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Iterative series for calculating the scattering of waves from a hard corrugated surface

C. Lopez and F. J. Yndurain
Departamento de Fisica Teorica, Universidad Autonoma de Madrid, Canto Blanco (Madrid), Spain

N. García*
Physics Department, University of Virginia, Charlottesville, Virginia 22901
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We present an iterative series expansion in closed form that satisfies all the analytical equations proposed for solving the scattering of waves from a hard corrugated surface. The series converges to the good solution up to $h \lesssim 0.20$ when the corrugation of the surface is $D(x) = 2\pi h \cos 2\pi x$.

Different methods for solving the scattering of waves from a hard corrugated surface[1] (HCS) have been developed,[2-7] each using different approaches: (i) the Rayleigh approximation,[1-3] valid only up to a certain limit of the corrugation strength; (ii) the solution based on the extinction theorem[4-6] first obtained by Masel, Merrill, and Miller[4] (MMM) and generalized by Goodman[5]; and (iii) the self-consistent solution obtained by Garcia and Cabrera[7] (GC). The last two solutions are shown to be exact by using Green's theorem (i.e., Huygen's principle). It has been shown that even if the MMM solution is analytically exact the matrices obtained for solving the equations are numerically inconvenient,[7] i.e., they may become ill-conditioned,[8] so that it may not be possible to obtain numerical solutions for strong corrugations. For example, if the corrugation is of the form

$$D(x) = 2\pi h \cos 2\pi x\,, \tag{1}$$

the MMM matrices become inconvenient for $h > \sim 0.25$. This limit is much larger than the Rayleigh[8] one ($h \simeq 0.072$) but still the method cannot solve cases of very-large-amplitude corrugations as the GC self-consistent solution does[7] (good solutions with $h \simeq 1$ have been obtained).

The purpose of this paper is to present an iterative-series-expansion solution in closed form that is easy to handle numerically and does not require inverting matrices. This series solution presents a unified approach which will satisfy the equations generated by the three methods mentioned above. While we cannot determine analytically the radius of convergence we shall show numerical agreement with the exact methods up to $h \simeq 0.20$.

Green's theorem leads to the following integral equation when an incident plane wave hits a periodic hard corrugated surface $z = \alpha D(x)$ (where α is the strength of the corrugation):

$$e^{-ik_z \alpha D(x)} = \sum_G \frac{e^{i2\pi Gx}}{k_{Gz}} \times \int_{-1/2}^{1/2} f(x', \alpha) e^{-i2\pi Gx'} \times e^{ik_{Gz}\alpha |D(x) - D(x')|}\, dx'\,, \tag{2}$$

where we have considered for simplicity normal incidence $\vec{k}_i = (K, k_z)$ with $K = 0$. The G are reciprocal vectors and $k_{Gz}^2 = k_i^2 - G^2$. Equation (2) is obtained by setting the total wave function at the surface equal to zero (see Ref. 7). By applying the extinction theorem, the wave function vanishes at any place below the surface, so we can have the MMM equation[4,5] in simple form

$$-\delta_{G,0} = \frac{1}{k_{Gz}} \int_{-1/2}^{1/2} f(x, \alpha) e^{-i2\pi Gx} e^{ik_{Gz}\alpha D(x)}\, dx\,. \tag{3}$$

Toigo *et al.*[6] have proved that both Eqs. (2) and (3) lead to the *exact analytical solution and that this solution is unique.*

By making certain formal manipulations in Eq. (3) and in the Rayleigh approach it is possible to have the following transformed equations[10]:

$$e^{-ik_z\alpha D(x)} = \sum_G \frac{e^{i2\pi Gx}}{k_{Gz}} \int_{-1/2}^{1/2} dx' f(x', \alpha)\, e^{-i2\pi Gx'} \times e^{ik_{Gz}\alpha[D(x') - D(x)]} \tag{4}$$

$$= \sum_G \frac{e^{i2\pi Gx}}{k_{Gz}} \int_{-1/2}^{1/2} dx' f_R(x'\alpha)\, e^{i2\pi Gx'} \times e^{-ik_{Gz}\alpha[D(x') - D(x)]}\,, \tag{5}$$

where (4) corresponds to (3) and (5) corresponds to the Rayleigh approach. [Note that Eqs. (2), (4), and (5) are practically the same except for the modulus and the change in sign in the exponents.]

It should be said that these two formal transformations are correct only if the series (4) and (5) converge with the order of summation given. Beeby[10] claims to prove that Eqs. (2)–(5) are the same, but his proof is incorrect because he interchanges the summation and integration when the series diverges. However, the claim of Beeby is correct in the sense that in the particular cases in which series (4) and (5) are convergent, the solution is the same for Eqs. (2)–(5). We will find here the solution that is unique owing to Green's theorem.[6]

We start by making the formal expansion in powers of α,

$$f(x,\alpha)=\sum_{n=0}^{\infty} f^{(n)}(x,0)\,\frac{\alpha^n}{n!}\ , \tag{6}$$

where $f^{(n)}(x,0)$ is the nth derivative with respect to α at $\alpha=0$. This solution is good only if the series is convergent for a given α. As $f^{(n)}(x,0)$ is periodic, we can define

$$f_G^{(n)}=\int_{-1/2}^{1/2} dx\, e^{-i2\pi Gx} f^{(n)}(x,0)\,. \tag{7}$$

Expanding both sides of Eq. (4) and equating powers in α we obtain the recursive formula

$$f_G^{(n)}=-\sum_{\nu=1}^{n}\binom{n}{\nu}(ik_{Gz})^{\nu}\{f^{(n-\nu)}(x,0)[D(x)]^{\nu}\}_G \tag{8}$$

and

$$f_G^{(0)}=-ik_{Gz}\delta_{G,0}\,. \tag{9}$$

It is easy to show that (8) and (9) satisfy the exact integral equations (2) and (3) as well as the Rayleigh one (5). Conversely, Eqs. (8) and (9) can be obtained easily by expanding in Eq. (3) and equating coefficients of α^n

$$-\delta_{G,0}=\frac{1}{k_{Gz}}\int_{-1/2}^{1/2} dx\, e^{-i2\pi Gx}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\sum_{j=0}\binom{n}{j} f^{(j)}(x,0)[ik_{Gz}D(x)]^{n-j}$$
$$=\frac{1}{k_{Gz}}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\sum_{j=0}\binom{n}{j}(ik_{Gz})^{n-j}\{f^{(j)}(x,0)[D(x)]^{n-j}\}_G\,. \tag{10}$$

The scattering amplitudes are obtained[4-7] from

$$A_G(\alpha)=\frac{1}{k_{Gz}}\int_{-1/2}^{1/2} dx\, f(x,\alpha)e^{-i2\pi Gx}e^{-ik_{Gz}\alpha D(x)} \tag{11}$$

which becomes, by expanding again as in (6),

$$A_G(\alpha)=\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}A_G^{(n)}\,, \tag{12}$$

with

$$A_G^{(n)}=\left.\frac{d^nA_G(\alpha)}{d\alpha^n}\right|_{\alpha=0}$$
$$=-\frac{1}{k_{Gz}}\sum_{\nu=1}^{n}\binom{n}{\nu}(ik_{Gz})^{\nu}[f^{(n-\nu)}(x,0)D^{\nu}(x)]_G$$
$$\times[1-(-1)^{\nu}]\,, \tag{13}$$

$$A_G^{(0)}=\delta_{G,0}\,. \tag{14}$$

The diffraction probabilities are given by

$$P_G(\alpha)=(k_{Gz}/k_z)|A_G(\alpha)|^2\,. \tag{15}$$

It is interesting to note that at the threshold condition, $k_{Gz}\to 0$ so $P_G(\alpha)\to 0$, but the beam appears or disappears with a vertical tangent, as has been proved before.[11,12]

As we mentioned above, we do not know the convergence limit of our series and we shall test its validity by comparing numerical calculations with MMM and GC calculations.[4-7] We make these computations for the cosinelike corrugation (1) ($\alpha=2\pi h$) and obtain the solution

$$f_G^{(n)}=-\sum_{\nu=1}^{n}\binom{n}{\nu}\left(\frac{ik_{Gz}}{2}\right)^{\nu}\sum_{r=0}^{\nu}\binom{\nu}{r}f_{G+\nu-2r}^{(n-\nu)}\,. \tag{16}$$

The numerical advantages of this series are that it is not necessary to invert matrices, thus avoiding ill-conditioning problems, and that once we have the $f_G^{(n)}$ for one type of corrugation, the value $f(x,\alpha)$ for each α is obtained by summing the series (6).

The computations are made using two summation procedures: (i) First, we use formulas (12)–(14) for $A_G^{(n)}$. The diffraction probabilities are given in Table I, and are the same as those obtained with the MMM and GC formalisms, yielding convergent solutions for $h\lesssim 0.16$. (ii) We make the change in the variable α

TABLE I. Diffraction probabilities for $2\pi k_i = 20$ at normal incidence. (a) GC and MMM exact calculations using the RR' method (Ref. 7); (b) series expansion in this paper. Corrugation $\alpha D(x) = 2\pi h \cos 2\pi x$. n is the number of terms used in the expansion (16). F are the outgoing beams that must satisfy the unitary conditions. Note that for $h \simeq 0.16$ unitarity starts falling down.

	$h = 0.04$		$h = 0.08$		$h = 0.16$	
Beam	(a)	(b) $n = 14$	(a)	(b) $n = 49$	(a)	(b) $n = 71$
0	0.2281	0.2281	0.0890	0.0883	0.2954	0.2794
±1	0.3321	0.3321	0.1046	0.1045	0.1528	0.1615
±2	0.0528	0.0528	0.3169	0.3167	0.0118	0.0116
±3	0.0009	0.0009	0.0344	0.0347	0.1887	0.1856
$\Sigma_F P_F$	1.0000	1.0000	1.0000	1.0000	1.0000	0.9968

TABLE II. Diffraction probabilities as in Table I. Results (b) obtained using the transformation (17). Note the improved convergence in comparison with Table I.

	$h = 0.16$		$h = 0.18$		$h = 0.20$	
Beam	(a)	(b) $n = 71$	(a)	(b) $n = 71$	(a)	(b) $n = 71$
0	0.2954	0.2954	0.6161	0.6161	0.6513	0.6355
±1	0.1528	0.1528	0.0254	0.0254	0.0442	0.0416
±2	0.0108	0.0108	0.0133	0.0133	0.0159	0.0183
±3	0.1887	0.1887	0.1528	0.1527	0.1162	0.1135
$\Sigma_F P_F$	1.0000	1.000	1.0000	0.9998	1.0000	0.9827

$$\beta = \frac{\alpha}{\alpha + 2/|k_{Gz}|} \tag{17}$$

and then

$$A_G(\alpha) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \left. \frac{d^n A_G(\beta)}{d\beta^n} \right|_{\beta=0} . \tag{18}$$

This procedure will render the series (18) convergent even if (12)–(14) do not converge because of a singularity in $A_G(\alpha)$ at $\alpha_s = -1/|k_{Gz}|$. In Table II we present calculations using this procedure that converge up to $h \simeq 0.20$ although they do so very slowly having some small oscillations for $n = 71$.

In conclusion, we have presented an iterative series expansion in a closed form that satisfies the Rayleigh approach as well as the exact equations for the scattering of waves from a HCS.[4-7] We have been unable to find the radius of convergence (α_{max}) of the series but we prove its numerical validity up to $h \simeq 0.20$, where the computations agree with the GC and MMM numerical results. This radius of convergence is more than twice that obtained with the Rayleigh approach[8] $h \simeq 0.072$. Also, the series provides in certain cases a simplification of the computation procedure in relation with other methods. The extension of the series to a more general hard-wall potential (e.g., HCS plus an attractive well) is straightforward, but still it is necessary to compare with the exact result or find the radius of convergence in order to claim a good solution to the problem.

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*Permanent address: Departamento de Fisica Fundamental, Universidad Autonoma de Madrid, Canto Blanco (Madrid), Spain.

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