On Integral Equation and Least Squares Methods for Scattering by Diffraction Gratings

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Abstract. In this paper we consider the scattering of a plane acoustic or electromagnetic wave by a one-dimensional, periodic rough surface. We restrict the discussion to the case when the boundary is sound soft in the acoustic case, perfectly reflecting with TE polarization in the EM case, so that the total field vanishes on the boundary. We propose a uniquely solvable first kind integral equation formulation of the problem, which amounts to a requirement that the normal derivative of the Green's representation formula for the total field vanish on a horizontal line below the scattering surface. We then discuss the numerical solution by Galerkin's method of this (ill-posed) integral equation. We point out that, with two particular choices of the trial and test spaces, we recover the so-called SC (spectral-coordinate) and SS (spectral-spectral) numerical schemes of DeSanto et al., *Waves Random Media*, **8**, 315-414, 1998. We next propose a new Galerkin scheme, a modification of the SS method that we term the SS* method, which is an instance of the well-known *dual least squares Galerkin method*. We show that the SS* method is always well-defined and is optimally convergent as the size of the approximation space increases. Moreover, we make a connection with the classical least squares method, in which the coefficients in the Rayleigh expansion of the solution are determined by enforcing the boundary condition in a least squares sense, pointing out that the linear system to be solved in the SS* method is identical to that in the least squares method. Using this connection we show that (reflecting the ill-posed nature of the integral equation solved) the condition number of the linear system in the SS* and least squares methods approaches infinity as the approximation space increases in size. We also provide theoretical error bounds on the condition number and on the errors induced in the numerical solution computed as a result of ill-conditioning. Numerical results confirm the convergence of the SS* method and illustrate the ill-conditioning that arises.

Key words: Helmholtz equation; first kind integral equation; spectral method; condition number.

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1   Introduction

We consider the scattering of a plane acoustic or electromagnetic wave by a perfectly reflecting, periodic surface. Adopting Cartesian coordinates $Oxyz$ we assume that the surface is invariant in the y direction and periodic in the x direction, specified by the equation $z = f(x)$, for some given continuous function f. The mathematical problem to be solved is two-dimensional. We assume throughout that the incident wave is time-harmonic ($e^{-i\omega t}$ time dependence), so that the total wave field u^t is a solution of the Helmholtz equation

$$\Delta u^t + k^2 u^t = 0 \quad \text{in } \Omega, \tag{1.1}$$

where $\Omega := \{\mathbf{r} = (x, z) \in \mathbb{R}^2 : z > f(x)\}$ is that part of the Oxz plane above the scattering surface. Throughout, we will assume that f is periodic with period $L > 0$ and that the incident field u^i is the plane wave

$$u^i(\mathbf{r}) = \exp(ik[x \sin\theta - z \cos\theta]), \tag{1.2}$$

where θ is the angle of incidence, measured from the z-axis, with $-\pi/2 < \theta < \pi/2$. It is the goal to determine the scattered field $u := u^t - u^i$ given the boundary condition

$$u^t = u^i + u = 0 \qquad \text{on } \partial\Omega, \tag{1.3}$$

where $\partial\Omega = \{(x, f(x)) : x \in \mathbb{R}\}$, and given that an appropriate radiation condition on u holds, expressing that u is outgoing from $\partial\Omega$. This problem models scattering of electromagnetic plane waves by a perfectly conducting diffraction grating in the TE polarization case. The same mathematics models acoustic scattering by a one-dimensional periodic sound soft surface.

Many different methods have been proposed for solving this problem. Alternative boundary integral equation methods to those proposed here are discussed in [1, 29, 35], standard differential equation (coupled-mode) based methods in [4, 31, 33], a coordinate-transformation-based differential equation method in [20, 21], and a method of variation of boundaries based on analytic continuation arguments in [5]. Many different specific surface examples are available [12] as well as the first treatment of the problem using spectral methods [13]. An extensive recent review of many of the different computational methods available is made in [14]. A classical method for solving this problem, on which we throw new light in Section 5, is the least squares method [28, 30], in which the scattered field is expressed as a linear combination of solutions of the Helmholtz equation (the Rayleigh expansion (2.1) below) and the coefficients in this expansion are determined by requiring that the boundary condition holds in a least squares sense. We note that, in the context of determining eigenfunctions of the Laplacian in 2D domains, the least squares method has recently been revived by Betcke and Trefethen [3]. The problem can also be tackled via a variational formulation in a part of the domain, truncated by the Rayleigh expansion which provides a non-local boundary condition, with the variational problem solved numerically by standard finite element methods (see e.g. [2, 17, 18]).