I. THE PHYSICAL PROBLEM

This presentation is based on the book *Scattering Theory for Diffraction Gratings* by Wilcox. In this book, the author studied the propagation of two-dimensional acoustic and electromagnetic fields in bounded planar regions whose boundaries, which are the diffraction gratings, lie between two parallel lines and are periodic. In each case, the medium filling the region is assumed to be either rigid or acoustically soft. In the electromagnetic case, it is assumed to be perfectly conduction. In both cases, the sources of the field are assumed to be localized in space and time.

II. THE MATHEMATICAL FORMULATION

The plane diffraction gratings are the boundaries of the class of planar domains $G$ defined by the following properties

(1) $G$ is contained in a half-plane,

(2) $G$ contains a smaller half-plane,

(3) $G$ is invariant under translation through a distance $a > 0$.

Domains with these properties are called grating domains. The half-plane of (2) is necessarily parallel to that of (1), and the translation of (3) is necessarily parallel to the edges of these half-planes. The smallest $a > 0$ in (3) is called the primitive grating period. It exists for all gratings except the degenerate grating for which $G$ is a half-plane.

We shall use the Cartesian coordinates $X = (x, y) \in \mathbb{R}^2$ in the plane of $G$ such that the x-axis is parallel to the edges of the half-planes of (1) and (2). We identify $G$ with the corresponding domain (open connected set) $G \subset \mathbb{R}^2$. 
Figure 1. Grating with Source Region and Incident Pulse

Source: "Scattering Theory for Diffraction Gratings" by Wileox.
Figure 2. Grating Domain with Coordinate System

Source: "Scattering Theory for Diffraction Gratings by Wilcox."
Define \( \mathbb{R}^2_c = \{ X \in \mathbb{R}^2 \mid y > c \} \), then for a suitable orientation of the coordinate axes, conditions (1) and (2) are equivalent to \( \mathbb{R}^2_h \subset G \subset \mathbb{R}^2_0 \) for some \( h > 0 \). Condition (3) is equivalent to \( G + (a, 0) = G \). We shall choose \( a = 2\pi \) as a convenient normalization.

The acoustic or electromagnetic field in \( G \) can be described by a real-valued function \( u = u(t, X) \) that is a solution of the initial boundary value problem

\[
D_t^2 u - \Delta u = 0 \text{ for all } t > 0 \text{ and } X \in G,
\]

and either the Neumann boundary condition

\[
D_n u \equiv \vec{v} \cdot \nabla u = 0 \text{ for all } t \geq 0 \text{ and } X \in \partial G,
\]

or the Dirichlet boundary condition

\[
u = 0 \text{ for all } t \geq 0 \text{ and } X \in \partial G.
\]

and

\[
u(0, X) = g_1(X) \text{ and } D_t u(0, X) = g_2(X) \text{ for all } X \in G.
\]

Here \( t \) is the time coordinate, \( D_t = \frac{\partial}{\partial t}, D_x = \frac{\partial}{\partial x}, D_y = \frac{\partial}{\partial y}, \nabla u = (D_x u, D_y u), \Delta u = D_x^2 + D_y^2 \) is the Laplacian, \( \partial G \) denotes the boundary of \( G \), and \( \vec{v} = \vec{v}(X) \) is a unit normal vector to \( \partial G \) at \( X \).

In the acoustic case, \( u(t, X) \) is interpreted as a potential for an acoustic field with velocity \( \vec{v} = -\nabla u \) and the acoustic pressure \( p = D_t u \). Then the boundary condition corresponds to an acoustically hard (i.e., \( D_n u = 0 \)) or soft (i.e., \( u = 0 \)) boundary.

The functions \( g_1(X) \) and \( g_2(X) \) characterize the initial state of the field. They are assumed to be given or calculated from the prescribed wave sources and to be localized:

\[
\text{supp} g_1 \cup \text{supp} g_2 \subset \{ X : x^2 + (y - y_0)^2 \leq \delta_0^2 \}, \text{ where } y_0 > h + \delta_0.
\]

In both the acoustic and the electromagnetic cases, the integral
\[ E(u, X, t) = \int_K \left( |\nabla u(t, X)|^2 + |D_t u(t, X)|^2 \right) dX \]

is interpreted as the wave energy in the set \( K \) at time \( t \) \( (dX = dx dy) \). Under both boundary conditions, solutions of the wave equation satisfy the energy conservation law

\[ E(u, G, t) = E(u, G, 0). \]

We will assume that the initial state has finite energy

\[ \int_K \left( |\nabla g_1(X)|^2 + |g_2(X)|^2 \right) dX < \infty. \]

III. MATHEMATICAL THEORY

1) The Reference Problem and Its Eigenfunction

Let \( \mathbb{R}^2_0 \) be the degenerate grating, then the initial value problem with Neumann boundary condition will be called the reference problem. The corresponding reference propagator is the operator \( A_0 = -\Delta \) in \( \mathcal{H}_0 = L_2(\mathbb{R}^2_0) \). The solution of the scattering problem for non-degenerate gratings is developed below as a perturbation of the reference problem.

Recall the initial value problem

\[ D^2_t u - \Delta u = 0 \text{ for all } t > 0 \text{ and } X \in \mathbb{R}^2_0. \]

We will solve this equation by separation of variables and seek solutions of the form

\[ u(t, x, y) = \psi_1(x)\psi_2(y)e^{-\lambda t}. \]

Then the differential equation becomes
\[- \omega^2 \psi_1(x) \psi_2(y) e^{-i\omega t} - \psi''_1(x) \psi_2(y) e^{-i\omega t} - \psi_1(x) \psi''_2(y) e^{-i\omega t} = 0. \]

We divide this equation by \( u(t, x, y) \) to obtain

\[
\frac{\psi''_1(x)}{\psi_1(x)} + \frac{\psi''_2(y)}{\psi_2(y)} + \omega^2 = 0.
\]

Let \((p, q) \in \mathbb{R}^2\) such that \(p^2 + q^2 = \omega^2(p, q)\), then we have a system of equations

\[
\frac{\psi''_1(x)}{\psi_1(x)} = -p^2, \quad \frac{\psi''_2(y)}{\psi_2(y)} = -q^2
\]

which has the solutions

\[
\psi_1(x) = c_1 e^{ipx} \text{ and } \psi_2(y) = c_2 e^{iqy} + c_3 e^{-iqy},
\]

and the general solution is

\[
\psi_0(x, y, p, q) = C_1 e^{i(px + qy)} + C_2 e^{i(px - qy)}.
\]

and

\[
D_x \psi_0(x, y, p, q) = 0 = D_y \psi_0(x, y, p, q) \text{ on } \partial \mathbb{R}^2_0
\]

since \(\psi_0\) satisfies the Neumann boundary condition.

The \(\psi^{inc}(x, y, p, q) = \frac{1}{2\pi} e^{i(px - qy)}\) represents a plane wave incident on the plane boundary in the direction \((p, -q)\), while the \(\psi^{sc}(x, y, p, q) = \frac{1}{2\pi} e^{i(px + qy)}\) represents the reflection by a grating of a plane wave propagating in the direction \((p, q)\).

Note that

\[
\psi^{inc}(x + 2\pi, y, p, q) = e^{2\pi ip} \psi^{inc}(x, y, p, q).
\]
2) Rayleigh-Bloch Waves

A function $\psi$ is said to be a Rayleigh-Bloch (R-B) wave for $G$ if and only if there exist numbers $p \in \mathbb{R}$ and $\omega \geq 0$ such that

$$\psi(x + 2\pi, y) = e^{2\pi ip} \psi(x, y), \quad (6)$$

$$\Delta \psi + \omega^2 \psi = 0 \text{ in } G, \text{ and} \quad (7)$$

$$\psi(x, y) \text{is bounded in } G \quad (8)$$

The parameter $p$ is called the x-momentum and $\omega$ is called the frequency of the R-B wave. The x-momentum that satisfies $-\frac{1}{2} < p \leq \frac{1}{2}$ will be called the reduced x-momentum of $\psi$.

The property (6) is sometimes called quasi-periodicity or p-periodicity. It is equivalent to the property that

$$\psi(x, y) = e^{ipx} \phi(x, y) \text{ for all } (x, y) \in G$$

where

$$\phi(x + 2\pi, y) = \phi(x, y) \text{ for all } (x, y) \in G.$$  

(7) is the Helmholtz equation, and its solutions are known to be analytic functions. In particular, each R-B wave satisfies $\psi \in C^\infty(G)$. Hence, the function $\phi(x, y) \in C^\infty(G)$ and has period $2\pi$ in $x$ since $\mathbb{R}_h^2 \in G$. Then for $(x, y) \in \mathbb{R}_h^2$, $\psi$ has an expansion

$$\psi(x, y) = \sum_{l \in \mathbb{Z}} \psi_l(y)e^{i(px+lx)}.$$

The series converges absolutely and uniformly on compact subsets of $\mathbb{R}_h^2$. Moreover, we may differentiate $\psi$ term-by-term, and hence the partial derivatives of $\psi$ also have expansions of the same form and have the same convergence properties.
Recall that \( p^2 + q^2 = \omega^2(p, q) \). For \( y > h \), the coefficients \( \psi_i(y) \) must satisfy

\[
\psi_i''(y) + (\omega^2 - (p + l)^2)\psi_i(y) = 0.
\]

**Case 1:** \( \omega > |p + l| \).

Let \( p_i = p + l \), \( q_i^2 = \omega^2 - (p + l)^2 > 0 \), then we have the ordinary differential equation

\[
\psi_i''(y) + q_i^2\psi_i(y) = 0.
\]

So there exist constants \( c_i^+ \) and \( c_i^- \) such that

\[
\psi_i(y) = c_i^+e^{i\omega_i y} + c_i^-e^{-i\omega_i y},
\]

and hence

\[
\psi(x, y) = \sum_{l \in \mathbb{Z}} \psi_i(y)e^{i(p+l)x} = \sum_{l \in \mathbb{Z}} c_i^+e^{i(p+l)x+q_i y} + \sum_{l \in \mathbb{Z}} c_i^-e^{i(p+l)x-q_i y}.
\]

These two terms describe the plane waves propagating in the directions \((p_i, \pm q_i)\). Also, since \( p_i^2 + q_i^2 = \omega^2 \), these vectors lie on the circle of radius \( \omega \) with center at the origin and their x-components differ by integers.

If \( c_i^- = 0 \) for all \( l \) such that \( \omega > |p + l| \), then we obtain an **outgoing R-B wave** for \( G \), i.e,

\[
\psi^{+\infty}_{\omega}(x, y, p, q) = \sum_{l \in \mathbb{Z}} c_i^+e^{i(p+l)x+q_i y}.
\]

If \( c_i^+ = 0 \) for all \( l \) such that \( \omega > |p + l| \), then we have an **incoming R-B wave** for \( G \), i.e,

\[
\psi^{-\infty}_{\omega}(x, y, p, q) = \sum_{l \in \mathbb{Z}} c_i^-e^{i(p+l)x-q_i y}.
\]

If \( c_i^- = c_i^+ \) for all \( l \) such that \( \omega > |p + l| \), then \( \psi \) will be said to be an **R-B surface wave** for \( G \).
**Case 2:** $\omega < |p + l|$. Then $(p + l)^2 - \omega^2 > 0$ and

$$
\psi''_l(y) - ((p + l)^2 - \omega^2)\psi_l(y) = 0.
$$

Since $\psi(x)$ is assumed to be bounded in $G$, it follows that there exists constant $c_l$ such that

$$
\psi_l(y) = c_l e^{-((p+l)^2-\omega^2)^{1/2}y}
$$

and hence

$$
\psi(x, y) = \sum_{l \in \mathbb{Z}} c_l e^{-((p+l)^2-\omega^2)^{1/2}y} e^{i(p+l)x}.
$$

In the application to diffraction gratings, terms of this type will be interpreted as **surface waves**.

**Case 3:** $\omega = |p + l|$.

Then $\psi''_l(y) = 0$. In this limiting case, the boundedness condition (8) implies that there exists constant $c_l$ such that $\psi_l(y) = c_l$, and hence

$$
\psi(x, y) = \sum_{l \in \mathbb{Z}} c_l e^{i(p+l)x}.
$$

This describes a plane wave that propagates parallel to the grating; i.e., the grazing wave. These waves divide the plane waves in case 1 from the surface waves in case 2.

The frequencies \( \{\omega = |p + l| \mid l \in \mathbb{Z}\} \) are called the cut-off frequencies for R-B waves with x-momentum $p$.

Note that the plane waves $\psi_{l}^{inc}(x, y, p, q) = \frac{1}{2\pi} e^{i(px - qy)}$ and $\psi_{l}^{inc}(x, y, p, -q) = \frac{1}{2\pi} e^{i(px + qy)}$ are incoming and outgoing R-B waves, respectively, with x-momentum $p$ and frequency $\omega = \omega(p, q) = \sqrt{p^2 + q^2}$. The scattering of these waves by a grating will
produce outgoing and incoming R-B waves, respectively, with the same x-momentum \( p \) and frequency \( \omega \). This leads to the following

**Definition:** An outgoing R-B diffracted plane wave for \( A \) with momentum \( (p, q) \in \mathbb{R}_0^2 \) is a function \( \psi_+(x, y, p, q) \) such that

\[
\psi_+(x, y, p, q) = \psi^{inc}_+(x, y, p, q) + \psi^sc_+(x, y, p, q)
\]

where \( \psi^sc_+(x, y, p, q) \) is an outgoing R-B wave for \( G \).

Note that

\[
\psi_-(x, y, p, q) = \psi_+(x, y, -p, q).
\]

In the half plane \( \mathbb{R}_h^2 \) above the grating, the \((p_l, q_l) = (p + l, \sqrt{p^2 + q^2 - (p + l)^2}) \in \mathbb{R}_0^2 \) defines the momentum of the reflected plane wave of order \( l \). The R-B waves \( \psi_\pm \) has the expansion

\[
\psi_+(x, y, p, q) = \frac{1}{2\pi} e^{i(px - qy)} + \frac{1}{2\pi} \sum_{(p+l)^2 < p^2 + q^2} c_l^+(p, q)e^{i(p_l x + q_l y)} \\
+ \frac{1}{2\pi} \sum_{(p+l)^2 > p^2 + q^2} c_l^-(p, q)e^{i(p_l x) e^{-\sqrt{(p+l)^2 - p^2 - q^2}}}
\]

and

\[
\psi_-(x, y, p, q) = \frac{1}{2\pi} e^{i(px + qy)} + \frac{1}{2\pi} \sum_{(p+l)^2 < p^2 + q^2} c_l^-(p, q)e^{i(p_l x + q_l y)} \\
+ \frac{1}{2\pi} \sum_{(p+l)^2 > p^2 + q^2} c_l^+(p, q)e^{i(p_l x) e^{-\sqrt{(p+l)^2 - p^2 - q^2}}}
\]

Since \( \psi_-(x, y, p, q) = \overline{\psi_+(x, y, -p, q)} \), it follows that for all \((p, q) \in \mathbb{R}_0^2 \) and \( l \in \mathbb{Z} \),
\[ c_i^- (p, q) = c_i^+ (-p, q). \]

Note that \( \omega^2 (p_l, q_l) = p_l^2 + q_l^2 = p^2 + q^2 = \omega^2 (p, q) \), hence the wave frequency is preserved under scattering.

The terms in the second sum are surface waves for the grating since they propagate in the \( x \)-direction, parallel to the grating, and are exponentially decreasing functions in \( y \), except in the case \( \omega (p, q) = \sqrt{p^2 + q^2} = |p + l| \) for some \( l \in \mathbb{Z} \). These are precisely the cut-off frequencies.

We may rewrite the R-B waves \( \psi_\pm \) as

\[ \psi_\pm (x, y, p, q) = \psi_{\pm}^{\text{inc}} (x, y, p, q) + \psi_{\pm}^{\text{sc}} (x, y, p, q). \]

Hence we may express the R-B wave eigenfunctions for \( G \) as a perturbations of those for \( \mathbb{R}^2_0 \).