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# Diffraction spectrum of a finite grating section from the sole diffraction S-matrix of the infinite grating

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**Abstract**—The possibility is demonstrated to obtain the diffraction pattern at infinity in the Fraunhofer zone of a finite section of a grating from the diffraction S-matrix of a plane wave by the infinite grating without limitation on the surface corrugation depth. A truncated plane wave impinges on the grating section which may consist of an integer number of periods of an actually periodic grating, or a finite section of an aperiodic surface corrugation repeated periodically, considered as the period of a virtual grating. Concrete examples illustrate the usefulness of the method and its highlighting physical meaning.

*OCIS codes:* (290.5880) Scattering, rough surfaces, (050.0050) Diffraction and gratings, (260.2110) Electromagnetic optics, (260.0260), Computational electromagnetic

## I. INTRODUCTION

Scattering of electromagnetic waves by rough surfaces occurs in many areas: optics, radar detection, telecommunications and more recently in computer graphics for the characterization of textures of materials [1,2,3,4,5,6,7]. If scattering surfaces are perfectly conducting, the equations are dimensionless and therefore apply regardless of the frequency used.

According to the geometry of the surface, methods used to solve are of different types depending on the value of the radius of curvature with respect to the wavelength. They appeal to geometrical optics for very large radii of curvature, physical optics or geometrical theory of diffraction for large curvatures and electromagnetism to the curvatures of the order of magnitude of the wave length. Scalar Kirchhoff approximation theory (KA) is the most widely used theory in the wave scattering from rough surfaces [1]. The advantage of this method is that it is easy to implement from the physical optics and leads to relatively simple analytical expressions for scattered field amplitudes. The basic feature of the KA is the assumption that the wave field on the surface of a scatterer is approximated as follows: each point of the surface is considered as a point of an infinite plane parallel to the local tangent surface. The interaction of the wave field with the surface is treated as the interaction of that field with that plane. KA gives good results in a rather large domain, but when the roughness becomes large, it appears multiple reflections; then it's necessary to use rigorous electromagnetic methods. In this paper, we propose a new approach to this problem in the resonant domain based on the resolution of the diffraction by gratings, for which there are rigorous numerical models and computer gratings codes (GC) that are very effective [8,9,10]. For the sake of simplicity we have chosen to limit our study to perfectly conducting surfaces.

In practice, for numerical modeling, it is impossible to take into account any infinite and aperiodic cylindrical rough surface  $\Sigma$ , described by a profile function  $y = f(x)$  with  $x \in \mathbb{R}$  and  $h = \max(f(x)) - \min(f(x))$  the height of the roughness. Numerical modeling is only possible for a finite window  $W$  of width  $D$  with  $x \in [-D/2, +D/2]$ . An immediate and very important consequence

of this limitation is that all rough surfaces  $\Sigma$  which are identical only inside the window  $W$  gives the same results, let  $\Sigma_D$  the infinite set of these surfaces. A consequence of this spatial restriction to  $W$  is that results given by the numerical modeling are valid for any surface  $\Sigma$  and in particular valid for the periodic surface of period  $D$  ie a grating  $\Gamma \in \Sigma_D$  described with a periodic profile function  $f_D(x)$ , such as  $f_D(x + D) = f_D(x)$  which coincides with  $f(x)$  in the window  $W$ :  $f_D(x) = f(x)$  if  $|x| < D/2$  and  $f_D(x) \neq f(x)$  if  $|x| \geq D/2$ . It is this properties, direct consequence of windowing, which is generally used to model the diffraction by any rough surfaces  $\Sigma \in \Sigma_D$  by assimilating the surface  $\Sigma$  to a grating  $\Gamma \in \Sigma_D$ . Currently, there are many rigorous and very efficient numerical codes GC to model the diffraction of electromagnetic waves by a periodic surface  $\Gamma$ . These codes provide a solution as accurate as desired for  $\Gamma$ . It must be present in the mind that if this resolution is rigorous for  $\Gamma$  with  $x \in \mathbb{R}$  it is only an approximate resolution for  $\Sigma$  when the space is reduced to  $x \in [-D/2, +D/2]$ . The rigorous solution for  $\Gamma$  with  $x \in \mathbb{R}$  contains much more information than those that is accessible only for a window  $W$ . For example, compared to the solution for  $\Sigma$  in the approximation  $W$  the rigorous solution for the grating contains systematic errors due to multiple scattering between different patterns of the grating if the finite size of  $W$  is not taken in account. These multiple scattering involve electromagnetic interactions between the part of  $\Gamma$  inside the window  $W$  and the part outside  $W$ . These interactions appear naturally in the modeling of diffraction by an infinite grating for  $x \in \mathbb{R}$  which should not be taken into account in the modeling for  $\Sigma \in \Sigma_D$  because it is contrary to the starting hypothesis which is to reduce the study to  $W$ . If the height of roughness is small, effect of these multiple scattering is negligible and the method is then very close to a perturbation method. An attractive way for suppressing multiple scattering is, in the numerical model, to place between each patterns of the infinite grating  $\Gamma$  a barrier made with a fictitious material (Perfect Matching Layer) perfectly absorbing for electromagnetic waves thus enabling each pattern of  $\Gamma$  to be decoupled from its neighbors [11]. We propose here another very simply method much easier to implement than PML to suppress these multiple scattering in the rigorous solution for  $\Gamma$ .

In order to understand how to eliminate the multiple scattering in the rigorous solution valid only for the grating  $\Gamma \in \Sigma_D$  and not for any surface  $\Sigma \in \Sigma_D$ , we deliberately restricted our work to the study of diffraction of a beam by a grating  $\Gamma$ . This systematic analysis makes it possible to understand and thus to be able to eliminate the obstacles encountered with the modeling of the diffraction by aperiodic surfaces [Réf Hal]. We show how it is easy to ignore the effects of periodization of the surface  $\Gamma$  which introduces multiple scattering between patterns, that do not exist for a single pattern. We show that, with our method, it is perfectly possible to determine rigorously the diffraction pattern of a single period of the grating illuminated by an electromagnetic wave. This diffraction pattern is identical to the response of aperiodic surface  $\Sigma \in \Sigma_D$  reduced to its inner part  $W$ . Once the finite width  $D$  of the modeling window  $W$  is defined, the method we propose gives the best results that can be obtained with the spatial approximation  $D$  for any aperiodic rough surface  $\Sigma \in \Sigma_D$ .

In section 2, we recall results relative to the diffraction of a plane wave by an infinite grating. Then we introduce the notion of an extended grating problem (EGP) when the incident wave is not only a plane wave but a pseudo-periodic wave, ie represented by a Rayleigh development. After that we show how to analytically and rigorously solve the problem of diffraction of an electromagnetic beam by a grating.

In section 3, we show how the discretization of an aperiodic incident beam leads to its numerical periodization; the beam is then transformed into a Rayleigh development ie a pseudo periodic wave. By using the linearity of the Maxwell equations we deduce the response of the grating to a truncated plane wave (TPW). This allows us to analyze in detail the response of any part of the elementary pattern ie one period of the grating to an incident plane wave. This approach is similar to that of the Huygens-Fresnel principle where an electromagnetic wave is decomposed into an infinite sum of point sources; the sum of the elementary responses naturally gives the response of the grating to the initial plane wave. Finally we show how the application of the stationary phase approximation makes it possible to determine the radiation pattern at infinity in the Fraunhofer zone of any part of  $\Gamma$  illuminated by a TPW.

To demonstrate the effectiveness of our approach we give some numerical results in sections 4 and 5. We have chosen two canonical profiles, triangular and parabolic, for which it is simple to interpret results from geometrical optics and physical optics. We show that our results are in very good agreement with those obtained by the completely different methods of classical optics. In section 4 we study the case of the hollow triangular profile when the angle between the facets is  $90^\circ$ . In this very particular case with a double reflection, the geometrical optics shows that there is retro-reflection, ie. the light is totally reflected in the direction of incidence. We show that the results obtained by our electromagnetic method using diffraction by gratings are in perfect agreement with predicted results by geometric optics.

## II. DIFFRACTION BY A GRATING

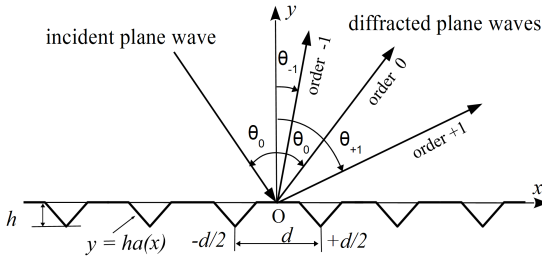


Figure 1. Diffraction of a plane wave by a grating

### A. Diffraction of a plane wave by a grating

Let us consider a grating whose surface coincides with a cylindrical surface, described in rectangular Cartesian coordinate system  $Oxyz$  by a periodic profile function  $y = ha(x)$  with period  $d$  (Fig. 1.). The grating is illuminated from the vacuum by an incident monochromatic plane wave with wavelength  $\lambda$  with the incident angle  $\theta_0$ . The time dependence is  $\partial/\partial t \rightarrow i\omega$  where  $\omega$  is the angular frequency [8,9]. Although the method is applicable to any grating, for the sake of simplicity, we consider only the case of perfectly conducting grating.

For 2D problems ( $\partial/\partial z \rightarrow 0$ ) there are two kinds of solutions **TE** and **TM**. In both cases the electromagnetic field is completely determined by the knowledge of its component along  $Oz$ ; we note that component  $F(x, y)$  with  $F = E_z$  for **TE** polarization and  $F =$

$H_z$  for **TM** polarization. The field of the incident plane wave is written:  $F^-(x, y) = A_0^- e^{-ik\alpha_0 x} e^{+ik\beta_0 y}$  with  $\alpha_0 = \sin \theta_0$  and  $\beta_0 = \cos \theta_0$ . Above the grating,  $y > \max(ha(x))$ , the diffracted wave has the form of a Rayleigh development which consists of a sum of plane waves and the total field is:

$$F(x, y) = A_0^- e^{-ik\alpha_0 x} e^{+ik\beta_0 y} + \sum_{n=-\infty}^{+\infty} A_n^+ e^{-ik\alpha_n x} e^{-ik\beta_n y}, \quad (1)$$

with:  $\alpha_n = \alpha_0 + n \frac{\lambda}{d}$ .

If  $|\alpha_n| < 1$  then  $A_n^+$  correspond to outgoing propagating wave with angle  $\theta_n$  so that  $\alpha_n = \sin \theta_n$  and if  $|\alpha_n| > 1$  to an evanescent wave. With our notations the propagation constant  $\beta_n$  according to  $Oy$  is given by:

$$\beta_n = \begin{cases} \sqrt{1 - \alpha_n^2} = \cos \theta_n & \text{if } |\alpha_n| < 1 \\ -i\sqrt{\alpha_n^2 - 1} & \text{if } |\alpha_n| > 1 \end{cases}. \quad (2)$$

Far from the grating, in the Fresnel zone, evanescent waves vanished, the diffracted wave is only composed of a finite set of propagative plane waves with angles  $\theta_n$  so that:

$$\begin{aligned} \alpha_n &= \sin \theta_n = \sin \theta_0 + n \frac{\lambda}{d}, \\ \beta_n &= \cos \theta_n, \end{aligned} \quad (3)$$

with  $n \in U_d = \{n \in \mathbb{Z} \mid |\sin \theta_0 + n \frac{\lambda}{d}| < 1\}$ .

The far diffracted field can therefore be written:

$$F^+(x, y) = \sum_{n \in U_d} A_n^+ e^{-ik \sin \theta_n x} e^{-ik \cos \theta_n y}. \quad (4)$$

The boundary conditions on the grating surface are used to calculate the diffracted amplitudes  $A_n^+$  in the directions  $\theta_n$  and therefore fractions of energy diffracted in these directions or efficiencies:  $W_n = (|A_n^+|^2 / |A_0^-|^2) (\cos \theta_n / \cos \theta_0)$ .

For numerical modeling we use the C-method or Chandezon method [10,12,13,14] developed in our Laboratory from the late 70s. This is a differential method of solving Maxwell's equations in a curvilinear translation coordinate system  $(u, v)$  adapted to the geometry of the surface such that the surface  $v = 0$  coincides with the grating surface.

### B. The extended grating problem

In fact, numerical modeling gives the solution of a more general problem called here extended grating problem (EGP). This is where the incident wave is not a single plane wave, but a sum of incoming plane propagating waves and evanescent waves in accordance with  $\alpha_n$ . These waves are correlated with each other and have complex amplitudes  $A_n^-$ . Propagation constants  $\alpha_n$  obey to grating equation (Eq. (1)). For  $y > \max(ha(x))$  the total field is written:

$$F(x, y) = \sum_{n=-\infty}^{+\infty} e^{-ik\alpha_n x} \left[ A_n^- e^{+ik\beta_n y} + A_n^+ e^{-ik\beta_n y} \right]. \quad (5)$$

The first sum represents the incoming waves and the second outgoing waves. In the numerical approximation of order  $M$  where  $-M \leq n \leq +M$  we keep only  $2M + 1$  terms in this development. The writing of boundary conditions on the surface  $y = ha(x)$  allows to determine the linear relationship between the  $2M + 1$  amplitudes of the incoming waves  $A_m^-$  assumed to be known, and those of the  $2M + 1$  amplitudes of outgoing waves  $A_n^+$ :

$$A_n^+ = \sum_{m=-M}^{+M} S_{m,n} A_m^-. \quad (6)$$



is an integer, then the period of modeling is  $Nd$ . The calculations for the incidences  $\alpha_p = \alpha_0 + p\Delta\alpha$  are then interpreted as EGP for the period  $Nd$ . Considering that the grating is of period  $Nd$  leads to make  $N$  independent calculations with EGP for the period  $d$  with  $N$  different angles of incidence  $\theta_{0,q}$  such as:

$$\sin \theta_{0,q} = \sin \theta_0 + q \frac{\lambda}{Nd} \text{ with } q = 0, 1, \dots, N-1. \quad (19)$$

After discretization the aperiodic initial problem of the diffraction of a beam by a grating (AP) is replaced by another one which is periodic (PP): diffraction of pseudo periodic incoming wave of period  $D = Nd$  by a grating of period  $d$ . The solution of PP is an approximate solution of AP only for  $|x| < D/2$ . The solution for PP better approximate AP when  $D$  is large

To obtain a good approximate numerical solution of AP one must choose  $N$  sufficiently large in such a way that the calculated values  $A_p^+ = A^+(\alpha_p)$  are sufficiently close to obtain, after linear interpolation, a continuous curve  $A^+(\alpha)$ . It is noted that for a given value of  $N$ , the calculation involves multiple diffractions between the incident beam and  $N$  patterns of the grating: if  $N = 1$  no multiple diffraction between patterns is taken into account.

### C. Analysis of diffracted wave

We have shown that for a given value of  $N$  we solve numerically and rigorously PP for the period  $D = Nd$ . The electromagnetic field calculated in this way in the space portion  $\tilde{D} = \{x \in [-D/2, +D/2], y \in \mathbb{R}^+\}$  is an approximation of the desired solution of AP in  $\tilde{D}$ . In the plane  $y = 0$  located immediately above the grating the diffracted wave  $F_0^+(x) = F^+(x, y = 0)$  is a pseudo periodic function of period  $D$ . Only the part of the field calculated in the domain  $x \in \tilde{D}$  corresponds to the approximate solution discretized in  $\alpha$  of AP in approximation  $N$ . When  $N$  increases, this increases the accuracy of the calculation for AP ( $\Delta\alpha$  decreases) and the range of validity  $\tilde{D}$  increases. Only the field calculated in  $\tilde{D}$  must be taken into account to calculate the radiated energy at infinity for AP. For this, and as we did for the incident wave, we write that  $F_0^+(x)$  can be expressed as the sum of two "complementary" aperiodic functions  $F_D^+(x)$  and  $F_{D^*}^+(x)$  of width  $D$  centered at  $x = 0$ :

$$\begin{cases} |x| < D/2 & F_D^+ = F_0^+ \text{ and } F_{D^*}^+ = 0 \\ |x| > D/2 & F_D^+ = 0 \text{ and } F_{D^*}^+ = F_0^+ \end{cases} \quad (20)$$

$F_D^+(x)$  is the rigorous field of PP restricted to  $x \in \tilde{D}$ ; it is also the best approximation for the field of AP for  $x \in \tilde{D}$ . If one is only interested in the far field, ie the plane waves propagating one can write:

$$F_D^+(x, y) = \Pi\left(\frac{x}{D}\right) \sum_{n \in U_D} A_n^+ e^{-ik\alpha_n x} e^{-ik\beta_n y}. \quad (21)$$

with:

$$U_D = \{n \in \mathbb{Z} \mid |\sin \theta_0 + n \frac{\lambda}{D}| < 1\}. \quad (22)$$

In the plane  $y = 0$  the TPW of width  $D$  associated to the plane wave of order  $n$  of the previous Rayleigh development is written:

$$F_{D,n}^+(x, y = 0) = \Pi\left(\frac{x}{D}\right) A_n^+ e^{-ik\alpha_n x}. \quad (23)$$

Let us write this expression in the form of a Fourier integral:

$$F_{D,n}^+(x, y = 0) = \int_{\alpha=-\infty}^{+\infty} A_n^+(\alpha) e^{-ik\alpha x} d\alpha, \quad (24)$$

with:

$$A_n^+(\alpha) = A_n^+ \frac{D}{\lambda} \text{sinc}(\pi(\alpha - \alpha_n)D/\lambda). \quad (25)$$

Finally, the approximate diffracted field of AP for all TPW associated to real orders of diffraction for the period  $D$  is written:

$$\begin{aligned} F_D^+(x, y) &= \sum_{n \in U_D} F_{D,n}^+(x, y), \\ &= \sum_{n \in U_D} \int_{\alpha=-\infty}^{+\infty} A_n^+(\alpha) e^{-ik\alpha_n x} e^{-ik\beta_n y} d\alpha. \end{aligned} \quad (26)$$

For AP, in the approximation  $N$ , this expression is, a priori, only valid for  $x \in \tilde{D}$ . It is nevertheless possible to use it as an extrapolation relation to determine the field at infinity outside  $\tilde{D}$ . It then expresses, as for the principle of Huygens, the radiation of the portion of width  $D$  of the electromagnetic wave which exists in the plane  $y = 0$  and approximately the radiation of the portion  $D$  of the diffraction grating.

### D. Radiation in Fraunhofer zone

Consider an observation point P (Fig. 2.) in Fraunhofer zone. This point is situated far from the origin at the distance  $r = \sqrt{x^2 + y^2}$  in the direction  $\theta$ . From P the radiating element of width  $D$  is seen from an angle  $\Delta\theta \simeq D/(r \cos \theta)$  let  $\Delta(\sin \theta) \simeq D/r$ . The discretization in  $\alpha$  of AP is done every  $\Delta\alpha = \lambda/D$ . If  $\Delta(\sin \theta) \ll \Delta\alpha$  ie if  $r \gg D^2/\lambda$  then the width part  $D$  of the grating is seen from P as a point at infinity: P is in the Fraunhofer domain.

At point P the diffracted wave is a locally plane wave whose amplitude decreases as  $1/\sqrt{r}$ , it is possible to calculate its amplitude by evaluating by the method of the stationary phase (Appendix 2) the integrals intervening in the expression of the field in P (Eq.26). It is then shown that for each diffraction order  $n$  the diffracted field  $F_n^+(x, y)$  expressed as a function of  $r$  and  $\theta$  is written:

$$F_n^+(r, \theta) = B_n^+(\theta) \frac{e^{-ikr}}{\sqrt{r}}, \quad (27)$$

with:

$$B_n^+(\theta) = \cos \theta A_n^+(\theta) \sqrt{2\pi} e^{-i\pi/4}. \quad (28)$$

For all the orders of the grating, the field radiated by the portion  $D$  of the grating is written:

$$F_D^+(r, \theta) = \sum_{n \in U_D} \cos \theta A_n^+(\theta) \sqrt{2\pi} e^{-i\pi/4} \frac{e^{-ikr}}{\sqrt{r}}. \quad (29)$$

At point P in Fraunhofer domain, in the chosen approximation  $\Delta\alpha$ , all outgoing waves can be considered as coming from a single source point located at the distance  $r$  from P, they are therefore in phase. We can therefore write that the resulting field radiated in P is written:

$$\begin{aligned} F_D^+(r, \theta) &= \sum_{n \in U_D} \cos \theta |A_n^+(\theta)| \sqrt{2\pi} \frac{e^{-ikr}}{\sqrt{r}}, \\ &= \sqrt{2\pi} \cos \theta \frac{e^{-ikr}}{\sqrt{r}} \sum_{n \in U_D} |A_n^+(\theta)|. \end{aligned} \quad (30)$$

Locally the diffracted wave has the structure of a plane wave of direction  $\vec{r}$ , the energy  $\Delta W(\theta)$  radiated by this wave in angle  $\Delta\theta$ :

$$\Delta W(\theta) = \frac{2\pi \cos^2 \theta}{r} \sum_{n \in U_D} (|A_n^+(\theta)|)^2 r \Delta\theta. \quad (31)$$

The normalized angular power density  $W(\theta)$  defined as:

$$W(\theta) = \frac{1}{2\pi} \frac{\Delta W(\theta)}{\Delta\theta}, \quad (32)$$

is written:

$$W(\theta) = \cos^2 \theta \sum_{n \in U_D} (|A_n^+(\theta)|)^2. \quad (33)$$

$$W(\theta) = \cos^2 \theta \left( \frac{D}{\lambda} \right)^2 \sum_{n \in U_D} |A_n^+|^2 \text{sinc}^2(\pi(\sin \theta - \sin \theta_0) \frac{D}{\lambda}) \quad (34)$$

#### E. Numerical examples

Provided we know the S matrix associated to the grating then, from a single calculation, it is possible to analyze in detail the response of this grating when only a part of a pattern is illuminated by a plane wave. The C-method we use applies to a very wide range of profiles in terms of period, height and shape. In order to show the interest of our analysis, in this paper, we studied two geometrically simple profiles: triangular hollow and parabolic. These canonical profiles were selected because it is very easy to obtain for comparisons approximate results with the classical methods of geometrical optics and physical optics. For all the numerical examples we have chosen a study window  $W$  whose width  $D$  is equal to the period of the associated grating  $D = d$ ,  $N = 1$ .

#### IV. DIFFRACTION BY TRIANGULAR HOLLOW GRATING

For this example the elementary pattern ABCDE of the grating is a hollow triangle in a plane (Fig. 3) the period is  $d = 12.8\lambda$ . It consists of four planar facets AB, BC, CD and DE such that the projections of each facet on the  $x$ -axis is equal to  $b = d/4 = 3.2\lambda$ . The height of the grating is  $h = b/\sqrt{3} = 1.85\lambda$  then  $\varphi = 30^\circ$  (angle between the BC and CD facets with the horizontal). This pattern is illuminated by a plane wave under normal incidence  $\theta_0 = 0^\circ$ .

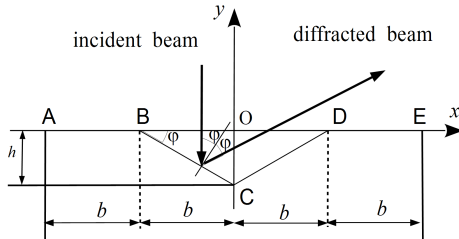


Figure 3. Triangular hollow pattern

The Fig. 4, shows, in dotted line, the angular distribution of the energy at infinity for this pattern in Fraunhofer domain calculated from the  $S$  matrix obtained by the C-method (results for the two polarizations **TE** and **TM** are very similar).

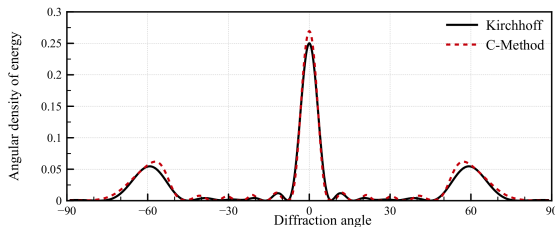


Figure 4. Triangular profile: angular density of energy at infinity calculated by C-method (dotted line) and by the Kirchhoff approximation (solid line), angle in degrees.

#### A. Interpretation from geometrical optics

The laws of reflection of geometrical optics show that light is reflected in three directions:

- $\theta = 0^\circ$  : reflection on AB and DE,
- $\theta = +60^\circ$  : reflection on BC,
- $\theta = -60^\circ$  : reflection on CD.

In Fig. 4, it can be seen that there is a maximum of energy diffracted in each of these three directions.

#### B. Interpretation from Kirchhoff approximation

With this approximation it is considered that the light is diffracted at each point of a surface as if it was reflected on the plane tangent to the surface at this point. We make the approximation which consists in assuming that each facet of the chosen triangular pattern diffracts like a plane ribbon. The angle  $\varphi = 30^\circ$  has been chosen in such a way that there is no multiple reflections and that it is possible to neglect the interferences between the beams diffracted by each of the facets. With these assumptions, the beam diffracted by ABCDE is the sum of three independent beams: AB+DE, BC and CD.

- Incident beam

The part of the normalized incident plane wave such that  $\theta_0 = 0^\circ$  illuminating a part of width  $L$  of the complete pattern ABCDE is a TPW of width  $L$  which, in the plane  $y = 0$  is written:

$$F^-(x, y = 0) = \int_{-\infty}^{+\infty} A^-(\alpha) e^{-ik\alpha x} d\alpha, \quad (35)$$

with  $A^-(\alpha) = \frac{L}{\lambda} \text{sinc}(\pi(\alpha - \alpha_0) \frac{L}{\lambda})$  (appendix 1).

The normalized energy  $W_i$  associated with this incident wave whose amplitude is taken as a unit is proportional to  $\int_{-\infty}^{+\infty} |A^-(\alpha)|^2 d\alpha$ , let:

$$W_i = \left( \frac{L}{\lambda} \right)^2 \int_{-\infty}^{\infty} \text{sinc}^2(\pi\alpha \frac{L}{\lambda}) d\alpha = \frac{L}{\lambda}. \quad (36)$$

For the entire pattern ABCDE of width  $L = d$  the associated incident energy is  $W_i = d/\lambda$ .

- Diffraction by AB and DE

The diffracted amplitude  $A^+(\alpha)$  by the two facets AB and DE is equivalent to the diffraction of a horizontal ribbon of width  $L = d/2$  is:

$$A_{AB+DE}^+(\alpha) = \frac{d}{2\lambda} \text{sinc}(\pi\alpha \frac{d}{2\lambda}). \quad (37)$$

The associated diffracted energy is then  $W_{AB+DE} = d/(2\lambda) = W_i/2$  ie half of the incident energy.

- Diffraction by BC

The facet BC makes the angle  $\varphi$  with the horizontal, as a consequence of this inclination, the diffraction by BC corresponds to the diffraction of a facet of width  $L = BC = d/(4 \cos \varphi)$  illuminated under the incidence  $\varphi$  by a plane wave of amplitude  $\sqrt{\cos \varphi}$  receiving therefore the incident energy  $W_i/4$ , finally:

$$A_{BC}^+(\alpha) = \frac{d}{4\lambda\sqrt{\cos \varphi}} \text{sinc}(\pi(\alpha - \sin \varphi) \frac{d}{4\lambda \cos \varphi}), \quad (38)$$

with:

$$W_{BC} = \int_{-\infty}^{+\infty} A_{BC}^2(\alpha) d\alpha = W_i/4. \quad (39)$$

which corresponds to a quarter of the incident energy.

- For the CD segment the result is the same by changing  $\varphi$  into  $-\varphi$ :

$$A_{CD}^+(\alpha) = \frac{d}{4\lambda\sqrt{\cos \varphi}} \text{sinc}(\pi(\alpha + \sin \varphi) \frac{d}{4\lambda \cos \varphi}). \quad (40)$$



The wave diffracted by the complete pattern ABCDE consists of three beams separated from each other by an angle of  $60^\circ$  which do not interfere practically with each other, hence the response for all facets is approximately equal to the sum of the illuminations for each facet. On the other hand, we seek the angular radiation of light at an observation point P located at the infinity of the pattern. The theorem of the stationary phase then makes it possible to write the angular density of energy diffracted by the locally plane wave in the direction  $\theta$ :

$$W(\theta) = [4A_{AB+DE}^2(\theta) + A_{BC}^2 + A_{CD}^2(\theta)] \cos^2(\theta)/16. \quad (41)$$

In Fig. 4, is represented in solid line the angular distribution of the energy at infinity computed by the Kirchhoff approximation to compare with results obtained by our method (dotted line). We see that there is an excellent agreement between the two types of results obtained by totally different methods.

### C. Double reflection and phenomenon of the retro-reflector

Like in the preceding paragraph the pattern studied is triangular but with a height  $h = b = 3.2\lambda$  such that there exists, in geometrical optics, a double reflection between the facets BC and CD. The angle  $\varphi = 45^\circ$  is chosen in such a way that, after double reflection, an incident ray emerges in the direction of incidence. The plane wave that illuminates the pattern arrives at an incidence  $\theta_0 = 10^\circ$ . Fig. 5a, shows the diffraction at infinity when the pattern is fully illuminated by the plane wave. Note that there are two very pronounced peaks, one for  $\theta = +10^\circ$  corresponding to the reflection on the AB and DE facets and the other for  $\theta = -10^\circ$  corresponding to the retro-reflection on the facets BC and CD. There is also a third peak not very pronounced for  $\theta = -70^\circ$  corresponding to the part of the incident plane wave which has only undergone a simple reflection on CD.

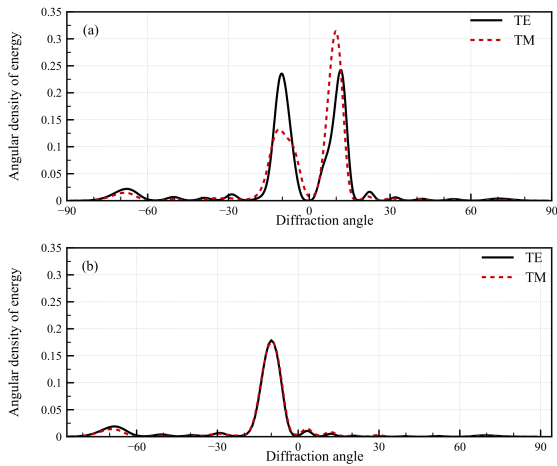


Figure 5. Triangular hollow pattern with  $\theta_0 = 10^\circ$  and  $\varphi = 45^\circ$ : (a) fully illuminated,  $L = d$ . (b) only the groove BD is illuminated,  $L = d/2$ .

Fig. 5b, corresponds to the diffraction at infinity when only the central part BD is illuminated and where almost all the light is retro-reflected in the direction of incidence ( $\theta = -10^\circ$ ). It is observed that the two polarizations give practically the same results, whereas this was not true in the previous case where ABCDE was fully illuminated (Fig.5a) because there is interference between the waves diffracted by the horizontal and inclined facets. There is also another small peak for  $\theta = -70^\circ$  corresponding to the part of the incident wave that undergoes a simple reflection on CD.

## V. DIFFRACTION BY A PARABOLA

The equation describing the profile of a parabolic pattern of width  $D$  is written:

$$y(x) = 4h \left( \frac{x}{D} \right)^2 \quad (42)$$

This parabolic mirror is illuminated by a TPW of width  $L$  (Fig. 6). The focus  $F$  of the parabola is at the distance  $f$  from the origin  $O$  such that the focal length is:  $OF = f = D^2/(16h) = L^2/(16h_i)$

The reflection of a plane wave by a parabolic mirror is a canonical example that is known to be treated by geometrical optics: after reflection, all the incident rays parallel to  $Oy$  composing the incident TPW converge at the focus  $F$  of the parabola (Fig. 6.). Another property is that all rays which constitute the output beam have the same amplitude. Then the distribution of the angular energy density in the output beam has the form of a rectangle function.

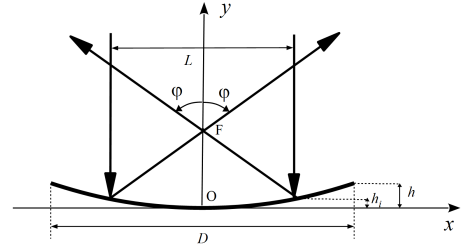


Figure 6. Parabolic pattern

If a TPW of width  $L$  illuminates the parabola the reflected beam has an aperture  $2\varphi$  (Fig. 6) such that:

$$\tan \varphi = \frac{L}{2(f - h_i)} \text{ with } h_i = h \left( \frac{L}{D} \right)^2 \quad (43)$$

### A. Example 1 : fully illuminated parabola

Parabola of width  $D = 21.3\lambda$ , with  $L = D$ ,  $h_i = h = 3.2\lambda$ , then focal length is:  $f = 8.86\lambda$ , the opening of output beam is:  $\varphi = 62.00^\circ$ . Period of the associated grating is  $d = D$ . Fig. 7a, shows the angular energy densities for the TE and TM polarizations and for the geometrical optics hypothesis (rectangular solid line).

In this example, it can be seen that the diffracted energy is concentrated between the predicted angles:  $-62^\circ < \varphi < 62^\circ$ . The angular density of energy has the appearance of the Fourier transform of the rectangle function with Gibbs phenomenon near limits of the diffraction domain.

### B. Example 2 : partially illuminated parabola

The pattern is identical to that of the previous example  $D = 21.3\lambda$  then the focal length is the same  $f = 8.86\lambda$ . This pattern is only partially illuminated over a width:  $L = 14.2\lambda < D = d$ , then  $h_i = h = 1.42\lambda$ . Then, the opening of the reflected beam is  $\varphi = 43.67^\circ$ .

Here again for TE and TM the diffracted energy (Fig. 7b) is concentrated between the predicted angles:  $-43.7^\circ < \varphi < 43.7^\circ$ .

### C. Example 3 comparison of results between fully and partially illuminated parabolas

The pattern consists of a portion of width  $D = d = 14.2\lambda$  of the previous parabolic profile (example1) with the same focal length  $f = 8.86\lambda$ . This pattern is fully illuminated then  $L = D$ . In these conditions the height is  $h = 1.42\lambda$ . Results are given in Fig. 7c.

From the point of view of geometrical optics the results Fig. 7b, and Fig. 7c, should be the same.

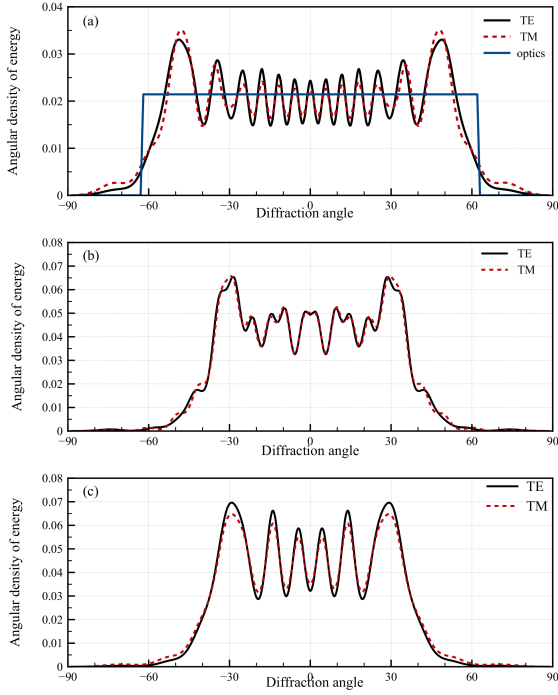


Figure 7. Parabolic pattern of focal length  $f = 8.86\lambda$ . (a) fully illuminated:  $L = D = 21.3\lambda$ . (b) partially illuminated  $L = 14.2\lambda$ ,  $D = 21.3$ . (c) smaller parabola of same focal length:  $D = L = 14.2\lambda$ , fully illuminated.

The differences in Fig. 7b and Fig. 7c, arise that in Example 2 account is taken of edge effects for a larger parabola,  $D = 21.3\lambda$  which is not totally illuminated  $L = 14.2\lambda$  whereas in Example 3 the parabola is narrower  $D = 14.2\lambda$  but fully illuminated,  $L = D = 14.2\lambda$ .

#### D. Spatial distribution of the energy diffracted by a parabolic mirror, highlighting the focus of mirror

In electromagnetic optics the focal point of the parabola is not a point where the energy is infinite but a zone of space where there is an important reinforcement of the electromagnetic field. To highlight this zone, we chose a parabolic profile grating of period  $d = 8.4\lambda$  with an output windows of width  $D = d$  and input window of width  $l = 1.8\lambda$ . The focal length of this parabola is  $f = 4.01\lambda$  and the opening of output beam is  $\varphi = 53.35^\circ$ .

In Fig. 8, we have plotted, in arbitrary unit, the density  $W$  of electromagnetic energy as a function of  $u = x$  and  $v = y - ha(x)$ . We note that there is, in the vicinity of the focus F, the expected maximum of energy.

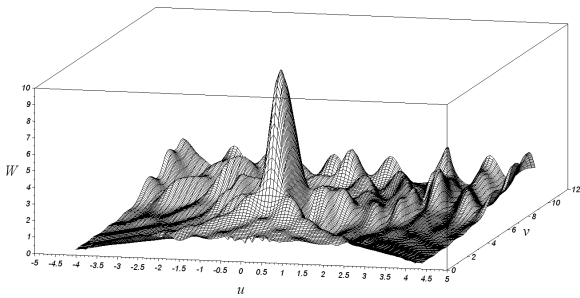


Figure 8. Energy density for TE polarization (arbitrary unit)

## VI. CONCLUSION

Currently, there are rigorous numerical modeling methods to determine the diffraction of a plane wave by a grating. One may not think that the results obtained for a grating formed by an infinite repetition of an elementary patterns contain the results for the diffraction of the plane wave by a single element of those patterns. However it is this approach that we have adopted to investigate the diffraction of a plane wave by a window  $W$  of width  $D$  of a periodic surface. The relevance of this approach is confirmed by the overall results obtained: our numerical results show that one finds well the expected results that are given by geometrical optics and optical physics.

The results of Fig. 4, concerning a weakly modulated plane are in perfect agreement with those provided by KA which assumes that surface is planar in the vicinity of each point. When the height of roughness increases multiple reflections appear and when both sides of the pattern are at right angles we find the phenomena of retro-reflection provided by geometrical optics. This phenomenon persists in the resonant domain as can be seen in Fig. 5.

We used the linearity of Maxwell's equations to decompose the incident plane wave and the diffracted plane waves as a sum of a TPW. This is in perfect agreement with the Huygens-Fresnel principle of assuming that at each point the wavefront can be considered as the limit of isotropic radiative point source. In our modeling the incident plane wave is decomposed into a sum of TPW with very small width and found that the diffracted wave as the sum of the small contributions, obeyed Huygens-Fresnel principle.

A final argument in favor of our approach lies in the Heisenberg uncertainty principle [15]. If we are interested by the corpuscular aspect of light it is possible to interpret efficiencies of a grating such as the probability of finding in the direction  $\theta_n$  an incident photon associated to a plane wave with the incidence  $\theta_0$ . If one restricts the study of the diffracted wave only to incident photons which interact with only a single period  $d$  of the grating they are diffracted in a direction  $\theta$  with a probability density  $A(\theta)\overline{A(\theta)}$ . There is an information on the position of the diffracted photons which come from a point of the pattern ( $-d/2 < x < d/2$ ) which, by virtue of the uncertainty principle, induces an uncertainty in their direction. In the plane  $y = 0$  the uncertainty relation is written  $\Delta p_x \cdot \Delta x \geq \hbar$  where  $\hbar$  is Planck's constant,  $\Delta p_x$  the uncertainty of the momentum of the photon according  $Ox$  and  $\Delta x = d$  the uncertainty of the position. For a photon, momentum is written  $p = h\nu/c = \hbar/\lambda$  with  $\Delta p_x = \Delta(p \sin \theta) = (\hbar/\lambda)\Delta \sin \theta$  which leads to an angular uncertainty  $\Delta \sin \theta \geq \lambda/d$ . From the point of view of the uncertainty principle, once fixed the width  $d$ , to make additional measures for an angular resolution  $\Delta(\sin \theta)$  less than  $\lambda/d$  adds no additional information. It is therefore possible to determine  $A(\theta)$  only from measurements  $A_n = A(\theta_n)$  made for angles obeying the grating formula  $\sin \theta_n = \sin \theta_0 + n\lambda/d$ , where  $\theta_0$  is an arbitrary origin angle.

If the uncertainty principle should be applied to measurements, it also applies to numerical modeling. If we are looking for the Fraunhofer diffraction pattern of width  $d$  illuminated by a plane wave, all information that is possible to know is contained in the diffracted amplitudes in directions  $\theta_n$  of associated grating. If additional calculations are made outside these directions, this gives no additional information for diffraction window of width  $d$ . If, for example, calculations are made to an angular resolution  $\Delta \sin \theta = \lambda/2d < \lambda/d$  the new calculated points are only valid for a window  $W$  of width  $D = 2d$ , they contain the contributions of multiple diffractions between two patterns which are not consistent to the originally posed problem. If roughness is of very low amplitude the effect of multiple diffractions become negligible then, in such a



case, these results would approximately correspond to the problem we have initially posed however but are useless in nature.

For the sake of simplicity we have chosen to study in this paper only the case of the perfectly conducting grating. The extension of our formalism to the case of finite conductivity should not pose particular problems. Indeed, with the C-method, taking into account the conductivity presents no difficulties.

Our rigorous method, proposed here, analyzing in detail the diffraction of a plane wave by a single pattern of a grating can be explicitly extended to the numerical modeling of the diffraction of a plane wave by a rough surface. It shows how, once the study window of width  $D$  of the infinite rough surface is chosen, this problem can best be modeled as diffraction by an elementary pattern of an associated grating.

Our method also applies to the case of diffraction of plane wave by a non planar perfectly conducting ribbon of width  $D$  and the complementary problem (Babinet's theorem) of the diffraction by an infinitely thin metallic grating with a slit of width  $D$ .

#### Appendix 1: The truncated plane wave TPW

Consider a plane wave of unit amplitude, with an incidence  $\theta_0$  propagating in the direction of  $y > 0$ , which is written:

$$F(x, y) = e^{-ik \sin \theta_0 x} e^{-ik \cos \theta_0 y}. \quad (44)$$

We call truncated plane wave (TPW) a wave, whose electromagnetic field  $F_L(x, y)$  in the plane  $y = 0$  coincides with that of a plane wave over an interval of width  $L$  situated at the distance  $l$  from the origin and which is zero outside:

$$F_L(x, y = 0) = \Pi\left(\frac{x-l}{L}\right) e^{-ik\alpha_0 x}, \quad (45)$$

where  $\Pi(x)$  is the rectangular function such that:

$$\Pi\left(\frac{x-l}{L}\right) = \begin{cases} 1 & \text{if } x \in ]-L/2 + l, +L/2 + l[ \\ 0 & \text{otherwise} \end{cases}. \quad (46)$$

For  $y = 0$ , the field  $F_L(x, y = 0)$  can be written as a Fourier integral:

$$F_L(x, y = 0) = \int_{\alpha=-\infty}^{+\infty} A(\alpha) e^{-ik\alpha x} d\alpha, \quad (47)$$

with:

$$A(\alpha) = \frac{1}{\lambda} \int_{x=-\infty}^{+\infty} F_L(x, y = 0) e^{+i2\pi\alpha x/\lambda} dx, \quad (48)$$

which, by setting  $\alpha_0 = \sin \theta_0$  is written:

$$A(\alpha) = \frac{L}{\lambda} \text{sinc}(\pi(\alpha - \alpha_0)L/\lambda) e^{+i2\pi(\alpha - \alpha_0)l/\lambda}. \quad (49)$$

Finally, at any point of space, this TPW may be written:

$$F_L(x, y) = \int_{\alpha=-\infty}^{+\infty} A(\alpha) e^{-ik\alpha x} e^{-ik\beta y} d\alpha. \quad (50)$$

When  $y \rightarrow +\infty$  evanescent waves disappear and this expression reduces to:

$$F_L(x, y) = \int_{\alpha=-1}^{+1} A(\alpha) e^{-ik\alpha x} e^{-ik\beta y} d\alpha. \quad (51)$$

#### Appendix 2 : Method of the stationary phase

Consider an integral of the form:

$$F(r) = \int_{\alpha_1}^{\alpha_2} f(\alpha) e^{-irg(\alpha)} d\alpha, \quad (52)$$

The stationary phase method [16,17] gives an asymptotic expression of this integral when  $r \rightarrow +\infty$  ie when the phase of the exponential

varies very rapidly with  $\alpha$ . It can be shown that if the derivative of the function  $g(\alpha)$  vanishes at a point  $\alpha = \alpha_s$  ie if  $g'(\alpha_s) = 0$  then there is an asymptotic expression for  $F(r)$ :

$$F(r) \sim \sqrt{\frac{2\pi}{r|g''(\alpha_s)|}} f(\alpha_s) e^{-irg(\alpha_s)} e^{i\sigma\pi/4}, \quad (53)$$

where  $\sigma = \text{sgn}(g''(\alpha_s))$ .

At infinity, at a point  $P$  of coordinates  $(x, y)$ , the electromagnetic field of a beam is composed of a continuous set of plane waves, it is written:

$$F(x, y) = \int_{\alpha=-1}^{+1} A(\alpha) e^{-ik\alpha x} e^{-ik\sqrt{1-\alpha^2}y} d\alpha, \quad (54)$$

putting  $x = r \sin \varphi$  et  $y = r \cos \varphi$ , then:

$$F(r, \varphi) = \int_{\alpha=-\infty}^{+\infty} A(\alpha) e^{-ik\alpha \sin \varphi r} e^{-ik \cos \varphi \sqrt{1-\alpha^2}r} d\alpha, \quad (55)$$

let:

$$F(r, \varphi) = \int_{\alpha=-\infty}^{+\infty} A(\alpha) e^{-ikrg(\alpha)} d\alpha, \quad (56)$$

with  $g(\alpha) = \alpha \sin \varphi + \cos \varphi \sqrt{1-\alpha^2}$ . The relation of the stationary phase gives the asymptotic expression of this field:

$$g'(\alpha) = \sin \varphi - \alpha \frac{\cos \varphi}{\sqrt{1-\alpha^2}}. \quad (57)$$

$g'(\alpha) = 0$  if  $\alpha_s = \sin \varphi$  ie  $\varphi = \theta$  and  $g''(\alpha_s) = -1/\cos^2(\varphi) < 0$ .

Then the final result is:

$$F(r, \theta) \sim \cos \theta \sqrt{\frac{2\pi}{r}} A(\theta) e^{-ikr} e^{-i\pi/4}. \quad (58)$$

Finally, at the point P situated at the distance  $r$  from the origin, in the direction  $\theta$ , the electromagnetic field has the properties of a locally plane cylindrical wave whose amplitude decreases in  $1/\sqrt{r}$  when  $r$  tends to infinity. By omitting the phase term  $e^{-i\pi/4}$  this equation is written:

$$F(r, \theta) \sim \cos \theta \sqrt{\frac{2\pi}{r}} A(\theta) e^{-ikr}. \quad (59)$$

This relationship applied to a TPW gives:

$$F(r, \theta) \sim \cos \theta \sqrt{\frac{2\pi}{r}} \frac{L}{\lambda} \text{sinc}(\pi(\sin \theta - \sin \theta_0)L/\lambda) e^{-ikr}. \quad (60)$$

The angular energy density  $W(\theta)$  is expressed as:

$$W(\theta) \sim \cos^2 \theta |A(\theta)|^2. \quad (61)$$

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