How can a reflection grating or a grating reflector be analyzed? Let us consider the simplest model of a reflection grating, a perfectly reflecting metal surface lying in the x-z plane, with parallel grooves running in the z direction, where the grooves are periodically spaced with period $a$. Let us specifically consider grooves with a triangular profile, so that the grating surface is like a staircase where each step has a height $a = p/2$. Let us introduce

$$x' = (x + y)/\sqrt{2} \quad \text{and} \quad y' = (-x + y)/\sqrt{2}. \quad (1)$$

Let the z axis be along one of the top edges of the grating, so that the surface of the grating is given by

$$y' = 0 \text{ for } -a/2 < x < 0,$$
$$x' = 0 \text{ for } 0 < x < a/2,$$
and $y' = -a' = -a/\sqrt{2}$ for $a/2 < x < a$.

Let us consider waves with angular repetency

$$k_0 = \omega/c, \quad (2)$$

and the case with incoming and reflected waves propagating in the x-y plane, so that we may limit our attention to the transverse magnetic (TM) case with $H_z = 0$ and a z-polarized field with

$$E_z (x, y, t) = \text{Re} \left[ \varphi (x, y) e^{-j\omega t} \right]. \quad (3)$$

Outside the metal, $\varphi$ satisfies the equation called the Helmholtz equation,

$$\left( \partial^2_x + \partial^2_y + k_0^2 \right) \varphi = 0. \quad (4)$$

With a perfectly reflecting metal, the E field parallel to the metal surface must vanish at the metal surface.

Since the structure is periodic in the x direction, there must be solutions of equation (4) that are Bloch waves propagating in the x direction,

$$\varphi(k_x, x, y) = \exp(ik_x x) u(k_x, x, y), \quad (5)$$

where $u(k_x, x, y)$ is periodic in the x direction, and $k_x$ is the x component of the Bloch vector lying in the x-y plane. For $y > 0$ we may then write

$$u(k_x, x, y) = \sum_{p=-\infty}^{+\infty} u_p(k_x, y) \exp(2\pi i px/a). \quad (6)$$

**Problem 1.**

Show that $\varphi(k_x, x, y)$ satisfies the Helmholtz equation, if the terms of the Fourier series (6) have the form

$$u_p(k_x, y) = \exp(i k_{yp} y) u_{p0}, \quad (7)$$

with $k_{yp} = \sqrt{k_0^2 - (k_x + 2p\pi/a)^2}. \quad (8)$
Problem 2

A real \( k_{yp} \) represents a propagating wave, whereas an imaginary \( k_{yp} \) represents an evanescent field, i.e., a field that decays or grows exponentially with increasing distance from the grating surface. A real \( k_{yp} \) as defined in (8) is positive and hence represents outgoing waves propagating away from the grating. To represent incoming waves propagating towards the grating, we need negative \( k_{yp} \).

The total field \( \varphi(k_x, x, y) \) above the grating (for \( y > 0 \)) has one single incoming plane wave

\[
\varphi_0(x, y) = \exp(ik_xx - ik_y0y)
\]

plus one reflected Bloch wave

\[
\varphi_+(k_x, x, y) = \sum_{p=-\infty}^{+\infty} u_{p+} \exp \left[ i(kx + 2\pi p/a)x + ik_{yp}y \right].
\]

The incoming wave (9) has an angle of incidence \( \theta \) given by

\[
sin \theta = k_x/k_0.
\]

\( k_{yp} \) as given by (8) is imaginary for all values of \( p \), except for a few values of \( p \) near zero. In addition to the propagating outgoing plane waves that we get for \( p \) near zero, we need terms in (10) with \( ik_{yp} < 0 \), to represent evanescent fields that ‘cling to’ the grating and decay exponentially as we go away from the grating, \( k_y0 \) is always real, and represents the directly reflected wave. If we have nonzero values of \( p \) that yield real \( k_{yp} \), we have more than one outgoing plane wave from the grating. The larger the frequency (or equivalently, the greater the grating period), the more values of \( p \) can be found with a real \( k_{yp} \), and the more orders of diffraction we get.

Let us first consider the low-frequency limit with \( k_0a \ll 1 \). Then \( k_{yp} \) is imaginary for all nonzero \( p \), there is no diffraction, and only one term is needed to describe the reflected waves. In addition we need one small contribution from the field inside the groove. A simple expression that has a form similar to \( \varphi_+(k_x, x, y) \), is zero at the metal surface, and satisfies the Helmholtz equation (4) is

\[
\varphi_-(x, y) = u_{1-} \sin(k_0x'/\sqrt{2}) \sin(k_0(y' + a')/\sqrt{2}) \approx u_{1-} k_{0}^{a'/2} (y' + a')/2.
\]

At any point on the x axis, \( \varphi \) and \( \partial \varphi/\partial y \) must be continuous if we cross the x axis in the y direction (for \( y = 0 \)).

Use this fact to set up a set of equations for the unknown coefficients \( u_{0+} \) and \( u_{1-} \). Do the field matching at \( x = a/2 \), and compute \( \varphi(x = a/2, y = 0) \). Find the phase shift that the reflected waves \( \varphi_+(k_x, x, y = 0) \) have relative to the incoming plane waves \( \varphi_0(x, y = 0) \).

Problem 3 (Matlab)

Let us finally consider the general case with many terms in the series expansions for the field, below and above the z-x plane. We would like to have the field inside a grating groove, in the triangular area defined by \( y < 0, x' > 0 \) and \( y' > -a' = -a/\sqrt{2} \), expressed as a series expansion similar to what we have for \( y > 0 \). There are many ways of doing this, but one possibility is to use Bessel functions of even order, centered in the bottom of the groove. This field satisfies the Helmholtz equation (4) and can be chosen to be zero at the metal surface:

\[
\varphi_-(x, y) = \sum_{q=1}^{\infty} u_{q-} J_{2q}(k_0r) \sin(2qy'),
\]
where

\[ r = \sqrt{(x - a/2)^2 + (y + a/2)^2} \quad \text{og} \quad \cos \varphi' = x'/r. \quad (14) \]

To solve such a field matching problem in Matlab, we must set up a set of linear equations to solve. To this end we require the field and the \( y \) derivative of the field to be the same in \( P \) equidistant points along the \( x \) axis, for the two series expansions (10) and (13).

Hint: A system of linear equations can be solved in Matlab with the help of the matrix divide operation.

To be specific, do the field matching in the seven points spaced a distance \( a/7 \) along the \( x \) axis, for \( x = a/14, 3a/14, 5a/14, \ldots, 13a/14 \), and include seven terms in the series expansion (13) for the field below the \( x-z \) plane. The last term in the expansion then has three and a half oscillations per period \( a \), and the next to last term has three oscillations. Over the \( x-z \) plane we must also have seven terms in the series expansion (10) for \( \varphi_+ (k_x, x, 0) \), and then we should include the terms with the greatest \( k_{yp}^2 \). Let \( p = p_0 \) be the value with the greatest \( k_{yp}^2 \). Then we have two terms in (10) with \( p = p_\pm = p_0 \pm 3 \) that both have three oscillations along the \( x \) axis inside the period \( a \), so we get about the same number of oscillations in the two series expansions (10) and (13), something we need to get good numerical results with few terms included in the series.

Do the calculation with an angle of incidence \( \theta = \pi/4 \), so that \( k_x = k_{y0} = k_0/\sqrt{2} \), and consider the two frequencies that make \( k_0 a' = \pi \) and \( k_0 a' = 2\pi \). Compute the seven coefficients \( u_{p+} \) and the seven \( u_{q-} \), and compare the results for the two frequencies. Please note that for frequencies such that \( k_0 a' \) is a large integer multiple of \( \pi \), the triangular grooves are perfectly spaced to reflect all of the light back towards the source, with no light in the zeroth order of diffraction (with no direct reflection from the grating).

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