0.1 Recent Progress on Time-harmonic Elastic Wave Scattering Problems for Diffraction Gratings

Johannes Elschner, Guanghui Hu

A diffraction grating is an optical device consisting of a surface with many parallel (periodic) grooves. It can be used to produce the spectrum of a beam of light (or other electromagnetic radiation) by dispersing it into its wavelengths. In recent years, increasing application of diffractive optics has driven a rigorous electromagnetic theory of gratings, not only to precisely predict scattering performance but also to carry out optimal design of new grating structures (see [1]). The elastic wave propagation in periodic structures have also a wide field of applications, particularly in geophysics, nondestructive testing and seismology. For instance, identifying fractures in sedimentary rocks can have significant impact on the production of underground gas and liquids by employing controlled explosions. The rock under question can be regarded as a homogeneous transversely isotropic elastic medium with periodic vertical fractures that can be extended to infinity in one of the horizontal directions (see Figure 1). Using the elastic plane wave as an incoming source, this can be formulated as an inverse problem of shape identification from the knowledge of near-field data measured above the periodic structure (see Figure 2). Analogous inverse problems also arise from the use of transient elastic waves to measure the elastic properties as well as flaws and cracks of solid speciments, especially in the nondestructive evaluation of concrete structures. As an example, we mention the nondestructive elastic-wave test of foundation slabs in important office buildings put under the ground water level. In addition, the problem of elastic pulse transmission and reflection through the earth is fundamental to both the investigation of earthquakes and the utility of seismic waves in search for oil and ore bodies. These applications motivate us to rigorously investigate the elastic wave scattering through unbounded interfaces and the associated inverse problems, a vast literature of which by far has only come from engineering community.

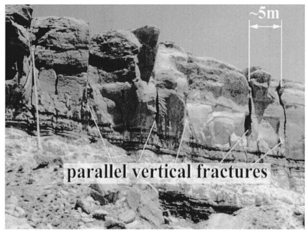

Fig. 1: *Vertical fractures in sandstone. Source: [5, page 3013]*

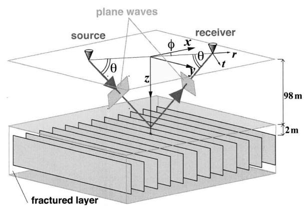

Fig. 2: *Identify periodic fractures using incident sources and receivers. Source: [5, page 3018]*

Compared to acoustic and electromagnetic scattering, the elasticity problem is more complicated because of the coexistence of compressional and shear waves that propagate at different speeds. These two waves are coupled at interfaces where boundary or transmission conditions depending on the elastic medium are imposed. The research at WIAS on the DFG project *Direct and inverse scattering problems for elastic waves* (07. 2009-07.2012) aims to investigate existence and uniqueness of solutions for non-smooth (periodic and rough) unbounded interfaces based on variational formulations, as well as uniqueness and inversion algorithms for the inverse problem of determining the scattering object by near and far field measurements. Emphasis of this report will be placed on progress on elastic scattering by diffraction gratings (periodic structures).

Consider a time-harmonic elastic plane pressure or shear wave u^i with the incident angle $\theta \in (-\pi/2, \pi/2)$ incident on a 2π -periodic grating surface Λ from the region Ω_Λ above the grating. Let the mass density of the elastic medium in Ω_Λ be one. Then, the total displacement $u(x_1, x_2)$, which is the sum of the incident field u^i and the scattered field u^s, satisfies the Navier equation

$$(\Delta^* + \omega^2)\, u = 0 \quad \text{in} \quad \Omega_\Lambda\,, \qquad \Delta^* := \mu\,\Delta + (\lambda+\mu)\,\text{grad div}\,. \tag{1}$$

Here, λ and μ are the *Lamé constants* satisfying $\mu > 0$ and $\lambda + \mu > 0$, and $\omega > 0$ denotes the angular frequency of the harmonic motion. If the medium below Λ is impenetrable, we assume one of the first (Dirichlet), second (Neumann), third and fourth kind boundary conditions is imposed on Λ (see [6]); For penetrable homogeneous medium, the transmissions conditions ensuring the continuity of the displacement and the stress are considered on Λ. The periodicity of Λ together with the form of u^i implies the α-quasiperiodicity of u (this will be rigorously justified in a future work, following the corresponding arguments in acoustics by Chandler-Wilde and Elschner (2012)) , i.e., $u(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi)u(x_1, x_2)$ for $(x_1, x_2) \in \Omega_\Lambda$, where the parameter α coincides with the quasiperiodicity of the incoming wave. In $x_2 > \Lambda^+ := \max_{(x_1,x_2)\in\Lambda} x_2$, we have the Rayleigh expansion of u^s into outgoing plane elastic waves as follows:

$$u^s(x) = \sum_{n\in\mathbb{Z}} \left\{ A_{p,n}(\alpha_n, \beta_n)^\top \exp(i\alpha_n x_1 + i\beta_n x_2) + A_{s,n}(\gamma_n, -\alpha_n)^\top \exp(i\alpha_n x_1 + i\gamma_n x_2) \right\}, \tag{2}$$

where the constants $A_{p,n}, A_{s,n} \in \mathbb{C}$ are called *Rayleigh coefficients* and $\alpha_n := \alpha + n$, $\beta_n := \sqrt{k_p^2 - \alpha_n^2}$, with the branch of a square root chosen such that its imaginary part is always positive. The parameter $\gamma_n := \gamma_n(\theta)$ is defined analogously as β_n with k_p replaced by k_s. Note that only a finite number of plane waves in (2) propagate into the far field, with the remaining evanescent waves (or surface waves) decaying exponentially as $x_2 \to +\infty$. Our direct and inverse diffraction problems for an impenetrable grating can be formulated as

(DP): Given a grating profile curve $\Lambda \subset \mathbb{R}^2$ and an incident field u^i with the incident angle θ, find the quasiperiodic function $u = u(x;\theta) = u^i + u^s \in H^1_{loc}(\Omega_\Lambda)^2$ that satisfies the Navier equation (1), the expansion (2) and the corresponding essential boundary condition on Λ.

(IP): Determine Λ from the near-field data $u(x_1, b; \theta)$ for all $x_1 \in (0, 2\pi)$ and some $b > \Lambda^+$, such that the Dirichlet boundary condition is satisfied on Λ.

Solvability results for direct scattering problems

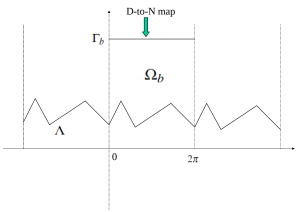

Fig. 3: *The variational formulation is posed in one periodic cell Ω_b*

Existence and uniqueness of quasiperiodic solutions to the Dirichlet problem was first established by T. Arens (1999) for grating profiles given by C^2-smooth graphs. The existence proof is based on the integral equation methods where the solution is sought as a superposition of single and double layer potentials. The C^2-regularity assumption in integral equation methods, we think, could be weekened to Lipschitz ones, with complicated arguments for justifying Fredholm properties of the integral system. To deal with (DP), we have proposed an equivalent variational formulation posed in a bounded periodic cell involving a nonlocal boundary operator defined on the artifical boundary $\Gamma_b := \{(x_1, b) : 0 \le x_1 \le 2\pi\}$ for some $b > \Lambda^+$; see Figure 3. The variational method appears to be well adapted to the analytical analysis and numerical approximation of rather general periodic diffractive structures involving complex materials in Lipschitz domains. Let V_α be an appropriate α-quasiperiodic variational space for (DP). By the first Betti formula, the problem (DP) is equivalent to the variational problem of finding $u \in V_\alpha$ such that

$$\int_{\Omega_b} \left(a(u, \overline{\varphi}) - \omega^2 u \cdot \overline{\varphi}\right) dx - \int_{\Gamma_b} \overline{\varphi} \cdot \mathcal{T} u \, ds = \int_{\Gamma_b} (T u^i - \mathcal{T} u^i) \cdot \overline{\varphi} \, ds, \quad \forall \varphi \in V_\alpha, \tag{3}$$

with $\mathcal{T}$ being the Dirichlet-to-Neumann map and the symmetric bilinear form $a(\cdot,\cdot)$ defined by

$$\begin{aligned} a(u,\varphi) \quad := \quad & (2\mu+\lambda)\,(\partial_1 u_1\,\partial_1\varphi_1 + \partial_2 u_2\,\partial_2\varphi_2) + \mu\,(\partial_2 u_1\,\partial_2\varphi_1 + \partial_1 u_2\,\partial_1\varphi_2) \\ & + \lambda\,(\partial_1 u_1\,\partial_2\varphi_2 + \partial_2 u_2\,\partial_1\varphi_1) + \mu\,(\partial_2 u_1\,\partial_1\varphi_2 + \partial_1 u_2\,\partial_2\varphi_1)\,. \end{aligned}$$

Similar variational formulations have been used in the literature for the Helmholtz equation by Kirsch (1993) and for Maxwell's equations by Abboud (1993). In contrast to the acoustic scattering, the D-to-N map $\mathcal{T}$ for the Navier equation, which can be explicitly represented via $n \times n$ matrices in $\mathbb{R}^n$ $(n = 2,3)$, does not have a definite real part. Thanks to the periodicity of the domain, one can apply the compact imbedding arguments to one periodic cell. This combined with the decomposition of $\mathrm{Re}\,(-\mathcal{T})$ into the sum of a positive-definite operator and a finite dimensional operator gives rise to the strong ellipticity of the sesquilinear form on the left hand side of (3). By Fredholm alternative we finally verified the following uniqueness and existence results for (DP).

Theorem 0.1.1 *(i) If the grating profile Λ is a Lipschitz curve, then there always exists a solution of (DP) under the boundary conditions of the first, second, third and fourth kind. Moreover, uniqueness holds for small frequencies, and for all frequencies excluding a discrete set with the only accumulation point at infinity. (ii) If Λ is the graph of a Lipschitz function, then for any frequency $\omega > 0$ there exists a unique solution of (DP) under the Dirichlet boundary condition.*

We have also proved uniqueness and existence of solutions under the mixed Dirichlet and Robin boundary conditions for any frequency of incidence, provided Λ is a Lipschitz curve. Moreover, these solvability results have been generalized to the more practical case of 3D, and the first assertion of Theorem 0.1.1 has been even applied to transmission problems in both 2D and 3D. The proof of the second assertion relies heavily on the use of periodic Rellich identities for the Navier equation, which is applicable only for grating profiles given by graphs where the Dirichlet boundary condition is imposed. Non-uniqueness examples under the second, third or fourth kind boundary conditions have been reported for flat gratings in the resonance case ([2]), and those for transmission problems can be found in the book by J. D. Achenbach (1973).

Rigorous numerical treatment using finite element or integral equation methods have been extensively studied for both acoustic and electromagnetic grating diffraction problems. To compute the scattered field for the Dirichlet boundary problem, we solved a first kind integral equation by using the discrete Galerkin method proposed by Atkinson (1988). The implementation of this method is easier than the integral equation method with a second kind integral equation that involves the computation of the stress operator on the profile. The proposed first kind integral equation has been proved uniquely solvable in $L^2(\Lambda)^2$, based on the decomposition of the quasi-periodic fundamental solution $\Pi(x,y)$ of the Navier equation into a logarithmically singular part and a smooth part. For piecewise linear gratings where the scattered field may be singular at corner points, a mesh grading transformation has been adopted to parameterize the grating profile.

Inversion algorithms and uniqueness to (IP)

The inverse scattering problem of determining the shape of an obstacle is highly nonlinear, since the measured near or far field data do not depend linearly on the shape. It is also severely ill-posed in the sense of Hadamard, whereas the direct problem is well-posed. A survey on the state of the art of inverse time-harmonic acoustic and electromagnetic scattering by bounded obstacles can be found in the monograph by D. Colton and R. Kress (1998). Traditional approach in shape identification is to formulate the problem as a least squares optimization problem according to the given boundary conditions and then solve the shape parameters by *iterative schemes*, e.g., Gauss-Newton and Levenberg-Marquardt methods. Based on the Kirsch-Kress optimization scheme, we applied a two-step inversion algorithm to (IP). Assume that Λ is the graph of a C^2-smooth 2π-periodic function f lying between $x_2 = 0$ and $x_2 = b$ for some $b > 0$. The first step is to reconstruct the scattered field from the near-field $u^s(x_1, b)$. We represent u^s as a single-layer potential and then solve the unknown density function φ from the first kind integral equation

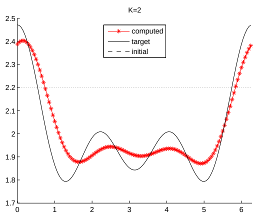

Fig. 4: *K=2, reconstruction from only partial propagating modes*

$$\frac{1}{2\pi}\int_0^{2\pi} \Pi(x_1, b; t, 0)\,\varphi(t)\,dt = u^s(x_1, b), \quad x_1 \in (0, 2\pi). \tag{4}$$

This step is linear but severely ill-posed, and can be easily achieved by employing Tikhonov regularization and the singular value decomposition of the operator on the right-hand side of (4). The second step, which is nonlinear but well-posed, is to determine f by minimizing the defect

$$||u^i(x_1, f(x_1)) + \frac{1}{2\pi}\int_0^{2\pi} \Pi(x_1, f(x_1); t, 0)\,\varphi(t)\,dt||_{L^2(0,2\pi)^2} \to \inf_{f\in\mathcal{M}} \tag{5}$$

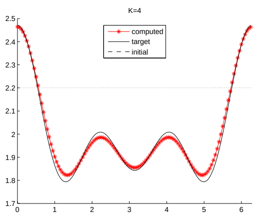

Fig. 5: *K=4, reconstruction from all propagating modes (i.e., far-field data)*

over some admissible set $\mathcal{M}$ of profile functions. We have discretized the objective functional in (5) by the trapezoidal rule and solved the resulting minimization problem in a finite dimensional space. Figure 4, Figure 5 and Figure 6 illustrate the numerical results for reconstructing a Fourier grating, where the number of wave modes involved in calculation is $2K+1$. We have also applied it to piecewise linear grating profiles with a finite number of corners and adapted it to the case of several incident angles or a finite number of incident frequencies. In principle it can be extended to the Neumann boundary value problem and the transmission problem in $\mathbb{R}^n$ $(n = 2, 3)$, with an increased computational complexity. A Dirichlt grating profile in 3D can be also recovered from only the shear part of near field corresponding to incident plane shear waves.

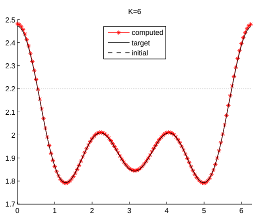

Fig. 6: *K=6, reconstruction from all propagating modes and six additional evanescent modes*

The two-step algorithm is easily implemented, and satisfactory reconstructions can be obtained for suitable initial values of grating parameters. Since no direct scattering problems need to be solved, it reduces the computational effort of the original Kirsch-Kress scheme which was based on a combined cost functional that requires the determination of two unknown functions. However, the two-step algorithm shows only local (but fast) convergence properties, and a rigorous convergence analysis is still missing. This is not only due to the high non-linearity of the inverse scattering problems but also the ill-posedness of their linearalizations.

We now turn to the uniqueness issue to (IP), i.e., whether the near field data provides enough information to completely determine an unknown grating profile. A positive answer to such a question guarantees by theory the validity of the inverse solution computed from the given data. For bounded (non-periodic) scatterers, it is still an open problem whether the uniqueness from the far-field pattern holds with one incoming plane wave. Nevertheless, we cannot expect the same global uniqueness in wave diffraction by general periodic structures, because a finite number of propagating modes without any decaying at infinity are involved in the Rayleigh expansion 2 and non-uniqueness examples can be readily reconstructed for flat gratings. It was shown by A. Charalambopoulos, etc. (2001) that a Dirichlet C^2-smooth surface can be uniquely determined from the scattered elastic fields corresponding to a finite number of incoming pressure wavenumbers, provided some a priori information about the height of the grating is available. To investigate global uniqueness with one plane wave, we have restricted ourselves to the kind of polygonal grating profiles and only studied the third and fourth kind boundary value problems. Relying on the reflection principle for the Navier equation by J. Elschner and M. Yamamoto (2009), we have proved that global uniqueness holds except for several extremely rare sets of grating profiles, each of them can be explicitly defined; see, e.g., Figure 7 and Figure 8 for the grids on which the unidentifiable grating profiles for the incident pressure plane wave with $\theta = -\frac{\pi}{6}$ and $k_p = 2$ are located. Thus we obtained global uniqueness with one incoming wave within the polygonal periodic structures excluding all unidentifiable sets. The inverse problems in 3D turn out to be more complicated than 2D, with several extra unidentifiable sets. The inverse Dirichlet problem seems challenging, due to the lack of reflection principle for the Navier equation under the Dirichlet boundary condition.

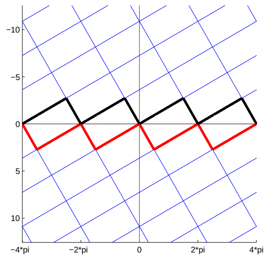

Fig. 7: *Unidentifiable grating profiles under the boundary conditions of the fourth kind*

Outlook

The elastic scattering by unbounded non-periodic surfaces will be our interest in the future. The compact imbedding theory, which has considerably simplified our arguments in periodic case, cannot be applied to rough surface scattering problems. Based on the perturbation arguments for semi-Fredholm operators, a progress has been made in [4] for the scattering due to an inhomogeneous source term whose support lies within a finite distance above the rough surface. We shall proceed with the solvability for elastic plane waves and spherical or cylindrical waves in appropriate weighted Sobolev spaces. In grating diffraction problems, this will also help us to interpret the quasiperiodicity of the scattered field corresponding to one single pressure or shear wave and to describe solution spaces for rather general non-quasiperiodic incoming elastic waves.

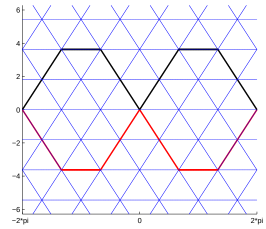

Fig. 8: *Unidentifiable grating profiles under the boundary conditions of the third kind*

References

[1] G. Bao, L. Cowsar, W. Masters, *Mathematical Modeling in Optical Science*, Philadelphia, USA, 2001.

[2] J. Elschner, G. Hu, *An optimization method in inverse elastic scattering for one-dimensional grating profiles*, Commun. Comput. Phys., **12** (2012), pp. 1434-1460.

[3] J. Elschner, G. Hu, *Scattering of plane elastic waves by three-dimensional diffraction gratings*, Math. Mode. Meth. Appl. Sci., **22** (2012), 1150019.

[4] J. Elschner, G. Hu, *Elastic scattering by unbounded rough surfaces*, WIAS Preprint no. 1677, 2012, to appear in: SIAM. J. Math. Anal., 2013.

[5] S. Nakagawa, K. T. Nihei, L. R. Myer and E. L. Majer, *Three-dimensional elastic wave scattering by a layer containing vertical periodic fractures*, J. Acoust. Soc. Am., **113** (2003), pp. 3012–3023.

[6] V. D. Kupradze et al, *Three-dimensional Problems of the Mathematical Theory of Elasticity and Thermoelasticity*, North-Holland, Amsterdam, 1979.