$

where  $\mathbf{v}$  is the particle velocity at an arbitrary field point  $(x, z)$ . Then the first boundary value problem, represented by Eq. (2), corresponds to a physical problem in which  $\zeta(x)$  is a pressure release surface. Furthermore, from Eq. (6) it is evident that the second boundary value problem corresponds to the physical problem in which  $\zeta(x)$  is a rigid surface. For problems involving electromagnetic radiation on the other hand,  $\zeta(x)$  is assumed to be a perfectly conducting surface. Then for an incident plane wave which has its propagation vector lying in the  $x$ - $z$ -plane and which is polarized so that the electric vector is perpendicular to the  $x$ - $z$ -plane, one chooses the boundary condition given by Eq. (2) where it is supposed that the electric field, which has but a single Cartesian component, is given by the function  $\phi$ . Finally, for incident radiation polarized so that the electric field lies in the  $x$ - $z$ -plane one lets  $\phi$  represent the (single Cartesian component) magnetic field and chooses the boundary condition given by Eq. (3).

II. REPRESENTATION OF THE REFLECTED FIELD

In order to make progress toward a solution of the foregoing class of problems, Rayleigh<sup>8</sup> and others<sup>9,10</sup> have chosen to represent the reflected field by an infinite set of plane-wave solutions of the wave equation. In addition to homogeneous, one must choose inhomogeneous waves. The waves must be chosen in such a way that they are either outgoing or exponentially damped as  $z \rightarrow -\infty$ . Furthermore the fact that the boundary is periodic implies that one needs only a discrete set of such waves. Thus, one is led to expect that the reflected field  $\phi$  can be represented by the following type of sum:

$$\sum_{\nu=-\infty}^{\infty} A_{\nu} \exp[-ik \sin\theta_{\nu} x - ik \cos\theta_{\nu} z] \tag{7}$$

where

$$\begin{aligned} \sin\theta_{\nu} &= \nu K/k - \sin\theta_i; \\ \cos\theta_{\nu} &= [1 - \sin^2\theta_{\nu}]^{1/2}, \end{aligned} \tag{8}$$

where  $K = 2\pi/\Lambda$  (see Fig. 1), and where the coefficients,  $A_{\nu}$ , are to be determined through the use of the boundary condition. The angles  $\theta_{\nu}$  of the various reflected orders are just those obtained from the ordinary grating equation.

Lippmann<sup>11</sup> has questioned the validity of the representation given by the expression (7) in the region

<sup>8</sup> Lord Rayleigh, *Theory of Sound* (Dover Publications, New York, 1945), second edition, Vol. II, p. 89.

<sup>9</sup> U. Fano, *Phys. Rev.* **51**, 288 (1937).

<sup>10</sup> K. Artmann, *Z. Physik* **119**, 529 (1942).

<sup>11</sup> B. A. Lippmann, *J. Opt. Soc. Am.* **43**, 408 (1953).

$\zeta^M < z < \zeta(z)$ , at the same time confirming its validity in the region  $z < \zeta^M$ . The  $\zeta^M$  is defined as the maximum displacement of the surface (see Fig. 2).

By using the Helmholtz formula<sup>12</sup> to represent the field, and upon utilizing Sommerfeld's contour integral representation for the Hankel function appearing in that formula, one arrives at the following representation for the reflected field:

$$\phi_r(P) = \sum_{\nu=-\infty}^{\infty} A_{\nu} \exp[-ik \sin\theta_{\nu} x_P - ik \cos\theta_{\nu} z_P], \tag{9}$$

when  $z_P - \zeta^M < 0$ , and where

$$\begin{aligned} A_{\nu} &= \frac{K}{\pi k \cos\theta_{\nu}} \int_0^{\Lambda} \left[ -\frac{1}{4i} \frac{ds_1}{dx_1} \frac{\partial\phi(1)}{\partial\nu_1} \right] \\ &\quad \times \exp[i \sin\theta_{\nu} k x_1 + ik \cos\theta_{\nu} \zeta(x_1)] dx_1. \end{aligned} \tag{10}$$

Further

$$\begin{aligned} \phi_r(P) &= \sum_{\nu=-\infty}^{\infty} \{ A_{\nu}^{-}(z_P) \exp[-ik \sin\theta_{\nu} x_P - ik \cos\theta_{\nu} z_P] \\ &\quad + A_{\nu}^{+}(z_P) \exp[-ik \sin\theta_{\nu} x_P + ik \cos\theta_{\nu} z_P] \}, \end{aligned} \tag{11}$$

when  $\zeta^M < z_P < \zeta(x)$ , where,

$$\begin{aligned} A_{\nu}^{\pm}(z_P) &= \frac{K}{\pi k \cos\theta_{\nu}} \int_{C^{\pm}} \left[ -\frac{1}{4i} \frac{ds_1}{dx_1} \frac{\partial\phi(1)}{\partial\nu_1} \right] \\ &\quad \times \exp[i \sin\theta_{\nu} k x \mp ik \cos\theta_{\nu} \zeta(x_1)] dx_1 \end{aligned} \tag{12}$$

and with  $C^{\pm}(z_P)$  defined in Fig. 3. The symbol  $\partial/\partial\nu_1$  represents the derivative with respect to the outward-drawn normal (see Fig. 2). The  $(x_P, z_P)$  are the rectangular coordinates of  $(P)$ .

The plausibility of the assertions made above concerning the reflected field now becomes evident. From Eq. (9) it is seen that when the point  $(P)$  is removed from the surface, the reflected field is composed of plane-wave solutions which either proceed in the negative  $z$ -direction or die out exponentially in that direction. Furthermore, when  $\zeta^M < z_P < \zeta(x_P)$  one sees from Eq. (11) that the field may be represented in a form

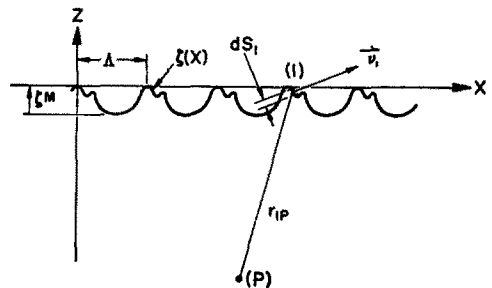


FIG. 2. The figure shows the symbols used in the Helmholtz formula and subsequent development.

<sup>12</sup> Baker and Copson, see reference 1, Chaps. I and II.

which appears to be a combination of waves moving in both the plus and the minus  $z$ -directions with coefficients dependent upon  $z_p$ . Of course in the latter case, individual terms of the series are not solutions of the wave equation.

For certain problems it may turn out that the representation given in Eq. (11) is merely an alternate (and more complicated) form for the representation of the type given by Eq. (9). Indeed this is the case for one special problem which can be solved exactly. The problem is one in which the field satisfies the boundary condition given by Eq. (3). It is supposed that the incident wave falls normally upon one of the faces of the representative groove form (see Fig. 4); in the figure,  $n$  is an integer. The reflected field for this problem obviously consists of a single plane wave moving in a direction opposed to that of the incident wave and with amplitude unity. This solution is valid in the entire region  $z \leq \zeta$ .

To summarize the work in this section, it is evident that for some problems one can represent the reflected field by a sum of plane waves proceeding in the negative  $z$ -direction even in the region  $\zeta^M < z < \zeta(x)$ . However, although to the author's knowledge an exact solution indicating the necessity of using a more complicated representation of the type given by Eq. (11) is lacking, it seems reasonable to suppose that in general the plane-wave representation is not sufficient in the region near the reflecting surface.

III. VARIATIONAL METHOD

It will be convenient to define

$$\phi_r = \phi_{rP} + \phi_{rNP}, \tag{13}$$

where

$$\phi_{rP} = - \sum_{\nu=-\infty}^{\infty} A_{\nu} \exp[-ik \sin\theta_{\nu}x - ik \cos\theta_{\nu}z], \tag{14}$$

valid in the region  $z \leq \zeta(x)$  with  $A_{\nu}$  constant, and  $\phi_{rNP}$  represents that part of the reflected field which cannot be written in that form. For the purposes of the present paper, attention is restricted to those problems for which

$$|\phi_{rNP}| \ll |\phi_{rP}|. \tag{15}$$

Lippmann and Oppenheim<sup>13</sup> have proposed a sufficient

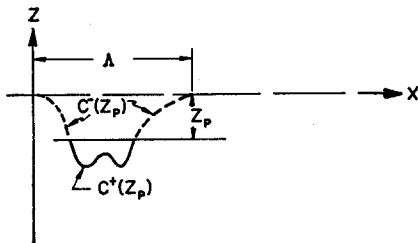


FIG. 3. Diagram defining the contours  $C^{\pm}(z_p)$ .

<sup>13</sup> B. A. Lippmann and A. Oppenheim, Technical Research Group, 56 West 45 Street, New York 36. Final Report on Contract No. AF18(600)-954.

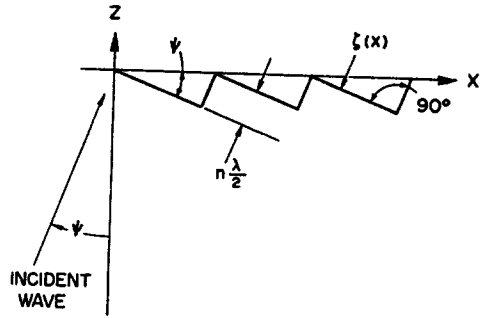


FIG. 4. Figure showing a simple reflection problem which can be solved exactly.

condition for the validity of the relation (15). It is:

$$|\zeta^M|/\lambda \ll 1, \tag{16}$$

when  $\Lambda$  and  $\lambda$  are of the same order of magnitude. The results given in Sec. IV make it evident that this condition is too restrictive for the present work, probably because of the minimal formulation of the problem.

It is possible, through a detailed consideration of the images contained in the region  $\zeta(x) < z \leq 0$ , to estimate the function  $\phi_{rNP}$  using a method essentially the same as that outlined below. Problems for which such a treatment is necessary will be considered in a later paper. In order to simplify notation it will be assumed hereafter that  $\phi_{rNP} = 0$ . Furthermore, only the first boundary value problem [the boundary condition is given in Eq. (2)] will be considered in detail. It is not difficult to alter the formulation for the second boundary value problem.

To proceed, upon using Eqs. (2), (4), (5), (13), and (14) one finds the following relation for the determination of the constants  $A_{\nu}$ :

$$\begin{aligned} & \exp(ik[\sin\theta_{\nu}x + \cos\theta_{\nu}\zeta(x)]) \\ & - \sum_{\nu=-\infty}^{\infty} A_{\nu} \exp(-ik[\sin\theta_{\nu}x + \cos\theta_{\nu}\zeta(x)]) = 0 \end{aligned} \tag{17}$$

and upon applying Eq. (8), and dividing by the common factor  $\exp(ik \sin\theta_{\nu}x)$ , this becomes

$$\begin{aligned} & \exp[ik \cos\theta_{\nu}\zeta(x)] \\ & - \sum_{\nu=-\infty}^{\infty} A_{\nu} \exp[-i\nu Kx - ik \cos\theta_{\nu}\zeta(x)] = 0. \end{aligned} \tag{18}$$

To render the treatment of Eq. (18) more systematic let

$$\begin{aligned} F_1(x) &= \exp(0) \\ F_2(x) &= \exp(1) \\ F_3(x) &= \exp(-1) \\ F_4(x) &= \exp(2) \\ &\vdots \\ &\vdots \\ &\vdots \end{aligned}$$

and

$$\begin{aligned} \bar{A}_1 &= A_0 \\ \bar{A}_2 &= A_1 \\ \bar{A}_3 &= A_{-1} \\ &\vdots \\ &\vdots \end{aligned} \tag{19}$$

where, in Eq. (19),

$$\exp(\mathbf{v}) = \exp[-i\nu Kx - ik \cos\theta_\nu \zeta(x)];$$

further let

$$\bar{\phi}_i = \exp[ik \cos\theta_\nu \zeta(x)]. \tag{20}$$

Then Eq. (18) becomes,

$$\bar{\phi}_i(x) - \sum_{k=1}^{\infty} \bar{A}_k F_k(x) = 0. \tag{21}$$

If the series in Eq. (21) is broken off after the  $N$ th term, as must be done in many problems, the left side of that equation is not in general equal to zero. It is proposed that in such a case, the constants  $\bar{A}_k$  be chosen in a way such that the integral over the surface  $\zeta$  of the absolute square of the left side of Eq. (21) is minimized. Since all quantities in that equation are periodic with period  $\Lambda$ , it is sufficient to carry the integral from  $x=0$  to  $x=\Lambda$ . It is easily seen from Eq. (17) that this minimization is equivalent to carrying out the corresponding minimization of the error in the boundary condition. It is not difficult to show that if one chooses the coefficients  $\bar{A}_k$  so that they satisfy the set of equations (with  $l=1,2,\dots,N$ )

$$\sum_{k=1}^N \bar{A}_k (F_l, F_k) = (F_l, \bar{\phi}_i) \tag{22}$$

when the inner product of two functions,  $(g, h)$ , is defined by

$$(g, h) = \frac{1}{\Lambda} \int_0^\Lambda g^* h dx, \tag{23}$$

then the foregoing indicated minimization is accomplished.

Rather than approach the inversion of the set of Eqs. (22) directly, it has proved convenient for the purposes of computation to use an equivalent though less direct method. To see this method, let Eq. (21) be considered again. One observes that the problem is equivalent to finding that linear combination of functions  $F_k$  which is equal to the given function  $\bar{\phi}_i$ .<sup>14</sup> Thus functions  $F_k$  are not in general mutually orthogonal. This suggests that one proceed by constructing an orthonormal set of functions from linear combinations of the given set  $F_k$ . There is a well-known method for doing this.<sup>15</sup>

<sup>14</sup> Setting  $\phi_{rNP}$  [of Eq. (13)] equal to zero is equivalent to assuming that this is possible.

<sup>15</sup> For a reference concerning representations in terms of systems of functions see R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1953), Vol. I, Chap. II, Secs. 2 and 3.

Let the desired orthonormal set be  $G_k$ ; then one can write

$$G_k = \sum_{l=1}^k \Gamma_l^{(k)} F_l, \tag{24}$$

with

$$(G_m, G_n) = \delta_{mn}$$

when  $\delta_{mn}$  is equal to one or zero depending on whether or not  $m=n$  and where the coefficients  $\Gamma_l^{(k)}$  are determined as follows. Let  $G_1$  be equal to  $F_1$  divided by its norm. The norm of  $F_1$  is defined as  $(F_1, F_1)^{1/2}$ . One then takes that linear combination of  $F_1$  and  $F_2$  which is orthogonal to  $G_1$ , divides it by its norm and sets it equal to  $G_2$ . Upon proceeding in this way the following recursion relations for the coefficients in Eq. (24) are easily obtained:

$$\Gamma_l^{(k)} = \frac{\gamma_l^{(k)}}{N_k^{1/2}} \tag{25}$$

where

$$l < k, \quad \gamma_l^{(k)} = - \sum_{\beta=l}^{k-1} \sum_{\alpha=1}^{\beta} \Gamma_\alpha^{(\beta)*} (F_\alpha, F_k) \Gamma_l^{(\beta)}, \tag{26}$$

$$l = k, \quad \gamma_l^{(k)} = 1$$

and where

$$N_k = \sum_{\mu=1}^k \sum_{\nu=1}^k \gamma_\mu^{(k)*} (F_\mu, F_\nu) \gamma_\nu^{(k)}, \tag{27}$$

when the star indicates the complex conjugate.

Now let

$$\bar{\phi}_i^{(N)}(x) = \sum_{k=1}^N B_k G_k(x), \tag{28}$$

where  $\bar{\phi}_i^{(N)}$  represents the  $N$ th approximation to  $\bar{\phi}_i$  and where  $B_k$  are defined by

$$B_k = (G_k, \bar{\phi}_i) \tag{29}$$

or upon using Eq. (24),

$$B_k = \sum_{\alpha=1}^k \Gamma_\alpha^{(k)*} (F_\alpha, \bar{\phi}_i). \tag{30}$$

Then by using Eq. (24) in connection with Eq. (28) one can write,

$$\bar{\phi}_i^{(N)}(x) = \sum_{k=1}^N \bar{A}_k' F_k \tag{31}$$

when

$$\bar{A}_k' = \sum_{\alpha=k}^N B_\alpha \Gamma_k^{(\alpha)}. \tag{32}$$

That

$$\bar{A}_k' = \bar{A}_k \tag{33}$$

where  $\bar{A}_k$  are defined implicitly in Eq. (22) can be seen by observing that the  $B_k$  as defined in Eq. (29) are the Fourier coefficients of the function  $\bar{\phi}_i$  with the set

$G_k$ . It follows then that the quantity

$$\frac{1}{\Lambda} \int_0^\Lambda |\bar{\phi}_i - \bar{\phi}_i^{(N)}|^2 dx \quad (34)$$

is minimized and therefore that the coefficients  $\bar{A}_k'$ , as obtained from the coefficients  $B_k$  in Eq. (32), must also minimize the expression (34). But Eq. (22) governing the quantities  $\bar{A}_k$  was obtained by minimizing the quantity Eq. (34). Hence Eq. (33) must follow. Indeed one can verify Eq. (33) directly by substituting Eq. (32) in Eq. (22).

One of the advantages of the foregoing procedure toward the solution of Eq. (22) is that one obtains an estimate of the error incurred by breaking off the infinite system of equations at  $N$ , this error being combined with the error involved in the assumption that  $\phi_{rNP} = 0$ . The estimate is obtained in a way similar to that by which one ordinarily obtains Bessel's inequality.<sup>16</sup> One finds that

$$\frac{1}{\Lambda} \int_0^\Lambda |\bar{\phi}_i - \bar{\phi}_i^{(N)}|^2 dx = (\bar{\phi}_i, \bar{\phi}_i) - \sum_{k=1}^N |B_k|^2, \quad (35)$$

or by observing the definition of  $\bar{\phi}_i$  given by Eq. (20),

$$\text{M.S.E.} = 1 - \sum_{k=1}^N |B_k|^2, \quad (36)$$

where M.S.E. stands for the mean square error in the boundary condition [the expression (34)]. The error arises both as a result of considering only a finite number of diffracted waves and as a result of neglecting  $\phi_{rNP}$ .

There is a relation which follows from the conservation of energy which can also be used as a check on the accuracy of the calculation. By considering the energy balance within the region of the  $x$ - $z$ -plane bounded by  $\zeta(x)$ ,  $x=0$ ,  $x=\Lambda$ , and  $z=-C$ , where  $C$  is large and positive, one obtains the following relation for the exact solution:

$$\cos\theta_i = \sum_{\nu} \cos\theta_{\nu} |A_{\nu}|^2 \quad (37)$$

where the summation is carried over those values of  $\nu$  for which  $\cos\theta_{\nu}$  is real and where the notation of Eq. (14) is used again, remembering the changes made by Eqs. (19).

A third relation which can be used to check the accuracy of the calculation arises from the reciprocity theorem.<sup>16</sup> To obtain this expression one treats first the problem of the reflection of radiation from a periodic surface which is finite in extent in the  $x$ -direction, using the Helmholtz formula. This problem is then compared with the corresponding problem involving an infinite periodic surface. By allowing the finite surface to extend to greater and greater distances in the  $x$ -direc-

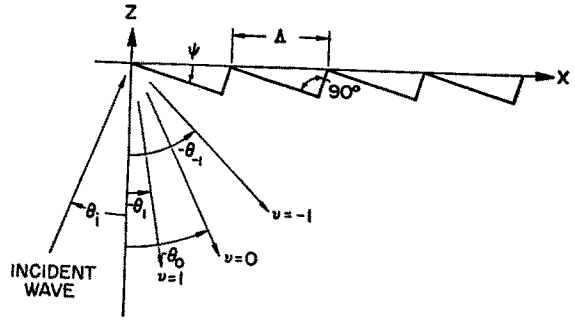


FIG. 5. Figure showing the type of surface for which computations have been made.

tion, one finds the following relation governing the plane-wave reflection coefficients,

$$\cos\theta_{\nu} A_{\nu}(\theta_i) = \cos\theta_i A_{\nu}(\theta_{\nu}), \quad (38)$$

where  $A_{\nu}(\theta_i)$  represents, as before, the reflection coefficient of the  $\nu$ th order wave but with the incident direction explicitly indicated. From Eq. (38) it is seen that the zeroth order (specular component) should be symmetrical about  $\theta_i=0$ , regardless of whether or not the surface is symmetrical.

To sum up the results of this section, one uses Eq. (32) to obtain estimates of the reflection coefficients of the various diffracted waves. The quantities  $B_k$  are defined in Eq. (30). The quantities  $\Gamma_i^{(k)}$  which are also needed are defined in Eqs. (25), (26), and (27). Finally, it is a simple matter to alter Eqs. (30), (25), (26), and (27) for the second boundary value problem.

#### IV. RESULTS OF CALCULATIONS AND CONCLUSIONS

Calculations based upon the method presented in the foregoing have been carried out for surfaces of the class shown in Fig. 5, and for the first boundary value problem. Hence, since the field function vanishes at the surface in such a case, the solutions are appropriate for acoustic problems involving free surfaces or for electromagnetic problems involving incident energy polarized with electric vector perpendicular to the page in Fig. 5.

In the figure three representative reflected wave directions are shown, although they have not been chosen to fit any particular case.

The surface was chosen for calculation for two reasons. First, it is of some physical interest. The sea surface assumes a shape reminiscent of that shown in the figure under conditions of high wind, so that the treatment of the problem may be helpful in attaining an understanding of the distribution of acoustic or electromagnetic energy reflected from such a surface. Furthermore, the surface is of the type known as an echelette grating which is used in optical and infrared spectral work. The second reason for choosing the indicated type of surface for the calculations is that the calculations are somewhat simplified.

<sup>16</sup> See reference 8, Vol. 2, Sec. 294.

The integrals shown in Eq. (23) can be evaluated in terms of exponentials when the surface is composed of straight line elements.

The entire problem, starting with the calculation of the inner products  $(F_k, F_m)$  and  $(F_k, \phi_i)$  through the calculation of the quantities  $\Gamma_l^{(k)}$  and including the calculation of the estimates of the reflection coefficients  $\bar{A}_k$  (or  $A_r$ ) has been programmed for MIDAC, the University of Michigan digital computer. The cyclical form of the central part of the calculation, the central part being the computation of the quantities  $\Gamma_l^{(k)}$  given by Eqs. (25), (26), and (27), renders the formulation easily adaptable to a digital machine. The capacity of the machine limited the calculation to ten diffracted waves ( $N=10$ ).

For the calculation presented in Fig. 6 a surface of the type shown in Fig. 5 was chosen with  $\psi=10^\circ$  and with  $\Lambda=1.155\lambda$ . This ratio of  $\Lambda$  to  $\lambda$  implies that for a given incident angle, at most three diffracted orders appear. The plus second diffracted order never exceeds 0.38% and is too small to show on the graph. It is noted from Fig. 6(a) that the energy deficit of the calculation [as computed from the right side of Eq. (37)] averages about 2.5% and never exceeds 5%; furthermore, the M.S.E. is less than 0.025. From these two checks, it seems reasonable to expect that the error for a given order is less than 5% (of its value). It is seen that the calculation is more accurate for incident angles nearer grazing.

As suggested in Sec. III, the reciprocity relation can also be used to check the accuracy of the calculation.

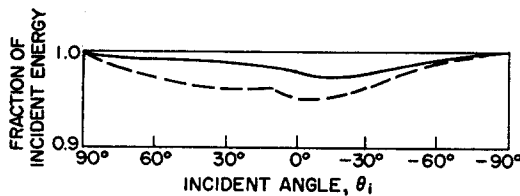


FIG. 6(a). The solid curve shows 1-M.S.E. (where M.S.E. is the mean square error in the boundary condition). The dashed curve shows the ratio of the total calculated, reflected energy to the incident energy.

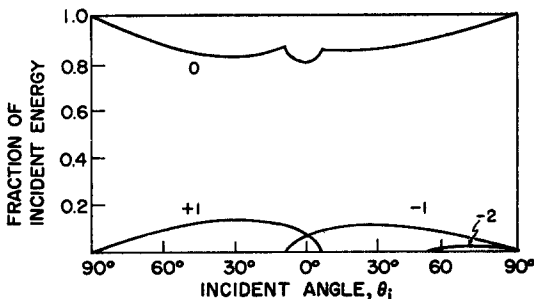


FIG. 6(b). The curves show the fraction of the total incident energy which is contained within a given diffracted order when a plane wave is incident upon the periodic surface with an angle, measured from the normal as indicated by the abscissas. The reflecting surface is described by  $\psi=10^\circ$  and  $\Lambda=1.155\lambda$ .

It was deduced from Eq. (38) that the reflection coefficient for the zeroth order should be symmetrical about the normal. It follows then from the energy relation given by Eq. (27) that the percentage of the total incident energy in the zeroth order should also be symmetrical. It is seen from Fig. 6(b) that this order is symmetrical within a few percent, the assigned error. All other reciprocity checks carried out also agree within a few percent. For instance one should have,

$$\cos 60^\circ A_1(0^\circ) = \cos 0^\circ A_1(60^\circ), \quad (39)$$

and

$$\cos 9^\circ 8' A_1(45^\circ) = \cos 45^\circ A_1(9^\circ 8'). \quad (40)$$

Actually, the numbers from the calculation are  $-0.1485 + 0.1449i$  and  $-0.1562 + 0.1525i$  for the left and right sides of Eq. (39), respectively;  $-0.1787 + 0.2312i$  and  $-0.1735 + 0.2242i$  for the left and right sides of Eq. (40), respectively.

From Fig. 6(b) it is seen that the main part of the reflected energy is carried by the zeroth, or specular order. This component never drops below 80%.

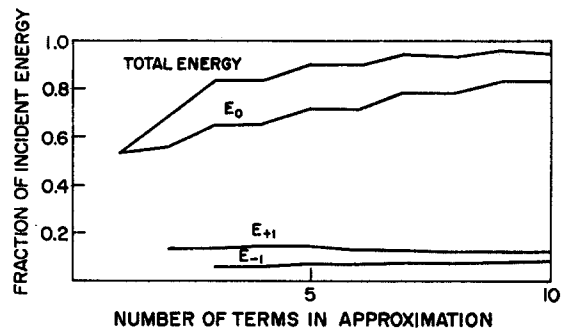


FIG. 7. The graph shows the successive approximations to the energy contained in the various orders appearing when a plane wave is normally incident upon a surface with  $\psi=10^\circ$  and with  $\Lambda=1.23\lambda$ . The total calculated energy is also shown.

Discontinuities of the type shown in the zeroth order at  $\theta \approx \pm 8^\circ$  are known as Wood anomalies<sup>17</sup> and have often observed experimentally for perpendicular-polarized radiation. Rayleigh<sup>18</sup> showed that the positions of the anomalies were connected with those angles at which diffracted orders appear. Both Wood and Rayleigh concluded that the anomalies appeared only for (electromagnetic) radiation incident with electric vector perpendicular to the generating element of the reflecting surface (the second boundary value problem) and that for parallel-polarized radiation no such anomalies occurred. Recent work by Palmer<sup>19</sup> has shown that the anomalies can occur for parallel-polarized radiation as well. Palmer concluded however that in this case the anomalies would not appear for shallow surfaces, where the angle  $\psi$  is small. The present calculation shows that they are to be expected even

<sup>17</sup> R. W. Wood, *Phil. Mag.* 4, 396 (1902).

<sup>18</sup> Lord Rayleigh, *Phil. Mag.* 14, 60 (1907).

<sup>19</sup> C. H. Palmer, Jr., *J. Opt. Soc. Am.* 42, 268 (1952).

TABLE I. A comparison of the results of the Kirchhoff formulation with those obtained using the variational method for normal incidence.

Theory	Zeroth	Plus first	Minus first	Total energy
Kirchhoff	$-0.248 + 0.720i$	$0.1900 - 0.313i$	$-0.1397 + 0.1546i$	67%
Variational	$-0.1875 + 0.879i$	$0.297 - 0.290i$	$-0.0916 + 0.329i$	95%

for such surfaces, although the effect here is not large, about 5%.

It is to be remarked that the problem of calculating the shape of the anomalies has proved difficult in the past. It is seen in Fig. 6 that the anomaly shows a sharp edge on the side where a new order first appears, as is often observed experimentally.<sup>19</sup> Existence of this edge is connected with the fact that the energy contained within an order falls off rapidly as the angle of the order approaches  $90^\circ$  (as the order disappears). In fact it can be shown through the use of a perturbation treatment such as Rayleigh's,<sup>2</sup> the treatment being useful for near grazing incidence, in conjunction with an application of the reciprocity theorem<sup>16</sup> that it is to be expected that the slope of the curve is infinite at this point. Indeed it is just this discontinuity, and its attendant effect upon the other orders through the conservation of energy requirement, that gives rise to the Wood anomalies.

It is of interest to compare the results of the present calculation with those obtained for the same problem using other methods. One might first consider Rayleigh's perturbation treatment. However it turns out that the method, at least in first order, is not applicable, since one requirement for its validity is that  $k\xi^M \ll 1$  whereas here  $k\xi^M \sim 1$ . Secondly, one might consider using Kirchhoff's approximation.<sup>1</sup> The results obtained using this approximation are essentially the same as those obtained from Eckart's<sup>4</sup> and Brekhovskikh's<sup>5</sup> formulations. Kirchhoff's method gives results which are considerably in error. For example the complex reflection coefficient using Kirchhoff's approximation is

compared with the corresponding results using the present formulation in Table I. The surface chosen is the same as that used in Fig. 6.

Finally, the question of the rate of convergence of the calculation is taken up. In Fig. 7 are shown the successive approximations to the values of the reflection coefficients, as each new diffracted wave is introduced in the calculation. It seems to be reasonable to deduce from the results shown that including more terms (more diffracted inhomogeneous plane waves) in the calculation is not likely to significantly improve the result. One then concludes that the residual error arises from the incomplete form of the representation of the reflected field, as explained in Sec. II. Hence, further improvement can be expected only through the introduction of images in the region  $\xi < z \leq 0$ . However, it seems that for surfaces whose average absolute slope is small (sections of surface of large slope may be included) and whose maximum displacement is not too many wavelengths, the formulation as presented is accurate to a few percent.

#### V. ACKNOWLEDGMENTS

The author wishes to take this opportunity to thank Mr. Gordon Grant for performing some of the early hand calculations. He also wishes to acknowledge the patient help of Mr. J. H. Brown who offered many helpful suggestions and criticisms concerning the programming of the problem for MIDAC. Finally, it is a pleasure to thank Professor C. W. Peters for many helpful discussions, in particular with regard to pertinent experimental results.