A Couple of Topics in Numerical Analysis of Diffraction by a Metal Grating Using Yasuura's Method of Modal Expansion

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Abstract— Assuming the progress of numerical solution of grating problems by Yasuura's method of modal expansion, we pick up a couple of issues that require our countermeasure, state our step, and give our opinion if appropriate. Here we take up: choice of modal functions; observation of condition number in least-squares boundary matching; and use of refractive indices of Au taken from references.

1. INTRODUCTION

In solving the problem of scattering or diffraction on a computer, we often encounter small issues that require us to take some action. Assuming the process of numerical solution (mainly) of grating problems by Yasuura's method of modal expansion [1–4], we pick up a few of such issues or topics and state our countermeasures or opinion. The issues are:

1) Choice of modal functions: In the method we define an approximate solution in terms of a finite linear-combination of modal functions. The choice of a set of modal functions from among possible set of functions is an important issue because the effectiveness of the method depends on the choice.
2) Observation of the condition number: We employ the orthogonal decomposition of the Jacobian matrix in solving the least-squares problem and the nature of the matrix given by the condition number is important.
3) Refractive index of Au: The index of a metal is of a great interest in application to plasmonics. Here we show a couple of examples of plasmon resonance absorption predicted by our computer program using four different values of Au index.

2. A BRIEF INTRODUCTION TO YASUURA'S METHOD OF MODAL EXPANSION

Before taking up the issues, we briefly see the process of solution by the method. Figure 1 shows the geometry of a sample problem: 2-D E-wave (s-polarization) scattering by a perfectly conducting grating. We denote the cross section of the grating by C and assume the semi-infinite region below C is filled with a perfect conductor. The cross section C is periodic in X with a period d. We represent a point on C by $s(x, y)$, assume $y = \eta(x)$ ($\eta(x+d) = \eta(x)$), and let a point in the free space region S above C be $\mathbf{r}(X, Y)$. Let us consider the problem to find the diffracted field when an E-polarized plane wave

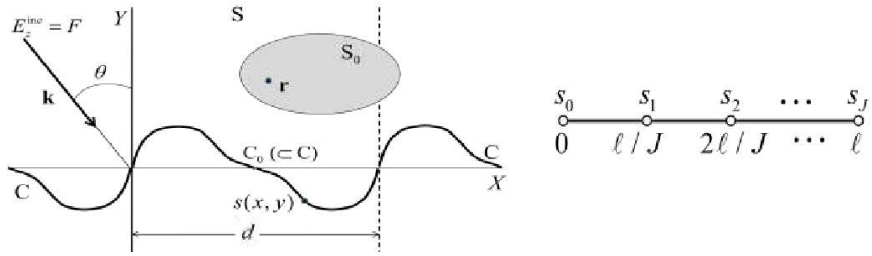
$$\mathbf{E}^{\mathrm{i}}(\mathbf{r}) = \mathbf{u}_Z F(\mathbf{r}) = \mathbf{u}_Z \exp(i\,\alpha_0 X - i\,\beta_0 Y), \quad \alpha_0 = k\sin\theta, \quad \beta_0 = k\cos\theta \tag{1}$$

is incident. Here, the time factor $e^{-i\omega t}$ is suppressed and $\mathbf{u}_Z$ denotes a unit vector in Z-direction.

The solution to this problem, $E_z^s(\mathbf{r}) = \Psi(\mathbf{r})$, should satisfy the following conditions:

D1. 2-D Helmholtz's equation in S, $\nabla^2\Psi(\mathbf{r}) + k^2\Psi(\mathbf{r}) = 0$;
D2. Pseudo-periodicity condition, $\Psi(X+d, Y) = \exp(i\,\alpha_0 d)\,\Psi(X, Y)$;
D3. 1-D radiation condition that $\Psi(X, Y)$ propagates or attenuates in the positive Y-direction;
D4. The boundary condition on a perfectly conducting surface, $\Psi(s)+F(s) = \Psi(x, \eta(x))+F(x, \eta(x)) = 0$.

To solve this problem by using Yasuura's method of modal expansion, we first need to define a set of modal functions $\{\varphi_m(\mathbf{r}) : m = 1, 2, \ldots\}$ that satisfies the requirements:



(a) (b)

Figure 1: (a) Geometry of a sample problem: E-wave (s-polarization) scattering by a grating made of a perfectly-conducting metal. C is the cross section and S is a semi-infinite region above C. C_0 is the first period of C and S_0 is an arbitrary closed subregion of S. (b) Equally located sampling points on C_0. s_j are the points whose s-coordinates are $j\ell/J$. Ed: Frame lines are for reference; please delete them.

M1. Each $\varphi_m(\mathbf{r})$ satisfies the conditions **D1**, **D2**, and **D3**.

M2. The set of boundary values $\{\varphi_m(s) : m = 1, 2, \ldots\}$ is complete in the function space $\mathrm{L}^2(\mathrm{C}_0)$ consisting of all the square integrable functions defined on C_0, the first period of C.

Next, we define an approximate solution in terms of a *finite* linear combination of the modal functions

$$\Psi_M(\mathbf{r}) = \sum\nolimits_{m=1}^{M} A_m(M)\, \varphi_m(\mathbf{r}) \tag{2}$$

where $A_m(M)$ means that the A_m-coefficient depends on the number of truncation M. Because the solution satisfies the conditions **D1**, **D2**, and **D3**, we determine the coefficients in order that the solution meets the boundary condition **D4** approximately. In Yasuura's method we employ the least-squares method:

Problem C. Find the set of A_m-coefficients that minimizes a normalized mean-squares boundary residual

$$\Omega_M^{\mathrm{C}} = \|\Psi_M + F\|^2 \Big/ \|F\|^2 = \int_{s=0}^{\ell} |\Psi_M(s) + F(s)|^2 ds \Big/ \int_{s=0}^{\ell} |F(s)|^2 ds \tag{3}$$

Here, ℓ denotes the length of C_0. In a shallow grating, a definition $\|f\|^2 = \int_{x=0}^{d} |f(x, \eta(x))|^2 dx$ also works.

In numerical solution on a computer we need (**i**) the method of discretization and (**ii**) the method for solving the discretized problem. Discretization can be made in the following way: First, we locate equally-spaced $J = 2M$ sampling points on C_0 and denote them by $\{s_0, s_1, \ldots, s_J\}$. Although this set includes $J+1$ points, s_0 and s_J share common information (except for the $\alpha_0 d$ phase difference; see Section 3.1) and we can regard them as one point. Second, we define J-dimensional column vectors whose members are boundary values of modal functions.

$$\boldsymbol{\varphi}_m = (\varphi_m(s_1)\ \varphi_m(s_2)\ \ldots\ \varphi_m(s_J))^{\mathrm{T}} \quad (m = 1, 2, \ldots, M) \tag{4}$$

Then, we set up a $J \times M$ Jacobian matrix

$$\Phi = [\boldsymbol{\varphi}_1\ \boldsymbol{\varphi}_2\ \ldots\ \boldsymbol{\varphi}_M] \tag{5}$$

Finally, defining an M-dimensional solution vector

$$\mathbf{A} = (A_1(M)\ A_2(M) \ldots A_M(M))^{\mathrm{T}} \tag{6}$$

we have a least-squares problem in a J-dimensional complex-valued vector space, a discretized form of **Problem C**.

Problem D. Find a solution vector $\mathbf{A}$ that minimizes the discretized boundary residual

$$\Omega_M = \|\Phi\mathbf{A} + \mathbf{F}\|^2 \Big/ J = \left\| \sum\nolimits_{m=1}^{M} A_m(M)\, \boldsymbol{\varphi}_m + \mathbf{F} \right\|^2 \Big/ J \tag{7}$$

Here, $\mathbf{F}$ is a discretized incident wave, $\|\mathbf{f}\|$ denotes the Euclidean norm of a J-dimensional vector, the denominator J comes from the line element $ds \simeq \ell/J$, and this ℓ has been canceled by the denominator of (3). In solving **Problem D**, we usually employ the QR decomposition. In case if we need the condition number of the Jacobian matrix, we use the singular-value decomposition.

We can prove that the sequence of approximate solutions $\{\Psi_1(\mathbf{r}), \Psi_2(\mathbf{r}), \ldots, \Psi_M(\mathbf{r}), \ldots\}$ with the coefficients obtained by solving **Problem D** converges to the true solution $\Psi(\mathbf{r})$ uniformly in any closed sub-region S_0 in S.

3. TOPICS IN THE SOLUTION PROCESS

Here we employ three representative topics/issues that emerge in the process of numerical analysis by Yasuura's method of modal expansion.

3.1. Choice of Modal Functions

If the cross section is simple like a sinusoid, is shallow, and if the period is comparable to the wavelength, the problems are easy to solve with the commonly-employed set of separated solutions satisfying the periodicity (**D2**) and radiation condition (**D3**). They are referred to as the Floquet or grating modes and are given by

$$\begin{aligned}&\varphi_m(X,Y) = \exp(i\alpha_m X + i\beta_m Y),\\&\alpha_m = \alpha_0 + 2m\pi/d, \quad \beta_m = \sqrt{k^2 - \alpha_m^2} \quad (\mathrm{Re}\beta \geq 0,\ \mathrm{Im}\beta \geq 0;\ m = 0,\ \pm 1,\ \pm 2, \ldots)\end{aligned} \tag{8}$$

In using this set of modal functions, we should modify the summations in (2) and (7) to $\Sigma_{m=-N}^{N}$ and the total number of unknowns is $M = 2N + 1$. In addition, we use the functions

$$\tilde{\varphi}_m(x,\, y) = \exp(-i\alpha_0 x)\, \varphi_m(x, y) \quad \text{and} \quad \tilde{F}(x,\, y) = \exp(-i\alpha_0 x)\, F(x,\, y) \tag{9}$$

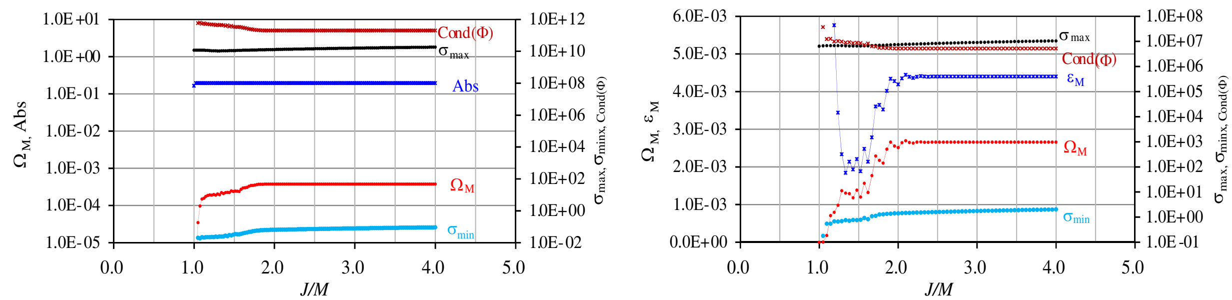
instead of $\varphi_m(x,\, y)$ and $F(x, y)$. Because the modified functions are periodic in x and s, this modification would accelerate the convergence of the solutions [5]. Further, the periodicity of functions means that the discretized boundary residual (7) is a trapezoidal approximation to (3).

Conversely, if the cross section is complicated, deep, or is electrically large, the problem is difficult and the method with Floquet modal functions often fails [6]. The same problem arises also in other methods employing modal expansion and many researchers have endeavored to develop methods of analysis that can solve the difficult problems. A lot of works can be found and we refer only a few examples [7–9]. We also have tried two approaches, which are understood as the use of alternative sets of modal functions:

(**i**) Location of line sources in S^c (the complement of S). This is the same as the equivalent-sources method and is useful when combined with a technique of concentrating the poles near the convex part of the obstacle. In scattering by a cylindrical obstacle $\rho = a(1 - 0.2\cos 3\theta)$ [10], we compared three types of modal functions: separated solutions (sep), fields from monopoles located equally on an analogous curve inside the boundary (pel), and fields from monopoles densely located near the peaks of the curve (pdp). At $ka = 10$, both (pel) and (pdp) works well and the energy errors at $M = 70$ are 9×10^{-5} and 1×10^{-5}%. It is difficult for (sep) to give good solutions for the error is 4%. At $ka = 30$, the energy errors of the solutions with $M = 100$ are 2×10^{-1}% (pel), 5×10^{-3}% (pdp), and 7% (sep). A similar choice of modal functions in grating problems seems to be more powerful than the Floquet modes. (**ii**) Employment of up- and down-going Floquet modes and normalization by vertical separation of groove regions. We have developed this scheme based on the following ideas: (a) Although it is commonly accepted that the diffracted field over the surface C can be represented in terms of up-going modes alone independently of the validity of the Rayleigh hypothesis, it is not unreasonable to assume down-going waves in the groove region; (b) Higher-order grating modes are often the origin of trouble in numerical computations because they oscillate in x strongly and increase/decrease in y rapidly. Hence, the scheme is a combination of (a) and (b) in the frame of Yasuura's modal expansion. The effectiveness of this method is as follows [11]: for both perfect-conductor and dielectric case, we can get solutions with high accuracy for deep gratings (sinusoidal, $1 < 2h/d < 2.4$) by separating the groove region into 20 layers.

3.2. Observation of the Condition Number

As we have mentioned after **Problem D**, we usually employ the QR decomposition (QRD) in solving the discretized problem. This is because the computational complexity of the solution by the QRD is much smaller than that of a method using the singular-value decomposition (SVD) in both time and storage. When running a computer program for a new problem for the first time, however, we employ a method using the SVD because we would like to know the nature of the Jacobian matrix. In particular we need J dependence of cond(Φ) for a fixed M and rank deficiency check [12]. The dependence of cond(Φ) and the smallest singular value on computational parameters are also meaningful and are important sometimes. In Figure 2 we show examples of the J-dependence of a few significant quantities.



(a) (b)

Figure 2: (a) J dependence of cond(Φ), Ω_M, maximum and minimum singular values. Conical mounting with azimuth $\varphi = 30°$ and polar angle $\theta = 10°$, p-wave. Au-sinusoidal grating, $d = 556\,\text{nm}$, $2h = 166.8\,\text{nm}$, $\lambda = 670\,\text{nm}$, and $n_{\text{Au}} = (0.17393, -3.61253)$. $N = 20$, $M = 2N + 1 = 41$, total number of unknowns is 82. (b) J dependence of cond(Φ), Ω_M, maximum and minimum singular values, and energy error ε_M. Conical mounting with $\varphi = 30°$ and $\theta = 10°$. BK7-sinusoidal grating, $d = 556\,\text{nm}$, $2h = 222.4\,\text{nm}$, $\lambda = 670\,\text{nm}$, and $n = 1.5139$. $N = 20$, $M = 2N + 1 = 41$, total number of unknowns is 82.

3.3. Refractive Index of Au

The refractive index (or permittivity) of a noble metal is an important material constant today because of the recent development of plasmonics: the plasmon wavenumber is closely related to the index. In computer simulation of a plasmonic structure, we usually employ an index value taken from a reference. Here sometimes arises a problem: In sensor application, for example, we need a precise value of the index with more than six- or seven-digit significant figures. Such a numerical value, however, is not placed in a reference available easily. Consequently, we should use an approximate value in our simulation. To see how the small difference in refractive index influences the resonance absorption, we made numerical computation about the index values from four references and compared the result in Figure 3. As we see the difference between the reflection efficiency curves cannot be neglected, which may have an influence on the fourth or fifth column of the result of an index measurement. Hence, it is an important issue for those working in plasmonics to study how to cope with the difficult situation.

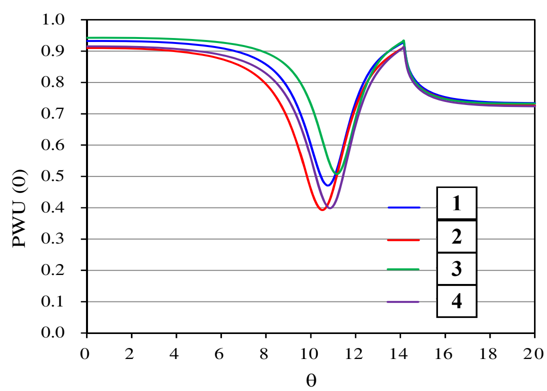


Figure 3: Comparison of the 0th order efficiency curves near the plasmon resonance absorption using Au index taken from four references. The sources are listed in Table 1. The grating is sinusoidal with $d = 556\,\text{nm}$ and $2h = 70\,\text{nm}$. Conical mounting with $\varphi = 30°$, p-wave. The abscissa shows polar angle θ and the ordinate is the 0th order reflection efficiency including both pand s-polarized wave. Note that the s-polarized component is dominant near the absorption peak ($\theta \simeq 11°$). Note also that the Au index is obtained through spline interpolation when necessary.

Table 1: Refractive indices of Au for $\lambda = 670$ nm taken from four sources.

	n	k	$\|n\_\mathrm{Au}\|$	sources of references
1	0.13179	3.56261	3.56505	[13]
2	0.16077	3.43942	3.44318	[14]
3	0.13225	3.79379	3.79609	[15]
4	0.17408	3.6123	3.61649	[16]

4. CONCLUSIONS

We have seen the solution process of Yasuura's method of modal expansion and have taken a few issues that require us to devise a countermeasure. Although most of the topics taken here might have been discussed elsewhere, we should consider the old topics together with many similar subjects again now to make good use of them. This is because such matters are inadequately forgotten in today's progressed computer environment.

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5. Recall that: the mth Fourier coefficient of a continuous and periodic function is in proportion to m^{-2}; while that of a discontinuous periodic function is m^{-1}.
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