The Rayleigh hypothesis in the theory of reflection by a grating

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In this paper, the Rayleigh hypothesis in the theory of reflection by a grating is investigated analytically. Conditions are derived under which the Rayleigh hypothesis is rigorously valid. A procedure is presented that enables the validity of the Rayleigh hypothesis to be checked for a grating whose profile can be described by an analytic function. As examples, we consider some grating profiles described by a finite Fourier series. Numerical results are then presented.

I. INTRODUCTION

The Rayleigh hypothesis has been employed by a number of authors to solve the problem of the reflection of a plane wave by a grating.[1] Under this hypothesis, the discrete set of reflected, propagating, and evanescent, spectral waves (together with the incident field) is assumed to yield a description of the total field that is sufficient to satisfy the boundary condition to be imposed on the surface of the grating. It has been argued by Lippmann,[2] that the Rayleigh

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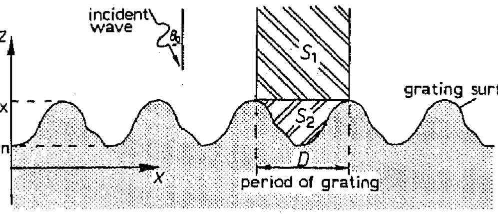

FIG. 1. Grating configuration and incident wave. S_1 denotes a single period of the domain $z_{max} < z < \infty$; S_2 denotes a single period of the domain $z_{min} < z < z_{max}$ (valley of the groove).

assumption seems unrealistic, for in between the corrugations, both incoming and outgoing secondary waves (as well as the corresponding exponentially growing and evanescent waves) are expected to exist.

Following Petit and Cadilhac,[3] Millar[4] investigated the conditions under which the Rayleigh hypothesis can be used for a sinusoidal grating. His basic problem involves the location of the singularities in the representation of the solution of the wave problem and he relates these to the singularities and the critical points in the Green's function of the corresponding potential problem. Further progress as regards the location of the singularities in the solution of the wave problem has been made in later papers by Nevière and Cadilhac[5] and Millar.[6]

In the present paper, we show in a fairly simple way, under which conditions the Rayleigh hypothesis holds. The method applies to an arbitrary grating profile, provided that it can be described by an analytic function of the arc length. As examples, we consider some grating profiles described by a finite Fourier series, hence for a limited sum of sinusoids.[7] Numerical results are then presented.

II. FORMULATION OF THE GRATING PROBLEM

Let the time-harmonic plane wave (with wave number k_0), $u^i(x,z) = \exp(i\alpha_0 x - i\gamma_0 z)$ with $\alpha_0 = k_0 \sin\theta_0$ and $\gamma_0 = k_0 \cos\theta_0$, be incident from $z > 0$ upon the periodic surface Λ shown in Fig. 1. The time-dependence factor $\exp(-i\omega t)$ is suppressed. The reflected field in $z > z_{\max}$ may be written as[8]

$$u^r(x,z) = \sum_{n=-\infty}^{\infty} \rho_n \exp(i\alpha_n x + i\gamma_n z), \quad z > z_{\max}, \tag{1}$$

in which $\alpha_n = \alpha_0 + 2\pi n/D$, $\gamma_n = (k_0^2 - \alpha_n^2)^{1/2}$ with $\mathrm{Re}(\gamma_n) \geq 0$ and $\mathrm{Im}(\gamma_n) \geq 0$. We suppose that the total field $u = u^i + u^r$ vanishes on Λ (the Dirichlet boundary condition), though this is inessential for our procedure and both the Neumann boundary condition and the impedance boundary condition could be imposed as well.

In the earliest attempts to analyze this problem rigorously, Rayleigh made the assumption that the series in Eq. (1) was a valid representation for u^r not only in $z > z_{\max}$ (S_1), but also in the valley of the groove (S_2). Let us write the Rayleigh solution of the boundary-value problem ($u^r = -u^i$ on Λ) as

$$u_R^r(x,z) = \sum_{n=-\infty}^{\infty} R_n \exp\{i\alpha_n x + i\gamma_n z\}, \quad (x,z) \in (S_1 + S_2). \tag{2}$$

Millar[4] has shown that a necessary and sufficient condition for the Rayleigh assumption to hold is that the series in Eq. (2) is an analytic function[9] of x and z for $(x,z) \in (S_1 + S_2)$. The proof is rather simple. Since (i) the series in Eq. (2) is an analytic solution of the Helmholtz equation $(\partial_x^2 + \partial_z^2 + k_0^2)u_R^r = 0$ in $S_1 + S_2$, (ii) u_R^r satisfies the radiation condition as $z \to \infty$, (iii) u_R^r satisfies the boundary condition on Λ, where Λ is an analytic surface (without edges), we are then dealing with a unique solution of the boundary-value problem. Because of this uniqueness, the coefficients R_n in Eq. (2) are equal to the coefficients ρ_n in Eq. (1) for all n. Hence, under the assumption of the analyticity, Eq. (2) is the exact solution.[10]

We directly observe that the series in Eq. (2) is analytic in $S_1 + S_2$, if the series is uniformly convergent as $z = z_{\min}$, or

$$\begin{aligned} &\lim_{n\to\infty} \inf |R_n|^{-1/n} \exp(2\pi z_{\min}/D) > 1, \\ &\lim_{n\to-\infty} \inf |R_n|^{1/n} \exp(2\pi z_{\min}/D) > 1, \end{aligned} \tag{3}$$

where we have used the relations $\lim_{n\to\infty}\gamma_n = i\alpha_0 + i2\pi n/D$ and $\lim_{n\to-\infty}\gamma_n = -i\alpha_0 - i2\pi n/D$. In order to investigate the analyticity of Eq. (2), we need the behavior of $|R_n|$ for $|n| \to \infty$. This behavior of the reflection factors will be discussed in Sec. III.

III. BEHAVIOR OF THE REFLECTION FACTORS

If, now, the Rayleigh hypothesis were to hold exactly for some type of grating profile, at least the Rayleigh method ($u_R^r = -u^i$ on Λ) should lead to an analytic single-valued reflected wave function upon approaching the grating surface. We represent the latter by $x = f(s)$ and $z = g(s)$, where $f(s)$ and $g(s)$ are assumed to be analytic functions of the (real valued) arc length s ($0 \leq s \leq L$). Let us define $u^i(x,z)$ on Λ as $u^i(s)$, then, the Rayleigh hypothesis yields

$$-u^i(s) = \sum_{n=-\infty}^{\infty} R_n u_n(s), \ \mathrm{Im}(s) = 0, \tag{4}$$

in which $u_n(s) = \exp[i\alpha_n f(s) + i\gamma_n g(s)]$.

Now, the dominant behavior of $|u_n(s)|$ as $|n| \to \infty$ is given by

$$\begin{aligned} &\lim_{n\to\infty} |u_n|^{1/n} = |w_1|, \\ &\lim_{n\to-\infty} |u_n|^{-1/n} = |w_2|^{-1}, \end{aligned} \tag{5}$$

where $w_1 = \exp\{2\pi[if(s) - g(s)]/D\}$, and $w_2 = \exp\{2\pi[if(s) + g(s)]/D\}$.

Let the maximum value of $|w_1(s)|$, $\mathrm{Im}(s) = 0$, be denoted by $|w_{1,\max}|$ and let the minimum value of $|w_2(s)|$, $\mathrm{Im}(s) = 0$, be denoted by $|w_{2,\min}|$. The series in Eq. (4) has to be a uniformly convergent series for real s. This property restricts the behavior of $|R_n|$ as $|n| \to \infty$ to

$$\begin{aligned} &\lim_{n\to\infty} \sup |R_n|^{1/n} |w_{1,\max}| < 1, \\ &\lim_{n\to-\infty} \sup |R_n|^{-1/n} |w_{2,\min}|^{-1} < 1, \end{aligned} \tag{6}$$

in which $|w_{1,\max}| = |w_{2,\min}|^{-1}$.

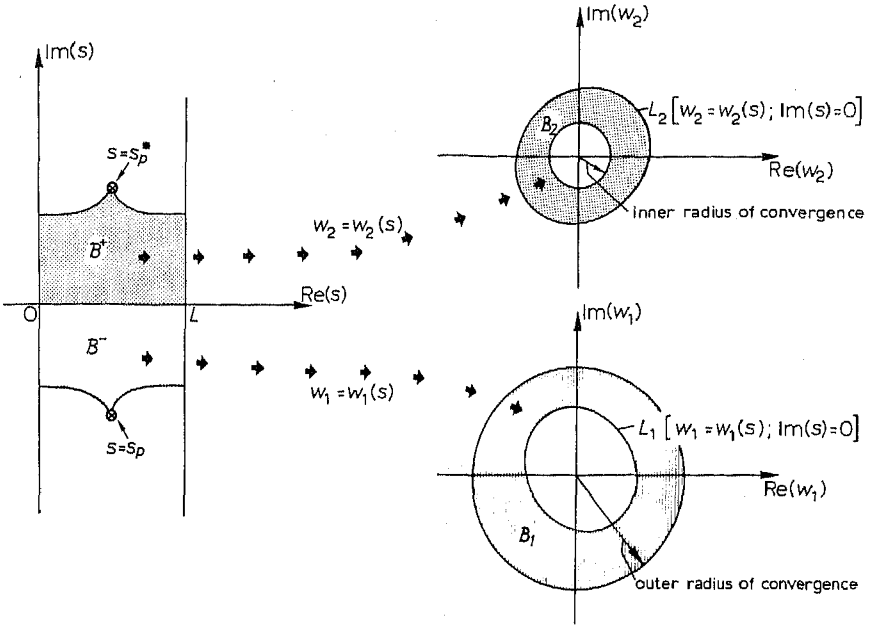

FIG. 2. Conformal transformations. s_p is either a zero of dw_1/ds or a singularity of either $f(s)$ or $g(s)$, or both.

More insight into the behavior of $|R_n|$ as $|n| \to \infty$ is obtained as follows. Let $f(s)$ and $g(s)$ be analytic functions of the complex variable s in a domain A of the complex s plane, containing the real axis. Then, Eq. (4) can be written as

$$-u^i(s) = \sum_{n=-\infty}^{\infty} R_n u_n(s), \quad s \in B, \tag{7}$$

in which B denotes the subdomain of A where the series in the right-hand side of Eq. (7) converges uniformly.[11] Since $\lim_{n\to\infty}|u_n|^{1/n} = |w_1|$ and $\lim_{n\to-\infty}|u_n|^{1/n} = |w_2|$ for all $s \in A$, B is also the domain where both series

$$v_1(s) = \sum_{n=0}^{\infty} R_n w_1^n$$

and (8)

$$v_2(s) = \sum_{n=-\infty}^{0} R_n w_2^n$$

converge uniformly. In order to obtain the behavior of $|R_n|$ as $|n| \to \infty$, we need the location of the boundary of B in the complex s plane. Let the real s axis divide the domain B into B^+ and B^- (see Fig. 2). Since $f(s)$ and $g(s)$ are real on the real s axis, $f(s)$ and $g(s)$ take conjugate values at conjugate points (principle of reflection; cf. Titchmarsh,[12] p. 155). It is easily verified that

$$w_2^*(s) = [w_1(s^*)]^{-1}, \quad s \in A, \tag{9}$$

in which the asterisk denotes the complex-conjugate value. From Eq. (9), it follows that if the convergence properties of the first series of Eq. (8) determine the lower boundary of B^-, the convergence properties of the second series determine the upper boundary of B^+. An easy procedure to investigate the domain of convergence of the two series of Eq. (8) is to carry out the analysis in the complex w_1 plane and the w_2 plane.

To this end, we employ a conformal mapping of the domain A in the s plane into the complex w_1 plane. Let the image of the arc $[0 \leq \mathrm{Re}(s) \leq L, \mathrm{Im}(s) = 0]$ be denoted by L_1 (see Fig. 2). Let further B^- in the s plane be mapped into the domain B_1 in the complex w_1 plane. Then, B_1 is the domain in the w_1 plane bounded by L_1 and the circle of convergence of the power series

$$v_1(w_1) = \sum_{n=0}^{\infty} R_n w_1^n. \tag{10}$$

Note that L_1 is always located completely inside this circle of convergence, because of Eq. (6). Now, this circle of convergence passes through the singularity of $v_1(w_1)$ nearest to the origin. Let $s = s_p$ ($\mathrm{Im}(s) < 0$) correspond to this singularity, then $s = s_p$ is either a zero of dw_1/ds [at this point the function $v_1(w_1)$ has a nonexisting derivative, since $dv_1/dw_1 = (dv_1/ds)/(dw_1/ds)$] or a singularity of either $f(s)$ or $g(s)$, or both. The zero's of dw_1/ds follow from

$$(d/ds)[if(s) - g(s)] = 0, \quad \mathrm{Im}(s) < 0. \tag{11}$$

The radius of convergence of the power series in the right-hand side of Eq. (10) is then given by

$$\liminf_{n\to\infty} |R_n|^{-1/n} = |w_1(s_p)| = |\exp\{2\pi[if(s_p) - g(s_p)]/D\}|. \tag{12}$$

Using a conformal mapping of the domain A in the s plane into the complex w_2 plane, a procedure similar to the one used earlier, but now with respect to the second series of Eq. (8), yields

$$\liminf_{n\to-\infty} |R_n|^{1/n} = |w_2(s_p^*)|^{-1} = |\exp\{2\pi[if(s_p) - g(s_p)]/D\}|. \tag{13}$$

Eqs. (12) and (13) specify the behavior of $|R_n|$ as $|n| \to \infty$, provided that the Rayleigh hypothesis is used.

IV. VALIDITY OF THE RAYLEIGH HYPOTHESIS

From Eqs. (3), (12), and (13), we observe that the series (2) is analytic for $z > z_{\min}$ if and only if

$$\mathrm{Re}[if(s_p) - g(s_p) + z_{\min}] > 0. \tag{14}$$

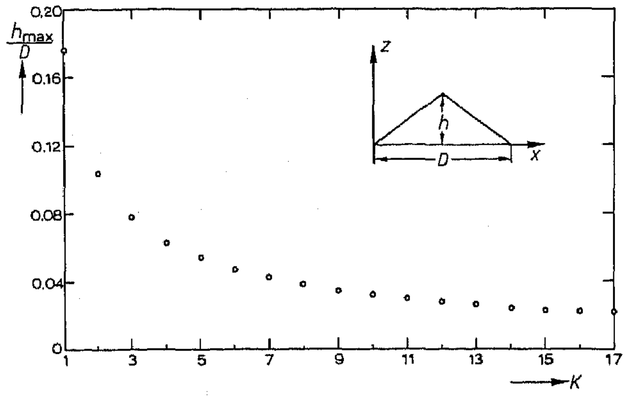

FIG. 3. h_{max} as a function of K when the grating profile is given by

$$z = h/2 - h \sum_{j=1}^{K} [4/\pi^2(2j-1)^2] \cos\{2\pi(2j-1)x/D\}$$

(= approximation to a triangular profile).

Equation (14), now, is the condition under which the Rayleigh hypothesis holds, if it ever does.

Instead of the representation of the grating profile in the arc length s, we now restrict ourselves to single-valued functions of x, say $z = z(x)$.

It is convenient to write

$$z = h\zeta(x);\ z_{\min} = h\zeta_{\min}, \quad h > 0, \tag{15}$$

where h is the depth of the grooves of the grating, i.e. $h = z_{max} - z_{\min}$. Eqs. (11) and (14) are then replaced by

$$i - h d\zeta(x)/dx = 0, \tag{16}$$

$$\mathrm{Re}\{ix_p - h\zeta(x_p) + h\zeta_{\min}\} > 0. \tag{17}$$

Let us assume that $h = h_{max}$ is the *smallest* value of h, where

$$\mathrm{Re}[ix_p - h_{max}\zeta(x_p) + h_{max}\zeta_{\min}] = 0. \tag{18}$$

For this value of $h = h_{max}$, the Rayleigh hypothesis does not hold. We then want to investigate whether the Rayleigh hypothesis still does not hold when $h > h_{max}$. To this end, we consider the expression

$$\frac{d}{dh}\mathrm{Re}[ix_p - h\zeta(x_p) + h\zeta_{\min}] = \begin{cases} \mathrm{Re}[-\zeta(x_p) + \zeta_{\min}], \\ \text{when } x_p \text{ is a singular point of } \zeta(x), \\ \mathrm{Re}\left(i\frac{dx_p}{dh} - h\frac{d\zeta(x_p)}{dx_p}\frac{dx_p}{dh} - \zeta(x_p) + \zeta_{\min}\right), \\ \text{when } x_p \text{ is a root of Eq. (16).} \end{cases}$$

Using Eq. (16), we observe that

$$\frac{d}{dh}\mathrm{Re}[ix_p - h\zeta(x_p) + h\zeta_{\min}] = \mathrm{Re}[-\zeta(x_p) + \zeta_{\min}], \tag{19}$$

where x_p is either a singular point of $\zeta(x_p)$ or a root of Eq. (16). Since $\mathrm{Im}(x_p) < 0$, it follows from Eq. (18) that the right-hand side of Eq. (19) is negative for $h = h_{max}$, and hence

$$\mathrm{Re}[ix_p - h\zeta(x_p) + h\zeta_{\min}] < 0 \quad \text{for } h = h_{max} + \Delta, \tag{20}$$

in which Δ is a sufficiently small positive number. Since $\mathrm{Im}(x_p)$ is always negative, it follows from Eq. (20) that the right-hand side of Eq. (19) is still negative for $h = h_{max} + \Delta$. Repeating this process, we observe that Eq. (20) holds for all $h > h_{max}$. Hence, Eq. (17) does not hold for $h > h_{max}$ and the Rayleigh hypothesis is valid only for $0 < h < h_{max}$, in which h_{max} is the smallest value of h where Eq. (18) applies.

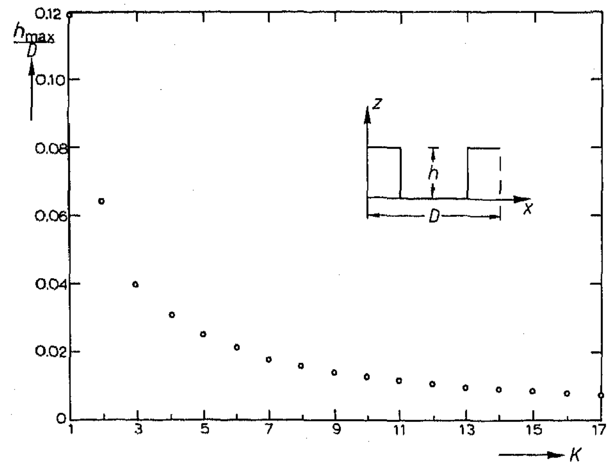

FIG. 4. h_{max} as a function of K when the grating profile is given by

$$z = h/2 - h \sum_{j=1}^{K} [2(-)^j/\pi(2j-1)] \cos\{2\pi(2j-1)x/D\}$$

(= approximation to a rectangular profile).

V. NUMERICAL RESULTS

We shall now present some numerical results pertaining to h_{max} for different grating profiles. These results are obtained by a numerical solution of Eqs. (16) and (18). We note that such a root of Eqs. (16) and (18) has been taken, that leads to the smallest value of h_{max}. This implies a careful investigation of the Eqs. (16) and (18) in the complex x plane ($0 \leqslant \mathrm{Re}(x) < D$, $\mathrm{Im}(x) < 0$). Further, we have investigated that for $0 < h < h_{max}$ Eq. (17) applies; in this way the validity of the Rayleigh hypothesis has been established.

(*i*) *sinusoidal profile:* $z = (h/2)\cos(2\pi x/D)$. We then have

$$\zeta(x) = \tfrac{1}{2}\cos(2\pi x/D)$$

and

$$\zeta_{\min} = -\tfrac{1}{2}.$$

We then arrive at $h_{max}/D = 0.142\,521$. The same result was already obtained by Petit and Cadilhac[3] and Millar.[4]

(*ii*) *approximation to a triangular profile* (see Fig. 3). For the triangular profile, the Rayleigh hypothesis is never valid,[13] since there is a singularity of $z(x)$ on the real x axis and, then, Eq. (17) does not hold. But, the Rayleigh hypothesis can hold when we approximate this profile by a finite Fourier series $z = h\zeta(x)$,[7] in which

$$\zeta(x) = \tfrac{1}{2} - \sum_{j=1}^{K} \frac{4}{\pi^2(2j-1)^2}\cos[2\pi(2j-1)x/D]$$

and

$$\zeta_{\min} = \tfrac{1}{2} - \sum_{j=1}^{K} \frac{4}{\pi^2(2j-1)^2}.$$

The approximation is better the larger K is. The values of h_{max} as a function of K are presented in Fig. 3. For all values of $0 < h < h_{max}$, we have found that the Rayleigh hypothesis is valid. From our computations we observe that as $K \to \infty$, hence for a triangular profile, the Rayleigh hypothesis never holds.

(*iii*) *approximation to a rectangular profile* (see Fig. 4). For the rectangular profile, the Rayleigh hypothesis is also never valid,[13] but the Rayleigh hypothesis can hold when we approximate this profile by a finite Fourier series $x = h\zeta(x)$, where

$$\zeta(x) = \tfrac{1}{2} - \sum_{j=1}^{K} \frac{2(-)^j}{\pi(2j-1)} \cos[2\pi(2j-1)x/D]$$

and

$$\zeta_{\min} = \tfrac{1}{2} + \sum_{j=1}^{K} \frac{2(-)^j}{\pi(2j-1)}.$$

The approximation is better the larger K is. The values of h_{max} as a function of K are presented in Fig. 4. For all values of $0 < h < h_{max}$, we have found that the Rayleigh hypothesis is valid. From our computations we also observe that as $K \to \infty$, hence for a rectangular profile, the Rayleigh hypothesis never holds.

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[1]Lord Rayleigh (J. W. Strutt), Proc. Roy. Soc. Lond. A, **79**, 399–416 (1907).

[2]B. A. Lippmann, J. Opt. Soc. Am., **43**, 408 (1953).

[3]R. Petit and M. Cadilhac, C. R. Acad. Sci. B, **262**, 468–471 (1966).

[4]R. F. Millar, Proc. Camb. Philos. Soc., **65**, 773–791 (1969).

[5]M. Nevière and M. Cadilhac, Opt. Commun., **2**, 235–238 (1970).

[6]R. F. Millar, Proc. Camb. Philos. Soc., **69**, 175–188 (1971).

[7]It has been pointed out that the results of the invalidity of the Rayleigh hypothesis for these types of profile can be done by an elementary extension of the work of Petit and Cadilhac.[3] We remark that the analyticity of the Rayleigh solution (and hence the validity) for some type of grating profile cannot be derived from their work.

[8]R. Petit, Revue d'Optique, **6**, 249–276 (1966).

[9]The conception of an analytic function is related to complex variables. We define that a function of a real variable is analytic when it can be expanded in a convergent power series (Ref. 12, p. 83).

[10]We remark that only uniqueness is investigated; no attempt is made to prove an existence theorem.

[11]The subdomain B may not exist. In that case the Rayleigh hypothesis never holds.

[12]E. C. Titchmarsh, *The theory of functions*, 2nd ed., (Oxford University, New York, 1939).

[13]One exception has to be made. It is possible that the series (1) is a finite one. Then, the Rayleigh hypothesis is true. This can occur in the case of dealing with a Neumann boundary condition and a certain angle of incidence. For instance, we refer to the Maréchal and Stroke position of the triangular grating [A. Maréchal and G. W. Stroke, C. R. Acad. Sci. (Paris), **249**, 2042 (1959)]. The same kind of exception also apply to gratings of rectangular profile.