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A two-step algorithm for the reconstruction of perfectly reflecting periodic profiles

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Abstract

We consider the inverse problem of recovering a 2D periodic structure from scattered waves measured above the structure. First, following [5], the inverse problem is reformulated as an optimization problem which consists of two parts: a linear severely ill–posed problem and a nonlinear well–posed one. Then, contrary to [5], here the two problems are solved separately to diminish the computational effort by exploiting their special properties. Numerical results for exact and noisy data demonstrate the practicability of the inversion algorithm.

1 Introduction

The scattering theory for periodic structures has many applications in micro-optics, where periodic structures are often called diffraction gratings. For an introduction to the direct problem of calculating the electromagnetic scattering produced by periodic interfaces, we refer to the monograph [19]. The inverse problem of recovering the periodic structure or the shape of the grating profile from the scattered field is also of great practical importance in modern diffractive optics, e.g., in quality control and design of diffractive elements with prescribed far field patterns (see [2, 22]).

As in [5], we shall restrict our attention to two-dimensional perfectly conducting gratings and consider the profile reconstruction problem for Dirichlet boundary conditions. Uniqueness results and local stability estimates were obtained in [1, 3, 13, 16], and a result on conditional (global) stability was proved in [4].

The goal of this paper is to present reconstruction algorithms based on the optimization method of [5] in the following three cases: (i) gratings given by a truncated Fourier series, (ii) binary gratings, (iii) piecewise linear gratings.

To this end first an unknown density function is computed from measured near–field data, which allows to represent the scattered field as a single layer potential. This is a severely ill-posed linear problem with a known singular value decomposition that helps to solve it with a low numerical expense. Then the computed density function is used as input to a nonlinear least squares problem which determines the unknown profile as the location of the zeros of the total field and is solved by the Gauss–Newton method. This approach, originally due to Kirsch and Kress in the case of acoustic obstacle scattering, avoids the solution of a direct problem in each iteration. Additionally, since only the grating parameters need be improved in each Gauss–Newton step, the linear system is of low dimension.

In the case when the minimization of the Tikhonov functional for the linear problem and the defect minimization of the Dirichlet condition is combined into one cost functional, the mathematical foundation of the optimization method together with its numerical performance are discussed in [5]; see also [10].

Numerical results are reported for various smooth and nonsmooth grating profiles, where the data are generated by the direct solver of [21]. The computations demonstrate the practicability of our method, showing its accuracy and low expense.

This paper is organized as follows:

- Section 2. Direct and inverse diffraction problems
- Section 3. The reconstruction method
- Section 4. The linear severely ill–posed part
- Section 5. The nonlinear part. Reconstruction algorithm for
  (i)Fourier gratings,
  (ii)Binary gratings,
  (iii)Piecewise linear gratings.
- Section 6. Numerical results.

2 Direct and inverse diffraction problems

The scattering of time-harmonic electromagnetic waves in the TE (transverse electric) mode by two-dimensional perfectly reflecting periodic structures is modelled by the Dirichlet problem for the Helmholtz equation. Let the profile of the diffraction grating be described by the curve

$$\Lambda_f := \{(x_1, f(x_1)) : x_1 \in \mathbb{R}\}$$

with a periodic function f of period 2π. If nothing else is said we always assume that $f \in C^{0,1}(\mathbb{R})$, i.e. f is a Lipschitz function. Let

$$\Omega_f := \{x \in \mathbb{R}^2 : x_2 > f(x_1),\ x_1 \in \mathbb{R}\}$$

be filled with a material whose index of refraction (or wave number) k is a positive constant, where $k = \omega c^{-1}(\mu\epsilon)^{1/2}$. Here ω is the angular frequency, c the speed of light, μ the magnetic permeability which is assumed to be 1 everywhere, and ϵ is the dielectric coefficient. Suppose that a plane wave given by

$$u^{in}(x) = \exp(i\alpha x_1 - i\beta x_2)$$

is incident on Λ_f from the top, where $\alpha = k\sin\theta$, $\beta = k\cos\theta$, and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. Then the direct scattering problem is to find the scattered field $u \in C^2(\Omega_f) \cap C(\overline{\Omega}_f)$ such that

$$\Delta u + k^2 u = 0 \quad \text{in} \quad \Omega_f, \quad u = -u^{in} \quad \text{on} \quad \Lambda_f, \tag{2.1}$$

and (as the incident wave) u is assumed to be α-quasiperiodic:

$$u(x_1 + 2\pi, x_2) = \exp(2\pi i\alpha) u(x_1, x_2). \tag{2.2}$$

Moreover, we require that u satisfies a radiation (or outgoing wave) condition, i.e., u is composed of bounded outgoing plane waves:

$$u(x) = \sum_{n\in\mathbb{Z}} A_n \exp\{i(n+\alpha)x_1 + i\beta_n x_2)\},\ x_2 > \|f\|_{C(\mathbb{R})} \tag{2.3}$$

with $\beta_n := (k^2 - (n+\alpha)^2)^{1/2}$ for $|n+\alpha| \le k$, $\beta_n := i((n+\alpha)^2 - k^2)^{1/2}$ for $|n+\alpha| > k$ and the Rayleigh coefficients $A_n \in \mathbb{C}$. We further exclude resonances by assuming $\beta_n \neq 0$ for all $n \in \mathbb{Z}$ throughout the paper. Then the sum over the finite index set

$$\mathcal{U} := \{n \in \mathbb{Z} : |n+\alpha| < k\},$$

i.e. $\beta_n > 0$ for $n \in \mathcal{U}$, corresponds to the propagating modes of the scattered field, whereas the terms in (2.3) for $n \in \mathbb{Z} \setminus \mathcal{U}$ represent evanescent (exponentially decaying) waves. For general Lipschitz grating profiles, the existence of a unique solution to the Dirichlet problem (2.1)–(2.3) is established in [10].

Our goal in this paper is to study the inverse problem of profile reconstruction. More precisely, given the incident wave u^{in} and $b > \|f\|_{C(\mathbb{R})}$, we introduce the 'output' operator

$$A : f \to u(x_1, b),$$

which maps the profile function f onto the trace of the scattered field on the line $x_2 = b$. In terms of this operator, given the exact scattered field on $x_2 = b$ (or, equivalently, the Rayleigh coefficients A_n for all $n \in \mathbb{Z}$), the inverse problem consists just in solving the nonlinear equation

$$A(f) = u_b := u(x_1, b) \tag{2.4}$$

for the unknown profile function f. As observed in [2],[4], solving the equation (2.4) is a severely ill-posed problem. Hence it is quite natural to apply regularization methods to this equation.

3 The reconstruction method

Assume, that we have the a priori information about our inverse periodic diffraction problem (2.4) that, without loss of generality, the unknown profile Λ_f lies above the line $x_2 = 0$ and below $x_2 = b$. We try to represent the scattered field as a single layer potential

$$u(x) = \int_0^{2\pi} \varphi(t) G(x_1, x_2, t, 0)\, dt \tag{3.1}$$

with an unknown density function $\varphi \in X = L^2(0, 2\pi)$ and the free space quasiperiodic Green function (cf., e.g., [15])

$$G(x, y) = \frac{i}{2\pi} \sum_{n \in \mathbb{Z}} \frac{1}{\beta_n} \exp(i(n+\alpha)(x_1 - y_1) + i\beta_n |x_2 - y_2|), \; x \neq y. \tag{3.2}$$

The function (3.2) is well defined since we assumed $\beta_n \neq 0$ for all $n \in \mathbb{Z}$. For fixed f, introduce the linear operators $T, S_f : X \to X$ by

$$\begin{aligned} T\varphi(x_1) &= \int_0^{2\pi} \varphi(t) G(x_1, b, t, 0)\, dt, \\ S_f\varphi(x_1) &= \int_0^{2\pi} \varphi(t) G(x_1, f(x_1), t, 0)\, dt. \end{aligned} \tag{3.3}$$

Note that $T\varphi$ approximates the output Af of the scattered field u on $x_2 = b$, whereas $S_f\varphi$ (which is nonlinear with respect to f) represents an approximation of u on the profile

Λ_f. Here and in the following we identify the (α-quasiperiodic) space $L^2(\Lambda_f)$ with X via $v \to v \circ f$

$$(v \circ f)(t) = v(t, f(t)), \quad t \in [0, 2\pi],$$

such that

$$\|v \circ f\|_X = \frac{1}{2\pi}(\int_0^{2\pi} |v(t, f(t))|^2 dt)^{1/2}, v \in L^2(\Lambda_f)$$

is a uniformly equivalent norm when f varies in a set of profile functions with uniformly bounded $C^{0,1}$ norm. If φ is given as a Fourier series

$$\varphi(t) = \sum_{n \in \mathbb{Z}} \varphi_n \exp(i(\alpha + n)t) \in X, \ \varphi_n \in \mathbb{C},$$

then from (3.2) and (3.3) we obtain

$$\begin{aligned} T\varphi(t) &= i \sum_{n \in \mathbb{Z}} \varphi_n \beta_n^{-1} \exp(i(\alpha + n)t + i\beta_n b), \\ S_f\varphi(t) &= i \sum_{n \in \mathbb{Z}} \varphi_n \beta_n^{-1} \exp(i(\alpha + n)t + i\beta_n f(t)). \end{aligned} \tag{3.4}$$

Because of $|\beta_n| \sim |n|$ as $n \to \infty$ and our a priori assumption on Λ_f, the series in (3.4) are convergent in any α-quasiperiodic Sobolev norm. Moreover, it can be easily checked that $T : X \to X$ is an injective compact operator with dense range and with the exponentially decreasing singular values $|\beta_n^{-1} \exp(i\beta_n b)|$. Hence, given the output u_b of the scattered field, the determination of the density φ from u_b by solving the first kind equation $T\varphi = u_b$ is a severely ill-posed problem.

We may solve its Tikhonov regularized version

$$\gamma\varphi + T^*T\varphi = T^*u_b, \tag{3.5}$$

with regularization parameter $\gamma > 0$. Given the solution $\varphi_\gamma \in X$ of (3.5) and the corresponding approximation u_γ of the scattered field, we can then seek the profile Λ_f of the grating by minimizing the defect

$$\|u^{in} + u_\gamma\|_{L^2(\Lambda_f)}, \ f \in \mathcal{M}, \tag{3.6}$$

over a class of admissible curves Λ_f.

Here a class $\mathcal{M}$ of profile functions is called admissible if the norm $\|f\|_{C^{0,1}}$ is uniformly bounded for all $f \in \mathcal{M}$; see [10].

To cover the practically important case of binary gratings, where the profile is given by a step function, the above approach has to be generalized slightly. In that case the defect (3.6) should be minimized over an admissible class of periodic Lipschitz curves Λ_f with parametrization

$$f(t) = (f^1(t), f^2(t)), \ 0 \le t \le 2\pi,$$

where f^1 and f^2 are uniformly bounded Lipschitz functions and the corresponding domains Ω_f (above Λ_f) satisfy an ε-cone property uniformly in $f \in \mathcal{M}$; see, e.g., [20], chap.3, for definition. Note that under these conditions the norm $\|v\|_{L^2(\Lambda_f)}$ is equivalent to

$$\left(\int_0^{2\pi} |v(f^1(t), f^2(t)|^2 dt\right)^{1/2},$$

uniformly in $f \in \mathcal{M}$. Then the convergence results of [5], [10] can be carried over to this more general class of grating profiles.

However, in Sections 5 and 6 we shall apply an alternative method to binary gratings, regarding the step functions as the graph of functions with a finite number of discontinuities and performing the defect minimization only over the horizontal segments. Though this approach is not justified by the convergence theory, it produces satisfactory numerical results.

4 The linear severely ill–posed part

Consider the Hilbert space $X = L^2(0, 2\pi)$ with the scalar product

$$< x, y >= \frac{1}{2\pi} \int_0^{2\pi} x(t)\overline{y(t)}dt,$$

the norm $\|x\| = \sqrt{< x, x >}$ and the orthonormal basis $v_n,\ n \in \mathbb{Z}$,

$$v_n(t) = \exp(i(\alpha + n)t).$$

Then

$$Tv_n = \sigma_n v_n,\ n \in \mathbb{Z},$$

where

$$\sigma_n = i\beta_n^{-1} \exp(i\beta_n b),\ n \in \mathbb{Z}.$$

The adjoint operator T^* satisfies

$$T^* v_n = \overline{\sigma_n} v_n.$$

Defining

$$u_n = \frac{\sigma_n}{|\sigma_n|} v_n,$$

a singular value decomposition of T is given by

$$\{|\sigma_n|, v_n, u_n,\ n \in \mathbb{Z}\}.$$

Now, consider the exact near–field (cf. (2.3) and (2.4))

$$u_b = \sum_{n \in \mathbb{Z}} y_n^b u_n,$$

where

$$y_n^b = A_n \exp(i\beta_n b) \frac{|\sigma_n|}{\sigma_n}.$$

Then $u_b \in \mathcal{D}(T^\dagger)$ if and only if the Picard condition

$$\sum_{n \in \mathbb{Z}} \frac{|y_n^b|^2}{|\sigma_n|^2} = \sum_{n \in \mathbb{Z}} |A_n|^2 |\beta_n|^2 < \infty,$$

is fulfilled (cf.[11], p.38), which cannot be guaranteed in general. Here $\mathcal{D}(T^\dagger)$ denotes the domain of the generalized inverse of T. Moreover, usually u_b will not be given exactly but perturbed by measurement errors. So instead of the problem

$$\|T\varphi - u_b\|^2 \to \inf_{\varphi \in X},$$

which is not solvable in general, let us consider its Tikhonov regularized version

$$||T\varphi - u_b||^2 + \gamma||\varphi||^2 \to \inf_{\varphi \in X}$$

for a suitable $\gamma > 0$. Its solution φ_γ can be represented as (cf. [11], p.117)

$$\varphi_\gamma = \sum_{n\in\mathbb{Z}} \frac{|\sigma_n|}{|\sigma_n|^2+\gamma} < u_b, u_n > v_n = \sum_{n\in\mathbb{Z}} a_n^\gamma < u_b, v_n > v_n,$$

where

$$a_n^\gamma = \begin{cases} \frac{-i\beta_n^{-1}\exp(-i\beta_n b)}{\beta_n^{-2}+\gamma} & \text{if } n \in \mathcal{U} \\ \frac{|\beta_n|^{-1}\exp(-|\beta_n|b)}{|\beta_n|^{-2}\exp(-2|\beta_n|b)+\gamma} & \text{if } n \in \mathbb{Z}\backslash\mathcal{U} \end{cases}.$$

One may expect a fast convergence of this series such that only a short part, say $|n| \leq N$, will be necessary in the implementation. In our numerical examples N will be always chosen such that $\mathcal{U} \subseteq \{n \in \mathbb{Z},\ |n| \leq N\}$.

Notice that each term appearing in this section (including $\beta, \beta_n, v_n, u_n, \sigma_n, u_b, \gamma, \varphi_\gamma, N$) may depend on the characteristics k, θ of the incoming wave u^{in}. So, if one wants to incorporate measurements u_b for n_r different experiments, one must perform n_r computations for the quantities φ_γ.

5 The nonlinear part

Now let us investigate the nonlinear problem

$$||u^{in} \circ f + S_f\varphi_\gamma||^2 \to \inf_{f\in\mathcal{M}},$$

where φ_γ is the input, computed in the previous section, and the admissible set $\mathcal{M}$ will be specified later. Using the explicit representations of the incoming wave u^{in} and the operator S_f (cf. (3.4)) and the input φ_γ as

$$\varphi_\gamma = \sum_{|n|\leq N} a_n^\gamma < u_b, v_n > v_n,$$

where $\gamma \geq 0$ and $N \in \mathbb{N}$ have to be chosen suitably, the problem takes the form

$$||\exp(-i\beta f(.)) + \sum_{|n|\leq N} Z_n \exp(i\beta_n f(.))v_n||^2 \to \inf_{f\in\mathcal{M}}. \tag{5.1}$$

Here

$$Z_n = i\beta_n^{-1} a_n^\gamma < u_b, v_n > . \tag{5.2}$$

In the case of n_r inputs φ_γ one has to minimize a sum of n_r functionals (5.1), where Z_n depends on the respective input.

Before specifying types of admissible sets for the profile function f let us go to describe the further treatment in an abstract way, confining ourselves to a single input. For more than one input one has to modify the functional (5.1) in a straightforward way.

Let us suppose that f depends smoothly on finitely many real parameters $p_\mu,\ \mu = 1, ..., M$

$$f(t) = f[p_1, ..., p_M](t),$$

and that

$$F = \| \exp(-i\beta f(.)) + \sum_{|n| \le N} Z_n \exp(i\beta_n f(.)) v_n \|^2$$

can be represented as

$$F = \sum_{1 \le j \le K} r_j^2,$$

where

$$r_j = r_j[p_1, ..., p_M] \in \mathbb{R}_+$$

depends smoothly on $p_1, ..., p_M$. In the case where the sum of n_r functionals (5.1) is to be minimized, K is the number of all residuals involved.

Consider the vectors

$$\underline{r} = (r_1, ..., r_K), \quad \underline{p} = (p_1, ..., p_M)$$

and the matrix

$$J = (\partial r_j / \partial p_\mu),$$

with K row indices j and M column indices μ.

Then the least squares problem

$$\sum_{1 \le j \le K} r_j^2 \to \inf_p$$

can be solved by the Gauss–Newton method iteratively via

$$\underline{p}_{new} = \underline{p}_{old} + \lambda \underline{q},$$

where $\underline{q}$ solves the linear system

$$J^T J \underline{q} = -J^T \underline{r}$$

and λ is a suitably chosen positive real number less or equal 1 (cf.[18]).

Defining

$$F_j = r_j^2,$$

we have $\partial r_j / \partial p_\mu = \frac{1}{2} F_j^{-1/2} \partial F_j / \partial p_\mu$, and the linear system takes the form

$$\frac{1}{4} \sum_{1 \le \nu \le M} \left(\sum_{1 \le j \le K} F_j^{-1} \frac{\partial F_j}{\partial p_\nu} \frac{\partial F_j}{\partial p_\mu} \right) q_\nu = -\frac{1}{2} \sum_{1 \le j \le K} \frac{\partial F_j}{\partial p_\mu}, \quad \mu = 1, ..., M,$$

which is used in the implementation. Notice that the matrix and right hand side are computed by only using the known parameter vector p_{old}.

In our cases the Hessian

$$\nabla^2 F = \left(\sum_{1 \le j \le K} \frac{\partial^2 F_j}{\partial p_\mu \partial p_\nu} \right)_{1 \le \mu, \nu \le M}$$

can be computed without much expense. So, as an alternative for updating the parameters, we can also use the Newton correction $\underline{q}$, i.e. the solution of the linear system

$$(\nabla^2 F)\underline{q} = -\nabla F,$$

where

$$\nabla F = \left(\sum_{1 \le j \le K} \frac{\partial F_j}{\partial p_\mu} \right)_{1 \le \mu \le M}.$$

Now we consider 3 types of admissible sets for the profile function f.

(i) Fourier gratings.

Let f be given as

$$f(t) = a_0 + 2 \sum_{1 \le \nu \le m} (c_\nu \cos(\nu t) + d_\nu \sin(\nu t)),$$

where m is considered to be fixed. Then

$$M = 2m + 1,$$

and the (bounded) set of real parameters characterizing f is

$$a_0, c_1, ..., c_m, d_1, ..., d_m.$$

Let K be a natural number and

$$s_j = \frac{2\pi}{K}(j-1), \quad j = 1, ..., K,$$

an equidistant partition of $[0, 2\pi]$. Then, using the trapezoidal rule, the functional F can be approximated by

$$F \cong \sum_{1 \le j \le K} F_j, \quad F_j = \frac{1}{K} | \exp(-i\beta f(s_j)) + \sum_{|n| \le N} Z_n \exp(i\beta_n f(s_j)) v_n(s_j)|^2,$$

where $f(s_j) = f_j[a_0, c_1, ..., c_m, d_1, ..., d_m]$ should be noticed.

(ii) Binary gratings.

Let here

$$M = 2n_0,$$

$n_0 \ge 1$ a fixed natural number. Consider the parameters

$$t_1, t_2, ..., t_{2n_0-1}, h,$$

such that $0 < t_1 < ... < t_{2n_0-1} < 2\pi$ and $0 < g < h$ hold, g given. Let $t_0 = 0, t_{2n_0} = 2\pi$ and define

$$f(t) = \begin{cases} h & \text{if } t_{2j-2} \le t \le t_{2j-1}, \quad j = 1, ..., n_0 \\ g & \text{if } t_{2j-1} < t < t_{2j}, \quad j = 1, ..., n_0 \end{cases}.$$

Vividly, n_0 can be interpreted as the number of 'towers' of the grating of height $h - g$ over the level g, and t_{2j-2} and t_{2j-1} are the positions of the 'walls' of the j-th tower.

Then

$$F = \sum_{1 \le j \le M} F_j,$$

i.e. $K = M$, and

$$F_j = \int_{t_{2j-2}}^{t_{2j-1}} |\exp(-i\beta h) + \sum_{|n| \le N} Z_n \exp(i\beta_n h) v_n(t)|^2 dt, \quad j = 1, ..., n_0,$$

$$F_{n_0+j} = \int_{t_{2j-1}}^{t_{2j}} |\exp(-i\beta g) + \sum_{|n| \le N} Z_n \exp(i\beta_n g) v_n(t)|^2 dt, \quad j = 1, ..., n_0.$$

(iii) Piecewise linear gratings.

Now, let $\ell \ge 1$ be a given natural number and let us take as parameters $\ell - 1$ partition points

$$0 < t_1 < t_2 < ... < t_{\ell-1} < 2\pi$$

and ℓ positive, bounded real numbers

$$d_1, d_2, ..., d_\ell.$$

Denote $t_0 = 0, t_\ell = 2\pi, d_0 = d_\ell$, and take the profile f as piecewise linear with the property

$$f(t_\mu) = d_\mu, \quad \mu = 0, ..., \ell.$$

Then

$$F = \sum_{1 \le j \le \ell} F_j,$$

so that we have $M = 2\ell - 1,\ K = \ell$ in this case. Furthermore,

$$F_j = \int_{t_{j-1}}^{t_j} |\exp(-i\beta(x_j t + y_j)) + \sum_{|n| \le N} Z_n \exp(i\beta_n(x_j t + y_j)) v_n(t)|^2 dt, \quad j = 1, ..., \ell,$$

where

$$x_j = \frac{d_j - d_{j-1}}{t_j - t_{j-1}}, \quad y_j = \frac{d_{j-1} t_j - d_j t_{j-1}}{t_j - t_{j-1}}, \quad j = 1, ..., \ell.$$

In the special case $\ell = 4\ell_0$ and

$$h = d_0 = d_1 = d_4 = d_5 = ... = d_{\ell-4} = d_{\ell-3},$$

$$g = d_2 = d_3 = d_6 = d_7 = ... = d_{\ell-2} = d_{\ell-1},$$

$h > g > 0$, the profile will be called a linear ℓ_0- tower profile of height $h - g$ over the level g.

To obtain an admissible set of grating profiles for the minimization problem in the cases (ii) and (iii), we have to assume that the heights h resp. d_j are uniformly bounded and that the minimal distance between partition points t_j remains uniformly bounded from below.

6 Numerical results

Here we present the results of numerical experiments using our method with exact and noisy data. The near field measurements u_b are simulated by first solving the direct problem by a finite element like method ([21]) and then disturbing with random errors:

$$u_b(r_\nu) + \delta\omega_\nu, \quad |\omega_\nu|^2 \le 1, \tag{6.1}$$

where $\delta \ge 0$ is the noise level and $\{r_\nu\}$ is an equidistant partition of $[0, 2\pi]$ used as discretization in the computation of the data Z_n via (5.2). Data where only the propagating modes (i.e. $n \in \mathcal{U}$) are taken into account will be called far–field data.

In the following experiments, if nothing else is mentioned, the unknown profile will be probed by the single incoming wave with characteristics $k = 4.45, \theta = 0$, where

$$\mathcal{U} = \{n \in \mathbb{Z}, \ |n| \le 4\},$$

i.e. the propagating modes correspond to $|n| \le 4$.

(i)*Fourier gratings.*

In the case of a Fourier grating the profile function $f(t)$ is given as a trigonometric polynomial. We performed numerical experiments for the following two profile functions, chosen as in the examples discussed in [14] and [12] :

$$f_0(t) = 2 + \zeta(\cos(t) + \cos(2t) + \cos(3t))\,, \tag{6.2}$$

$$f_1(t) = 1.5 + 0.2e^{\sin(3t)} + 0.3e^{\sin(4t)}\,. \tag{6.3}$$

Concerning the case (6.2) take ζ as a measure of the profile steepness. As was found in [5] the reconstruction becomes worse when the steepness of the profile increases. In [5] we obtained satisfactory results for $\zeta \le 0.05\pi$. Here, our improved algorithm allowed treating the case $\zeta \le 0.1\pi$. We used undisturbed far-field data without regularization and updated 7 parameters in each of 50 iterations. The results are given in Table 1.

	a_0	c_1	c_2	c_3	d_1	d_2	d_3
target	2.00	.157	.157	.157	0	0	0
initial	1.80	0	0	0	0	0	0
calcul	2.04	.165	.131	.112	-.001	-.001	-.002

Table 1: Case (6.2) for $\zeta = 0.1\pi$

Instead of (6.3) we used its truncated Fourier series

$$f_1(t) = < f_1, v_0 > +2 \sum_{1 \le \nu \le 8} (Re\{< f_1, v_\nu >\} \cos(\nu t) + Im\{< f_1, v_\nu >\} \sin(\nu t)),$$

which can be approximated by

$$f(t) = 2.133 + 2[-0.02715 \cos(6t) - 0.0407 \cos(8t) + 0.11303 \sin(3t) + 0.1695 \sin(4t)]. \tag{6.4}$$

In our computations given in Table 2, for $N = 4$ the outgoing modes were used, while for $N = 5$ two additional modes only appearing in the near–field were taken into account. In both cases a regularization parameter $\gamma = 0.1$ was appropriate yielding the result given in Table 2. Moreover, again using $\gamma = 0.1$ perturbations (6.1) with $\delta = 0.1$ of the near–field corresponding to a noise of 5.3% led to deviations of about 10% in the result.

The computations were performed assuming a priori that all coefficients not appearing in the (unknown) target vanish so that only 5 parameters had to be updated in the iterations. To reach stationarity 400 iterations were enough, taking two or three seconds all together on a workstation. Without the a priori information satisfactory results could be achieved only for suitable start values.

	a_0	c_6	c_8	d_3	d_4
target	2.13	-.027	-.040	.113	.169
initial	2.13	0	0	0	0
calcul	2.20	-.004	-.049	.036	.130

Table 2: Case (6.3)

(ii) Binary gratings.

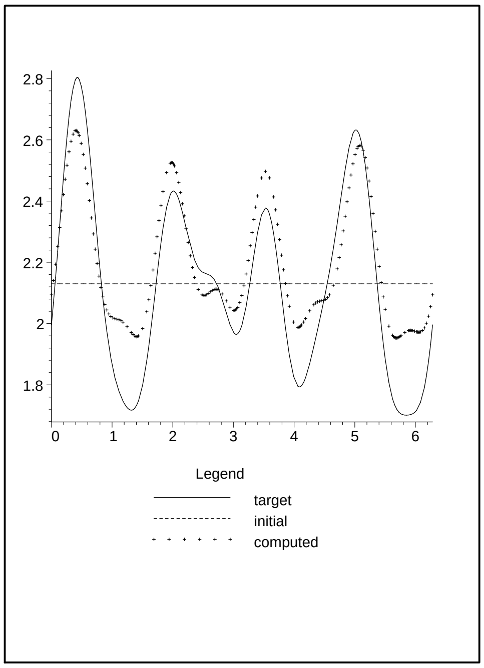
Here we used undisturbed far–field data without regularization from the three incoming waves for $k = 4.45$ and $\theta = 0, 45, -45$ degrees. We calculated a two-tower profile of height 1.2 over the level 2. After 200 iterations with $\lambda = 0.1$ the computation became stationary till the 12th digit. The results, given in Table 3, proved to be stable when the initial values for t_1, t_2, t_3 were changed coarsely, but turned out to be rather sensitive with respect to h.

	t_1	t_2	t_3	h
target	1.000	3.000	5.000	3.200
initial	0.5	1.5	5.5	3.0
initial	0.5	1.5	3.0	3.2
calcul1	1.069	2.881	5.371	2.958
initial	0.5	1.5	3.0	3.4
initial	0.5	1.5	3.0	4.0
initial	0.5	1.5	6.0	4.0
calcul2	1.074	2.957	5.082	3.830

Table 3: Binary grating, 2-tower profile

(iii) Piecewise linear gratings.

We considered a linear two-tower profile of fixed height 1 over the bottom level 2 given by the 7 target parameters $t_1, ..., t_7$ specified in Table 4. We made calculations with undisturbed and disturbed data. For $N = 4$, also for disturbed data a regularization was not necessary, while for $N = 5$ we had to regularize with $\gamma = 10^{-5}$ or greater even in the undisturbed case. For $\gamma = 10^{-7}$ the calculation became unstable. Starting at different initial values, we made calculations with 1000 iterations each and $\lambda = 0.01$ leading for exact data to identical results given in Table 4. For diminishing the rather large number of iterations we combined each iteration with a line-search (cf.[18]), but this gave no improvement compared to the constant step length λ as chosen.



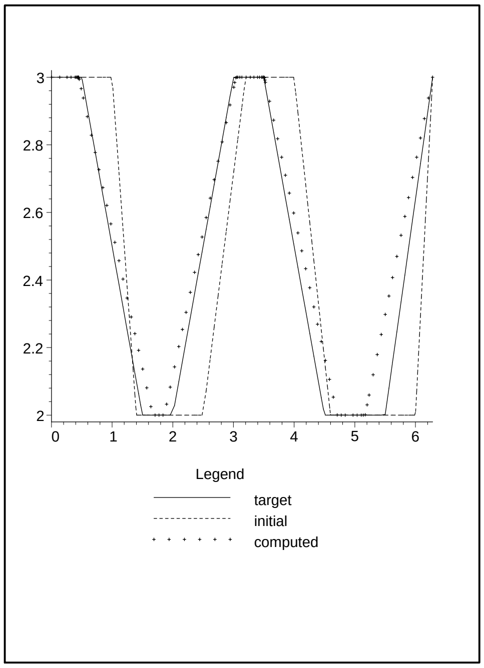


Figure 1: Fourier grating, case (6.3)

Figure 2: Linear grating

The results became stationary till the fourth digit and proved rather unsensible against changes of initial values.

We considered perturbations (6.1) with $\delta = 0.1$ corresponding to a noise of 3.4% leading to a deviation in the result of less than 1%.

	t_1	t_2	t_3	t_4	t_5	t_6	t_7
target	0.5	1.5	2.0	3.0	3.5	4.5	5.5
initial	0.5	1.5	2.0	3.0	3.5	4.5	5.5
initial	1.0	1.4	2.5	3.2	4.0	4.6	6.0
calcul	0.45	1.67	1.86	3.04	3.51	4.71	5.17

Table 4: Linear 2-tower profile

To the reader's convenience, some of our computational results presented in the Tables are additionally drawn in Figures 1–4.

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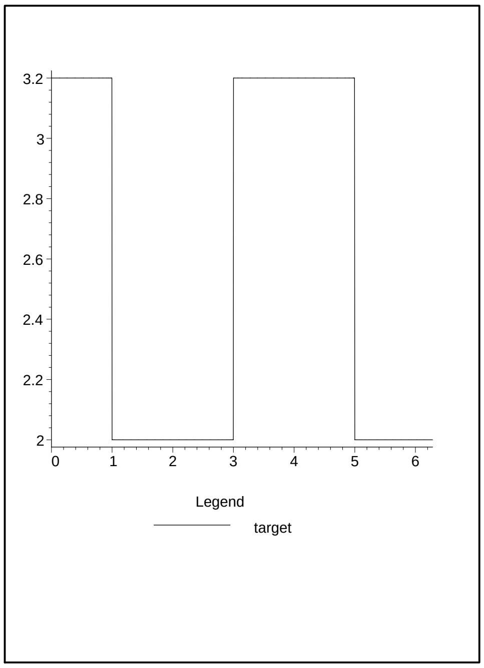

Figure 3: Binary grating, target

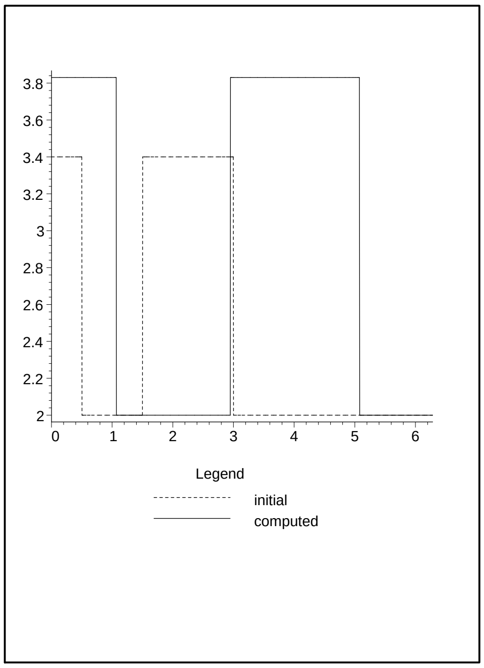

Figure 4: Binary grating, calcul2

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