Army Research Laboratory

# Light Scattering from a Sphere Near a Plane Interface

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#### Abstract

Scattered light from particles near a plane interface has important implications for many branches of science. Applications range from radar detection and remote sensing to clean-room monitoring and quality control in the manufacture of silicon wafers. The most fundamental system of this type is that of a sphere near a plane interface. Calculating the scattering is complicated because the boundary conditions at the sphere and plane surfaces must be satisfied simultaneously, and these two systems represent two fundamentally different geometries. In this report we present an analytical solution to this problem that retains the physics and may be used as a basis for more numerically intensive techniques necessary when the system constituents become irregular.

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#### 1. Scattering System

Physically, we can consider four field components that interact with the system of a sphere near a plane interface shown in figure 1. For one component, the incident light strikes the sphere and is scattered into the far-field region beneath the plane interface. For a second component, the incident light reflects off the plane interface before it is scattered by the sphere into the far-field region beneath the plane interface. For a third component, the incident light strikes the sphere and is scattered toward the plane interface, which reflects this light toward the far-field region beneath the plane interface. And for a fourth component, the incident light reflects off the plane interface before it is scattered by the sphere toward the plane interface; the plane interface reflects this light toward the far-field region beneath the plane interface. The total scattered field can be found as the superposition of these four components, since it is widely known how a plane wave interacts with isolated spheres and plane interfaces. However, this "double interaction" model does not include the interaction fields, i.e., fields that are scattered by the sphere, reflected off the plane interface, and are once again incident upon the sphere. To include the effects of this interaction, we must use more complicated models.

In this report, we discuss a multipole solution, based on image theory, to the problem of a sphere in proximity to a plane interface. This type of solution is valuable, since it retains the individual field components interacting with the individual system components that many numerical techniques cannot. In this way, the physics is preserved. The incident, scattered, and interaction fields are expanded in terms of vector spherical harmonics about coordinate systems centered on the sphere and its image. The boundary conditions on each subsystem can then be satisfied individually. Because the field expansions are in terms of vector spherical harmonics, it is relatively easy to satisfy the boundary conditions on the spherical interface. To satisfy the boundary conditions at the plane interface, an image (or interaction) field is introduced that is physically equivalent to the scattered field from the sphere that reflects off the plane interface and is incident upon the sphere. For a perfectly conducting plane interface, this interaction field is the image of the scattered field from the sphere. When the half-space not encompassing the particle is dielectric or lossy, some approximation or numerical technique must be used to represent this interaction field.

Figure 1. Diagram of scattering system. A sphere of radius  $r_{\rm sph}$ , complex refractive index  $m_{\rm sph},$  lies a distance dbeneath a plane interface separating a medium of refractive index  $m_1$  below interface  $(z_1 < d)$  from a region of complex refractive index  $m_2$  above interface  $(z_1 > d)$ . A plane wave, whose wave vector lies in the  $x_1 - z_1$  plane and is oriented at angle  $\theta_{\circ}$ with respect to  $z_1$  axis, is incident upon system. To help satisfy boundary conditions, an image coordinate system  $(x_2, y_2, z_2)$  is introduced a distance 2d above coordinate system centered on sphere.



#### 2. Field Expansions

Figure 1 shows the scattering system. The isotropic, homogeneous sphere of refractive index  $m_{\rm sph}$  and radius  $r_{\rm sph}$  is located in air, centered on the  $(x_1, y_1, z_1)$  coordinate system located a distance d beneath a plane interface separating region 2 of complex refractive index  $m_2$   $(z_1 > d)$  from region 1 of real refractive index  $m_1$   $(z_1 < d)$ . We denote  $k_1$ ,  $k_2$ , and  $k_{\rm sph}$  to be the propagation constants of waves in region 1, region 2, and within the sphere. To satisfy the boundary conditions at the plane interface, we introduce an image coordinate system  $(x_2, y_2, z_2)$ , located a distance d above the plane interface on the  $z_1$  axis. This coordinate system is the source of the image or interaction fields. Incident upon the scattering system is a plane wave of wavelength  $\lambda$  whose wavevector  $\mathbf{k}_{\circ}$  is oriented in the  $x_1 - z_1$  plane at angle  $\theta_{\circ}$  with respect to the  $z_1$  axis. The electromagnetic fields may be expanded in terms of the vector spherical harmonics centered about the j coordinate system (j = 1, 2):

$$\mathbf{M}_{mn}^{(\rho)}\left(k\mathbf{r}_{j}\right) = \hat{\theta}_{j}\left[z_{n}^{(\rho)}(kr_{j})\mathrm{i}\tilde{\pi}_{mn}\left(\cos\theta_{j}\right)\exp\left(\mathrm{i}m\phi_{j}\right)\right]$$

$$-\hat{\phi}_{j}\left[z_{n}^{(\rho)}(kr_{j})\tilde{\tau}_{mn}\left(\cos\theta_{j}\right)\exp\left(\mathrm{i}m\phi_{j}\right)\right],$$

$$(1)$$

$$\mathbf{N}_{mn}^{(\rho)}\left(k\mathbf{r}_{j}\right) = \hat{\mathbf{r}}_{j}\left[\frac{1}{kr_{j}}z_{n}^{(\rho)}(kr_{j})n(n+1)\tilde{P}_{n}^{m}(\cos\theta_{j})\exp\left(\mathrm{i}m\phi_{j}\right)\right]$$

$$+ \hat{\theta}_{j}\left\{\frac{1}{kr_{j}}\frac{d}{dr_{j}}\left[r_{j}z_{n}^{(\rho)}(kr_{j})\right]\tilde{\tau}_{mn}\left(\cos\theta_{j}\right)\exp\left(\mathrm{i}m\phi_{j}\right)\right\}$$

$$+ \hat{\phi}_{j}\left\{\frac{\mathrm{i}}{kr_{j}}\frac{d}{dr_{j}}\left[r_{j}z_{n}^{(\rho)}(kr_{j})\right]\tilde{\pi}_{mn}\left(\cos\theta_{j}\right)\exp\left(\mathrm{i}m\phi_{j}\right)\right\},$$

$$(2)$$

where  $z_n^{(\rho)}(kr_j)$  are the spherical Bessel functions of the first, second, third, or fourth kind ( $\rho = 1, 2, 3, 4$ ), and

$$\tilde{\pi}_{mn}\left(\cos\theta\right) = \frac{m}{\sin\theta}\tilde{P}_{n}^{m}(\cos\theta) \tag{3}$$

$$\tilde{\tau}_{mn}\left(\cos\theta\right) = \frac{d}{d\theta}\tilde{P}_{n}^{m}(\cos\theta) \tag{4}$$

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$$\tilde{P}_{n}^{m}(\cos\theta) = \sqrt{\frac{(2n+1)(n-m)!}{2(n+m)!}} P_{n}^{m}(\cos\theta),$$
(5)

where  $P_n^m(\cos\theta)$  are the associated Legendre polynomials. We assume a time dependence of  $\exp(-i\omega t)$  throughout.

To satisfy the boundary conditions, we use the linearity property of the electromagnetic fields and consider the components of the electromagnetic field individually. These components are each expressed as a multipole expansion of vector spherical harmonics, and the boundary conditions at the interfaces of the sphere and of the plane are satisfied simultaneously. We first consider the incident fields.

#### 3. Incident Field

The incident electric field that strikes the sphere is expanded in vector spherical harmonics about the sphere coordinate system as

$$\mathbf{E}_{\rm inc} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} a_{mn}^{(1)} \mathbf{M}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right) + a_{mn}^{(2)} \mathbf{N}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right), \tag{6}$$

where  $a_{mn}^{(j)}$  are the incident field coefficients. This component of the electric field is made up of two parts: (1) the plane wave that strikes the sphere directly and (2) the plane wave that strikes the sphere after it is reflected off the plane interface. We consider these subcomponents individually, and because we are dealing with a linear system, the incident field coefficients are each composed of two elements:

$$a_{mn}^{(j)} = a_{mn}^{(j)\circ} + a_{mn}^{(j)R},\tag{7}$$

where  $a_{mn}^{(j)\circ}$  are the coefficients of the incident plane wave that strike the sphere directly, and  $a_{mn}^{(j)R}$  are the coefficients of the incident plane wave that were reflected off the plane substrate. In general, we consider two different polarization states of the incident field: (1) A unit-normalized TE-incident (transverse electric) plane wave of the form  $\mathbf{E}^{TE} = \exp ik_1(z_1 \cos \theta_{\circ} + x_1 \sin \theta_{\circ})\hat{\mathbf{y}}_1$  and (2) a unit-normalized TM-incident (transverse magnetic) plane wave of the form  $\mathbf{E}^{TM} = \exp ik_1(z_1 \cos \theta_{\circ} + x_1 \sin \theta_{\circ}) \times (\hat{\mathbf{x}}_1 \cos \theta_{\circ} - \hat{\mathbf{z}}_1 \sin \theta_{\circ})$ . We denote the coefficients for these two cases with an additional superscript:  $a_{mn}^{(j)\circ,TE}$  and  $a_{mn}^{(j)\circ,TM}$ . We can find these coefficients using the orthogonality properties of the vector spherical wave functions. The first coefficient can be expressed as

$$a_{mn}^{(1)\circ,\text{TE}} = \frac{\int \mathbf{E}^{\text{TE}} \cdot \mathbf{M}_{mn}^{(1)*}(k_1\mathbf{r}_1) \, dV}{\int \mathbf{M}_{mn}^{(1)}(k_1\mathbf{r}_1) \cdot \mathbf{M}_{mn}^{(1)*}(k_1\mathbf{r}_1) \, dV},\tag{8}$$

where the asterisk denotes the complex conjugate and the integral is taken over all space. With a little bit of algebra and calculus, we find

$$a_{mn}^{(1)\circ,\mathrm{TE}} = \frac{-2\mathbf{i}^n}{n\left(n+1\right)}\tilde{\tau}_{mn}(\cos\theta_\circ).$$
(9)

Similarly, the coefficients

$$a_{mn}^{(2)\circ,\text{TE}} = \frac{\int \mathbf{E}^{\text{TE}} \cdot \mathbf{N}_{mn}^{(1)*}(k_1\mathbf{r}_1) \, dV}{\int \mathbf{N}_{mn}^{(1)}(k_1\mathbf{r}_1) \cdot \mathbf{N}_{mn}^{(1)*}(k_1\mathbf{r}_1) \, dV} = \frac{-2i^n}{n(n+1)} \tilde{\pi}_{mn}(\cos\theta_\circ).$$
(10)

It is a simple exercise of Maxwell's equations to show that

$$a_{mn}^{(1)\circ,\text{TM}} = ia_{mn}^{(2)\circ,\text{TE}}$$
 (11)

and

$$a_{mn}^{(2)\circ,\text{TM}} = ia_{mn}^{(1)\circ,\text{TE}}.$$
 (12)

Finally, we must determine the reflected components of the incident field coefficients. The solution to the scatter of a plane wave by an infinite plane interface is a classic problem of electromagnetism solved by Fresnel in the nineteenth century. The amplitude and phase of the reflected plane wave are dependent on its polarization state, incident angle, and the refractive index of the media at either side of the interface. The Fresnel reflection coefficients for a plane wave incident at angle  $\alpha$  on the interface, traveling from medium *i* and reflecting off the interface at medium *j*, are

$$R_{ij}^{\text{TE}}(\alpha) = \frac{m_i \cos \alpha - m_j \sqrt{1 - (m_i/m_j)^2 \sin^2 \alpha}}{m_i \cos \alpha + m_j \sqrt{1 - (m_i/m_j)^2 \sin^2 \alpha}}$$
(13)

$$R_{ij}^{\rm TM}(\alpha) = -\frac{m_j \cos \alpha - m_i \sqrt{1 - (m_i/m_j)^2 \sin^2 \alpha}}{m_j \cos \alpha + m_i \sqrt{1 - (m_i/m_j)^2 \sin^2 \alpha}},$$
(14)

where the superscripts on the reflection coefficients denote the polarization state of the incident field. It should be noted that these particular sets of equations are valid when the reflected electric field component is pointed in the same direction as the incident electric field component for both TE and TM polarization states when  $\alpha = 0$ . From the relation

$$\tilde{P}_{n}^{m}(-x) = (-1)^{n+m} \,\tilde{P}_{n}^{m}(x), \tag{15}$$

we find

$$\tilde{\pi}_{mn}\left(-x\right) = \left(-1\right)^{n+m} \tilde{\pi}_{mn}\left(x\right) \tag{16}$$

and

$$\tilde{\tau}_{mn}\left(-x\right) = \left(-1\right)^{n+m+1} \tilde{\tau}_{mn}\left(x\right).$$
(17)

Using these expressions, we can write the coefficients of the reflected field in terms of the coefficients of the direct field:

$$a_{mn}^{(j)\text{TE}} = a_{mn}^{(j)\circ,\text{TE}} (-1)^{j+n+m} R_{12}^{\text{TE}} (\theta_{\circ}) \exp\left(2ik_1 d\cos\theta_{\circ}\right)$$
(18)

for the TE-incident plane wave, and

$$a_{mn}^{(j)\text{TM}} = a_{mn}^{(j)\circ,\text{TM}} \, (-1)^{j+n+m} \, R_{12}^{\text{TM}} \, (\theta_{\circ}) \exp\left(2ik_1 d\cos\theta_{\circ}\right) \tag{19}$$

for the TM-incident plane wave. The total incident field coefficients can be written as

$$a_{mn}^{(j)\text{TE}} = a_{mn}^{(j)\circ,\text{TE}} \left[ 1 + (-1)^{j+n+m} R_{12}^{\text{TE}} \left(\theta_{\circ}\right) \exp\left(2ik_{1}d\cos\theta_{\circ}\right) \right]$$
(20)

for the TE-incident plane wave, and

$$a_{mn}^{(j)\text{TM}} = a_{mn}^{(j)\circ,\text{TM}} \left[ 1 + (-1)^{j+n+m} R_{12}^{\text{TM}} \left(\theta_{\circ}\right) \exp\left(2ik_{1}d\cos\theta_{\circ}\right) \right]$$
(21)

for the TM-incident plane wave. Equations (20) and (21) are the vector spherical harmonic expansion coefficients for the total field of a plane wave reflecting off a plane interface, and are nothing more than Fresnel theory expressed in a spherical coordinate system. The phase term  $\exp(2ik_1d\cos\theta_{\circ})$  exists in these expressions because the coordinate system from which the waves are expanded is located a distance *d* beneath the plane interface.

#### 4. Fields at the Spherical Interface

The next step in the derivation is to satisfy the boundary conditions at the spherical interface. All the components of the electromagnetic field must be expanded in vector spherical harmonics as we did in the previous section for the incident field. The scattered field component is expanded as

$$\mathbf{E}_{\text{sca}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} b_{mn}^{(1)} \mathbf{M}_{mn}^{(3)} \left(k_1 \mathbf{r}_1\right) + b_{mn}^{(2)} \mathbf{N}_{mn}^{(3)} \left(k_1 \mathbf{r}_1\right).$$
(22)

For the chosen time dependence, the spherical Hankel functions  $z_n^{(3)}(k_1r_1) = h_n^{(1)}(k_1r_1)$  represent outgoing spherical waves and satisfy the boundary conditions at infinity. Because there is a pole at the origin, this expansion can only be used in the region exterior to the spherical interface.

The electric fields inside the sphere volume  $(r_1 < r_{sph})$  are expanded in vector spherical harmonics about the sphere coordinate system as

$$\mathbf{E}_{\rm sph} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn}^{(1)} \mathbf{M}_{mn}^{(1)} \left( k_{\rm sph} \mathbf{r}_1 \right) + c_{mn}^{(2)} \mathbf{N}_{mn}^{(1)} \left( k_{\rm sph} \mathbf{r}_1 \right),$$
(23)

where  $c_{mn}^{(j)}$  are the internal field coefficients. The radial dependence of the vector spherical harmonic expansion must be in terms of Bessel functions  $z_n^{(1)} (k_{\rm sph} r_1) = j_n (k_{\rm sph} r_1)$ .

Finally, an image or interaction field must be introduced to help satisfy the boundary conditions at the plane interface. This field is expanded in a series of outgoing spherical waves centered on the  $(x_2, y_2, z_2)$  coordinate system:

$$\mathbf{E}_{\text{ima}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} d_{mn}^{(1)} \mathbf{M}_{mn}^{(3)} \left( k_1 \mathbf{r}_2 \right) + d_{mn}^{(2)} \mathbf{N}_{mn}^{(3)} \left( k_1 \mathbf{r}_2 \right).$$
(24)

Physically, this field corresponds to the interaction of the sphere with the plane interface: the scattered field from the sphere reflects off the plane interface and interacts with the sphere again. To satisfy the boundary conditions on the spherical interface, it is convenient to expand this image field on the  $(x_1, y_1, z_1)$  coordinate system. Such a transformation of coordinate systems can be performed, since the vector spherical harmonics represent a complete orthogonal expansion. We discuss details of this expansion and

satisfying the boundary conditions on the plane interface in the next sections. Because there is no pole in the interaction field when  $\mathbf{r}_1 = 0$ , the radial dependence of the vector spherical harmonic expansion must be in terms of Bessel functions  $z_n^{(1)}(k_1r_1) = j_n(k_1r_1)$ :

$$\mathbf{E}_{\text{ima}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} e_{mn}^{(1)} \mathbf{M}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right) + e_{mn}^{(2)} \mathbf{N}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right).$$
(25)

Satisfying the boundary conditions at the spherical interface is a relatively straightforward process. This has been done well in so many texts that it would be tedious to repeat the process. Since many applications call for scattering from nonspherical particles, it is worthwhile to outline a more general formulation of this scattering solution. The solution when the particle is spherical will then be provided. We express the fields incident upon and scattered by the particle in vector spherical harmonics. Any field incident upon a three-dimensional particle

$$\mathbf{E}_{\rm inc} = p_{mn}^{(1)} \mathbf{M}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right) + p_{mn}^{(2)} \mathbf{N}_{mn}^{(1)} \left( k_1 \mathbf{r}_1 \right)$$
(26)

has a corresponding scattered field, which can be expanded in terms of vector spherical harmonics

$$\mathbf{E}_{\text{sca}} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \left[ p_{mn}^{(1)} T_{mnm'n'}^{11} + p_{mn}^{(2)} T_{mnm'n'}^{12} \right] \mathbf{M}_{m'n'}^{(3)} \left( k_1 \mathbf{r}_1 \right)$$

$$+ \left[ p_{mn}^{(1)} T_{mnm'n'}^{21} + p_{mn}^{(2)} T_{mnm'n'}^{22} \right] \mathbf{N}_{m'n'}^{(3)} \left( k_1 \mathbf{r}_1 \right);$$
(27)

that is, the scattered field coefficients  $b_{mn}^{(j)}$  are related to the incident field coefficients via some transition matrix (or T-matrix)  $T_{mnm'n'}^{jk}$ :

$$b_{mn}^{(j)} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} p_{mn}^{(1)} T_{mnm'n'}^{j1} + p_{mn}^{(2)} T_{mnm'n'}^{j2}.$$
 (28)

In a multiple system like that of a sphere and a plane interface, the total field incident upon the particle is composed of the incident plane wave and the interaction field, and the scattered field coefficients are expressed as

$$b_{mn}^{(j)} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[ a_{mn}^{(1)} + e_{mn}^{(1)} \right] T_{mnm'n'}^{j1} + \left[ a_{mn}^{(2)} + e_{mn}^{(2)} \right] T_{mnm'n'}^{j2}.$$
 (29)

This equation expresses the scattering coefficients in terms of the T-matrix of the isolated particle. This is convenient, since T-matrix routines are readily available for many particle systems. For certain types of particles, the T-matrix can be simplified. The T-matrix of axially symmetric particles obeys  $T_{mnm'n'}^{jk} = \delta_{mm'}T_{mnm'n'}^{jk}$ . For radially symmetric particles,  $T_{mnm'n'}^{jk} = \delta_{nn'}\delta_{mm'}T_{mnm'n'}^{jk}$ , and there is no mode mixing, i.e.,  $T_{mnm'n'}^{12} = T_{mnm'n'}^{21} = 0$ . Spheres are a subgroup of this latter particle type, and the T-matrix is simply composed of the Mie scattering coefficients  $f_n^j$ :

$$T_{mnmn}^{11} = f_n^1$$

$$= -\frac{k_{\rm sph}\psi_n'(k_{\rm sph}r_{\rm sph})\psi_n(k_1r_{\rm sph}) - k_1\psi_n'(k_1r_{\rm sph})\psi_n(k_{\rm sph}r_{\rm sph})}{k_{\rm sph}\psi_n'(k_{\rm sph}r_{\rm sph})\xi_n(k_1r_{\rm sph}) - k_1\psi_n'(k_1r_{\rm sph})\xi_n(k_{\rm sph}r_{\rm sph})},$$
(30)

and

$$T_{mnmn}^{22} = f_n^2$$
(31)  
=  $-\frac{k_1 \psi'_n (k_{\rm sph} r_{\rm sph}) \psi_n (k_1 r_{\rm sph}) - k_{\rm sph} \psi'_n (k_1 r_{\rm sph}) \psi_n (k_{\rm sph} r_{\rm sph})}{k_1 \psi'_n (k_{\rm sph} r_{\rm sph}) \xi_n (k_1 r_{\rm sph}) - k_{\rm sph} \psi'_n (k_1 r_{\rm sph}) \xi_n (k_{\rm sph} r_{\rm sph})},$ 

where  $\psi_n(x) = xj_n(x)$  and  $\xi_n(x) = xh_n^{(1)}(x)$  are the Riccati-Bessel functions and the primes denote derivatives with respect to the argument. The other terms of the T-matrix are zero.

#### 5. Translation Addition Theorem

The translation addition theorem is used to translate a set of vector spherical harmonics from one coordinate system onto another coordinate system. We need to find in this derivation a relationship between the two sets of interaction coefficients given by equations (24) and (25). The fields expressed by these equations are identical, but they are expanded about different coordinate systems. For a translation along the negative  $z_1$  axis a distance 2dwith no rotation, the vector spherical harmonics are related by

$$\mathbf{M}_{mn}^{(3)}(k_1\mathbf{r}_2) = \sum_{n'=1}^{\infty} A_{n'}^{(m,n)} \mathbf{M}_{mn'}^{(1)}(k_1\mathbf{r}_1) + B_{n'}^{(m,n)} \mathbf{N}_{mn'}^{(1)}(k_1\mathbf{r}_1)$$
(32)

and

$$\mathbf{N}_{mn}^{(3)}(k_1\mathbf{r}_2) = \sum_{n'=1}^{\infty} B_{n'}^{(m,n)} \mathbf{M}_{mn'}^{(1)}(k_1\mathbf{r}_1) + A_{n'}^{(m,n)} \mathbf{N}_{mn'}^{(1)}(k_1\mathbf{r}_1).$$
(33)

This relationship is valid in the region where  $r_1 < |2d|$ , i.e., out to the pole located at  $r_2 = 0$ . We can use these equations to find the relationship between the  $d_{mn}^{(j)}$  and  $e_{mn}^{(j)}$  coefficients. Substituting equations (32) and (33) into equation (24) and comparing with equation (25) yields

$$e_{mn}^{(1)} = \sum_{n'=1}^{\infty} d_{mn'}^{(1)} A_n^{(m,n')} + d_{mn'}^{(2)} B_n^{(m,n')}$$
(34)

and

$$e_{mn}^{(2)} = \sum_{n'=1}^{\infty} d_{mn'}^{(1)} B_n^{(m,n')} + d_{mn'}^{(2)} A_n^{(m,n')},$$
(35)

and for a spherical particle, equation (29) can now be expressed as

$$b_{mn}^{(j)} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left\{ a_{mn}^{(1)} + \sum_{n'=0}^{\infty} \left[ d_{mn'}^{(1)} A_n^{(m,n')} + d_{mn'}^{(2)} B_n^{(m,n')} \right] \right\} f_n^1 \\ + \left\{ a_{mn}^{(2)} + \sum_{n'=0}^{\infty} \left[ d_{mn'}^{(1)} B_n^{(m,n')} + d_{mn'}^{(2)} A_n^{(m,n')} \right] \right\} f_n^2 .$$
(36)

It is beyond the scope of this report to provide a complete derivation of the vector translation coefficients  $A_{n'}^{(m,n)}$  and  $B_{n'}^{(m,n)}$ ; however, it is certainly

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worthwhile to write out a set of relations from which these may be calculated. The vector translation coefficients can be expressed in terms of the scalar translation coefficients  $C_{n'}^{(m,n)}$  that are used to translate the spherical harmonics from one coordinate system onto another coordinate system:

$$h_n^{(1)}(kr_2)\tilde{P}_n^m(\cos\theta_2)\exp(im\phi_2) = \sum_{n'=0}^{\infty} C_{n'}^{(m,n)} j_{n'}(kr_1)\tilde{P}_{n'}^m(\cos\theta_1)\exp(im\phi_1) .$$
(37)

The scalar translation coefficients can be found via various recursion relations. The starting point for calculating the scalar coefficients is

$$C_{n'}^{(0,0)} = \sqrt{2n' + 1} h_{n'}^{(1)}(2k_1 d),$$
(38)

which results from the expression

$$h_0^{(1)}(k_1 r_2) = \sum_{n'=0}^{\infty} \left(2n'+1\right) j_{n'}(k_1 r_1) h_n^{(1)}(2k_1 d).$$
(39)

From here, the relation

$$C_{n'}^{(0,n+1)} = \frac{1}{(n+1)} \sqrt{\frac{2n+3}{2n'+1}} \left\{ n' \sqrt{\frac{2n+1}{2n'-1}} C_{n'-1}^{(0,n)} + n \sqrt{\frac{2n'+1}{2n-1}} C_{n'}^{(0,n-1)} - (n'+1) \sqrt{\frac{2n+1}{2n'+3}} C_{n'+1}^{(0,n)} \right\}$$
(40)

can be used to calculate the elements  $C_{n'}^{(0,n)}$ . The remaining terms in the matrix can be calculated using the relation

$$C_{n'}^{(m,n)} = \sqrt{\frac{(n'-m+1)(n'+m)(2n'+1)}{(n-m+1)(n+m)(2n'+1)}} C_{n'}^{(m-1,n)}$$

$$- 2k_1 d \sqrt{\frac{(n'-m+2)(n'-m+1)}{(n-m+1)(n+m)(2n'+1)(2n'+3)}} C_{n'+1}^{(m-1,n)}$$

$$- 2k_1 d \sqrt{\frac{(n'+m)(n'+m-1)}{(n-m+1)(n+m)(2n'+1)(2n'-1)}} C_{n'-1}^{(m-1,n)}.$$
(41)

It should be noted that

$$C_{n,n}^{(n,n)} = C_{n'}^{(-m,n)}.$$
 (42)

We can find the vector translation coefficients using

 $C_{n'}^{(m)}$ 

$$A_{n'}^{(m,n)} = C_{n'}^{(m,n)} - \frac{2k_1 d}{n'+1} \sqrt{\frac{(n'-m+1)(n'+m+1)}{(2n'+1)(2n'+3)}} C_{n'+1}^{(m,n)} - \frac{2k_1 d}{n'} \sqrt{\frac{(n'-m)(n'+m)}{(2n'+1)(2n'-1)}} C_{n'-1}^{(m,n)},$$
(43)

$$B_{n'}^{(m,n)} = -\frac{2ik_1md}{n'(n'+1)}C_{n'}^{(m,n)}.$$
(44)

Finally, from equations (42) to (44), the following relations are valid:

$$A_{n'}^{(-m,n)} = A_{n'}^{(m,n)},$$
(45)

$$B_{n'}^{(-m,n)} = B_{n'}^{(m,n)}.$$
(46)

#### 6. Plane Interface

The boundary conditions at the plane interface are the most difficult to satisfy because all the field expansions are in terms of vector spherical harmonics. In general terms, we can introduce another transition matrix  $U_{mnm'n'}^{ij}$ , which, for our purposes, transforms any set of expanding spherical waves centered on coordinate system  $(x_1, y_1, z_1)$  incident on the plane interface:

$$\mathbf{E}_{\rm inc}^{\rm plane} = q_{mn}^{(1)} \mathbf{M}_{mn}^{(3)} \left( k_1 \mathbf{r}_1 \right) + q_{mn}^{(2)} \mathbf{N}_{mn}^{(3)} \left( k_1 \mathbf{r}_1 \right), \tag{47}$$

to its scattering response, a set of expanding spherical waves centered on coordinate system  $(x_2, y_2, z_2)$  that are reflected by the plane interface:

$$\mathbf{E}_{\text{sca}}^{\text{plane}} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \left[ q_{mn}^{(1)} U_{mnm'n'}^{11} + q_{mn}^{(2)} U_{mnm'n'}^{12} \right] \mathbf{M}_{m'n'}^{(3)} \left( k_1 \mathbf{r}_2 \right) \\ + \left[ q_{mn}^{(1)} U_{mnm'n'}^{21} + q_{mn}^{(2)} U_{mnm'n'}^{22} \right] \mathbf{N}_{m'n'}^{(3)} \left( k_1 \mathbf{r}_2 \right),$$
(48)

that is, any field incident on the plane interface expressed by equation (47) is scattered by a field expressed by equation (48). For a plane interface, all elements  $U_{mnm'n'}^{ij} = \delta_{mm'} U_{mnm'n'}^{ij}$  because of the system symmetry.

We first treat the case of a perfectly conducting plane interface. At the interface ( $r_2 = r_1$ ,  $\theta_2 = \pi - \theta_1$ ,  $\phi_2 = \phi_1$ ), the tangential components of the electric and magnetic fields must be continuous. We can achieve this by making the scattered field the mirror image of the incident field. Using equations (1), (2), (16), and (17), we can easily show that the boundary conditions are satisfied if the scattered field is of the form

$$\mathbf{E}_{\text{sca}}^{\text{plane}} = q_{mn}^{(1)} \, (-1)^{n+m+1} \, \mathbf{M} \, (-1)^{n+m} \, \mathbf{N}_{mn}^{(3)} \, (k_1 \mathbf{r}_2) \tag{49}$$

or

$$U_{mnm'n'}^{jk} = \delta_{nn'}\delta_{mm'}\delta_{jk} \left(-1\right)^{n+m+j}.$$
(50)

This is equivalent to the following relationship between the scattering and interaction coefficients

$$d_{mn}^{(j)} = -\left(-1\right)^{n+m+j} b_{mn}^{(j)} \tag{51}$$

and equation (36) can now be written as

$$b_{mn}^{(j)} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left\{ a_{mn}^{(1)} + \sum_{n'=1}^{\infty} (-1)^{n'+m} \left[ b_{mn'}^{(1)} A_n^{(m,n')} - b_{mn'}^{(2)} B_n^{(m,n')} \right] \right\} f_n^1 \\ + \left\{ a_{mn}^{(2)} + \sum_{n'=1}^{\infty} (-1)^{n'+m} \left[ b_{mn'}^{(1)} B_n^{(m,n')} - b_{mn'}^{(2)} A_n^{(m,n')} \right] \right\} f_n^2 .$$
(52)

Equation (52) represents the final solution to the scattering problem of a sphere near a perfectly conducting interface. The scattering coefficients  $b_{mn}^{(j)}$  are written in terms of a set of known quantities: translation coefficients  $A_n^{(m,n')}$  and  $B_n^{(m,n')}$ , incident field coefficients  $a_{mn}^{(j)}$ , and Mie coefficients  $f_n^j$ . By truncating the infinite series, we can find a solution through matrix inversion techniques. The number of terms necessary for convergence depends on the required accuracy. We can obtain adequate results by carrying the summation in n to

$$N = x_{\rm sph} + 4x_{\rm sph}^{1/3} + 2 \tag{53}$$

terms, where  $x_{sph}$  is the size parameter of the sphere. Note that this formula is independent of the separation distance d.

Many real-world interfaces are not perfectly conducting. To solve this more general problem, we must either make some approximation or resort to numerical techniques. The simplest approximation one can make is to assume that, for the purposes of the interaction only, the image fields are proportional to the scattered fields, i.e.,

$$U_{mnm'n'}^{jk} = \delta_{nn'} \delta_{mm'} \delta_{jk} \, (-1)^{n+m+j} \, R_{12}^{\text{TE}} \, (0) \,. \tag{54}$$

The factor of proportionality chosen is the Fresnel coefficient at normal incidence. This means that the scattered fields from the sphere that reflect off the plane interface and strike the sphere again, strike the plane interface at normal incidence. Geometrically, there is some justification to this argument: rays emanating from the center of the sphere reflecting off the plane interface and striking the sphere can have a maximum incident angle on the plane interface of 30°, and the Fresnel reflection coefficients remain nearly constant at near-normal incident angles. Equation (54) is equivalent to the following relationship between the scattering and interaction coefficients

$$d_{mn}^{(j)} = -\left(-1\right)^{n+m+j} R_{12}^{\text{TE}}\left(0\right) b_{mn}^{(j)}$$
(55)

and equation (36) can now be written as

$$b_{mn}^{(j)} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (56)$$

$$\left\{ a_{mn}^{(1)} + \sum_{n'=1}^{\infty} (-1)^{n'+m} R_{12}^{\text{TE}}(0) \left[ b_{mn'}^{(1)} A_n^{(m,n')} - b_{mn'}^{(2)} B_n^{(m,n')} \right] \right\} f_n^1$$

$$+ \left\{ a_{mn}^{(2)} + \sum_{n'=1}^{\infty} (-1)^{n'+m} R_{12}^{\text{TE}}(0) \left[ b_{mn'}^{(1)} B_n^{(m,n')} - b_{mn'}^{(2)} A_n^{(m,n')} \right] \right\} f_n^2.$$

An exact solution for the scattering from a sphere located near an arbitrary half space requires considerably more effort; however, we can find one using the derivation above. The only requirement is finding the matrix elements  $U_{mnm'n'}^{jk}$ . One way to do this is by expanding the individual vector spherical harmonics given by equation (47) as an angular spectrum of plane waves. The reflected field is also expressed as an angular spectrum of plane waves and the angle-dependent amplitudes of the reflected field are equal to those of the incident field, mulitplied by the appropriate Fresnel reflection coefficient. Finding the matrix elements  $U_{mnm'n'}^{jk}$  requires expressing the reflected angular spectrum in terms of the vector spherical harmonics. This final step is a minor variation on equations (8) and (10). Note that with little modification, the equations of this report can also be modified to accommodate irregularly shaped particles and roughness on the "plane" interface. The only knowledge required is the appropriate T-matrix of these constituents.

#### 7. Scattered Field

For many applications, only the far-field region is of interest, where

$$h_n^{(1)}(kr) = \frac{(-i)^n \exp(ikr)}{ikr}.$$
(57)

The scattered far fields can be expressed in terms of a scattering amplitude matrix that contains all the polarization information of the scattered light,

$$\begin{pmatrix} E_{\text{sca}}^{\theta} \\ E_{\text{sca}}^{\phi} \end{pmatrix} = \frac{\exp\left[\mathrm{i}k_{1}r_{1}\right]}{-\mathrm{i}k_{1}r_{1}} \begin{bmatrix} S_{2} & S_{3} \\ S_{4} & S_{1} \end{bmatrix} \begin{pmatrix} E_{\text{inc}}^{\text{TM}} \\ E_{\text{inc}}^{\text{TE}} \end{pmatrix},$$
(58)

where  $E_{\text{inc}}^{\text{TE}}$  and  $E_{\text{inc}}^{\text{TM}}$  are the amplitudes of incident TE and TM plane waves, and  $E_{\text{sca}}^{\theta}$  and  $E_{\text{sca}}^{\phi}$  are the  $\hat{\theta}_1$  and  $\hat{\phi}_1$  components of the scattered electric field. The total scattered field is composed of the linear superposition of the scattered field from the sphere  $\mathbf{E}_{\text{sca}}$  and from its image  $\mathbf{E}_{\text{ima}}$ . We have provided only an explicit expression for  $\mathbf{E}_{\text{ima}}$  when the interface is perfectly conducting (for the dielectric half space, the approximate coefficients given are only valid for the purpose of the interaction). However, the contribution of the image field in the far field is equivalent to the image of the scattered field multiplied by the Fresnel reflection coefficient  $R_{\text{TE}}(\pi - \theta_1)$ or  $R_{\text{TM}}(\pi - \theta_1)$ , and a phase shift  $\exp(-2ikd\cos\theta_1)$ . We can express the image of the scattered field in terms of the scattered field using equations (16) and (17). Separating the individual vector components of equation (22) yields the following:

$$S_{1} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (-i)^{n} \exp(im\phi_{1})$$

$$\times \left\{ \left[ 1 + R_{12}^{TE} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) \right] b_{nm}^{(2)TE} \tilde{\pi}_{mn} (\cos\theta_{1})$$

$$+ \left[ 1 - R_{12}^{TE} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) b_{nm}^{(1)TE} \tilde{\tau}_{mn} (\cos\theta_{1}) \right] \right\},$$
(59)

$$S_{2} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (-i)^{n+1} \exp(im\phi_{1})$$

$$\times \left\{ \left[ 1 + R_{12}^{\text{TM}} \left( \pi - \theta_{1} \right) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) \right] b_{nm}^{(1)\text{TM}} \tilde{\pi}_{mn} \left( \cos\theta_{1} \right) \right. \\ \left. + \left[ 1 - R_{12}^{\text{TM}} \left( \pi - \theta_{1} \right) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) b_{nm}^{(2)\text{TM}} \tilde{\tau}_{mn} \left( \cos\theta_{1} \right) \right] \right\},$$
(60)

$$S_{3} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (-i)^{n+1} \exp(im\phi_{1})$$

$$\times \left\{ \left[ 1 + R_{12}^{\text{TM}} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) \right] b_{nm}^{(1)\text{TE}} \tilde{\pi}_{mn} (\cos\theta_{1}) \right.$$

$$\left. + \left[ 1 - R_{12}^{\text{TM}} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) b_{nm}^{(2)\text{TE}} \tilde{\tau}_{mn} (\cos\theta_{1}) \right] \right\},$$
(61)

$$S_{4} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (-i)^{n} \exp(im\phi_{1})$$

$$\times \left\{ \left[ 1 + R_{12}^{\text{TE}} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) \right] b_{nm}^{(2)\text{TM}} \tilde{\pi}_{mn} (\cos\theta_{1})$$

$$+ \left[ 1 - R_{12}^{\text{TE}} (\pi - \theta_{1}) (-1)^{n+m} \exp(-2ikd\cos\theta_{1}) b_{nm}^{(1)\text{TM}} \tilde{\tau}_{mn} (\cos\theta_{1}) \right] \right\}.$$
(62)

The superscripts on the scattering coefficients  $b_{nm}^{(j)\text{TE}}$  and  $b_{nm}^{(j)\text{TM}}$  are the scattering field coefficients when the system is illuminated by TE and TM plane waves. These expressions represent the far-field solution to the problem of a sphere near a plane interface. Scattering amplitudes are convenient, theoretically, because they can be manipulated to produce measureable quantities like scattering intensities and polarization states. Figure 2 shows the scatter in the plane of incidence ( $\phi_1 = 0^\circ$ ) of  $r = 0.55 \ \mu m$  spheres resting on a substrate illuminated at  $\theta_{\circ} = 30^{\circ}$  and  $\lambda = 0.6328 \ \mu m$ . This figure demonstrates the sensitivity of the scatter to system parameters. The TM polarization intensities are especially sensitive to a change in the halfspace complex refractive index  $(m_2)$ , since the TM Fresnel reflection amplitudes are more sensitive than the TE amplitudes. Many sizing routines are based on the positions and spacing of the maxima and minima intensities. This graph demonstrates that care must be taken when applying such techniques to particles located on substrates. The spacings remain fairly constant for the TE illumination of figure 2, but change drastically for TM illumination.



Figure 2. Light scattering intensities calculated for  $r=0.55~\mu m$  spheres on a substrate illuminated at  $\lambda=0.6328~\mu m$ ,  $\theta_\circ=30^\circ$ ,  $\phi_1=0^\circ$ , and  $d=0.55~\mu m$ . Results are shown when system is composed entirely of gold ( $m_{\rm sph}=0.226+3.32i$ ) and when system is perfectly conducting.

#### 8. Conclusion

We derived a solution for the scattering from a spherical particle near a perfectly conducting plane interface. The analytical solution is in terms of a vector spherical harmonic expansion. The equations can be modified to accommodate an irregular particle near an irregular interface if the scattering T-matrix is known for these isolated subsystems. Additionally, the equations may also accommodate a nonperfectly conducting half space. We provided an approximate solution for this latter case, based on a normal-incident Fresnel reflection of the interaction field.

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