7 T-Matrix Method for Light Scattering from a Particle on or Near an Infinite Surface

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Abstract. The problem of light scattering by a particle on or near a surface is treated using the field decomposition method and the free-field T-matrix method. The model takes into account that the incident field strikes the particle either directly or after interacting with the surface, while the fields emanating from the particle may also reflect off the surface and interact with the particle again. The reflection of the scattered and incident fields are determined in the context of a T-operator formalism which enables us to compute scattering by infinite surfaces. The solution for a plane interface is obtained as a special case of this general formalism. An approximate solution is also given by assuming that the scattered field, reflecting off the surface and interacting with the particle, is incident upon the surface at near-normal incidence. The range of validity of the approximate and rigorous method is checked from a numerical point of view.

1 Introduction

Particle contamination characterization of a silicon wafer surface is of great importance in semiconductor manufacturing. As semiconductor device dimensions become smaller, there is a need for wafer surface inspection systems to detect the size of microcontaminations to as low as 0.1 μm or even smaller. To expand the current detection ability an efficient mathematical model and computer simulation technique is needed.

Calculation of light scattering from particles deposited upon a surface is of great interest in the simulation, development and calibration of a surface scanner. Several studies have addressed this problem with the use of widely differing methods.

Some simplified theoretical models have been developed on the basis of Mie light-scattering theory and Fresnel surface reflection [1–4]. These approaches represent an extension of Mie theory and are focussed on the light scattering problem of a sphere on or near a plane surface. A coupled-dipole algorithm has also been employed for the scattering problem [5,6]. In this case a three dimensional array of dipoles is used to model a feature shape and its composition. In order to take the presence of the unbounded space into account the Sommerfeld integrals for interaction between a dipole and a surface are introduced.

A model based on the discrete source method was given by Eremin and Orlov [7,8]. In this approach the transmission conditions at the half-space

F. Moreno and F. González (Eds.): Lectures 1998, LNP 534, pp. 113−132, 2000.

interface are taken into account in an analytical manner so that the algorithm does not need to satisfy them numerically. This is done by using the Green tensor components for the interface to construct the fields of discrete sources.

Similar scattering problems were considered by Kristensson and Ström [9], and Hackmann and Sammelmann [10] in the context of the extended boundary condition method. Acoustic scattering from a buried inhomogeneity is discussed by Kristensson and Ström by assuming that the free-field T-matrix of the particle modifies the free-field T-operator of the arbitrary surface. By projecting the free-field T-operator of the surface onto a spherical basis the authors derive an infinite system of linear equations to determine the coupling of the free-field T-matrix of the particle at each order of perturbation theory. In contrast, for the acoustic scattering from an elastic shell in a waveguide Hackmann and Sammelmann consider that the free-field T-operator of the surface modifies the free-field T-matrix of the particle. In this context, the free-field T-matrix of the particle is projected onto a rectangular basis and an integral equation for the spectral amplitudes of the fields even in zeroth order perturbation theory is derived.

In the present contribution we use the field decomposition method and the free-field T-matrix approach [11] to analyze scattering from a particle situated on or near an infinite surface. The method takes into account that the incident field strikes the particle either directly or after interacting with the surface, while the fields emanating from the particle may also reflect off the surface and interact with the particle again. The reflected scattered field or the interacting field is computed in the context of a T-operator formalism using the integral representation of spherical vector wave functions over plane waves. For these fields we assume expansions in terms of regular or radiating spherical vector wave functions. The transition matrix, or the free-field T-matrix relates the expansion coefficients of the incident fields to the scattered field. However, for some special scattering configurations such an approach is expected to fail as a consequence of the geometrical constraints of the T-matrix method. The expansion of the scattered field in terms of radiating multipoles is valid outside the circumscribed sphere of the scatterer, and in general this fact generates restrictions in applying the T-matrix method for analyzing multiple scattering problem. For example, in the case of an oblate particle situated upon a wafer surface the circumscribed sphere intersects the plane interface, and consequently the geometrical constraints of the T-matrix method are violated.

2 Geometry of the Scattering Problem

The geometry of the scattering system is shown in Fig. 1. An axisymmetric particle is situated above an infinite surface S. The surface S separates the two half-spaces D_0 and D_1, and is assumed to be sufficiently regular for application of Green's theorem. We choose the origin of a rectangular coordinate system $Oxyz$ at a distance z_0 above the mean plane Σ of the surface S, and assume that the surface is bounded by two parallel planes $z = z_>$ and $z = z_<$. The normal to these planes defines the z axis. We assume that the z axis is directed into D_0 and coincides with the particle symmetry axis. The half-spaces D_0 and D_1 are considered to be isotropic, homogeneous, and non-magnetic, i.e. $\mu_0 = \mu_1 = \mu$. The incident radiation is a plane wave traveling in the xz plane, oriented at angle β_{inc} with respect to the z axis. The wave-numbers in each region are denoted by $k_0 = \omega(\varepsilon_0\mu)^{1/2}$ and $k_1 = \omega(\varepsilon_1\mu)^{1/2}$, respectively.

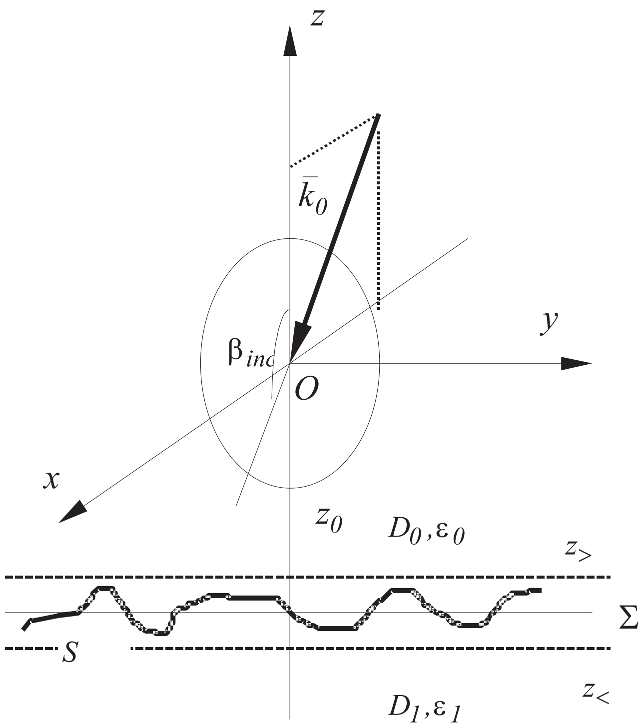

Fig. 1. Geometry of the scattering system.

3 Scattering by Infinite Surfaces

Before analyzing the multiple scattering problem we digress and present in this section the fundaments of the T-operator formalism for solving the scattering problem by infinite surfaces. This approach will be used latter for computing the scattering characteristics of an axisymmetric particle in the presence of an infinite surface. Our presentation closely follows the guidelines given by Kristensson [12].

3.1 Notations and Mathematical Formulation of the Scattering Problem

Let us consider the scattering problem of an infinite surface S illuminated by the incident wave field $(\mathbf{E}_{inc}(\mathbf{r}), \mathbf{H}_{inc}(\mathbf{r}))$. The mathematical formulation of the boundary value problem consists in Maxwell's equations

$$\begin{aligned} \nabla \times \mathbf{E}_p(\mathbf{r}) &= j\omega\mu\, \mathbf{H}_p(\mathbf{r}) \\ \nabla \times \mathbf{H}_p(\mathbf{r}) &= -j\omega\varepsilon_p \mathbf{E}_p(\mathbf{r}), \quad p = 0, 1 \end{aligned} \tag{1}$$

the boundary condition at the surface S

$$\begin{aligned} \mathbf{n} \times [\mathbf{E}_0(\mathbf{r}) + \mathbf{E}_{inc}(\mathbf{r}) - \mathbf{E}_1(\mathbf{r})] &= 0 \\ \mathbf{n} \times [\mathbf{H}_0(\mathbf{r}) + \mathbf{H}_{inc}(\mathbf{r}) - \mathbf{H}_1(\mathbf{r})] &= 0 \end{aligned} \tag{2}$$

and the radiation/attenuation conditions for the fields in the half-spaces at infinity. Here, $\mathbf{n}$ is the unit normal vector to the interface pointing into region D_0. Assuming $Im(k_{0,1}) > 0$ then, there is a unique solution of the boundary value problem (1)-(2).

In the following we will extensively use representations of electromagnetic fields in terms of vector plane waves. We briefly recall the definitions and the basic properties of scalar and vector plane waves [13]. The scalar plane wave is defined by

$$\chi(\mathbf{r}, \mathbf{K}_\pm) = \exp(j\mathbf{K}_\pm \cdot \mathbf{r}) = \exp[j(K_x x + K_y y \pm K_z z)] \tag{3}$$

where $\mathbf{K}_\pm = K_x \mathbf{e}_x + K_y \mathbf{e}_y \pm K_z \mathbf{e}_z$. Using the notation $\lambda = \sqrt{K_x^2 + K_y^2}$, K_z can be expressed as $K_z = \sqrt{k^2 - \lambda^2}$, where the square root is always chosen to have a positive imaginary part. For real k , K_z is given by $K_z = \sqrt{k^2 - \lambda^2}$, if $\lambda \leq k$, and by $K_z = j\sqrt{\lambda^2 - k^2}$ if $\lambda > k$. The case $\lambda \leq k$ corresponds to harmonic propagating waves, while the case $\lambda > k$ corresponds to evanescent waves.

The vector waves $\mathbf{M}(\mathbf{r}, \mathbf{K}_\pm)$ and $\mathbf{N}(\mathbf{r}, \mathbf{K}_\pm)$ are defined in terms of the scalar plane waves as

$$\begin{aligned} \mathbf{M}(\mathbf{r}, \mathbf{K}_\pm) &= \nabla \times [\mathbf{e}_z \chi(\mathbf{r}, \mathbf{K}_\pm)] / \lambda = j(\mathbf{K}_T / |\mathbf{K}_T|) \chi(\mathbf{r}, \mathbf{K}_\pm) \\ \mathbf{N}(\mathbf{r}, \mathbf{K}_\pm) &= \nabla \times \mathbf{M}(\mathbf{r}, \mathbf{K}_\pm)/k = -\left[(\mathbf{K}_\pm / |\mathbf{K}_\pm|) \times (\mathbf{K}_T / |\mathbf{K}_T|)\right] \chi(\mathbf{r}, \mathbf{K}_\pm) \end{aligned} \tag{4}$$

Here, $\mathbf{K}_T = \mathbf{K}_\pm \times \mathbf{e}_z = K_y \mathbf{e}_x - K_x \mathbf{e}_y$ is the transverse component of the wave vector $\mathbf{K}_\pm$. The orthogonality relations

$$\begin{aligned} \int_\Sigma \mathbf{M}(\mathbf{r}, \mathbf{K}_\pm) \mathbf{M}(-\mathbf{r}, \mathbf{K}_\pm^{'})\, dxdy &= (2\pi)^2 \delta(K_x - K_x^{'}, K_y - K_y^{'}) \\ \int_\Sigma \mathbf{N}(\mathbf{r}, \mathbf{K}_\pm) \mathbf{N}(-\mathbf{r}, \mathbf{K}_\pm^{'})\, dxdy &= (2\pi)^2 \delta(K_x - K_x^{'}, K_y - K_y^{'}) \\ \int_\Sigma \mathbf{M}(\mathbf{r}, \mathbf{K}_\pm) \mathbf{N}(-\mathbf{r}, \mathbf{K}_\pm^{'})\, dxdy &= \int_\Sigma \mathbf{N}(\mathbf{r}, \mathbf{K}_\pm) \mathbf{M}(-\mathbf{r}, \mathbf{K}_\pm^{'})\, dxdy = 0 \end{aligned} \tag{5}$$

hold on a plane Σ, $z = const$, where $|\mathbf{K}_{\pm}|^2 = |\mathbf{K}'_{\pm}|^2 = k^2$, $\mathbf{M}(-\mathbf{r}, \mathbf{K}_{\pm}) = \nabla \times \left[\mathbf{e}_z \chi(-\mathbf{r}, \mathbf{K}_{\pm})\right] / \lambda$ and $\mathbf{N}(-\mathbf{r}, \mathbf{K}_{\pm}) = \nabla \times \mathbf{M}(-\mathbf{r}, \mathbf{K}_{\pm})/k$. We note here the alternative expressions for the vector plane waves: $\mathbf{M}(\mathbf{r}, \mathbf{K}_{\pm}) = -j\mathbf{e}_{\alpha}\chi(\mathbf{r}, \mathbf{K}_{\pm})$ and $\mathbf{N}(\mathbf{r}, \mathbf{K}_{\pm}) = -\mathbf{e}_{\beta}\chi(\mathbf{r}, \mathbf{K}_{\pm})$, where $(\mathbf{e}_k, \mathbf{e}_{\beta}, \mathbf{e}_{\alpha})$ are the spherical unit vectors in the $\mathbf{K}$-space.

Now, let us apply the Huygens principle or the extinction theorem to a surface consisting of a finite part of S and a lower half sphere. Let the radius of the sphere go to infinity and assume the integrals over S exist, and furthermore that the integrals over the lower half-space vanish (radiation conditions). We get

$$\left.\begin{matrix}\mathbf{E}(\mathbf{r}) \\ 0\end{matrix}\right\} = \mathbf{E}_{inc}(\mathbf{r}) + \int_S \left[\mathbf{n} \times \mathbf{E}_1(\mathbf{r}')\right] \cdot \nabla' \times \overline{\overline{\mathbf{G}}}{}^0_{e0}(\mathbf{r}', \mathbf{r}) + \left[\mathbf{n} \times \nabla \times \mathbf{E}_1(\mathbf{r}')\right] \cdot \overline{\overline{\mathbf{G}}}{}^0_{e0}(\mathbf{r}', \mathbf{r})\, dS\,, \quad \left\{\begin{matrix}\mathbf{r} \in D_0 \\ \mathbf{r} \in D_1\end{matrix}\right. \tag{6}$$

Here, $\mathbf{E}(\mathbf{r}) = \mathbf{E}_{inc}(\mathbf{r}) + \mathbf{E}_0(\mathbf{r})$ is the total field in region D_0 and $\overline{\overline{\mathbf{G}}}{}^0_{e0}(\mathbf{r}', \mathbf{r})$ is the free-space dyadic Green function of wavenumber k_0. The superscript (0) indicates that the free-space dyadic corresponds to region D_0. Since the T-matrix formalism is based on suitable expansions of the Green's dyadic we use the plane wave expansion. This type of expansion has been extensively analyzed in the literature [12,13] and is of the form

$$\overline{\overline{\mathbf{G}}}{}^0_{e0}(\mathbf{r}', \mathbf{r}) = \frac{j}{8\pi^2} \int_{R^2} \left[\mathbf{M}(-\mathbf{r}', \mathbf{K}^0_+)\,\mathbf{M}(\mathbf{r}, \mathbf{K}^0_+) + \mathbf{N}(-\mathbf{r}', \mathbf{K}^0_+)\,\mathbf{N}(\mathbf{r}, \mathbf{K}^0_+)\right] \frac{dK^0_x dK^0_y}{K^0_z} \tag{7}$$

when $z > z'$, and

$$\overline{\overline{\mathbf{G}}}{}^0_{e0}(\mathbf{r}', \mathbf{r}) = \frac{j}{8\pi^2} \int_{R^2} \left[\mathbf{M}(-\mathbf{r}', \mathbf{K}^0_-)\,\mathbf{M}(\mathbf{r}, \mathbf{K}^0_-) + \mathbf{N}(-\mathbf{r}', \mathbf{K}^0_-)\,\mathbf{N}(\mathbf{r}, \mathbf{K}^0_-)\right] \frac{dK^0_x dK^0_y}{K^0_z} \tag{8}$$

when $z < z'$.

3.2 T-Operator Formalism

We now turn to the derivation of a set of basic equations which will be used to compute the scattered field. The entire analysis can conveniently be broken down into the following steps:

(I) The external problem consisting in the null-field condition (6), for $\mathbf{r} \in D_1$, is analyzed. This problem is called the external problem, because the fields external to S are the same as in the original problem. The null-field condition asserts that for all points below the surface, the field due to the sources distributed over the surface must exactly extinguish the incident wave. Mathematically, the null-field condition gives an expression for the unknown surface current densities in terms of the incident wave. These equations are put in a form suitable for numerical solution by expansion of the various field quantities into plane waves.

(II) Once the surface current densities are determined the scattered field in the region D_0 is obtained by using the field representation (6), for $\mathbf{r} \in D_0$. We note that (6) simply asserts that, above the surface, the total field is the sum of the incident field and the radiation due to the sources distributed over the surface.

We begin by considering the null-field condition in the region D_1 and represent the incoming field as a superposition of plane waves, i.e.

$$\mathbf{E}_{inc}(\mathbf{r}) = \int\limits_{R^2} \left[A(\mathbf{K}_-^0)\,\mathbf{M}(\mathbf{r},\mathbf{K}_-^0) + B(\mathbf{K}_-^0)\,\mathbf{N}(\mathbf{r},\mathbf{K}_-^0)\right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0} \tag{9}$$

Assume that the integral representation is valid at least for $z < z_<$. The incoming field is as usual a prescribed field, whose sources are assumed to be situated in D_0. This means that in any case the sources are above the fictitious plane $z = z_<$ and an expansion of the incident field as in (9) can be found for a wide class of sources.

For an $\mathbf{r} \in D_1$ satisfying $z < z_<$, we insert the plane wave expansion of the Green's dyadic in (6) and due to the orthogonality properties of the plane vector waves (5) we get

$$\begin{aligned} A(\mathbf{K}_-^0) &= -\tfrac{jk_0^2}{8\pi^2} \int\limits_S \Big\{ \Big[\mathbf{n} \times \mathbf{E}_1(\mathbf{r}')\Big] \cdot \mathbf{N}(-\mathbf{r}',\mathbf{K}_-^0) \\ &\quad + (1/k_0)\Big[\mathbf{n}\times\nabla\times\mathbf{E}_1(\mathbf{r}')\Big] \cdot \mathbf{M}(-\mathbf{r}',\mathbf{K}_-^0)\Big\}\, dS \\ B(\mathbf{K}_-^0) &= -\tfrac{jk_0^2}{8\pi^2} \int\limits_S \Big\{ \Big[\mathbf{n} \times \mathbf{E}_1(\mathbf{r}')\Big] \cdot \mathbf{M}(-\mathbf{r}',\mathbf{K}_-^0) \\ &\quad + (1/k_0)\Big[\mathbf{n}\times\nabla\times\mathbf{E}_1(\mathbf{r}')\Big] \cdot \mathbf{N}(-\mathbf{r}',\mathbf{K}_-^0)\Big\}\, dS. \end{aligned} \tag{10}$$

The next step of the T-matrix formalism is the expansion of the surface current density $\mathbf{n} \times \mathbf{E}_1(\mathbf{r}')$ into a suitable complete sets of functions. By means of these expansion, an algorithm for eliminating the surface fields can be constructed. In this context we use the well known result which states that the tangential plane vector waves $\{\mathbf{n} \times \mathbf{M}(\mathbf{r},\mathbf{K}_-^1), \mathbf{n} \times \mathbf{N}(\mathbf{r},\mathbf{K}_-^1)\}$, with $K_x, K_y \in R^2$, are complete on $L^2(S)$ [9,12]. Hence, we represent the surface current density as a superposition of down-going plane waves, i.e.

$$\begin{aligned} \mathbf{n} \times \mathbf{E}_1(\mathbf{r}') = \int\limits_{R^2} & \left\{C(\mathbf{K}_-^1)\,c(\mathbf{K}_-^1)\ \left[\mathbf{n} \times \mathbf{M}(\mathbf{r},\mathbf{K}_-^1)\right]\right. \\ & \left. + D(\mathbf{K}_-^1)\,d(\mathbf{K}_-^1)\ \left[\mathbf{n} \times \mathbf{N}(\mathbf{r},\mathbf{K}_-^1)\right]\right\} dK_x^1 dK_y^1. \end{aligned} \tag{11}$$

We explicitly write the plane wave transmission coefficients in (11),

$$\begin{aligned} c &= 2K_z^0/(K_z^0 + K_z^1)\exp[-j(K_z^0 - K_z^1)z_0] \\ d &= 2mK_z^0/(m^2 K_z^0 + K_z^1)\exp[-j(K_z^0 - K_z^1)z_0] \end{aligned} \tag{12}$$

where m denotes the relative index of refraction of the half-space D_1, and the wave vectors $\mathbf{K}_-^0$ and $\mathbf{K}_-^1$ are related to each other by the Snell's law:

$$\lambda = \lambda_0 = \lambda_1 = \sqrt{(K_x^0)^2 + (K_y^0)^2} = \sqrt{(K_x^1)^2 + (K_y^1)^2}. \tag{13}$$

This expansion can now be inserted into Eq.(10) and we get

$$\begin{bmatrix} A(\mathbf{K}_-^0) \\ B(\mathbf{K}_-^0) \end{bmatrix} = \int_{R^2} \left[Q(\mathbf{K}_-^0, \mathbf{K}_-^1)\right] \begin{bmatrix} C(\mathbf{K}_-^1) \\ D(\mathbf{K}_-^1) \end{bmatrix} dK_x^1 dK_y^1 \tag{14}$$

where

$$\left[Q(\mathbf{K}_-^0, \mathbf{K}_-^1)\right] = \begin{bmatrix} Q^{11}(\mathbf{K}_-^0, \mathbf{K}_-^1) & Q^{12}(\mathbf{K}_-^0, \mathbf{K}_-^1) \\ Q^{21}(\mathbf{K}_-^0, \mathbf{K}_-^1) & Q^{22}(\mathbf{K}_-^0, \mathbf{K}_-^1) \end{bmatrix} \tag{15}$$

and

$$\begin{aligned} Q^{11}(\mathbf{K}_-^0, \mathbf{K}_-^1) &= -\tfrac{jk_0^2}{8\pi^2} c(\mathbf{K}_-^1) \int_S \Big\{ \left[\mathbf{n} \times \mathbf{M}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{N}(-\mathbf{r}', \mathbf{K}_-^0) \\ &\quad + m^2 \left[\mathbf{n} \times \mathbf{N}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{M}(-\mathbf{r}', \mathbf{K}_-^0) \Big\} dS \\ Q^{12}(\mathbf{K}_-^0, \mathbf{K}_-^1) &= -\tfrac{jk_0^2}{8\pi^2} d(\mathbf{K}_-^1) \int_S \Big\{ \left[\mathbf{n} \times \mathbf{N}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{N}(-\mathbf{r}', \mathbf{K}_-^0) \\ &\quad + m^2 \left[\mathbf{n} \times \mathbf{M}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{M}(-\mathbf{r}', \mathbf{K}_-^0) \Big\} dS \\ Q^{21}(\mathbf{K}_-^0, \mathbf{K}_-^1) &= -\tfrac{jk_0^2}{8\pi^2} c(\mathbf{K}_-^1) \int_S \Big\{ \left[\mathbf{n} \times \mathbf{M}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{M}(-\mathbf{r}', \mathbf{K}_-^0) \\ &\quad + m^2 \left[\mathbf{n} \times \mathbf{N}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{N}(-\mathbf{r}', \mathbf{K}_-^0) \Big\} dS \\ Q^{22}(\mathbf{K}_-^0, \mathbf{K}_-^1) &= -\tfrac{jk_0^2}{8\pi^2} d(\mathbf{K}_-^1) \int_S \Big\{ \left[\mathbf{n} \times \mathbf{N}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{M}(-\mathbf{r}', \mathbf{K}_-^0) \\ &\quad + m^2 \left[\mathbf{n} \times \mathbf{M}(\mathbf{r}', \mathbf{K}_-^1)\right] \cdot \mathbf{N}(-\mathbf{r}', \mathbf{K}_-^0) \Big\} dS\,. \end{aligned} \tag{16}$$

An inspection of (16) reveals that $Q^{\alpha\beta}(\mathbf{K}_-^0, \mathbf{K}_-^1)$, $\alpha, \beta = 1, 2$, are in general not functions in the usual sense and relations involving $Q^{\alpha\beta}(\mathbf{K}_-^0, \mathbf{K}_-^1)$ should be understood in a distributional sense. For a plane surface we have

$$Q^{11(plane)}(\mathbf{K}_-^0, \mathbf{K}_-^1) = Q^{22(plane)}(\mathbf{K}_-^0, \mathbf{K}_-^1) = (k_0 K_z^0)\delta(K_x^1 - K_x^0, K_y^1 - K_y^0) \tag{17}$$

and

$$Q^{12(plane)}(\mathbf{K}_-^0,\mathbf{K}_-^1) = Q^{21(plane)}(\mathbf{K}_-^0,\mathbf{K}_-^1) = 0. \tag{18}$$

In this case the system of integral equations (14) reduces to a system of algebraic equations

$$\begin{aligned} A(\mathbf{K}_-^0) &= (k_0 K_z^0) C(\mathbf{K}_-^1) \\ B(\mathbf{K}_-^0) &= (k_0 K_z^0) D(\mathbf{K}_-^1) \end{aligned} \tag{19}$$

where the wave vectors $\mathbf{K}_-^0$ and $\mathbf{K}_-^1$ are related to each other by the Snell's law. Obviously for solving the general case of an arbitrary surface, one has to invert a system of two-dimensional integral transforms and this usually constitutes a formidable analytic and numerical problem. We can formally assume that the inverse integral transform exists and consequently the solution to (14) may be written as

$$\begin{bmatrix} C(\mathbf{K}_-^1) \\ D(\mathbf{K}_-^1) \end{bmatrix} = \int\limits_{R^2} \left[Q(\mathbf{K}_-^0,\mathbf{K}_-^1)\right]^{-1} \begin{bmatrix} A(\mathbf{K}_-^0) \\ B(\mathbf{K}_-^0) \end{bmatrix} dK_x^0 dK_y^0. \tag{20}$$

We consider now the expression of the scattered field in the region D_0 given by (6). Expanding the dyadic Green function in terms of plane waves and inserting this expansion in Eq. (6) we get, for $z > z_>$,

$$\mathbf{E}_0(\mathbf{r}) = \int\limits_{R^2} \left[F(\mathbf{K}_+^0)\,\mathbf{M}(\mathbf{r},\mathbf{K}_+^0) + G(\mathbf{K}_+^0)\,\mathbf{N}(\mathbf{r},\mathbf{K}_+^0)\right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0}. \tag{21}$$

The vector amplitudes $F(\mathbf{K}_+^0)$ and $G(\mathbf{K}_+^0)$ are given by

$$\begin{aligned} F(\mathbf{K}_+^0) = \tfrac{jk_0^2}{8\pi^2} \int\limits_S & \Big\{ \left[\mathbf{n}\times\mathbf{E}_1(\mathbf{r}^{'})\right]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_+^0) \\ & +(1/k_0)\left[\mathbf{n}\times\nabla\times\mathbf{E}_1(\mathbf{r}^{'})\right]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_+^0)\Big\}\,dS \\ G(\mathbf{K}_+^0) = \tfrac{jk_0^2}{8\pi^2} \int\limits_S & \Big\{ \left[\mathbf{n}\times\mathbf{E}_1(\mathbf{r}^{'})\right]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_+^0) \\ & +(1/k_0)\left[\mathbf{n}\times\nabla\times\mathbf{E}_1(\mathbf{r}^{'})\right]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_+^0)\Big\}\,dS. \end{aligned} \tag{22}$$

Using the representation of the surface current densities $\mathbf{n}\times\mathbf{E}_1(\mathbf{r}^{'})$ in terms of down-going plane waves (11), we obtain a relation between the amplitudes of the field in the region D_0, $F(\mathbf{K}_+^0)$ and $G(\mathbf{K}_+^0)$, and the amplitudes of the field in the region D_1, $C(\mathbf{K}_-^1)$ and $D(\mathbf{K}_-^1)$, i.e.

$$\begin{bmatrix} F(\mathbf{K}_+^0) \\ G(\mathbf{K}_+^0) \end{bmatrix} = \int\limits_{R^2} \left[P(\mathbf{K}_+^0,\mathbf{K}_-^1)\right] \begin{bmatrix} C(\mathbf{K}_-^1) \\ D(\mathbf{K}_-^1) \end{bmatrix} dK_x^1 dK_y^1 \tag{23}$$

where

$$\left[P(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\right]=\begin{bmatrix}P^{11}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\ P^{12}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\\ P^{21}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\ P^{22}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\end{bmatrix} \tag{24}$$

and

$$\begin{aligned}
P^{11}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= \tfrac{jk_0^2}{8\pi^2}c(\mathbf{K}_{-}^{1})\int\limits_{S}\Big\{\Big[\mathbf{n}\times\mathbf{M}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\\
&\quad +m^2\Big[\mathbf{n}\times\mathbf{N}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\Big\}\,dS\\
P^{12}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= \tfrac{jk_0^2}{8\pi^2}d(\mathbf{K}_{-}^{1})\int\limits_{S}\Big\{\Big[\mathbf{n}\times\mathbf{N}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\\
&\quad +m^2\Big[\mathbf{n}\times\mathbf{M}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\Big\}\,dS\\
P^{21}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= \tfrac{jk_0^2}{8\pi^2}c(\mathbf{K}_{-}^{1})\int\limits_{S}\Big\{\Big[\mathbf{n}\times\mathbf{M}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\\
&\quad +m^2\Big[\mathbf{n}\times\mathbf{N}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\Big\}\,dS\\
P^{22}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= \tfrac{jk_0^2}{8\pi^2}d(\mathbf{K}_{-}^{1})\int\limits_{S}\Big\{\Big[\mathbf{n}\times\mathbf{N}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{M}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\\
&\quad +m^2\Big[\mathbf{n}\times\mathbf{M}(\mathbf{r}^{'},\mathbf{K}_{-}^{1})\Big]\cdot\mathbf{N}(-\mathbf{r}^{'},\mathbf{K}_{+}^{0})\Big\}\,dS.
\end{aligned} \tag{25}$$

Combining (20) and (23) we are led to

$$\begin{aligned}
&\begin{bmatrix}F(\mathbf{K}_{+}^{0})\\ G(\mathbf{K}_{+}^{0})\end{bmatrix}\\
&=\int\limits_{R^2}\int\limits_{R^2}\left[P(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\right]\left[Q(\mathbf{K}_{-}^{\prime 0},\mathbf{K}_{-}^{1})\right]^{-1}\begin{bmatrix}A(\mathbf{K}_{-}^{\prime 0})\\ B(\mathbf{K}_{-}^{\prime 0})\end{bmatrix}dK_x^{\prime 0}dK_y^{\prime 0}dK_x^{1}dK_y^{1}\\
&=\int\limits_{R^2}\left[T(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{\prime 0})\right]\begin{bmatrix}A(\mathbf{K}_{-}^{\prime 0})\\ B(\mathbf{K}_{-}^{\prime 0})\end{bmatrix}dK_x^{\prime 0}dK_y^{\prime 0}
\end{aligned} \tag{26}$$

where

$$\left[T(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{\prime 0})\right]=\int\limits_{R^2}\left[P(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})\right]\left[Q(\mathbf{K}_{-}^{\prime 0},\mathbf{K}_{-}^{1})\right]^{-1}dK_x^{1}dK_y^{1} \tag{27}$$

is the $T-$operator of the infinite surface. For a plane surface we have

$$\begin{aligned}
P^{11(plane)}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= (k_0K_z^0)a(\mathbf{K}_{+}^{0})\delta(K_x^1-K_x^0,K_y^1-K_y^0)\\
P^{22(plane)}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1}) &= (k_0K_z^0)b(\mathbf{K}_{+}^{0})\delta(K_x^1-K_x^0,K_y^1-K_y^0)
\end{aligned} \tag{28}$$

and

$$P^{12(plane)}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})=P^{21(plane)}(\mathbf{K}_{+}^{0},\mathbf{K}_{-}^{1})=0. \tag{29}$$

Here,

$$\begin{aligned} a(\mathbf{K}_+^0) &= (K_z^0 - K_z^1)/(K_z^0 + K_z^1)\exp(-2jK_z^0 z_0) \\ b(\mathbf{K}_+^0) &= (m^2K_z^0 - K_z^1)/(m^2K_z^0 + K_z^1)\exp(-2jK_z^0 z_0) \end{aligned} \tag{30}$$

are the reflection coefficients for a plane interface. In this case we get

$$\begin{aligned} F(\mathbf{K}_+^0) &= (k_0K_z^0)a(\mathbf{K}_+^0)C(\mathbf{K}_-^1) = a(\mathbf{K}_+^0)A(\mathbf{K}_-^0) \\ G(\mathbf{K}_+^0) &= (k_0K_z^0)b(\mathbf{K}_+^0)D(\mathbf{K}_-^1) = b(\mathbf{K}_+^0)B(\mathbf{K}_-^0) \end{aligned} \tag{31}$$

and clearly,

$$\begin{aligned} T^{11(plane)}(\mathbf{K}_+^0, \mathbf{K}_-'^0) &= a(\mathbf{K}_+^0)\delta(K_x^0 - K_x'^0, K_y^0 - K_y'^0) \\ T^{22(plane)}(\mathbf{K}_+^0, \mathbf{K}_-'^0) &= b(\mathbf{K}_+^0)\delta(K_x^0 - K_x'^0, K_y^0 - K_y'^0). \end{aligned} \tag{32}$$

In (31) the wave vectors $\mathbf{K}_-^0$, $\mathbf{K}_+^0$ and $\mathbf{K}_-^1$ are related to each other by Snell's law. Actually, if $\mathbf{K}_-^0$ is an arbitrary incident wave vector, then $\mathbf{K}_+^0$ and $\mathbf{K}_-^1$ represents the reflected and the transmitted wave vectors, respectively.

We conclude this section by noting the expansion of an electromagnetic field expressed as a superposition of plane waves, i.e.

$$\mathbf{E}_0(\mathbf{r}) = \int_{R^2} \left[F(\mathbf{K}_+^0)\,\mathbf{M}(\mathbf{r},\mathbf{K}_+^0) + G(\mathbf{K}_+^0)\,\mathbf{N}(\mathbf{r},\mathbf{K}_+^0)\right] \frac{dK_x^0 dK_y^0}{k_0K_z^0} \tag{33}$$

in terms of regular spherical vector wave functions. We assume that the integral converges for $z > z_{\min}$, where $z_{\min} < 0$, and transform the integration over the rectangular components of the wave vector into an integration over polar angles, i.e.

$$\mathbf{E}_0(\mathbf{r}) = -\int_0^{2\pi}\int_{C_+} [jF(\alpha,\beta)\mathbf{e}_\alpha + G(\alpha,\beta)\mathbf{e}_\beta] \exp\left(\mathbf{K}_+^0 \cdot \mathbf{r}\right) \sin\beta d\beta d\alpha. \tag{34}$$

Here $\mathbf{K}_+^0 = (k_0\sin\beta\cos\alpha, k_0\sin\beta\sin\alpha,\ k_0\cos\beta)$, and the complex angle β belongs to the curve C_+ . The contour C_+ corresponds to an integration path in the complex plane from 0 to $\pi/2 - j\infty$. Each plane wave in the integrand (34) can be expanded in terms of spherical vector wave functions,

$$\begin{aligned} \begin{pmatrix} \mathbf{e}_\beta \\ \mathbf{e}_\alpha \end{pmatrix} \exp\left(\mathbf{K}^0 \cdot \mathbf{r}\right) = -\sum_{n=1}^{\infty}\sum_{m=-n}^{n} 4j^n D_{mn} &\left[\begin{pmatrix} jm\pi_n^{|m|}(\beta) \\ \tau_n^{|m|}(\beta) \end{pmatrix} \mathbf{M}_{mn}^1(k\mathbf{r}) \right. \\ &\left. + \begin{pmatrix} j\tau_n^{|m|}(\beta) \\ m\pi_n^{|m|}(\beta) \end{pmatrix} \mathbf{N}_{mn}^1(k\mathbf{r}) \right] e^{-jm\alpha} \end{aligned} \tag{35}$$

where $\pi_n^{|m|}(\theta) = P_n^{|m|}(\cos\theta)/\sin\theta, \tau_n^{|m|}(\theta) = dP_n^{|m|}(\cos\theta)/d\theta,$ and $P_n^{|m|}(\cos\theta)$ are the associated Legendre polynomials. This expansion is valid not only for propagating waves, but also for evanescent waves when the analytic continuation of the Legendre functions for complex arguments is evaluated on the physical Riemann sheet. Consequently, the desired spherical waves expansion is

$$\mathbf{E}_0(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} D_{mn} \left[a_{mn} \mathbf{M}^1_{mn}(k\mathbf{r}) + b_{mn} \mathbf{N}^1_{mn}(k\mathbf{r}) \right] \tag{36}$$

where

$$\begin{aligned} a_{mn} &= 4j^{n+1} \int_0^{2\pi} \int_{C_+} \left[F(\alpha,\beta)\tau_n^{|m|}(\beta) + G(\alpha,\beta) m\pi_n^{|m|}(\beta) \right] e^{-jm\alpha} \sin\beta d\beta d\alpha \\ b_{mn} &= 4j^{n+1} \int_0^{2\pi} \int_{C_+} \left[F(\alpha,\beta) m\pi_n^{|m|}(\beta) + G(\alpha,\beta)\tau_n^{|m|}(\beta) \right] e^{-jm\alpha} \sin\beta d\beta d\alpha. \end{aligned} \tag{37}$$

Note, that if the radius of convergence for the series (36) is $R_{\max}$, then (36) is a valid representation for the electromagnetic field (33) if $R_{\max} \leq |z_{\min}|$.

4 T-Matrix Method

In this section we consider the multiple scattering problem of a particle in the presence of an infinite surface. Using the field decomposition method we simplify the boundary value problem to single scattering problems.

4.1 Formal Solution for an Arbitrary Interface

Let us return to our original scattering problem depicted in Fig. 1. The incident plane wave strikes the particle either directly or after interacting with the surface. We assume that the direct field and the reflected incident field can be expressed as a series of regular spherical vector wave functions (SVWF) $\mathbf{M}^1_{mn_1}(k_0\mathbf{r})$ and $\mathbf{N}^1_{mn_1}(k_0\mathbf{r})$, i.e.

$$\mathbf{E}_{inc}(\mathbf{r}) = \sum_{n_1=1}^{\infty} \sum_{m=-n_1}^{n_1} D_{mn_1} [a_{mn_1} \mathbf{M}^1_{mn_1}(k_0\mathbf{r}) + b_{mn_1} \mathbf{N}^1_{mn_1}(k_0\mathbf{r})] \tag{38}$$

and

$$\mathbf{E}^R_{inc}(\mathbf{r}) = \sum_{n_1=1}^{\infty} \sum_{m=-n_1}^{n_1} D_{mn_1} [a^R_{mn_1} \mathbf{M}^1_{mn_1}(k_0\mathbf{r}) + b^R_{mn_1} \mathbf{N}^1_{mn_1}(k_0\mathbf{r})]. \tag{39}$$

Here, D_{mn_1} is a normalization constant and is given by

$$D_{mn_1} = \frac{2n_1+1}{4n_1(n_1+1)} \cdot \frac{(n_1-|m|)!}{(n_1+|m|)!}. \tag{40}$$

Explicit expressions for the expansion coefficients a_{mn_1} and b_{mn_1} corresponding to a plane wave incidence in the $(0, \beta_{inc})$ direction can be found in [14].

The scattered field is also expressed in terms of radiating SVWF:

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} D_{mn}[e_{mn}\mathbf{M}^3_{mn}(k\mathbf{r}) + f_{mn}\mathbf{N}^3_{mn}(k\mathbf{r})] \tag{41}$$

and this expansion is valid outside a sphere enclosing the scatterer.

In addition to the three fields described by (38), (39) and (41), a fourth field exists in the ambient medium. This field, which for convenience is called the interacting field, is a result of the scattered field reflecting off the surface and striking the particle again. The interacting field can be expressed in the following form

$$\mathbf{E}^R_{sca}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} D_{mn}[e_{mn}\mathbf{M}^{3,R}_{mn}(k\mathbf{r}) + f_{mn}\mathbf{N}^{3,R}_{mn}(k\mathbf{r})] \tag{42}$$

where $\mathbf{M}^{3,R}_{mn}(k\mathbf{r})$ and $\mathbf{N}^{3,R}_{mn}(k\mathbf{r})$ denote the radiating SVWF reflected by the surface. For $\mathbf{r}$ inside a sphere enclosed in the particle and a given azimuthal mode m the reflected SVWF are given by:

$$\begin{pmatrix} \mathbf{M}^{3,R}_{mn}(k\mathbf{r}) \\ \mathbf{N}^{3,R}_{mn}(k\mathbf{r}) \end{pmatrix} = \sum_{n_1=1}^{\infty} D_{mn_1} \left[\begin{pmatrix} \alpha_{mnn_1} \\ \gamma_{mnn_1} \end{pmatrix} \mathbf{M}^1_{mn_1}(k\mathbf{r}) + \begin{pmatrix} \beta_{mnn_1} \\ \delta_{mnn_1} \end{pmatrix} \mathbf{N}^1_{mn_1}(k\mathbf{r}) \right]. \tag{43}$$

Substituting (43) into (42) we get a representation of the interacting field in terms of regular SVWF, i.e.

$$\mathbf{E}^R_{sca}(\mathbf{r}) = \sum_{n_1=1}^{\infty} \sum_{m=-n_1}^{n_1} D_{mn_1}[e^R_{mn_1}\mathbf{M}^1_{mn_1}(k\mathbf{r}) + f^R_{mn_1}\mathbf{N}^1_{mn_1}(k\mathbf{r})] \tag{44}$$

where

$$\begin{pmatrix} e^R_{mn_1} \\ f^R_{mn_1} \end{pmatrix} = \sum_{n_1=1}^{\infty} D_{mn} \left[\begin{pmatrix} \alpha_{mnn_1} \\ \gamma_{mnn_1} \end{pmatrix} e_{mn} + \begin{pmatrix} \beta_{mnn_1} \\ \delta_{mnn_1} \end{pmatrix} f_{mn} \right]. \tag{45}$$

In the T-matrix method the scattered field coefficients are related to the expansion coefficients of the fields striking the particle by the transition matrix. For an axisymmetric particle the equations become decoupled, permitting a separate solution for each azimuthal mode. For a fixed azimuthal mode

m we truncate the expansions given in (38), (39), (41) and (44) and get the following matrix equation for the scattering problem:

$$\begin{bmatrix} e_{mn} \\ f_{mn} \end{bmatrix} = [T_{mnn_1}] \cdot \left(\begin{bmatrix} a_{mn_1} \\ b_{mn_1} \end{bmatrix} + \begin{bmatrix} a^R_{mn_1} \\ b^R_{mn_1} \end{bmatrix} + \begin{bmatrix} e^R_{mn_1} \\ f^R_{mn_1} \end{bmatrix} \right) . \tag{46}$$

Here, $m = \overline{-M, M}$ and $n, n_1 = \overline{1, N}$, where M is the number of azimuthal modes and N is the truncation index. The explicit form of the transition matrix $[T_{mnn_1}]$ can be found in [12]. The expansion coefficients of the interacting field are related to the scattered field coefficients by a so called reflection matrix

$$\begin{bmatrix} e^R_{mn_1} \\ f^R_{mn_1} \end{bmatrix} = [A_{mn_1n}] \cdot \begin{bmatrix} e_{mn} \\ f_{mn} \end{bmatrix} \tag{47}$$

where, accordingly to (45)

$$[A_{mn_1n}] = \begin{bmatrix} D_{mn}\alpha_{mnn_1} & D_{mn}\gamma_{mnn_1} \\ D_{mn}\beta_{mnn_1} & D_{mn}\delta_{mnn_1} \end{bmatrix} \tag{48}$$

The scattered field coefficients e_{mn} and f_{mn} are obtained by combining matrix equations (46) and (47).

The main problem which must be solved is the calculation of the reflection matrix. In order to master this problem it is necessary to compute the reflection of a plane wave and a radiating spherical vector wave function by the infinite surface. Thus, we have to solve the single scattering problem of an infinite surface. Actually, we need not only to compute the reflected fields $\mathbf{E}^R_{inc}$ and $\mathbf{M}^{3,R}_{mn}$ and $\mathbf{N}^{3,R}_{mn}$, but also to expand these fields in terms of regular spherical vector wave functions. Essentially, this can be done by using the T-operator formalism discussed in Sect. 2. It is noted that application of the T-operator formalism requires the representation of incident fields as integrals over plane waves.

In this context, let us write the incident plane wave as

$$\begin{aligned} \mathbf{E}_{inc}(\mathbf{r}) &= (E_{\beta_{inc}}\mathbf{e}_{\beta_{inc}} + E_{\alpha_{inc}}\mathbf{e}_{\alpha_{inc}}) \exp\left(j\mathbf{K}^{0inc}_{-} \cdot \mathbf{r}\right) \\ &= \int\limits_{R^2} \left[A_{inc}(\mathbf{K}^0_-)\,\mathbf{M}(\mathbf{r}, \mathbf{K}^0_-) + B_{inc}(\mathbf{K}^0_-)\,\mathbf{N}(\mathbf{r}, \mathbf{K}^0_-)\right] \frac{dK^0_x dK^0_y}{k_0 K^0_z} \end{aligned} \tag{49}$$

where

$$\begin{aligned} A_{inc}(\mathbf{K}^0_-) &= jE_{\alpha_{inc}}\left(k_0 K^0_z\right) \delta(K^0_x - K^{0inc}_x, K^0_y - K^{0inc}_y) \\ B_{inc}(\mathbf{K}^0_-) &= -E_{\beta_{inc}}\left(k_0 K^0_z\right) \delta(K^0_x - K^{0inc}_x, K^0_y - K^{0inc}_y) \end{aligned} \tag{50}$$

Then, the corresponding reflected field takes on the form

$$\mathbf{E}^R_{inc}(\mathbf{r}) = \int\limits_{R^2} \left[F_{inc}(\mathbf{K}^0_+)\,\mathbf{M}(\mathbf{r}, \mathbf{K}^0_+) + G_{inc}(\mathbf{K}^0_+)\,\mathbf{N}(\mathbf{r}, \mathbf{K}^0_+)\right] \frac{dK^0_x dK^0_y}{k_0 K^0_z} . \tag{51}$$

In (49) $E_{\beta_{inc}}$ and $E_{\alpha_{inc}}$ are the parallel and perpendicular component of the electric field, respectively. The spectral amplitudes $F_{inc}(\mathbf{K}_{+}^{0})$ and $G_{inc}(\mathbf{K}_{+}^{0})$ are computed according to (26).

Now, we write the radiating SVWF as integrals over plane waves traveling into various directions [12,15]

$$\begin{pmatrix} \mathbf{M}_{mn}^{3}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3}(k\mathbf{r}) \end{pmatrix} = \int_{R^2} \left[\begin{pmatrix} A_s(\mathbf{K}_{-}^{0}) \\ B_s(\mathbf{K}_{-}^{0}) \end{pmatrix} \mathbf{M}(\mathbf{r}, \mathbf{K}_{-}^{0}) + \begin{pmatrix} B_s(\mathbf{K}_{-}^{0}) \\ A_s(\mathbf{K}_{-}^{0}) \end{pmatrix} \mathbf{N}(\mathbf{r}, \mathbf{K}_{-}^{0}) \right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0} \tag{52}$$

where

$$\begin{aligned} A_s(\mathbf{K}_{-}^{0}) &= \tfrac{1}{2\pi j^{n+1}} \tau_n^{|m|}(\beta) e^{jm\alpha} \\ B_s(\mathbf{K}_{-}^{0}) &= \tfrac{1}{2\pi j^{n+1}} m \pi_n^{|m|}(\beta) e^{jm\alpha} \end{aligned} \tag{53}$$

and $\mathbf{K}_{-}^{0} = (k_0 \sin\beta \cos\alpha,\ k_0 \sin\beta \sin\alpha, -k_0 \cos\beta)$. Representations (52) are valid for $z < 0$ since only then the integrals converge. Hence, application of $T-$operator formalism leads to

$$\begin{pmatrix} \mathbf{M}_{mn}^{3R}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3R}(k\mathbf{r}) \end{pmatrix} = \int_{R^2} \left[\begin{pmatrix} F_s(\mathbf{K}_{+}^{0}) \\ G_s(\mathbf{K}_{+}^{0}) \end{pmatrix} \mathbf{M}(\mathbf{r}, \mathbf{K}_{+}^{0}) + \begin{pmatrix} G_s(\mathbf{K}_{+}^{0}) \\ F_s(\mathbf{K}_{+}^{0}) \end{pmatrix} \mathbf{N}(\mathbf{r}, \mathbf{K}_{+}^{0}) \right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0} \tag{54}$$

where the spectral amplitudes $F_s(\mathbf{K}_{+}^{0})$ and $G_s(\mathbf{K}_{+}^{0})$ are computed according to (26). Analog to the previous case the expansion coefficients in (43) are given by (37) and therefore the reflection matrix can be computed according to (48). The solution given above is formal and in practice of limited use since we assumed the invertibility of the integral equation (14). As stated before equations with a continuous variable often lead to inversion of integral equations which is a delicate problem for numerical calculations. The usefulness of the formalism in numerical applications will to a large degree depend upon the possibility of discretizing (14) in a suitable way. This can be done for a class of simple infinite surfaces as for example the plane surface or surfaces with periodic roughness and small amplitude roughness. In the following we specialize the above formalism to scattering from a plane surface for which an exact solution is obtained.

4.2 Exact Solution for a Plane Interface

For a plane surface, (14) and (23) will degenerate to just simple algebraic expressions and the inversion is trivial. Accounting of (19) and (31) we get the following expression for the reflected incident field:

$$\mathbf{E}_{inc}^{R}(\mathbf{r}) = \int_{R^2} \left[A_{inc}(\mathbf{K}_-^0) a(\mathbf{K}_+^0)\, \mathbf{M}(\mathbf{r},\mathbf{K}_+^0) + B_{inc}(\mathbf{K}_-^0) b(\mathbf{K}_+^0)\, \mathbf{N}(\mathbf{r},\mathbf{K}_+^0)\right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0}. \tag{55}$$

Here $\mathbf{K}_-^0$ and $\mathbf{K}_+^0$ are related to each other by Snell's law, that means $\mathbf{K}_\pm^0 = \left(K_x^0, K_y^0, \pm K_z^0\right)$. As expected, denoting by $\mathbf{K}_+^{0inc}$ the reflected wave vector corresponding to the incident wave vector $\mathbf{K}_-^{0inc}$, and by $\alpha_{inc,r}$ and $\beta_{inc,r}$ the angular spherical coordinates of $\mathbf{K}_+^{0inc}$, where $\alpha_{inc,r} = \alpha_{inc}$ and $\beta_{inc,r} = \pi - \beta_{inc}$, we find

$$\mathbf{E}_{inc}^{R}(\mathbf{r}) = \left(E_{\beta_{inc}} b(\beta_{inc,r}) \mathbf{e}_{\beta_{inc,r}} + E_{\alpha_{inc}} a(\beta_{inc,r}) \mathbf{e}_{\alpha_{inc,r}}\right) \exp\left(j\mathbf{K}_+^{0inc} \cdot \mathbf{r}\right). \tag{56}$$

In this context, the coefficients $a_{mn_1}^R$ and $b_{mn_1}^R$ appearing in (39) are the expansion coefficients of a plane wave traveling in the $(0, \beta_{inc,r})$ direction.

We turn now our attention to the reflection of a spherical multipole in the case of a plane interface. The simplified expressions for $\mathbf{M}_{mn}^{3R}(k\mathbf{r})$ and $\mathbf{N}_{mn}^{3R}(k\mathbf{r})$ take on the forms

$$\begin{pmatrix} \mathbf{M}_{mn}^{3R}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3R}(k\mathbf{r}) \end{pmatrix} = \int_{R^2} \left[\begin{pmatrix} A_s(\mathbf{K}_-^0) \\ B_s(\mathbf{K}_-^0) \end{pmatrix} a(\mathbf{K}_+^0)\, \mathbf{M}(\mathbf{r},\mathbf{K}_+^0) + \begin{pmatrix} B_s(\mathbf{K}_-^0) \\ A_s(\mathbf{K}_-^0) \end{pmatrix} b(\mathbf{K}_+^0) \mathbf{N}(\mathbf{r},\mathbf{K}_+^0) \right] \frac{dK_x^0 dK_y^0}{k_0 K_z^0}. \tag{57}$$

Denoting the angular coordinates of $\mathbf{K}_+^0$ and $\mathbf{K}_-^0$ by (α_r, β_r) and (α, β), respectively, where $\alpha = \alpha_r$ and $\beta = \pi - \beta_r$, and transforming the integration over the rectangular components of the wave vector into an integration over polar angles, we get

$$\begin{pmatrix} \mathbf{M}_{mn}^{3R}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3R}(k\mathbf{r}) \end{pmatrix} = -\frac{1}{2\pi j^{n+1}} = \int_0^{2\pi} \int_{C_-} \left[\begin{pmatrix} m\pi_n^{|m|}(\beta) \\ \tau_n^{|m|}(\beta) \end{pmatrix} b(\beta_r) \mathbf{e}_{\beta_R} + j \begin{pmatrix} \tau_n^{|m|}(\beta) \\ m\pi_n^{|m|}(\beta) \end{pmatrix} a(\beta_r) \mathbf{e}_{\alpha_R} \right] \times \exp(jm\alpha) \exp(j\mathbf{K}_+^0 \cdot \mathbf{r}) \sin\beta d\beta d\alpha \tag{58}$$

It is noted that the contour C_- corresponds to an integration path in the complex plane from $\pi/2 + j\infty$ to π. Clearly, each elementary plane wave in the integrand of (58) represents the reflection of the corresponding elementary incident wave in the integrand of (52), taking into account the Fresnel reflection coefficients at the interface. Making use of the spherical waves expansion (43), we find that the elements of the reflection matrix are given by

$$\begin{aligned}
\alpha_{mnn_1} &= 4j^{n_1-n} \int\limits_{C_-} \Big[m^2 \pi_n^{|m|}(\beta) \pi_{n_1}^{|m_1|}(\pi-\beta) b(\pi-\beta) \\
&\quad + \tau_n^{|m|}(\beta) \tau_{n_1}^{|m_1|}(\pi-\beta) a(\pi-\beta) \Big] \sin\beta d\beta \\
\beta_{mnn_1} &= 4j^{n_1-n} \int\limits_{C_-} m \Big[\pi_n^{|m|}(\beta) \tau_{n_1}^{|m_1|}(\pi-\beta) b(\pi-\beta) \\
&\quad + \tau_n^{|m|}(\beta) \pi_{n_1}^{|m_1|}(\pi-\beta)(\pi-\beta) \Big] \sin\beta d\beta \\
\gamma_{mnn_1} &= 4j^{n_1-n} \int\limits_{C_-} m \Big[\tau_n^{|m|}(\beta) \pi_{n_1}^{|m_1|}(\pi-\beta) b(\pi-\beta) \\
&\quad + \pi_n^{|m|}(\beta) \tau_{n_1}^{|m_1|}(\pi-\beta) a(\pi-\beta) \Big] \sin\beta d\beta \\
\delta_{mnn_1} &= 4j^{n_1-n} \int\limits_{C_-} \Big[\tau_n^{|m|}(\beta) \tau_{n_1}^{|m_1|}(\pi-\beta) b(\pi-\beta) \\
&\quad + m^2 \pi_n^{|m|}(\beta) \pi_{n_1}^{|m_1|}(\pi-\beta) a(\pi-\beta) \Big] \sin\beta d\beta .
\end{aligned} \tag{59}$$

4.3 Approximate T-Matrix Method

An approximate expression for the reflected spherical waves can be found if one assumes that the interacting radiation strikes the surface at normal incidence. A Fresnel reflection at normal incidence is used to account for the reflection loss at the interface. Writing

$$\begin{aligned}
a(\beta_r) &= \widehat{a}(\beta_r) \exp(-2jk_0 z_0 \cos\beta_r) \\
b(\beta_r) &= \widehat{b}(\beta_r) \exp(-2jk_0 z_0 \cos\beta_r)
\end{aligned} \tag{60}$$

assuming

$$r(0) = \widehat{a}(\beta_r) = -\widehat{b}(\beta_r), \tag{61}$$

changing the integration variable from β to $\beta_R = \pi - \beta,$ and using

$$\begin{aligned}
\pi_n^{|m|}(\pi-\beta_R) &= (-1)^{n-|m|} \pi_n^{|m|}(\beta_R) \\
\tau_n^{|m|}(\pi-\beta_R) &= (-1)^{n-|m|+1} \tau_n^{|m|}(\beta_R)
\end{aligned} \tag{62}$$

we obtain the following simplified integral representations for the reflected SVWF:

$$\begin{pmatrix} \mathbf{M}_{mn}^{3,R}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3,R}(k\mathbf{r}) \end{pmatrix} = -\frac{(-1)^{n-|m|}r(0)}{2\pi j^{n+1}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} \times \int_0^{2\pi}\int_{C_-} \left[\begin{pmatrix} m\pi_n^{|m|}(\beta_R) \\ \tau_n^{|m|}(\beta_R) \end{pmatrix} \mathbf{e}_{\beta_R} + j \begin{pmatrix} \tau_n^{|m|}(\beta_R) \\ m\pi_n^{|m|}(\beta_R) \end{pmatrix} \mathbf{e}_{\alpha_R} \right] \times \exp(jm\alpha_R)\exp(-2jkz_0\cos\beta_R)\exp(j\mathbf{K}_+^0 \cdot \mathbf{r})\sin\beta_R d\beta_R d\alpha_R. \tag{63}$$

Let us introduce the image coordinate system $O^{'}x^{'}y^{'}z^{'}$ by shifting the original coordinate system a distance $2z_0$ along the negative z axis. The point $O^{'}$ is the image of the point O with respect to the surface Σ. With the notation $\mathbf{K}_+^0 \cdot \mathbf{r}^{'} = \mathbf{K}_+^0 \cdot \mathbf{r} - 2kz_0\cos\beta_R$, where $\mathbf{r}^{'} = (x^{'}, y^{'}, z^{'})$, we identify in (63) the integral representation over the plane waves of the radiating SVWF in the half-space $z' > 0$. Thus,

$$\begin{pmatrix} \mathbf{M}_{mn}^{3,R}(k\mathbf{r}) \\ \mathbf{N}_{mn}^{3,R}(k\mathbf{r}) \end{pmatrix} = (-1)^{n-|m|}r(0) \begin{pmatrix} -\mathbf{M}_{mn}^{3}(k\mathbf{r}^{'}) \\ \mathbf{N}_{mn}^{3}(k\mathbf{r}^{'}) \end{pmatrix}. \tag{64}$$

In this case the interaction field is the image of the scattered field. The expansion (43) can be obtained by using the addition theorem for spherical vector wave functions. The elements of the reflection matrix, which essentially represents the translation coefficients can be computed recursively. Recurrence relations for the translation coefficients of vector multipoles field are available in the literature [2–4,16]. As a result, the amount of computer time to solve the electromagnetic scattering problem is greatly reduced.

The approximate scattering model consisting in computation of reflected spherical vector waves according to (64) is based on the assumption that the interacting field is incident on the surface at near-normal incidence. In the context of a ray tracing model this assumption is justified by the fact that the maximum angle at which a ray emanating from the center of the image coordinate system strikes the surface is small (30° for a sphere), and the Fresnel coefficients are fairly constant from normal incidence up to this angle [2–4]. In view of the above justification we note that the maximum angle is large for particles with strongly deformed surfaces, such as oblates, and decreases with increasing the distance between the particle and the surface. Furthermore, an inspection of (59) reveals that for particles with high size parameters the matrix equation includes Legendre polynomials with high order. In this case the integrands are highly oscillating functions and the assumption that the Fresnel coefficients are constant can lead to erroneous result.

Next, we perform computer simulations in order to investigate the validity of the approximate model. Essentially, we compute the normalized differential scattering cross section (DSCS) of polystyrene particles with a refractive index of 1.59 deposited on a silicon substrate with a refractive index of 3.88+0.02j. Assuming the incident field to have unit amplitude we evaluate the normalized DSCS in the azimuthal plane $\varphi = 0°$, which corresponds to the plane of incidence. The wavelength of the incident wave is chosen to be $\lambda = 0.6328$ μm. The excitation light is a P-polarized plane wave having an inclination from the normal of 60°.

Figure 2 shows the normalized DSCS of spherical particles with different radii a deposited on the substrate. The curves correspond to the methods which use the exact and the approximate reflection matrix. It is obvious that the relative errors of the normalized DSCS computed by the approximate method increases with the diameter of the particle.

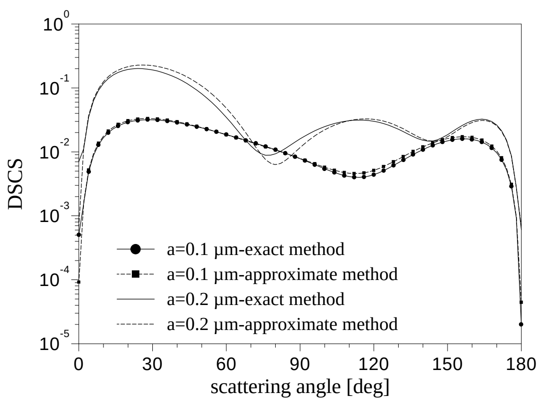

Fig. 2. Normalized differential scattering cross section (DSCS) of spherical particles with different radii a deposited on the substrate. The DSCS is normalized by πa^2 and is evaluated in the azimuthal plane $\varphi = 0°$. The wavelength of the incident wave is $\lambda = 0.6328$ μm, and the excitation light is a P-polarized plane wave having an inclination from the normal of 60°.

In Fig. 3 we consider a spherical particle with $a = 0.3$ μm situated on the surface and at a distance $z_0 = 0.4$ μm above the surface. The plotted data show that the approximate method leads to accurate results when the distance between the particle and the substrate increases.

The results plotted in Fig. 4 correspond to an oblate with semiaxes $a = 0.1$ μm and $b = 0.2$ μm. Two situations are considered: $z_0 = 0.1$ μm and $z_0 = 0.2$ μm. Again, the relative errors of the normalized DSCS are significant when the particle is on the substrate and decrease with increasing the distance z_0.

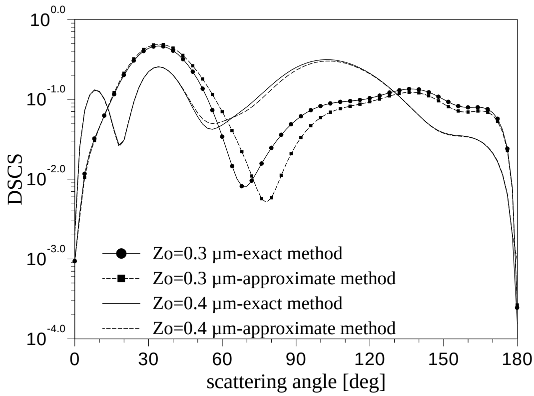

Fig. 3. Normalized differential scattering cross section (DSCS) of a spherical particle with $a = 0.3$ μm situated on the surface and at a distance $z_0 = 0.4$ μm above the surface. The DSCS is normalized by πa^2 and is evaluated in the azimuthal plane $\varphi = 0°$. The wavelength of the incident wave is $\lambda = 0.6328$ μm, and the excitation light is a P-polarized plane wave having an inclination from the normal of 60°.

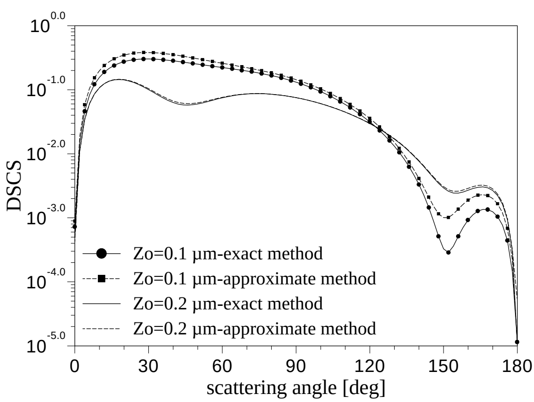

Fig. 4. Normalized differential scattering cross section (DSCS) of an oblate with semiaxes $a = 0.1$ μm and $b = 0.2$ μm. Two situations are considered: $z_0 = 0.1$ μm and $z_0 = 0.2$ μm. The DSCS is normalized by πa^2 and is evaluated in the azimuthal plane $\varphi = 0°$. The wavelength of the incident wave is $\lambda = 0.6328$ μm, and the excitation light is a P-polarized plane wave having an inclination from the normal of 60°.

We conclude this section by noting that the approximate model can leads to erroneous results for 1) particles with extreme geometries, when 2) the particle is deposited on the surface, or when 3) the main dimension of the particle is comparable with the incident wavelength.

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