New method for solving the scattering of waves from a periodic hard surface: Solutions and numerical comparisons with the various formalisms

N. García
Departamento de Física Fundamental, Universidad Autónoma de Madrid, Canto Blanco (Madrid), Spain and Departamento de Matemáticas, Universidad Nacional de Education a Distancia, Ciudad Universitaria, Madrid, Spain

N. Cabrera
Departamento de Física Fundamental, Universidad Autónoma de Madrid, Canto Blanco (Madrid), Spain
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In this paper we present a formalism and a numerical method, called CG and *RR'*, respectively, which lead to the exact solution of the scattering of waves from a periodic hard corrugated surface. The relation of this formalism to those previously in use [Rayleigh hypothesis and Masel, Merrill, and Miller (MMM) formalism] is also discussed. Numerical computations show that his formalism seems to give always a convergent numerical solution for any shape and strength of the corrugations. On the other hand, the other two formalisms give also convergent numerical solutions for small values of the corrugation strength. Numerical results show that the MMM formalism, *although analytically exact,* converges very slowly as the corrugation strength increases and it may become ill-conditioned. This formalism seems to be an inconvenient way of writing the boundary conditions on the scattered wave function. In particular, the theoretical validity of the Rayleigh hypothesis is numerically confirmed for a shape corrugation $D(x) = b\cos\kappa x$ when $\kappa b \leq 0.448$. When the computed diffraction probabilities satisfy unitarity, they are the same no matter what formalism is used. The *RR'* numerical method proposed here allows the calculation of diffracted intensities for large corrugation strengths.

I. INTRODUCTION

The scattering of waves from a periodic hard corrugated surface (HCS) was first studied by Rayleigh[1] in 1907, in connection with other types of waves, scalar or vectorial, in different fields of physics. Recently, the scattering of atoms from crystal surfaces has been considered from the same point of view and it is with this problem that we will be mainly concerned in this paper.

To avoid complications we will consider the simplest scattering problem, namely, an atom beam incident on a one-dimensional corrugated surface, and will attempt to find a definite answer to the question of whether or not there is a method of solution which can be applied to any kind and any strength of the corrugation. We will also attempt to compare this exact method to other methods that have already been proposed. The one-dimensional corrugation is not just an academic problem, as it is a good approximation to the behavior of a vicinal crystal surface, consisting of a periodic distribution of atomic steps separated by close-packed terraces, which has attracted recently considerable attention both experimentally[2] and theoretically.[3]

The first method to treat our problem was the one proposed by Rayleigh[1] himself. He assumed that the asymptotic wave function valid at large distance from the corrugated surface can be extended down to the "selvedge" region (Fig. 1) containing the corrugated surface. The so-called "Rayleigh hypothesis" permits the determination of scattering amplitudes provided the corrugation is sufficiently smooth. This basic conclusion was reached after a long series of papers among which we will mention those by Lippmann,[4] Petit and

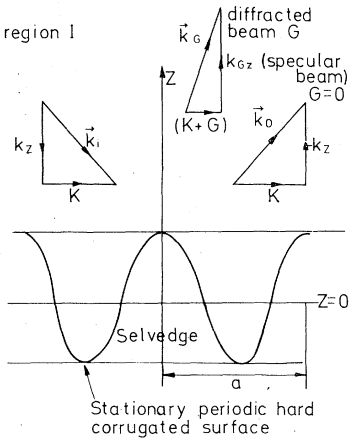

FIG. 1. Representation of the incident wave vector $\vec{k}_i$ and the diffracted beam G from the stationary periodic hard corrugated surface. The upper region I and the inner region II, as well as the selvedge oscillating region are indicated.

Cadilhac,[5] Uretsky,[6] and Millar.[7-9] In the specific field of atom scattering, the Rayleigh hypothesis was first proposed by Garibaldi *et al.*[10] and studied in further detail by Chow and Thompson,[11] García *et al.*,[12] and García.[13,14] (A detailed study of the applicability of the model to the scattering of atoms from crystal surfaces is presented in the paper by García.[14]) In all of these investigations the corrugation has been assumed to be a sinusoidal or nearly sinusoidal one. There is an open question as to whether or not the method is applicable to other corrugations both in kind and in strength. We will attempt to answer these questions by numerical computations.

Recently, other methods have been considered based on Huygens' principle from which one derives integral equations basically correct and applicable to any corrugation. Waterman[15] and De Santo[16] claimed to have solved the problem exactly, but the application to different corrugation shapes and strengths has not been tested and we will not discuss these methods here. More recently, Masel *et al.*,[17] Goodman,[18] and Toigo *et al.*[19] simplified the integral equation based on Huygens' principle by applying the extinction theorem. This method is exact and seems to "simplify" the scattering equations but converges very slowly and the numerical results fall down for large corrugation strengths.

Finally, and very recently, Cabrera and García[20] have set up a method based on the above unmodified integral equation, called "CG *formalism*." This method appears to have the great advantage of rapid convergence and validity without restriction. By numerical computations we will show that the method leads to a solution for corrugations which cannot be solved numerically by the Masel, Merrill, and Miller (MMM) and Rayleigh methods.

In Sec. II we will present first the CG formalism and discuss the characteristics of the solutions obtained for any corrugation. Second, we will discuss the MMM formalism and show its connection to the CG formalism. Both formalisms are correct but the MMM appears to be a very inconvenient way of writing the boundary conditions and is not able to obtain solutions for large corrugations. Finally, we will consider the approximation deduced from the Rayleigh hypothesis, and show rapidly its connection with the other two methods.

In Sec. III, numerical procedures will be set up for the three methods, so that in Sec. IV results will be presented for four different kinds of corrugations with variable amplitudes: (i) sinusoidal, (ii) sum of sinusoidals, (iii) sawtooth profiles, and (iv) spherical profiles.

Finally, in Sec. V we will present a set of conclusions derived from the analysis of the three methods in Sec. II and the results of the numerical computations considered in Secs. III and IV. The overall conclusion is that the CG formalism and the RR' method (consisting in solving the equations in the real space R, R') give always good numerical solutions for the scattering amplitudes, while the other two lead to numerical solutions only for smooth corrugations, and whenever the solutions of the three methods are convergent the obtained scattering probabilities are the same.

II. CG, MMM, AND RAYLEIGH FORMALISMS

The potential energy of the particle scattered from a one-dimensional hard corrugated surface (HCS) model of a crystal surface is

$$\begin{aligned} &V(x,z)=0, \quad D(x)<z\,, \\ &V(x,z)=\infty, \quad z\leq D(x)\,, \end{aligned} \tag{1}$$

where $z=D(x)$ represents the one-dimensional corrugation function. We restrict ourselves to one dimension for simplicity, and we assume $D(x)$ to be periodic with periodicity a, so that $D(x+a)=D(x)$.

The wave function $\psi(x,z)$ of the particle can be described by the Lippmann-Schwinger[21] integral equation

$$\psi(x,z)=e^{i(Kx-k_{Gz}z)}+\int_{-\infty}^{\infty}dz'\int_{-a/2}^{a/2}dx'\,R_0^+(x-x',z-z') \times V(x',z')\psi(x',z')\,. \tag{2}$$

The first term of Eq. (2) represents the incident particle, with the incident wave vector $\vec{k}_i=(K,k_z)$, $R_0^+(x,z)$ is the outgoing-free-particle propagator. The propagator for a periodic surface can be written

$$R_0^+(x-x',z-z')=-\frac{iM_p}{\hbar^2 a}\sum_G \frac{e^{i(K+G)(x-x')}}{k_{Gz}}\,e^{ik_{Gz}|z-z'|}\,, \tag{3}$$

where M_p is the mass of the particle, k_{Gz} are the normal components of the outgoing wave vectors corresponding to each $G=2\pi n/a$ $(-\infty<n<\infty)$ reciprocal vector. As we are considering an elastic problem, energy conservation requires

$$\begin{aligned} &K'=K+G\,, \\ &k_{Gz}^2=k_i^2-(K+G)^2\,. \end{aligned} \tag{4}$$

We use all throughout this paper the notation introduced by Cabrera *et al.*[22] Namely, the F vectors correspond to the propagating waves $(k_{Fz}^2\geq 0)$, and the E vectors correspond to the evanescent waves $(k_{Ez}^2<0)$.

The potential energy defined by (1) requires that

$\psi(x,z)\equiv 0$ *everywhere for* $z\leq D(x)$, so that if we defined

$$F(x,z)=-(iM_p/\hbar^2 a)V(x,z)\psi(x,z) \tag{5}$$

we can write, following Masel *et al.*,[17] that

$$F(x,z)=f(x)\delta(z-D(x)), \tag{6}$$

where $f(x)$ is still to be determined.

Introducing (3) and (6) into (2) and integrating over z' we obtain

$$\left.\begin{matrix} D(x)<z, & \psi(x,z) \\ D(x)>z, & 0 \end{matrix}\right\} = e^{i(Kx-k_z z)} + \int_{-a/2}^{a/2} dx' f(x') M(x',x,z), \tag{7,8}$$

where

$$M(x',x,z)=\sum_G \frac{e^{i(K+G)(x-x')}}{k_{Gz}} e^{ik_{Gz}|z-D(x')|}. \tag{9}$$

The still undetermined function $f(x)$ acts as a density of "sources" located on the surface $z=D(x)$ so that their "field" "extinguishes the total field" below $z=D(x)$.

Up to this point the wave function (7) and (8) is basic to the various formalisms developed to solve our problem. The differences will appear when we attempt to determine the function $f(x)$; in this respect, we will consider three methods:

(i) the CG formalism, which we believe always leads to the exact solution for any corrugation $z=D(x)$.

(ii) the MMM formalism, which gives analytical exact scattering equations by applying to the CG the extinction theorem, but unfortunately appears to give practical results only for small corrugations.

(iii) the Rayleigh hypothesis, which is only valid for sufficiently weak corrugations.

A. CG formalism

To determine the function $f(x)$ we require $\psi(x,z)$ to be continuous over the surface $z=D(x)$ so that the wave function must satisfy the condition

$$\psi(x,z=D(x))\equiv 0. \tag{10}$$

This condition permits the determination of $f(x)$ from the integral equation

$$\int_{-a/2}^{a/2} dx' f(x') M(x',x) + e^{i[Kx-k_z D(x)]} = 0, \tag{11}$$

$$M(x',x)=\sum_G \frac{e^{i(K+G)(x-x')}}{k_{Gz}} e^{ik_{Gz}|D(x)-D(x')|}.$$

This integral equation is complicated to handle analytically because of the absolute values $|D(x)-D(x')|$; on the other hand, the factor $\exp[ik_{Gz}|D(x)-D(x')|]$ becomes exponentially decreasing for large E ($k_{Ez}^2<0$) and makes the kernel $M(x',x)$ and its inverse $M^{-1}(x',x)$ well defined. We will show in Secs. III and IV that (11) can be numerically solved by a finite difference procedure using a finite number of terms G, which then converges to the exact solution as G becomes large. The evidence we now possess is that $f(x)$ can be determined from (11) for any $D(x)$.

To calculate the scattering amplitudes we consider the behavior of $\psi(x,z)$ in the domain I (Fig. 1) for which $D_{\max}<z$. Then $|z-D(x')|=z-D(x')$ and (7) can be written as

$$D_{\max}<z;\quad \psi_{\rm I}(x,z)=e^{i(Kx-k_z z)}+\sum_G A_G e^{i(K+G)x} e^{ik_{Gz} z}, \tag{12}$$

where the scattering amplitudes A_G are

$$A_G=\frac{1}{k_{Gz}}\int_{-a/2}^{a/2} dx\, f(x) e^{-i(K+G)x} e^{-ik_{Gz}D(x)}. \tag{13}$$

The formalism consists then in finding $f(x)$ from (11) and the A_G from (13). As is known, the scattering probabilities P_F corresponding to the propagating waves $F(k_{Fz}$ real) will satisfy the unitarity rule

$$P_F=\frac{k_{Fz}}{k_z}|A_F|^2,\quad \sum_F P_F=1. \tag{14}$$

As proved by Cabrera and Solana[23] and by Garcia,[24] the intensity P_F of a new wave must increase from zero with a vertical tangent as k_i and θ_i vary through the threshold condition ($k_{Fz}=0$). This condition, together with the unitarity rule, should be satisfied by any credible elastic theory of scattering from a hard corrugated surface. The proof of the correct behavior of the P_F's is given in Appendix A, and it is demonstrated numerically in Sec. IV.

It is also very illuminating to consider the wave function (8) in the domain II (Fig. 1, $z<D_{\min}$). In this case $|z-D(x')|=D(x')-z$ so that (8) can be written as

$$z<D_{\min}:\quad 0=\sum_G (\delta_{G,0}+B_G) e^{i(K+G)x} e^{-ik_{Gz}z}, \tag{15}$$

where

$$B_G=\frac{1}{k_{Gz}}\int_{-a/2}^{a/2} dx\, f(x) e^{-i(K+G)x} e^{ik_{Gz}D(x)} \tag{16}$$

and is to be computed once $f(x)$ has been determined from (11).

At this point we would like to make the following comments on Eqs. (10)–(16).

(a) The integral equation (11) does not depend on the position of $D(x)$, that is to say it is the same for $D(x)$ or $D(x)\pm\alpha$ as it should be from physical arguments, provided that f is changed to $fe^{-ik_z\alpha}$. This change does not affect the following considerations.

(b) Then, by changing $D(x)$ to $D(x)+\alpha$ the values of A_G and B_G [Eq. (13) and (15)] will change to $A_G e^{-ik_{Gz}\alpha}$ and $B_G e^{ik_{Gz}\alpha}$.

(c) Equation (15) describes a Fourier series of the zero function, then its coefficients must be zero,

$$(\delta_{G,0}+B_G)e^{-ik_{Gz}z}=0 \tag{17}$$

for all G and $z\leq D_{\min}$. Then the analytical exact solution implies

$$\delta_{G,0}+B_G=0\,. \tag{18}$$

(d) As a consequence, any numerical procedure will make Eq. (15) approximately zero, but not exactly zero. This implies that the numerical value of Eq. (17) will read, for $z\leq D_{\min}$,

$$(\delta_{G,0}+B_G)e^{-ik_{Gz}z}\approx 0\,. \tag{19}$$

Now Eq. (18) does not have to be satisfied and B_G is not the interesting quantity because by considering (b) above it can be as large or as small as we wish and it will not change Eq. (19). We point out that varying α is like changing $z=D_{\min}$. It is interesting to note that for F waves

$$\delta_{F,0}+B_F\approx 0 \tag{20}$$

because of the propagating property of $e^{ik_{Fz}z}$, but for $E\to\infty$ we have

$$\lim_{E\to\infty} B_E e^{+ED_{\min}}=0\,. \tag{21}$$

If this is satisfied, the same is also true for $z\leq D_{\min}$. Depending on the origin of $D(x)$ the $\lim_{E\to\infty}B_E$ can be either zero or large and still satisfy Eq. (19), and consequently the wave function vanishes approximately for $z\leq D_{\min}$, $\psi(x,z\leq D_{\min})\approx 0$.

(e) Finally, the behavior of A_E must satisfy $\lim_{z\to\infty}A_E e^{-Ez}=0$ because no other condition is imposed on the wave function (7).

B. MMM formalism

This formalism was developed as an exact method by various authors, in particular Masel, Merrill, and Miller[17] and Goodman[18] and also discussed by Toigo *et al.*[19] It consists in using the more strict conditions of Eq. (18).

We return to the correct wave function (8) for $z<D(x)$. In order to determine the function $f(x)$, instead of using the boundary condition (10) the method imposes as a consequence of the extinction theorem the equivalent boundary condition (19),

$$\psi(x,z=\text{const})=0,\quad z=\text{const}<D_{\min} \tag{22}$$

This condition, as discussed above, can be written in the form (15) and leads directly to $\delta_G+B_G=0$ [Eq. (18)]. Once this condition has been accepted, using (16) we deduce the set of equations

$$\int_{-a/2}^{a/2} f(x)\,dx\, e^{-i(K+G)x}e^{ik_{Gz}D(x)}=-k_{Gz}\delta_{G,0} \tag{23}$$

to determine $f(x)$. Finally the scattering amplitudes A_F are computed from (13).

Alternatively, one can Fourier transform equation (23) and determine the Fourier components of $f(x)$, $f(x)=\sum_{G'} f_{G'} e^{iG'x}$, from the system of equations

$$\sum_G f_G M_{GG'}=-k_{Gz}\delta_{G,0},$$
$$M_{G'G}=\int_{-a/2}^{a/2} dx\, e^{i(G'-G)x}e^{ik_{Gz}D(x)}\,. \tag{24}$$

In principle, it seems that the set of integral equations (23) is much simpler than that of the CG formalism (11), although the MMM equations are a consequence of the latter one, as we have seen in Sec. IIA. However, the numerical solution of (23) is again satisfied approximately. Then the condition $\delta_{G,0}+B_G\approx 0$ is a very restrictive condition, as we discussed previously. We like to say that it is a very inconvenient way of introducing the boundary condition in the problem because it does not include the factor $e^{ik_{Gz}z}$ on the B_G. Attempts to solve Eq. (20) (MMM formalism) have been made besides the one we propose in this paper, but unfortunately none has reached a convergent numerical solution for large values of the corrugation strength,[25] regardless of the numerical method used. So the MMM formalism is exact, it is deduced in a straightforward manner from CG, but it seems "not good" for obtaining numerical results. It becomes ill-conditioned.

C. Rayleigh hypothesis

We now proceed to describe very quickly the Rayleigh hypothesis that has been discussed in almost all references on the subject.[1,4,5-15] This consists in assuming that the convergence of the wave function $\psi_{\rm I}$ can be extended from domain I down to the selvedge domain. Then, one can obtain an equation for the scattering amplitudes by imposing the boundary condition

$$\psi_{\rm I}(x,z=D(x))=0 \tag{25}$$

that reads as

$$\sum_G A_G e^{i(k_{Gz}+k_z)} e^{iGx} = -1 \tag{26}$$

This method is simpler than the other two because it allows one to obtain A_G directly without knowing $f(x)$; on the other hand, it clearly has limited validity for the proposed scattering problem. In general, the series might be divergent because of the increasing exponential $e^{ik_{Gz}D(x)}$. The limitations as well as the validity of equation (26) have been extensively discussed in Refs. 1, 4, and 5–15. Unfortunately, these discussions have been limited to a cosinelike corrugated surface,

$$D(x) = b\cos\kappa x\,. \tag{27}$$

Petit and Cadilhac[5] showed that the Rayleigh hypothesis is invalid if $\kappa b > 0.448$. Later, Millar[8] has shown that it is valid if $\kappa b < 0.448$. In Ref. 9, Millar seems to prove also that the hypothesis can be always valid by determining coefficients A_G satisfying the boundary conditions in a least-square sense. In all of these investigations no numerical computations were presented. Recently García *et al.*[12] have discussed the characteristics of the different methods to solve Eq. (26), showing that the limit of convergence of the series depends on the method of summation used. In this sense, the so-called *GR* method is the easiest one to use and gives a larger range of validity for b, being in agreement with the results in Ref. 8. A detailed application of the *GR* method to a two-dimensional corrugation is presented in Refs. 12–14. In particular, Ref. 14 gives an extensive application for the case of all scattering parameters varying.

III. RR′ NUMERICAL METHOD

In order to solve the integral equation (11) to obtain the source density $f(x)$ and the scattering amplitude A_G [Eq. (13)], we have developed a numerical algorithm called *RR′* after the procedure used.

This consists basically of a finite-difference method, to substitute the integral signs by discrete summations. $\int \to (1/L_n)\sum$, where $1/L_n$ is the elementary unit volume considered, i.e., L_n is the number of points over which the function is integrated.

To determine the function $f(x)$ we use a set of linear equations in which the unknown are the values of the function at the discrete points (see Fig. 2) and are constant in the elementary unit volume

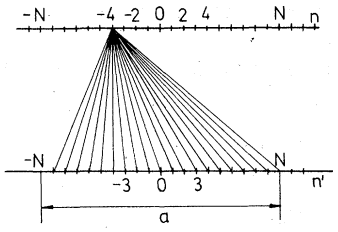

FIG. 2. Scheme of the *RR′* numerical procedure. For each point n we determine $2N$ unknown values of $f(n')$ and as $2N$ value of nn exists, we have a set of $2N$ unknowns by $2N$ equations.

that surrounds each point. The matrix elements are taken as the values of the kernel $M(x,x')$ (Eq. (9) at the points defining $f(x')$; the independent term consists of the values of the first term in the same equation. Note that we are conjugating the points x and x' (for which reason we call this the *RR′* numerical method because R, R' are vectors in real space.) and in the set of linear equations we write an equation in the unknowns $f(x')$ for each value of x, taking as many values of x as of x' in units of $a/2\pi$ and the reciprocal magnitudes k_i in units of $2\pi/a$. Equation (11) reads

$$\sum_{n'=-N+1}^{N} \frac{f(n')}{2N} M(n,n') = -e^{-ik_z D(n)} e^{i\pi Kn/N}\,, \tag{28}$$

where $x = 2\pi n/2N$ and $2N$ is the number of equidistant points in the unit cell a. As mentioned before, we have an equation for each $n (n = -N+1, \ldots, N)$ and $f(n')$ unknowns for $n' = -N+1, \ldots, 0, 1, \ldots, N$ (The values at $n = -N$ and N are the same since the kernel is invariant because of translational symmetry). Then we have a set of $2N \times 2N$ unknowns and equations.

Now the "discretized" kernel may be written

$$M(n,n') = \sum_G \frac{\exp i\pi(K+G)(n'-n)/N}{k_{Gz}} \times \exp ik_{Gz}\left|D(n) - D(n')\right| \quad \text{if } n \neq n'\,. \tag{29}$$

The summation over G is extended until the value obtained is close "enough" to the case $G \to \infty$. For example, at normal incidence ($K = 0$) the sum should be $-M_1 < G \leq M_1$ because of the symmetry conditions, and M_1 is such that the difference with respect to the sum $-(M_1+1) \leq G \leq M_1 + 1$ is "small" enough. In the case $n = n'$, the matrix elements are calculated in linear approximation of $\left|D(n) - D(n')\right|$ and written

$$M_{nn} = \sum_G \frac{2N}{k_{Gz}} \left(\frac{\exp\{i[2\pi(K+G) + \left|D'(n)\right| k_{Gz}]n/4N\} - 1}{i[(K+G) + \left|D'(n)\right| k_{Gz}]} + \frac{1 - \exp\{-i[2\pi(K+G) - \left|D'(n)\right| k_{Gz}]n/4n\}}{i[(K+G) - \left|D'(n)\right| k_{Gz}]} \right). \tag{30}$$

(In Appendix A we present a proof of the value of this matrix.)

element, as well as of the convergent behavior of the series when $G \to \infty$.

Now the scattering amplitudes A_G can be easily obtained when $f(n)$ is determined by Eq. (28),

$$A_G = \frac{1}{k_{Gz}} \sum_{n=-N+1}^{N} \frac{f(n)}{2N} e^{-i\pi(K+G)n/N} e^{-ik_{Gz}D(n)} . \quad (31)$$

Note that the behavior $\lim_{G\to\infty} A_G \to \infty$ is satisfied in general because of the increasing behavior character of the exponential $e^{-ik_{Gz}D(n)}$. We calculate and use $f(n)/2N$ and because of this the factor $2N$ appears in Eq. (30). The application of the above "discretized" formula allows us to calculate the scattered probabilities P_F and to solve for wave scattering from an HCS having finite matrix elements for any summation over G.

Analogous to the procedure used in the GR[12-14] method in which the equations are solved by using vectors in the reciprocal space G and in real space R to calculate the A_G amplitudes from the Rayleigh hypothesis, it is possible to proceed with Eq. (23) of the MMM formalism to calculate $f(x)$. This consists in relating the x and G vectors and setting up a system of linear equations in x, and G, one equation for each G. This procedure will be called the RG (R for real space and G for reciprocal space) method. The resulting equations are

$$-\sum_{n} \frac{f(n)}{2N} e^{-i(K+G)\pi n/N} e^{ik_{Gz}D(n)} = \delta_{G,0} k_{Gz} . \quad (32)$$

In the case of the Rayleigh hypothesis, the GR method establishes an equation for each R. Again, this method of calculating $f(n)/2N$ has computational simplicity over others[17,18] that Fourier transform Eq. (23) and allows one to calculate the Fourier components of the periodic function $f(x)$. However, it seems to give a convergent solution for a smaller corrugation strength than suggested by others[25] and depends critically on the number of points used.

The Rayleigh hypothesis represents a great simplification when there is convergence because then it is not necessary to solve the equations for $f(x)$, since one obtains directly the scattering amplitudes by solving Eq. (26). As a consequence, the computation is simplified, as has been pointed out in Refs. 12, 14, and 18, but with this approach it is not possible to calculate the sources function.

IV. NUMERICAL RESULTS

To appreciate how the different numerical methods proposed in Sec. III work out, we have solved the "discretized" equations corresponding to the three formalisms of Sec. II for four different corrugation functions and a wide range of strength amplitudes. Figs. 3a–d show the corrugation profiles described by the following analytical expressions:

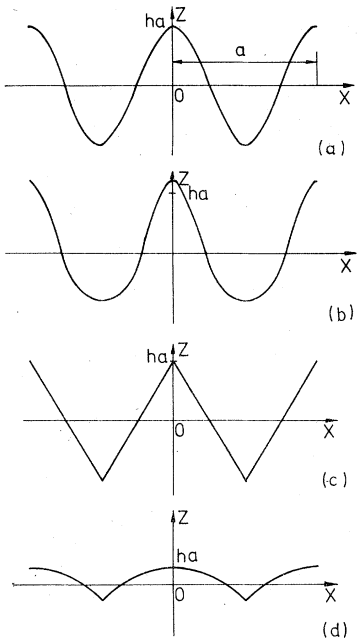

FIG. 3. Different corrugations used in the calculations. Parts (a), (b), (c), and (d) correspond to the formulas (33a) (33b), (33c), and (33d), repectively.

$$D(n) = 2\pi h \cos(\pi n/N) , \quad (33a)$$

$$D(n) = 2\pi h \cos(\pi n/N) + 2\pi(0.2h)\cos(2\pi n/N) , \quad (33b)$$

$$D(n) = 2\pi h(-|2n/N| + 1) , \quad (33c)$$

$$D(n) = (R^2 - \pi n/N)^{1/2} - R + 2\pi h , \quad (33d)$$

$$R = \pi(1 - 16h^2)/8h ;$$

h is equal to the value of the difference between the maximum and the minimum of the corrugation divided by twice the surface periodicity in the (a), (c), and (d) cases. Formula (33d) corresponds to a surface of hard spheres in which $R \to \infty$ implies zero corrugation (plane surface) and the maximum value of $h = 0.25$ is that for a sphere of radius equal to one-half of the periodicity parameter. This is independent of the surface periodicity.

We present now systematic computations for the four cases using the GR method described elsewhere[12-14] with the Rayleigh hypothesis, the RG method [Eq. (32)] with the MMM formalism, and the RR' method [Eq. (28)] with the CG formalism.

In each case, and for a given value of h, one looks for a convergent solution by trying out in the computation larger and larger sets of points, i.e., larger matrices. Convergence is obtained

TABLE I. Diffraction probabilities at normal incidence for $2\pi k_i = 20$. *GR* method (Rayleigh hypothesis). The asterisk indicates that symmetry between P_n and P_{-n} hardly exists. The result is not valid and unitarity is not verified. The notation $\alpha(n)$ means $\alpha \times 10^n$.

Beam \ h	0.02	0.04	0.06	0.08*	0.1
			Corrugation (33a), $2N = 40$		
0	7.2877 (-1)	2.2813 (-1)	1.032 (-3)	8.61 (-2)	1.41 (-1)
1	1.3143 (-1)	3.2110 (-1)	3.1090 (-1)	1.01 (-1)	5. (-4)
2	4.160 (-3)	5.2883 (-2)	1.8004 (-1)	3.18 (-1)	3.41 (-1)
3	1.691 (-5)	9.469 (-3)	8.578 (-3)	3.4 (-2)	8.2 (-2)
$\Sigma_F P_F$	1.0000	1.0000	1.0000	0.991	0.993
h	0.02	0.04	0.06	0.08	0.1
			Corrugation (33b)		
0	7.2145 (-1)	2.2249 (-1)	3.3994 (-2)	1.82 (-1)	...
1	1.3092 (-1)	3.2659 (-1)	2.9790 (-1)	9.1 (-2)	...
2	8.086 (-3)	5.7901 (-2)	1.6394 (-1)	2.6 (-1)	...
3	2.609 (-4)	4.225 (-3)	2.0977 (-2)	6.2 (-2)	
$\Sigma_F P_F$	0.9999	0.9999	0.9999	1.01	2.5

when unitarity [Eq. (14)] and geometrical symmetry in the diffraction probabilities (P_F) are verified. We will find that for the Rayleigh and the MMM methods numerical solutions are possible only for h sufficiently small, while for the CG method there seems to be no limit in the values of h.

The notation $\alpha(n)$ means $\alpha \times 10^n$.

A. GR computations (Rayleigh hypothesis)

Tables I and II show the results obtained by solving the Rayleigh hypothesis [Eq. (26)] and using the *GR* method, for the shape corrugation functions (33a)–(33d) corresponding to Figs. 3(a)–(d). The calculation is for normal incidence and the energy $2\pi k_i = 20$. The asterisk indicates that the symmetry $P_n = P_{-n}$ is not well satisfied and unitarity is not very good. Dots indicate that convergence does not exist no matter how many points are used. We take $2N = 40$ points but the same result is obtained using $2N$ from 20 to 80. We observe that a good solution is obtained for all corrugations up to $h \simeq 0.08$ for the cosinelike cases (33a) and 33(b) and $h \simeq 0.06$ for the sawtooth and the hard-sphere corrugations of (33c) and (33d).

TABLE II. Diffraction probabilities for $2\pi k_i = 20$. *GR* method (Rayleigh hypothesis).

Beam \ h	0.02	0.04	0.06	0.08	0.1
			Corrugation (33c), $2N = 40$		
0	8.0264 (-1)	3.8572 (-1)	7.37 (-2)	...	...
1	9.5131 (-2)	2.6675 (-1)	3.04 (-1)	...	...
2	2.996 (-3)	3.9542 (-2)	1.54 (-1)	...	...
3	5.846 (-4)	7.425 (-4)	5.9 (-4)	...	...
$\Sigma_F P_F$	1.0000	0.9998	0.9935	1.87	...
h	0.02	0.04	0.06	0.08	0.1
			Corrugation (33d)		
0	8.0831 (-1)	4.0816 (-1)	1.8650 (-1)	...	...
1	8.8894 (-2)	2.5437 (-1)	3.2596 (-1)	...	...
2	8.083 (-3)	3.9421 (-2)	1.0870 (-1)	...	...
3	4.130 (-4)	2.827 (-3)	6.325 (-3)	...	...
$\Sigma_F P_F$	0.9999	0.9999	1.0006	1.5	...

Since the case (33a) has been specially studied[3-9] finding a theoretical limit $h \simeq 0.072$, we have made an extra analysis of this corrugation by varying the corrugation h and the incident angle θ_i, as presented in Table III, by using $2N = 40$. Observe that the validity of the solution is better for small incident angles. However, Refs. 4–9 set up the theoretical limit $h \simeq 0.072$ independent of the angle or incidence. The difference can be a consequence of the number of points used in the approximate numerical solution. In Table IV we present calculations using $2N = 140$ to establish the limit of validity of the Rayleigh hypothesis and it seems clear that for $0.071 < h < 0.073$ we do observe disappearing of unitarity in the solution, which gives the limiting case. We do not know what happens for larger numbers of points. This result shows that the *GR* method is a numerical method that converges very satisfactorily, as has been previously mentioned in the cases of two-dimensional corrugations.[12-14]

TABLE III. Analysis of the unitarity obtained with the *GR* method for corrugation (33a) and using $2N = 40$.

h \ θ_i	0°	20°	40°	60°	80°
0.01	7[a] 1.0000[b]	7 1.0000	7 1.0000	6 1.0000	7 1.0000
0.02	7 1.0000	7 1.0000	7 1.0000	6 1.0000	1.0000
0.03	7 1.0000	7 1.0000	7 1.0000	6 1.0000	7 1.0000
0.04	7 1.0000	7 1.0000	7 1.0000	6 1.0000	7 1.0000
0.05	7 0.9999	7 0.9999	7 0.9999	6 0.9999	7 0.9998
0.06	7 1.0000	7 1.0000	7 1.0014	6 0.9998	7 0.9964
0.07	7 1.0003	7 0.9998	7 0.9997	6 0.9961	7 1.0120
0.08	7 0.9915	7 1.0042	7 1.0993	6 0.9194	7 1.0368
0.09	7 0.9333	7 1.0047	7 1.0740	6 1.0455	7 1.0519
0.10	7 0.9928	7 0.9434	7 2.0495	6 1.5865	7 2.0155

[a] Number of F vectors. [b] Unitarity.

B. RG computations (MMM formalism)

Tables V and VI show the computations, using the *RG* method [formula (32)] for obtaining $f(x)$ and formula (31) to calculate A_G, for the corrugations (33a), (33c), and (33d) at normal incidence and $2\pi k_i = 20$. We use the same notation used in previous tables. We notice that the solution obtained has a pronounced dependence on the number of points used throughout the computations, as shown in Table VII, contrary to what happens with the *GR* method. We do think this is because of the numerical procedure used. Goodman[25] has communicated to us that for small $h (h \leq 0.12)$ he obtains convergent solutions. Note that the MMM formalism implies $B_G = -\delta_{G,0}$ and Eq. (23) may be very difficult to satisfy because of the form of the integral when $G \to \infty$. As we argued before, these are very severe boundary conditions to be verified numerically. We have also made computations by increasing the incident wave vector k_i, that is to say, by increasing the number of F vectors, and we find that the number of points used must then be larger in order to obtain a convergent solution and that the convergence limit h increases slowly.

It should be stressed that when unitarity is achieved the Rayleigh hypothesis and MMM formalism give the same diffraction probabilities, as shown in Tables I, II, V, and VI in which the results are practically the same except perhaps for small numerical deviations.

On the other hand, it seems that the *RG* method gives poorer results than others which have been proposed,[17,18] even if it is simpler to use.

TABLE IV. Unitarity obtained with the *GR* method using $2N = 140$ at normal incidence, $2\pi k_i = 20$ with varying h. Notice that the analytical limit $h \cong 0.072$ is satisfied by the numerical results. The number of F vectors is 7.

	Corrugation (33a)									
h	0.07	0.071	0.072	0.073	0.074	0.075	0.076	0.077	0.078	0.079
Unitarity	0.9999	0.9997	0.9985	0.9991	0.9965	0.9943	1.0132	1.0998	1.1254	1.1843

TABLE V. Diffraction probabilities for $2\pi k_i = 20$. *RG* method (MMM formalism).

Beam \ h	0.02	0.04	0.06	0.08	0.1	
	Corrugation (33a), $2N = 10$					
0	7.2877 (-1)	2.2813 (-1)	1.033 (-3)	8.8125 (-2)	1.436 (-1)	
1	1.3143 (-1)	3.2111 (-1)	3.1089 (-1)	1.0456 (-1)	3.66 (-4)	
2	4.161 (-3)	5.2875 (-2)	1.7996 (-1)	3.1590 (-1)	3.362 (-1)	
3	1.690 (-5)	9.469 (-4)	8.627 (-3)	3.5622 (-2)	9.443 (-2)	
$\Sigma_F P_F$	1.0000	1.0000	1.0000	1.0000	1.006	
h	0.02	0.04	0.06	0.08	0.02	0.04
	Corrugation (33a), $2N = 8$				Corrugation (33a), $2N = 14$	
0	7.2877 (-1)	2.2813 (-1)	1.039 (-3)	8.773 (-2)	7.2877 (-1)	2.2813 (-1)
1	1.3143 (-1)	3.3205 (-1)	3.1014 (-1)	1.018 (-1)	1.3143 (-1)	3.3211 (-1)
2	4.161 (-3)	5.3015 (-2)	1.8249 (-1)	3.312 (-1)	4.161 (-3)	5.2876 (-2)
3	1.655 (-5)	8.691 (-4)	7.089 (-3)	2.487 (-2)	1.691 (-5)	9.46 (-4)
$\Sigma_F P_F$	1.0000	1.0000	1.0005	1.004	1.0000	1.0001

C. RR′ computations (CG exact formalism)

We shall now discuss the results obtained for the diffraction probabilities by applying the *RR′* numerical procedure [Eqs. (28)–(31)] to the CG exact formalism [Eqs. (11)–(13)].

Tables VIII–X present these results for $2\pi k_i = 20$, normal incidence, and for the four corrugations (33a)–(33d). We use the number of points, $2N$, necessary to achieve convergence, that is to say unitarity, and this depends on the shape and strength of the corrugations. For larger values of $2N$ unitarity remains valid. The number of G vectors used in the sums of matrix elements [Eqs. (28) and (29)] is the one needed to obtain unitarity and is not given explicitly. We find no limitations on the shape and strength of the corrugations and if we do not present calculations for larger values of h it is because we do not believe it necessary or have reached the maximum limit [Eq. (33d)]. We do, however, present convergent solutions for $h = 1$ in the cosine-like case [corrugation (33a)], which is a value 10 times larger, to our knowledge, than for any other calculated case, and for $h = 0.3$ for the sawtooth corrugation (33c).

Computations of $f(n)$ are presented for the corrugations (33a) and (33c) in Figs. 4 and 5. Note that when $h = 0.01$ the result is practically constant, $-f(n) \simeq k_z$, as it should be for the case

TABLE VI. Diffraction probabilities for $2\pi k_i = 20$. *RG* method (MMM formalism). These computations correspond to the number of points ($2N$) that give a convergent solution for a higher value of h.

Beam \ h	0.02	0.04	0.06	0.08	0.1
	Corrugation (33c), $2N = 10$				
0	8.0264 (-1)	3.8561 (-1)	7.3418 (-2)	1.779 (-3)	5.3240 (-1)
1	9.5131 (-2)	2.6751 (-1)	3.2094 (-1)	2.1049 (-1)	6.6416 (-2)
2	2.996 (-3)	3.9486 (-2)	1.4402 (-1)	2.8411 (-1)	3.6759 (-1)
3	5.846 (-4)	7.346 (-4)	6.301 (-4)	7.631 (-3)	3.5078 (-2)
$\Sigma_F P_F$	1.0000	1.001	1.004	1.006	0.992
h	0.02	0.04	0.06	0.08	0.1
	Corrugation (33d), $2N = 10$				
0	7.9568 (-1)	3.8703 (-1)	1.0856 (-1)	7.3066 (-2)	...
1	9.3431 (-2)	2.5866 (-1)	3.1762 (-1)	2.3505 (-1)	...
2	8.040 (-3)	4.4729 (-2)	1.1934 (-1)	2.1038 (-1)	...
3	6.674 (-4)	2.800 (-3)	7.9941 (-3)	2.1066 (-2)	...
$\Sigma_F P_F$	0.9999	0.9998	0.998	1.006	1.2

TABLE VII. Values of h for which the MMM formalism and the RG method give a convergent solution as the number of points ($2N$) used in the RG method is increased. The incident wave vector is $2\pi k_i = 20$ at normal incidence. The number of F vectors is 7.

	Corrugation (33a)					
$2N$	8	10	12	14	16	20
h	0.08	0.1	0.08	0.04	0.02	<0.01

$h \to 0$. This shows that the numerical procedure used is satisfactory. On the other hand, when h increases $f(n)$ oscillates strongly. We stress the difficulty of satisfying equation (23) for such a behavior of $f(x)$ for large strengths. We do not know if in these oscillations $f(x)$ goes to infinity because no computer solutions can answer this question. However, we note that by increasing the number of points $2N$, $f(n)$ remains practically unchanged.

It should be stressed again that no matter when unitarity is reached with the Rayleigh, MMM, and CG formalisms, the *diffraction probabilities* are the same as shown in the above tables. However, the only one that always gives a convergent numerical solution is the CG formalism with the RR' numerical procedure. This has been proved numerically, not only in the cases presented here, but in many other calculations, varying the energy, the incident angle θ_i, and corrugation, as for example in the case of the scattering of thermal atomic He beams from stepped surfaces for which $2\pi k_i \simeq 100$.[3,20]

D. Some comments on the A_G and B_G values obtained with the three formalisms

We have compared in Secs. A–C the diffraction probabilities obtained within the three formalisms which give the same values when unitarity is satisfied; however they are calculated with formula (15) which only requires the modulus of the F-vector amplitudes. Other questions remain open, as for example: (i) What happens with the A_G values for F and E vectors? (ii) What happens with the B_G values obtained with the MMM and CG formalisms? (iii) Is the CG calculated wave function zero at $z \leq D(x)$? (iv) Do the diffraction probabilities obey a vertical-tangent law at threshold conditions?

The following numerical answers can be given:

(i) Regarding the A_F calculated with the GR and RR' methods (Table XI), they have the same real part, while the imaginary parts are smaller in both cases, but those of the Rayleigh hypothesis are two orders of magnitude smaller. These differences, perhaps due to numerical procedures, are such that there are no appreciable changes in the diffraction probabilities P_F. The A_E are small when E increases if h is small enough, but those of Rayleigh are much smaller. This is necessary to achieve a convergent solution with his hypothesis. Observe that when h increases from 0.02 to 0.06 the CG formalism gives larger values of A_E for $E \to \infty$, while the Rayleigh approximation fails to do this. Finally, in Table XII the h values are large enough that the approximation does not give a convergent solution, and this is because the A_E values tend to infinity as $E \to \infty$ but slower than

TABLE VIII. Diffraction probabilities for $2\pi k_i = 20$. RR' method (CG formalism).

Beam \ h	0.02	0.06	0.08	0.12	0.20	0.25
	Corrugation (33a), $2N = 40$					
0	7.3000 (-1)	1.017 (-3)	8.9057 (-2)	3.825 (-2)	6.5127 (-1)	9.132 (-2)
1	1.3197 (-1)	3.1158 (-1)	1.0467 (-1)	1.0665 (-1)	4.4214 (-2)	2.7359 (-1)
2	4.053 (-3)	1.8028 (-1)	3.1794 (-1)	2.3042 (-1)	1.5889 (-2)	8.113 (-2)
3	1.395 (-5)	8.510 (-3)	3.4404 (-2)	1.4485 (-1)	1.1623 (-1)	9.902 (-2)
$\Sigma_F P_F$	1.0000	1.0000	1.0000	1.0000	1.0000	0.9998
	$2N = 40$	$2N = 40$	$2N = 80$	$2N = 80$		
h	0.30	0.36	0.5	1.0		
	Corrugation (33a)					
0	2.9369 (-1)	5.4917 (-1)	5.7857 (-1)	5.8301 (-1)		
1	6.4021 (-2)	7.1992 (-2)	6.3764 (-2)	1.2139 (-1)		
2	2.4936 (-1)	6.2265 (-2)	4.6360 (-2)	5.3673 (-2)		
3	4.0191 (-2)	9.8006 (-2)	9.9403 (-2)	6.5871 (-2)		
$\Sigma_F P_F$	1.0008	1.0005	0.9999	0.9998		

TABLE IX. Diffraction probabilities for $2\pi k_i = 20$. RR' method (CG formalism).

Beam \ h	0.02	0.04	0.06	0.08	0.10	0.12
			Corrugation (33b), $2N = 60$			
0	7.1806 (-1)	2.1618 (-1)	3.3111 (-2)	1.8249 (-1)	2.6604 (-1)	1.2718 (-1)
1	1.3273 (-1)	3.2979 (-1)	2.9830 (-1)	9.4874 (-2)	1.2303 (-2)	1.2687 (-1)
2	7.959 (-3)	5.7936 (-2)	1.6418 (-1)	2.5268 (-1)	2.2981 (-1)	1.2031 (-1)
3	2.619 (-4)	4.222 (-3)	2.0960 (-1)	6.1115 (-2)	1.2471 (-1)	1.8877 (-1)
$\Sigma_F P_F$	1.0000	1.0000	1.0000	1.0000	0.9999	0.9999

e^{Bx}. For example for $h = 0.1550$, $\mathrm{Re}A_{20} = 7.421(2)$ and $\mathrm{Im}A_{20} = 1.605(2)$ or for $h = 0.250$, $\mathrm{Re}A_{20} = -9.559(6)$ and $\mathrm{Im}A_{20} = -1.122(8)$. It is clear and obvious that for this behavior of A_E it is impossible to obtain a solution with the Rayleigh hypothesis [Eq. (26)]. Note that we still have the property $\lim_{E\to\infty} A_E e^{-Bx} = 0$.

(ii) In the numerical calculations we do not need $B_G \approx 0$, but better, $B_G e^{ik_{Gx} D_{\min}} \approx 0$. So, as we discussed previously in Sec. II A, the possibility exists of having the latter condition with $B_E \neq 0$. In our calculation method, the B_E have no real physical sense. Observe that we impose a boundary condition on each point on the surface and then we must test the value of the wave function at each point. As shown in Table XIII, B_E can be large and $\psi(x, z) \approx 0$. In any case, not much attention should be paid to the B_E values and we may make some numerical errors in calculating the integral (16) given the oscillating character of $f(x)$ for large h. On the contrary, it is interesting to observe that $B_F \approx 0$ must always be satisfied in order to make the wave function go to zero; this is because of the propagating character of the F waves. The numerical errors for F waves are smaller than for E large.

(iii) Even if the B_E obtained with the CG formalism are not zero, the value of the wave function below the surface $z = D(x)$ is practically zero, as implied by the condition (6) imposed on the density of sources $f(x)$. The last two lines of Table XIII give values practically zero for $\psi(\vec{r}_1)$ and $\psi(\vec{r}_2)$, for $h = 0.01$ and $h = 0.25$, at the points $\vec{r}_1 = (0, -2\pi h)$ and $\vec{r}_2 = (0, -4\pi h)$. In all the calculated cases $|\psi(r)|^2 < 10^{-5}$. We should stress here that we have recalculated the wave function for points $(x_p, D(x_p))$ at which boundary conditions were not imposed on each point; that is to say we impose boundary conditions on the points $x_0, x_1, \ldots, x_N$ and then the wave function is zero. However, it turns out that if the result is unitary then the value of the wave function at intermediate points x_p is also practically zero. This also happens with the Rayleigh hypothesis.

(iv) Figure 6 shows the correct behavior of the beams at threshold conditions obtained with the GR and RR' numerical methods, varying θ_i for $2\pi k_i = 20$ and $h = 0.06$. Computations by Masel *et al.*[26] within the MMM formalism do not show this correct behavior (Figs. 4 and 5 from Ref. 26).

TABLE X. Diffraction probabilities for $2\pi k_i = 20$. RR' method (CG formalism).

Beam \ h	0.02	0.06	0.12	0.15	0.18	0.30
			Corrugation (33c), $2N = 60$			
0	8.0265 (-2)	8.902 (-2)	7.3732 (-2)	4.638 (-3)	8.2151 (-2)	3.2631 (-1)
1	9.5131 (-2)	3.2945 (-1)	3.0541 (-2)	8.7612 (-2)	1.3406 (-1)	1.7959 (-1)
2	2.996 (-3)	1.2554 (-1)	3.6565 (-1)	1.9664 (-1)	4.5550 (-2)	6.5091 (-2)
3	5.852 (-4)	6.128 (-4)	9.7013 (-2)	2.1343 (-1)	2.7932 (-1)	8.8462 (-2)
$\Sigma_F P_F$	1.0000	1.0000	1.0000	1.0000	1.0000	0.9995
h	0.02	0.06	0.10	0.16	0.19	0.22
			Corrugation (33d), $2N = 40$			
0	8.1272 (-1)	1.2820 (-1)	1.5851 (-1)	2.9963 (-1)	2.5149 (-1)	1.9140 (-1)
1	8.6003 (-2)	3.2224 (-1)	1.2710 (-1)	4.5916 (-2)	1.2606 (-1)	1.8406 (-1)
2	6.333 (-3)	1.0479 (-1)	2.6260 (-1)	2.4206 (-1)	1.8015 (-1)	1.4571 (-1)
3	4.251 (-4)	6.501 (-3)	2.7860 (-2)	6.2205 (-2)	6.8040 (-2)	6.9316 (-2)
$\Sigma_F P_F$	0.9999	0.9999	0.9999	1.0000	1.0000	1.0001

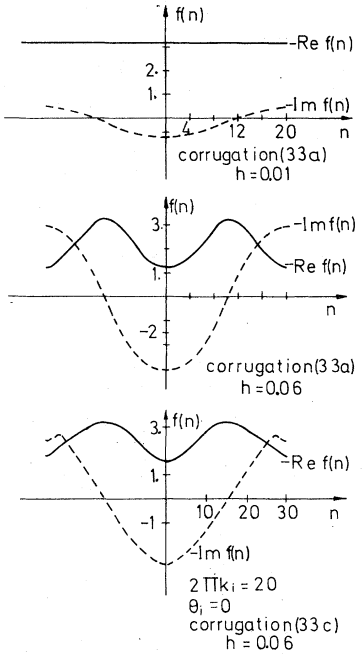

FIG. 4. Values of $f(n)$ (RR' method) for different shapes and strengths of the corrugations indicated in the figure. Observe that for $h=0.01$, -Ref $(n) \simeq k_z$ and Imf (n) is small; in the limit $h=0$, -Ref $(n)=k_z$ and Imf $(n)=0$. As h increases, $f(n)$ varies more.

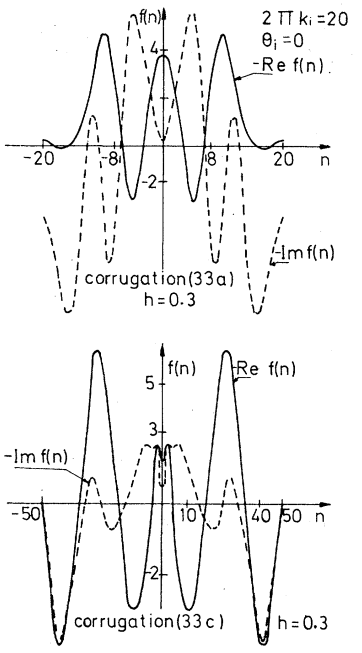

FIG. 5. Same as Fig. 4 for larger values of h. Note the strong oscillations of $f(n)$ for these relatively high values of the strength h.

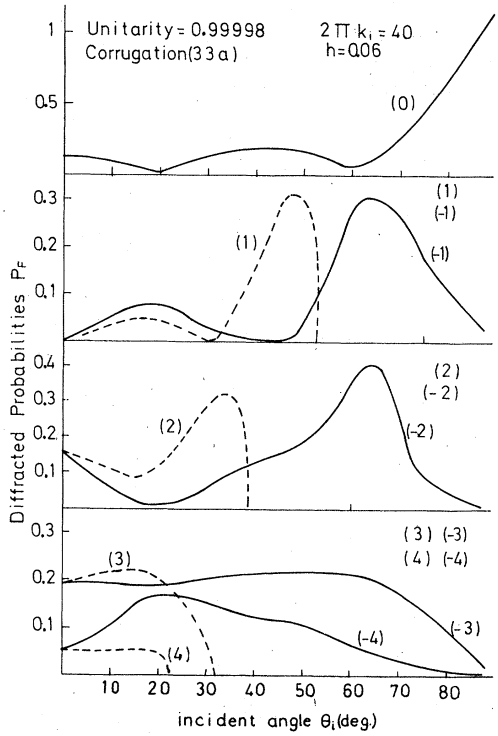

FIG. 6. Diffraction probablities calculated with the GR and RR' methods varying θ_i. Observe the correct behavior at threshold conditions of beams–4.

V. CONCLUSIONS

Due to the results presented in Sec. IV, we reach the following conclusions.

(i) The only formalism that leads to the exact numerical solution, when this exists, is the "new" formalism, the numerical method RR' yields a convergent approximate solution. The above formalism, based on Huygens' principle, is "new" in the sense that we stress its validity as well as establish the RR' numerical procedure to solve it. This is the first time that such numerical solutions are presented.

(ii) We believe that imposing a boundary condition on the correct wave function $\psi(x, z=D_{\min}) \equiv 0$ (extinction theorem) we reach the same solution as with the CG formalism, that is to say the extinction theorem also yields a correct solution in all cases.

(iii) The conditions $\delta_{G,0}+B_G=0$ imposed by the MMM formalism are exact but this is not a "practical" way of writing boundary conditions from the numerical point of view. Until now convergent solutions have not been obtained for $h \gtrsim 0.2$.[25] In our opinion there is no possibility of solving this equation for large values of h. We are now trying to solve the equations within the MMM formalism but with the condition $(\delta_{G,0}+B_G)\, e^{ik_{Gz}D_{\min}} \approx 0$ by imposing some behavior law on the B_G values.

TABLE XI. Scattering amplitudes A_G for $2\pi k_i = 20$. Note that even if the outgoing intensities are the same in both formalisms, the amplitudes are different for large G.

	$h = 0.02$ Corrugation (33a)				$h = 0.06$			
	GR Rayleigh		*RR'* CG Formalism		*GR* Rayleigh		*RR'* CG Formalism	
Beam	ReA_G	ImA_G	ReA_G	ImA_G	ReA_G	ImA_G	ReA_G	ImA_G
0	-8.537 (-1)	-3.246 (-7)	-8.527 (-1)	5.320 (-4)	-3.206 (-2)	-3.973 (-5)	-3.121 (-2)	2.710 (-3)
2	7.313 (-2)	6.413 (-7)	7.211 (-2)	3.270 (-5)	4.811 (-1)	3.201 (-4)	4.809 (-1)	-2.686 (-2)
8	-2.615 (-8)	2.037 (-7)	-1.888 (-3)	6.314 (-6)	-6.302 (-4)	5.031 (-4)	3.544 (-3)	1.133 (-2)
14	2.491 (-7)	-5.850 (-8)	-2.699 (-3)	1.039 (-5)	7.878 (-5)	-2.038 (-4)	-3.482 (-2)	8.431 (-2)
20	-4.350 (-8)	1.001 (-7)	-4.467 (-3)	1.677 (-5)	2.314 (-5)	2.231 (-5)	-3.340 (-1)	6.312 (-1)

(iv) The Rayleigh hypothesis works out for small corrugations. The numerical range of validity seems to be consistent with the condition that A_E is small as E increases. In this sense the analytical limit $h = 0.072$,[5-9] for a cosinelike corrugation, seems to be confirmed numerically in Table IV when the number of points in the calculation is large ($2N = 140$).

(v) The numerical procedures called *GR* previously introduced for a two-dimensional corrugation,[12-14] and the *RG* and *RR'* procedures for solving the Rayleigh, MMM, and CG equations simplify the computations carried out by others[10,11,17,18] and seem to behave satisfactorily, although the *RG* method seems to reduce the range of h for convergent solutions.

(vi) The main conclusion to be stressed is that wherever unitarity is verified the diffraction probabilities are the same independently of the formalism used.

Finally, we mentioned that the CG formalism and the *RR'* numerical method allow one to treat problems that could not be handled with other formalisms, as, for example, the case of He thermal beams scattered from stepped surfaces[20] and from impure surfaces. Work is now in progress along these lines as well as for two-dimensional corrugations for which the generalization is trivial.

TABLE XII. Scattering amplitudes for $2\pi k_i = 20$. *RR'* method (CG formalism). Note that A_G increases very quickly as $G \to \infty$ and h increases.

	$h = 0.1550$		$h = 0.250$	
Beam	ReA_G	ImA_G	ReA_G	ImA_G
	Corrugation (33a)			
0	-4.593 (-1)	-1.331 (-2)	1.458 (-2)	-3.111 (-1)
2	1.464 (-1)	5.281 (-2)	3.268 (-1)	-2.386 (-2)
8	5.233 (0)	3.335 (0)	-1.899 (1)	8.515 (1)
14	1.588 (2)	6.724 (1)	-3.775 (3)	7.835 (3)
20	7.421 (4)	1.605 (4)	-9.959 (6)	-1.122 (8)
$\Sigma_F P_F$	1.0000		0.9998	

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APPENDIX A: PROOF OF THE VERTICAL TANGENT OF THE DIFFRACTION PROBABILITIES AT THE THRESHOLD CONDITION

To prove this property the necessary and sufficient condition [see formula (14)] is that the threshold beam F_T satisfy[23,24] $A_{F_T} = \text{const}$. For any $l(x)$, we now define

$$l_{K+F_T} = \int_{-a/2}^{+a/2} l(x)\, e^{-i(K+F_T)x}\, dx\,, \tag{A1}$$

that is to say the $K+F_T$ Fourier component of $l(x)$.

Because of the absolute value in the exponential term of Eq. (11), it is possible to interchange the integral and the summation sign,[27] and then Eq. (11) reads

$$\sum_G \frac{e^{i(K+G)x}}{k_{Gx}} \int_{-a/2}^{a/2} f(x')\, e^{-i(K+G)x'} e^{ik_{Gz}|D(x)-D(x')|} = -e^{i(Kx-k_{iz}z)}\,. \tag{A2}$$

Note that a term of the series at the threshold condition $k_{F_{Tz}} \to 0$ is

$$\frac{e^{i(K+F_T)x}}{k_{F_{Tx}}}\left[f_{K+F_T} + ik_{F_{Tz}}(f|D-D'|)_{K+F_T} + \cdots\right], \tag{A3}$$

where the dots represent small terms. Then, in order to satisfy (A3) we need at least $f_{K+F_T} \simeq \alpha k_{F_{Tz}}$; if this is not so, Eq. (11) will have an infinity.

From the expression for the scattering amplitudes [Eq. (13)], we have for $k_{F_{Tz}} \to 0$,

$$A_{F_T} = (1/k_{F_{Tz}})[f_{K+F_T} - ik_{F_{Tz}}(fD)_{K+F_T} + \cdots] \tag{A4}$$

and, as $f_{K+F_T} \simeq \alpha k_{F_{Tz}}$,

$$A_{F_T} \simeq [\alpha - i(fD)_{K+F_T} + \cdots] = \text{const}\,. \tag{A5}$$

TABLE XIII. B_G values for $2\pi k_i = 20$. These values increase quickly when $G \to \infty$ and h increases. RR' method (CG formalism). The value of the wave function at $\vec{r}_1 = (0, -2\pi h)$ and $\vec{r}_2 = (0, -4\pi h)$ is also given (even though $B_E \neq 0$ the wave function is nearly zero).

	$h = 0.01$		$h = 0.02$		$h = 0.25$	
Beam	$\mathrm{Re}B_G$	$\mathrm{Im}B_G$	$\mathrm{Re}B_G$	$\mathrm{Im}B_G$	$\mathrm{Re}B_G$	$\mathrm{Im}B_G$
			Corrugation (33a), $2N = 40$			
0	-9.998 (-1)	6.031 (-4)	-9.991 (-1)	6.197 (-4)	-1.001	8.638 (-3)
1	-3.053 (-5)	4.650 (-6)	-5.822 (-5)	8.803 (-6)	-9.407 (-4)	-9.830 (-4)
2	-1.181 (-4)	6.491 (-5)	-1.110 (-4)	1.162 (-4)	2.873 (-5)	-1.173 (-3)
3	1.332 (-5)	1.285 (-5)	3.221 (-5)	2.326 (-5)	4.645 (-4)	-1.962 (-3)
8	-1.584 (-3)	-9.795 (-5)	-1.941 (-3)	-4.712 (-4)	3.892 (-1)	1.212 (0)
14	-1.373 (-4)	-1.781 (-4)	-2.723 (-3)	-9.916 (-4)	4.835 (3)	1.197 (4)
20	-1.440 (-3)	-2.588 (-4)	-4.329 (-3)	-1.794 (-3)	4.589 (7)	1.319 (8)
$\psi(\vec{r}_1)$	-6.194 (-5)	-1.450 (-5)			8.707 (-4)	1.047 (-3)
$\psi(\vec{r}_2)$	-7.538 (-5)	1.638 (-4)			5.790 (-4)	3.999 (-4)

This proves the correct behavior of the diffraction probabilities at threshold conditions.

APPENDIX B: CALCULATION OF THE MATRIX ELEMENTS M_{nn} [Eq. (30)].

The M_{nn} cannot be calculated from the general formula (32) because for $n = n'$ the series diverges as $\sum_G (1/G)$.

From (11) and for the interval $-\frac{1}{2}\epsilon + x, \frac{1}{2}\epsilon x$ we can write

$$\sum_G \frac{1}{k_{Gz}} \int_{x-\epsilon/2}^{x+\epsilon/2} dx' f(x') e^{i(K+G)(x-x')} \times e^{ik_{Gz}|D(x)-D(x')|}, \tag{B1}$$

where $\epsilon = 1/2N$ and $f(x') = f(x) = \text{const}$ in the interval.

Then by retaining only the linear term in $|D(x) - D(x')|$,

$$|D(x) - D(x')| \simeq |D'(x)|\,|x - x'|, \tag{B2}$$

integrating (B1), and for discrete x, we obtain formula (32). Note that for $G \to \infty$ formula (30) for $2N$ fixed behaves as $1/G^2$.

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