# DIFFRACTION GRATING PROFILE RECONSTRUCTION: SIMPLE APPROACHES TO SOLVING APPLIED PROBLEMS

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## ABSTRACT

R.J.Wombell and J.A.De Santo have presented in their paper (Wombell and De Santo, 1991) the computational scheme which implementation made possible sufficiently good reconstruction of one-dimensional rough-surface profile with small roughness when a single frequency and a single viewing angle are used. The basic idea of the method (quasilinearization of integral relations of potential theory) turns out to be reasonably universal with respect to numerically solvable inverse boundary value problems and can give rise a large body of simple algorithms being efficient both in long wavelength and resonance frequency regions. Certain of these potentialities are analyzed in our paper. Reflecting grating with an arbitrary profile (a classical object in wave scattering theory) has been chosen as a model structure.

## 1. DIRECT PROBLEM OF THE DIFFRACTION GRATING

Consider a grating (see Fig.1, the structure is uniform in $x$-direction) placed in the field of a plane $E$-polarized electromagnetic wave $U^i(y,z) = E_x^i = \exp[i(\Phi_0 y - \Gamma_0 z)]$, $E_y = E_z = H_x = 0$. The direct diffraction problem is reduced to determination in the region $Q = \{\{y,z\} : -\infty < y < \infty;\, f(y) < z < \infty\}$ of twice continuously differentiable function $U(y,z) = E_x = U^i + U^s$ (the total field) which is the solution of the homogeneous Helmholtz equation

$$\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + k^2\right)U(y,z) = 0, \qquad \{y,z\} \in Q, \tag{1}$$

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with boundary conditions

$$\left\{U, \frac{\partial U}{\partial y}\right\}(y+2\pi, z) = e^{i2\pi\Phi_0}\left\{U, \frac{\partial U}{\partial y}\right\}(y, z); \quad U(y, f(y)) = 0 \tag{2}$$

and radiation conditions

$$U(y,z) = U^i(y,z) + \sum_{n=-\infty}^{\infty} a_n e^{i(\Phi_n y + \Gamma_n z)}, \qquad z \geq 0. \tag{3}$$

$E_{(...)}$ and $H_{(...)}$ are the components of electric and magnetic field strength vectors; $\Gamma_n = \sqrt{k^2 - \Phi_n^2}$, $\mathrm{Im},\mathrm{Re}\Gamma_n \geq 0$; $\Phi_n = n + \Phi_0$, $n = 0, \pm 1, \ldots$; $\Phi_0 = k \sin\alpha$; $k = 2\pi/\lambda$ is a frequency parameter; $\lambda$ and $\alpha$ are wavelength and angle of incidence of a plane wave; $f(y)$ is $2\pi$-periodic real function. The problem is considered in the dimensionless space-time coordinates, in which the period of the structure is $2\pi$ and the time dependence is defined by the factor $\exp(-ikt)$.

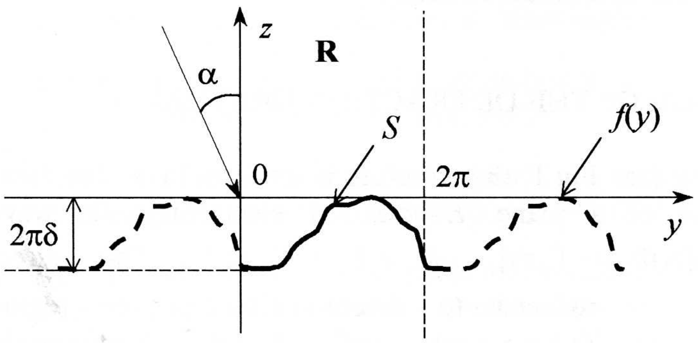



FIGURE 1. Perfectly conducting grating.

The problem (1)-(3) is uniquely resolvable for all real $k$ except a countable set of $k$ that may has accumulation points only at infinity (Shestopalov and Sirenko, 1989). It is known (Shestopalov and Sirenko, 1989, Colton and Kress, 1983) that its solution everywhere in $\mathrm{R} \setminus S$

($R = \{\{y,z\} : 0 \le y \le 2\pi\}$, $S = \{\{y,z\} : z = f(y),\ 0 \le y \le 2\pi\}$ is a scatterer's boundary) can be represented as a single layer potential

$$U^s(y,z) = -\int_S \eta(y_0,z_0) G(y,z;y_0,z_0)\,dS; \qquad \{y,z\} \in R \setminus S, \tag{4}$$

if only the continuous density $\eta(y_0,z_0)$ is the solution of the following singular integral equation:

$$\int_S \eta(y_0,z_0) G(y,z;y_0,z_0)\,dS = U^i(y,z); \quad \{y,z\} \in S, \tag{5}$$

where $G(y,z;y_0,z_0) = -i(4\pi)^{-1} \sum_{n=-\infty}^{\infty} \Gamma_n^{-1} \exp\left[i\left(\Phi_n(y-y_0) + \Gamma_n|z-z_0|\right)\right]$ is a quasiperiodic Green's function of a uniform Floquet channel. From the physically evident condition $U(y,z) \equiv 0$ for all $z < f(y)$ we can obtain one more expression for scattered field which is akin to (3):

$$U^s(y,z) = -\sum_{n=-\infty}^{\infty} \delta_0^n \,e^{i(\Phi_n y - \Gamma_n z)}, \qquad z < f(y). \tag{6}$$

## 2. INVERSE PROBLEM OF THE DIFFRACTION GRATING

The inverse problem (the grating profile reconstruction problem) is to determine the boundary $S$ from the total field $U(y,z)$, which is given for $z > 0$ by its complex amplitudes $\{a_n\}$. Let $\alpha$ and $k$ are fixed. It is also assumed the function $f(y)$ is single-valued. However, this requirement is not essential in constructing the algorithms and can be removed through a proper parametrization of the contour $S$.

Substituting the expression for $G$ into (4) and using (3) and (6), we obtain the following relations:

$$b_n = 2\pi\Gamma_n(a_n + \delta_n^0) \approx$$
$$\approx \int_0^{2\pi} \mu(y_0) \left[ \Gamma_n f(y_0) + \ldots + (-1)^{N+1} \frac{[\Gamma_n f(y_0)]^{2N-1}}{(2N-1)!} \right] e^{-iny_0}\,dy_0, \tag{7}$$

$$c_n = -2\pi i\Gamma_n(a_n - \delta_n^0) \approx$$

$$\approx \int_0^{2\pi} \mu(y_0)\left[1 - \frac{\Gamma_n{}^2 f^2(y_0)}{2!} + \ldots + (-1)^{N-1}\frac{[\Gamma_n f(y_0)]^{2(N-1)}}{(2(N-1))!}\right] \mathrm{e}^{-iny_0} dy_0,$$

$$\mu(y_0) = \eta(y_0, f(y_0))\left[1 + \left(\frac{d}{dy_0} f(y_0)\right)^2\right]^{1/2} \exp(-i\Phi_0 y_0), \quad n = 0, \pm 1, \ldots \ .$$

The smoothness of these functions is determined by the number of terms taken into account in the expansion of $\exp(\pm i\Gamma_n f(y_0))$ in powers of arguments. In this case $2N$ terms are considered.

By introducing new variables $a_n$

$$a_n^{(m)} = \int_0^{2\pi} \mu(y_0) f^m(y_0) e^{-iny_0}, \quad m = 0,1,\ldots,2N-1, \quad n = 0, \pm 1, \ldots \qquad (8)$$

we come to the following quasilinear problem which is equivalent to (7):

$$\begin{cases} a^{(m)} = (a^{(m-1)} * f), \quad m = 1,2,\ldots,2N-1, \\ b \approx D^{(1)}a^{(1)} - D^{(3)}a^{(3)} + \ldots + (-1)^{N+1} D^{(2N-1)} a^{(2N-1)}, \\ c \approx a^{(0)} - D^{(2)}a^{(2)} + \ldots + (-1)^{N-1} D^{(2N-2)} a^{(2N-2)}, \end{cases} \qquad (9)$$

where $a^{(m)} = \{a_n^{(m)}\}_n$, $b = \{b_n\}_n$, $c = \{c_n\}_n$, $f = \{f_n\}_n$, $f_n$ are the Fourier coefficients of $f(y)$, $D^{(m)} = \{\delta_n^p (\Gamma_n)^m / m!\}_{n,p}$. The asterisk signifies the convolution operation in the space of infinite sequences, i.e. $(a * b) = \{\sum_p a_{n-p} b_p\} = \{\sum_p b_{n-p} a_p\}$. The complete system (9) consisting of $2N+1$ equations for unknown vectors $f$, $a^{(0)}$, $a^{(1)},\ldots,a^{2N-1}$ is suggested as a base for constructing the numerical inverse algorithms under consideration.

At $N = 1$ (this approximation has been used by R.J.Wombell and J.A.De Santo in their paper (Wombell and De Santo, 1991)) the system (9) is solvable with respect to $f(y)$ in the explicit form:

$$f(y) \approx \hat{f}(y) = \mathrm{Re}\left\{ i \sum_n (a_n + \delta_n^0) e^{iny} \Big/ \sum_n \Gamma_n (a_n - \delta_n^0) e^{iny} \right\}. \qquad (10)$$

The numerical implementation of (10) allows one to estimate beforehand the real potentialities of the algorithms resulting from (9).

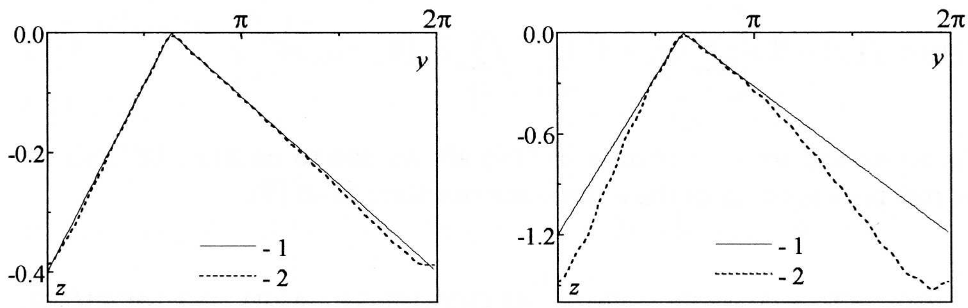
## 3. REFINEMENT OF THE ALGORITHM AND NUMERICAL EXAMPLES

The input data for computational experiments (complex amplitudes $a_n$) in Fig.2-7 have been obtained from numerical solution of the associated direct problems by the method of analytical regularization of singular integral equations (5) (Shestopalov and Sirenko, 1989, Krutin' et al., 1992). This method ensures the required accuracy of the input values in the considered range of parameters $k, \alpha$ and $\delta$. So, one can be sure that the input data correspond to a real scatterer. By this means the question about existence of the inverse problem solution which is not unique in the general case is removed.

The relative grating depth (parameter $k\delta$) and period (parameter $k$) have a pronounced effect on the accuracy of the inverse problem solution in the approximation being used. The relative error in the determination of $f(y)$ in a uniform metric (by maximal deviation) on the period ($0 < y < 2\pi$) for $k < 2$, $\alpha < 80°$, and $\delta$ up to about 0.15 does not exceed 6% for actually any profiles (see Fig.2a, Fig.3b).

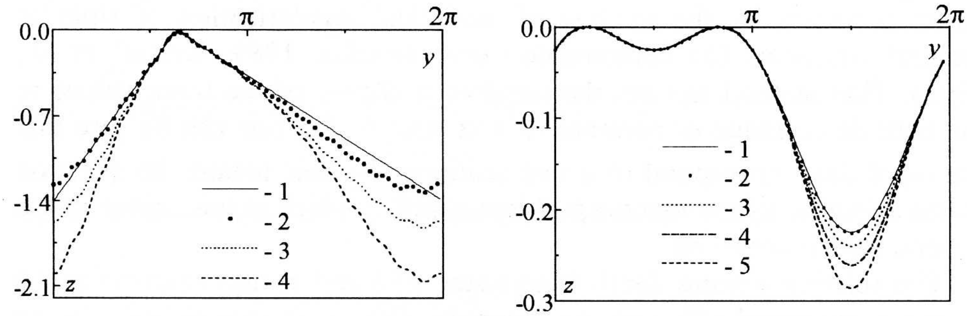
The growth of the error through increase of $k$ goes on more rapidly than its reduction when decreasing the value $\delta$. This is observed also in the cases when $k\delta$ does not increase (see Fig.2b, Fig.3). The decrease of the grating depth in an integral metric, even with its increase in a uniform one, allows one to move the limit of acceptable accuracy of the reconstruction towards the greater values of $\delta$ and $k$. The curves in Fig.4b and Fig.3b, where the integral norm of the proper profile $f(y)$ is sufficiently large, confirm this conclusion: the reconstruction error both in a uniform and in an integral metric is distinctly higher than in the case from the Fig.4a, in spite of considerable decrease in $\delta$.

The case when $N = 1$ and $\delta$ is large (or in more general situation: at high integral norm of the reconstructed function $f(y)$) can be used efficiently in the framework of the following iteration procedure. The function $\hat{f}(y)$ given by (10) acts as starting approximation allowing one



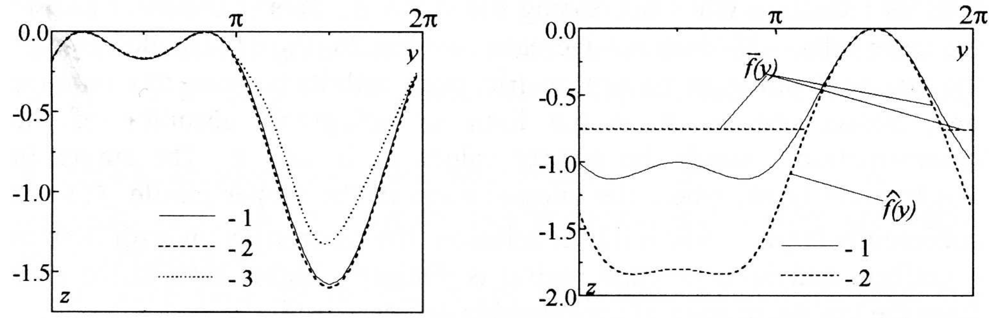

a b

FIGURE 2. Results of solving the inverse problem for echelettes of various depth with $\alpha = 0°$ and $k = 1.2$. 1: true profile $f$. 2: $\hat{f}$.




a b

FIGURE 3. Results of one-step procedure of the profile reconstruction with $\alpha = 0°$ and various $k$. 1: true profile. 2: computed profile with $k = 0.8$ (a); $k = 1.4$ (b). 3: $k = 1.05$ (a); $k = 2.4$ (b). 4: $k = 1.2$ (a); $k = 3.2$ (b). 5: $k = 3.8$.




a b

FIGURE 4. The effect of $k$ and $\alpha$ on the reconstruction of gratings with different depth and $k = 1.2$. (a) 1: true profile $f$. 2: $\hat{f}$ with $\alpha = 0°$. 3: $\hat{f}$ with $\alpha = 80°$. (b) $\alpha = 0°$. 1: $f$. 2: $\hat{f}$.

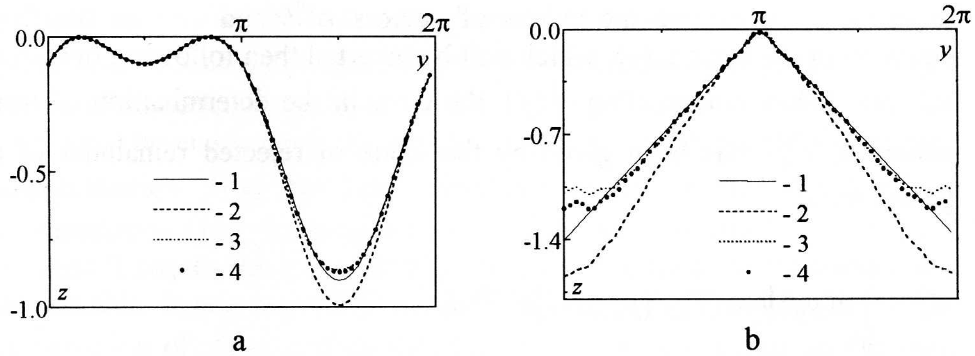



FIGURE 5. The use of $\hat{f}$ as starting approximation in the iterative process for reconstructing $f$ with $\alpha = 0°$. 1: $f$. 2: $\hat{f}$. 3: $\hat{f}1[\hat{f}]$. 4: $\hat{f}2[\hat{f}1]$. (a) $k = 1.4$. (b) $k = 1.05$.

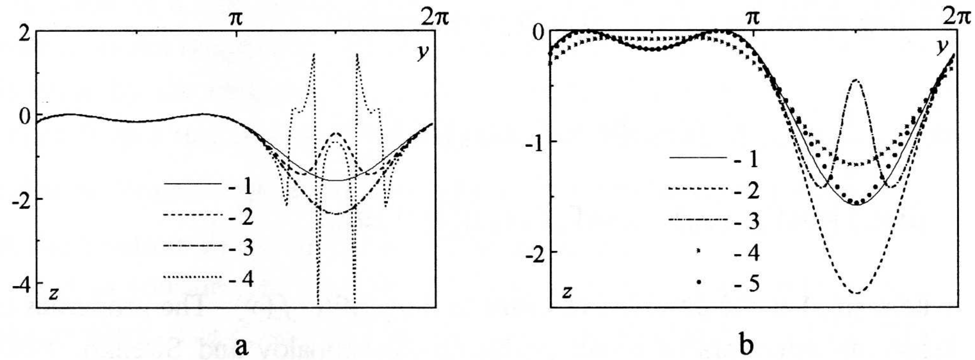



FIGURE 6. The regularization of the iterative scheme with $\alpha = 0°$ and $k = 1.4$. (a) direct scheme. 1: $f$. 2: $\hat{f}$. 3: $\hat{f}1[\hat{f}]$. 4: $\hat{f}2[\hat{f}1]$. (b) modified scheme. 1: $f$. 2: $\hat{f}$. 3: $\hat{f}1[\hat{f}]$. 4: $\overline{f1}[\hat{f}]$. 5: $\hat{f}2[\overline{f1}]$.

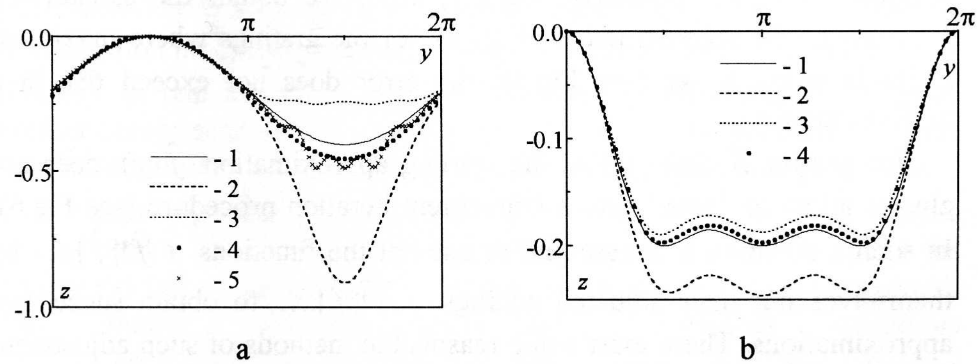



FIGURE 7. Results of the iteration procedure with $N = 2$ and $\alpha = 0°$. 1: $f$. 2: $\hat{f}$. 3: $\hat{f}1[\hat{f}]$. 4: $\hat{f}2[\hat{f}1]$. (a) $k = 3.2$. (b) $k = 3.8$.

to make more precise the values of vectors $a^{(0)}$ and $a^{(1)}$ in the first equation of the system (9), which will be inverted then following the same scheme. When constructing $\hat{f}(y)$ the error in the determination of true values of $a_n^{(0)}$ has been given by the value of rejected remainder of a power series:

$$d_n^0 = \int_0^{2\pi} \mu(y_0)\left[\cos(\Gamma_n f(y_0)) - 1\right] e^{-iny_0} dy_0 .$$

In the next step it is suggested the replacement (not the rejection) of this remainder by the analogous one appropriate to the found function $\hat{f}(y)$. As a result the error in the determination of $a^{(0)}$ with rather "good" starting approximation $\hat{f}(y)$ will be reduced to

$$\hat{d}_n^{(0)} = \int_0^{2\pi} \{[\mu(y_0) - \hat{\mu}(y_0)][\cos(\Gamma_n f(y_0)) - 1] +$$
$$+ \hat{\mu}(y_0)\left[\cos\Gamma_n f(y_0) - \cos(\Gamma_n \hat{f}(y_0))\right]\} e^{-iny_0} dy_0 ,$$

where $\hat{\mu}(y)$ is the potential relevant to the profile $\hat{f}(y)$. The properties of resolving operators of direct problems (Shestopalov and Sirenko, 1989, Krutin' et al., 1992) let us to assert that in this case the computational procedures realizing such scheme will be convergent. Our calculations confirm drawn conclusion: even in the second step when determining $\hat{f}1(y)$ through $a_n^{(0)}$ and $a_n^{(1)}$ corrected with the help of $\hat{f}(y)$ (we note this relation as $\hat{f}1[\hat{f}]$, similarly $\hat{f}2[\hat{f}1]$, etc.), we obtain the satisfactory accuracy of the reconstruction of $f(y)$ for the gratings where maximum depth is twice larger (see Fig.5); the error does not exceed 6% in a uniform metric.

For greater $\delta$ and (or) $k$ the starting approximation $\hat{f}(y)$ does not always allow to "enter" into a convergent iteration procedure (see Fig.6). In such a situation it is essential to use not the functions $\hat{f}, \hat{f}1[\hat{f}], \ldots$ by themselves but their adjusted analogs $\bar{f}, \overline{f1}[\hat{f}], \ldots$ to obtain successive approximations. There exist some reasonable methods of such adjustment (one simple version is presented in Fig.4b). We shall consider the following method in greater detail. The method takes account of the peculiar features of the basic algorithm. It also considers the behaviour of $\hat{f}(y)$ and its successive approximations which have been revealed in the course of numerical experiments.

It must be emphasized that the first artificial adjustment of the starting approximation $\hat{f}(y)$ has been performed yet in the framework of the representation (10): the imaginary part of the solution has been discarded because it causes the error accumulation and the iteration procedure will be unstable. It is a reasonable step in the search for a real function. The construction of $\bar{f}(y)$ and the subsequent procedure is based on the same principle: the elimination beforehand of those factors which lead to accumulation of the error. The following facts provide the background for this action. Firstly, the sections of graphs of any reconstructed profile the maximum depth of which is under some fixed value are coincident with the graph of a real profile. This fixed value correlates for each iteration with a certain range of $k$. Such, for example, for $\hat{f}(y)$ at $k<2$ the depth is given by the inequality $z \geq -0.5$. Secondly, the greatest deviations of $\hat{f}(y)$ from a real profile $f(y)$ in the region where $|f(y)|$ is of maximum value are conditioned by the errors in the determination of amplitudes $\hat{f}_n$ of the function $\hat{f}(y)$ higher Fourier components.

Let us consider one example (Fig.6) suggesting the correct solution of the problem. The direct iteration procedure on the third step ($\hat{f}2[\hat{f}1]$) is starting to get away from the desired solution in the interval $4<y<5.5$ (Fig.6a). As this take place $f_n = 0$ for $|n|>2$; $(\hat{f}1[\hat{f}])_n$ reach the value about $0.5 \cdot 10^{-2}$. The amplitudes of basic components ($n = 0, \pm 1, \pm 2$) are changed moderately with each iteration. Having interrupted the process after receiving $\hat{f}1[\hat{f}]$ and having constructed $\overline{f1}[\hat{f}]$ we obtain on the next iteration practically precise coincidence with a desired function $f(y)$ (Fig.6b). In real instead of model conditions the determination of basic Fourier components is not a complicated computational problem, because Fourier amplitudes remain relatively stable under step by step procedure.

For adjusting values of the vectors $a^{(0)}$ and $a^{(1)}$ the following scheme can be used . The subsystem of $2N$ linear operator equations from the system (9) (all equations with the exception of the first one) is inverted. The matrix operators of the convolution equations $a^{(m)} = (a^{(m-1)} * \hat{f})$, $m = 2, \ldots, 2N-1$ are given by the Fourier coefficients of the obtained function $\hat{f}(y)$. The next approximation

$\hat{f}1[\hat{f}]$ is determined by the formula $a^{(1)} = (a^{(0)} * \hat{f}1)$, where vector $\hat{f}1$ consists of the Fourier coefficients of function $\hat{f}1[\hat{f}]$. The process is repeated many times until the required accuracy of the reconstruction is achieved. The accuracy can be checked against the error in the reconstruction of the input data $\{a_n\}$. In any step of the process the next approximation can be adjusted by artificial means, specifically by using the method outlined above. For large $\delta$ the suggested scheme turns out to be not as efficient as the previous one. However, it gives the desired result more rapidly if the integral norm of $f(y)$ and $k$ are large and $\delta$ is not too large (see Fig.7). Thus, apparently that both of these schemes can be used in the framework of one algorithm: one can turn from one scheme to another taking into account the results of earlier steps.

We can not indicate right now the boundary values of $\delta$ and $k$ at which the starting approximation $\hat{f}(y)$ for $N = 1$ become invalid: we have got satisfactory results even when period length is five times larger than $\lambda$ and grating depth was $2\lambda$. However it is clear that the range of $\delta$ and $k$ where the starting approximation $\hat{f}(y)$ matches our requirements is bounded. So we have to seek for alternative procedures for constructing $\hat{f}(y)$ for increasing $k$ and $\delta$. One of supposed procedures is associated with direct inversion of the quasilinear system (9) for $N > 1$. The idea of quasilinearization is rather fruitful and may serve as a basis for several computational schemes. Such schemes undoubtedly deserve certain attention because they do not utilize any additional input data even in such important issue as starting approximation, they rely only on basic numerical techniques that are flexible and easily adjustable for required parameter range. Their capabilities allows one to solve a number of important applied problems in optics (holographic grating diagnostics), solid state electronics and diffraction electronics (synthesis of dispersion open resonators with selective mirrors), and radiolocation (synthesis of effectively reflecting and absorbing coatings) (Shestopalov and Sirenko, 1989), where small depth of the structure is the frequently occurring process requirement. Besides, the gratings in relevant devices usually has to bring into existence not a large number of spreading harmonics.

In conclusion we should like to point out one rather important particularity of algorithms described. The choice of starting approximation $\hat{f}(y)$ as it has been made for $N = 1$ regularizes in essence the ill-posed profile reconstruction problem. It is known that the uniqueness of the solution in the mode of one frequency and one position probing can not be ensured. However, the precise starting “getting into” on the sections of $y$

where $|f(y)|$ is not too large "cuts off" immediately all alternative possibilities. So if the iterative process converges then it does converge to the true profile $\hat{f}(y)$.

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