# GRATINGS: THEORY AND NUMERIC APPLICATIONS

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ISBN: 978-2-8539-9860-4
www.fresnel.fr/numerical-grating-book

**ISBN: 978-2-8539-9860-4**

First Edition, 2012, Presses universitaires de Provence (PUP)

**World Wide Web:**

www.fresnel.fr/numerical-grating-book

Institut Fresnel, Université d'Aix-Marseille, CNRS
Faculté Saint Jérôme,
13397 Marseille Cedex 20,
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Gratings: Theory and Numeric Applications, Evgeny Popov, editor (Institut Fresnel, CNRS, AMU, 2012)

# Chapter 3:

# Spectral Methods for Gratings

John A. DeSanto

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# Chapter 3

# Spectral Methods for Gratings

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## Abstract

We present a unified formal treatment of spectral methods applied to scattering from penetrable gratings for both acoustic (scalar) and electromagnetic (vector) problems. These are derived from coordinate space representations for both acoustic problems for a one-dimensional grating, and full electromagnetic problems for a two-dimensional grating. The coordinate space representations are also derived here. By unified we mean that the electromagnetic results use a scalar analogy, in that the boundary unknowns are the electric field and its normal derivative.

In coordinate space, the kernels of either the integral representations or integral equations have two variables, the first relating to the field coordinate (which, for an integral equation, has been evaluated on the surface), and the second evaluated on the surface as part of the surface integration. We refer to this procedure as coordinate in both variables or simply a *CC* method. Partial spectral results involve a spectral replacement of the first coordinate variable, and we refer to these methods as *SC*. Full spectral methods involve an additional replacement of the second (always surface) coordinate variable by a spectral one and we refer to these as *SS* methods, or in the case of a conjugate Rayleigh basis as $SS^*$.

For both scalar and electromagnetic cases, the partial spectral results are derived without the use of Green's functions. Instead we use plane wave states in Green's theorem. The partial spectral results are also used to generate surface inversion methods involving perturbation theory and the Kirchhoff approximation. For the full spectral scalar case three spectral expansions are considered, a physical optics modified Fourier expansion, a Floquet-Fourier expansion, and an expansion in conjugate Rayleigh basis functions. All are Floquet- or quasi-periodic. For the full spectral electromagnetic case only the conjugate Rayleigh basis expansion is presented.

## 3.1 Introduction

In this paper we present formal equations in spectral space to describe the scattering from periodic surfaces or gratings. We do this both for the acoustic case in one dimension for the direct scattering problem (Secs.4,5,7) and the inverse problem(Sec.6), and in two dimensions for the general electromagnetic problem (Secs.9,10,11). In order to do this and justify the validity of the spectral representations in various regions, we derive in each case the coordinate-space representations for the scattering (Secs.4,9). This includes the two- and three-dimensional periodic Green's function (Sec.3) necessary to describe the coordinate-space scattering, and the development of plane wave expansions in periodic media (Sec.2) which are used throughout the paper.

For the partial spectral-space equations it is not necessary to use the Green's function. Instead we describe a method using plane waves and Green's theorem in the periodic cell of the surface to derive the spectral equations directly and simply. One can describe the coordinate-space integral representations or integral equations to solve the boundary unknowns as equations in two coordinate spaces, the space of the source or integrated coordinate, and the space of the field or exterior coordinate. For clarity, we refer to this as a coordinate-coordinate (CC) representation. Spectral can then refer to one or both of these coordinate spaces transformed, a partial spectral space when one is transformed (Secs.5,10) where we use first the transform of the exterior coordinate (following from the plane waves and Green's theorem) so we are in a spectral-coordinate (SC) representation which we treat extensively, including its use in the inverse problem, the problem of surface reconstruction from (known) scattered field data. A second version (CS) is referred to[93] but not extensively discussed. Using SC we can then represent the integrated coordinate in spectral space (SS) where we reference extensive computational results[36,37,38,39]. What has become of interest lately[3] is the transform of the coordinate-space of integration into the conjugate spectral space $S^{\star}$, and we describe this $SS^{\star}$ method extensively (Secs.8,11) for acoustic and electromagnetic results respectively. Formally this is equivalent to a dual least squares method.

It is important to define what we mean by the word "spectral"[28]. In a general context, this could mean just Fourier space, and boundary function expansions in pure Fourier series. However, in our context, this is not correct. The reason is that the boundary fields are limits of Floquet- or quasi-periodic functions and must themselves be Floquet- or quasi-periodic. This reflects the nature of the incident field being, in general, incident off the normal. The periodic surface has right-left symmetry, but the boundary value problem does not (unless the field is incident normally). By "spectral" we thus mean here three kinds of expansions, a physical-optics modified Fourier expansion (Sec.7) where a single plane wave modulates the Fourier series, an expansion which we term Floquet-Fourier which preserves the quasi-periodicity but without the modulating plane wave (Sec.7), and an expansion in conjugate plane wave states on the boundary (Secs.8,11) where plane waves modulate each term in the expansion. These latter are Rayleigh or Bloch wave type expansions and are useful because, at least in some degenerate cases, they lead to self-adjoint problems. All expansions are quasi-periodic. Relation of the results to Rayleigh and Waterman expansions is discussed.

Using the partial spectral methods developed in Sec.5 for the direct scattering problem, we discuss in Sec.6 how they can be used to find the periodic surface profile from the incident and scattered fields. Two methods are presented, one based on perturbation theory and the other on the Kirchhoff approximation, both for the scalar case. Both surface inversion methods were initially applied to truncated random surfaces[111,112] with good results, and the methodology is here applied to gratings.

The electromagnetic equations we present are not done in the conventional formalism[61] using boundary currents, but are based on earlier work of ours[35] which rely on a scalar analogue of the electromagnetic problem, so the boundary unknowns we use are the electric field and its normal derivative. The resulting equations become a direct scalar analogue in terms of different boundary unknowns for the electromagnetic problem. We also do not discuss the computational solutions of the equations but rely on references where available. Some related equations have been solved, and we point out the references where appropriate, but a full discussion of computational issues would require a separate paper.

A very large number of references are cited in the text. Many of these references, some not specifically attuned to spectral methods, nevertheless contain spectral components in the development or in reference to expansions, in particular to the Rayleigh expansion[11,12,14,48,50,54,56,57,64,66,70,76,80,81,82,94,99,100,104], the Waterman expansion[105], both[4,5,23,24,109], or a combination of the two expansions[62]. The gratings we consider are infinite, although spectral methods have been applied to finite gratings also[84], and our gratings are purely deterministic although random gratings have also been considered[83]. Newer results on gratings apply surface integral methods to periodic nanostructures[43], indicating the generality of the methods we describe. We are mainly interested in scattering methods which produce the scattered and transmitted fields and their use in inversion, although others prefer to consider the dispersion relation for surface plasmons and polaritons propagating along the grating[46,47,63]. Other rigorous theoretical and computational developments are also available[2,6,7,8,16,44,45,49,67,68,77,78,79,87,92,96,113], as well as approximations[65,110], applications[9,13,42,51,71,75], and other methodology[1,85].

There are very many papers (our many references do not scratch the surface), reviews[10,40,69,88,89,91,98] and books[52,103,108] on scattering from gratings, not the least of them being the important book edited by Petit[90] in honor of which this paper is contributed.

## 3.2 Plane Waves in Periodic Media

In two dimensions $\vec{x} = (x,z)$, we write a plane wave as

$$\phi(\vec{x}) = \exp[ik(\alpha_0 x + \gamma_0 z)], \tag{3.1}$$

where $\alpha_0 = \sin(\theta)$, $\gamma_0 = \cos(\theta) = \sqrt{1-\alpha_0^2}$, and $\theta$ is measured clockwise from the positive $z$ axis. With the time convention $\exp(-i\omega t)$, where $\omega$ is circular frequency, this is thus an up-going plane wave, and satisfies the two-dimensional Helmholtz equation

$$(\nabla_2^2 + k^2)\phi(\vec{x}) = 0, \tag{3.2}$$

where $k$ is the wavenumber (here considered to be strictly real). On a one-dimensional surface $z = h(x)$ we have

$$\phi(\vec{x}_h) = \exp[ik(\alpha_0 x + \gamma_0 h(x))], \tag{3.3}$$

where $\vec{x}_h = (x, h(x))$. This is referred to as a Rayleigh function. For one-dimensional periodic media (here the surface), $h(x+L) = h(x)$, where $L$ is the period, we have the relation

$$\phi(x+L, h(x+L)) = \exp(ik\alpha_0 L)\phi(x, h(x)). \tag{3.4}$$

The same result is true even off the surface, i.e.

$$\phi(x+L, z) = \exp(ik\alpha_0 L)\phi(x,z). \tag{3.5}$$

These results are referred to as Floquet- or quasi-periodicity. The field scattered from this periodic surface, $\psi^{sc}$, satisfies the same Helmholtz equation, and is also quasi-periodic because the ratio $\frac{\psi^{sc}}{\phi}$ is periodic, i.e.

$$\frac{\psi^{sc}(x+L,z)}{\phi(x+L,z)} = \frac{\psi^{sc}(x,z)}{\phi(x,z)}, \tag{3.6}$$

so that

$$\psi^{sc}(x+L,z) = \exp(ik\alpha_0 L)\psi^{sc}(x,z), \tag{3.7}$$

and the same is true on the surface $z = h(x)$. In general for any field function $\psi$ satisfying (3.2) and shifted an integer $n$ number of periods we have

$$\psi(x+nL,z) = \exp(ik\alpha_0 nL)\psi(x,z). \tag{3.8}$$

The same is of course true on the surface $z = h(x)$.

In three dimensions any field function which satisfies the three-dimensional Helmholtz equation

$$(\nabla_3^2 + k^2)\psi(\vec{x}) = 0, \tag{3.9}$$

where $\vec{x} = (x,y,z)$, and is quasi-periodic in $x$ with period $L_1$ and in $y$ with period $L_2$ satisfies

$$\psi(x+n_1L_1, y+n_2L_2, z) = \exp[ik(\alpha_0 n_1 L_1 + \beta_0 n_2 L_2)]\psi(x,y,z), \tag{3.10}$$

where $\alpha_0 = \sin(\theta)\cos(\varphi)$ and $\beta_0 = \sin(\theta)\sin(\varphi)$ with $\theta$ the polar angle, $\varphi$ the azimuthal angle, and $n_1$ and $n_2$ are integers. In three dimensions the up-going plane wave is now written as

$$\phi(\vec{x}) = \exp[ik(\alpha_0 x + \beta_0 y + \gamma_0 z)], \tag{3.11}$$

where $\gamma_0 = \sqrt{1-\alpha_0^2-\beta_0^2}$. Although we use some of the same notation in both two and three dimensions the interpretation will be clear from the context.

We consider the periodic surface $z = h(x)$ in one dimension and $z = h(x,y) = h(\vec{x}_\perp)$ in two dimensions which separates two media with wavenumbers $k_1$ for $z > h$ (the upper region 1) and $k_2$ for $z < h$ (the lower region 2). Notationally, subscripts are used to identify the region, e.g. $\phi$ becomes $\phi_1$ or $\phi_2$, $\gamma_0$ becomes $\gamma_{10}$ or $\gamma_{20}$, etc. The paper has a lot of notation, and we have tried to keep it as clear as possible.

### 3.3 Green's Functions in Periodic Media

In two dimensions the free-space Green's function is

$$G^{(2)}(\vec{x}',\vec{x}) = \frac{i}{4}H_0^{(1)}(k_0|\vec{x}'-\vec{x}|), \tag{3.12}$$

where $H_0^{(1)}$ is the Hankel function, and $k_0$ is a generic wave number. It satisfies the equation

$$(\nabla_2^2 + k_0^2)G^{(2)}(\vec{x}',\vec{x}) = -\delta(\vec{x}'-\vec{x}). \tag{3.13}$$

Its representation as a Fourier transform is

$$G^{(2)}(\vec{x}',\vec{x}) = \frac{1}{(2\pi)^2}\iint \frac{\exp[ik_x(x'-x)+ik_z(z'-z)]}{k^2-k_{0+}^2}dk_x dk_z, \tag{3.14}$$

where the integrals run from $-\infty$ to $\infty$. We have given $k_0$ a small positive imaginary part to define the integral, and $k^2 = k_x^2 + k_z^2$. If we choose a specific direction, here the fixed direction $z$, we can evaluate the $k_z$ integration using complex variables. The result is the Weyl representation[34] for $G^{(2)}$

$$G^{(2)}(\vec{x}',\vec{x}) = \frac{i\pi}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{\exp[ik_x(x'-x)+iK_0|z'-z|]}{K_0}dk_x, \tag{3.15}$$

where $K_0 = \sqrt{k_0^2 - k_x^2}$ for $k_0^2 > k_x^2$, and $= i\sqrt{k_x^2 - k_0^2}$ for $k_x^2 > k_0^2$.

We have two regions. In region 1, we let $k_0 = k_1$ in (3.15), scale the integral using $k_x = k_1\alpha$, and we get the Green's function for region 1 (subscript) in (2)-dimensions (superscript)

$$G_1^{(2)}(\vec{x}',\vec{x}) = \frac{i\pi}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{\exp[ik_1(\alpha(x'-x)+\gamma_1(\alpha)|z'-z|)]}{\gamma_1(\alpha)}d\alpha, \tag{3.16}$$

where

$$\gamma_1(\alpha) = \sqrt{1-\alpha^2}, \quad (\alpha^2 < 1) \tag{3.17}$$

$$= +i\sqrt{\alpha^2-1}, \quad (\alpha^2 > 1). \tag{3.18}$$

In region 2, let $k_0 = k_2$ in (3.15) and scale using $k_x = k_1\alpha$ (the same scaling as in region 1) to get the Green's function in region 2 (subscript) in (2)-dimensions (superscript)

$$G_2^{(2)}(\vec{x}',\vec{x}) = \frac{i\pi}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{\exp[ik_1(\alpha(x'-x)+\gamma_2(\alpha)|z'-z|)]}{\gamma_2(\alpha)}d\alpha, \tag{3.19}$$

where

$$\gamma_2(\alpha) = \sqrt{K^2-\alpha^2}, \quad (\alpha^2 < K^2) \tag{3.20}$$

$$= +i\sqrt{\alpha^2-K^2}, \quad (\alpha^2 > K^2), \tag{3.21}$$

and $K = k_2/k_1$, the ratio of wavenumbers. The same scaling in both regions can be thought of as simply a result of Snell's Law since the $x$-components of the phases of both functions must match at a flat interface.

The Green's functions above are for an infinite space or, in our case, an infinite surface. To find the periodic Green's function for a single cell of the surface we use the single or double layer potentials which occur in Sec.4. For example, define the single layer potential on an infinite surface $h(x)$ as

$$(S\psi)(\vec{x}_h') = \int_{-\infty}^{\infty} G^{(2)}(\vec{x}_h',\vec{x}_h)\psi(\vec{x}_h)dx, \tag{3.22}$$

where $\psi$ is any field function (here it is the normal derivative). The result can be written as a sum over periodic cells

$$(S\psi)(\vec{x}_h') = \sum_{n=-\infty}^{\infty} I_n(x'), \tag{3.23}$$

where

$$I_n(x') = \int_{(2n-1)L/2}^{(2n+1)L/2} G^{(2)}(\vec{x}_h',\vec{x}_h)\psi(\vec{x}_h)dx. \tag{3.24}$$

Use (3.16) or (3.19) in (3.24), shift the integration by defining $x'' = x - nL$, and use the Floquet property of the field function to rewrite (3.22) as

$$(S\psi)(\vec{x}_h') = \int_{-L/2}^{L/2} G^{(2p)}(\vec{x}_h',\vec{x}_h)\psi(\vec{x}_h)dx, \tag{3.25}$$

where the two-dimensional periodic Green's function ($(2p)$-superscript) is given by

$$G^{(2p)}(\vec{x}'_h,\vec{x}_h) = \frac{i\pi}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{\exp[ik_1(\alpha(x'-x)+\gamma(\alpha)|h(x')-h(x)|)]}{\gamma(\alpha)}S(\alpha)d\alpha, \tag{3.26}$$

where the sum $S$ is given by

$$S(\alpha) = \sum_{n=-\infty}^{\infty}\exp[ink_1L(\alpha_0-\alpha)], \tag{3.27}$$

and can be evaluated using the Poisson sum[95] to be

$$S(\alpha) = \frac{2\pi}{ik_1}\sum_{j=-\infty}^{\infty}\delta(\alpha-\alpha_j), \tag{3.28}$$

where $\delta$ represents the delta function and $\alpha_j = \alpha_0 + j\lambda/L$ is the grating equation. The result substituted in (3.26) yields the periodic Green's function for region 1

$$G_1^{(2p)}(\vec{x}'_h,\vec{x}_h) = \frac{i}{2k_1L}\sum_{j=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\gamma_{1j}|h(x')-h(x)|)]}{\gamma_{1j}}, \tag{3.29}$$

where

$$\gamma_{1j} = \sqrt{1-\alpha_j^2}, \quad (\alpha_j^2 < 1), \tag{3.30}$$

$$= +i\sqrt{\alpha_j^2-1}, \quad (\alpha_j^2 > 1), \tag{3.31}$$

and the periodic Green's function for region 2

$$G_2^{(2p)}(\vec{x}'_h,\vec{x}_h) = \frac{i}{2k_1L}\sum_{j=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\gamma_{2j}|h(x')-h(x)|)]}{\gamma_{2j}}, \tag{3.32}$$

where

$$\gamma_{2j} = \sqrt{K^2-\alpha_j^2}, \quad (\alpha_j^2 < K^2) \tag{3.33}$$

$$= +i\sqrt{\alpha_j^2-K^2}, \quad (\alpha_j^2 > K^2). \tag{3.34}$$

We have listed the Green's functions of both regions to stress the exterior scaling $k_1$ for both. The result is the residual of the $k_1$ in the phase of both terms, Snell's law, and the same Poisson sum.

The Green's functions satisfy the differential equations

$$(\nabla_2^2 + k_l^2)G_l^{(2p)}(\vec{x}',\vec{x}) = -\sum_{n=-\infty}^{\infty}\delta(x'-x_n)\delta(z'-z), \tag{3.35}$$

where $x_n = x + nL$ and $l = 1,2$. The periodic Green's function can also be written as a phased array of Hankel functions, e.g. for region 1

$$G_1^{(2p)}(\vec{x}',\vec{x}) = \frac{i}{4}\sum_{n=-\infty}^{\infty}\exp(ik_1\alpha_0 nL)H_0^{(1)}(k_1\sqrt{(x'-x_n)^2+(z'-z)^2}). \tag{3.36}$$

The periodic Green's functions are also Floquet-periodic. For either Green's function, using (3.29) or (3.32) we have that

$$G^{(2p)}(\vec{x}',\vec{x}_n) = \exp(-ik_1\alpha_0 nL)G^{(2p)}(\vec{x}',\vec{x}), \tag{3.37}$$

where $\vec{x}_n = \vec{x} + \hat{i}nL$. Since the Floquet condition on any field function (3.8) has the conjugate phase of (3.37), the product of any Green's function times any field function $\psi$ is periodic,

$$G^{(2p)}(\vec{x}',\vec{x}_n)\psi(\vec{x}_n) = G^{(2p)}(\vec{x}',\vec{x})\psi(\vec{x}). \tag{3.38}$$

This result will be used later to cancel vertical integrals in Green's theorem for the coordinate-space representation.

The three-dimensional Green's function in free space is given by

$$G^{(3)}(\vec{x}',\vec{x}) = \frac{1}{4\pi}\frac{\exp(ik_0|\vec{x}'-\vec{x}|)}{|\vec{x}'-\vec{x}|}, \tag{3.39}$$

where $k_0$ is a generic wave number. It satisfies the equation

$$(\nabla_3^2 + k_0^2)G^{(3)}(\vec{x}',\vec{x}) = -\delta(\vec{x}'-\vec{x}), \tag{3.40}$$

where $\vec{x} = (x,y,z)$. Its Fourier representation is

$$G^{(3)}(\vec{x}',\vec{x}) = \frac{1}{(2\pi)^3}\iiint \frac{\exp[ik_x(x'-x)+ik_y(y'-y)+ik_z(z'-z)]}{k^2-k_{0+}^2}dk_x dk_y dk_z, \tag{3.41}$$

with $k^2 = k_x^2 + k_y^2 + k_z^2$. Use complex integration on the preferred $z$-direction to yield

$$G^{(3)}(\vec{x}',\vec{x}) = \frac{i\pi}{(2\pi)^3}\iint \frac{\exp[ik_x(x'-x)+ik_y(y'-y)+iK_0|z'-z|]}{K_0}dk_x dk_y, \tag{3.42}$$

where

$$K_0 = \sqrt{k_0^2-k_x^2-k_y^2}, \quad (k_x^2+k_y^2<k_0^2) \tag{3.43}$$

$$= +i\sqrt{k_x^2+k_y^2-k_0^2}, \quad (k_x^2+k_y^2>k_0^2). \tag{3.44}$$

In the upper region, let $k_0 = k_1$ in (3.42), and scale the wavenumbers as $k_x = k_1\alpha$ and $k_y = k_1\beta$. This yields the three-dimensional Green's function for region 1 in the Weyl representation

$$G_1^{(3)}(\vec{x}',\vec{x}) = \frac{i\pi k_1}{(2\pi)^3}\iint \frac{\exp[ik_1(\alpha(x'-x)+\beta(y'-y)+\gamma_1(\alpha,\beta)|z'-z|)]}{\gamma_1(\alpha,\beta)}d\alpha d\beta, \tag{3.45}$$

where

$$\gamma_1 = \sqrt{1-\alpha^2-\beta^2}, \quad (\alpha^2+\beta^2<1), \tag{3.46}$$

$$= +i\sqrt{\alpha^2+\beta^2-1}, \quad (\alpha^2+\beta^2>1). \tag{3.47}$$

In the lower region, let $k_0 = k_2$ in (3.42), scale the wavenumbers the same (two-dimensional Snell's law) to yield the three-dimensional Green's function for region 2 in the Weyl representation

$$G_2^{(3)}(\vec{x}',\vec{x}) = \frac{i\pi k_1}{(2\pi)^3}\iint \frac{\exp[ik_1(\alpha(x'-x)+\beta(y'-y)+\gamma_2(\alpha,\beta)|z'-z|)]}{\gamma_2(\alpha,\beta)}d\alpha d\beta, \tag{3.48}$$

where

$$\gamma_2 = \sqrt{K^2-\alpha^2-\beta^2}, \quad (\alpha^2+\beta^2<K^2), \tag{3.49}$$

$$= +i\sqrt{\alpha^2+\beta^2-K^2}, \quad (\alpha^2+\beta^2>K^2). \tag{3.50}$$

The above results are for an infinite surface. To illustrate the reduction to a single cell of a two-dimensional periodic surface we choose a single layer potential (for either region) with density $\psi$ which is any field function (here the normal derivative of the velocity potential)

$$(S\psi)(\vec{x}'_h) = \iint_{-\infty}^{\infty} G^{(3)}(\vec{x}'_h,\vec{x}_h)\,\psi(\vec{x}_h)dxdy. \tag{3.51}$$

Here the surface is doubly periodic (period $L_1$ in $x$ and $L_2$ in $y$)

$$h(\vec{x}_\perp+\vec{x}_{n_1n_2}) = h(\vec{x}_\perp), \tag{3.52}$$

where $n_1$ and $n_2$ are integers and $\vec{x}_{n_1n_2} = \hat{i}n_1L_1+\hat{j}n_2L_2$. The field function is Floquet-periodic in two dimensions, see (3.10). We can thus write (3.51) as a double sum over periodic cells

$$(S\psi)(\vec{x}'_h) = \sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty} I_{n_1n_2}(\vec{x}'_h), \tag{3.53}$$

where

$$I_{n_1n_2}(\vec{x}'_h) = \int_{(2n_2-1)L_2/2}^{(2n_2+1)L_2/2}\int_{(2n_1-1)L_1/2}^{(2n_1+1)L_1/2} G^{(3)}(\vec{x}'_h,\vec{x}_h)\,\psi(\vec{x}_h)dxdy. \tag{3.54}$$

Use the Weyl representation (3.45) or (3.48) for $G^{(3)}$, shift the integrations using $x''=x-n_1L_1$ and $y''=y-n_2L_2$ to yield

$$(S\psi)(\vec{x}'_h) = \int_{-L_2/2}^{L_2/2}\int_{-L_1/2}^{L_1/2} G^{(3p)}(\vec{x}'_h,\vec{x}_h)\,\psi(\vec{x}_h)dxdy, \tag{3.55}$$

where the three-dimensional periodic Green's function is given by

$$G^{(3p)}(\vec{x}'_h,\vec{x}_h) = \frac{i\pi k_1}{(2\pi)^3}\iint \frac{\exp[ik_1(\alpha(x'-x)+\beta(y'-y)+\gamma|h(\vec{x}'_\perp)-h(\vec{x}_\perp)|)]}{\gamma(\alpha,\beta)}P_1P_2\,d\alpha d\beta, \tag{3.56}$$

with the Poisson sums

$$P_1(\alpha) = \sum_{n_1=-\infty}^{\infty}\exp[in_1k_1L_1(\alpha_0-\alpha)] = \frac{2\pi}{k_1L_1}\sum_{j=-\infty}^{\infty}\delta(\alpha_j-\alpha), \tag{3.57}$$

and

$$P_2(\beta) = \sum_{n_2=-\infty}^{\infty}\exp[in_2k_1L_2(\beta_0-\beta)] = \frac{2\pi}{k_1L_2}\sum_{j'=-\infty}^{\infty}\delta(\beta_{j'}-\beta). \tag{3.58}$$

The grating equations are now $\alpha_j = \alpha_0 + j\lambda/L_1$ and $\beta_{j'} = \beta_0 + j'\lambda/L_2$. The result is the three-dimensional periodic Green's function for region 1 with both coordinates on the surface

$$G_1^{(3p)}(\vec{x}'_h,\vec{x}_h) = \frac{i}{2k_1L_1L_2}\sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\beta_{j'}(y'-y)+\gamma_{1jj'}|h(\vec{x}'_\perp)-h(\vec{x}_\perp)|)]}{\gamma_{1jj'}}, \tag{3.59}$$

where

$$\gamma_{1jj'} = \sqrt{1-\alpha_j^2-\beta_{j'}^2}, \quad (\alpha_j^2+\beta_{j'}^2 < 1) \tag{3.60}$$

$$= +i\sqrt{\alpha_j^2+\beta_{j'}^2-1}, \quad (\alpha_j^2+\beta_{j'}^2 > 1). \tag{3.61}$$

The three-dimensional periodic Green's function for region 2 is given by

$$G_2^{(3p)}(\vec{x}_h',\vec{x}_h) = \frac{i}{2k_1L_1L_2}\sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\beta_{j'}(y'-y)+\gamma_{2jj'}|h(\vec{x}_\perp')-h(\vec{x}_\perp)|)]}{\gamma_{2jj'}}, \tag{3.62}$$

where

$$\gamma_{2jj'} = \sqrt{K^2-\alpha_j^2-\beta_{j'}^2}, \quad (\alpha_j^2+\beta_{j'}^2 < K^2) \tag{3.63}$$

$$= +i\sqrt{\alpha_j^2+\beta_{j'}^2-K^2}, \quad (\alpha_j^2+\beta_{j'}^2 > K^2). \tag{3.64}$$

We use these Green's functions later for three-dimensional electromagnetic problems. Note again that the scaling is $k_1$ in front of both (3.59) and (3.62). Note also the obvious remark that for a two-dimensional surface $h(\vec{x}_\perp)$ we have two spectral parameters, $j$ and $j'$.

Both Green's functions satisfy a two-dimensional Floquet condition

$$G^{(3p)}(\vec{x}_h',\vec{x}_h+\vec{x}_{n_1n_2}) = \exp[-ik_1(\alpha_0n_1L_1+\beta_0n_2L_2)]G^{(3p)}(\vec{x}_h',\vec{x}_h). \tag{3.65}$$

Combined with the two-dimensional Floquet condition on any field function (3.10), the product of any Green's function times a field function is periodic

$$G^{(3p)}(\vec{x}_h',\vec{x}_h+\vec{x}_{n_1n_2})\psi(\vec{x}_h+\vec{x}_{n_1n_2}) = G^{(3p)}(\vec{x}_h',\vec{x}_h)\psi(\vec{x}_h). \tag{3.66}$$

We use this property later to cancel side integrals in Green's theorem. Techniques for computing these periodic Green's functions are available[101,102].

### 3.4 Integral Methods in Coordinate Space for Scalar Problems

We first present the coordinate-space representation of the scattering from a periodic surface as comparison and contrast to that of the spectral representations in later sections. In addition, these yield rigorous representations for the scattered field above the highest surface excursion and for the transmitted field below the lowest surface excursion, as well as projections on lines above and below the surface.

The total field in region 1, $\psi_1$, equals the sum of incident plus scattered fields, $\psi_1 = \psi^{in}+\psi^{sc}$, and it satisfies the scalar Helmholtz equation

$$(\nabla_2^2+k_1^2)\psi_1(\vec{x}) = 0, \tag{3.67}$$

as do both incident and scattered fields. We do Green's theorem using $\psi_1$ and $G_1^{(2p)}$. Cross multiply (3.67) and (3.35), multiply by the characteristic function of region 1

$$\Theta_1(\vec{x}) = \theta(L/2-x)\theta(x+L/2)\theta(z-h(x))\theta(H_1-z), \tag{3.68}$$

where $\theta$ is the step function, $\theta(x) = 1$ when $x > 0$, and $\theta(x) = 0$ when $x < 0$, and integrate by parts. To express the results conveniently, introduce the bracket notation

$$[G_1^{(2p)}, \psi_1; \vec{x}', S] = \iint_S [G_1^{(2p)}(\vec{x}', \vec{x}_S)\partial_l \psi_1(\vec{x}_S) - \partial_l G_1^{(2p)}(\vec{x}', \vec{x}_S)] n_l ds, \tag{3.69}$$

where $\partial_l$ is the partial derivative ($\partial_x$ for $l = 1$ and $\partial_z$ for $l = 2$), $n_l$ is the non-unit surface normal, and $ds$ the arc length along the surface. Repeated subscripts are summed. There are four surfaces $S$: $x = \pm L/2$ ($h < z < H_1$), $z = h$, and $z = H_1$, both with $-L/2 < x < L/2$. The result is

$$\psi_1(\vec{x}')\Theta_1(\vec{x}') = [G_1^{(2p)}, \psi_1; \vec{x}', L/2] - [G_1^{(2p)}, \psi_1; \vec{x}', -L/2] + [G_1^{(2p)}, \psi_1; \vec{x}', H_1] - [G_1^{(2p)}, \psi_1; \vec{x}', h]. \tag{3.70}$$

Using (3.38), the first two brackets on the right hand side of (3.70) cancel by Floquet periodicity. For the moment assume the integral on $H_1$ represents the incident field (proof below), i.e.

$$\psi^{in}(\vec{x}') = [G_1^{(2p)}, \psi_1; \vec{x}', H_1]. \tag{3.71}$$

We thus have three results. Inside region 1, $h(x') < z' < H_1$, $\Theta_1 = 1$, we have

$$\psi_1(\vec{x}') = \psi^{in}(\vec{x}') - [G_1^{(2p)}, \psi_1; \vec{x}', h]. \tag{3.72}$$

Outside region 1, where $\Theta_1 = 0$, we have from (3.70)

$$\psi^{in}(\vec{x}') = [G_1^{(2p)}, \psi_1; \vec{x}', h], \tag{3.73}$$

which is an Extinction Theorem, and on the surface $z' = h(x')$, taking into account the discontinuity of the double layer potential in (3.72), we have

$$\frac{1}{2}\psi_1(\vec{x}'_h) = \psi^{in}(\vec{x}'_h) - [G_1^{(2p)}, \psi_1; \vec{x}'_h, h]. \tag{3.74}$$

In particular, we can write the scattered field above the highest surface excursion, $z' > max(h)$, using (3.72). The absolute value in the Green's function in (3.72) is not present, i.e. we use the representation

$$G_1^{(2p)}(\vec{x}', \vec{x}_h) = \frac{i}{2k_1 L} \sum_{j=-\infty}^{\infty} \frac{\exp[ik_1(\alpha_j(x'-x) + \gamma_{1j}(z' - h(x)))]}{\gamma_{1j}}. \tag{3.75}$$

The result is that the scattered field above the highest surface excursion can be written exactly as a plane wave expansion of upgoing waves

$$\psi^{sc}(\vec{x}') = \sum_{j=-\infty}^{\infty} A_j \exp[ik_1(\alpha_j x' + \gamma_{1j} z')], \tag{3.76}$$

where $A_j$ can be written as the integral

$$A_j = \frac{1}{L}\int_{-L/2}^{L/2} A(j,x) \exp[-ik_1(\alpha_j x + \gamma_{1j} h(x))] dx, \tag{3.77}$$

and the integrand $A(j,x)$ is in terms of the boundary unknowns

$$A(j,x) = \frac{-i}{2k_1\gamma_{1j}}\left\{\frac{\partial\psi_1}{\partial n}(\vec{x}_h) + ik_1(\gamma_{1j} - \alpha_j h'(x))\psi_1(\vec{x}_h)\right\}. \tag{3.78}$$

We have written $A(j,x)$ as a function of two variables, the first a discrete spectral (S) variable $j$ which has replaced the field coordinate variable, and the second a continuous coordinate (C) variable $x$, which is the surface integration variable. This is the basis for the spectral-coordinate (SC) approach used in Sec. 5.

There remains to prove (3.71). This time the representation for the Green's function evaluated on $z = H_1$ is with $\vec{x}_1 = (x, H_1)$

$$G_1^{(2p)}(\vec{x}', \vec{x}_1) = \frac{i}{2k_1 L}\sum_{j=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x) + \gamma_{1j}(H_1 - z'))]}{\gamma_{1j}}. \tag{3.79}$$

Using (3.79) in (3.71) and the representation (3.76) for the scattered field it is straighforward to show that

$$[G_1^{(2p)}, \psi^{sc}; \vec{x}', H_1] = 0. \tag{3.80}$$

Further, if we assume a general plane wave decomposition of the incident field in terms of downgoing waves

$$\psi^{in}(\vec{x}) = \sum_n I_n \exp[ik_1(\alpha_n x - \gamma_{1n} z)], \tag{3.81}$$

the relation

$$[G_1^{(2p)}, \psi^{in}; \vec{x}', H_1] = \psi^{in}(\vec{x}'), \tag{3.82}$$

follows immediately. Alternatively, one can view the integrand in (3.71)

$$\frac{\partial\psi_1}{\partial z}(x, H_1) - ik_1\gamma_{1j}\psi_1(x, H_1), \tag{3.83}$$

as projecting out only the downgoing waves and canceling the scattered waves. The combination of (3.80) and (3.82) is the proof of (3.71).

In the region below the surface, region 2, the total field $\psi_2$ satisfies the Helmholtz equation

$$(\nabla_2^2 + k_2^2)\psi_2(\vec{x}) = 0, \tag{3.84}$$

where the wavenumber $k_2 = Kk_1$ is written in terms of a scale factor $K$. The region is defined by the characteristic function

$$\Theta_2(\vec{x}) = \theta(L/2 - x)\theta(x + L/2)\theta(h(x) - z)\theta(z - H_2). \tag{3.85}$$

The Green's function $G_2^{(2p)}$ is given by

$$G_2^{(2p)}(\vec{x}', \vec{x}) = \frac{i}{2k_1 L}\sum_{j=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x) + \gamma_{2j}|z'-z|)]}{\gamma_{2j}}, \tag{3.86}$$

where $\gamma_{2j}$ is defined in (3.33). Green's theorem in this region, the cancellation of integrals along $x = \pm L/2$ by Floquet periodicity, and the vanishing of the integral along $H_2$ since at this value of $z$ the total field consists of downward propagating waves, yields the result

$$\psi_2(\vec{x}')\Theta_2(\vec{x}') = [G_2^{(2p)}, \psi_2; \vec{x}', h]. \tag{3.87}$$

On the boundary, the limit of (3.87) is

$$\frac{1}{2}\psi_2(\vec{x}'_h) = [G_2^{(2p)}, \psi_2; \vec{x}'_h, h]. \tag{3.88}$$

For $z' < min(h)$, (3.87) yields a representation of the total field in region 2 in terms of downward propagating plane waves

$$\psi_2(\vec{x}') = \sum_{j=-\infty}^{\infty} B_j \exp[ik_1(\alpha_j x' - \gamma_{2j} z')], \tag{3.89}$$

where

$$B_j = \frac{1}{L}\int_{-L/2}^{L/2} B(j,x)\exp[-ik_1(\alpha_j x - \gamma_{2j} h(x))]dx, \tag{3.90}$$

and $B(j,x)$ is in terms of the boundary values from region 2

$$B(j,x) = \frac{i}{2k_1\gamma_{2j}}\left\{\frac{\partial\psi_2(\vec{x}_h)}{\partial n} - ik_1(\gamma_{2j} + \alpha_j h'(x))\psi_2(\vec{x}_h)\right\}. \tag{3.91}$$

We have assumed that $\psi$ is a velocity potential. Then the continuity conditions at the boundary are written as the continuity of velocity

$$\frac{\partial\psi_2}{\partial n}(\vec{x}_h) = \frac{\partial\psi_1}{\partial n}(\vec{x}_h) \doteq N(\vec{x}_h), \tag{3.92}$$

and continuity of pressure

$$\rho_2\psi_2(\vec{x}_h) = \rho_1\psi_1(\vec{x}_h), \tag{3.93}$$

where $\rho_j$ are the densities. In (3.92) we defined the normal derivative boundary unknown as $N$, and we define the surface field boundary unknown as $\psi(\vec{x}_h) = \psi_1(\vec{x}_h)$, so that $\psi_2(\vec{x}_h) = \frac{1}{\rho}\psi(\vec{x}_h)$ where $\rho = \rho_2/\rho_1$. Using these unknowns, (3.78) and (3.91) become

$$A(j,x) = \frac{-i}{2k_1\gamma_{1j}}[N(\vec{x}_h) + ik_1(\gamma_{1j} - \alpha_j h'(x))\psi(\vec{x}_h)], \tag{3.94}$$

and

$$B(j,x) = \frac{i}{2k_1\gamma_{2j}}[N(\vec{x}_h) - \frac{ik_1}{\rho}(\gamma_{2j} + \alpha_j h'(x))\psi(\vec{x}_h)]. \tag{3.95}$$

We can summarize these results using single($S$) and double($D$) layer potentials

$$(S_j u)(\vec{x}') = \int_{-L/2}^{L/2} G_j^{(2p)}(\vec{x}', \vec{x}_h)u(\vec{x}_h)dx, \tag{3.96}$$

and

$$(D_j v)(\vec{x}') = \int_{-L/2}^{L/2} \frac{\partial G_j^{(2p)}}{\partial n}(\vec{x}', \vec{x}_h)v(\vec{x}_h)dx, \tag{3.97}$$

and write the integral equations (3.74) and (3.88) in symbolic form as

$$\frac{1}{2}\psi = \psi^{in} - (S_1 N) + (D_1\psi), \tag{3.98}$$

and

$$\frac{1}{2}\psi = \rho(S_2N) - (D_2\psi). \tag{3.99}$$

Various combinations of these equations and integral equations formed by first taking the normal derivative of the field representations (3.72) and (3.87) and passing to the surface limit can be used to solve for the boundary unknowns $\psi$ and $N$. For the Dirichlet problem, $\psi = 0$ and $\rho = 0$ so (3.99) disappears and (3.98) is an integral equation of first kind for $N$. For the Neumann problem, first divide (3.99) by $\rho$, then let $\rho \to \infty$ and set $N = 0$.

Direct integral equation methods have been used to computationally solve this problem[21,22,67]. Other integral equation solutions[36,37,38,39] have been compared to the solutions of spectral methods presented later in this paper. Other methods have also been employed[18,19,20,73,74,86]. Point collocation questions arise[10,25,53,60,72] for any coordinate based method.

### 3.5 Partial Spectral Methods for Scalar Problems

In this section we use a direct method to generate integral equations in a partial spectral representation. The method uses Green's theorem again, but not the Green's function. Define the up- and down-going plane wave states in region 1

$$\phi_{1j}^{\pm}(\vec{x}) = \exp[ik_1(-\alpha_j x \pm \gamma_{1j} z)], \tag{3.100}$$

which satisfy the same Helmholtz equation as $\psi_1$, (3.67),

$$(\nabla_2^2 + k_1^2)\phi_{1j}^{\pm}(\vec{x}) = 0. \tag{3.101}$$

For convenience, in (3.100) we have chosen the conjugate in the $x$-coordinate. In the Green's function this occurs naturally. Cross multiply (3.67) and (3.101) and subtract the results, multiply by $\Theta_1$ from (3.68), integrate over all space, and then integrate by parts. Since all fields are Floquet periodic, the integrals along $x = \pm L/2$ cancel. The results can be expressed with the collapsed bracket notation

$$[u, v; S] = \int_S [u(\vec{x}_S)\partial_l v(\vec{x}_S) - v(\vec{x}_S)\partial_l u(\vec{x}_S)] n_l ds, \tag{3.102}$$

where, unlike the bracket notation in Sec.4, no exterior coordinate-space variable appears. There are two surfaces, $z = h$ with $-L/2 < x < L/2$, and $z = H_1$ with $-L/2 < x < L/2$. The result is

$$[\phi_{1j}^{\pm}, \psi_1; h] = [\phi_{1j}^{\pm}, \psi_1; H_1]. \tag{3.103}$$

The result can be thought of as an analytic continuation from the periodic surface $z = h$ to a flat plane $z = H_1$ above the surface. The right hand side of (3.103) can be evaluated explicitly using (3.76) and (3.81) to give

$$[\phi_{1j}^{\pm}, \psi_1; H_1] = 2ik_1 L\gamma_{1j}\{{}^{-I_j}_{A_j}\}. \tag{3.104}$$

Here the up-going plane waves $\phi_{1j}^{+}$ project out the down-going spectral components of the incident wave $I_j$, and the down-going plane waves $\phi_{1j}^{-}$ project out the up-going spectral components of the scattered waves $A_j$. Combining this with the left hand side of (3.103) we get the set of equations for region 1

$$\frac{1}{L}\int_{-L/2}^{L/2} \phi_{1j}^{\pm}(\vec{x}_h) U_j^{\pm}(\vec{x}_h) dx = \gamma_{1j}\{{}^{-I_j}_{A_j}\}, \tag{3.105}$$

where

$$U_j^{\pm}(\vec{x}_h) = \frac{1}{2ik_1}[N(\vec{x}_h) - ik_1(\pm\gamma_{1j} + \alpha_j h'(x))\psi(\vec{x}_h)]. \quad (3.106)$$

We have incorporated the boundary unknowns defined following (3.92). Note that $U_j^- = \gamma_{1j}A(j,x)$ from (3.94).

In region 2, the up- and down-going plane waves are given by

$$\phi_{2j}^{\pm}(\vec{x}) = \exp[ik_1(-\alpha_j x \pm \gamma_{2j} z)], \quad (3.107)$$

which satisfy the Helmholtz equation

$$(\nabla_2^2 + k_2^2)\phi_{2j}^{\pm}(\vec{x}) = 0. \quad (3.108)$$

Cross multiply (3.84) and (3.108), multiply the result by $\Theta_2$ from (3.85), integrate over all space, then integrate by parts. The Floquet periodicity cancels the integrals on $x = \pm L/2$ and the result is the analytic continuation

$$[\phi_{2j}^{\pm}, \psi_2; h] = [\phi_{2j}^{\pm}, \psi_2; H_2]. \quad (3.109)$$

The right hand side of (3.109) can be evaluated using (3.89) for $\psi_2$ to yield

$$[\phi_{2j}^{\pm}, \psi_2; H_2] = -2ik_1 L\gamma_{2j}\left\{ {B_j \atop 0} \right\}. \quad (3.110)$$

Combined with (3.109), and incorporating the definitions of the boundary values following (3.92) yields the equations from the lower region

$$\frac{1}{L}\int_{-L/2}^{L/2} \phi_{2j}^{\pm}(\vec{x}_h) L_j^{\mp}(\vec{x}_h) dx = -\gamma_{2j}\left\{ {B_j \atop 0} \right\}. \quad (3.111)$$

where

$$L_j^{\pm}(\vec{x}_h) = \frac{1}{2ik_1}[N(\vec{x}_h) - \frac{ik_1}{\rho}(\pm\gamma_{2j} + \alpha_j h'(x))\psi(\vec{x}_h)]. \quad (3.112)$$

The lower equation in (3.111) is a spectral version of the Extinction Theorem.

The procedure is to solve the combined $U^+$ equation in (3.105) and the $L^-$ equation in (3.111) for the boundary unknowns $N$ and $\psi$, and to evaluate the $U^-$ and $L^+$ equations for the scattered ($A_j$) and transmitted ($B_j$) amplitudes. The scattered and transmitted fields can be then found from (3.76) and (3.89) respectively. In order to find field values in the surface wells, we must use these boundary unknowns in (3.72) and (3.87) respectively.

The advantage of the method is that there are no Green's functions to compute. Instead, the results are projected onto plane wave based basis functions (really Rayleigh functions since they're on the surface). The Green's function does this in an alternate way.

It is useful with any theory to check simple special cases. It is also necessary that the general results reduce to simple solvable cases. Here we take the flat surface limit ($h = 0$), and derive from them the Fresnel reflection and transmission coefficients as a necessary check on the general results. For $h = 0$, let $L \to \infty$, so that for any finite $j$, $\lim_{L\to\infty}\alpha_j = \alpha_0$, so that the only surviving waves are the $0^{th}$ order reflection ($A_0$) and transmission ($B_0$) amplitudes. The surface fields $N$ and $\psi$ thus have two different flat-surface field representations which are

$$\psi_1(x,0) = (I_0 + A_0)\exp[ik_1\alpha_0 x], \quad (3.113)$$

$$N_1(x,0) = -ik_1\gamma_{10}(I_0 - A_0)\exp[ik_1\alpha_0 x], \tag{3.114}$$

$$\psi_2(x,0) = B_0\exp[ik_1\alpha_0 x], \tag{3.115}$$

and

$$N_2(x,0) = -ik_1\gamma_{20}B_0\exp[ik_1\alpha_0 x]. \tag{3.116}$$

From (3.105) and (3.111) we have

$$A_0 = \frac{1}{2ik_1\gamma_{10}}\lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2}[N(x,0) + ik_1\gamma_{10}\psi(x,0)]\exp[-ik_1\alpha_0 x]dx, \tag{3.117}$$

and

$$B_0 = \frac{-1}{2ik_1\gamma_{20}}\lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2}[N(x,0) - \frac{ik_1}{\rho}\gamma_{20}\psi(x,0)]\exp[-ik_1\alpha_0 x]dx. \tag{3.118}$$

If we use the flat-surface field representations on the surface from region 1, ($N_1$ and $\psi_1$), in the $A_0$ equation, and the flat-surface field representations from region 2, ($N_2$ and $\psi_2$), in the $B_0$ equation, we just get identities. Instead, use the opposite procedure, i.e. write $A_0$ and $B_0$ as

$$A_0 = \frac{1}{2ik_1\gamma_{10}}\lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2}[N_2(x,0) + ik_1\gamma_{10}\psi_2(x,0)]\exp[-ik_1\alpha_0 x]dx, \tag{3.119}$$

and

$$B_0 = \frac{-1}{2ik_1\gamma_{20}}\lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2}[N_1(x,0) - \frac{ik_1}{\rho}\gamma_{20}\psi_1(x,0)]\exp[-ik_1\alpha_0 x]dx. \tag{3.120}$$

Using (3.113) through (3.116) in (3.119) and (3.120) we get two equations

$$A_0 = \frac{\rho\gamma_{10} - \gamma_{20}}{2\gamma_{10}}B_0, \tag{3.121}$$

and

$$B_0 = \frac{\gamma_{10}[I_0 - A_0] + (\gamma_{20}/\rho)[I_0 + A_0]}{2\gamma_{10}}. \tag{3.122}$$

These can be solved to yield the Fresnel reflection coefficient

$$\frac{A_0}{I_0} = \frac{\rho\gamma_{10} - \gamma_{20}}{\rho\gamma_{10} + \gamma_{20}}, \tag{3.123}$$

and the Fresnel transmission coefficient

$$\frac{B_0}{I_0} = \frac{2\gamma_{10}}{\rho\gamma_{10} + \gamma_{20}}. \tag{3.124}$$

Finally we have that

$$1 + \frac{A_0}{I_0} = \rho\frac{B_0}{I_0}, \tag{3.125}$$

as expected.

## 3.6 Surface Inversion Using the Partial Spectral Method

We can use the partial spectral results from Sec.5 to develop simple algorithms to reconstruct the surface height $h(x)$ from the knowledge of the incident and scattered field amplitudes $I_j$ and $A_j$. For simplicity, we choose the Dirichlet problem, $\psi(\vec{x}_h) = 0$. This is a perfectly reflecting case, and (3.111) vanishes identically (multiply it by $\rho$, and then set $\rho = 0$). The resulting equations (3.105) become

$$\frac{1}{L}\int_{-L/2}^{L/2} \phi_{1j}^{\pm}(\vec{x}_h)N(\vec{x}_h)dx = 2ik_1\gamma_{1j}\{{}^{-I_j}_{A_j}\}. \tag{3.126}$$

We describe two methods, the first is perturbation theory in the surface height, and the second is the use of the Kirchhoff approximation for the normal derivative $N$. The full details of both methods with numerical results were presented in[111,112]. There the methods were applied to truncated rough surfaces. Some other methods can be found in[59] for uniqueness questions and[17] for more detailed reconstruction algorithms.

For perturbation theory (3.100) is used on the surface, and becomes

$$\phi_{1j}^{\pm}(\vec{x}_h) \approx \exp[-ik_1\alpha_j x](1 \pm ik_1\gamma_{1j}h(x)). \tag{3.127}$$

Substituting (3.127) in (3.126), and adding and subtracting the resulting equations yields the two results

$$\frac{1}{L}\int_{-L/2}^{L/2} \exp[-ik_1\alpha_j x]N(\vec{x}_h)dx = -ik_1\gamma_{1j}(I_j - A_j), \tag{3.128}$$

and

$$\frac{1}{L}\int_{-L/2}^{L/2} \exp[-ik_1\alpha_j x]N(\vec{x}_h)h(x)dx = -(I_j + A_j). \tag{3.129}$$

Fourier inverting both equations yields

$$N(\vec{x}_h) = -ik_1 \sum_{j=-\infty}^{\infty} \exp[ik_1\alpha_j x](I_j - A_j), \tag{3.130}$$

and

$$N(\vec{x}_h)h(x) = -\sum_{j=-\infty}^{\infty} \exp[ik_1\alpha_j x](I_j + A_j). \tag{3.131}$$

Divide (3.131) by (3.130) (so that we factor out the boundary condition) and take the real part to get the approximation to the surface profile $h_{PT}$ produced by perturbation theory

$$h_{PT}(x) = \frac{1}{k_1} Im \left\{ \frac{\sum_{j=-\infty}^{\infty}(I_j + A_j] \exp[ik_1\alpha_j x]}{\sum_{j=-\infty}^{\infty}(I_j - A_j) \exp[ik_1\alpha_j x]} \right\}. \tag{3.132}$$

where $(Im)$ is the imaginary part. The equation simplifies for a single incident wave $(I_j = \delta_{j0}I_0)$ to be

$$h_{PT}(x) = \frac{1}{k_1} Im \left\{ \frac{I_0 + \sum_{j=-\infty}^{\infty} A_j \exp[i2\pi jx/L]}{I_0 - \sum_{j=-\infty}^{\infty} A_j \exp[i2\pi jx/L]} \right\}. \tag{3.133}$$

These equations (3.132) and (3.133) express the surface in terms of the amplitudes of the incident and scattered fields.

For the Kirchhoff approximation (KA), assume a single plane wave incidence

$$\psi^{in}(\vec{x}) = I_0 \exp[ik_1(\alpha_0 x - \gamma_{10} z)], \tag{3.134}$$

and approximate the normal derivative on the surface in (3.126) by twice the normal derivative of the incident field

$$N(\vec{x}_h) \approx N^{KA}(\vec{x}_h) = 2n_l \partial_l \psi^{in}(\vec{x}_h). \tag{3.135}$$

For the lower equation in (3.126) this yields

$$\frac{1}{L}\int_{-L/2}^{L/2} [\gamma_{10} + \alpha_0 h'(x)] \exp[-ik_1(p_j x + q_j h(x))] dx = -\gamma_{1j} A_j / I_0, \tag{3.136}$$

where

$$p_j = \alpha_j - \alpha_0, \tag{3.137}$$

and

$$q_j = \gamma_{1j} + \gamma_{0j}. \tag{3.138}$$

The $h'(x)$ term in (3.136) can be integrated by parts to yield

$$\frac{1}{L}\int_{-L/2}^{L/2} \exp[-ik_1(p_j x + q_j h(x))] dx = -f_j^- A_j / I_0, \tag{3.139}$$

where

$$f_j^- = \frac{\gamma_{1j}(\gamma_{1j} + \gamma_{10})}{\gamma_{1j}\gamma_{10} + (1 - \alpha_j \alpha_0)}. \tag{3.140}$$

We can re-express $p_j$ and $q_j$ using trig identities as

$$p_j = \sin(\theta_j^{sc}) - \sin(\theta^{in}) = 2\cos\left\{\frac{\theta_j^{sc} + \theta^{in}}{2}\right\} \sin\left\{\frac{\theta_j^{sc} - \theta^{in}}{2}\right\}, \tag{3.141}$$

and

$$q_j = \cos(\theta_j^{sc}) + \cos(\theta^{in}) = 2\cos\left\{\frac{\theta_j^{sc} + \theta^{in}}{2}\right\} \cos\left\{\frac{\theta_j^{sc} - \theta^{in}}{2}\right\}. \tag{3.142}$$

We thus have that $p_j$ and $q_j$ are confined to an Ewald circle

$$p_j^2 + q_j^2 \leqslant 4. \tag{3.143}$$

and we further have $|p_j| \leqslant 2$ and $|q_j| \leqslant 2$. This restricts the acceptable $j$ values to a set $J$ and correspondingly restricts the acceptable scattering angles (modulo the incident angle), and thus the scattered amplitudes and fields used for the inversion. For fixed $q_j$, say $q_{j_1}$, (3.139) is a periodic Fourier transform restricted in $p_j$ and thus restricted in the set $J$. As $q_{j_1}$ increases, $p_j$ decreases, which is equivalent to a low-pass filter. As $q_{j_1}$ decreases, more data near grazing illumination and scattering is involved, where the Kirchhoff approximation gets worse. For fixed $q_{j_1}$, assume the integral in (3.139) can be approximately inverted to yield

$$\exp[-ik_1 q_{j_1} h(x)] = \frac{-1}{I_0} \sum_J f_j^- A_j \exp[ik_1 p_j x] \doteq \mathscr{R}(x). \tag{3.144}$$

Taking the real *Re* and imaginary *Im* parts of (3.144) (and neglecting periodic phase shifts) yields $h_{KA}$, the Kirchhoff approximation of the surface height

$$h_{KA}(x, q_{j_1}) = \frac{1}{k_1 q_{j_1}} \arctan\left\{ \frac{-Im(\mathscr{R}(x))}{Re(\mathscr{R}(x))} \right\}, \tag{3.145}$$

which again produces the surface height function in terms of the scattered field amplitudes this time modulated by the Kirchhoff components. Each $q_{j_1}$ produces a different value of $h_{KA}$. For a non-periodic truncated random surface the method was used successfully to reconstruct ensemble surface height functions with approximately twice the rms height as for perturbation theory[112]. The cited paper also contains a discussion of the various angle combinations for different reconstructions.

## 3.7 Full Spectral Methods for Scalar Problems: Physical Optics Modified Fourier Basis and Floquet-Fourier Expansions

In Sec.4, both the exterior and interior (integration) variables were in coordinate space. The equations generated were formally exact for the solution of the boundary values $\psi(\vec{x}_h)$ and $N(\vec{x}_h)$. Once the boundary values were found, the scattered and transmitted fields anywhere away from the surface wells could be evaluated via either direct transforms or summation methods in the resulting plane wave cum evanescent wave expansions. The periodic Green's function was used and had to be computed. Acceleration methods to do this are available[101,102].

In Sec.5, we used plane/evanescent waves to derive another set of equations, again formally exact, for the boundary unknowns which avoided the use of the periodic Green's functions. The equations to be solved were similar to the equations to be evaluated in the sense that both involved a close interplay between spectral and coordinate parameters in "parallel" as distinct from the "serial" presentation of methods in Sec.4.

Solution of the boundary unknowns in Secs.4 and 5 using direct discretization methods involves matrix inversion where the rows and columns of the matrix are both sampled in coordinate space, and the sampling methods are flexible. In Sec.5 the columns are sampled in coordinate space, but the rows are sampled in spectral space, and this is proscribed in terms of the Bragg waves. Convergence and the usefulness of the two sets of solutions have been discussed[36,37,38,39]. The major point is that the limits of convergence, stability and errors are numerical and directly related to the solution of *exact formal equations* and not to any strictly "physical" approximations.

That changes when we attempt to approximate the surface fields in some spectral basis, and thus to write equations fully in spectral space. The first question is what do we mean by spectral space in this context? The second is what do we know about possible expansions? The main thing we know is that the surface fields are the limits of Floquet-periodic functions, so they must also be Floquet-periodic. In particular, they should not be expanded in a pure Fourier series (no matter the temptation) since the latter are only valid for normal incidence ($\alpha_0 = 0$), where the Floquet periodicity reduces to ordinary periodicity. The validity of a pure Fourier expansion deteriorates for non-normal incidence.

In this section we briefly describe the use of a pure Floquet type expansion which defines "spectrum" in one particular way. It is also a physical optics (PO) expansion explained below. From this we are able to infer the results for what we refer to as a Floquet-Fourier (FF) expansion, and these latter results are presented at the end of the section. The PO expansions for the boundary unknowns are

$$\psi(\vec{x}_h) = \exp[-ik_1\gamma_{10}h(x)] \sum_{j'=-\infty}^{\infty} \psi_{j'}^{(PO)} \exp[ik_1\alpha_{j'}x], \tag{3.146}$$

or, written in another form

$$\psi(\vec{x}_h) = \exp[ik_1\alpha_0 x - ik_1\gamma_{10}h(x)] \sum_{j'=-\infty}^{\infty} \psi_{j'}^{(PO)} \exp[i2\pi j'x/L], \tag{3.147}$$

where the term outside the summation can be written using the complex conjugate of (3.100)

$$\exp[ik_1\alpha_0 x - ik_1\gamma_{10}h(x)] = \bar{\phi}_{10}^{+}(\vec{x}_h). \tag{3.148}$$

The term is the physical optics or Kirchhoff approximation of a down-going plane wave evaluated on the boundary. It serves to modulate the remaining Fourier series, and can be viewed as a precursor to more general Waterman-type expansions[105] in terms of down-going waves. (If the $h$ term is not present in (3.146), the expansion is still a Floquet-periodic expansion, and, since it is a generalization of the Fourier expansion, has the advantage of being invertible. Its result can be inferred from the results below, and are presented at the end of this section.) The normal derivative is similarly expanded

$$N(\vec{x}_h) = ik_1 \exp[-ik_1\gamma_{10}h(x)] \sum_{j'=-\infty}^{\infty} N_{j'}^{(PO)} \exp[ik_1\alpha_{j'}x]. \tag{3.149}$$

Here we have scaled the normal derivative term by $ik_1$ for convenience. The expansion was initially introduced as a physical optics modified Fourier expansion[31,32,33], and used by several others[15,26,27,55,106,107]. The reference[33] can be viewed as the exact version of the approximate Rayleigh-Fano equations[97] valid in perturbation theory for shallow surfaces. The expansions can be substituted into (3.105) and (3.111) to yield

$$\sum_{j'=-\infty}^{\infty} M_{1jj'}^{\pm}(PO)[N_{j'}^{(PO)} \mp \gamma_{1j}\psi_{j'}^{(PO)}] - \alpha_j \sum_{j'=-\infty}^{\infty} \tilde{M}_{1jj'}^{\pm}(PO)\psi_{j'}^{(PO)} = 2\gamma_{1j}\left\{\begin{smallmatrix} -I_j \\ A_j \end{smallmatrix}\right\}, \tag{3.150}$$

and

$$\sum_{j'=-\infty}^{\infty} M_{2jj'}^{\pm}(PO)[N_{j'}^{(PO)} \mp \frac{ik_1}{\rho}\gamma_{2j}\psi_{j'}^{(PO)}] - \frac{ik_1}{\rho}\alpha_j \sum_{j'=-\infty}^{\infty} \tilde{M}_{2jj'}^{\pm}(PO)\psi_{j'}^{(PO)} = -2\gamma_{2j}\left\{\begin{smallmatrix} B_j \\ 0 \end{smallmatrix}\right\}, \tag{3.151}$$

where the physical optics $(PO)$ matrix elements are $(p = 1, 2)$

$$M_{pjj'}^{\pm}(PO) = \frac{1}{L}\int_{-L/2}^{L/2} \exp(ik_1[(\pm\gamma_{pj} - \gamma_{10})h(x) + (\alpha_{j'} - \alpha_j)x])dx, \tag{3.152}$$

(note that $M_{10j'}^{+}(PO) = \delta_{j'0}$) and

$$\tilde{M}_{pjj'}^{\pm}(PO) = \frac{1}{L}\int_{-L/2}^{L/2} h'(x)\exp(ik_1[(\pm\gamma_{pj} - \gamma_{10})h(x) + (\alpha_{j'} - \alpha_j)x])dx. \tag{3.153}$$

The latter is written in such a way that integration by parts is obvious. Using integration by parts, the equations reduce to a simple form

$$\sum_{j'=-\infty}^{\infty} M^{\pm}_{1jj'}(PO)[N^{(PO)}_{j'} \mp a^{\pm}_{1jj'}\psi^{(PO)}_{j'}] = 2\gamma_{1j}\{^{-I_j}_{A_j}\}, \tag{3.154}$$

where

$$a^{\pm}_{1jj'} = \frac{\pm(1-\alpha_j\alpha_{j'}) - \gamma_{1j}\gamma_{10}}{\pm\gamma_{1j} - \gamma_{10}}, \tag{3.155}$$

and

$$\sum_{j'=-\infty}^{\infty} M^{\pm}_{2jj'}(PO)[N^{(PO)}_{j'} \mp a^{\pm}_{2jj'}\psi^{(PO)}_{j'}] = -2\gamma_{2j}\{^{B_j}_{0}\}, \tag{3.156}$$

where

$$a^{\pm}_{2jj'} = \frac{\pm(K^2-\alpha_j\alpha_{j'}) - \gamma_{2j}\gamma_{10}}{\rho(\pm\gamma_{2j} - \gamma_{10})}. \tag{3.157}$$

Finally, it is useful to rewrite the physical optics matrix elements as

$$M^{\pm}_{pjj'}(PO) = \frac{1}{L}\int_{-L/2}^{L/2} \exp[-i2\pi(j-j')x/L + ik_1(\pm\gamma_{pj} - \gamma_{10})h(x)]dx, \tag{3.158}$$

which displays the Fourier part explicitly. Note that for a flat surface, the only elements of (3.158) which survive are the diagonal elements $j = j'$ (which equal 1). Further, $\tilde{M}^{\pm}_{pjj'}(PO) = 0$, $a^{\pm}_{1jj'} = \gamma_{1j}$, $a^{\pm}_{2jj'} = \gamma_{2j}/\rho$, and, for a single plane wave incidence ($I_j = \delta_{j0}$), the usual flat surface limit of (3.154) and (3.156) follows directly.

A Floquet-Fourier (FF) expansion for the boundary unknowns can be written as

$$\psi(\vec{x}_h) = \sum_{j'=-\infty}^{\infty} \psi^{(FF)}_{j'} \exp(ik_1\alpha_{j'}x), \tag{3.159}$$

and

$$N(\vec{x}_h) = ik_1 \sum_{j'=-\infty}^{\infty} N^{(FF)}_{j'} \exp(ik_1\alpha_{j'}x). \tag{3.160}$$

The equations corresponding to (3.154) and (3.156) are thus

$$\sum_{j'=-\infty}^{\infty} M^{\pm}_{1jj'}(FF)[N^{(FF)}_{j'} \mp a_{1jj'}\psi j'^{(FF)}] = 2\gamma_{1j}\{^{-I_j}_{A_j}\}, \tag{3.161}$$

and

$$\sum_{j'=-\infty}^{\infty} M^{\pm}_{2jj'}(FF)[N^{(FF)}_{j'} \mp a_{2jj'}\psi^{(FF)}_{j'}] = -2\gamma_{2j}\{^{B_j}_{0}\}, \tag{3.162}$$

where

$$a_{1jj'} = \frac{1-\alpha_j\alpha_{j'}}{\gamma_{1j}}, \tag{3.163}$$

$$a_{2jj'} = \frac{K^2-\alpha j\alpha_{j'}}{\rho\gamma_{2j}}, \tag{3.164}$$

and, for $p=1,2$, the matrix elements are

$$M^{\pm}_{pjj'}(FF)=\frac{1}{L}\int_{-L/2}^{L/2}\exp[-i2\pi(j-j')x/L\pm ik_1\gamma_{pj}h(x)]dx. \tag{3.165}$$

The FF equations follow from (3.154) through (3.158) by setting the $\gamma_{10}$ term to zero. These provide an alternative set of equations to solve for the alternative boundary function coefficients to produce the same coefficients for the scattered and transmitted fields[58].

## 3.8 Full Spectral Methods for Scalar Problems: Conjugate Rayleigh Basis

A further spectral expansion consists in modifying the physical optics expansion by making the single physical optics plane wave dependent on the Bragg mode, so that the phase height term is dependent on the mode, and this leads to a conjugate Rayleigh (CR) expansion using the complex conjugate of the plane wave states (3.100) evaluated on the surface as

$$\psi(\vec{x}_h)=\sum_{j'=-\infty}^{\infty}\psi^{(CR)}_{j'}\exp[ik_1\alpha_{j'}x-ik_1\bar{\gamma}_{1j'}h(x)]=\sum_{j'=-\infty}^{\infty}\psi^{(CR)}_{j'}\bar{\phi}^{+}_{1j'}(\vec{x}_h), \tag{3.166}$$

and the scaled expansion for the normal derivative

$$N(\vec{x}_h)=ik_1\sum_{j'=-\infty}^{\infty}N^{(CR)}_{j'}\bar{\phi}^{+}_{1j'}(\vec{x}_h), \tag{3.167}$$

where the overbar is complex conjugation. Substituting these expansions in (3.105) and (3.111), and carrying out the integration by parts necessary to simplify the slope terms as in Sec.7 yields equations similar in form to (3.154) and (3.156). For the upper region equation we get

$$\sum_{j'=-\infty}^{\infty}M^{\pm}_{1jj'}(CR)[N^{(CR)}_{j'}\mp b^{\pm}_{1jj'}\psi^{(CR)}_{j'}]=2\gamma_{1j}\{{}^{-I_j}_{A_j}\}, \tag{3.168}$$

where

$$b^{\pm}_{1jj'}=\frac{1-\alpha_j\alpha_{j'}\mp\gamma_{1j}\bar{\gamma}_{1j'}}{\gamma_{1j}\mp\bar{\gamma}_{1j'}}, \tag{3.169}$$

and the matrix elements are defined as

$$M^{\pm}_{1jj'}(CR)=\frac{1}{L}\int_{-L/2}^{L/2}\exp[-i2\pi(j-j')x/L+ik_1(\pm\gamma_{1j}-\bar{\gamma}_{1j'})h(x)]dx=<\phi^{\pm}_{1j},\phi^{+}_{1j'}>. \tag{3.170}$$

It is obvious that $M^{+}_{1jj'}(CR)$ is self-adjoint, positive definite and thus invertible, and this fact was used with success in solving the Dirichlet problem[3]. That is,

$$[M^{+}_{1jj'}]^{\star}(CR)=M^{+}_{1jj'}(CR), \tag{3.171}$$

where the symbol $\star$ represents the adjoint.

The same expansion for the equations in region 2 yields the equations

$$\sum_{j'=-\infty}^{\infty}M^{\pm}_{2jj'}(CR)[N^{(CR)}_{j'}\mp b^{\pm}_{2jj'}\psi^{(CR)}_{j'}]=-2\gamma_{2j}\{{}^{B_j}_{0}\}, \tag{3.172}$$

where

$$b^{\pm}_{2jj'} = \frac{1}{\rho}\frac{K_2 - \alpha_j\alpha_{j'} \mp \gamma_{2j}\bar{\gamma}_{1j'}}{\gamma_{2j} \mp \bar{\gamma}_{1j'}}, \tag{3.173}$$

and the matrix elements are

$$M^{\pm}_{2jj'}(CR) = \frac{1}{L}\int_{-L/2}^{L/2} \exp[-i2\pi(j-j')x/L + ik_1(\pm\gamma_{2j} - \bar{\gamma}_{1j'})h(x)]dx =< \phi^{\pm}_{2j}, \phi^{+}_{1j'} > . \tag{3.174}$$

## 3.9 Integral Equation Methods in Coordinate Space for Electromagnetic Problems

Up to now we have considered one-dimensional surfaces and acoustic problems. These correspond directly to electromagnetic scattering problems where there is no change in polarization for the scattered and transmitted fields. The general electromagnetic problem for a periodic dielectric interface is for a two-dimensional surface $z = h(\vec{x}_\perp) = h(x,y)$ which separates media of different dielectric constants $\varepsilon_j$ for $j = 1,2$ and permeability $\mu_j$. The wave numbers for the two regions are $k_j = k_0\sqrt{\varepsilon_j\mu_j}$ where $k_0 = \omega/c$, $\omega$ is the circular frequency and $c$ the speed of light. There is now a change in polarization in the scattered and transmitted fields.

For the source-free electric field $\partial_i E_i = 0$, and each component of the electric field $E_i$ with $i = 1,2,3$ satisfies the same Helmholtz equation as the scalar field, viz. in region 1

$$(\nabla_3^2 + k_1^2)E_{1i}(\vec{x}) = 0, \tag{3.175}$$

where $E_{1i}$ is the $i^{th}$ electric field component in region 1, and the Laplacian is three-dimensional. This is just the vector analogue of (3.67). We can use this to write the vector analogues of the scalar equations in Sec.4, using Green's theorem, the three-dimensional periodic Green's functions $G^{(3p)}$ from (3.59) and (3.62), the two-dimensional Floquet periodicity of the field, and the characteristic function defining the region, e.g. for region 1

$$\Theta_1(\vec{x}) = \theta(L_1/2 - x)\theta(x + L_1/2)\theta(L_2/2 - y)\theta(y + L_2/2)\theta(z - h(\vec{x}_\perp))\theta(H_1 - z). \tag{3.176}$$

In region 1 the result is

$$E_{1i}(\vec{x}')\Theta_1(\vec{x}') = E_i^{in}(\vec{x}') - [G_1^{(3p)}, E_{1i}; \vec{x}', h], \tag{3.177}$$

where $E_i^{in}$ is the incident field, and the two-dimensional bracket is explicitly

$$[G_1^{(3p)}, E_{1i}; \vec{x}', h] = \iint_D [G_1^{(3p)}(\vec{x}', \vec{x}_h)N_{1i}(\vec{x}_h) - N_1^{(3p)}(\vec{x}', \vec{x}_h)E_{1i}(\vec{x}_h)]d\vec{x}_\perp, \tag{3.178}$$

where $\vec{x}_\perp = (x,y)$, the domain of integration $D$ is $x\varepsilon[-L_1/2, L_1/2]$, $y\varepsilon[-L_2/2, L_2/2]$, and the normal derivatives are

$$N_{1i}(\vec{x}_h) = n_l(\vec{x}_\perp)\partial_l E_{1i}(\vec{x}_h), \tag{3.179}$$

and

$$N_1^{(3p)}(\vec{x}', \vec{x}_h) = n_l(\vec{x}_\perp)\partial_l G_1^{(3p)}(\vec{x}', \vec{x}_h), \tag{3.180}$$

the normal derivatives of the boundary unknown and the periodic Green's function respectively. From (3.177), the field representation in $D$ is found by setting $\Theta_1 = 1$, the Extinction Theorem by setting $\Theta_1 = 0$, the scattered field is just the bracket term

$$E_{1i}^{sc}(\vec{x}') = -[G_1^{(3p)}, E_{1i}; \vec{x}', h], \tag{3.181}$$

and the boundary integral equation is

$$\frac{1}{2}E_{1i}(\vec{x}'_h) = E_i^{in}(\vec{x}'_h) - \iint_D [G_1^{(3p)}(\vec{x}'_h,\vec{x}_h)N_{1i}(\vec{x}_h) - N_1^{(3p)}(\vec{x}'_h,\vec{x}_h)E_{1i}(\vec{x}_h)]d\vec{x}_\perp, \tag{3.182}$$

with the boundary unknowns $E_{1i}$ and its normal derivative $N_{1i}$.

Green's theorem in region 2 yields the representation for the total transmitted field

$$E_{2i}(\vec{x}')\Theta_2(\vec{x}') = [G_2^{(3p)}, E_{2i}; \vec{x}', h], \tag{3.183}$$

where $\Theta_2 = 1 - \Theta_1$, and the boundary integral equation becomes

$$\frac{1}{2}E_{2i}(\vec{x}'_h) = \iint_D [G_2^{(3p)}(\vec{x}'_h,\vec{x}_h)N_{2i}(\vec{x}_h) - N_2^{(3p)}(\vec{x}'_h,\vec{x}_h)E_{2i}(\vec{x}_h)]d\vec{x}_\perp, \tag{3.184}$$

with boundary unknowns $E_{2i}$ and its normal derivative $N_{2i}$. Equations (3.182) and (3.184) are similar to the scalar equations (3.74) and (3.88), but the fields and their normal derivatives are not the usual electromagnetic boundary values, the latter being typically written in terms of normal field components and currents[61]. So to continue we must relate these usual boundary conditions to our boundary unknowns.

For the electric field on the boundary we have the continuity condition of the normal component of the displacement vector $\vec{D} = \varepsilon\vec{E}$ which becomes

$$\varepsilon\vec{n}\cdot\vec{E}_2 = \vec{n}\cdot\vec{E}_1, \tag{3.185}$$

where $\varepsilon = \varepsilon_2/\varepsilon_1$, and the continuity of the magnetic current

$$\vec{n}\times\vec{E}_2 = \vec{n}\times\vec{E}_1. \tag{3.186}$$

These are four equations, three of which are independent. These three can be solved directly, or the four equations solved using a Moore-Penrose pseudo inverse to yield the boundary conditions on the electric field (in index notation) as

$$E_{2i}(\vec{x}_h) = C_{ij}(\vec{x}_h)E_{1j}(\vec{x}_h), \tag{3.187}$$

with repeated subscripts summed from 1 to 3 and

$$C_{ij}(\vec{x}_h) = \delta_{ij} + (\varepsilon^{-1} - 1)\hat{n}_i\hat{n}_j, \tag{3.188}$$

with $\hat{n}$ representing the unit normal. These boundary conditions were introduced some time ago[35] and used successfully for scattering from a body of revolution[41].

The continuity conditions on the normal derivative components are more involved. The full details are in[35]. Briefly we introduce the bracket notation for when we set the field on the surface first and then differentiate

$$\{E_m\} \doteq E_m(x,y,h(x,y)). \tag{3.189}$$

Then the transverse ("t") derivatives ($x$ and $y$) are given by

$$\partial_x\{E_m\} = \{\partial_x E_m\} + h_x\{\partial_z E_m\}, \tag{3.190}$$

and

$$\partial_y\{E_m\} = \{\partial_y E_m\} + h_y\{\partial_z E_m\}. \tag{3.191}$$

Using this notation and the continuity of the electric surface current $\vec{K}^e = -\vec{n} \times \vec{H}$, where $\vec{H}$ is the magnetic field, in index form

$$K^e_{2i}(\vec{x}_h) = K^e_{1i}(\vec{x}_h), \tag{3.192}$$

we can write the continuity condition for the normal derivative as[35]

$$\{N_{2i}\} = \mu\{N_{1i}\} + (\varepsilon^{-1} - 1)V_i(\vec{x}_h), \tag{3.193}$$

where $V_i$ can be written in terms of transverse partial derivatives involving the normal components of the electric field as

$$V_i(\vec{x}_h) = n_m \partial_{it}\{\hat{n}_m \hat{n}_j E_{1j}\} - n_i \partial_{qt}\{\hat{n}_{qt} \hat{n}_j E_{1j}\}. \tag{3.194}$$

This $V_i$ term looks awkward, but it can be integrated by parts. First, choose the boundary unknowns as

$$E_{1i}(\vec{x}_h) = \{E_{1i}\} \doteq \{E_i\}, \tag{3.195}$$

and

$$N_{1i}(\vec{x}_h) = \{N_{1i}\} \doteq \{N_i\}. \tag{3.196}$$

Then we can write the equation for the upper region (3.182) as

$$\frac{1}{2}\{E'_i\} + \iint_D [G_1^{(3p)}(\vec{x}'_h, \vec{x}_h)\{N_i\} - N_1^{(3p)}(\vec{x}'_h, \vec{x}_h)\{E_i\}] d\vec{x}_\perp = E_i^{in}(\vec{x}'_h). \tag{3.197}$$

Here $\{E'_i\}$ means the exterior primed variable placed on the surface, i.e. $\vec{x}'_h$. The equation (3.197) is diagonal in the index. The coupling is from the lower equation (3.184) written using (3.193) through (3.196) as

$$\frac{1}{2}C_{ij}(\vec{x}'_h)\{E'_j\} = \iint_D [G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)(\mu\{N_i\} + (\varepsilon^{-1} - 1)V_i(\vec{x}_h)) - N_2^{(3p)}(\vec{x}'_h, \vec{x}_h)C_{ij}(\vec{x}_h)\{E_j\}] d\vec{x}_\perp. \tag{3.198}$$

The $V_i$ term can be integrated by parts to yield

$$\iint_D G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)V_i(\vec{x}_h) d\vec{x}_\perp = \iint_D V_{ij}(\vec{x}'_h, \vec{x}_h)\{E_i\} d\vec{x}_\perp, \tag{3.199}$$

where

$$V_{ij}(\vec{x}'_h, \vec{x}_h) = \partial_{qt}\{n_i G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\}\hat{n}_{qt}\hat{n}_j - \partial_{it}\{n_m G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\}\hat{n}_m \hat{n}_j. \tag{3.200}$$

We can simplify (3.200) to yield

$$V_{ij}(\vec{x}'_h, \vec{x}_h) = N_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\hat{n}_i \hat{n}_j - \{\partial_i G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\}n_j, \tag{3.201}$$

where now the derivative of the Green's function is taken first, and then the result set on the surface. Combining these results we can rewrite (3.198) as

$$\frac{1}{2}C_{ij}(\vec{x}'_h)\{E'_j\} = \iint_D [G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\mu\{N_i\} - W_{ij}(\vec{x}'_h, \vec{x}_h)\{E_j\}] d\vec{x}_\perp, \tag{3.202}$$

where

$$W_{ij}(\vec{x}'_h, \vec{x}_h) = N_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\delta_{ij} + (\varepsilon^{-1} - 1)\{\partial_i G_2^{(3p)}(\vec{x}'_h, \vec{x}_h)\}n_j. \tag{3.203}$$

Note that (3.197) and (3.202), if put in matrix form, are diagonal in three of the four matrix blocks multiplying the six-dimensional vector of boundary unknowns $[\{E_i\},\{N_i\}]^T$ where $T$ is transpose. The only coupling occurs in the single block of the electric fields from (3.202). We note this in contrast to pre-conditioning methods used to sparsify matrix inversion problems. Here the results are exact and highly sparse as formulated. They have been used computationally to treat the scattering from a body of revolution[41].

We can use these representations to write plane wave representations for the scattered and transmitted fields, above and below the largest surface excursions. From (3.177) we can write the scattered field above the highest surface excursion ($z' > max(h)$) as

$$E_i^{sc}(\vec{x}') = -\iint_D [G_1^{(3p)}(\vec{x}',\vec{x}_h)\{N_i\} - N_1^{(3p)}(\vec{x}',\vec{x}_h)\{E_i\}]d\vec{x}_\perp, \tag{3.204}$$

where now the Green's function is, following (3.59), with the field point above the surface

$$G_1^{(3p)}(\vec{x}',\vec{x}_h) = \frac{i}{2k_1L_1L_2}\sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\beta_{j'}(y'-y)+\gamma_{1jj'}(z'-h(\vec{x}_\perp))]}{\gamma_{1jj'}}, \tag{3.205}$$

and

$$N_1^{(3p)}(\vec{x}',\vec{x}_h) = n_q\partial_q G_1^{(3p)}(\vec{x}',\vec{x}_h). \tag{3.206}$$

Combining these results we can write the scattered field exactly above the highest surface excursion as a plane wave expansion in terms of purely up-going waves as

$$E_i^{sc}(\vec{x}') = \sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty} A_{ijj'}\exp[ik_1(\alpha_j x' + \beta_{j'}y' + \gamma_{1jj'}z')], \tag{3.207}$$

where

$$A_{ijj'} = \frac{1}{L_1L_2}\iint_D A_{ijj'}(\vec{x}_\perp)\exp[-ik_1(\alpha_j x + \beta_{j'}y + \gamma_{1jj'}h(\vec{x}_\perp))]d\vec{x}_\perp, \tag{3.208}$$

and

$$A_{ijj'}(\vec{x}_\perp) = \frac{-i}{8\pi^2k_1\gamma_{1jj'}}[\{N_i\} + ik_1(\gamma_{1jj'} - \alpha_j h_x - \beta_{j'}h_y)\{E_i\}], \tag{3.209}$$

in terms of the boundary unknowns.

Similarly, from (3.183), we have the transmitted field below the lowest surface excursion ($z' < min(h)$)

$$E_{2i}(\vec{x}') = \iint_D [G_2^{(3p)}(\vec{x}',\vec{x}_h)N_{2i}(\vec{x}_h) - N_2^{(3p)}(\vec{x}',\vec{x}_h)E_{2i}(\vec{x}_h)]d\vec{x}_\perp, \tag{3.210}$$

where now

$$G_2^{(3p)}(\vec{x}',\vec{x}_h) = \frac{i}{8\pi^2k_1L_1L_2}\sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty}\frac{\exp[ik_1(\alpha_j(x'-x)+\beta_{j'}(y'-y)-\gamma_{2jj'}(z'-h(\vec{x}_\perp))]}{\gamma_{2jj'}}, \tag{3.211}$$

and

$$N_2^{(3p)}(\vec{x}',\vec{x}_h) = n_q\partial_q G_2^{(3p)}(\vec{x}',\vec{x}_h). \tag{3.212}$$

The result is the plane wave spectral representation for the transmitted field below the lowest surface excursion in terms of purely down-going waves as

$$E_{2i}(\vec{x}') = \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} B_{ijj'} \exp[ik_1(\alpha_j x' + \beta_{j'} y' - \gamma_{2jj'} z')], \tag{3.213}$$

where

$$B_{ijj'} = \frac{1}{L_1 L_2} \iint_D B_{ijj'}(\vec{x}_\perp) \exp[-ik_1(\alpha_j x + \beta_{j'} y - \gamma_{2jj'} h(\vec{x}_\perp))] d\vec{x}_\perp, \tag{3.214}$$

and

$$B_{ijj'}(\vec{x}_\perp) = \frac{i}{8\pi^2 k_1 \gamma_{2jj'}} [N_{2i}(\vec{x}_h) - ik_1(\gamma_{2jj'} + \alpha_j h_x + \beta_{j'} h_y) E_{2i}(\vec{x}_h)], \tag{3.215}$$

written in terms of the boundary values from the lower region. Using the boundary conditions (3.187) and (3.193) and integration by parts we can rewrite (3.215) in terms of the boundary unknowns as

$$B_{ijj'}(\vec{x}_\perp) = \frac{i}{8\pi^2 k_1 \gamma_{2jj'}} [\mu\{N_i\} - W_{ijj'l}(\vec{x}_\perp)\{E_l\}], \tag{3.216}$$

where

$$W_{ijj'l}(\vec{x}_\perp) = ik_1[\alpha_j h_x + \beta_{j'} h_y + \gamma_{2jj'})\delta_{il} - (\varepsilon^{-1} - 1)(\delta_{i1}\alpha_j + \delta_{i2}\beta_{j'} - \delta_{i3}\gamma_{2jj'})n_l]. \tag{3.217}$$

Equations (3.207) and (3.213) are the exact plane wave representations in the appropriate regions. In the next section we write general partial spectral representations of the fields, and show the relations between them and the plane wave spectral representations here which are valid in limited domains.

### 3.10 Partial Spectral Methods for Electromagnetic Problems

We develop this section in analogy with the scalar results in Sec.5. This is the electromagnetic version of the Spectral-Coordinate approach. We define the three-dimensional plane wave states in the upper region 1 for up$^{(+)}$- and down$^{(-)}$-going waves as

$$\phi^{\pm}_{1jj'}(\vec{x}) = \exp[ik_1(-\alpha_j x - \beta_{j'} y \pm \gamma_{1jj'} z), \tag{3.218}$$

where $\gamma_{1jj'}$ is defined following (3.59). The function satisfies the three-dimensional Helmholtz equation

$$(\nabla_3^2 + k_1^2)\phi^{\pm}_{1jj'}(\vec{x}) = 0. \tag{3.219}$$

The incident electric field can be written as a general plane wave expansion of down-going waves

$$E_i^{in}(\vec{x}) = \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} I_{ijj'} \exp[ik_1(\alpha_j x + \beta_{j'} y - \gamma_{1jj'} z)]. \tag{3.220}$$

Apply Green's theorem in the domain defined by $\Theta_1$ in (3.176) to $\phi^{\pm}_{1jj'}$ and $E_{1i}$, use the two-dimensional Floquet conditions to cancel the side integrals as in Sec.9 and the result is

$$\frac{1}{L_1 L_2} \iint_D \phi^{\pm}_{1jj'}(\vec{x}_h) U^{\pm}_{ijj'}(\vec{x}_h) d\vec{x}_\perp = \gamma_{1jj'} \left\{ {-I_{ijj'} \atop A_{ijj'}} \right\}, \tag{3.221}$$

where $U$ is defined as

$$U^{\pm}_{ijj'}(\vec{x}_h) = \frac{1}{2ik_1}[\{N_i\} - ik_1(\pm\gamma_{1jj'} + \alpha_j h_x + \beta_{j'} h_y)\{E_i\}]. \tag{3.222}$$

The $A_{ijj'}$ are the spectral coefficients of the scattered field from (3.207). Recall that the scattered field is evaluated on a flat surface ($z = H_1$) above the highest surface excursion, so the representation (3.207) is rigorously valid and not a Rayleigh approximation. We also used the boundary values (3.195) and (3.196). In (3.221), the up-going plane wave states $\phi^+$ project out the down-going incident field spectral components $I_{ijj'}$, and the down-going plane wave states $\phi^-$ project out the up-going scattered field spectral components $A_{ijj'}$. Equations (3.221) and (3.222) are the vector generalizations of (3.105) and (3.106).

For the lower region 2, the three-dimensional up- and down-going plane wave states are defined as

$$\phi^{\pm}_{2jj'}(\vec{x}) = \exp[ik_1(-\alpha_j x - \beta_{j'} y \pm \gamma_{2jj'} z)], \tag{3.223}$$

where $\gamma_{2jj'}$ is defined following (3.62). The functions satisfy the three-dimensional Helmholtz equation

$$(\nabla_3^2 + k_2^2)\phi^{\pm}_{2jj'}(\vec{x}) = 0. \tag{3.224}$$

Green's theorem on $\phi^{\pm}_{2jj'}$ and the total transmitted field $E_{2i}$ in the domain defined by $\Theta_2(\vec{x}) = 1 - \Theta_1(\vec{x})$ yields the relations

$$\frac{1}{L_1 L_2}\iint_D \phi^{\pm}_{2jj'}(\vec{x}_h) L^{\pm}_{ijj'}(\vec{x}_h) d\vec{x}_\perp = -\gamma_{2jj'}\left\{{B_{ijj'} \atop 0}\right\}, \tag{3.225}$$

where

$$L^{\pm}_{ijj'}(\vec{x}_h) = \frac{1}{2ik_1}[N_{2i}(\vec{x}_h) - ik_1(\pm\gamma_{2jj'} + \alpha_j h_x + \beta_{j'} h_y)E_{2i}(\vec{x}_h)], \tag{3.226}$$

in terms of the boundary values from the lower region. Using the boundary values (3.195) and (3.196) and integration by parts, (3.226) can be rewritten as

$$L^{\pm}_{ijj'}(\vec{x}_h) = \frac{1}{2ik_1}[\mu\{N_i\} - W^{\pm}_{ijj'l}(\vec{x}_h)\{E_l\}], \tag{3.227}$$

with a sum over $l = (1,2,3)$ and where

$$W^{\pm}_{ijj'l}(\vec{x}_h) = ik_1[(\alpha_j h_x + \beta_{j'} h_y \pm \gamma_{2jj'})\delta_{il} - (\varepsilon^{-1} - 1)(\alpha_j \delta_{i1} + \beta_{j'}\delta_{i2} \mp \gamma_{2jj'}\delta_{i3})n_l]. \tag{3.228}$$

Note that $W^{+}_{ijj'l}$ is just $W_{ijj'l}$ from (3.217). Equations (3.225) and (3.227) are the vector generalizations of (3.111) and (3.112). The procedure is to solve the upper equation (3.221) and the lower equation (3.225) for the boundary unknowns $\{Ni\}$ and $\{E_i\}$ and evaluate the remaining equations for the scattered and transmitted amplitudes.

## 3.11 Full Spectral Methods for Electromagnetic Problems

In this section we develop the full spectral methods using the conjugate Rayleigh basis in analogy with Sec.8 for the scalar case. In (3.221) and (3.225) we use the following expansions in the conjugate Rayleigh basis,

$$\{E_i\} = \sum_{l=-\infty}^{\infty}\sum_{l'=-\infty}^{\infty} E_{ill'}\bar{\phi}^{+}_{1ll'}(\vec{x}_h), \tag{3.229}$$

and

$$\{N_i\} = ik_1 \sum_{l=-\infty}^{\infty} \sum_{l'=-\infty}^{\infty} N_{ill'} \bar{\phi}^{+}_{1ll'}(\vec{x}_h), \tag{3.230}$$

with the normal derivative on the boundary scaled by $ik_1$ and where $\phi^{+}_{1ll'}$ is from (3.218). The overbar is complex conjugation. Integrate the slope terms by parts as for example

$$< \phi^{\pm}_{1jj'}, h_x \phi^{+}_{1ll'} >= \frac{\alpha_j - \alpha_l}{\pm\gamma_{1jj'} - \bar{\gamma}_{1ll'}} < \phi^{\pm}_{1jj'}, \phi^{+}_{1ll'} >, \tag{3.231}$$

and the equations for the upper region can be written using (3.221) as

$$\sum_{l=-\infty}^{\infty} \sum_{l'=-\infty}^{\infty} < \phi^{\pm}_{1jj'}, \phi^{+}_{1ll'} > [N_{ill'} - U^{\pm}(jj', ll')E_{ill'}] = 2\gamma_{1jj'} \{^{-I_{ijj'}}_{A_{ijj'}}\}, \tag{3.232}$$

where

$$U^{\pm}(jj', ll') = \frac{1 - \alpha_j \alpha_l - \beta_{j'} \beta_{l'} \mp \gamma_{1jj'} \bar{\gamma}_{1ll'}}{\pm\gamma_{1jj'} - \bar{\gamma}_{1ll'}}. \tag{3.233}$$

We have written the double spectral values $jj'$ and $ll'$ as arguments of $U$ in illustration of the fact that they are each replacing coordinate sampling/integration along two-dimensional surfaces denoted by $\vec{x}'_h$ and $\vec{x}_h$ respectively, as well as to indicate that the equations (3.232) are diagonal in the vector index $''i''$. That is, the $i^{th}$ component of $A$ is related to the $i^{th}$ components of $N$ and $E$. There is no coupling in this index for the equations from region 1. It can be shown that the matrix $< \phi^{+}_{1jj'}, \phi^{+}_{1ll'} >$ is self-adjoint, positive definite and hence invertible.

For the lower region 2 these same expansions and integration of the slope terms yields from (3.225)

$$\sum_{l=-\infty}^{\infty} \sum_{l'=-\infty}^{\infty} < \phi^{\pm}_{2jj'}, \phi^{+}_{1ll'} > [\mu N_{ill'} - L^{\pm}_{ip}(jj', ll')E_{pll'}] = -2\gamma_{2jj'} \{^{B_{ijj'}}_{0}\}, \tag{3.234}$$

where there is an implicit sum over the repeated subscript $p = (1,2,3)$. The full coupling of these equations resides in this summation. Here the $L$ term can be written as

$$L^{\pm}_{ip}(jj', ll') = \frac{M^{\pm}_{ip}(jj', ll')}{\pm\gamma_{2jj'} - \bar{\gamma}_{1ll'}}, \tag{3.235}$$

where $M$ can be written as a diagonal ($D$) part and a full ($F$) part, the latter of which contains the coupling,

$$M^{\pm}_{ip}(jj', ll') = D^{\pm}(jj', ll')\delta_{ip} + F^{\pm}_{ip}(jj', ll'), \tag{3.236}$$

where

$$D^{\pm}(jj', ll') = K^2 - \alpha_j \alpha_l - \beta_{j'} \beta_{l'} \mp \gamma_{2jj'} \bar{\gamma}_{1ll'}, \tag{3.237}$$

and

$$F^{\pm}_{ip}(jj', ll') = (\varepsilon^{-1} - 1)(\alpha_j \delta_{i1} + \beta_{j'} \delta_{i2} \mp \gamma_{2jj'} \delta_{i3})[(\alpha_j - \alpha_l)\delta_{p1} + (\beta_{j'} - \beta_{l'})\delta_{p2} - (\pm\gamma_{2jj'} - \bar{\gamma}_{1ll'})\delta_{p3}]. \tag{3.238}$$

The procedure is to solve the upper equation (3.232) and the lower equation (3.234), which is a spectral extinction equation, for the unknown expansion coefficients $N_{ill'}$ and $E_{ill'}$, and evaluate the remaining equations for the scattered $A_{ijj'}$ and transmitted $B_{ijj'}$ spectral coefficients.

### 3.12 Summary

We have derived exact formal sets of equations, in both coordinate and various spectral domains, to describe the scattering from deterministic gratings. Both acoustic scalar one-dimensional problems and full electromagnetic two-dimensional problems were considered. Both involved a grating surface separating two homogeneous regions of space. Both involved coordinate-space representations from which proceeded rigorous plane wave spectral representations valid for the scattered field above the highest surface excursion and for the transmitted field below its lowest excursion. The electromagnetic development was treated in analogy with the scalar problem, with boundary conditions derived for the electric field and its normal derivative from the standard boundary conditions on currents and the normal components of the displacement vector.

From these coordinate representations we proceeded first to partial spectral representations where the word ”partial” refers to the field variables. These could be derived in a straightforward way just using plane waves and Green’s theorem, and without involving the Green’s function explicitly. We stress again that the equations are exact. In addition, these led to surface inversion examples for the scalar case using perturbation theory (where the boundary values could be factored out), and the Kirchhoff approximation (where the boundary values were approximated).

The full spectral equations involved expanding the boundary unknowns in some set of functions, and it is here where the Rayleigh and Waterman assumptions come into play. For the scalar case we presented three expansions. The first was a physical optics modified Fourier expansion with a single plane wave modulating the surface fields. The second was what we referred to as a Floquet-Fourier basis which modulated the Fourier expansion by still preserving the Floquet-periodicity of the surface fields but without the full plane waves, and the third was an expansion in the conjugate Rayleigh basis where each term in the expansion could be thought of as modulated by a plane wave. For the electromagnetic case only the expansion in the conjugate Rayleigh basis was considered. Since we used a scalar analogy for the electromagnetic problem the resulting equations were formally analogous to the scalar equations with the additional complication being first a vector problem, and second the Bragg modal sampling in two two-dimensional spaces, the spaces of boundary and field points.

We pointed out in the paper where any of these equations have been solved, but we repeat that the full computational results and the comparisons of different computational results for this problem require at least a separate paper if not a separate book.

## Appendix 3.A. A Note on Matrix Elements

For the fully spectral methods in Secs.7 and 8 for the acoustic case and Sec.11 for the electromagnetic case, the matrix elements have a characteristic form. In the one-dimensional case, after projection on the various basis sets considered in this paper, (see (3.158), (3.165), (3.170), and (3.174)), they have the general form

$$M(a,b) = \frac{1}{L}\int_{-L/2}^{L/2} \exp[iax + ik_1 bh(x)]dx. \tag{3.239}$$

For all the cases in question, $a = 2\pi(j' - j)/L$ which is the Fourier part common to all, and $b = \pm\gamma_{pj} - \gamma_{10}$ for the physical optics case with one overall plane wave, $b = \pm\gamma_{pj}$ for the Floquet-Fourier case with no plane waves modulating the field expansion, and $b = \pm\gamma_{pj} - \bar{\gamma}_{1j'}$ for the conjugate Rayleigh case with plane waves related to each Bragg mode in the sum. They have a general validity in surface scattering problems due to the presence of Green's functions or plane wave type expansions. For example, for a random surface, these functions $M$ were referred to as interaction functions in a Feynman diagram expansion[114,29,30], essentially a perturbation expansion in the functions.

In addition, for many surfaces, not necessarily analytic ones, the integral can be expressed in closed form in terms of special functions. For example, a cosine surface yields Bessel functions for $M$, a symmetric sawtooth function yields simple exponentials, a quadratic surface yields Fresnel integrals, a vortex-like surface involving a logarithm yields cosine integrals which can be evaluated in closed form (or, in a different form, confluent hypergeometric functions), a cycloid can be evaluated in terms of Bessel functions, a full-wave rectified surface in terms of a Bessel series, and a periodic array of semicircular cylinders (bosses)[98] in terms of a Bessel series. These closed form solutions can be useful in computations or for approximations. The details can be found in[32]. Two-dimensional integrals occurring in the electromagnetic problem can be developed in a similar way for egg-crate surfaces of the form $h(x,y) = h_1(x) + h_2(y)$.

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