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PROPAGATIVE AND EVANESCENT WAVES DIFFRACTED BY PERIODIC SURFACES: PERTURBATION METHOD

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Abstract—The propagation equation, written in a curvilinear coordinate system, is solved by using a perturbation method inspired from quantum physics and extended to imaginary eigenvalues and evanescent waves. The parameter of perturbation is the groove depth which is small compared to the period. The method is expanded up to second order for the non-degenerate problem. In this way the solutions have analytical form compared to a numerical method. They present the advantage to put in evidence the evolution of the energy distribution for different diffraction orders as a function of the magnitude of the perturbation. The efficiencies which are deduced from these analytical solutions are compared of those obtained by the curvilinear coordinate method. The good agreement between the two methods occurs for a groove depth with respect to the wavelength less than or equal to 0.16. Thus, this new approach opens a new range of applications for inverse problems.

1. INTRODUCTION

The curvilinear coordinate method is a well known method for modelling wave diffraction at a periodic surface. The main feature of this method is the use of a translation coordinate system that maps the profile to a plane and enables to express the problem as an eigenvalue problem which can be easily numerically solved by standard algorithms [1–4]. The eigenvalues correspond to diffracted directions and the eigenfunctions correspond to fields of diffracted waves in these directions. The system which must be solved is generally of infinite

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dimension but can be limited to a problem of finite lower dimension when the diffracting surface is not very different from a plane. In this case it is possible to obtain the solution by a perturbation method inspired by quantum physics methods. Our approach is comparable to that of Malischewsky in the field of seismology [5, 6].

Historically, the perturbation method has its roots in early celestial mechanics and it was first used to solve algebraic equations, before being applied to the operator theory, especially in quantum mechanics version. In this case the calculations are easier than the corresponding classical perturbation techniques presented by Goldstein et al. [7].

The perturbation theory is widely used in electromagnetism. For instance it has been recently used to calculate the sensitivity of chirowaveguides to circular birefringence [8] and to investigate the plane wave diffraction by a semi-infinite parallel-plate waveguide with sinusoidal wall corrugation [9, 10].

Here, we are interested in the analysis of diffraction by shallow gratings. In a first paper [11] we have combined the theory of perturbation with the method of curvilinear coordinates. However, this work was inspired by text book [12] widely used in quantum mechanics. In that field, the perturbation method has been established from Hamiltonian operator which is a hermitian operator of which the eigenvalues (energy levels) are real and the eigenvectors form an orthonormal basis in the case of non-degenerate states. That's why we had only considered propagative waves. This preliminary study paved the way for the general case that should also include evanescent waves.

Thus, the main purpose of the present paper is to propose the general case that considers both propagative and evanescent waves corresponding to real and imaginary eigenvalues. For that, we relate in detail the different states of the analytical calculation of the perturbation method applied to a simple case: a sinusoidal surface the groove depth of which is small with respect to the period of the profile. The analytical solutions, eigenvalues and eigenfunctions, are obtained from known eigensolutions of the unperturbed problem that is a plane surface. The amplitudes of eigenfunctions are determined from boundary conditions. The domain of validity of the perturbation method is obtained by comparison with rigorous numerical method. We have calculated with both methods the diffracted efficiencies of a given perfectly conducting sinusoidal grating. Let us recall that efficiencies correspond to the fraction of incident energy scattered in discrete directions. For the case under consideration the relative uncertainty for efficiencies was less than 8% for groove depth to wavelength ratio smaller than 0.16.

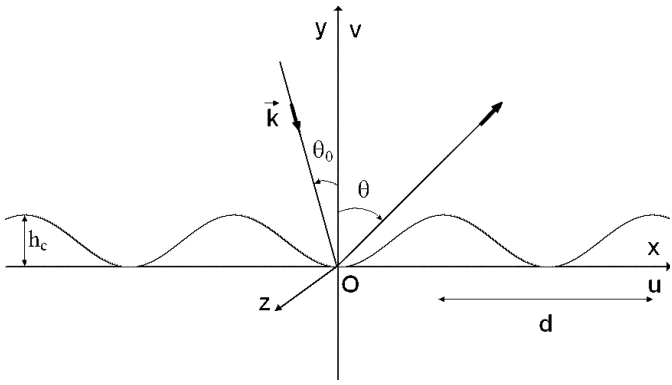

Figure 1. Sinusoidal grating with incident and diffracted waves.

2. FORMULATION OF THE PROBLEM

In Cartesian coordinate $(Oxyz)$, we assume a cylindrical surface whose generatrix, parallel to the Oz axis, is on the line $y = h_c a(x)$ localised in the (xOy) plane with $y \geq 0$ (Figure 1).

The periodic function $a(x)$ with period d is assumed continuously differentiable. This surface represents the interface between the vacuum and a perfectly conductor medium. It is illuminated by a monochromatic plane wave of angular frequency ω, wavelength λ and wave number $k = 2\pi/\lambda$.

Our study is related to a sinusoidal grating which the profile $a(x) = 1/2 \sin 2\pi x/d$. This profile is normalized so that the groove depth h_c is the maximal deviation from the y-axis with: $\max a(x) - \min a(x) = 1$.

The incidence angle θ_o varying from $-\pi/2$ to $\pi/2$ is positively counted as shown in Figure 1. The diffraction angles θ are oriented in the reverse trigonometric sense.

We wish to calculate the distribution of diffracted energy as a function of the angle θ when h_c is small with respect to the period d.

The time dependence of the electromagnetic field is such that:

$$i\partial/\partial t = \omega \tag{1}$$

The problem presents an invariance according to z-axis translation, that is:

$$\partial/\partial z = 0 \tag{2}$$

For 2D problems there are two types of solution according to whether the z-component of electrical or magnetic field is parallel to the z-axis.

One can summarize:

$$TE \text{ polarization for :} \quad E_z \neq 0 \Rightarrow E_x = E_y = 0 \tag{3}$$

$$H_z = 0 \Rightarrow H_x \neq 0, \quad H_y \neq 0 \tag{4}$$

$$TM \text{ polarization for :} \quad E_z = 0 \Rightarrow E_x \neq 0, \quad E_y \neq 0 \tag{5}$$

$$H_z \neq 0 \Rightarrow H_x = H_y = 0 \tag{6}$$

Let us denote $F(x, y)$ the E_z or H_z component according to TE or TM polarization. In this case, $F(x, y)$ is solution of the following propagation equation which is deduced from Maxwell's equations:

$$\left[(\partial/\partial x)^2 + (\partial/\partial y)^2 + k^2\right] F(x, y) = 0 \tag{7}$$

with a medium with refractive index equal to unity.

The other components of electromagnetic field can be calculated from $F(x, y)$.

3. PERIODIC SURFACE WITH h_c CLOSE TO ZERO

Let consider the special case of a periodic surface $y = h_c a(x)$ with h_c close to zero.

The propagation Equation (7) is an eigenvalue equation of the form:

$$\left[(-i\partial/\partial x)^2 + (-i\partial/\partial y)^2\right] F(x, y) = k^2 F(x, y) \tag{8}$$

According to the wave-particle duality and corresponding relations introduced in quantum physics, we associate to wave vector $\mathbf{k}\,(k_x, k_y)$ of the (xOy) plane the operator:

$$\underline{\mathbf{k}}\,(\underline{k}_x = -i\partial/\partial x, \quad \underline{k}_y = -i\partial/\partial y) \tag{9}$$

Let $k\alpha$ and $k\beta$ the eigenvalues of k_x and k_y, with real values (fundamental rule in quantum physics).

The Equation (8) implies:

$$\alpha^2 + \beta^2 = 1 \tag{10}$$

According to the incidence angle θ_0 and the diffraction angles θ (Figure 1) the eigenfunction $F(x, y)$ of Equation (8), is written to within a constant A^- or A^+ and one has:

- for the incoming incident wave:

$$F^-(x, y) = A^- \exp(ik\alpha_0 x) \exp(-ik\beta_0 y) \tag{11}$$

- for outgoing diffracted wave:

$$F^+(x, y) = A^+ \exp(ik\alpha x) \exp(+ik\beta y) \tag{12}$$

From the periodicity of the rough surface we have shown in [11] the quantification of diffracted beam directions.

Let $U^p = \{m/|\alpha_m| < 1\}$, then it is possible to define the angles θ_m so that:

$$\alpha_m = \sin\theta_m = \sin\theta_0 + m\lambda/d \quad \text{with} \quad m = 0, \pm 1, \pm 2, \ldots, \pm N_p \tag{13}$$

and:

$$\pm\beta_m = \pm(1 - \alpha_m^2)^{1/2} = \pm\cos\theta_m \quad \text{with} \quad -N_p \leq m \leq N_p \tag{14}$$

For simplification of analytical calculations we consider the same diffracted real order number on both sides of zero-order.

Consequently, the eigenfunctions $F_m^{p+}(x,y)$ and $F_m^{p-}(x,y)$ associated to each of m-th direction of $\mathbf{k}$ (also called m-th order) representing outgoing and incoming progressive waves respectively are:

$$F_m^{p\pm}(x,y) = A_m^{p\pm} \exp(\pm ik\beta_m y) \exp(ik\alpha_m x) \tag{15}$$

In the case where

$$m \notin U^p, \quad \text{set} \quad U^{ev} = \{m'/|\alpha_{m'}| > 1\}, \tag{16}$$

then:

$$\alpha_{m'} = \alpha_0 + m'\lambda/d \quad \text{with} \quad m' = \pm(N_p + 1), \ldots, \pm N \tag{17}$$

and:

$$\pm i\beta_{m'} = \pm i\left(\alpha_{m'}^2 - 1\right)^{1/2} \quad \text{with} \quad N_p + 1 \leq |m'| \leq N \tag{18}$$

N being the truncature order for numerical calculations.

The corresponding waves denote the evanescent waves (or exponentially decaying waves) which decrease quickly when y increases by positive value (negative sign in exponential) or y increases by negative value (positive sign in exponential):

$$F_{m'}^{ev\pm}(x,y) = A_{m'}^{ev\pm} \exp(\mp k\beta_{m'} y) \exp(ik\alpha_{m'} x) \tag{19}$$

To the incoming incident field (11) corresponds the diffracted field $F^+(x,y)$ which is the sum of the outgoing progressive plane waves and outgoing evanescent waves:

$$\begin{aligned} F^+(x,y) \;=\; & \sum_{m \in U^p} A_m^{p+} \exp(ik\beta_m y) \exp(ik\alpha_m x) \\ & + \sum_{m' \in U^{ev}} A_{m'}^{ev+} \exp(-k\beta_{m'} y) \exp(ik\alpha_{m'} x) \end{aligned} \tag{20}$$

Denote $U = U^p \cup U^{ev}$. The set U is to $2N + 1$ dimensional.

4. THE PROPAGATION EQUATION FROM THE TRANSLATION COORDINATE SYSTEM

4.1. The Differential Operators

Our goal is to determinate the scattered field defined as the difference between the total electromagnetic field and the incident field. The field must satisfy the far-field radiation conditions and the boundary conditions along the interface. In order to express the latter simply, we use the so-called "translation coordinate system" (u, v, w) [1] defined from Cartesian coordinates as follows:

$$\begin{aligned} u &= x \\ v &= y - h_c a(x) \\ w &= z \end{aligned} \tag{21}$$

In this case the diffracting surface corresponds to $v = 0$. Note that the z-component of electrical or magnetic field (E_z or H_z) is unchanged in the new coordinate system. We it call $F(u, v)$ and it is considered as an unknown function.

One must write the differential operators in the translation coordinate system:

$$\begin{aligned} \partial/\partial x &= \partial/\partial u - h_c a' \partial/\partial v \\ \partial/\partial y &= \partial/\partial v \end{aligned} \tag{22}$$

where: $a' = da/dx$.

The propagation Equation (7) is changed to:

$$\begin{aligned} &\left\{(\partial/\partial u)^2 - h_c \left[(\partial/\partial u)a' + a'(\partial/\partial u)\right](\partial/\partial v)\right. \\ &\left.+(h_c^2 a'^2 + 1)(\partial/\partial v)^2 + k^2\right\} F(u, v) = 0 \end{aligned} \tag{23}$$

In this equation, it is not the profile function $a(x)$ which appears but its derivative $a'(x)$. This shows the invariance of problem by translation with respect to the variable v.

In order to use reduced quantities, we define:

$h = 2\pi h_c/d$: the normalized magnitude

and: $\ddot{a} = da'(x)/2\pi$: the normalized derivative of the profile which is a periodic function of period d.

Then, the Equation (23) becomes:

$$\begin{aligned} &\left\{(\partial/\partial u)^2 - h\left[(\partial/\partial u)\ddot{a} + \ddot{a}(\partial/\partial u)\right](\partial/\partial v)\right. \\ &\left.+(h^2\ddot{a}^2 + 1)(\partial/\partial v)^2 + k^2\right\} F(u, v) = 0 \end{aligned} \tag{24}$$

It is an equation with constant coefficients according to v and periodical coefficients according to u.

Consequently:

$$F(u,v) = \sum_m F_m(v) \cdot \exp(ik\alpha_m u) \tag{25}$$

with α_m satisfying (13) and (17) by analogy to the previous case of a surface with periodicity d in the u-direction,
and:

$$F_m(v) = F_m \exp(ik\rho v) \tag{26}$$

where F_m and ρ are unknowns of problem.

4.2. Dirac Notation

The set of pseudo-periodic functions $F(u,v)$ provided with scalar produce form a subspace $\mathbb{E}_m$ of the Hilbert functional space $\mathbb{E}$.

In order to simplify the writing of equations it is very useful to represent the vectors of this space with Dirac notation as in quantum physics:

- an element of space $\mathbb{E}$ is noted by the column vector $|f\rangle$ or "ket",
- an element of dual space $\mathbb{E}^\dagger$ is a row vector $\langle f|$ or "bra".

The "bra" is the adjoint (noted †) of the "ket":

$$\langle f| = [|f\rangle]^\dagger \tag{27}$$

For $-N < m < +N$, the set of functions $\exp(ik\alpha_m u)$, represent also the orthonormal Fourier's basis of $2N+1$ dimension denoted $\{|\exp(ik\alpha_m u) >\}$ (or $\{|e_m\rangle$ to simplify) of the subspace $\mathbb{E}_m$ of the Hilbert functional space $\mathbb{E}$. In $\mathbb{E}_m$ the scalar produce is defined as "bracket":

$$\langle \exp(ik\alpha_m u)|\exp(ik\alpha_n u)\rangle = \frac{1}{d}\int_0^d (\exp(ik\alpha_m u))^\dagger \cdot \exp(ik\alpha_n u)du = \delta_{mn} \tag{28}$$

where δ_{mn}, the Kronecker symbol, equal to unit for $m = n$ and to zero for $m \neq n$.

4.3. Matrix Form of the Propagation Equation

In Hilbert subspace $\mathbb{E}_m$ we can associated to each functional operator $(-i\partial/\partial u)$ a square matrix of $2N+1$ dimension noted $[-i\partial/\partial u]$.

The coefficients of propagation Equation (24) are independent of the variable v, then according to (26) the differential operator $(-i\partial/\partial v)$ behaves as a single multiplication.

Furthermore in this basis, the components $F_m(v)$ of the function $F(u,v)$ are regrouped in $|f\rangle$. Then, in this basis $\{|\exp(ik\alpha_m u)\rangle\}$, the Equation (24) is written in matrix form:

$$\begin{aligned}&\left\{[-i\partial/\partial u]^2 - h\left([-i\partial/\partial u][\ddot{a}] + [\ddot{a}][-i\partial/\partial u]\right)(-i\partial/\partial v)\right.\\&\left.+\left(h^2[\ddot{a}]^2 + [I]\right)(-i\partial/\partial v)^2 - k^2\right\}|f\rangle = 0\end{aligned} \tag{29}$$

with:

$[-i\partial/\partial u] = k[\alpha]$ where $[\alpha]$ is a diagonal matrix so that: $\alpha_{m,m} = \alpha_m$ as defined in Equations (13) and (17) (that is $m \in U$) and $\alpha_{m,n} = 0$ if $m \neq n$.

$(-i\partial/\partial v) = k\rho$ where ρ is a numerical factor.

$[I]$ is an identity matrix,

$[\ddot{a}]$ is a Toeplitz matrix associated to the normalized derivative of profile function. It is formed by the Fourier coefficients $\ddot{a}_{m,n}$ of $\ddot{a}(x)$ so that:

$$(\ddot{a})_{m,n} = (\ddot{a})_{m-n} = \frac{1}{d}\int_0^d \ddot{a}(x)\exp\left[i(m-n)\frac{2\pi}{d}x\right]dx \tag{30}$$

Thus, the Equation (29) is written as:

$$\left[-([I]-[\alpha]^2) - h([\alpha][\ddot{a}] + [\ddot{a}][\alpha])\rho + (h^2[\ddot{a}]^2 + [I])\rho^2\right]|f\rangle = 0 \tag{31}$$

From diagonal matrix $[\alpha]$, set a new diagonal matrix $[\beta]$ so that:

$$[\beta]^2 = [I] - [\alpha]^2 \tag{32}$$

The diagonal elements β_m of $[\beta]$ are writing:

$$\beta_m^2 = 1 - \alpha_m^2 \tag{33}$$

By convention, we set:

- for $m \in U^p$

$$\beta_m = +(1-\alpha_m^2)^{1/2} \text{ if } |\alpha_m| < 1 \text{ and } -N_p \leq m \leq N_p \tag{34}$$

- for $m' \in U^{ev}$

$$i\beta_{m'} = +i(\alpha_{m'}^2 - 1)^{1/2} \text{ if } |\alpha_{m'}| > 1 \text{ and } N_{p+1} \leq |m'| \leq N \tag{35}$$

5. CONVERSION OF THE PROPAGATION EQUATION INTO EIGENVALUES EQUATION

5.1. The Eigenvalues Equation

In order to calculate eigenvalues on the one hand and to get a series expansion in h on the other hand we propose to calculate ρ by introducing an auxiliary function: $F'(v) = \rho F(v)$ [3]. The associated vector is $|f'\rangle$ of which terms are the components $F'_m(v)$ of $F'(v)$ in the basis $\{|\exp(ik\alpha_m u)\rangle\}$.

Thus, in the doubled subspace $\mathbb{C}_m \oplus \mathbb{C}_m$ with the basis B: $\{|\exp(ik\alpha_m u)\rangle, |\exp(ik\alpha_m u)\rangle\}$ we obtain the following system:

$$\begin{bmatrix} -h[\beta]^{-2}([\alpha][\ddot{a}] + [\ddot{a}][\alpha]) & [\beta]^{-2}(h^2[\ddot{a}]^2 + [I]) \\ [I] & 0 \end{bmatrix} \begin{bmatrix} |f\rangle \\ |f'\rangle \end{bmatrix} = \rho^{-1} \begin{bmatrix} |f\rangle \\ |f'\rangle \end{bmatrix} \quad (36)$$

which appears as a $2(2N+1)$ dimensional system where ρ^{-1} is the eigenvalue and

$$|\varphi\rangle = \begin{bmatrix} |f\rangle \\ |f'\rangle \end{bmatrix} \text{ is the eigenvector.} \quad (37)$$

The Equation (36) is written in the following form:

$$\left(M^{(0)} + hM^{(1)} + h^2 M^{(2)}\right) |\varphi\rangle = \rho^{-1} |\varphi\rangle \quad (38)$$

with:

$$M^{(0)} = \begin{bmatrix} 0 & [\beta]^{-2} \\ [I] & 0 \end{bmatrix} \quad (39)$$

$$M^{(1)} = \begin{bmatrix} -[\beta]^{-2}[A] & 0 \\ 0 & 0 \end{bmatrix} \quad (40)$$

$$M^{(2)} = \begin{bmatrix} 0 & [\beta]^{-2}[B] \\ 0 & 0 \end{bmatrix} \quad (41)$$

setting:

$$[A] = [\alpha][\ddot{a}] + [\ddot{a}][\alpha] \quad (42)$$

$$[B] = [\ddot{a}]^2 \quad (43)$$

5.2. Principe of the Perturbation Method

We wish to solve the eigenvalues Equation (38) written in the form:

$$M |\varphi\rangle = \rho^{-1} |\varphi\rangle \quad (44)$$

with:

$$M = M^{(0)} + hM^{(1)} + h^2 M^{(2)} \quad (45)$$

Such a problem cannot be solved exactly with rigorous mathematics. Therefore, as many physical problems, it can be solved approximately. We propose a perturbation method inspired by quantum physics methods for non degenerate states [12]. The solutions that we obtain have analytical expressions.

The matrix M (Equation (45)) is split into three terms: an unperturbed matrix $M^{(0)}$ and two terms of perturbation $hM^{(1)}$ and $h^2M^{(2)}$ depending of the parameter h. This small dimensionless parameter h, shows the intensity of the perturbation with regard to plane surface:

h: first-order perturbation;

h^2: second-order perturbation.

The solutions of the perturbed problem are obtained from those known eigensolutions of the unperturbed problem (that is for $h = 0$). In this case the translation coordinate system is the same as the Cartesian system.

The principle of the method is as follows:

- to calculate exactly eigenvalues and eigenfunctions for the unperturbed problem (that is for $h = 0$).
- to verify that eigenfunctions form an orthonormal basis.
- to write the matrix M in the eigenbasis of unperturbed problem. It will be denoted M.
- to determine the corrective terms that must to be added to the known eigensolutions of unperturbed problem in order to obtain the approximate solutions of M according to an expansion in powers of h to second-order.

6. UNPERTURBED PROBLEM ($h = 0$): PERIODIC PLANE SURFACE

6.1. Eigensolutions of Unperturbed Problem

Calculate eigenvalues and eigenvectors of unperturbed operator $M^{(0)}$, written in the basis B, satisfying the equation:

$$M^{(0)} \begin{bmatrix} |e_m\rangle \\ |e_m\rangle \end{bmatrix} = (\rho_m^{(0)})^{-1} \begin{bmatrix} |e_m\rangle \\ |e_m\rangle \end{bmatrix} \tag{46}$$

To simplify the expression, let:

$$(\rho_m)^{-1} = r_m \tag{47}$$

To zero-order, the eigenvalues, given in a matrix form, are:

$$[r^{(0)\pm}] = \pm[\beta^{-1}] \tag{48}$$

The corresponding basis eigenvectors denoted: $|e_m^{\pm}\rangle$ have their components grouped in the following matrix T:

$$T = \begin{bmatrix} [I] & [I] \\ [\beta] & -[\beta] \end{bmatrix} \tag{49}$$

This is the matrix of B to $B^{\pm}$ basis change, such that:

$$\begin{bmatrix} |e_m^+\rangle \\ |e_m^-\rangle \end{bmatrix} = {}^tT \begin{bmatrix} |e_m\rangle \\ |e_m\rangle \end{bmatrix} \tag{50}$$

where ${}^tT$ denotes the transpose of T matrix. According to the condition of normalization of basis vectors $\langle e_m^{\pm}|e_m^{\pm}\rangle = 1$, the new basis $B^{\pm}$: $\{|e_m^+\rangle_{normalized}, |e_m^-\rangle_{normalized}\}$ in under space $\mathbb{E}_m^+ \oplus \mathbb{E}_m^-$ is identical to the initial basis B: $\{|e_m\rangle, |e_m\rangle\}$.

In this basis $B^{\pm}$: $\{|\exp(ik\alpha_m u)\rangle, |\exp(ik\alpha_m u)\rangle\}$ the matrix of eigenvalues is:

$$[r^{(0)}] = \begin{bmatrix} [\beta^{-1}] & 0 \\ 0 & -[\beta^{-1}] \end{bmatrix} \tag{51}$$

and the matrix associated eigenfunctions is:

$$\left|\psi^{(0)}\right\rangle = \begin{bmatrix} |\psi^{(0)+}\rangle \\ |\psi^{(0)-}\rangle \end{bmatrix} \tag{52}$$

To components of $|\psi^{(0)+}\rangle$ and $|\psi^{(0)-}\rangle$ we associate respectively the components $F_m^{(0)+}(v)$ and $F_m^{(0)-}(v)$ of eigenfunctions $F^{(0)+}(v)$ and $F^{(0)-}(v)$ in the basis $B^{\pm}$ when $m \in U$ varies in the range $(-N, +N)$. These components are:

- for $m \in U^p$ $\quad F_m^{p(0)\pm}(v) = F_m^{p(0)\pm} \exp(\pm ik\beta_m v)$ (53)
- for $m' \in U^{ev}$ $\quad F_{m'}^{ev(0)\pm}(v) = F_{m'}^{ev(0)\pm} \exp(\mp k\beta_{m'} v)$ (54)

with respective amplitudes $F_m^{p(0)\pm}$ and $F_{m'}^{ev(0)\pm}$.

Thus, to zero-order the analytical solutions corresponding to the unperturbed problem are written in the following form:

- for $m \in U^p$ $\quad F_m^{p(0)\pm}(u,v) = F_m^{p(0)\pm} \exp(\pm ik\beta_m v) \exp(ik\alpha_m u)$ (55)
- for $m' \in U^{ev}$ $\quad F_{m'}^{ev(0)\pm}(u,v) = F_{m'}^{ev(0)\pm} \exp(\mp k\beta_{m'} v) \exp(ik\alpha_{m'} u)$ (56)

They represent respectively the same plane waves given in (15) and evanescent waves given in (19).

6.2. Propriety of Eigenfunctions of Unperturbed Problem

The perturbation method requires that eigenfunctions of unperturbed problem in under space $\mathbb{C}_m^+ \oplus \mathbb{C}_m^-$ form an orthonormal basis. For more generality we note respectively $|\psi_m^{p(0)\pm}\rangle$ and $|\psi_{m'}^{ev(0)\pm}\rangle$ these solutions given by (55) and (56) when their amplitude is equal to the unity.

According to $m \in U^p$ and $m' \in U^{ev}$ when m and m' vary within the range $(-N, +N)$, these new basis functions needful to solve the perturbed problem are respectively:

$$\text{- for } \mathbb{C}_m^+ : \left|\psi_m^{(0)+}\right\rangle = \begin{bmatrix} \left|\psi_{m'}^{ev(0)+}\right\rangle \\ \left|\psi_m^{p(0)+}\right\rangle \\ \left|\psi_{m'}^{ev(0)+}\right\rangle \end{bmatrix} = \begin{bmatrix} \exp(-k\beta_{m'}v)\,|\exp(ik\alpha_{m'}u)\rangle \\ \exp(ik\beta_m v)\,|\exp(ik\alpha_m u)\rangle \\ \exp(-k\beta_{m'}v)\,|\exp(ik\alpha_{m'}u)\rangle \end{bmatrix} \quad (57)$$

$$\text{- for } \mathbb{C}_m^- : \left|\psi_m^{(0)-}\right\rangle = \begin{bmatrix} \left|\psi_{m'}^{ev(0)-}\right\rangle \\ \left|\psi_m^{p(0)-}\right\rangle \\ \left|\psi_{m'}^{ev(0)-}\right\rangle \end{bmatrix} = \begin{bmatrix} \exp(+k\beta_{m'}v)\,|\exp(ik\alpha_{m'}u)\rangle \\ \exp(-ik\beta_m v)\,|\exp(ik\alpha_m u)\rangle \\ \exp(+k\beta_{m'}v)\,|\exp(ik\alpha_{m'}u)\rangle \end{bmatrix} \quad (58)$$

and for $\mathbb{C}_m^+ \oplus \mathbb{C}_m^-$ we set:

$$\left|\psi_m^{(0)}\right\rangle = \begin{bmatrix} \left|\psi_m^{(0)+}\right\rangle \\ \left|\psi_m^{(0)-}\right\rangle \end{bmatrix} \quad (59)$$

With regard to basis vectors of $B^{\pm}\{|\exp(ik\alpha_m u)\rangle, |\exp(ik\alpha_m u)\rangle\}$, these new functions $\{|\psi_m^{(0)+}\rangle, |\psi_m^{(0)-}\rangle\}$ are estimated to within a phase term $\exp(\pm ik\beta_m v)$ for propagative waves and amplitude term $\exp(\mp k\beta_{m'}v)$ for evanescent waves of which decrease quickly when v increases respectively by positive or negative values.

Each set of functions $\{|\psi_m^{(0)+}\rangle\}$ on the one hand and $\{|\psi_m^{(0)-}\rangle\}$ on the other hand form an orthonormal basis of $2N+1$ dimension for each under space $\mathbb{C}_m^+$ and $\mathbb{C}_m^-$.

From the definition of scalar produce (28), summarize the normalization calculation of $|\psi_m^{(0)+}\rangle$ on the one hand and $|\psi_m^{(0)-}\rangle$ on the other hand in each under space $\mathbb{C}_m^+$ and $\mathbb{C}_m^-$:

- for propagative waves it is easy to show the next relations:

$$\text{with } m,n \in U^p \quad \left\langle \psi_m^{p(0)+} \middle| \psi_n^{p(0)+} \right\rangle = \left\langle \psi_m^{p(0)-} \middle| \psi_n^{p(0)-} \right\rangle = \delta_{mn} \quad (60)$$

- for evanescent waves, from the relation: $(\partial/\partial v)^\dagger = -(\partial/\partial v)$ we find that:

$$(\exp(\pm k\beta_{m'}v))^\dagger = \exp(\mp k\beta_{m'}v) \quad (61)$$

Taking into account (61), with m', $n' \in U^{ev}$ we find that:

$$\left\langle \psi_{m'}^{ev(0)+} \middle| \psi_{n'}^{ev(0)+} \right\rangle = \left\langle \psi_{m'}^{ev(0)-} \middle| \psi_{n'}^{ev(0)-} \right\rangle = \delta_{m'n'} \quad (62)$$

- For a mixing of propagative wave and evanescent wave we obtain:

with $m \in U^p$ and $n' \in U^{ev}$

$$\left\langle \psi_m^{p(0)+} \middle| \psi_{n'}^{ev(0)+} \right\rangle = \left\langle \psi_{n'}^{ev(0)+} \middle| \psi_m^{p(0)+} \right\rangle = \delta_{mn'} \quad (63)$$

and

$$\left\langle \psi_m^{p(0)-} \middle| \psi_{n'}^{ev(0)-} \right\rangle = \left\langle \psi_{n'}^{ev(0)-} \middle| \psi_m^{p(0)-} \right\rangle = \delta_{mn'} \quad (64)$$

In fact, when $m = n'$ the two waves are of the same kind and relations (63) and (64) are identical either to (60) or to (62).

Taking into account results of (60), (62)–(64) we point out that it is not necessary to do the distinction between $m \in U^p$ and $m' \in U^{ev}$. Then, later on we shall take the same letter m not primed on the union U of U^p and U^{ev} with $-N < m < +N$.

Then the same set of relations (60), (62)–(64) can be summarized by:

$$\left\langle \psi_m^{(0)\pm} \middle| \psi_n^{(0)\pm} \right\rangle = \delta_{mn} \quad (65)$$

This last relation shows that each set of functions $\{|\psi_m^{(0)+}\rangle\}$ on the one hand and $\{|\psi_m^{(0)-}\rangle\}$ on the other hand determine an orthonormal basis of $2N+1$ dimension for each of them $\mathbb{E}_m^+$ and $\mathbb{E}_m^-$.

But in space $\mathbb{E}_m^+ \oplus \mathbb{E}_m^-$, the set $\{|\psi_m^{(0)+}\rangle, |\psi_m^{(0)-}\rangle\}$ forms only an orthogonal basis of $2(2N+1)$ dimension. In fact, the different species of scalar produce which appear give the next results:

- for m, $n \in U^p$:

$$\left\langle \psi_m^{p(0)\pm} \middle| \psi_n^{p(0)\mp} \right\rangle = 0 \text{ with } m \neq n \quad (66)$$

$$\left\langle \psi_m^{p(0)\pm} \middle| \psi_n^{p(0)\mp} \right\rangle = \exp[\mp ik(\beta_m + \beta_n)v] \text{ with } m = n \quad (67)$$

- for $m', n' \in U^{ev}$:

$$\left\langle \psi_{m'}^{ev(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = 0 \text{ with } m' \neq n' \tag{68}$$

$$\left\langle \psi_{m'}^{ev(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = \exp[\pm k(\beta_{m'} + \beta_{n'})v] \text{ with } m' = n' \tag{69}$$

- for $m \in U^p$, $n' \in U^{ev}$:

$$\left\langle \psi_{m}^{p(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = 0 \text{ with } m \neq n' \tag{70}$$

$$\left\langle \psi_{m}^{p(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = \left\langle \psi_{m}^{p(0)\pm} \middle| \psi_{m}^{p(0)\mp} \right\rangle = \exp[\mp ik(\beta_m + \beta_m)v] \text{ with } n' = m \tag{71}$$

$$\left\langle \psi_{m}^{p(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = \left\langle \psi_{n'}^{ev(0)\pm} \middle| \psi_{n'}^{ev(0)\mp} \right\rangle = \exp[\pm k(\beta_{n'} + \beta_{n'})v] \text{ with } m = n' \tag{72}$$

As previously, we can summarize the set of results given by Equations (66)–(72) by following relations:

- for $m, n \in U$

$$\left\langle \psi_{m}^{(0)\pm} \middle| \psi_{n}^{(0)\mp} \right\rangle = 0 \quad \text{with} \quad m \neq n \tag{73}$$

$$\left\langle \psi_{m}^{(0)\pm} \middle| \psi_{n}^{(0)\mp} \right\rangle \neq 1 \quad \text{with} \quad m = n \tag{74}$$

Then the basis $\{|\psi_m^{(0)+}\rangle, |\psi_m^{(0)-}\rangle\}$ is an orthogonal basis.

But for $v = 0$, on the perfectly conducting surface, the functions which depend on v into relations (67), (69), (71), (72) take the value one. Therefore in this case, the relations (73), (74) are spelt:

- for $m, n \in U$

$$\left\langle \psi_{m}^{(0)\pm} \middle| \psi_{n}^{(0)\mp} \right\rangle = \delta_{mn} \tag{75}$$

Then, in this case ($v = 0$), the basis $\{|\psi_m^{(0)+}\rangle, |\psi_m^{(0)-}\rangle\}$ is an orthonormal basis identical to the basis $B^{\pm}$: $\{|\exp(ik\alpha_m u)\rangle, |\exp(ik\alpha_m u)\rangle\}$.

7. PERTURBED PROBLEM ($h \neq 0$): PERIODIC ROUGH SURFACE

7.1. Writing of the Matrix M in the Eigenbasis $B^{\pm}$ of the Unperturbed Problem

In basis $B^{\pm}$ the matrix M is changed to M according to the following relation:

$$\mathrm{M} = T^{-1} M T \tag{76}$$

Thus, M appears in the form:

$$\mathrm{M} = \mathrm{M}^{(0)} + h\mathrm{M}^{(1)} + h^2\mathrm{M}^{(2)} \tag{77}$$

with:

$$\mathrm{M}^{(0)} = \begin{bmatrix} [\beta^{-1}] & 0 \\ 0 & -[\beta^{-1}] \end{bmatrix} \tag{78}$$

$$\mathrm{M}^{(1)} = \begin{bmatrix} [C] & [C] \\ [C] & [C] \end{bmatrix} \tag{79}$$

$$\mathrm{M}^{(2)} = \begin{bmatrix} [D] & -[D] \\ [D] & -[D] \end{bmatrix} \tag{80}$$

setting:

$$[C] = -[\beta^{-2}][A]/2 \tag{81}$$

$$[D] = [\beta^{-2}][B][\beta]/2 \tag{82}$$

7.2. Solutions of Perturbed Problem

The eigenstates of the perturbed problem must satisfy the equation:

$$\mathrm{M}\,|\psi_m\rangle = r_m\,|\psi_m\rangle \tag{83}$$

with M given by (77) and:

$$|\psi_m\rangle = \begin{bmatrix} |\psi_m^+\rangle \\ |\psi_m^-\rangle \end{bmatrix} \quad \text{in under space } \mathbb{E}_m^+ \oplus \mathbb{E}_m^- \tag{84}$$

The principle of perturbation theory is to expand eigenvalues r_m and eigenstates $|\psi_m\rangle$ in series of powers of h keeping only a finite number of terms. Here, we take expansions up to second-order in agreement with the writing of the operator M in Equation (77).

Furthermore, we suppose that the eigenstates $|\psi_m^{(0)}\rangle$ and the eigenvalues $r_m^{(0)}$ of the unperturbed operator $\mathrm{M}^{(0)}$ are known and satisfy the following equation:

$$\mathrm{M}^{(0)} \left|\psi_m^{(0)}\right\rangle = r_m^{(0)} \left|\psi_m^{(0)}\right\rangle \tag{85}$$

We consider the case $v = 0$ where the set of vectors $|\psi_m^{(0)}\rangle$ forms an orthonormal basis $\{|\psi_m^{(0)+}\rangle, |\psi_m^{(0)-}\rangle\}$ in the space of states $\mathbb{E}_m^+ \oplus \mathbb{E}_m^-$.

Let us apply the fundamental idea of perturbation theory and let us assume that both the eigenvalues and eigenvectors of M can be expanded in powers of the perturbation parameter h in order to determine the coefficients in the perturbation expansions:

$$r_m = r_m^{(0)} + hr_m^{(1)} + h^2 r_m^{(2)} \tag{86}$$

$$|\psi_m\rangle = \left|\psi_m^{(0)}\right\rangle + h\left|\psi_m^{(1)}\right\rangle + h^2\left|\psi_m^{(2)}\right\rangle \tag{87}$$

To go beyond the first approximation in a systematic method, we substitute the three expressions (77), (86) and (87) into (83) and compare coefficients of powers of h to obtain the successive approximation equations:

$$\mathrm{M}^{(0)} \left|\psi_m^{(0)}\right\rangle = r_m^{(0)} \left|\psi_m^{(0)}\right\rangle \tag{88}$$

and:

$$\mathrm{M}^{(0)} \left|\psi_m^{(1)}\right\rangle + \mathrm{M}^{(1)} \left|\psi_m^{(0)}\right\rangle = r_m^{(0)} \left|\psi_m^{(1)}\right\rangle + r_m^{(1)} \left|\psi_m^{(0)}\right\rangle \tag{89}$$

$$\mathrm{M}^{(0)} \left|\psi_m^{(2)}\right\rangle + \mathrm{M}^{(1)} \left|\psi_m^{(1)}\right\rangle + \mathrm{M}^{(2)} \left|\psi_m^{(0)}\right\rangle = r_m^{(0)} \left|\psi_m^{(2)}\right\rangle + r_m^{(1)} \left|\psi_m^{(1)}\right\rangle + r_m^{(2)} \left|\psi_m^{(0)}\right\rangle \tag{90}$$

If we denote the complete set of eigenstates of $\mathrm{M}^{(0)}$ by $|\psi_i^{(0)}\rangle$, then any function $|\psi_m^{(1)}\rangle$ and $|\psi_m^{(2)}\rangle$ can be expanded in terms of the $|\psi_i^{(0)}\rangle$:

$$\left|\psi_m^{(1)}\right\rangle = \sum_i a_{mi}^{(1)} \left|\psi_i^{(0)}\right\rangle \tag{91}$$

$$\left|\psi_m^{(2)}\right\rangle = \sum_i a_{mi}^{(2)} \left|\psi_i^{(0)}\right\rangle \tag{92}$$

We substitute expressions (91) and (92) into Equations (89) and (90). Then we project these later upon the basis functions $\{\langle\psi_m^{(0)+}|, \langle\psi_m^{(0)-}|\}$ of dual space $(\mathbb{E}_m^+ \oplus \mathbb{E}_m^-)^\dagger$ within the aim to do to appear the scalar produces as defined in (28).

Furthermore, it is necessary to use the normalization of corrected wave functions to each order. We choose the phase so that $\langle\psi_m^{(0)}|\psi_m\rangle$ has a real value. This requirement imposes the following conditions:

- to zero order, the conditions (65) and (75),
- to first order, $\langle\psi_m|\psi_m\rangle = 1$ that is $\langle\psi_m^{\pm}|\psi_m^{\pm}\rangle = 1$ and $\langle\psi_m^{\pm}|\psi_m^{\mp}\rangle = 1$ if the choice of the phase is such that:

$$\left\langle\psi_m^{(0)\pm}\right|\left.\psi_m^{(1)\pm}\right\rangle = \left\langle\psi_m^{(1)\pm}\right|\left.\psi_m^{(0)\pm}\right\rangle = 0 \tag{93}$$

and:

$$\left\langle\psi_m^{(0)\mp}\right|\left.\psi_m^{(1)\pm}\right\rangle = \left\langle\psi_m^{(1)\pm}\right|\left.\psi_m^{(0)\mp}\right\rangle = 0 \tag{94}$$

- to second order, $\langle\psi_m|\psi_m\rangle = 1$ if the choice of the phase is such that:

$$\left\langle\psi_m^{(0)\pm}\right|\left.\psi_m^{(2)\pm}\right\rangle = \left\langle\psi_m^{(2)\pm}\right|\left.\psi_m^{(0)\pm}\right\rangle = -1/2 \left\langle\psi_m^{(1)\pm}\right|\left.\psi_m^{(1)\pm}\right\rangle \tag{95}$$

$$\left\langle\psi_m^{(0)\mp}\right|\left.\psi_m^{(2)\pm}\right\rangle = \left\langle\psi_m^{(2)\pm}\right|\left.\psi_m^{(0)\mp}\right\rangle = -1/2 \left\langle\psi_m^{(1)\pm}\right|\left.\psi_m^{(1)\mp}\right\rangle \tag{96}$$

The set of algebraic calculations lead to results below for the mth perturbed eigenvalues r_m and the mth perturbed eigenvectors $|\psi_m\rangle$, correct to second order:

$$r_m = r_m^{(0)} + h\left\langle \psi_m^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle + h^2 \left[\left\langle \psi_m^{(0)} \left| \mathrm{M}^{(2)} \right| \psi_m^{(0)} \right\rangle + \sum_{i \neq m} \left| \left\langle \psi_i^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right|^2 / \left(r_m^{(0)} - r_i^{(0)} \right) \right] \quad (97)$$

$$\begin{aligned} |\psi_m\rangle = {} & \left|\psi_m^{(0)}\right\rangle + h \sum_{i \neq m} \left[\left(\left\langle \psi_i^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right) / \left(r_m - r_i^{(0)} \right) \right] \left|\psi_i^{(0)}\right\rangle \\ & + h^2 \left\{ \sum_{j \neq m} \sum_{i \neq m} \left[\left(\left\langle \psi_i^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right) / \left(r_m - r_i^{(0)} \right) \right] \right. \\ & \left[\left(\left\langle \psi_j^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_i^{(0)} \right\rangle \right) / \left(r_m^{(0)} - r_j^{(0)} \right) \right] \left|\psi_j^{(0)}\right\rangle \\ & - \sum_{j \neq m} \left[\left(\left\langle \psi_j^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right) \right. \\ & \left. \left(\left\langle \psi_m^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right) / \left(r_m^{(0)} - r_j^{(0)} \right)^2 \right] \left|\psi_j^{(0)}\right\rangle \\ & - 1/2 \sum_{i \neq m} \left| \left(\left\langle \psi_i^{(0)} \left| \mathrm{M}^{(1)} \right| \psi_m^{(0)} \right\rangle \right) / \left(r_m^{(0)} - r_i^{(0)} \right) \right|^2 \left|\psi_i^{(0)}\right\rangle \\ & \left. + \sum_{j \neq m} \left[\left(\left\langle \psi_j^{(0)} \left| \mathrm{M}^{(2)} \right| \psi_m^{(0)} \right\rangle \right) / \left(r_m^{(0)} - r_j^{(0)} \right) \right] \left|\psi_j^{(0)}\right\rangle \right\} \end{aligned} \quad (98)$$

The Equation (98) is of the form:

$$|\psi_m\rangle = \left|\psi_m^{(0)}\right\rangle + h \sum_i a_{mi}^{(1)} \left|\psi_i^{(0)}\right\rangle + h^2 \sum_i a_{mi}^{(2)} \left|\psi_i^{(0)}\right\rangle \quad (99)$$

In matrix notation, the Equation (98) is written:

$$|\psi\rangle = \left\{ [I] + h \left[a^{(1)} \right] + h^2 \left[a^{(2)} \right] \right\} \left|\psi^{(0)}\right\rangle \quad (100)$$

where $[a^{(1)}]$ and $[a^{(2)}]$ are the matrix of which elements given in (98) are respectively the coefficients $a_{mi}^{(1)}$ and $a_{mi}^{(2)}$ of developments (91) and (92) of $|\psi_m^{(1)}\rangle$ and $|\psi_m^{(2)}\rangle$ against $|\psi_i^{(0)}\rangle$.

8. RETURN TO INITIAL EIGENFUNCTIONS IN BASIS *B*

The initial eigenvector $|\varphi\rangle$ that we seek is obtained from $|\psi\rangle$ (relation (100)) and the matrix T (49) of B to $B^{\pm}$ basis change:

$$|\varphi\rangle = T\,|\psi\rangle \tag{101}$$

that is:

$$\begin{bmatrix} |f\rangle \\ |f'\rangle \end{bmatrix} = [T] \begin{bmatrix} |\psi^{+}\rangle \\ |\psi^{-}\rangle \end{bmatrix} \tag{102}$$

The sought eigenfunctions, solutions of Equation (38), are written in the matrix form according to a expanding in powers of perturbation parameter h. They are:

$$\begin{bmatrix} |f\rangle \\ |f'\rangle \end{bmatrix} = \left\{ \begin{bmatrix} [F^{(0)+}] & [F^{(0)-}] \\ [F'^{(0)+}] & [F'^{(0)-}] \end{bmatrix} + h \begin{bmatrix} [F^{(1)+}] & [F^{(1)-}] \\ [F'^{(1)+}] & [F'^{(1)-}] \end{bmatrix} + h^2 \begin{bmatrix} [F^{(2)+}] & [F^{(2)-}] \\ [F'^{(2)+}] & [F'^{(2)-}] \end{bmatrix} \right\} \begin{bmatrix} [\psi^{(0)+}] & 0 \\ 0 & [\psi^{(0)-}] \end{bmatrix} \begin{bmatrix} |A^{+}\rangle \\ |A^{-}\rangle \end{bmatrix} \tag{103}$$

with: $[F^{(0)+}] = [F^{(0)-}] = [I]$ since $|\psi_m^{(0)+}\rangle$ form an orthonormal basis as well as $|\psi_m^{(0)-}\rangle$,

$$[F'^{(0)+}] = [\beta][F^{(0)+}] \quad \text{and} \quad [F'^{(0)-}] = -[\beta][F^{(0)-}]$$

$[F^{(1)+}]$, $[F^{(1)-}]$, $[F^{(2)+}]$, $[F^{(2)-}]$ are matrices deduced from (100) and (102).

Each of these functions are defined to within an amplitude term which are the components of $|A^{+}\rangle$ and $|A^{-}\rangle$. They will be calculated in the next paragraph in order to satisfy the boundary conditions.

9. BOUNDARY CONDITIONS AT THE GRATING SURFACE

The boundary conditions at the perfectly conducting surface deals with the tangential component $E_t(u, v)$ of electrical field. It is equal to zero for $v = 0$ and all u.

9.1. *TE* polarization

In TE polarization the tangential component $E_t(u, v)$ of the electrical field is represented by the sum for all m-th orders of functions $F_m^{+}(u, v)$

for outgoing waves and $F_m^-(u,v)$ for incoming waves, each of them being affected with the arbitrary constants A_m^+ and A_m^- :

$$E_t(u,v) = \sum_m A_m^+ F_m^+(u,v) + A_m^- F_m^-(u,v) \tag{104}$$

The constants A_m^+ and A_m^- will be adjusted to satisfy the boundary condition for $v = 0$ and all u, that is with matrix notation:

$$[F^+][A^+] + [F^-][A^-] = 0 \tag{105}$$

For simplification, we set the magnitude of electric field of incident wave equal to unity for each incident and evanescent order.

$$[A^-] = [A^{(0)-}] = [I] \tag{106}$$

$[A^+]$ is expanding in powers of h:

$$[A^+] = [A^{(0)+}] + h[A^{(1)+}] + h^2[A^{(2)+}] \tag{107}$$

as:

$$[F^\pm] = [F^{(0)\pm}] + h[F^{(1)\pm}] + h^2[F^{(2)\pm}] \tag{108}$$

given by Equation (103).

We substitute the three expressions (106), (107) and (108) into (105). Then comparing coefficients in powers of h one gets the coefficients of the $[A^+]$ expansion which are:

$$[A^{(0)+}] = -[F^{(0)+}]^{-1}([F^{(0)-}][A^{(0)-}]) \tag{109}$$

$$[A^{(1)+}] = -[F^{(0)+}]^{-1}([F^{(1)-}][A^{(0)-}] + [F^{(1)+}][A^{(0)+}]) \tag{110}$$

$$[A^{(2)+}] = -[F^{(0)+}]^{-1}([F^{(2)-}][A^{(0)-}] + [F^{(2)+}][A^{(0)+}] + [F^{(1)+}][A^{(1)+}]) \tag{111}$$

9.2. *TM* Polarization

We still must write the continuity of the tangential component $E_t(u,v)$ of electric field on conductor surface ($v = 0$ and all u).

A classical calculation of $E_t(u,v)$ shows that it is proportional to a function $G(u,v)$:

$$E_t(u,v) = G(u,v) \cdot Z_0 \cos\varphi \tag{112}$$

with:

$$G(u,v) = h\ddot{a}\alpha F(u,v) - (1 + h^2\dot{a}^2)F'(u,v) \tag{113}$$

Z_0: vacuum impedance

φ: angle between the tangent to the profile and x-axis

Furthermore, to functions $F(u,v)$ and $F'(u,v)$ firstly defined in the basis B correspond in the normalized basis $B^\pm$ to:

- the functions $F^+(u,v)$ and $F'^+(u,v) = \beta F^+(u,v)$ for outgoing waves,
- the functions $F^-(u,v)$ and $F'^-(u,v) = -\beta F^-(u,v)$ for incoming waves.

Then, on the grating surface we write the continuity of the sum for all m-th orders of $G_m^+(u,v)$ and $G_m^-(u,v)$ each respectively multiplied by the arbitrary constants A_m^+ and A_m^-. These constants must be adjusted to satisfy the boundary condition $G(u,0) = 0$ for all u. In matrix notation one writes:

$$[G^+][A^+] + [G^-][A^-] = 0 \tag{114}$$

with:

$$[G^\pm] = h[\ddot{a}][\alpha][F^\pm] - \left([I] + h^2[\ddot{a}]^2\right)[F'^\pm] \tag{115}$$

and:

$$[F'^\pm] = \pm[F^\pm][\beta] \tag{116}$$

We apply the same method for $[A^-]$ which is taken equal to unity ($[A^-] = [A^{(0)-}] = [I]$).

Since $[F^\pm]$ and $[F'^\pm]$ are known to second order in powers of h (103) and (116), $[G^\pm]$ and $[A^+]$ will be expanded to fourth order in powers of h:

$$[A^+] = [A^{(0)+}] + h[A^{(1)+}] + h^2[A^{(2)+}] + h^3[A^{(3)+}] + h^4[A^{(4)}] \tag{117}$$

The coefficients of expansion of $[A^+]$ are calculated to fourth order in powers of h. They are given in matrix form below:

$$[A^{(0)+}] = -[G^{(0)+}]^{-1}\left([G^{(0)-}][A^{(0)-}]\right) \tag{118}$$

$$[A^{(1)+}] = -[G^{(0)+}]^{-1}\left([G^{(1)-}][A^{(0)-}] + [G^{(1)+}][A^{(0)+}]\right) \tag{119}$$

$$\begin{aligned}[A^{(2)+}] = -[G^{(0)+}]^{-1}\Big([G^{(2)-}][A^{(0)-}] + [G^{(2)+}][A^{(0)+}] \\ +[G^{(1)+}][A^{(1)+}]\Big)\end{aligned} \tag{120}$$

$$\begin{aligned}[A^{(3)+}] = -[G^{(0)+}]^{-1}\Big([G^{(3)-}][A^{(0)-}] + [G^{(3)+}][A^{(0)+}] \\ +[G^{(2)+}][A^{(1)+}] + [G^{(1)+}][A^{(2)+}]\Big)\end{aligned} \tag{121}$$

$$\begin{aligned}[A^{(4)+}] = -[G^{(0)+}]^{-1}\Big([G^{(4)-}][A^{(0)-}] + [G^{(4)+}][A^{(0)+}] \\ +[G^{(3)+}][A^{(1)+}]+[G^{(2)+}][A^{(2)+}]+[G^{(1)+}][A^{(3)+}]\Big)\end{aligned} \tag{122}$$

10. CALCULATION OF EFFICIENCY

It is interesting to define an efficiency P equal to the fraction of incident energy which is transmitted in each diffracted wave. This energy is obtained from the flow of Poynting vector through the unit surface perpendicular to y-axis.

Then:

$$P = |E|^2 \rho^+ / \beta^- \approx |E|^2 \beta^+ / \beta^-, \tag{123}$$

limiting the expansion of ρ^+ to the first-order of the perturbation in order to compare our results in the same direction as curvilinear coordinate method.

$$\text{For } TE \text{ polarization}: \ [P_{TE}] = [A^+][A^+]^* \left([\beta^+][\beta^-]^{-1}\right) \tag{124}$$

$$\text{For } TM \text{ polarization}: \ [P_{TM}] = [A^+][A^+]^* \left([\beta^+][\beta^-]^{-1}\right) \tag{125}$$

The values of P_{TE} and P_{TM} are calculated according to a fourth order expansion in powers of h for each of them:

$$P = P^{(0)} + hP^{(1)} + h^2 P^{(2)} + h^3 P^{(3)} + h^4 P^{(4)} \tag{126}$$

The expansion terms are analytically known:

- For P_{TE}, they are in matrix form:

$$\begin{aligned}[P_{TE}] = \Big\{ & [A^{(0)+}][A^{(0)+}]^* + h\left([A^{(1)+}][A^{(0)+}]^* + [A^{(0)+}][A^{(1)+}]^*\right) \\ & + h^2\left([A^{(2)+}][A^{(0)+}]^* + [A^{(1)+}][A^{(1)+}]^* + [A^{(0)+}][A^{(2)+}]^*\right) \\ & + h^3\left([A^{(2)+}][A^{(1)+}]^* + [A^{(1)+}][A^{(2)+}]^*\right) \\ & + h^4\left([A^{(2)+}][A^{(2)+}]^*\right)\Big\}\left([\beta^+][\beta^-]^{-1}\right)\end{aligned} \tag{127}$$

- For P_{TM}, they are in matrix form:

$$\begin{aligned}[P_{TM}] = \Big\{ & [A^{(0)+}][A^{(0)+}]^* + h\left([A^{(1)+}][A^{(0)+}]^* + [A^{(0)+}][A^{(1)+}]^*\right) \\ & + h^2\left([A^{(2)+}][A^{(0)+}]^* + [A^{(1)+}][A^{(1)+}]^* + [A^{(0)+}][A^{(2)+}]^*\right) \\ & + h^3\left([A^{(3)+}][A^{(0)+}]^* + [A^{(2)+}][A^{(1)+}]^* + [A^{(1)+}][A^{(2)+}]^*\right. \\ & \left. + [A^{(0)+}][A^{(3)+}]^*\right) + h^4\left([A^{(4)+}][A^{(0)+}]^* + [A^{(3)+}][A^{(1)+}]^*\right. \\ & \left. + [A^{(2)+}][A^{(2)+}]^* + [A^{(1)+}][A^{(3)+}]^* + [A^{(0)+}][A^{(4)+}]^*\right)\Big\} \\ & \left([\beta^+][\beta^-]^{-1}\right)\end{aligned} \tag{128}$$

11. VALIDITY CONDITIONS OF THE PERTURBATION METHOD

11.1. Theoretic Validity

The perturbation method applies to case where the first order perturbation $h\mathrm{M}^{(1)}$ and second order perturbation $h^2\mathrm{M}^{(2)}$ are very small with respect to $\mathrm{M}^{(0)}$. Then the result given by Equation (98) suggests that a suitable definition of "smallness" for the perturbations $h\mathrm{M}^{(1)}$ and $h^2\mathrm{M}^{(2)}$ is that the relevant matrix elements $|\langle\psi_i^{(0)}|h\mathrm{M}^{(1)}|\psi_m^{(0)}\rangle|$ and $|\langle\psi_i^{(0)}|h^2\mathrm{M}^{(2)}|\psi_m^{(0)}\rangle|$ should be small compared to the difference of corresponding eigenvalues $r_m^{(0)} - r_i^{(0)}$.

From (98) and (99) we can see that the perturbed wave vector $|\psi_m\rangle$ can be viewed as a linear combination of unperturbed eigenvector $|\psi_i^{(0)}\rangle$; the coefficients $a_{mi}^{(1)}$ and $a_{mi}^{(2)}$ tell us "how much" of the ith unperturbed vectors contribute to the mth perturbed vector. We say that the unperturbed vector $|\psi_i^{(0)}\rangle$ for a particular $i \neq m$ mix with $|\psi_m^{(0)}\rangle$ to form the perturbed vector $|\psi_m\rangle$.

Since $a_{mi}^{(1)}$ and $a_{mi}^{(2)}$ are inversely proportional to eigenvalues separation between the mth and ith unperturbed diffracted directions we expect directions that are closest together in diffracted directions to mix most strongly with $|\psi_m^{(0)}\rangle$. This fact provides a clue on how to avoid calculating the set of terms in Equation (98) depending on the degree of accuracy desired, we need only evaluate terms for the diffracted directions closest in mth direction. It is important to note that if any of these coefficients is large, then perturbation method might break down and the problem probably must be handled in another way.

Finally, it is apparent from (98) that this result is restricted to non-degenerate states only, for if some unperturbed vector, say $|\psi_i^{(0)}\rangle$, is degenerate with $|\psi_m^{(0)}\rangle$, then $r_m^{(0)} = r_i^{(0)}$ and the mth term in the summation of Equation (98) is infinite. This situation would not occur if $\langle\psi_i^{(0)}|h\mathrm{M}^{(1)}|\psi_m^{(0)}\rangle$ or if $\langle\psi_i^{(0)}|h^2\mathrm{M}^{(2)}|\psi_m^{(0)}\rangle$ happened to be zero, but such will not generally the case. Thus all degenerate states must be treated differently.

Moreover, the Equation (97) indicates that the mth perturbed eigenvalue r_m associated to the mth diffracted direction is given by the eigenvalue $r_m^{(0)}$ of the corresponding unperturbed problem plus the expectation values of the first order perturbation $h\mathrm{M}^{(1)}$ and second order perturbation $h^2\mathrm{M}^{(2)}$. These terms can be of either sign and thus can raise or lower the value r_m from the unperturbed value $r_m^{(0)}$.

11.2. Numerical Validity

The perturbation method is applied to a sinusoidal grating of infinite conductivity. The calculation of efficiencies P_{TE} and P_{TM} is tried on various values of parameters: incidence angle θ_0, period d, wavelength λ, groove depth h_c with a suitable number of space-harmonic N introducing evanescent waves and m-th real orders.

Especially, the values of d/λ and θ_0 being fixed we study the evolution of efficiencies P_{TE} and P_{TM} against parameter h_c/λ when it varies from 0 to 0.20 by steps of 0.04.

We have chosen two domains of study according to respective values of d and λ:

- The first study is done into domain of electromagnetism waves or resonant domain corresponding to d/λ near of value one, let $d/\lambda = 1.3$.

The chosen values for angles are $\theta_0 = 10°$ (three real orders), $\theta_0 = 30°$ (two real orders), $\theta_0 = 22.62°$ very near of Littrow (two real orders) and $\theta_0 = 1°$ very near normal incidence (three real orders).

- The second study is done near physical optics domain corresponding to d/λ large with respect to the value one, let $d/\lambda = 10.3$.

The chosen values for angles are $\theta_0 = 5°$ with the incident order $m = 0$ (five real diffracted orders -2, -1, 0, 1, 2, far from evanescent waves) and $\theta_0 = 5°$ with the incident order $m = 8$, let $\theta_8 = 59.7522°$ (five real diffracted orders, 5, 6, 7, 8, 9 or -3, -2, -1, 0, 1 by slipping of numbers, close to evanescent waves). In fact, when the number of eigenvalues is great, the calculation done for $\theta_0 = 5°$ gives also the results for all m-th incident orders such that $\sin\theta_m = \sin\theta_0 + m\lambda/d$.

11.2.1. Comparison of Efficiencies

In order to appreciate the numerical results obtained from algebraic expression of perturbation method we compare them with those obtained through the rigorous numerical method with same values of parameters. The curves representing the evolution of efficiencies P_{TE} and P_{TM} against parameter h_c/λ for the incident order $m = 0$ and the diffracted order $m = -1$ are then drawn on Figure 2 for $d/\lambda = 1.3$ and Figure 3 for $d/\lambda = 10.3$.

The comparison of numerical results obtained from two methods on the one hand and the comparison of corresponding curves on the other hand show that a good agreement is obtained up to a maximum value of parameter h_c/λ. This limit value defines the smallest domain of variation of groove depth compared to wavelength

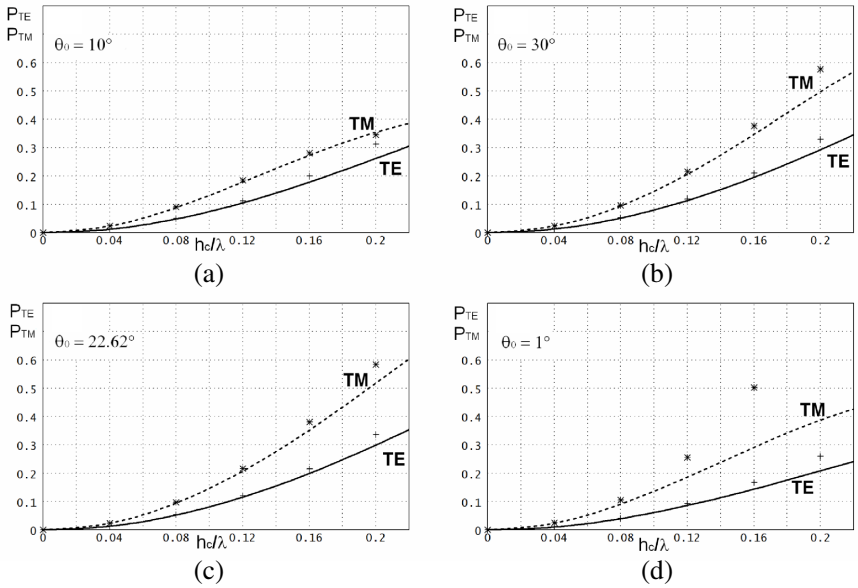

Figure 2. Efficiencies P_{TE} and P_{TM} versus groove depth h_c/λ for diffracted order $m = -1$ and period $d/\lambda = 1.3$. Crosses correspond to perturbation method and solid curve corresponds to numerical method for TE polarization. Asterisks correspond to perturbation method and dotted curve corresponds to numerical method for TM polarization. Incidence angles (a) $\theta_0 = 10°$, (b) $\theta_0 = 30°$, (c) $\theta_0 = 22.62°$ and (d) $\theta_0 = 1°$.

where the perturbation method must be applied. To this limit value of parameter h_c/λ we calculate the corresponding relative uncertainty of efficiencies $\Delta P_{TE}/P_{TE}$ and $\Delta P_{TM}/P_{TM}$ between the two methods for each TE and TM polarization:

$$\frac{\Delta P}{P} = \frac{\left|P_{(perturbation)} - P_{(numerical)}\right|}{P_{(numerical)}} \tag{129}$$

The Table 1 gives the limit value of parameter h_c/λ and corresponding uncertainties $\Delta P_{TE}/P_{TE}$ and $\Delta P_{TM}/P_{TM}$ for each set of parameters and m-th incident and diffracted orders written in thick character.

11.2.2. Comments

The angle $\theta_0 = 22.62°$ is very near degenerated point of 22.6198° that correspond to Littrow mounting obtained when $\theta_{-1} = -\theta_0 = \lambda/2d$.

Table 1. Values of parameters d/λ, θ_0, N used for calculations efficiencies. Relative uncertainty on efficiencies P_{TE}, P_{TM} and on the eigenvalue r_{-1} calculated for the limit value of h_c/λ with incident and diffracted orders written in thick character.

d/λ	θ_0	m-th incident order	N	m-th diffracted order
1.3	10°	**0**	3	**−1**, 0, 1
	30°	**0**	3	**−1**, 0
	22.62°	**0**	3	**−1**, 0
	1°	**0**	3	**−1**, 0, 1
10.3	5°	**0**	13	−2, **−1**, 0, 1, 2
	5°	**8**	13	−3, −2, **−1**, 0, 1
h_c/λ	$\frac{\Delta P_{TE}}{P_{TE}}$	$\frac{\Delta P_{TM}}{P_{TM}}$	$\frac{\Delta r_{-1}}{r_{-1}^{(0)}}$	-
≤ 0.16	≤ 0.12	≤ 0.03	≤ 0.037	-
≤ 0.16	≤ 0.08	≤ 0.08	≤ 0.037	-
≤ 0.16	≤ 0.08	≤ 0.08	≤ 0.037	-
≤ 0.12	≤ 0.08	≤ 0.37	≤ 0.021	-
≤ 0.12	≤ 0.15	≤ 0.17	≤ 0.0004	-
≤ 0.16	≤ 0.08	≤ 0.08	≤ 0.0006	-

In this case, the deviation is minimum for order $m = -1$. Thus for an angle difference $\Delta\theta = 2 \times 10^{-4}$ degree it appears an eigenvalue difference $\Delta\beta^{-1} = \beta_{-1}^{-1} - \beta_0^{-1} = 2 \times 10^{-6}$ which is sufficient for perturbation method to give results in agreement with numerical method (Figure 2(c)). This situation only occurs twice with matrix elements of $\mathrm{M}^{(1)}$, $\langle\psi_{-1}|h\mathrm{M}^{(1)}|\psi_0\rangle$ and $\langle\psi_0|h\mathrm{M}^{(1)}|\psi_{-1}\rangle$, and twice with matrix elements of $\mathrm{M}^{(2)}$, $\langle\psi_{-1}|h^2\mathrm{M}^{(2)}|\psi_0\rangle$ and $\langle\psi_0|h^2\mathrm{M}^{(2)}|\psi_{-1}\rangle$, which are small.

The angle $\theta_0 = 1°$ has been chosen near another degenerated point, the normal incidence. In fact, into normal incidence $\theta_0 = 0°$ that is $\alpha_0 = 0$, real and imaginary eigenvalues are twofold ($\pm\beta_3^{-1} = \pm\beta_{-3}^{-1}$, $\pm\beta_2^{-1} = \pm\beta_{-2}^{-1}$, $\pm\beta_1^{-1} = \pm\beta_{-1}^{-1}$) except β_0. In this case the perturbation method established for undegenerated states does not agree. However, near of normal incidence $\theta_0 = 1°$ (Figure 2(d)), the perturbation method gives results into good agreement with numerical method with $h_c/\lambda \leq 0.12$, smaller value than for other cases (Figures 2(a), (b), (c), let angles $\theta_0 = 10°$, 30°, 22.62°). The precision is better for TE polarization ($\Delta P_{TE}/P_{TE} \leq 0.08$) than for TM polarization ($\Delta P_{TM}/P_{TM} \leq 0.37$).

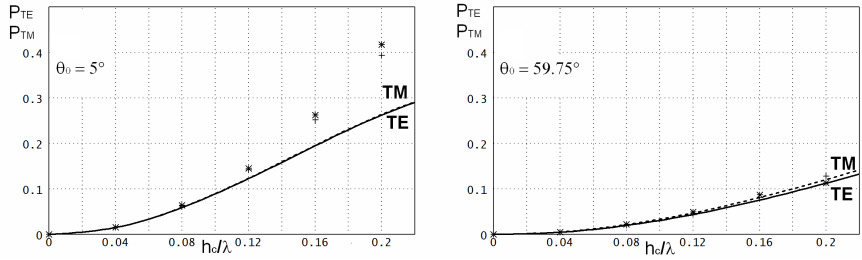

Figure 3. Efficiencies P_{TE} and P_{TM} versus groove depth h_c/λ for diffracted order $m = -1$ and period $d/\lambda = 10.3$. Crosses correspond to perturbation method and solid curve corresponds to numerical method for TE polarization. Asterisks correspond to perturbation method and dotted curve corresponds to numerical method for TM polarization. Incidence angles (a) $\theta_0 = 5°$ and (b) $\theta_0 = 59.75°$.

For $d/\lambda = 10.3$, period large with respect to wavelength, the two cases considered with incident angles $\theta_0 = 5°$ and $\theta_8 = 59.7522°$ give different results for limit value of h_c/λ and $\Delta P/P$ (Figure 3 and Table 1). In fact, the results are better with θ_8 than θ_0. We can explain this difference with regard to the influence of evanescent waves which is more important in second case (Figure 3(b)) than in first case (Figure 3(a)). Furthermore, the Figure 3 shows that values of efficiencies P_{TE} and P_{TM} are similar for each of them perturbation method and numerical method. Indeed, $d/\lambda = 10.3$ is near of physical optics domain where polarization effects disappear.

The Table 1 shows that the two chosen periods $d/\lambda = 1.3$ and $d/\lambda = 10.3$ lead to same limit value $h_c/\lambda \leq 0.16$ for example with the same uncertainties on efficiencies $\Delta P/P \leq 0.08$ deduced of limit good agreement of efficiencies between results obtained from perturbation method and rigorous numerical method. Now, it is from eigenfunctions that efficiencies are calculated. Consequently, on condition that $d/\lambda > 1$ it may be seen that parameter d/λ has a weak effect on eigenfunctions.

11.2.3. Comparison of Eigenvalues

According to (97), in our problem of a sinusoidal surface, we can observe that the eigenvalue $r_m (= r_m^{\pm})$ is independent of magnitude h because the matrix $\mathrm{M}^{(1)}$ has its diagonal terms equal to zero. The only dependence is in h^2. Therefore, the eigenvalues are independent

of sign of h when we stop the calculation to the first order in h^2 with $\mathrm{M}^{(2)}$ operator (97).

The perturbation method leads to $r_m \neq r_m^{(0)}$ with $r_m^{(0)} = \beta_m^{-1}$. Then, the rigorous numerical method gives $r_m = r_m^{(0)}$ in here considered cases for real eigenvalues. Consequently, to compare eigenvalues obtained with perturbation method and numerical method it is sufficient to compare r_m and $r_m^{(0)}$. Thus, for the same set of parameters and same m-th incident directions ($m = 0$ and $m = 8$) and diffracted direction $m = -1$ as indicated in Table 1, we calculate relative uncertainties $\Delta r_{-1}/r_{-1}^{(0)} = (r_{-1} - r_{-1}^{(0)})/r_{-1}^{(0)}$ for the limit values of h_c/λ given in Table 1. The obtained values for $\Delta r_{-1}/r_{-1}^{(0)}$ are given in Table 1.

We note that uncertainties $\Delta r_{-1}/r_{-1}^{(0)}$ vary as $(h_c/\lambda)^2$ for d/λ fixed and as $(\lambda/d)^2$ for h_c/λ fixed. These results are in agreement with the considered corrective term due to $h^2\mathrm{M}^{(2)}$ when we stop the calculation to the first order in h^2 (97) where h is of the form $h = 2\pi\frac{h_c}{\lambda} \times \frac{\lambda}{d}$.

11.3. Results for Domain of Validity

To point of view of efficiencies, it is the parameter h_c/λ which defines the domain of validity of perturbation method, let $0 < h_c/\lambda \leq 0.16$, with a period d satisfying $d/\lambda = 1.3$ (domain of electromagnetic waves) or $d/\lambda = 10.3$ (domain near to physical optics waves)

However the accuracy on eigenvalues is better for $d/\lambda = 10.3$ than for $d/\lambda = 1.3$. Here the calculation of efficiencies does not depend on of accuracy on eigenvalues. Generally the value of parameter d/λ is fixed by the choice of number diffracted orders.

The perturbation method presents some advantage with regard to the numerical method. It is principally an analytic method. Consequently, at each step of calculation it is possible to follow the influence of parameters. Furthermore, the last results of this work that is the efficiencies are also presented under analytic form.

12. CONCLUSION

The present work has been devoted to perturbation method relating to propagative and evanescent waves for undegenerated states in case of diffraction of electromagnetic waves by periodic surface. The propagation equation is a second order differential equation with first order term.

In the case of a surface with groove depth small compared to its period we have written the propagation equation in a translation coordinate system and we have associated operators to the different coefficients of the equation. This equation appears in matrix form according to an expansion in series of powers of h to second order. The small dimensionless parameter h, leads us to use the perturbation method to find an approximate solution of the eigenvalue equation. Unlike the quantum physics, our operator is not a hermitian operator. Consequently, there are also imaginary eigenvalues, then evanescent waves. For that, each of steps of calculation has been related in detail.

These analytical solutions, eigenvalues and eigenfunctions, are obtained from known eigensolutions of the unperturbed problem that is a plane surface. Furthermore, the efficiencies are expressed as a function of geometrical parameters.

From comparison of efficiencies deduced from perturbation method with those obtained with rigorous numerical method we have defined a validity domain of perturbation method. This domain relates to the groove depth h_c with regard to wave length λ. We obtain $0 < h_c/\lambda \leq 0.16$ with a period d satisfying $d/\lambda > 1$ (resonant domain) or $d/\lambda \gg 1$ (physics optics domain). Although the variation domain of h_c/λ may appear narrow, the perturbation method presents some interests. For instance it shows in a simple way that eigenvalues do not depend h parameter. Therefore up to the first order, eigenvalues are the same for surfaces $y = +ha(x)$ and $y = -ha(x)$. Furthermore it allows understand how the unperturbed vector $|\psi_i^{(0)}\rangle$ for a particular $i \neq m$ mixes with $|\psi_m^{(0)}\rangle$ to form the perturbed vector $|\psi_m\rangle$.

However, for exact values of incidence angle corresponding to normal incidence and Littrow mounting it will be necessary to develop the perturbation method for degenerated states. Indeed for these both cases, two different physical directions correspond to the same eigenvalue.

Our future work will be the generalization of the method. For example, starting from known numerical solutions associated to particular surface ($h \neq 0$), we will derive approximate solutions when this surface undergoes a periodic deformation.

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