Analyzing Diffraction Gratings by Neumann-to-Dirichlet Maps and Boundary Integral Equations

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Diffraction gratings [1] are important in many practical applications. Numerical methods are essential in the design, analysis and optimization of grating structures. Existing numerical methods include the finite element method (FEM) [2], the Fourier modal method (FMM) [3, 4], the boundary integral equation (BIE) method [5, 6], etc. The FEM is very general, but it gives rise to large, complex and indefinite linear systems that can be difficult to solve. The FMM is suitable if the grating is a layered structure, but it is not so efficient when a general grating structure with sloping interfaces must be approximated by a layered one. The BIE method is suitable if the grating structure involves a small number of interfaces and the refractive index is piecewise constant, but it is somewhat complicated to implement, since the integral operators are related to the quasi-periodic Green’s function which requires lattice sums to evaluate. Recently, Huang and Lu [7] developed a Dirichlet-to-Neumann (DtN) map method for scattering of periodic arrays of cylinders. Existing numerical methods for diffraction gratings are applicable to the problem studied in [7], but special methods taking advantage of the geometry features, such as the multipole method [8] and the DtN-map method, are often more efficient. Unlike the multipole method, the DtN-map method [7] does not require lattice sums.

In this paper, we extend the DtN-map method to general diffraction grating problems. For 2D cases where the structure and the fields do not depend on z, the governing equation is

\[ q\partial_z(q^{-1}\partial_z u) + q\partial_y(q^{-1}\partial_y u) + k_0^2 n^2 u = 0, \tag{1} \]

where \( k_0 \) is the free space wavenumber, \( q = 1 \) or \( q = n^2 \) for the TE or TM polarization, respectively. For a plane incident wave, and if the refractive index profile \( n(x, y) \) is periodic in \( x \) with period \( L \) and is constant for \( y < 0 \) and \( y > D \), then the problem can be reduced to a rectangle \( G \) given by \( 0 < x < L \) and \( 0 < y < D \), with a quasi-periodic condition in the \( x \) direction and some boundary conditions at \( y = 0 \) and \( y = D \) [1].

We divide \( G \) into sub-domains \( \Omega_1, \Omega_2, \ldots, \Omega_m \), where \( \Omega_j \) is bounded by two curves \( \Gamma_{j-1} \) and \( \Gamma_j \), and two vertical lines at \( x = 0 \) and \( x = L \). On \( \Gamma_j \), we let \( \nu \) be the outward unit normal vector of \( \Omega_j \). The DtN-map method solves the diffraction grating problem by manipulating two operators from \( \Gamma_0 \) to \( \Gamma_m \). On \( \Gamma_j \), we define the global DtN operator \( Q_j \) and fundamental solution operator \( Y_j \) by

\[ Q_j u|_{\Gamma_j} = q^{-1}\partial_y u|_{\Gamma_j}, \quad Y_j u|_{\Gamma_j} = u|_{\Gamma_j}, \tag{2} \]

where \( u \) is any solution of Eq. (1) satisfying the quasi-periodic condition and the boundary condition at \( y = 0 \). On \( \Gamma_0 \), we know \( Q_0 \) from the boundary condition and \( Y_0 = I \). If \( Q_m \) and \( Y_m \) are obtained, we can find the reflected and transmitted waves as in [7]. The key step is to march these two operators from \( \Gamma_{j-1} \) to \( \Gamma_j \). This requires the NtD map \( \Lambda \) of the sub-domain \( \Omega_j \) and the quasi-periodic condition. In \( \Omega_j \), the refractive index \( n \) is a constant. Using the fundamental solution of the Helmholtz equation \( G(x, y) = \frac{1}{4} H_0^{(1)}(k_0 n|x - y|) \), we define the integral operators \( S \) and \( K \) as

\[ (S\phi)(x) := 2 \int_{\partial\Omega_j} G(x, y)\phi(y)ds(y), \quad (K\phi)(x) := 2 \int_{\partial\Omega_j} \frac{\partial G(x, y)}{\partial\nu(y)}\phi(y)ds(y), \quad x \in \partial\Omega_j, \tag{3} \]

where \( \phi \) is an arbitrary function defined on \( \partial\Omega_j \). Then, on the boundary of \( \Omega_j \), we have \((1 + K)u = S\partial_{\nu} u\). Therefore, the NtD map of \( \Omega_j \) is \( \Lambda = (1 + K)^{-1}S \). In practice, \( \Lambda \) is approximated by a matrix. We discretize the integral equation by a Nyström method using a graded mesh.

For an example, we consider the structure shown in Fig. 1(a). The refractive indices of the top, the thin film and the substrate are \( n_0 = 1 \), \( n = 2.25 \) and \( n_s = 1.46 \), respectively. The parameters in Fig. 1(a) are \( d = 2L \) and \( \Delta d = 0.4L \). The reflectance of the zeroth order mode is shown in Fig. 1(b) as a function of the scaled wavelength \( \lambda_0 = 1.2\pi/(k_0 L) \), where \( L = 0.6\lambda_0 \). Our results agree well with those in [9].

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Figure 1: (a): a grating structure with a thin film; (b): Reflectance of zeroth order mode as a function of the scaled wavelength.

References