Resonant Frequencies for Diffraction Gratings

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Abstract—This note is devoted to a study of resonance phenomena in electromagnetic gratings. In particular, a characterization of the scattering frequencies (the complex values of the frequency inducing resonant behaviors) is given by using a variational method. After the diffraction problem is reduced to a bounded domain, we extend it to complex values of the frequency. The existence of the resolvant of the diffraction problem is established in the upper complex half-plane. It is shown that this resolvant can be extended meromorphically to the domain $C\backslash R^+$. In addition, the scattering frequencies, which correspond to the poles of this extension, solve a nonlinear eigenvalue problem.

Keywords—Gratings, Resonance, Diffraction, Electromagnetics, Resolvant.

1. INTRODUCTION

One of the most exciting new developments in diffractive optics involves the integration of zero-order grating with a planar waveguide to create a resonance. Such structures, known as guided-mode resonance filters, have been demonstrated to yield ultra-narrow bandwidth filters for a selected center wavelength and polarization with $\approx 100\%$ reflectance [1–4]. With such extraordinary potential performance, these “resonant reflectors” have attracted attention for many applications, such as lossless spectral filters with arbitrarily narrow, controllable linewidth, efficient and low-power optical switch elements, 100% reflective narrow-band spectrally selective mirrors, polarization control, high-precision sensors, lasers, and integrated optics. This note is concerned with the analysis of the resonance behavior of diffraction gratings (periodic structures).

An integral equation approach has recently been developed in [5] to study resonant frequencies of a multislot grating structure. Variational approaches have also been introduced to study resonant states and poles by Shenk and Thoe [6] for perturbations of the Laplacian and by Lenoir et al. [7] for the scattering by a bounded obstacle. Here, we develop a variational approach in the spirit of [6,7] to obtain a characterization of the scattering frequencies of a general grating structure, which are the complex values of the frequency inducing a resonant state.

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2. THE DIFFRACTION PROBLEM

Let \((U, x_1, x_2, x_3)\) be an orthonormal system of coordinates in \(\mathbb{R}^3\). Consider a grating structure which is invariant in the \(x_3\)-direction, and periodic in the \(x_1\)-direction, with period \(d\).

The medium is characterized by its real valued refractive index \(n(x_1, x_2) \in L^\infty(\mathbb{R}^2)\), satisfying the periodicity condition \(n(x_1 + d, x_2) = n(x_1, x_2)\). It is assumed that the propagation medium is homogeneous for \(|x_2|\) large enough: \(n(x) = n_\infty\) for \(|x_2| > H_\infty\).

The grating is illuminated by a monochromatic plane wave \(U_i\) contained in the plane \((x_1, x_2)\). In other words, if we denote by \(k \in \mathbb{R}^+\) the wave number of the incident field and by \(\theta_i \in [0, \pi/2)\) its angle of incidence, we have \(U_i = U_0^i e^{i(ax_1 - \beta x_2)}\), where \(\alpha = k \sin \theta_i\) and \(\beta = k \cos \theta_i\).

Under these assumptions, solving Maxwell's equations amounts to solve the scalar TE (transverse electric) and TM (transverse magnetic) diffraction problems. In this note, attention will be restricted to the analysis of the TE case, since the analysis of the TM case can be treated analogously. In this context, the total field \(U\) satisfies

\[\Delta U + k^2 n^2 U = 0, \quad \text{in } \mathbb{R}^2.\]

Because of the unboundness of the grating in the \(x_1\)-direction, Sommerfeld's radiation condition is not anymore suitable to describe the behavior of the diffracted field when \(|x_2| \to +\infty\). The appropriate radiation condition in the \(x_2\)-direction can be derived (cf. [8]) using the fact that the diffracted field \(U^d\) and the total field \(U = U^d + U_i\) are quasiperiodic in \(x_1\) with a period \(d\), i.e., the functions

\[u^d(x_1, x_2) = e^{-i\alpha x_1} U^d(x_1, x_2), \quad u(x_1, x_2) = e^{-i\alpha x_1} U(x_1, x_2)\]

are periodic in \(x_1\) with period \(d\) for each \(x_2\). More precisely, the diffracted field has the following expansion (the Rayleigh expansion) in the homogeneous medium:

\[u^d(x_1, x_2) = \sum_{p \in \mathbb{Z}} A_p^\pm e^{i(p \alpha x_1 + \beta_p x_2)}, \quad \text{for } x_2 > H_\infty,\]

\[\sum_{p \in \mathbb{Z}} A_p^- e^{i(p \alpha x_1 - \beta_p x_2)}, \quad \text{for } x_2 < -H_\infty,\]

where \(A_p^\pm \in \mathbb{C}, \alpha_p = \alpha + (2p\pi/d)\) and

\[\beta_p = \begin{cases} \sqrt{k^2 n_\infty^2 - \alpha_p}, & \text{if } |\alpha_p| < kn_\infty, \\ i\sqrt{\alpha_p - k^2 n_\infty^2}, & \text{if } |\alpha_p| \geq kn_\infty. \end{cases}\]

Note that the values of \(p\) for which \(|\alpha_p| < kn_\infty\) correspond to the propagating modes of the diffracted field, while the others correspond to the surface waves (exponentially decreasing with respect to \(x_2\) far from the grating). The physical diffraction problem can then be set in the periodic cell of the grating \(\Omega' = \{(0 < x_1 < d, x_2 \in \mathbb{R})\}\) in terms of the \(x_1\)-periodic function \(u\) as follows:

\[\Delta_{x_1} u + k^2 u^{x_1^2} u = 0, \quad \text{in } \Omega',\]

\[u(0, x_2) = u(d, x_2), \quad \partial_{x_1} u(0, x_2) = \partial_{x_1} u(d, x_2),\]

\[u^d = u - u^i, \quad \text{satisfies (1)},\]

where \(\Delta_{x_1} = (\partial_{x_1} + i\alpha)^2 + (\partial_{x_2})^2\).

The next step is to transform this problem into an equivalent problem, set in the bounded domain \(\Omega = \{(0 < x_1 < d, |x_2| > H)\}\), where \(H > H_\infty\) is fixed. To derive a transparent boundary condition on the boundaries \(\Gamma^\pm = \{0 < x_1 < d, x_2 = \pm H\}\), we use the fact that the diffracted field \(u^d\) is given by (1) on \(\Gamma^\pm\). More precisely, let \(\mathcal{H}^s(\Gamma^\pm)\) be the functional space of \(x_1\)-periodic functions of period \(d\) defined by

\[\mathcal{H}^s(\Gamma^\pm) = \left\{ v = \sum_{p \in \mathbb{Z}} v_p e^{i(2p\pi/d)x_1}, \sum_{p \in \mathbb{Z}} \left(1 + \frac{4p^2\pi^2}{d^2}\right)^s |v_p|^2 < +\infty \right\},\]

where \(\beta_p\) is defined by (2) (here, \(v_p\) are the coefficients of the Fourier series expansion of \(v\)).
Consider the boundary operators $T^\pm$ on $\Gamma^\pm$ defined by

$$T^\pm(v) = \sum_{p \in \mathbb{Z}} i \beta_p v_p e^{i(2\pi p/d) x_1},$$

for $v = \sum_{p \in \mathbb{Z}} v_p e^{i(2\pi p/d) x_1}$.

One can easily check that $T^\pm$ are continuous from $H^{1/2}(\Gamma^\pm)$ to $H^{-1/2}(\Gamma^\pm)$.

Note that $H^{1/2}(\Gamma^\pm)$ (respectively, $H^{-1/2}(\Gamma^\pm)$) is the natural functional space for the trace (respectively, the normal derivative) of the periodic diffracted field $u^d$ on $\Gamma^\pm$. We will denote by $\langle \cdot, \cdot \rangle_{\Gamma^\pm}$ the duality between the spaces $H^{-1/2}(\Gamma^\pm)$ and $H^{1/2}(\Gamma^\pm)$. The boundary operators $T^\pm$ are the Dirichlet-to-Neumann operators of the problem. Thus, the following boundary conditions hold:

$$\partial_n u^d = T^\pm u^d \quad \text{on } \Gamma^\pm.$$ (3)

Setting $u^i(x_1, x_2) = e^{-i\alpha x_1} U^i(x_1, x_2)$, consider the following problem in $H^1(\Omega)$:

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

$$u(0, x_2) = u(d, x_2), \quad \partial_1 u(0, x_2) = \partial_1 u(d, x_2),$$

$$\partial_n u = \partial_n u^i + T^\pm (u - u^i), \quad \text{on } \Gamma^\pm.$$ (P)

Problems $(P')$ and $(P)$ are equivalent in the sense of the following proposition (see [8] for the proof).

**Proposition 1.1.**

(i) If $u$ is a solution of $(P')$, then its restriction to $\Omega$ solves $(P)$.

(ii) If $u$ solves $(P)$, then it can be uniquely extended into a solution of $(P')$.

Thus, to study the scattering frequencies of $(P')$, it suffices to study those of $(P)$.

3. THE DISSIPATIVE DIFFRACTION PROBLEM

Consider the so-called dissipative problem, obtained by extending the physical diffraction Problem $(P)$ to complex values of $k^2$.

Let $\nu = k^2 \in \mathbb{C}$ and set $\alpha(\nu) = \sqrt{\nu} n_{\infty} \sin \theta_i$, $\beta(\nu) = \sqrt{\nu} n_{\infty} \cos \theta_i$, where the square root of $\nu$ is defined by $\sqrt{\nu} = |\nu|^{1/2} e^{i \theta/2}$, where $\theta \in [0, 2\pi]$ is an argument of $\nu$. Then, set for any $p \in \mathbb{Z}$

$$\alpha_p(\nu) = \alpha(\nu) + \frac{2p\pi}{d}, \quad \beta_p(\nu) = \sqrt{\nu n_{\infty}^2 - \alpha_p^2(\nu)} = |\nu n_{\infty}^2 - \alpha_p(\nu)|^{1/2} e^{i \varphi_p(\nu)/2},$$ (4)

where $\varphi_p(\nu) \in [0, 2\pi]$ is an argument of the complex number $\nu n_{\infty}^2 - \alpha_p(\nu)$.

Note that because of this determination of the square root, we have $\text{Im} (\beta_p(\nu)) \geq 0$ for any $p \in \mathbb{Z}$.

The Dirichlet-to-Neumann boundary operators on $\Gamma^\pm$ take the form

$$T^\pm(v)(u) - \sum_{p \in \mathbb{Z}} i \beta_p(v) v_p e^{i(2\pi p/d) x_1},$$

for $v = \sum_{p \in \mathbb{Z}} v_p e^{i(2\pi p/d) x_1}$. Therefore, for any complex number $\nu$, the dissipative problem reads

$$\Delta_{\alpha(\nu)} u + \nu n^2 u = 0, \quad \text{in } \Omega,$$

$$u(0, x_2) = u(d, x_2), \quad \partial_1 u(0, x_2) = \partial_1 u(d, x_2),$$

$$\partial_n u - \partial_n u^i + T^\pm (u - u^i), \quad \text{on } \Gamma^\pm.$$ (P_u)

Here, $\Delta_{\alpha(\nu)}$ denotes the operator $(-\partial_{x_1}^2 + i \alpha(\nu))^2 + (\partial_{x_2})^2$. It is easily seen that $(P_u)$ has the variational formulation

$$\text{find } u \in H^1(\Omega) \text{ such that } \forall \nu \in H^1(\Omega), \quad \alpha_{\nu}(u, u) = L_{\nu}(u),$$

where $L_{\nu}(u)$ is a linear functional.
where $\mathcal{H}^1(\Omega)$ denotes the closure in $H^1(\Omega)$ of the functional space

$$C^{\infty, \text{per}}(\mathbb{R}^2) = \{ u|_{\Omega}, u \in C^\infty(\mathbb{R}^2), u \equiv 0 \text{ for large } |x_2|, u \text{ is } x_1 \text{-periodic of period } d \},$$

and $a_\nu(\cdot, \cdot)$ and $L_\nu(\cdot)$ are defined on $\mathcal{H}^1(\Omega)$ by the following formulas:

$$a_\nu(u, v) = \int_\Omega \left\{ \nabla_\nu u \cdot \nabla_\nu \bar{v} - \nu n^2 u \bar{v} \right\} - \langle T^+(\nu) u, v \rangle_{\Gamma^+} - \langle T^-(\nu) u, v \rangle_{\Gamma^-},$$

$$L_\nu(v) = \langle \partial_n u^i - T^+(\nu) u^i, v \rangle_{\Gamma^+} + \langle \partial_n u^i - T^-(\nu) u^i, v \rangle_{\Gamma^-}.$$

Let $A(\nu): \mathcal{H}^1(\Omega) \to \mathcal{H}^1(\Omega)$ be the continuous operator associated to the bilinear form $a_\nu$

$$(A(\nu)u, v)_{1, \Omega} = a_\nu(u, v), \quad \text{for } u, v \in \mathcal{H}^1(\Omega). \quad (5)$$

The following proposition shows that $A(\nu)$ is a Fredholm operator of the second kind.

**Proposition 2.1.** For any complex number $\nu$, the operator $A(\nu)$ admits a Fredholm decomposition, i.e., we have $A(\nu) = B(\nu) + C(\nu)$, where $B(\nu)$ is an automorphism of $\mathcal{H}^1(\Omega)$ and $C(\nu)$ a compact operator on $\mathcal{H}^1(\Omega)$.

**Proof.** Clearly

$$\int_\Omega \nabla_\nu u \cdot \nabla_\nu \bar{v} = \int_\Omega \nabla u \cdot \nabla \bar{v} + \alpha(\nu)^2 \int_\Omega u \bar{v} + \int_\Omega (u \partial_1 \bar{v} - \partial_1 u \bar{v}).$$

Set $a_\nu = b_\nu + c_\nu$, where the bilinear forms $b_\nu$ and $c_\nu$ are defined on $\mathcal{H}^1(\Omega) \times \mathcal{H}^1(\Omega)$ by

$$b_\nu(u, v) = \int_\Omega (\nabla u \cdot \nabla \bar{v} + u \cdot \bar{v}) - \langle T^+(\nu) u, v \rangle_{\Gamma^+} - \langle T^-(\nu) u, v \rangle_{\Gamma^-},$$

$$c_\nu(u, v) = -\int_\Omega (\nu n^2 + 1 - \alpha(\nu)^2) u \bar{v} + \int_\Omega (u \partial_1 \bar{v} - \partial_1 u \bar{v}).$$

Let $B(\nu)$ (respectively, $C(\nu)$) be the continuous operator of $\mathcal{H}^1(\Omega)$ associated to the bilinear form $b_\nu(\cdot, \cdot)$ (respectively, $c_\nu(\cdot, \cdot)$). Since

$$\text{Re } b_\nu(u, u) = \|u\|^2_{1, \Omega} + \sum_{p \in \mathbb{Z}} \text{Im } (\beta_p(\nu)) \left( |A_p^+|^2 + |A_p^-|^2 \right)$$

and $\text{Im } (\beta_p(\nu)) \geq 0$, $b_\nu$ is elliptic on $\mathcal{H}^1(\Omega)$, hence, $B(\nu)$ is an automorphism.

To prove the compactness of $C(\nu)$, for $u, v \in \mathcal{H}^1(\Omega)$, we have $\int_\Omega \partial_1 u \bar{v} = -\int_\Omega u \partial_1 \bar{v}$, and consequently,

$$(C(\nu)u, v)_{1, \Omega} = c_\nu(u, v) = -\int_\Omega (\nu n^2 + 1 - \alpha(\nu)^2) u \bar{v} + 2 i \alpha(\nu) \int_\Omega u \partial_1 \bar{v}.$$}

The compactness of $C(\nu)$ follows from the compactness of the embedding of $H^1(\Omega)$ into $L^2(\Omega)$. \hfill \blacksquare

We next define the resolvent operator of the diffraction problem. Indeed, using Green's formula, it is obvious that for $\text{Im } \nu \neq 0$, the homogeneous dissipative problem (i.e., with $U_0 = 0$) set in $\Omega'$ has only the trivial solution. Then, from Proposition 2.1, the following result holds.

**Proposition 2.2.** The operator $A(\nu)$ defined by (5) is an automorphism of $\mathcal{H}^1(\Omega)$ for $\text{Im } \nu \neq 0$. 

4. THE ANALYTIC CONTINUATION OF THE RESOLVANT

Let $H(\nu) = A(\nu)^{-1} : H^1(\Omega) \rightarrow H^1(\Omega)$ be the resolvent of the problem for $\text{Im} \nu > 0$ (the existence of $R(\nu)$ follows from Proposition 2.2). To determine the domain of the complex plane where $R(\nu)$ can be extended analytically, we first study the analyticity of the operators $A(\nu)$, $B(\nu)$, and $C(\nu)$. We have the following.

**Proposition 3.1.** The operators $B(\nu)$, $C(\nu)$, and $A(\nu) = B(\nu) + C(\nu)$ are holomorphic in the domain $C \setminus R^+$. 

**Proof.**

(i) To study the analyticity of $B(\nu)$, we have to study that of $T(\nu)$, which amounts to check the analyticity of $\beta_p(\nu)$ (defined in (4)) for $p \in \mathbb{Z}$. Because of the determination chosen for the square root, $\beta_p(\nu)$ is holomorphic for the values of $\nu$ satisfying $\nu n_\infty^2 - \alpha_p(\nu) \notin R^+$. It is then straightforward that

$$\nu n_\infty^2 - \alpha_p(\nu) \in R^+ \iff \nu \in [\nu_p, +\infty),$$

where $\nu_p$ is the smallest root of the equation $\nu n_\infty^2 = \alpha_p(\nu)$. A straightforward computation shows that $\nu_p = (2\pi n_\infty \cos \theta_i)^2 (1 - \sin \theta_i)^2 \geq 0 = \nu_0$, and thus, that the functions $(\beta_p(\nu))_{p \in \mathbb{Z}}$ are holomorphic in $C \setminus R^+$, and so is $B(\nu)$.

(ii) The expression of $c_\nu(\cdot, \cdot)$ shows that $C(\nu)$ is holomorphic when $Q(\nu) = \tan^{-1} \sin \theta_i$ is holomorphic, i.e., for $\nu \in C \setminus R^+$.

In particular, this proposition indicates that the following result holds for the resolvent $R(\nu)$.

**Corollary 3.2.** The resolvent operator $R(\nu) = A(\nu)^{-1}$ is holomorphic in the half plane $\text{Im} \nu > 0$.

We are now ready to present the main result of this note.

**Theorem 3.3.** The resolvent operator $R(\nu) = A(\nu)^{-1}$ can be extended meromorphically to $C \setminus R^+$. 

**Proof.** Writing $R(\nu)$ as $R(\nu) = (B(\nu) + C(\nu))^{-1} = B(\nu)^{-1} (I + C(\nu)B(\nu)^{-1})^{-1}$ shows that it suffices to prove the theorem for the operator $(I + C(\nu)B(\nu)^{-1})^{-1}$, since $B(\nu)^{-1}$ exists and is holomorphic in $C \setminus R^+$. But this is a direct consequence of Steinberg's theorem (cf. [9]) and Corollary 3.2, since $C(\nu)B(\nu)^{-1}$ is compact and holomorphic in $C \setminus R^+$. 

Furthermore, the poles of $R(\nu)$ (recall that these poles lie in the half plane $\text{Im} \nu \leq 0$) correspond to the values $\nu^*$ of $\nu$ for which $A(\nu) = B(\nu) + C(\nu)$ is not injective, or equivalently, to the values of $\nu$ for which $\sigma$ is an eigenvalue of the operator $B(\nu)^{-1}C(\nu)$. Consequently, the scattering frequencies of the diffraction problem are characterized by the following result.

**Theorem 3.4.** The scattering frequencies $\nu^*$ of the diffraction problem $(P_\nu)$ are the solutions of the nonlinear eigenvalue problem

$$\int_\Omega \left( \nabla_{\alpha(\nu^*)} u \cdot \nabla_{\alpha(\nu^*)} \bar{v} - \nu^* n_\infty^2 \bar{u} \right) - \left< T^+(\nu^*) u, v \right>_{T^+} - \left< T^-(\nu^*) u, v \right>_{T^-} = 0. \quad (6)$$

This nonlinear problem can be solved numerically by a fixed-point method. This result can also be used for solving the optimal design problem (of the structure and/or material), where the goal is to generate a resonance at some specified frequency. Numerical solution of this optimal design problem is currently in progress.

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