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The optical properties of particles deposited on a surface.

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by
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1. Outline of the research.

The motivation of this research stems from the need to detect and identify small particles deposited on a plane surface that is assumed to be otherwise clean. Such detection and identification is, in fact, relevant to all researches in which the cleannes of the surfaces is a fundamental prerequisite and to all the applications whose purpose is the deposition on a surface of particles of a given kind.

In the preceding years we addressed our research toward the study of the resonances from particles on account that the resonance spectra are widely known to give useful information both fer free particles and for particles on a surface. Nevertheless, our methods were restricted to the case of metallic surfaces because the latter are a good approximation to perfectly reflecting surfaces. In this case, in fact, the image method proved to be very efficient to yield useful information both on the presence and of the shape of the particles of interest.

In the last year our interest has been directed toward the properties of particles deposited on non-perfectly reflecting surfaces, i. e. on surfaces that separate two different dielectric media. Of course this new purpose of our research did not stopped our study of the shape resonances from particles on metallic surfaces, but our main aim has been toward the formulation of a theory applicable to particles on a surface of general dielectric properties.

2. Method of attack.

It is well known that the expansion of the field in terms of spherical vector multipoles is a good method to deal with the electromagnetic scattering from small particles even when the Rayleigh approximation does not apply. Therefore our starting point has been the formulation of a general theory to describe the reflection of a spherical vector multipole field on a plane surface. To this end we expanded a general vector multipole field as a superposition of polarized plane waves with complex propagation vectors that were the reflected on the surface through the Fresnel reflection rule. As a result we were led to define a matrix that transforms the original multipôle field into the reflected one. In this respect two point must be carefully stressed. First, the reflection of a single multipole field (either magnetic or electric) yields a superposition of both magnetic and electric multipole fields and, second, the reflected multipoles do not satisfy the radiation condition at infinity. While the first point has no further consequences than some complication of the algebra, the second point seem to imply that the reflected field cannot yield the field in the far zone where the observation is likely to take place. We were able, however, to show that this is a deciving appearence because of the fact that the expansion of a multipole field as an integral over plane waves has a domain of validity that does not extend to infinity. To gett the reflected field at infinity we remarked that the refelcted field can also be written as a superposition of vector multipole fields that satisfy the radiation condition and whose origin is at the image point of the origin of the incident multipoles. The whole theory is better described in the enclosed paper that has been submitted for publication.

A consequence of the research that has been outlined above is the possibility of studying the scattering both from a single sphere and from aggregated spheres in the presence of a surface of arbitrary dielectric properties. For the case of a single sphere the calculations have been completed whereas for aggregated spheres the calculations are still in progress. The results for a single sphere are better described in the second enclosed paper and may be summarized as follows. The calculated extonction patterns show an excellent agreement with the available experimental data as well as with the results of ab initio numerical simulations. Morover, unlike the existing theories, our approach yields a non-vanishing field that propagates along the surface. The latter esult was well known to radio engineers but in the past it was obtained only for dipole fields whereas our approach yield the correct result for fields of any multiplicity.

3. Resonances of hemispheres on a metal surface.

As we stated above, our work on the resonance spectra from particles on a metal surface has not been discontinued. We, in fact dealt with the properties of hemispheres on a perfectly reflecting surface because such hemispheres may be a good model for liquid droplets on a metal surface. Of course, in this case the method of choice has been the image theory whose efficiency has been proved in our preceding works. We also studied the case of aggregated droplets.

As a general comment to the results that are reported in the third enclosed paper, we can state that in the case of single hemispheres a reliable interpretation of the behavior of the observed resonances can be given on general grouds; for the case of aggregated hemispheres no general rule was found so that the interpretation of the resonance spectra requires a detailed analysis of the transition matrix of the aggregate of interest.

The problem is still under investigation and in particular a study of the case of hemispheres containig small inclusions is in progress.

4. List of publications.

1) E. Fucile, F. Borghese, P. Denti, R. Saija and O. I. Sindoni, "General reflection rule for electromagnetic multipole fields on a plane interface," Submitted to IEEE Trans on Antennas and Propagation.

2) F. Borghese, P. Denti, R. Saija, E. Fucile and O. I. Sindoni, "Resonance suppression in the extinction spectrum of single and aggregated hemispheres on a perfectly reflecting surface," submitted to Applied Optics

3) E. Fucile, P. Denti, F. Borghese, R. Saija and O. I. Sindoni, "Optical properties of a sphere in the vicinity of a plane surface," submitted to Journal of the Opti-

cal Society of America.

5. Partecipants to the research.

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General reflection rule for electromagnetic multipole fields on a plane interface.

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The general rule for reflection of a vector 2^l-pole field on a plane interface between two media of different dielectric properties is established starting from the expansion of the spherical multipole field as a linear combination of inhomogeneous vector plane waves. In fact, by considering vector multipole fields that satisfy the radiation condition at infinity we are able to define a matrix that effects their reflection on the plane interface. Such a matrix can also be used to reflect a superposition of many 2^l-pole fields and so can be useful to describe the effect of a plane surface near to a specified source or to a scattering particle.

1. Introduction

Several problems in electromagnetic wave propagation imply the reflection on the plane interface between two different media of the vector 2^l-pole fields emitted by a localized source: let us recall, for instance, the effect of earth on the propagation of the field emitted by an antenna[1,2] and the reflection on a plane interface of the light scattered by a particle.[3–5] The literature reports several papers that deal with some specific aspects of the subject, for instance the reflection of the field emitted by electric and magnetic dipoles,[6,7] but a general solution to the problem of the reflection of a spherical 2^l-pole field is still to come. This is not surprising because the mathematical structure of the vector multipole fields makes rather difficult the imposition of the boundary conditions across a plane interface.

In this paper we show how this difficulty can be overcome by combining together the expansion of a scalar spherical multipole field in terms of inhomogeneous scalar plane waves[3] and the definition of the vector multipole fields.[8] Since the components of a vector multipole field are indeed linear combinations of scalar multipole fields, we are able to build the vector equivalent of the expansion referred to above. The resulting formula gives, in fact, the expansion of a general vector multipole field that satisfy the radiation condition at infinity as a linear combination of inhomogeneous vector plane waves that can thus be reflected through the Fresnel reflection rule. By expanding the reflected vector plane waves into a series of vector multipole fields we are led to define a multipole reflection matrix that effects the transformation of the incident vector multipole field into a linear combination of reflected vector multipole fields. Close examination of the latter combination shows that the reflected multipoles appear as emitted by the mirror image of the original source with respect to the interface.

In Section 2 we establish the formula for the expansion of a vector 2^l-pole field in terms of vector plane waves and with the help of the Fresnel reflection rule define the matrix that effects the reflection of such a field on the plane interface. To this end we assume that the source of multipole fields be embedded within a homogeneous medium with real refractive index; also the medium beyond the interface is assumed to be homogeneous but its refractive index may possibly be complex. The theory also includes, as a limit, the case of a perfectly reflecting surface.

In Section 3 we show how the formal solution that has been established in Section 2 is actually suitable for numerical calculations. In particular, the elements of the multipole reflection matrix turn out to be given by integrals that can be evaluated through standard numerical methods.

In Section 4 the accuracy of the calculated elements of the multipole reflection matrix is tested by investigating the numerical stability of the intensity that would be detected in the far zone when a vector multipole field that satisfies the radiation condition at infinity is emitted by a point source located in the vicinity of the plane interface. Since, according to our previous remark, the reflected field is given by a series of vector multipole fields that appear as emitted by the image of the source with respect to the interface, we also check the convergence of the latter series as a function of the distance of the source from the interface.

A number of useful formulas and expansions are, for completeness, summarized in Appendix A and B.

2. Multipole reflection rule

The field emitted by a localized source, embedded in a homogeneous medium of refractive index n, can be expanded as a linear combination of spherical vector multipoles that satisfy the radiation condition at infinity.[2,9] In order to define such multipole fields we consider a cartesian frame of reference whose axes are characterized by the unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$. Then, by assuming that all the fields depend on time through the factor $\exp(-i\omega t)$, the appropriate vector 2^l-pole fields are[8]

$$\begin{aligned} \mathbf{H}_{lm}^{(1)}(\mathbf{r}, nk) &= h_l(nkr)\mathbf{X}_{lm}(\hat{\mathbf{r}}), \\ \mathbf{H}_{lm}^{(2)}(\mathbf{r}, nk) &= \frac{1}{nk}\nabla \times \mathbf{H}_{lm}^{(1)}(\mathbf{r}, nk), \end{aligned} \tag{1}$$

where, as usual, $k = \omega/c$ and the superscripts 1 and 2 are the values of the parity index p that distinguishes the magnetic multipoles ($p = 1$) from the electric ones ($p = 2$); the quantities h_l are spherical Hankel functions of the first kind and the vectors $\mathbf{X}_{lm}$ are vector spherical harmonics.[9] The latter are conveniently defined as

$$\mathbf{X}_{lm} = -\sum C(1,l,l;-\mu,m+\mu)Y_{l,m+\mu}(\vartheta,\varphi)\boldsymbol{\xi}_{-\mu}, \tag{2}$$

where the functions $Y_{lm}(\vartheta,\varphi)$ are (scalar) spherical harmonics,[9]

$$\boldsymbol{\xi}_0 = \hat{\mathbf{z}}, \quad \boldsymbol{\xi}_{\pm 1} = \mp\frac{1}{\sqrt{2}}(\hat{\mathbf{x}} \pm i\hat{\mathbf{y}}),$$

are the unit vectors of the spherical basis and the C are the Clebsch–Gordan coefficients[8]

$$\begin{aligned} C(1,l,l;\pm 1, m\mp 1) = c_{lm}^{(\mp 1)} &= \pm\sqrt{\frac{(l\pm m)(l\mp m+1)}{2l(l+1)}}, \\ C(1,l,l;0,m) = c_{lm}^{(0)} &= -\frac{m}{\sqrt{l(l+1)}}. \end{aligned}$$

Our present purpose is to establish a general rule for the reflection of the multipole fields $\mathbf{H}_{lm}^{(p)}$ on the plane interface between two media of different dielectric properties. It is easily understood, however, that the mathematical structure of the spherical multipole fields, Eqs. (1), makes rather difficult imposing the appropriate boundary conditions across the flat interface.[4] In order to face this problem we search for the vector equivalent of the integral expression[3]

$$h_l(nkr)Y_{lm}(\vartheta,\varphi) = \frac{(-i)^l}{2\pi}\int_0^{2\pi} d\varphi_k \int_0^{\frac{\pi}{2}-i\infty} d\vartheta_k \sin\vartheta_k Y_{lm}(\vartheta_k,\varphi_k)e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{3}$$

that, in the halfspace $z > 0$, gives the scalar multipole $h_l Y_{lm}$ as a superposition of plane waves with complex propagation vectors (inhomogeneous plane waves). It may be worth noticing that the range of integration in Eq. (3) is such that the real part of all the propagation vectors lies in the halfspace $z > 0$: thus the scalar multipole field $h_l(nkr)Y_{lm}(\vartheta,\varphi)$ turns out to be a superposition of inhomogeneous plane waves that come from the source at the origin and propagate through the halfspace $z > 0$. An analogous expansion, applicable to the halfspace $z < 0$, can be written by considering plane waves whose propagation vectors have a real part that lies in the latter region.

A. Reflected field

Let us now define a cartesian frame of reference whose origin O lies on the plane interface between two media. Without loss of generality we can assume that the interface coincides with the plane $z = 0$ and that a homogeneous medium of refractive index n' fills the half-space $z < 0$ whereas a different homogeneous medium of refractive index n'' fills the half-space $z > 0$ (see Fig. 1). We assume that a source of $\mathbf{H}$ multipole fields lies entirely within the half-space $z < 0$ and define a further frame of reference that is translated with respect to O and whose origin, O', lies within the source at a distance d from the interface. For our purposes it is also convenient to define a third frame of reference that is also translated with respect to O and whose origin, O'', is the mirror image of O' with respect to the interface. We will denote with $\mathbf{R}'$ and $\mathbf{R}''$ the vector position of the origins O' and O'' in the frame of reference with origin at O, respectively, whereas the vector position of the point of observation P in the three frames defined above will be denoted with $\mathbf{r}$, $\mathbf{r}'$ and $\mathbf{r}''$, respectively. Then, by applying Eq. (3) to each of the scalar multipole fields that appear in the definition of an $\mathbf{H}$ multipole field, Eqs. (1) and (2), the multipole field $\mathbf{H}_{lm}^{(p)}(\mathbf{r}', n'k)$ with origin at O' can be expanded as

$$\mathbf{H}_{lm}^{(p)}(\mathbf{r}', n'k) = \frac{(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}) \exp(i\mathbf{k}\cdot\mathbf{r}')\, d\hat{\mathbf{k}}, \tag{4}$$

where we define the transverse vector harmonics

$$\mathbf{Z}_{lm}^{(1)}(\hat{\mathbf{k}}) = \mathbf{X}_{lm}(\hat{\mathbf{k}}), \quad \mathbf{Z}_{lm}^{(2)}(\hat{\mathbf{k}}) = \mathbf{X}_{lm}(\hat{\mathbf{k}}) \times \hat{\mathbf{k}}, \tag{5}$$

$\mathcal{D}$ denotes the same integration domain as in Eq. (3) and $\mathbf{k} = n'k\hat{\mathbf{k}}$ is the propagation vector of the component plane wave.

Equation (4) is the vector equivalent of Eq. (3) that is suitable for our purposes as it states that any $\mathbf{H}$ multipole field can be written as a superposition of inhomogeneous vector plane waves, of amplitude $\mathbf{Z}_{lm}^{(p)}$, whose propagation vectors have a real part that points towards the flat interface: as a consequence, each of the component plane waves can be reflected according to the Fresnel reflection rule. To this end each component plane wave must be rewritten as a superposition of its polarized components that are parallel and perpendicular to the plane of incidence, that, as usual, is defined as the plane that contains both $\mathbf{k}$ and the z axis. Let us therefore define a pair of unit vectors, $\hat{\mathbf{u}}_\eta$, $(\eta = 1, 2)$, that are parallel $(\eta = 1)$ and perpendicular $(\eta = 2)$ to the plane of incidence and so oriented that

$$\hat{\mathbf{u}}_1 \times \hat{\mathbf{u}}_2 = \hat{\mathbf{k}}.$$

Now, since $\mathbf{r}' = \mathbf{r} - \mathbf{R}'$, Eq. (4) can be rewritten as

$$\mathbf{H}_{lm}^{(p)}(\mathbf{r}', n'k) = \frac{(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \sum_\eta [\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})]\, \hat{\mathbf{u}}_\eta \exp(i\mathbf{k}\cdot\mathbf{r}) \exp(-i\mathbf{k}\cdot\mathbf{R}')\, d\hat{\mathbf{k}}, \tag{6}$$

so that the integrand contains only plane waves referred to the origin at O. In fact, the term $\hat{\mathbf{u}}_\eta \exp(i\mathbf{k}\cdot\mathbf{r})$ in Eq. (6) is a vector inhomogeneous plane wave that is unitary at O and that can be reflected using the Fresnel reflection rule. As a result of the reflection we get the field

$$\mathbf{H}_{Rlm}^{(p)} = \frac{(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \sum_\eta F_\eta \left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right] \hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R\cdot\mathbf{r}) \exp(-i\mathbf{k}\cdot\mathbf{R}')\, d\hat{\mathbf{k}}, \tag{7}$$

where $\mathbf{k}_R$ and $\hat{\mathbf{u}}_{R\eta}$ are, respectively, the wave vector and the polarization unit vectors for the reflected wave and the quantities F_η are the Fresnel reflection coefficients[9]

$$F_1 = \frac{n^2\cos\vartheta_k - \beta}{n^2\cos\vartheta_k + \beta}, \quad F_2 = \frac{\cos\vartheta_k - \beta}{\cos\vartheta_k + \beta},$$

where

$$\beta = \sqrt{(n^2-1) + \cos^2\vartheta_k}$$

and $n = n''/n'$. The integrand in Eq. (7) can be referred back to the origin at O' by the phase factor $\exp(i\mathbf{k}_R\cdot\mathbf{R}')$ with the result

$$\mathbf{H}_{Rlm}^{(p)} = \frac{(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \sum_\eta F_\eta \left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right]$$
$$\hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R\cdot\mathbf{r}') \exp[i(\mathbf{k}_R - \mathbf{k})\cdot\mathbf{R}']\, d\hat{\mathbf{k}}. \tag{8}$$

Now, according to Appendix A, the multipole expansion of the vector inhomogeneous plane wave in Eq. (8) is

$$\hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R\cdot\mathbf{r}') = 4\pi \sum_{plm} i^{p+l-1}(-)^{m+1} \mathbf{Z}_{l,-m}^{(p)}(\hat{\mathbf{k}}_R)\cdot\hat{\mathbf{u}}_{R\eta} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', n'k), \tag{9}$$

where the multipole fields $\mathbf{J}_{lm}^{(p)}$ are identical to the $\mathbf{H}_{lm}^{(p)}$ except for the substitution of a spherical Bessel function j_l for the Hankel function h_l. Then, substitution of Eq. (9) into Eq. (8) leds us to write the reflected field as

$$\mathbf{H}_{Rlm}^{(p)} = \sum_{p'l'm'} \mathbf{J}_{l'm'}^{(p')}(\mathbf{r}', n'k)\mathcal{F}_{l'm'lm}^{(p',p)}, \tag{10}$$

where we define the quantities

$$\mathcal{F}_{l'm'lm}^{(p',p)} = 2i^{p'-p+l'-l}(-)^{m+1} \int_{\mathcal{D}} \sum_{\eta} F_\eta \left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right] \times \left[\hat{\mathbf{u}}_{R\eta} \cdot \mathbf{Z}_{l',-m'}^{(p')}(\hat{\mathbf{k}}_R)\right] \exp(2in'kd\cos\vartheta_k)\, d\hat{\mathbf{k}}, \tag{11}$$

that are the elements of the matrix F that effects the reflection of the spherical vector multipoles. Equation (10) is thus the formal solution of the problem at hand.

B. Far field

It may be surprising that Eq. (10) gives the reflected field $\mathbf{H}_{Rlm}^{(p)}$ in terms of multipole fields, namely the J fields, that do not satisfy the radiation condition at infinity. This is a deceiving appearance, however, because it must be borne in mind that the reflection has been performed on the terms of an expansion, Eq. (6), that is valid only in the half-space $z' > 0$: as a result the region of validity of Eq. (10) is still to be determined.

A simple way to asses this point is suggested by the fact that Eq. (8) can be rewritten in the form

$$\mathbf{H}_{Rlm}^{(p)} = \frac{(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \sum_{\eta} F_\eta \left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right] \hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R \cdot \mathbf{r}'')\, d\hat{\mathbf{k}}, \tag{12}$$

so that the integrand is expressed in terms of reflected plane waves that are referred to the origin O'': the phase factor

$$\exp[i(\mathbf{k}_R - \mathbf{k}) \cdot \mathbf{R}'] = \exp(2in'kd\cos\vartheta_k)$$

in Eq. (8) effects, indeed, the translation of origin from O'' to O'. With the help of Eqs. (A7) and (A8) in Appendix A it is an easy matter to see that the amplitudes of the incident and of the reflected wave are related by the equation[10]

$$\hat{\mathbf{u}}_{R\eta} \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}_R) = (-)^{\eta+p+l+m}\, \hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}), \tag{13}$$

so that Eq. (12) can be rewritten as

$$\mathbf{H}_{Rlm}^{(p)} = \frac{(-)^{p+l+m-1}(-i)^{p+l-1}}{2\pi} \int_{\mathcal{D}} \sum_{\eta} (-)^{\eta+1} F_\eta \left[\hat{\mathbf{u}}_{R\eta} \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}_R)\right] \times \hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R \cdot \mathbf{r}'')\, d\hat{\mathbf{k}}. \tag{14}$$

The interpretation of Eq. (14) is straightforward when the plane interface is perfectly reflecting. In this case, in fact, the Fresnel coefficients take on the limiting value

$$F_\eta = (-)^{\eta-1}$$

and Eq. (14) can be easily verified to represent, except for a sign, the multipole field $\mathbf{H}_{lm}^{(p)}(\mathbf{r}'', n'k)$, with origin at the image point O'': this representation is valid in the half-space $z'' < 0$. Let us thus assume that in the general case Eq. (14) represents, in the half-space $z'' < 0$, a linear combination of $\mathbf{H}$ multipole fields with origin at O'' such as

$$\mathbf{H}^{(p)}_{Rlm} = \sum_{p''l''m''} \mathbf{H}^{(p'')}_{l''m''}(\mathbf{r}'', n'k) a^{(p'',p)}_{l''m'',lm}. \tag{15}$$

In order to determine the amplitudes $a^{(p'',p)}_{l''m'',lm}$ we express each of the $\mathbf{H}$ multipole fields in Eq. (15) as a combination of multipoles centered at O' through the use of the appropriate addition theorem.[11] By defining $\mathbf{R} = \mathbf{R}' - \mathbf{R}''$, in the region inside the sphere with center at O' and of radius R (see Fig. 1), i. e. for $r' < R$, the addition theorem yields

$$\mathbf{H}^{(p)}_{Rlm} = \sum_{p''l''m''} \sum_{p'l'm'} \mathbf{J}^{(p')}_{l'm'}(\mathbf{r}', n'k) \mathcal{H}^{(p',p'')}_{l'm',l''m''}(\mathbf{R}, n'k) a^{(p'',p)}_{l''m'',lm}, \tag{16}$$

whereas, in the region outside this sphere, i. e. for $r' > R$, we get

$$\mathbf{H}^{(p)}_{Rlm} = \sum_{p''l''m''} \sum_{p'l'm'} \mathbf{H}^{(p')}_{l'm'}(\mathbf{r}', n'k) \mathcal{J}^{(p',p'')}_{l'm',l''m''}(\mathbf{R}, n'k) a^{(p'',p)}_{l''m'',lm}. \tag{17}$$

The quantities $\mathcal{H}^{(p',p'')}_{l'm',l''m''}(\mathbf{R}, n'k)$ and $\mathcal{J}^{(p',p'')}_{l'm',l''m''}(\mathbf{R}, n'k)$ are explicitly given in Appendix B. By comparing Eq. (16) and Eq. (10) we get for the coefficients $a^{(p'',p)}_{l''m'',lm}$ the expression

$$a^{(p'',p)}_{l''m'',lm} = \sum_{p'l'm'} (\mathcal{H}^{-1})^{(p'',p')}_{l''m'',l'm'} \mathcal{F}^{(p',p)}_{l'm',lm}, \tag{18}$$

that, when substituted into Eq. (17), yields the reflected field $\mathbf{H}_R$ in a form that is valid at large distance from the source and satisfy the radiation condition at infinity as it contains $\mathbf{H}$ multipole fields only.

3. Calculation of the reflected field

Equation (11), that defines the elements of the multipole reflection matrix, may seem to give only a formal solution to the problem of reflection. Nevertheless in this section we use the properties of the spherical multipole fields to put Eq. (11) into a form that is suitable for actual calculations. First by substituting Eq. (13) into Eq. (11) we eliminate the reflected wavevector $\mathbf{k}_R$ and the polarization vectors $\hat{\mathbf{u}}_{R\eta}$ so that the integrand depends on the dot product $\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{k}})$ only. The latter can be calculated by representing the polarization unit vectors on the spherical basis as

$$\hat{\mathbf{u}}_1 = \frac{\cos\vartheta_k \exp(i\varphi_k)}{\sqrt{2}} \boldsymbol{\xi}_{-1} - \sin\vartheta_k \boldsymbol{\xi}_0 - \frac{\cos\vartheta_k \exp(-i\varphi_k)}{\sqrt{2}} \boldsymbol{\xi}_1,$$

$$\hat{\mathbf{u}}_2 = \frac{i}{\sqrt{2}} \exp(i\varphi_k) \boldsymbol{\xi}_{-1} + \frac{i}{\sqrt{2}} \exp(-i\varphi_k) \boldsymbol{\xi}_1,$$

so that we get

$$\begin{aligned}\hat{\mathbf{u}}_1 \cdot \mathbf{Z}^{(1)}_{lm} = \Big[& -\frac{1}{\sqrt{2}} c^{(1)}_{lm} \overline{P}_{l,m+1}(\cos\vartheta_k) \cos\vartheta_k + \\ & + c^{(0)}_{lm} \overline{P}_{lm}(\cos\vartheta_k) \sqrt{1 - \cos^2\vartheta_k} + \\ & + \frac{1}{\sqrt{2}} c^{(-1)}_{lm} \overline{P}_{l,m-1}(\cos\vartheta_k) \cos\vartheta_k \Big] \exp(im\varphi_k),\end{aligned}$$

$$\hat{\mathbf{u}}_2 \cdot \mathbf{Z}^{(1)}_{lm} = \left[\frac{i}{\sqrt{2}} c^{(1)}_{lm} \overline{P}_{l,m+1}(\cos\vartheta_k) + \right.$$
$$\left. + \frac{i}{\sqrt{2}} c^{(-1)}_{lm} \overline{P}_{l,m-1}(\cos\vartheta_k)\right] \exp(im\varphi_k),$$

where we define the functions

$$\overline{P}_{lm}(z) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_{lm}(z)$$

in which $P_{lm}(z)$ denotes the Legendre functions of complex argument

$$P_{lm}(z) = (-)^m \frac{(1-z^2)^{m/2}}{2^l l!} \frac{d^{l+m}}{dz^{l+m}}(z^2-1)^l.$$

Then it can be easily verified that the relation $\hat{\mathbf{u}}_2 = \hat{\mathbf{k}} \times \hat{\mathbf{u}}_1$ and the definition of the transverse harmonics, Eq. (5), yield the rules

$$\hat{\mathbf{u}}_2 \cdot \mathbf{Z}^{(2)}_{lm} = -\hat{\mathbf{u}}_1 \cdot \mathbf{Z}^{(1)}_{lm} = -\hat{\mathbf{u}}_1 \cdot \mathbf{X}_{lm},$$
$$\hat{\mathbf{u}}_1 \cdot \mathbf{Z}^{(2)}_{lm} = \hat{\mathbf{u}}_2 \cdot \mathbf{Z}^{(1)}_{lm} = \hat{\mathbf{u}}_2 \cdot \mathbf{X}_{lm},$$

whereas, the properties of the vector spherical harmonics yield the relation

$$\hat{\mathbf{u}}_\eta \cdot \mathbf{X}_{l,-m} = (-)^{\eta+m} \hat{\mathbf{u}}_\eta \cdot \mathbf{X}_{l,m} \exp(-2im\varphi_k).$$

We are now able to perform at once the integration over the angle φ_k with the result

$$\int_0^{2\pi} \exp[i(m-m')\varphi_k] d\varphi_k = 2\pi\delta_{mm'},$$

so that the elements of the multipole reflection matrix $\mathcal{F}^{(p',p)}_{l'm',lm}$ with $m \neq m'$ do vanish. This property is conveniently expressed by the equation

$$\mathcal{F}^{(p',p)}_{l'm',lm} = \mathcal{F}^{(p',p)}_{l',l;m}\delta_{mm'}, \tag{19}$$

that, when introduced into Eq. (11) yields the useful relation

$$\mathcal{F}^{(p',p)}_{l',l;-m} = \mathcal{F}^{(p,p')}_{l,l';m}.$$

At this stage each element of the matrix F is given by an integral of the form

$$\int_0^{\frac{\pi}{2}-i\infty} f(\cos\vartheta_k) \exp(2in'kd\cos\vartheta_k) \sin\vartheta_k \, d\vartheta_k,$$

that, through the substitution $x = 2in'kd(1-\cos\vartheta_k)$ becomes

$$\frac{\exp(i2n'kd)}{i2n'kd} \int_0^{+\infty} f\left(1 - \frac{x}{2in'kd}\right) \exp(-x)\, dx, \tag{20}$$

and is thus suitable for numerical integration, e. g. through the Gauss–Laguerre method.[12] In practice, the implied formula is

$$\int_0^\infty f(x)\exp(-x)\,dx \approx \sum_{i=1}^N w_i f(x_i),$$

where the weights w_i are

$$w_i = \frac{(N!)^2 x_i}{(N+1)^2[L_N(x_{i+1})]^2},$$

x_i being the i-th zero of the Laguerre polynomial L_N. Thus to get reliable values of the elements of F the order N must be wisely chosen so as to ensure a fair convergence of the integrals.

Let us now recall that, according to Eqs. (15) and (18), the calculation of the reflected field requires the elements of the reflection matrix F as well as the quantities $(\mathcal{H}^{-1})^{(p'',p')}_{l''m'',l'm'}$. Since in the present case the translation vector $\mathbf{R}$ is parallel to the z axis, the elements of $\mathcal{H}$, according to Eq. (B3), vanish for $m \neq m'$. As a result also the quantities $(\mathcal{H}^{-1})^{(p'',p')}_{l''m'',l'm'}$ have the same property so that also the amplitudes $a^{(p'',p)}_{l''m'',lm}$ do vanish unless $m'' = m$, i. e.

$$a^{(p'',p)}_{l''m'',lm} = a^{(p'',p)}_{l'',l;m}\delta_{mm''},$$

with

$$a^{(p'',p)}_{l'',l;m} = \sum_{p'l'}(\mathcal{H}^{-1})^{(p'',p')}_{l'',l';m}\mathcal{F}^{(p',p)}_{l',l;m}. \tag{21}$$

4. Results and discussion

The main result of the theory that we developed in Section 2 is the introduction of the matrix F that effects the reflection of a $\mathbf{H}$ multipole field on a plane interface. The elements of this matrix were shown in Section 3 to be given by integrals that, though suitable for numerical calculations, require a careful check of their convergence. Nevertheless, considering the convergence of each of the elements of F only would be, in our opinion, of little significance because their numerical values, for fixed values of n', k and d, may have widely different values with varying pl, $p'l'$ and m. We thus resolved to make an indirect test of F by investigating the numerical stability of the field that would be observed in the far zone.

At any point in the half-space $z < 0$ the total field is the superposition of the field that is directly emitted by the source and of the field that is reflected by the surface. The physical situation is much the same as a detector that receives both the field from an emitting antenna and the field that is reflected by the surface of earth. According to Section 2B, the total field is the superposition of the original multipole field with origin at O' and of the reflected field that is given by a combination of multipole fields with origin at O'', Eq. (15): it is thus convenient to refer all the multipole fields to the same origin by resorting again to the addition theorem of ref. 11. For symmetry reasons we choose to refer all the multipole fields to the origin O on the interface (see Fig. 1) and get for the total field in the far zone

$$\begin{aligned}\mathbf{H}^{(p)}_{Tlm} &= \sum_{p'l'm'}\mathbf{H}^{(p')}_{l'm'}(\mathbf{r},nk)\mathcal{J}^{(p',p)}_{l'm',lm}(-\mathbf{R}',n'k)\\ &+ \sum_{p'l'm'}\sum_{p''l''}\mathbf{H}^{(p')}_{l'm'}(\mathbf{r},nk)\mathcal{J}^{(p',p'')}_{l'm',l''m}(-\mathbf{R}'',n'k)a^{(p'',p)}_{l'',l;m},\end{aligned}$$

where the arguments of the quantities $\mathcal{J}$ get a minus sign because the translations go towards O and are thus opposite both to $\mathbf{R}'$ and to $\mathbf{R}''$. By defining the amplitudes

$$A^{(p',p)}_{l'm',lm} = \mathcal{J}^{(p',p)}_{l'm',lm}(-\mathbf{R}',n'k) + \sum_{p''l''}\mathcal{J}^{(p',p'')}_{l'm',l''m}(-\mathbf{R}'',n'k)a^{(p'',p)}_{l'',l;m},$$

the total field becomes

$$\mathbf{H}^{(p)}_{Tlm} = \sum_{p'l'm'} \mathbf{H}^{(p')}_{l'm'}(\mathbf{r}, n'k) A^{(p',p)}_{l'm',lm},$$

so that at P it turns out to be a superposition of $\mathbf{H}$ multipole fields only. Now, if the receiver is far enough from O, it is sufficient to consider the asymptotic form of the field. On account of the limiting form of the spherical Hankel functions for large values of their argument[2] and of the transversality of the far field with respect to the direction of observation $\hat{\mathbf{r}}$, we can write

$$\mathbf{H}^{(p)}_{Tlm} = \frac{\exp(in'kr)}{r}\mathbf{f}^{(p)}_{lm},$$

where we define the vector amplitude

$$\mathbf{f}^{(p)}_{lm} = \frac{1}{n'k} \sum_{p'l'm'} (-i)^{p'+l'} \mathbf{Z}^{(p')}_{l'm'}(\hat{\mathbf{r}}) A^{(p',p)}_{l'm',lm}.$$

Accordingly, the waves that are polarized along the unit vector $\hat{\mathbf{u}}$ yield the intensity

$$I^{(p)}_{lm} = \frac{1}{r^2}|\mathbf{f}^{(p)}_{lm} \cdot \hat{\mathbf{u}}|^2,$$

where, by using the definition of the amplitudes $W^{(p')*}_{l'm'}$, Eq. (A8), we have

$$\mathbf{f}^{(p)}_{lm} \cdot \hat{\mathbf{u}} = -\frac{i}{4\pi n'k} \sum_{p'l'm'} W^{(p')*}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{r}}) A^{(p',p)}_{l'm',lm}.$$

The preceding equation can be greatly simplified by resorting to Eq. (B5). On account of the definition of the amplitudes $A^{(p',p)}_{l'm',lm}$ and of the fact that, as we stated in Section 1, the refractive index n' is assumed to be real we get

$$\mathbf{f}^{(p)}_{lm} \cdot \hat{\mathbf{u}} = -\frac{i}{4\pi n'k} \left[\exp(i\mathbf{k} \cdot \mathbf{R}') W^{(p)*}_{lm}(\hat{\mathbf{u}}, \hat{\mathbf{r}}) + \sum_{p''l''} \exp(i\mathbf{k} \cdot \mathbf{R}'') W^{(p'')*}_{l''m}(\hat{\mathbf{u}}, \hat{\mathbf{r}}) a^{(p'',p)}_{l'',l;m} \right], \tag{22}$$

that is the equation that we actually used to calculate the far field intensity.

Equation (22) shows that one has to extend the sum within the square brackets to a sufficiently high value of l'' to get reliable values for the observed intensity. It must be borne in mind, however, that one should also check the convergence of the amplitudes $a^{(p'',p)}_{l'',l;m}$ that, according to Eq. (21), imply a further sum over the intermediate index l'. We remark, however, that, whatever value of l' is needed to get the convergence of the amplitudes $a^{(p'',p)}_{l'',l;m}$, the calculation of the elements of $\mathcal{H}$ and thus of the elements of $\mathcal{H}^{-1}$ did not give any computational trouble: therefore the convergence of the sum in Eq. (21) stands on the values of the elements of F only.

On account of the preceding considerations we resolved to investigate the convergence of the quantity $r^2 I^{(p)}_{lm}$ for both values of p and for $l = 1$, 2 and 3. The field was calculated for polarization both parallel and perpendicular to the plane that contains the z axis and the direction of observation. We assumed that the source at O' were embedded in a medium with refractive index $n' = 1$ and that its distance from the interface were such that $kd = 0.5$, 1.0 and 1.5. The angle between the direction of observation and the z axis was assumed to be $\vartheta = 165°$: in fact, this choice ensures that the trigonometric functions that are involved in the elements of F do not assume particular values that may produce undue cancellation.

In Table 1 we report the result of our study of the convergence of the total field for $\lambda = 500\,\mathrm{m}$ and $n'' = 9$; this choice of the refractive index is, indeed, appropriate for water in the radiowave range.[2] More precisely we reported in Table 1 the value of N that ensures the convergence of all the relevant elements of F, Eq. (20). As regards the convergence of the sums in Eq. (21) and (22) we found that, in the worst case, it suffices to consider elements up to and including $l'' = l' = 7$ to ensure that the observed intensity be stable at least to two decimal digits.

In Table 2 we report similar information for $\lambda = 500\,\text{nm}$ and $n'' = 1.3$, the latter choice of the refractive index being appropriate in the visible range. Even in this case we had to retain, at worst, terms up to and including $l'' = l' = 7$ to get convergence of the calculated field at least to two decimal digits.

We notice that the values reported in the tables above apply to both values of p and to any choice of the polarization; in other words, the convergence of the calculated field is practically independent of these features. On the contrary, comparison of Table 1 and 2 show that the rate of convergence is quite different in the radiowave and in the optical range: the values of N in Table 1 decrease with increasing kd whereas the values in Table 2 are more or less independent of the choice of kd. Close examination of Eq. (11), that defines the elements of F, leads us to conclude that this different behavior is entirely due to the Fresnel coefficients F_η on account of their dependence on the ratio n''/n'. Our investigation on this point was further pursued by examining in detail the specific behavior of a few selected elements of F when they are calculated by means of Eq. (20). We found that the real and the imaginary part of the integral in Eq. (20) may converge at a different rate that depends on the choice of the refractive index n''. In particular, when $n'' = 9$, this difference of convergence rate may become large and leads to the highest values of N that are reported in Table 1.

5. Conclusions

The theory that we presented in the preceding sections is essentially based on two main ingredients: the extension to vector multipole fields of the plane-wave expansion of Bobbert and Vlieger[3] and the addition theorem for vector multipole fields.[11]

The first ingredient allowed us to formulate our theory in terms of vector fields only and thus to account for the reflection of both magnetic and electric multipole fields of arbitrary order and for the effect of the polarization.

The second ingredient, in turn, proved to be the key tool to define unambiguously the region within which the reflected field is given by $\mathbf{J}$ multipole fields and the region in which it is given by $\mathbf{H}$ multipole fields with origin at the actual source. As a result, we were able to get the reflected field at any point within the accessible half-space $z < 0$ without resort to any approximation. Moreover, the addition theorem allows us to introduce the image source in a quite natural way.

The formal solution to the multipole reflection problem is given in terms of the multipole reflection matrix F that proved to be suitable for numerical calculations; in fact, the discussion in Section 4 leds us to conlude that the elements of F that may be needed for particular applications can confidently be calculated without undue computational effort.

Appendix A: Multipole amplitudes of an inhomogeneous plane wave

The field of a plane wave of unit amplitude, (possibly complex) propagation vector $\mathbf{k} = nk\hat{\mathbf{k}}$ and polarization unit vector $\hat{\mathbf{u}}$ can be expanded into a series of spherical vector multipoles as

$$\mathbf{E} = \hat{\mathbf{u}} \exp(i\mathbf{k}\cdot\mathbf{r}) = \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk) W_{lm}^{(p)}(\hat{\mathbf{u}}, \hat{\mathbf{k}}), \tag{A1}$$

$$i\mathbf{B} = \frac{1}{k}\nabla \times \mathbf{E} = in(\hat{\mathbf{k}} \times \hat{\mathbf{u}}) \exp(i\mathbf{k}\cdot\mathbf{r}) = n \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk) W_{lm}^{(p'\neq p)}(\hat{\mathbf{u}}, \hat{\mathbf{k}}), \tag{A2}$$

where the amplitudes W depend only on the polarization and propagation unit vectors. Multiplication of Eqs. (A1) and (A2) by $(-)^{m+1}\mathbf{X}_{l,-m}(\hat{\mathbf{r}})$, integration over the solid angle and use of the well known orthonormality relation

$$(-)^{m+1}\int_\Omega \mathbf{X}_{lm}(\hat{\mathbf{r}})\cdot\mathbf{X}_{l,-m}(\hat{\mathbf{r}})d\hat{\mathbf{r}} = \delta_{ll'}\delta_{mm'}$$

yields

$$\hat{\mathbf{u}}\cdot\mathbf{w}_{lm}(\mathbf{k},r) = W_{lm}^{(1)}(\hat{\mathbf{u}},\hat{\mathbf{k}})j_l(nkr), \tag{A3}$$

$$i(\hat{\mathbf{k}}\times\hat{\mathbf{u}})\cdot\mathbf{w}_{lm}(\mathbf{k},r) = W_{lm}^{(2)}(\hat{\mathbf{u}},\hat{\mathbf{k}})j_l(nkr), \tag{A4}$$

where

$$\mathbf{w}_{lm}(\mathbf{k},r) = \int_\Omega (-)^{m+1}\mathbf{X}_{l,-m}(\hat{\mathbf{r}})\exp(i\mathbf{k}\cdot\mathbf{r})d\hat{\mathbf{r}}. \tag{A5}$$

Now, by inserting into Eq. (A5) the Bauer expansion of a scalar plane wave,[9]

$$\exp(i\mathbf{k}\cdot\mathbf{r}) = 4\pi\sum_{l'm'} i^{l'}(-)^{m'}Y_{l',-m'}(\hat{\mathbf{k}})Y_{l'm'}(\hat{\mathbf{r}})j_{l'}(kr).$$

we get

$$\mathbf{w}_{lm}(\mathbf{k},r) = 4\pi i^l(-)^{m+1}\mathbf{X}_{l,-m}(\hat{\mathbf{k}})j_l(kr), \tag{A6}$$

on account of the orthogonality relations for the (scalar) spherical harmonics and of the definition of the vector spherical harmonics, Eq. (2). Ultimately, from Eqs. (A3), (A4) and (A6) we get the expression

$$W_{lm}^{(p)}(\hat{\mathbf{u}},\hat{\mathbf{k}}) = 4\pi i^{p+l-1}(-)^{m+1}\mathbf{Z}_{l,-m}^{(p)}(\hat{\mathbf{k}})\cdot\hat{\mathbf{u}} \tag{A7}$$

that gives the multipole amplitudes of an inhomogeneous plane wave. We also need the complex conjugate of Eq. (A7) that is easily seen to be

$$W_{lm}^{(p)*}(\hat{\mathbf{u}},\hat{\mathbf{k}}) = 4\pi(-i)^{p+l-1}\mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\cdot\hat{\mathbf{u}}. \tag{A8}$$

Let us now recall that if the polar angles of the incident wavevector $\mathbf{k}$ are ϑ and φ we have[10]

$$\begin{array}{lll} \hat{\mathbf{k}}\equiv(\vartheta,\varphi), & \hat{\mathbf{u}}_1\equiv(\vartheta+\frac{\pi}{2},\varphi), & \hat{\mathbf{u}}_2\equiv(\frac{\pi}{2},\varphi+\frac{\pi}{2}), \\ \hat{\mathbf{k}}_R\equiv(\pi-\vartheta,\varphi), & \hat{\mathbf{u}}_{R1}\equiv(\vartheta+\frac{\pi}{2},\varphi+\pi), & \hat{\mathbf{u}}_{R2}\equiv(\frac{\pi}{2},\varphi+\frac{\pi}{2}), \end{array}$$

and that any unit vector $\hat{\mathbf{v}}\equiv(\vartheta,\varphi)$ can be represented on the spherical basis as[13]

$$\hat{\mathbf{v}} = \sum_\mu(-)^\mu v_\mu\xi_{-\mu} = \sum_\mu(-)^\mu\sqrt{\frac{4\pi}{3}}Y_{1\mu}(\vartheta,\varphi)\xi_{-\mu}.$$

Thus, representing both the incident and the reflected polarization and propagation unit vectors on the spherical basis it is an easy matter to see that the properties of the spherical harmonics under change of their arguments yield the relation

$$W_{lm}^{(p)}(\hat{\mathbf{u}}_{R\eta},\hat{\mathbf{k}}_R) = (-)^{\eta+p+l+m}W_{lm}^{(p)}(\hat{\mathbf{u}}_\eta,\hat{\mathbf{k}}), \tag{A9}$$

between the multipole amplitudes of the incident and of the reflected wave.

Appendix B: Addition theorem for multipole fields

The addition theorem of Ref. 11 gives a vector multipole field with origin at O'' as a linear combination of vector multipole fields with origin at a different point O'; in a sense it is thus a translation rule for the origin of a vector multipole. Let us denote with $\mathbf{R}'$ and $\mathbf{R}''$ the vector position of O' and O'', respectively, with respect to an arbitrary origin, O. Then, by defining $\mathbf{r}' = \mathbf{r} - \mathbf{R}'$, $\mathbf{r}'' = \mathbf{r} - \mathbf{R}''$ and $\mathbf{R} = \mathbf{R}' - \mathbf{R}''$ we get for an $\mathbf{H}$ field

$$\mathbf{H}_{lm}^{(p)}(\mathbf{r}'', nk) = \sum_{p'l'm'} \mathbf{J}_{l'm'}^{(p')}(\mathbf{r}', nk)\mathcal{H}_{l'm'lm}^{(p',p)}(\mathbf{R}, nk), \quad \text{for} \quad r' < R,$$

and

$$\mathbf{H}_{lm}^{(p)}(\mathbf{r}'', nk) = \sum_{p'l'm'} \mathbf{H}_{l'm'}^{(p')}(\mathbf{r}', nk)\mathcal{J}_{l'm'lm}^{(p',p)}(\mathbf{R}, nk), \quad \text{for} \quad r' > R.$$

In the preceding equations we define

$$\mathcal{H}_{l'm',lm}^{(p',p)} = \left[\delta_{pp'} + i\sqrt{\frac{2l'+1}{l'+1}}(1-\delta_{pp'})\right]$$
$$\times \sum_{\mu} C(1, l'-1+\delta_{pp'}, l'; -\mu, m'+\mu) G_{l'-1+\delta_{pp'},m'+\mu;l,m+\mu} C(1, l, l; -\mu, m+\mu), \tag{B1}$$

where

$$G_{l'm'lm} = 4\pi \sum_{\lambda} i^{l'-l+\lambda} \mathcal{I}_{\lambda}(l', m'; l, m) h_{\lambda}(nkR) Y_{\lambda, m'-m}^{*}(\hat{\mathbf{R}}). \tag{B2}$$

In Eq. (B2), in turn, the quantities $\mathcal{I}_{\lambda}$ are Gaunt integrals, whose expression in terms of the Clebsh–Gordan coefficients C is[13]

$$\mathcal{I}_{\lambda}(l', m'; l, m) = \sqrt{\frac{(2\lambda+1)(2l+1)}{4\pi(2l'+1)}}\, C(\lambda, l, l'; 0, 0) C(\lambda, l, l'; m'-m, m).$$

The quantities $\mathcal{J}_{l'm'lm}^{(p',p)}$ are identical to the quantities $\mathcal{H}_{l'm'lm}^{(p',p)}$ except that in Eq. (B2) the Bessel function j_{λ} must be substituted for the Hankel function h_{λ}. When the addition theorem is applied to a $\mathbf{J}$ field we get the result

$$\mathbf{J}_{lm}^{(p)}(\mathbf{r}'', nk) = \sum_{p'l'm'} \mathbf{J}_{l'm'}^{(p')}(\mathbf{r}', nk)\mathcal{J}_{l'm'lm}^{(p',p)}(\mathbf{R}, nk)$$

for any value of R. From the definitions above it can also be proved that, for real n, the elements $\mathcal{J}$ have the property

$$\mathcal{J}_{l'm',lm}^{(p',p)*}(\mathbf{R}, nk) = \mathcal{J}_{lm,l'm'}^{(p,p')}(-\mathbf{R}, nk) \tag{B3}$$

When the translation is parallel to the z axis, $\mathbf{R} = \pm R\hat{\mathbf{z}}$, and the above formulas assume a simple form that proves useful for the calculation of the far field. Since

$$Y_{\lambda, m'-m}(\pi, \varphi) = (-)^{\lambda} Y_{\lambda, m'-m}(0, \varphi) = (-)^{\lambda}\left(\frac{2\lambda+1}{4\pi}\right)^{1/2} \delta_{m'-m,0},$$

the quantities $\mathcal{H}$ and $\mathcal{J}$ do vanish unless $m' = m$. This property is conveniently expressed by the equations

$$\mathcal{H}^{(p',p)}_{l'm',lm}(\pm R\hat{\mathbf{z}}, nk) = \mathcal{H}^{(p',p)}_{l',l;m}(\pm R\hat{\mathbf{z}}, nk)\delta_{mm'}, \tag{B4}$$
$$\mathcal{J}^{(p',p)}_{l'm',lm}(\pm R\hat{\mathbf{z}}, nk) = \mathcal{J}^{(p',p)}_{l',l;m}(\pm R\hat{\mathbf{z}}, nk)\delta_{mm'}.$$

The addition theorem yields also a useful relation that we used in Section 4 to calculate the far field intensity. Let us, indeed, consider the vector plane wave $\hat{\mathbf{u}}\exp(i\mathbf{k}\cdot\mathbf{r}'')$ that is referred to the origin O''. With reference to the geometry that we described above we have

$$\begin{aligned}\hat{\mathbf{u}}\exp(i\mathbf{k}\cdot\mathbf{r}'') &= \exp[i\mathbf{k}\cdot\mathbf{R}]\hat{\mathbf{u}}\exp[i\mathbf{k}\cdot\mathbf{r}'] \\ &= \exp[i\mathbf{k}\cdot\mathbf{R}]\sum_{p'l'm'}\mathbf{J}^{(p')}_{l'm'}(\mathbf{r}', nk)W^{(p')}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{k}}),\end{aligned}$$

where we used the multipole expansion of Appendix A. On the other hand we also have

$$\begin{aligned}\hat{\mathbf{u}}\exp(i\mathbf{k}\cdot\mathbf{r}'') &= \sum_{p''l''m''}\mathbf{J}^{(p'')}_{l''m''}(\mathbf{r}'', nk)W^{(p'')}_{l''m''}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) \\ &= \sum_{p'l'm'}\mathbf{J}^{(p')}_{l'm'}(\mathbf{r}', nk)\sum_{p''l''m''}\mathcal{J}^{(p',p'')}_{l'm',l''m''}(\mathbf{R}, nk)W^{(p'')}_{l''m''}(\hat{\mathbf{u}}, \hat{\mathbf{k}}),\end{aligned}$$

where we used the addition theorem to translate the origin of each of the $\mathbf{J}$ multipole fields. Comparison of the preceding equations the yield the relation

$$\exp[i\mathbf{k}\cdot\mathbf{R}]W^{(p)}_{lm}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) = \sum_{p'l'm'}\mathcal{J}^{(p,p')}_{lm,l'm'}(\mathbf{R}, nk)W^{(p')}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{k}}).$$

By assuming n to be real, we can take the complex conjugate of the latter equation, written for $\mathbf{R} \to -\mathbf{R}$, and use Eq. (B3), that holds true for real n only, to get the required result

$$\exp[i\mathbf{k}\cdot\mathbf{R}]W^{(p)*}_{lm}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) = \sum_{p'l'm'}W^{(p')*}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{k}})\mathcal{J}^{(p',p)}_{l'm',lm}(\mathbf{R}, nk). \tag{B5}$$

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Fig. 1. Sketch of the geometry that has been adopted in the present paper. The axes of the three frames with origin at O, O' and O'' are parallel to each other. Both media are assumed to be homogeneous and the refractive index of the accessible half-space is assumed to be real, whereas the refractive index n'' is allowed to be complex. The axes z, z' and z'' are oriented from the medium of refractive index n' towards the medium of refractive index n''.

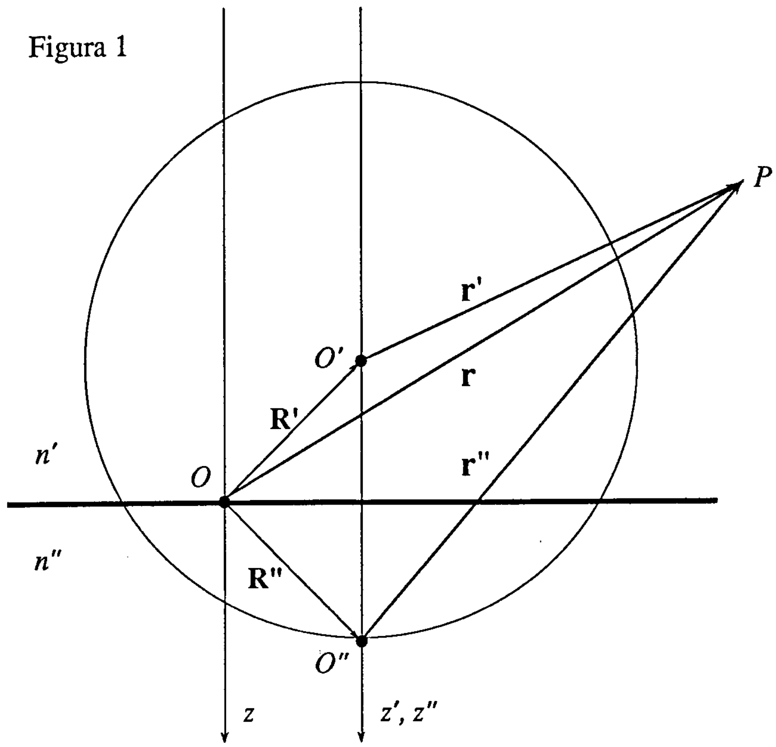
Table 1. Values of N that ensure the convergence of all the relevant elements of F that enter the calculated intensity for the indicated values of the distance of the source from the interface. The relevant parameters are $n' = 1$, $n'' = 9$, $\lambda = 500$ m, $l'' = l' = 7$; the angle between the direction of observation and the z axis is $\vartheta = 165°$. The convergence is ensured for both values of p and for polarization both parallel and perpendicular to the plane that contains the z axis and the direction of observation.

		$kd = 0.50$	$kd = 1.00$	$kd = 1.50$
$l = 1$	$m = 1$	14	10	10
	$m = 0$	14	14	10
$l = 2$	$m = 2$	18	10	10
	$m = 1$	34	22	10
	$m = 0$	24	22	10
$l = 3$	$m = 3$	26	10	10
	$m = 2$	30	10	10
	$m = 1$	38	18	10
	$m = 0$	38	18	10

Table 2. Values of N that ensure the convergence of all the relevant elements of F that enter the calculated intensity for the indicated values of the distance of the source from the interface. The relevant parameters are $n' = 1$, $n'' = 1.3$, $\lambda = 500$ nm, $l'' = l' = 7$; the angle between the direction of observation and the z axis is $\vartheta = 165°$. The convergence is ensured for both values of p and for polarization both parallel and perpendicular to the plane that contains the z axis and the direction of observation.

		$kd = 0.50$	$kd = 1.00$	$kd = 1.50$
$l = 1$	$m = 1$	10	10	10
	$m = 0$	10	10	10
$l = 2$	$m = 2$	10	10	10
	$m = 1$	12	10	10
	$m = 0$	12	10	10
$l = 3$	$m = 3$	10	10	10
	$m = 2$	10	10	12
	$m = 1$	10	10	10
	$m = 0$	10	10	10

Figura 1



Resonance suppression in the extinction spectrum of single and aggregated hemispheres on a perfectly reflecting surface

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The effect of a perfectly reflecting surface on the extinction spectrum from single and aggregated hemispheres whose flat face lies on the surface is investigated. When the spectrum of these particles is calculated in the framework of image theory some of the expected resonances are found to disappear for specific choices of the direction and polarization of the incident wave. This resonance suppressing effect is fully explained for the case of single hemispheres whereas for the case of aggregated hemispheres the guidelines for its explanation are given for the case of binary aggregates.

1. Introduction

The electromagnetic resonances are a well known feature of the extinction spectrum of a spherical scatterer. In the plot of the extinction cross section vs. the size parameter a resonance appears as a peak that can be explained in the framework of the Mie theory and of its extensions for radially non-homogeneous spheres.[1,2] The resonance spectra of spherical scatterers have been thoroughly investigated[3–8] and several methods have been proposed to relate the observed peaks to the actual size and shape of the scattering particles.[9–13] Resonances may also occur in the spectra from spheres in the vicinity of a plane substrate and of hemispheres with their flat face on a plane surface. The resonances of these systems have been investigated, though in the long wevelength limit,[14–17] on account of their relevance for the analysis of the cleannes and of the smoothness of surfaces.

Li and Chýlek[18] and Videen and Chýlek[19] observed that the resonances of spheres and cylindes can be enhanced or suppressed by illuminating such particles with two mutually coherent plane waves of fixed phase relation. In turn, Johnson[20,21] suggested to resort to the coherence of a plane wave and of its mirror image to study the scattering from a spherical particle coupled to a perfectly reflecting surface. As a matter of fact, refs. 18–21 are strictly related to the purpose of the present paper.

In this paper, indeed, we investigate how a perfectly reflecting surface yields, for specific choice of the direction of incidence, the suppression of some of the expected resonances. This will be done with reference to the extinction spectrum of hemispheres with their flat face on the reflecting surface because hemispheres may be an acceptable model for liquid droplets deposited on a metal surface. Our investigation will be performed in the framework of image theory according to which the scattering from a particle in the vicinity of a perfectly reflecting surface is equivalent to the dependent scattering from the compound object that includes both the actual particle and its image when illuminated by the superposition of the actual incident field and of the field that comes from the image source. Therefore, the extinction spectrum from hemispheres on a surface is equivalent to the spectrum from whole spheres illuminated by the superposition of two waves whose phase relation is dictated by the reflection condition. Hereafter we will refer to this superposition as the exciting field and to the whole sphere as the equivalent sphere. By comparing the calculated spectrum from a hemisphere on the surface with the spectrum from the equivalent sphere illuminanted by the incident field only we will show that some of the resonances in the latter spectrum may not appear in the spectrum of the hemisphere. More precisely, we will show that the resonance suppressing mechanism is effective only for particular choices of the direction and polarization of the incident wave.

In this paper we will also deal with a binary aggregate of identical hemispheres with their flat face on the perfectly reflecting surface: according to image theory, the equivalent scatterer is the aggregate of two spheres. The calculation of the dependent scattering from aggregated spheres is a well established procedure[23] whose results are in excellent agreement with the available experimental data,[24,25] so that no particular difficulty should be expected. However, the resonance spectrum from aggregated spheres is, in general, more complex that the superposition of the resonce spectra of the component spheres.[26,27] This circumstance may frustrate our attempt to asses how the resonance suppressing effect of the reflecting surface works on the spectrum of aggregated hemispheres. To overcome this difficulty, the radius of the component hemispheres was chosen to be small while the refractive index was assumed to be rather high. These choices result in a spectrum whose simplicity allows us to explain the behavior of the spectrum for this limiting case of non-spherical equivalent scatterers and gives the giudelines to understand the resonance-suppressing mechanism for more general cases. .

In Section 2 we revisit the reflection of a polarized plane wave on a perfectly reflecting surface in order to reformulate the problem in terms of spherical multipole fields. The conditions for the vanishing of some of the amplitudes of the exciting field are established on general grounds.

In Section 3 we discuss the scattering from particles in terms of the transition matrix and give a general definition of the extinction cross section that applies even when a perfectly reflecting surface is present.

In Section 4 the resonance spectra from homogeneous hemispheres and from the aggregates of two identical hemispheres that we mentioned above are compared with those of the equivalent sphere and of the aggregate of equivalent spheres, respectively, illuminated by the incident field only. The mechanism through which some of the resonances in the spectrum of the hemispheres disappear is also explained.

2. Exciting field

In the framework of the image theory,[28] the exciting field is the superposition of the actual incident field and of the field that comes from the image source: the latter, in turn, coincides with the field that is reflected by the interface in the absence of any scatterer. The reflection condition implies that the amplitude and the polarization of the incident and of the reflected wave satisfy a relation that will now be explicitly established within the formalism of the vector multipole fields. Similar relations are reported in several papers[22,29–32] but never in a form suitable for our present purposes. We want, in fact to show that as an effect of the condition of perfect reflection some of the multipole amplitudes of the exciting field are bound to vanish. To achieve our goal we will deal at first with the reflection on a plane surface that separates two media of general dielectric properties but we will specialize our results to the case of the perfectly reflecting interface when the need arises.

We consider a frame of reference whose cartesian axes are characterized by the unit vectors $\hat{\mathbf{u}}_x$, $\hat{\mathbf{u}}_y$ and $\hat{\mathbf{u}}_z$, and assume that the halfspace $z < 0$, the accessible half-space, is filled by a homogeneous medium of refractive index n while a different medium of refractive index n' fills the halfspace $z > 0$: thus the interface coincides with xy plane and its unit normal concides with $\hat{\mathbf{u}}_z$. The electromagnetic plane wave

$$\mathbf{E}_I = E_0 \hat{\mathbf{e}}_I \exp[i\mathbf{k}_I \cdot \mathbf{r}], \tag{1}$$

that propagates through the halfspace $z < 0$, is reflected by the interface into the plane wave

$$\mathbf{E}_R = E'_0 \hat{\mathbf{e}}_R \exp[i\mathbf{k}_R \cdot \mathbf{r}], \tag{2}$$

where $\hat{\mathbf{e}}_I$ and $\hat{\mathbf{e}}_R$ are the (unit) polarization vectors of the incident and of the reflected wave, respectively, $\mathbf{k}_I = nk\hat{\mathbf{k}}_I$ and $\mathbf{k}_R = nk\hat{\mathbf{k}}_R$ are the respective propagation vectors, and, as usual, $k = \omega/c$. The time dependence $\exp(-i\omega t)$ will be assumed throughout. We now introduce two pairs of unit vectors $\hat{\mathbf{u}}_{I\eta}$ and $\hat{\mathbf{u}}_{R\eta}$ whose index $\eta = 1, 2$ distinguish wether they are parallel ($\eta = 1$) or perpendicular ($\eta = 2$) to the plane of incidence, i. e. to the plane that contains $\mathbf{k}_I$, $\mathbf{k}_R$ and the z axis. The orientation is chosen so that $\hat{\mathbf{u}}_{R2} \equiv \hat{\mathbf{u}}_{I2}$ and

$$\hat{\mathbf{u}}_{I1} \times \hat{\mathbf{u}}_{I2} = \hat{\mathbf{k}}_I, \quad \hat{\mathbf{u}}_{R1} \times \hat{\mathbf{u}}_{R2} = \hat{\mathbf{k}}_R.$$

Then Eqs. (1) and (2) can be rewritten as

$$\begin{aligned} \mathbf{E}_I &= E_0 \sum_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \hat{\mathbf{u}}_{I\eta} \exp[i\mathbf{k}_I \cdot \mathbf{r}], \\ \mathbf{E}_R &= E'_0 \sum_\eta (\hat{\mathbf{e}}_R \cdot \hat{\mathbf{u}}_{R\eta}) \hat{\mathbf{u}}_{R\eta} \exp[i\mathbf{k}_R \cdot \mathbf{r}], \end{aligned} \tag{3}$$

and application of the reflection condition on the plane surface leads one to define the Fresnel coefficients F_η for the reflection of a plane wave with polarization along $\hat{\mathbf{u}}_{I\eta}$. The expression of the coefficients F_η in terms of the angle ϑ_I between $\hat{\mathbf{k}}_I$ and $\hat{\mathbf{u}}_z$ is[33]

$$\begin{aligned} F_1 &= \frac{n'^2 \cos\vartheta_I - n\sqrt{n'^2 - n^2 \sin^2\vartheta_I}}{n'^2 \cos\vartheta_I + n\sqrt{n'^2 - n^2 \sin^2\vartheta_I}}, \\ F_2 &= \frac{n \cos\vartheta_I - \sqrt{n'^2 - n^2 \sin^2\vartheta_I}}{n \cos\vartheta_I + \sqrt{n'^2 - n^2 \sin^2\vartheta_I}}, \end{aligned}$$

and their limiting value for the case of a perfectly reflecting surface is

$$F_\eta = (-)^{\eta - 1}.$$

In terms of the Fresnel coefficients the relation between the components of the incident and of the reflected field is

$$E'_0 \hat{\mathbf{e}}_R \cdot \hat{\mathbf{u}}_{R\eta} = E_0 F_\eta \hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta},$$

and, as a result, the reflected plane wave, Eq. (3), can be rewritten as

$$\mathbf{E}_{\mathrm{R}} = E_0 \sum_{\eta} F_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \hat{\mathbf{u}}_{R\eta} \exp[i\mathbf{k}_R \cdot \mathbf{r}].$$

At this stage we recall that the multipole expansion of a vector plane wave of wavevector $\mathbf{K} = K\hat{\mathbf{K}}$ is[34,35]

$$\mathbf{E} = E_0 \hat{\mathbf{u}} \exp[i\mathbf{K} \cdot \mathbf{r}] = E_0 \sum_{plm} W_{lm}^{(p)}(\hat{\mathbf{u}}, \hat{\mathbf{K}}) \mathbf{J}_{lm}^{(p)}(\mathbf{r}, K),$$

where we define the spherical vector multipoles

$$\mathbf{J}_{lm}^{(1)}(\mathbf{r}, K) = j_l(Kr)\mathbf{X}_{lm}(\hat{\mathbf{r}}), \quad \mathbf{J}_{lm}^{(2)}(\mathbf{r}, K) = \frac{1}{K}\nabla \times j_l(Kr)\mathbf{X}_{lm}(\hat{\mathbf{r}}),$$

and the amplitudes

$$W_{lm}^{(1)}(\hat{\mathbf{u}}, \hat{\mathbf{K}}) = 4\pi i^l \hat{\mathbf{u}} \cdot \mathbf{X}_{lm}^*(\hat{\mathbf{K}}), \quad W_{lm}^{(2)}(\hat{\mathbf{u}}, \hat{\mathbf{K}}) = 4\pi i^{l+1}(\hat{\mathbf{K}} \times \hat{\mathbf{u}}) \cdot \mathbf{X}_{lm}^*(\hat{\mathbf{K}}).$$

In the preceding equations the superscripts 1 and 2 are the values of a parity index p that distinguishes the magnetic multipoles ($p = 1$) from the electric ones ($p = 2$) and the functions $\mathbf{X}_{lm}$ are vector spherical harmonics.[33] Accordingly, the multipole expansions the incident and the reflected field are

$$\mathbf{E}_I = E_0 \sum_{\eta} (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \sum_{plm} W_{I\eta lm}^{(p)} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk)$$
$$\mathbf{E}_R = E_0 \sum_{\eta} F_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \sum_{plm} W_{R\eta lm}^{(p)} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk),$$

respectively, where we define

$$W_{I\eta lm}^{(p)} = W_{lm}^{(p)}(\hat{\mathbf{u}}_{I\eta}, \hat{\mathbf{k}}_I),$$
$$W_{R\eta lm}^{(p)} = W_{lm}^{(p)}(\hat{\mathbf{u}}_{R\eta}, \hat{\mathbf{k}}_R).$$

The vector spherical harmonics have useful transformation properties under change of their arguments that help us to to relate the multipole amplitudes of the reflected wave, $W_{R\eta lm}^{(p)}$, to those of the incident wave, $W_{I\eta lm}^{(p)}$. In fact, the following relation holdsbetween the multipole amplitudes of the incident and the reflected field

$$W_{R\eta lm}^{(p)} = (-)^{\eta+p+l+m} W_{I\eta lm}^{(p)}. \tag{4}$$

As a result the reflected field takes on the final form

$$\mathbf{E}_R = E_0 \sum_{\eta} F_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \sum_{plm} (-)^{\eta+p+l+m} W_{I\eta lm}^{(p)} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk), \tag{5}$$

that depends on the parameters of the incident wave only.

. Equation (5) allows us to write the exciting field, that is the superposition of the incident and of the reflected field, as

$$\mathbf{E}_E = \mathbf{E}_I + \mathbf{E}_R = E_0 \sum_{\eta} (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) \sum_{plm} [1 + (-)^{\eta+p+l+m} F_\eta] W_{I\eta lm}^{(p)} \mathbf{J}_{lm}^{(p)}(\mathbf{r}, nk). \tag{6}$$

For a surface of general dielectric properties $|F_\eta| \neq 1$, so that the term within square brackets in eq. (6) never vanishes. However, for a perfectly reflecting interface $F_\eta = (-)^{\eta-1}$: therefore, when $[1 - (-)^{p+l+m}] = 0$, i. e. when $p + l + m$ is even, the corresponding multipole is not present in the exciting field.

3. Scattered field and extinction cross section

The field that is scattered by any particle embedded in a homogeneous medium of refractive index n can be expanded in a series of spherical vector multipoles

$$\mathbf{E}_{S\eta} = \sum_{plm} A^{(p)}_{\eta lm} \mathbf{H}^{(p)}_{lm}(\mathbf{r}, nk), \tag{7}$$

where the multipole fields $\mathbf{H}^{(p)}_{lm}$ are identical to the multipoles $\mathbf{J}^{(p)}_{lm}$ except for the substitution of the spherical Hankel functions of the first kind, $h^{(1)}_l(kr)$, for the spherical Bessel functions, $j_l(kr)$. The label η that is attached to $\mathbf{E}_{S\eta}$ and to the amplitudes $A^{(p)}_{\eta lm}$ recalls that the scattered field depends on the state of polarization of the incident wave. According to Waterman,[36] the multipole amplitudes of the scattered field are related to the amplitudes of the exciting field through the equation

$$A^{(p)}_{\eta lm} = -\sum_{p'l'm'} S^{(p,p')}_{lm,l'm'} W^{(p')}_{E\,\eta l'm'}, \tag{8}$$

where the quantities $S^{(p,p')}_{lm,l'm'}$ are the elements of the so called transition matrix, S, that accounts for the morphology (structure and scattering power) and the orientation of the particle. In the absence of any substrate the amplitudes $W^{(p')}_{E\,\eta l'm'}$ concide with those of the incident plane wave and S is the transition matrix of the actual scattering particle. However, when a perfectly reflecting surface is present the amplitudes of the exciting field, according to the preceding section, are

$$W^{(p)}_{E\eta lm} = [1 - (-)^{p+l+m}] W^{(p)}_{I\eta lm}, \tag{9}$$

and S is the transition matrix appropriate to the compound object that includes both the actual particle and its image. In the latter case, according to Eq. (9), even a non vanishing incident amplitude $W^{(p)}_{I\eta lm}$ may yield a vanishing exciting amplitude $W^{(p)}_{E\eta lm}$ and thus affect the amplitudes of the scattered field up to the suppression of some of the characteristic resonance peaks.

We now need a definition of the extinction cross section that applies even in the presence of the reflecting surface. To this end we resort to the optical theorem that, according to van de Hulst,[1] can be proved by considering the field that is actually detected by an optical instrument. Let us recall that the scattering amplitude of any particle, $\mathbf{f}_\eta$, can be defined through the equation

$$\mathbf{E}_{S\eta} = \frac{\exp{(inkr)}}{r} E_0 \mathbf{f}_\eta(\hat{\mathbf{k}}_S, \hat{\mathbf{k}}_I),$$

where $\hat{\mathbf{k}}_S$ denotes the direction of observation, provided that the particle is at the origin and the distance of observation, r, is large. The scattering amplitude depends, in general, on the morphology as well as on the orientation of the scatterer with respect to the incident field and, once the amplitudes $A^{(p)}_{\eta lm}$ are known, its expression is[37]

$$\mathbf{f}_\eta = \frac{1}{nk} \sum_{lm} (-i)^{l+1} \left[A^{(1)}_{\eta lm} \mathbf{X}_{lm}(\hat{\mathbf{k}}_S) + i A^{(2)}_{\eta lm} \hat{\mathbf{k}}_S \times \mathbf{X}_{lm}(\hat{\mathbf{k}}_S) \right].$$

In terms of $\mathbf{f}_\eta$ the optical theorem reads

$$\sigma_\eta = \frac{4\pi}{k} \mathrm{Im}[f_{\eta\eta}(\hat{\mathbf{k}}_S = \hat{\mathbf{k}}_I, \hat{\mathbf{k}}_I)], \tag{10}$$

where σ_η is the extinction cross section; the index η recalls that, for an anisotropic scatterer, the cross section depends on the polarization and $f_{\eta,\eta'} = \mathbf{f}_\eta \cdot \hat{\mathbf{u}}^*_{S\eta'}$, so that

$$f_{\eta\eta}(\hat{\mathbf{k}}_I, \hat{\mathbf{k}}_I) = \frac{i}{4\pi nk} \sum_{plm} \sum_{p'l'm'} W^{(p)*}_{I\eta lm} S^{(p,p')}_{lm,l'm'} W^{(p')}_{I\eta l'm'}. \tag{11}$$

Now, according to van de Hulst,[1] Eq. (10) holds true even when a reflecting surface is present provided that the direction of observation be the direction of the reflected wave ($\hat{\mathbf{k}}_S \equiv \hat{\mathbf{k}}_R$): this is, indeed, the forward scattering direction when a reflecting surface is present. Nevertheless, one has to take account that, according to Section 2, when the incident wave is

$$\mathbf{E}_{I\eta} = E_0 \hat{\mathbf{u}}_{I\eta} \exp(i\mathbf{k}_I \cdot \mathbf{r}),$$

i. e. when $\mathbf{E}_{I\eta}$ is either parallel ($\eta = 1$) or perpendicular ($\eta = 2$) to the plane of incidence, the reflected wave is

$$\mathbf{E}_{R\eta} = E_0(-)^{\eta-1} \hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R \cdot \mathbf{r}).$$

Therefore, the total field that is detected by an optical instrument in the direction of reflection is

$$\mathbf{E}_{D\eta} = E_0[(-)^{\eta-1} \hat{\mathbf{u}}_{R\eta} \exp(i\mathbf{k}_R \cdot \mathbf{r}) + \frac{\exp(inkr)}{r} \mathbf{f}_\eta(\hat{\mathbf{k}}_R, \hat{\mathbf{k}}_I)],$$

and the optical theorem should read

$$\sigma_{R\eta} = \frac{4\pi}{k} \mathrm{Im}[(-)^{\eta-1} f_{R\eta,\eta}(\hat{\mathbf{k}}_R, \hat{\mathbf{k}}_I)], \tag{12}$$

where

$$f_{R\eta\eta}(\hat{\mathbf{k}}_R, \hat{\mathbf{k}}_I) = \frac{i}{4\pi nk} \sum_{plm} \sum_{p'l'm'} W^{(p)*}_{R\eta lm} S^{(p,p')}_{lm,l'm'} W^{(p')}_{E\eta l'm'}, \tag{13}$$

and the subscript R that is attached to f recalls that, on account of the presence of the reflecting surface, the exciting field is the superposition defined in Section 1 and the transition matrix S is that of the equivalent scatterer. The phase factor $(-)^{\eta-1}$ in Eq. (12) does not appear explicitly in the expression given by Johnson[20] because this author considers only normal incidence and includes the correct phase in the expression for the reflected plane wave.

When the particle of interest is a hemisphere whose flat face lies on the reflecting surface, the exciting field is the superposition of the incident and of the reflected field but the transition matrix is that appropriate to a single sphere. In this case S is diagonal,

$$S^{(p,p')}_{lm,l'm'} = \delta_{pp'} \delta_{ll'} \delta_{mm'} R^{(p)}_l,$$

and its elements are given by

$$R^{(p)}_l = \frac{(1+\overline{n}\delta_{p1}) u'_l(n_0 k\rho) u_l(nk\rho) - (1+\overline{n}\delta_{p2}) u_l(n_0 k\rho) u'_l(nk\rho)}{(1+\overline{n}\delta_{p1}) u'_l(n_0 k\rho) w_l(nk\rho) - (1+\overline{n}\delta_{p2}) u_l(n_0 k\rho) w'_l(nk\rho)}, \tag{14}$$

where

$$\overline{n} = \frac{n_0}{n} - 1, \quad u_l(x) = x j_l(x), \quad w_l(x) = x h^{(1)}_l(x).$$

The quantities $R^{(1)}_l$ and $R^{(2)}_l$ coincide with the Mie coefficients b_l and a_l, respectively, for a homogeneous sphere of radius ρ and refractive index n_0 embedded in a homogeneous medium of refractive index n. Therefore, when considering a hemisphere on a reflecting surface, Eqs. (11) and (13) can be rewritten as

$$f_{\eta\eta}(\hat{\mathbf{k}}_I, \hat{\mathbf{k}}_I) = \frac{i}{4\pi nk} \sum_{plm} W^{(p)*}_{I\eta lm} R^{(p)}_l W^{(p)}_{I\eta lm} \tag{15}$$

and

$$f_{R\eta\eta}(\hat{\mathbf{k}}_R, \hat{\mathbf{k}}_I) = \frac{i}{4\pi nk} \sum_{plm} W^{(p)*}_{R\eta lm} R^{(p)}_l W^{(p)}_{E\eta lm}.$$

Now, on account that the elements $R_l^{(p)}$ are independent of m, the relation[38,37]

$$\sum_m W_{I\eta lm}^{(p)*} W_{I\eta lm}^{(p)} = 2\pi(2l+1), \tag{16}$$

implies that $f_{\eta\eta}$, Eq. (15), in spite of the index η, be independent of the polarization. Moreover, it is meaningful to define the quantity

$$U_{\eta l}^{(p)} = \sum_m W_{R\eta lm}^{(p)*} W_{E\eta lm}^{(p)}, \tag{17}$$

that, with the help of Eqs. (4), (9) and (16) can also be put into the form

$$U_{\eta l}^{(p)} = (-)^{\eta-1} 2\pi(2l+1) + \sum_m (-)^{\eta+p+l+m} W_{I\eta lm}^{(p)*} W_{I\eta lm}^{(p)}. \tag{18}$$

The behavior of $U_{\eta l}^{(p)}$ as a function of the angle of incidence may give useful information for the interpretation of the resonance spectrum: for instance, any resonance of the equivalent sphere that is associated to a vanishing $U_{\eta l}^{(p)}$ is bound to disappear.

4. Results and discussion

Before we go to discuss the results of our specific calculations it may be useful to recall a few facts about the electromagnetic resonances. A resonance occurs in the extinction spectrum from a particle when, with varying wavelength, at least one of the elemnts of the transition matrix undergoes a fast change from a rather small value to a value of order unity. For a spherical scatterer, according to Section 3, the transition matrix is diagonal with non-vanishing elements given by Eq. (14), so that it is an easy matter to associate, according to Eq. (8), each resonance to one and only one of the elements of the matrix S. For a nonspherical scatterer, such as an aggregate of spheres, the transition matrix is no longer diagonal so that the association of the observed resonances to a particular element of the transition matrix requires a close examination of the behavior of all the relevant elements of S as a function of the wavelength. Anyway, we decided to label the resonances both of single and aggregated hemispheres as magnetic and electric resonances according to whether they are associated to the magnetic part, $S_{lm,l'm'}^{(1,1)}$, or to the electric part, $S_{lm,l'm'}^{(2,2)}$, of the appropriate transition matrix; in this respect let us remark that for the scatterers that we are going to describe never occurred that a resonance was associated with the mixed elements $S_{lm,l'm'}^{(1,2)}$ or $S_{lm,l'm'}^{(2,1)}$.

A. Single hemispheres

We report in Figs. 1 (a), (b), (c) and (d) the plots of $U_{\eta l}^{(p)}$ for $l \leq 4$, $\eta = 1, 2$ and $p = 1, 2$, as a function of ϑ_I. We notice in Figs. 1 (a) and (b) that at $\vartheta_I = 0°$ all the $U_{1l}^{(1)}$ vanish for even l whereas all the $U_{1l}^{(2)}$ do vanish for odd l. This result was expected because when $\vartheta_I = 0°$ the only non-vanishing amplitudes $W_{I\eta lm}^{(p)}$ are those with $m = \pm 1$. Therefore the above result is a consequence of the fact that the factor within square brackets in Eq. (6) reduces to $1 + (-)^{p+l}$. Although the preceding argument is based on the vanishing of the individual amplitudes $W_{E\eta lm}^{(p)}$ at $\vartheta_I = 0°$ the usefulness of the quantity $U_{\eta l}^{(p)}$ remains unaffected. In fact, the vanishing of $U_{1l}^{(2)}$ for $l = 2$ at $\vartheta_I = 45°$, Fig. 1 (b), is due to the sum over m in Eq. (17). The plots in Figs. 1 (c) and (d) show that the behavior of $U_{2l}^{(p)}$ is similar to that of $U_{1l}^{(p)}$. We remark that again all the $U_{2l}^{(1)}$ vanish at $\vartheta_I = 0°$ for even l whereas all the $U_{2l}^{(2)}$ vanish at the same incidence for odd l and, in particular, $U_{21}^{(2)}$ turns out to be identically zero: these features were expected on the ground of the structure of Eq. (18).

We report in Fig. 2 the quantity

$$\gamma_{R\eta} = 2k\mathrm{Im}[(-)^{\eta-1} f_{R\eta\eta}(\hat{\mathbf{k}}_R, \hat{\mathbf{k}}_I)],$$

for $\eta = 1$, for a hemisphere of radius ρ and (real) refractive index $n_0 = 3$ on the reflecting surface; the homogeneous medium that fills the accessible half-space was assumed to be the vacuum ($n = 1$). $\gamma_{R\eta}$ is plotted as a function of the size parameter $x = nk\rho$ in the range from $x = 1$ to $x = 3$. The angle of incidence is $\vartheta_I = 0°$ in Fig. 2 (a), 45° in Fig 2 (b) and 70° in Fig. 2 (c), the latter choice being suggested by the fact that, according to Figs. 1 (a) and (b), at this incidence none of the quantities $U_{1l}^{(1)}$ vanish although several of them assume a small value. The quantity $\gamma_{R\eta}$ is as meaningful as $\sigma_{R\eta}$ because it gives the extinction coefficient of a low density dispersion of identical scatterers[39].

Now, according to the discussion in Section 3, it is quite natural to compare the spectrum from a hemisphere on the reflecting surface with the spectrum from the equivalent sphere whose transition matrix is given by Eq. (14) illuminated by the actual incident field only. Therefore, in each of Figs. 2 (a), (b) and (c) we also report the plot of the quantity

$$\gamma = 2k\mathrm{Im}[f_{\eta\eta}(\hat{\mathbf{k}}_I, \hat{\mathbf{k}}_I)],$$

for the sphere illuminated by the incident field only. We recall that, in this case, $f_{\eta\eta}$ does not actually depend on the polarization so that the quantity γ need not carry the subscript η. We also stress that, for our purposes, $\gamma_{R\eta}$ is quite comparable to γ because both quantities refer to forward scattering, according to the discussion in Section 3. All the resonances were classified with the help of the well known formulas.[26,41]

The strict correspondence between the resonances that disappear and the vanishing of the respective $U_{1l}^{(p)}$ is so evident that, in our opinion, no further comment would be necessary. However, we call the attention of the reader on the simultaneous disappearence, in Fig. 2 (a), of the two resonances at $x = 1.3118$, that is associated to $p = 2$ and $l = 1$, and at $x = 1.437$, that is associated to $p = 1$ and $l = 2$: both peaks belong, in fact, to an odd value of $p + l$. The same mechanism explains also the simultaneous disappearence of the peaks at $x = 2.2$ and at $x = 2.28$. The former peak is associated with $p = 2$ and $l = 3$ whereas for the latter peak $p = 1$ and $l = 4$: again, both peaks belong to an odd value of $p + l$. Even the resonance spectrum for $\eta = 2$ strictly follows the behavior of the $U_{2l}^{(2)}$ so that we resolved not to report the specific plot that, in spite of its significance, do not add any further information worth of a separate comment.

B. Binary clusters

The lack of a general theory for the resonances of non-spherical particles makes rather difficult an unambiguous classification of their resonances. According to Eq. (8), the lack of diagonality of the transition matrix prevents a meaningful definition of a function analogous to the quantity $U_{\eta l}^{(p)}$ that we defined above. Even in the case of aggregated spheres the transition matrix is not a diagonal matrix so that there is no one-to-one association of the multipole amplitudes of the exciting field to those of the scattered field; nor there is a simple relation between the resonances of the component spheres and those of the aggregate as a whole. Nevertheless, Eq. (9) does not depend on the shape of the particles so that the vanishing of any of the amplitudes of the exciting field is expected to affect the resonances even of a non spherical particle. To show that this is, indeed, the case we resolved to investigate the resonance spectrum of an aggregate of two identical mutually contacting hemispheres of radius ρ on a perfectly reflecting surface and to compare the results with those from the aggregate of the equivalent spheres illuminated by the incident field only. In this respect we recall that the procedure for the calculation of the transition matrix of aggregated spheres is outlined in Ref. 22. Even in this case the medium that fills the accessible half-space was chosen to be the vacuum ($n = 1$); for the refractive index of the component hemispheres was assumed the unusually high value of $n_0 = 10\pi \approx 31.4$. According to Newton[39] and to our prevous experience[26], this choice makes the resonances of the aggregate as a whole, as well as of its components, to occur at so small values of $x = nk\rho$ that fully convergent values of the scattered field are obtained for $l = l' = 1$ only. As a result, the resonances of the aggregate as a whole can surely be associated to the multipole amplitudes with $l = 1$. In view of the anisotropy of any aggregate of spheres its orientation with respect to the incident field must be stated. The axis of the binary aggregates of spheres that we consider was chosen to be along the x axis of the frame of reference that we introduced in Section 2. The plane of incidence, in turn, always coincide with xz plane.

In Fig. 3 (a) we report, for both values of η, the quantity

$$\gamma_\eta = 2k\mathrm{Im}[f_{\eta,\eta}(\hat{\mathbf{k}}_I, \hat{\mathbf{k}}_I)],$$

for the aggregate of spheres referred to above illuminated by the incident field only, whereas in Fig. 3 (b) we report $\gamma_{R\eta}$ for the aggregate of hemispheres on the reflecting surface. All the plots are reported as a function of $x = nk\rho$ and the angle of incidence is $\vartheta_I = 70°$.

Figures 4 (a) and (b) are identical to Figs. 3 (a) and (b), respectively, except that the angle of incidence is $\vartheta_I = 0°$.

On the whole, Figs. 3 and 4 present three peaks at $x_1 = 0.09629$, $x_2 = 0.09813$ and $x_3 = 0.10183$. Since for $l = 1$ the component spheres have a single resonance at $x = 0.1$, Figs. 3 and 4 confirm our previous results[26,40] that the multiple scattering processes within an aggregate produce resonances whose location cannot be related to the locations of the resonances of the component spheres.

The dependence of the resonanace spectrum of an aggregate on the polarization of the incident light can be understood only through a close examinantion of the features of the transition matrix and of the amplitudes of the exciting field. In this respect it is important to recall that the matrix S does not depend on the polarization so that the dependence on the polarization of the spectra in Figs. 3 and 4 are entirely due to the properties of the incident amplitudes $W^{(p)}_{I\eta lm}$.

Now, at x_1 the largest elements of S are $S^{(1,1)}_{1,\pm1;1,-1} \approx -S^{(1,1)}_{1,\pm1;1,1}$ so that a magnetic resonance ($p = 1$) is expected; at x_2 the leading elements are $S^{(2,2)}_{1,0;1,0}$ and $S^{(2,2)}_{1,\pm1;1,-1} \approx S^{(2,2)}_{1,\pm1;1,1}$ so that an electric resonance ($p = 2$) is expected; finally at x_3 the leading elements of S are $S^{(1,1)}_{1,0;1,0}$ and $S^{(1,1)}_{1,\pm1;1,-1} \approx S^{(1,1)}_{1,\pm1;1,1}$ thus suggesting that this resonance is a magnetic one. Nevertheless by comparing Figs. 3 and 4 one sees that not all the possible resonances actually occur. This is due to the dependence of the amplitudes $W^{(p)}_{I\eta lm}$ both on the polarization and on the angle of incidence ϑ_I.

As an example let us discuss the behavior of the resonance at x_2 that appears in Fig. 3 (a) for any choice of the polarization. According to Eq. (8) the implied amplitudes of the incident field are the $W^{(2)}_{I\eta1,m}$, with $W^{(2)}_{I2,1,0} = 0$ and $W^{(2)}_{I\eta1,1} = (-)^\eta W^{(2)}_{I\eta1,-1}$. Therefore, when $\eta = 1$, the peak at x_2 belongs to $m = 0$ whereas for $\eta = 2$ it belongs to $m = \pm1$. When the reflecting surface is present, the implied amplitudes of the exciting field are the $W^{(2)}_{E\eta1,m}$, but only $W^{(2)}_{E1,1,0} \neq 0$. This is enough to explain why the peak at x_2 may appear in Fig. 3 (b) only for $\eta = 1$.

When $\vartheta_I = 0°$ the appropriate resonance spectra are those in Fig. 4. The behavior of the peak at x_2 is easily understood when one considers that at $\vartheta_I = 0°$ we have $W^{(2)}_{I1,1,0} = W^{(2)}_{E1,1,0} = 0$. Therefore this resonance can occur in Fig. 4 (a) for $\eta = 2$ only and cannot appear at all in Fig. 4 (b).

The behavior of the resonances at x_1 and at x_3 that appear in Figs. 3 and 4 can be understood through a quite similar analysis.

5. Conclusions

The results that we presented in Section 4 show that the resonance suppressing effect of a perfectly reflecting surface is effective both for single and for aggregated hemisferes.

For the case of single hemispheres the introduction of the function $U^{(p)}_{\eta l}$ yields a full and satisfactory explanation of the behavior of the extinction spectrum as a function of the direction of propagation and of the polarization of the incident wave.

For the case of aggregated hemispheres the effect of the dependent scattering gratly complicates the spectrum, so that, unlike the case of single hemispheres, the resonance suppressing mechanism cannot be discussed on general grounds. Nevertheless, the discussion of the limiting case that we dealt with in Section 4.B yields the guidelines for the dicussion of the problem for more complicated cases of aggregation and, in general, for anisotropic particles.

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Fig. 1. Plot of the quantity $U_{\eta l}^{(p)}(\vartheta_I)$ for $l \leq 4$. In (a) $p=1$ and $\eta=1$; in (b) $p=2$ and $\eta=1$; in (c) $p=1$ and $\eta=2$; in (d) $p=2$ and $\eta=2$. In this paper we adopted the convention that $p=1,2$ classifies the multipoles as magnetic or electric, respectively; in turn $\eta=1,2$ indicates that the polarization is parallel or orthogonal to the plane of incidence, respectively.

Fig. 2. $\gamma_{R\eta}$ (solid curve) for a homogeneous hemisphere of radius ρ and refractive index $n_0=3$ on a reflecting surface as a function of $x=nk\rho$ for $\eta=1$. The medium that fills the accessible half-space is assumed to be the vacuum ($n=1$). The angle of incidence is $\vartheta_I=0°$ in (a), $\vartheta_I=45°$ in (b) and $\vartheta_I=70°$ in (c). For comparison we also report γ (dotted curve) for the equivalent sphere illuminated by the incident wave only. The resonances are labelled with $(p,l)_n$, where n distinguishes different resonances with the same value of p and l.

Fig. 3. γ_η for the aggregate of two identical mutually contacting spheres of radius ρ and refractive index $n_0=31.4$ (a) and $\gamma_{R\eta}$ for the binary aggregate of hemispheres with the same radius and refractive index on a reflecting surface (b) as a function of $x=nk\rho$. The medium that fills the accessible half-space is assumed to be the vacuum ($n=1$). The axis of the aggregate lies in the xz plane and is parallel to the x axis. The plane of incidence coincides with the xz plane and the angle of incidence is $\vartheta_I=70°$. The solid and the dotted curves refer to polarization parallel and orthogonal to the plane of incidence, respectively. We notice that the spike at $x=0.09813$ in Fig. 3 (a) appears for both choices of the polarization, although they are hardly discernible on the scale of the figure.

Fig. 4. Same as Figure 3 except that the angle of incidence is here $\vartheta_I=0°$.

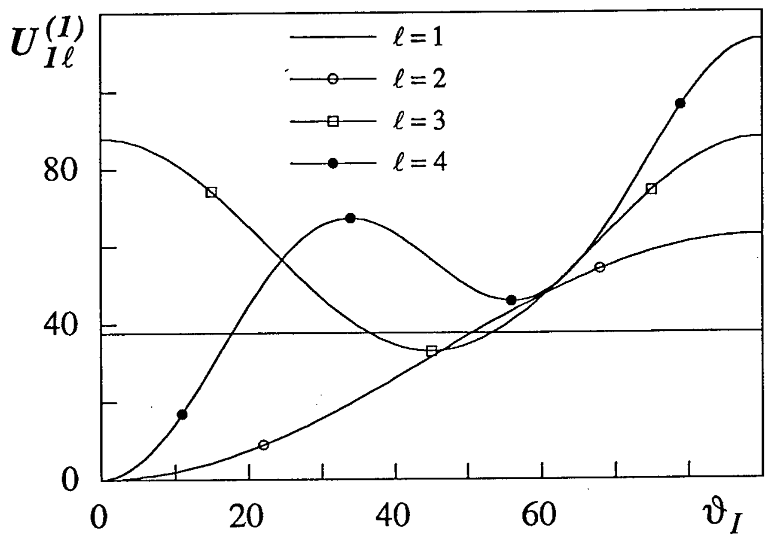


Fig 1a

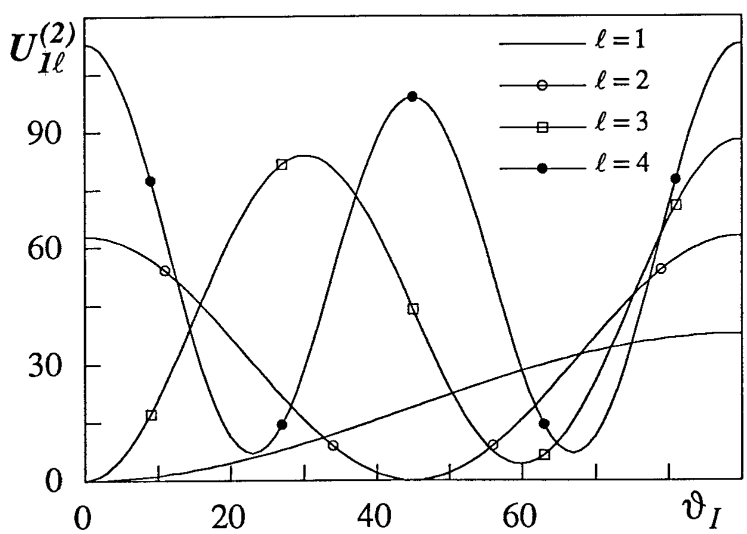


Fig 1 b

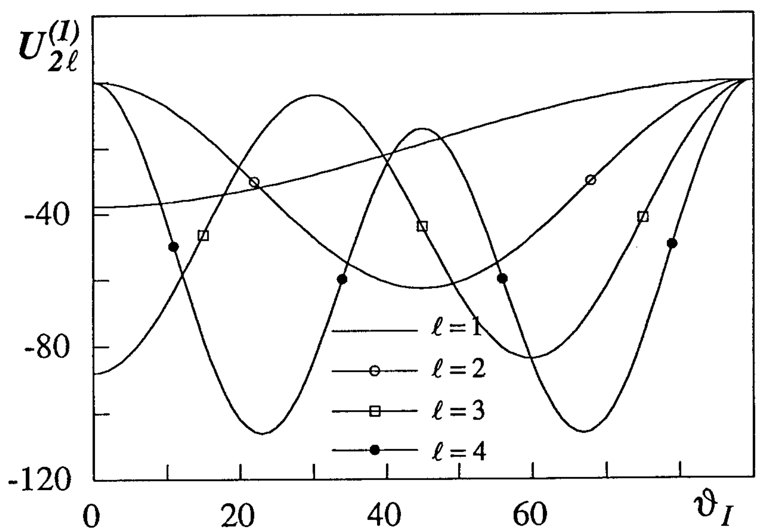


Fig 1c

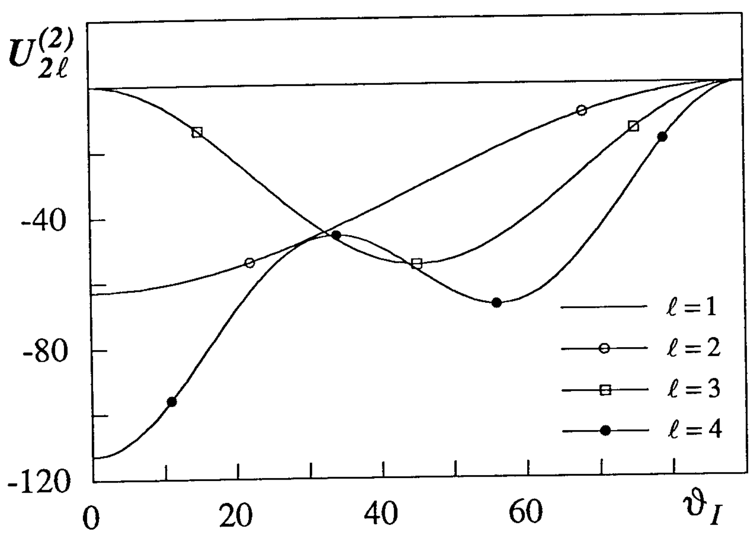
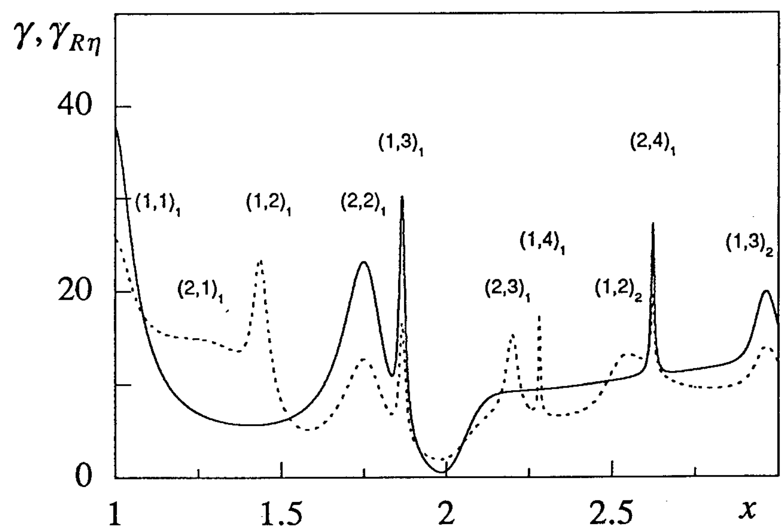


Fig 1d



$\gamma, \gamma_{R\eta}$
40
20
0
1
1.5
2
2.5
x
(1,1)$_1$
(2,1)$_1$
(1,2)$_1$
(2,2)$_1$
(1,3)$_1$
(2,3)$_1$
(1,4)$_1$
(1,2)$_2$
(2,4)$_1$
(1,3)$_2$

Fig 2a

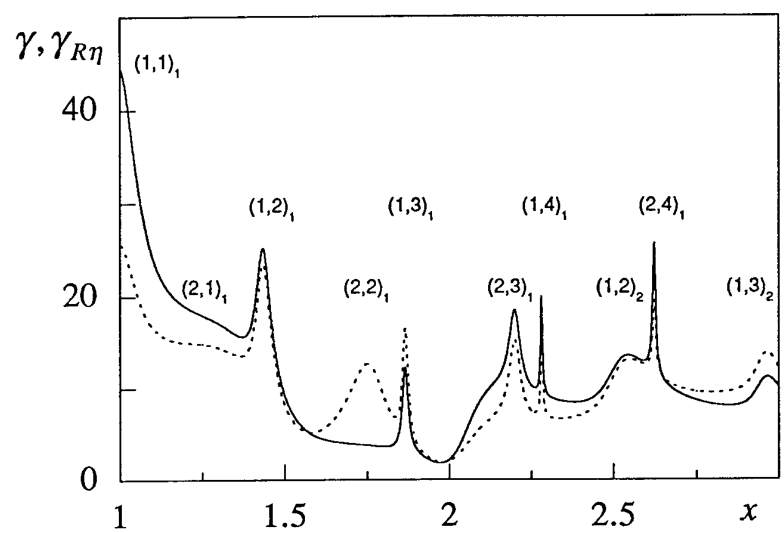
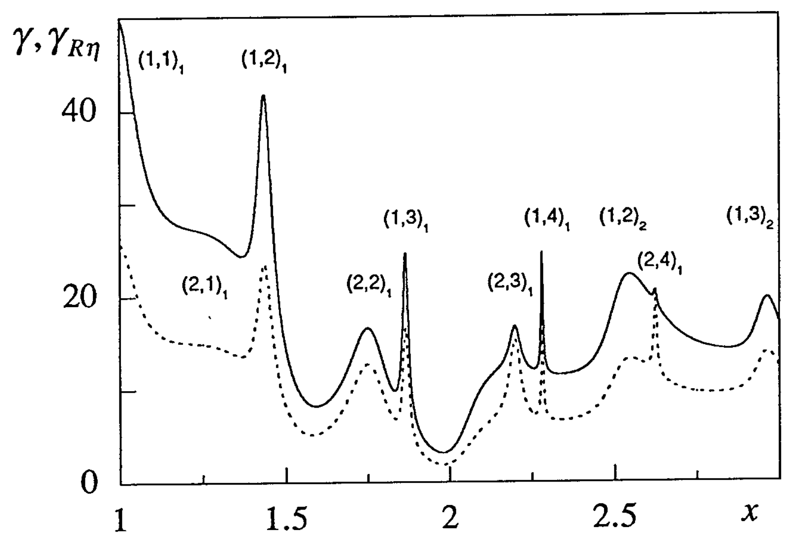

$\gamma, \gamma_{R\eta}$
40
20
0
1
1.5
2
2.5
x
(1,1)$_1$
(2,1)$_1$
(1,2)$_1$
(2,2)$_1$
(1,3)$_1$
(2,3)$_1$
(1,4)$_1$
(1,2)$_2$
(2,4)$_1$
(1,3)$_2$

Fig 2b


$\gamma, \gamma_{R\eta}$
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(1,2)$_1$
(2,1)$_1$
(2,2)$_1$
(1,3)$_1$
(2,3)$_1$
(1,4)$_1$
(1,2)$_2$
(2,4)$_1$
(1,3)$_2$
40
20
0
1
1.5
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x

Fig 2c

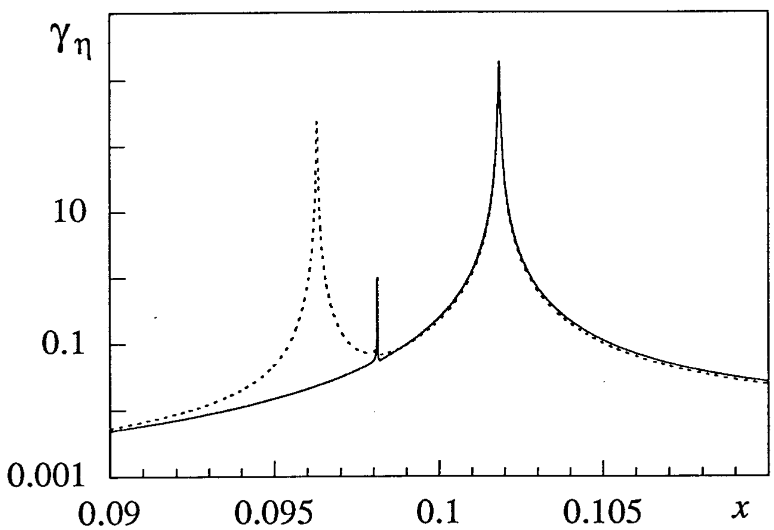

Fig 3a

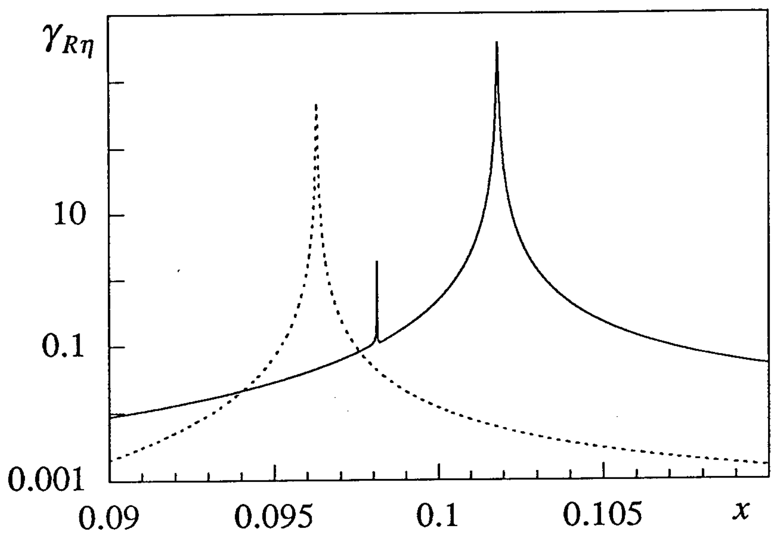

Fig 3 b

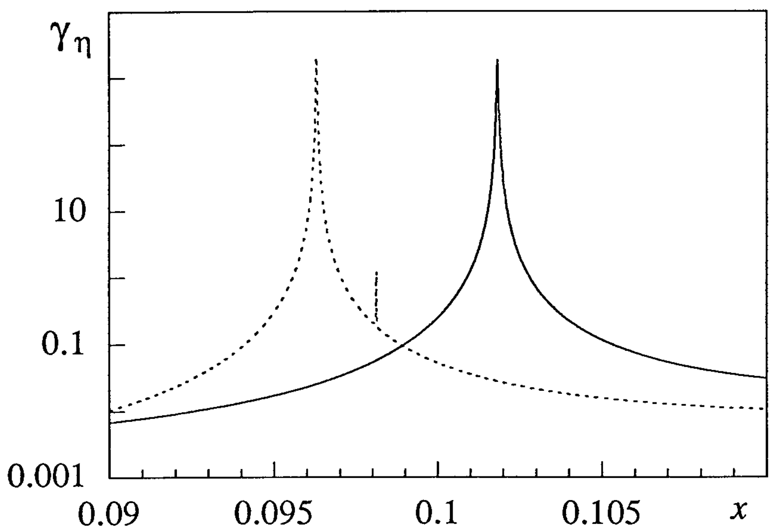

Fig 4a

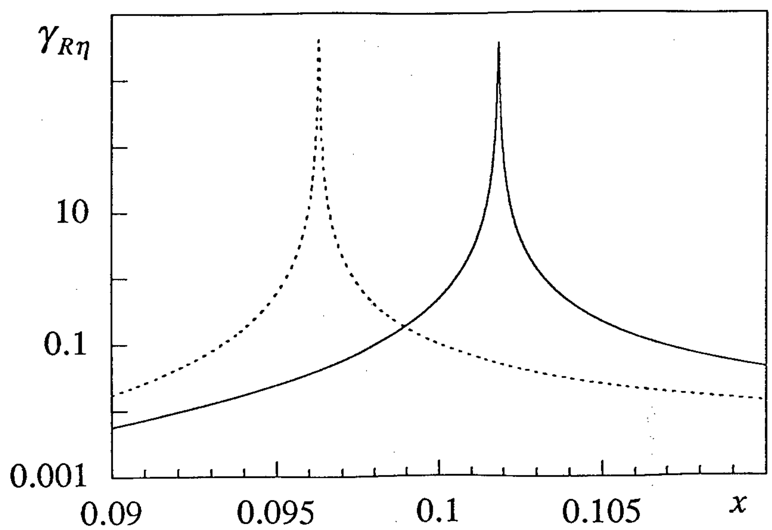

Fig 4b

Optical properties of a sphere in the vicinity of a plane surface

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The full scattering pattern from a sphere in the vicinity of a plane surface is calculated through an approach based on the expansion of the electromagnetic field in terms of vector multipole fields and on the imposition of the boundary conditions. Our approach does not invoke any approximation but can easily incorporate the simplifying assumptions of Bobbert and Vlieger [Physica **137**, 202–249 (1986)] and of Johnson [J. Opt. Soc. Am. A**13**, 326–337 (1996)] whose results are compared with our ones. A real progress is achieved as, unlike the previous theories but in agreement with the available experimental data, a non vanishing field is allowed to propagate along the surface even when the latter is non-perfectly reflecting .

1. Introduction

The optical properties of a particle in the vicinity of a plane surface are known to be rather different from the properties of the same particle in free space. The actual calculation of these properties requires to impose the boundary conditions both across the surface of the particle and across the plane surface so that one has to resort to more complicated approaches than those that are customarily used for isolated particles.[1] The mathematical development of such approaches is often so cumbersome that it is necessary to resort to suitable approximations or to restrict the investigation to limiting cases. For instance Bobbert and Vlieger[2] formulated a theory that succeeds in the exact calculation of the scattered field from a sphere near a non-perfectly reflecting plane surface; these authors, however, resort to a suitable approximation to get the observed field in the far zone. Johnson,[3] in turn, besides the approximation of Bobbert and Vlieger, resorts to the so-called Yousif-Videen[4,5] approximation to simplify the imposition of the boundary conditions on the surface of the scattering sphere; both Bobbert and Vlieger's approach and the approach of Johnson become exact in the limit of a perfectly reflecting surface. A quite different kind of approach is the one used by Lindell et al.[6] and by Muinonen et al.[7] to describe the scattering from a particle of arbitrary shape in the presence of a non-perfectly reflecting surface. They resort, in fact, to the exact-image theory[8] but they restrict their investigation to particles so small that the Rayleigh approximation applies. Anyway, their approach shares in common with the approaches of Bobbert and Vlieger and of Johnson the rather unphysical result that no field can propagate along the surface.

In the present paper we deal with the optical properties of a spherical scatterer in the vicinity of a plane surface through an approach that does not require to invoke any approximation. To perform our task, we make extensive use of the expansion of all the fields in terms of spherical vector multipoles[9,10] and of a general addition theorem that effects the translation of the origin of the spherical vector multipole fields according to the need.[11] We also use our generalization to vector multipole fields of a formula that yields the expansion of a spherical scalar multipole in terms of inhomogeneous plane waves.[2] The use of the above mentioned ingredients yields a theory that is suitable for actual calculations and that does not imply any approximation or any limitation to the refractive indices of the homogeneous isotropic media that are separated by the surface.

In Section 2 we describe our approach by recalling first how the problem of the reflection of a vector plane wave of arbitrary polarization can be formulated in terms of spherical vector multipole fields. Next, we consider the reflection on the plane surface of the field that is scattered by a sphere: as usual, the scattered field is assumed to be a superposition of spherical vector multipole fields that include only outgoing waves at infinity. The reflection of the scattered field is dealt with through the above mentioned expansion of a vector multipole field in terms of vector plane waves with complex propagation vectors.[12] Ultimately we are able to show that, in the vicinity of the surface of the sphere, the total field, i. e. the superposition of the incident, reflected, scattered and reflected-scattered fields, can be given as a linear combination of vector multipole fields with origin at the center of the sphere itself. Imposition of the boundary conditions across the surface of the sphere then yields a system of linear non-homogeneous equations for the multipole amplitudes of the scattered field.

In Section 3 we establish the exact expression of the far field by invoking our recent result[12] that each of the multipole fields that form the field scattered by the sphere yields, by reflection, a superposition, with known coefficients, of vector multipole fields with origin at the mirror image of the center of the sphere. Since all the implied multipole fields behave as outgoing waves at infinity, we get the far-zone expression of the reflected-scattered field without introducing any simplifying assumption. It is then an easy matter to get also the transition matrix[13] for a sphere in the presence of the plane surface in a form that is suitable for the extension to the case of aggregated spheres.

In Section 4 we show how the approximations that were used by Bobbert and Vlieger[2] and by Johnson[3] can readily be incorporated into our theory; therefore we were able to reproduce the approximate results of these authors and to compare them with the exact results of our approach.

In particular we show that, unlike the above mentioned theories, our approach yields a non-vanishing field that propagates along the surface. Finally, we present our specific results for the full scattering pattern from a sphere deposited on a surface: by considering three values of the refractive index we study the evolution of the pattern and show that the latter becomes identical to the pattern that is yielded by image theory when the surface becomes perfectly reflecting.[14]

In order to ensure a straightforward development of the theory, a number of related procedures and formulas are summarized in Appendices A and B.

2. Theory

Let us assume that a plane surface separates a semi-infinite homogeneous isotropic medium of real refractive index n' from another semi-infinite isotropic homogeneous medium of (possibly complex) refractive index n''. Hereafter we will refer to the region filled by the former medium as the accessible half-space. According to our statement in Section 1, our present purpose is the calculation of the scattering pattern from a particle embedded into the former medium. To this end, by assuming that a plane wave propagates in the accessible half-space, we need to determine the total field at any point P in the same half-space: we will refer to the total field either as $\mathbf{E}^{Int}$ or as $\mathbf{E}^{Ext}$ according to whether P is internal or external to the particle. Now, if no particle were present, the total field, $\mathbf{E}^{Ext}$, would be the superposition of the incident wave, $\mathbf{E}^{I}$, and of the field that has been reflected by the surface, $\mathbf{E}^{R}$; these fields are related to each other by the reflection conditions on the plane surface. To take account of the presence of a scattering particle we add to $\mathbf{E}^{I}$ and $\mathbf{E}^{R}$ the field that is scattered by the particle itself, $\mathbf{E}^{S}$, as well as the field that, after scattering by the particle, is reflected by the plane surface, $\mathbf{E}^{RS}$: even the latter two fields are related to each other by the reflection conditions. Ultimately, we have

$$\mathbf{E}^{Ext} = \mathbf{E}^{I} + \mathbf{E}^{R} + \mathbf{E}^{S} + \mathbf{E}^{RS}, \tag{1}$$

and $\mathbf{E}^{S}$ is determined by imposing to $\mathbf{E}^{Ext}$ the appropriate boundary conditions across the surface of the scattering particle. It is just the need to impose the latter boundary conditions that makes us restrict our present investigation to the determination of the scattering properties of a homogeneous sphere. The case of a radially non-homogeneous sphere requires our formalism to undergo minor changes that will be outlined at the end of Subsection 2.C.

The geometry that we adopt for our study is devised so as to make full use of the symmetry of the problem while preserving the generality of our approach. With reference to Fig. 1, the surface on which the reflection occurs coincides with the plane $z = 0$ of a cartesian frame of reference, of origin O, whose z axis is characterized by the unit vector $\hat{\mathbf{z}}$: the accessible half-space thus coincides with the region $z < 0$. We also define two further frames of reference whose respective axes are parallel to the axes with origin at O. The origin of the first frame, O', coincides with the center of the sphere at a distance a from the surface; the origin of the second frame, O'', is the mirror image of O' with respect to the surface. We will denote with $\mathbf{R}' = -a\hat{\mathbf{z}}$ and $\mathbf{R}'' = a\hat{\mathbf{z}}$ the vector position of the origins O' and O'' in the frame of reference with origin at O, respectively, whereas the vector position of a point P in the three frames defined above will be denoted with $\mathbf{r}$, $\mathbf{r}'$ and $\mathbf{r}''$, respectively.

A. Reflection of the incident plane wave

We assume that all the fields depend on time through the factor $\exp(-i\omega t)$ and define the propagation constant in vacuo $k = \omega/c$. The electromagnetic plane wave

$$\mathbf{E}^{I} = E_0\hat{\mathbf{e}}_I \exp[i\mathbf{k}_I \cdot \mathbf{r}], \tag{2}$$

that propagates through the halfspace $z < 0$, is reflected into the plane wave

$$\mathbf{E}^R = E_0'\hat{\mathbf{e}}_R \exp[i\mathbf{k}_R \cdot \mathbf{r}], \tag{3}$$

where $\hat{\mathbf{e}}_I$ and $\hat{\mathbf{e}}_R$ are the (unit) polarization vectors of the incident and of the reflected wave, respectively, and $\mathbf{k}_I = n'k\hat{\mathbf{k}}_I$ and $\mathbf{k}_R = n'k\hat{\mathbf{k}}_R$ are the respective propagation vectors. In order to impose the reflection condition on the surface we define two pairs of unit vectors, $\hat{\mathbf{u}}_{I\eta}$ and $\hat{\mathbf{u}}_{R\eta}$, whose index η distinguish whether they are parallel ($\eta = 1$) or perpendicular ($\eta = 2$) to the plane of incidence, i. e. to the plane that contains $\mathbf{k}_I$, $\mathbf{k}_R$ and the z axis; the orientation is chosen so that $\hat{\mathbf{u}}_{I2} \equiv \hat{\mathbf{u}}_{R2}$ and

$$\hat{\mathbf{u}}_{I1} \times \hat{\mathbf{u}}_{I2} = \hat{\mathbf{k}}_I, \qquad \hat{\mathbf{u}}_{R1} \times \hat{\mathbf{u}}_{R2} = \hat{\mathbf{k}}_R.$$

Accordingly, $\mathbf{E}^I$ and $\mathbf{E}^R$ can be rewritten as

$$\mathbf{E}^I = E_0 \sum_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta})\hat{\mathbf{u}}_{I\eta} \exp[i\mathbf{k}_I \cdot \mathbf{r}], \tag{4}$$

$$\mathbf{E}^R = E_0' \sum_\eta (\hat{\mathbf{e}}_R \cdot \hat{\mathbf{u}}_{R\eta})\hat{\mathbf{u}}_{R\eta} \exp[i\mathbf{k}_R \cdot \mathbf{r}], \tag{5}$$

i. e. as a superposition of components that are parallel and perpendicular to the plane of incidence. Then by imposing the reflection condition and denoting with ϑ_I the angle between $\mathbf{k}_I$ and $\hat{\mathbf{z}}$ we get the relation

$$E_0'\hat{\mathbf{e}}_R \cdot \hat{\mathbf{u}}_{R\eta} = E_0 F_\eta(\vartheta_I)\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}.$$

In the preceding equation the quantities $F_\eta(\vartheta_I)$ are the Fresnel coefficients[15] for the reflection of a plane wave with polarization along $\hat{\mathbf{u}}_{I\eta}$

$$F_1(\vartheta_I) = \frac{n^2 \cos\vartheta_I - \beta}{n^2 \cos\vartheta_I + \beta}, \quad F_2(\vartheta_I) = \frac{\cos\vartheta_I - \beta}{\cos\vartheta_I + \beta},$$

where $n = n''/n'$ and

$$\beta = \sqrt{(n^2 - 1) + \cos^2\vartheta_I}.$$

As a result, the reflected plane wave, Eq. (5), can be rewritten as

$$\mathbf{E}^R = E_0 \sum_\eta (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta}) F_\eta(\vartheta_I)\hat{\mathbf{u}}_{R\eta} \exp[i\mathbf{k}_R \cdot \mathbf{r}]. \tag{6}$$

Since $\mathbf{E}^I$ and $\mathbf{E}^R$ must satisfy the boundary conditions also on the surface of the scattering sphere, it is convenient to expand both fields in terms of spherical vector multipole fields with origin at the center of the sphere, O'. To this end we use the multipole expansion for a vector plane wave, Eq. (A1), and get the incident and reflected fields, Eqs. (4) and (6), in the form

$$\mathbf{E}^I = \exp(i\mathbf{k}_I \cdot \mathbf{R}') \sum_\eta E_{0\eta} \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', n'k) W_{lm}^{(p)}(\hat{\mathbf{u}}_{I\eta}, \hat{\mathbf{k}}_I), \tag{7}$$

$$\mathbf{E}^R = \exp(i\mathbf{k}_R \cdot \mathbf{R}') \sum_\eta F_\eta(\vartheta_I) E_{0\eta} \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', n'k) W_{lm}^{(p)}(\hat{\mathbf{u}}_{R\eta}, \hat{\mathbf{k}}_R), \tag{8}$$

respectively, where the vector multipole fields $\mathbf{J}_{lm}^{(p)}$ and the amplitudes $W_{lm}^{(p)}$ are defined in Eqs. (A2) and (A3), respectively, and $E_{0\eta} = (\hat{\mathbf{e}}_I \cdot \hat{\mathbf{u}}_{I\eta})E_0$; the phase factors $\exp(i\mathbf{k}_I \cdot \mathbf{R}')$ and $\exp(i\mathbf{k}_R \cdot \mathbf{R}')$ effect the transfer of origin from O to O'. We notice that the amplitudes $W_{lm}^{(p)}(\hat{\mathbf{u}}_{I\eta}, \hat{\mathbf{k}}_I)$ are related by Eq. (A6) to the amplitudes $W_{lm}^{(p)}(\hat{\mathbf{u}}_{R\eta}, \hat{\mathbf{k}}_R)$ so that the latter never need to be calculated explicitly.

B. Reflection of the scattered field

The field that is scattered by a particle that lies entirely in the accessible half-space can always be expanded in a series of vector multipole fields that satisfy the radiation condition at infinity. The component of the incident field that is polarized along $\hat{\mathbf{u}}_{I\eta}$ yields, indeed, a scattered field that, with respect to an origin O' within the particle, can be written as

$$\mathbf{E}_\eta^S = E_{0\eta} \sum_{plm} \mathbf{H}_{lm}^{(p)}(\mathbf{r}', n'k) A_{\eta lm}^{(p)}, \tag{9}$$

where the multipole fields $\mathbf{H}$ are identical to the $\mathbf{J}$ fields, Eq. (A2), except for the substitution of the spherical Hankel functions of the first kind $h_l(n'kr')$ for the Bessel functions $j_l(n'kr')$. The amplitudes A are as yet unknown but will be calculated by imposing the appropriate boundary conditions at the surface of the particle.[9] The scattered field incides on the plane surface and, by reflection, yields a field that can be obtained through a technique that we described elsewhere in full detail[12] and whose guidelines are summarized in Appendix B. Here we state the result that the reflected-scattered field in the vicinity of the surface of the particle can be written as the superposition of $\mathbf{J}$ multipole fields with origin at O'

$$\mathbf{E}_\eta^{RS} = E_{0\eta} \sum_{plm} \sum_{p'l'} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', n'k) \mathcal{F}_{l,l';m}^{(p,p')} A_{\eta l'm}^{(p')}, \tag{10}$$

where the quantities $\mathcal{F}$, whose expression is given in Eq. (B4), are the elements of a matrix that effects the reflection of the $\mathbf{H}$ multipole fields on the plane surface and thus yields the required relation between the scattered and the reflected-scattered field. We remark that in Eq. (10) we used the property, Eq. (B5a), that the elements $\mathcal{F}$ vanish unless $m' = m$.

C. Amplitudes of the scattered field

The results in Subsections 2.A and 2.B show that the fields that contribute to $\mathbf{E}^{Ext}$, Eq. (1), in the vicinity of the surface of the particle, according to Eqs. (7), (8), (9) and (10), are all expressed in terms of vector multipole fields with origin at O'; $\mathbf{E}^{Ext}$ is thus suitable for the imposition of the boundary conditions. The multipole expansion of the magnetic field $\mathbf{B}^{Ext}$, that is also needed to impose the boundary conditions, is readily obtained through the Maxwell equation[16]

$$i\mathbf{B}_\eta^{Ext} = \frac{1}{k} \nabla \times \mathbf{E}_\eta^{Ext}.$$

We now assume that the scattering particle is a homogeneous non-magnetic sphere with (possibly complex) refractive index n_0 and radius ρ. The field within the sphere must be regular at O' and can thus be taken in the form

$$\mathbf{E}_\eta^{Int} = E_{0\eta} \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', n_0 k) C_{\eta lm}^{(p)}, \tag{11}$$

and the corresponding magnetic field is

$$i\mathbf{B}_\eta^{Int} = \frac{1}{k} \nabla \times \mathbf{E}_\eta^{Int}.$$

In order to impose the boundary conditions across the surface of the scattering sphere we apply to $\mathbf{E}$ and $\mathbf{B}$ the procedure that we described elsewhere in full detail.[9] This procedure yields, for each p, l and m, four equations among which the amplitudes of the internal field C can be easily eliminated. As a result we get, for each m, a system of linear non-homogeneous equations for the amplitudes $A_{\eta lm}^{(p)}$

$$\sum_{p'l'}[\mathcal{M}^{-1}]^{(p,p')}_{l,l';m}A^{(p')}_{\eta l'm} = -\mathcal{W}^{(p)}_{\eta lm}, \tag{12}$$

where

$$[\mathcal{M}^{-1}]^{(p,p')}_{l,l';m} = (R^{-1})^{(p)}_l \delta_{pp'}\delta_{ll'} + \mathcal{F}^{(p,p')}_{l,l';m}, \tag{13}$$

$$\mathcal{W}^{(p)}_{\eta lm} = \left[\exp(i\mathbf{k}_I\cdot\mathbf{R}')W^{(p)}_{lm}(\hat{\mathbf{u}}_{I\eta},\hat{\mathbf{k}}_I) + F_\eta \exp(i\mathbf{k}_R\cdot\mathbf{R}')W^{(p)}_{lm}(\hat{\mathbf{u}}_{R\eta},\hat{\mathbf{k}}_R)\right], \tag{14}$$

and

$$R^{(p)}_l = \frac{(1+\overline{n}\delta_{p1})u'_l(n_0k\rho)u_l(n'k\rho) - (1+\overline{n}\delta_{p2})u_l(n_0k\rho)u'_l(n'k\rho)}{(1+\overline{n}\delta_{p1})u'_l(n_0k\rho)w_l(n'k\rho) - (1+\overline{n}\delta_{p2})u_l(n_0k\rho)w'_l(n'k\rho)}$$

with

$$\overline{n} = \frac{n_0}{n'} - 1, \quad u_l(x) = xj_l(x), \quad w_l(x) = xh_l(x).$$

The quantities $R^{(1)}_l$ and $R^{(2)}_l$ coincide with the Mie coefficients b_l and a_l, respectively, for a homogeneous sphere of refractive index n_0 embedded into a homogeneous medium of refractive index n'. We remark that our theory can easily deal also with radially nonhomogeneous spheres; even in this case, in fact, one gets Eq. (12) although the quantities $R^{(p)}_l$ in Eq. (13) must be redefined.[17,18]

3. Scattering amplitude and transition matrix

Once the amplitudes $A^{(p)}_{\eta lm}$ of $\mathbf{E}^S_\eta$ have been calculated by solving Eq. (12), the reflected-scattered field, $\mathbf{E}^{RS}_\eta$, is also determined by Eq. (10). The latter equation, however, gives an expression of $\mathbf{E}^{RS}_\eta$ that is valid only in the vicinity of the surface of the sphere as it includes multipole fields that do not satisfy the radiation condition at infinity. Nevertheless, our recent study of the reflection of spherical vector multipole fields on a plane surface,[12] whose guidelines are summarized in Appendix B, led us to conclude that, at any point of the accessible half-space, $\mathbf{E}^{RS}_\eta$ is given by the equation

$$\mathbf{E}^{RS}_\eta = E_{0\eta}\sum_{plm}\mathbf{H}^{(p)}_{lm}(\mathbf{r}'', n'k)\overline{A}^{(p)}_{\eta lm}, \tag{15}$$

where

$$\overline{A}^{(p)}_{\eta lm} = \sum_{p'l'} a^{(p,p')}_{l,l';m}A^{(p')}_{\eta l'm}. \tag{16}$$

The amplitudes a that are defined in Eq. (B9), are determined, with the help of a suitable addition theorem for vector multipole fields,[11] by the condition that the fields described by Eqs. (10) and (15) coincide on the surface of the scattering sphere. Therefore, the superposition of $\mathbf{E}^S_\eta$, Eq. (9), and of $\mathbf{E}^{RS}_\eta$, Eq. (15), yields the field that would be observed by an optical instrument in the far zone; the reflected field $\mathbf{E}^R_\eta$ would be observed in the direction of reflection only. Since $\mathbf{E}^S_\eta$ and $\mathbf{E}^{RS}_\eta$ are given as expansions in terms of $\mathbf{H}$ multipole fields with origin at O' and O'', respectively, it is convenient to use again the addition theorem of ref. 11 to refer both fields to a common origin that, for symmetry reasons, we choose to be the point O that is defined in Fig. 1. The observed field then becomes

$$\mathbf{E}^{Obs}_\eta = \sum_{plm}\mathbf{H}^{(p)}_{lm}(\mathbf{r}, n'k)\mathcal{A}^{(p)}_{\eta lm},$$

where

$$\mathcal{A}^{(p)}_{\eta lm} = \sum_{p'l'} \left[\mathcal{J}^{(p,p')}_{l,l';m}(a\hat{\mathbf{z}}, n'k) A^{(p')}_{\eta l'm} + \mathcal{J}^{(p,p')}_{l,l';m}(-a\hat{\mathbf{z}}, n'k) \overline{A}^{(p')}_{\eta l'm} \right]. \tag{17}$$

We notice that the quantities $\mathcal{J}$ in Eq. (17) are the elements of the matrix that effects the translation of origin of the vector multipole fields;[11,14] when, as in the present case, the translation takes place along the z axis they have the property

$$\mathcal{J}^{(p,p')}_{lm;l'm'}(\pm a\hat{\mathbf{z}}, n'k) = \mathcal{J}^{(p,p')}_{l,l';m}(\pm a\hat{\mathbf{z}}, n'k)\delta_{mm'}.$$

Then, on account of the asymptotic form of the $\mathbf{H}$ fields for large values of $n'kr$ and of their transversality in the far zone, we are led to write $\mathbf{E}^{Obs}_{\eta}$ as

$$\mathbf{E}^{Obs}_{\eta} = \frac{\exp(in'kr)}{r} E_{0\eta}\mathbf{f}_{\eta},$$

where we define the scattering amplitude[15] $\mathbf{f}_{\eta}$ that, in terms of the transverse vector harmonics $\mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{r}})$, Eq. (B4), reads

$$\mathbf{f}_{\eta} = \frac{1}{n'k} \sum_{plm} (-i)^{p+l} \mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{r}}) \mathcal{A}^{(p)}_{\eta lm}.$$

Therefore, the intensity that would be detected in the direction $\hat{\mathbf{k}}_O$ with polarization along $\hat{\mathbf{u}}_{O\eta'}$ is

$$I_{\eta'\eta} = \frac{1}{r^2}|E_{0\eta} f_{\eta'\eta}|^2 = \frac{1}{r^2} I_{O\eta} |f_{\eta'\eta}|^2,$$

where

$$f_{\eta'\eta} = \mathbf{f}_{\eta} \cdot \hat{\mathbf{u}}_{O\eta'} = -\frac{i}{4\pi n'k} \sum_{plm} W^{(p)*}_{lm}(\hat{\mathbf{u}}_{O\eta'}, \hat{\mathbf{k}}_O) \mathcal{A}^{(p)}_{\eta lm}. \tag{18}$$

The efficiency of Eq. (18) can be improved when, as we assumed throughout, the refractive index n' is real. In this case, indeed, a consequence of the addition theorem of ref. 11 is the pair of identities[12]

$$\exp[i\mathbf{k} \cdot \mathbf{R}] W^{(p)}_{lm}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) = \sum_{p'l'm'} \mathcal{J}^{(p,p')}_{lm,l'm'}(\mathbf{R}, n'k) W^{(p')}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{k}}), \tag{19a}$$

$$\exp[-i\mathbf{k} \cdot \mathbf{R}] W^{(p)*}_{lm}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) = \sum_{p'l'm'} W^{(p')*}_{l'm'}(\hat{\mathbf{u}}, \hat{\mathbf{k}}) \mathcal{J}^{(p',p)}_{l'm',lm}(-\mathbf{R}, n'k), \tag{19b}$$

where, as in Section 2, $\mathbf{k} = n'k\hat{\mathbf{k}}$. Equations (19) are valid for any choice of the translation vector $\mathbf{R}$ but, when the latter is parallel to the z axis the elements $\mathcal{J}$ do vanish unless $m' = m$, as we mentioned above. Now, with the help of Eq. (19b), the multipole transfer elements $\mathcal{J}$ that are included into the definition of the amplitudes $\mathcal{A}$ can be eliminated, so that Eq. (18) can be rewritten as

$$f_{\eta'\eta} = -\frac{i}{4\pi n'k} \sum_{plm} W^{(p)*}_{lm}(\hat{\mathbf{u}}_{O\eta'}, \hat{\mathbf{k}}_O) \left[\exp(i\mathbf{k}_O \cdot \hat{\mathbf{z}}a) A^{(p)}_{\eta lm} + \exp(-i\mathbf{k}_O \cdot \hat{\mathbf{z}}a) \overline{A}^{(p)}_{\eta lm} \right]. \tag{20}$$

Equation (20) is the one that we actually used for our calculations.

We proceed now to a further modification of Eq. (18) that leads to the definition of the transition matrix for a particle in the presence of a plane interface. To this end let us recall that the formal solution to Eq. (12) is

$$A_{\eta lm}^{(p)} = -\sum_{p'l'} \mathcal{M}_{l,l';m}^{(p,p')} \mathcal{W}_{\eta l'm}^{(p')}, \tag{21}$$

where $\mathcal{M}$ is the inverse to the matrix $\mathcal{M}^{-1}$, Eq. (13). In this respect we notice that, on account of the symmetry properties of the elements $\mathcal{F}$, Eq. (B5b), the inversion of the matrix $\mathcal{M}^{-1}$ need to be performed for $m \geq 0$ only. With the help of Eq. (19a) and of the relation between the amplitudes of $\mathbf{E}_\eta^I$ and $\mathbf{E}_\eta^R$, Eq. (A6), we transform the amplitudes $\mathcal{W}$, Eq. (14), into the form

$$\mathcal{W}_{\eta lm}^{(p)} = \sum_{p'l'} \mathcal{J}_{l,l';m}^{(p,p')}(-a\hat{\mathbf{z}}, n'k) W_{E\eta l'm}^{(p')},$$

where we define the multipole amplitudes of the exciting field

$$W_{E\eta lm}^{(p)} = W_{lm}^{(p)}(\hat{\mathbf{u}}_{I\eta}, \hat{\mathbf{k}}_I)\left[1 + (-)^{\eta+p+l+m} F_\eta(\vartheta_I)\right].$$

Substitution of the latter equation into Eq. (21) allows us to write the scattering amplitude as

$$f_{\eta'\eta} = \frac{i}{4\pi n'k} \sum_{pp'} \sum_{ll'} \sum_{m} W_{lm}^{(p)*}(\hat{\mathbf{u}}_{O\eta'}, \hat{\mathbf{k}}_O) S_{l,l';m}^{(p,p')} W_{E\eta l'm}^{(p')},$$

where the quantities

$$S_{l,l';m}^{(p,p')} = \sum_{qL} \sum_{q'L'} \Big[\mathcal{J}_{l,L;m}^{(p,q)}(a\hat{\mathbf{z}}, n'k) \mathcal{M}_{L,L';m}^{(q,q')} + \mathcal{J}_{l,L;m}^{(p,q)}(-a\hat{\mathbf{z}}, n'k) \sum_{q''L''} a_{L,L'';m}^{(q,q'')} \mathcal{M}_{L'',L';m}^{(q'',q')} \Big] \mathcal{J}_{L',l';m}^{(q',p')}(-a\hat{\mathbf{z}}, n'k)$$

can be interpreted as the elements of the transition matrix for the spherical scatterer in the presence of the plane surface.[13]

Using the transition matrix to get the observed field does not yield any advantage in the case that we deal with in this paper; in fact, as we stated above, Eq. (20) is computationally more effective. However, when dealing with non spherical particles such as, for instance, with aggregated spheres, the transition matrix proves to be a useful tool on account of its transformation properties under rotation. In practice, the transition matrix includes all the structural and orientational information of a nonspherical scatterer whereas all the information on the polarization and on the direction of incidence and of observation is included in the multipole amplitudes of the exciting field and of the observed field. As a result it is an easy matter to perform averages over the orientation of the particles along the lines of our preceding papers;[14,17,19,20] work on this subject is presently in progress.

4. Results and discussion

The theory that we developed in sections 2 and 3 will now be applied to the same systems that were dealt with by Bobbert and Vlieger[2] and by Johnson[3] in order to assess how the approximate results of these authors compare with our ones. In this respect we remark that, although our approach needs not invoke any simplifying assumption, it can readily incorporate the approximations that were described in refs. 2 and 3. We will also add to the comparison the results of two further approximations that we developed as variants to the approximations of the above mentioned authors. The results of Muinonen et al.[7] for small particles will also be compared with our ones.

According to the approximation devised by Bobbert and Vlieger (hereafter referred to as Approximation B0), the far zone expression of $\mathbf{E}_\eta^{RS}$ equals that of the scattered field, calculated for the direction $\pi - \vartheta_{Obs}$, where ϑ_{Obs} denotes the direction of observation, with its amplitude scaled by the factor $F_\eta(\pi - \vartheta_{Obs})$. Approximation B0 has been tested together with our variant (Approximation B1) that assumes that $\mathbf{E}_\eta^{RS}$ equals the field that is obtained by scaling by the factor $(-)^{\eta-1}F_\eta(\vartheta_{Obs})$, the field that would come from the image sphere with center at O'' if the surface were perfectly reflecting. In practice, this is achieved by calculating, for the direction ϑ_{Obs}, $\mathbf{E}_\eta^{RS}$ as given by Eqs. (15) and (16), but scaling by the factor $(-)^{\eta-1}F_\eta(\vartheta_{Obs})$ the amplitudes a, Eq. (B9), evaluated for a perfectly reflecting surface.

Next we considered the approach of Johnson who, beside using Approximation B0 to get the far zone expression of $\mathbf{E}^{RS}$, introduces a further approximation that affects the imposition of the boundary conditions that yield the equations for the amplitudes A, Eq. (12). In the framework of the present theory Johnson's procedure (hereafter referred to as Approximation J0) stems from the equation

$$\sum_{p''l''}\sum_{p'l'm'} \mathbf{J}_{l'm'}^{(p')}(\mathbf{r}', n'k)\mathcal{H}_{l',l'';m'}^{(p',p'')}(-2a\hat{\mathbf{z}}, n'k)\overline{A}_{\eta l''m'}^{(p'')}$$
$$= \sum_{plm}\sum_{p'l'} \mathbf{J}_{l'm}^{(p')}(\mathbf{r}', n'k)\mathcal{F}_{l',l;m}^{(p',p)}A_{\eta lm}^{(p)}, \tag{22}$$

that is a consequence of Eqs. (10) and (B8), and is valid on the surface of the scattering sphere. Equation (22) shows that the calculation of the elements $\mathcal{F}$ can be overcome provided that the amplitudes A and $\overline{A}$ can be related through some $\mathcal{F}$-independent equation. Johnson, by invoking the so-called Yousif-Videen approximation,[4,5] states such a relation in the form

$$\overline{A}_{\eta lm}^{(p)} = (-)^{\eta+p+l+m}A_{\eta lm}^{(p)}F_\eta(\vartheta = 0°),$$

that becomes exact in the limit of a perfectly reflecting interface. Johnson's Approximation J0 has been tested together with a variant (Approximation J1) that keeps in Eq. (B4) the Fresnel coefficients to the value $F_\eta(\vartheta_k = 0°)$ to get approximate values for the elements $\mathcal{F}$.

All the approximations that were described above, as well as our exact theory, where applied to the calculation of the scattered intensity from the systems that were considered by Johnson. Doing this has the further advantage that our results can also be compared with the experimental results of Wojcik, Vaughan and Galbraith[21] as well as with the ab initio simulation of Lee et al.[22] Accordingly, the scattered intensity from a sphere of radius $\rho = 0.27\,\mu$m, illuminated by a radiation of wavelength $\lambda = 0.6328\,\mu$m, is reported as a function of the angle of observation for parallel polarization in Fig. 2(a) and for perpendicular polarization in Fig. 2(b). Analogous results for a sphere of radius $\rho = 0.38\,\mu$m are reported in Figs. 3(a) and 3(b). In all the figures $\vartheta_I = 0°$, $n_0 = 1.59$, $n' = 1$ and $n'' = 3.8$; the angle of observation is measured from the negative z axis. The result that we report in Figs. 2 and 3 required to extend the multipole expansions up to $l_{Max} = 10$ to achieve an accuracy to four significant digits.

We first notice that Figs. 2(a) and 2(b) seem to report three curves only: in fact, the pair of Approximations B0-B1 and J0-J1 yield identical results to a high degree of precision. This is not surprising when one recalls how these approximations are defined. Anyway, the approximate results compare well with the results of our theory provided that ϑ_{Obs} is not near to 90° because our theory predicts the occurrence of a nonvanishing field that propagates along the interface. The situation is analogous in Figs. 3(a) and 3(b): even in this case our theory is the only one that gives a non vanishing field that propagates along the interface. Moreover, the minima of the intensity occur at different angles of observation when different approximations are used. The best coincidence with our results is attained by Approximation B0-B1 for both choices of the polarization. The different result yielded by Approximations J0-J1 was to be expected because the latter, besides including Approximation B0 to get the far zone expression of $\mathbf{E}^{RS}$, also resort to a further approximation to simplify the imposition of the boundary conditions.

When we come to compare our results with the experimental data of Wojcik, Vaughan and Galbraith[21] and the simulation of Lee et al.,[22] that Johnson reports in Figs. 3 and 4 of his paper, we see that a fair agreement is attained not only in the position of the minima but also in our prediction that the field along the surface does not vanish. Of course the computer time that is needed for our calculations is several orders of magnitude smaller than the time that is needed to complete the simulation.[22]

In Fig. 4 we report the results of the application of our theory as well as of Approximations B0, B1, J0 and J1 to the case of a small particle in the vicinity of a plane interface that Muinonen et al.[7] deal with by means of the exact-image theory. Actually, these authors consider a small sphere, with polarizability α, for several values of the distance from a plane surface that separates the vacuum from a homogeneous dielectric medium with $\varepsilon = 2.4$. The results are normalized so as to ensure their independence of the choice of α, the angle of incidence is held fixed at $\vartheta_I = 45°$ and the incident light is assumed to be unpolarized. The results that we report in Fig. 4 refer to a distance such that $ka = \pi/2$ and their convergency to four significant digits is ensured by including terms up to $l_{Max} = 6$ both in our exact theory and in the approximations B0, B1, J0 and J1. The need to use so high a value for l_{Max} in spite of the smallness of the scattering particle stems from the fact that the particle itself is not in contact with the surface. In fact, $\mathbf{E}^{RS}$ was shown to be a superposition of multipole fields with origin at the image point O'', Eq. (15) so that the larger the distance of this point from the surface the larger must be l_{Max} to get fairly convergent values for $\mathbf{E}^{RS}$ as seen from the point O on the surface, Eq. (17). This fact is quite analogous to the behaviour of the far field that we already discussed for the case of a perfectly reflecting surface.[14]

Actually, Fig. 4 seems to report two curves only but this is due to the almost perfect coincidence of all the approximate results that, in turn, agree fairly well with the results that Muinonen et al. report in Fig. 2 of ref. 7. In particular this coincidence suggests that the further approximation that is included in J0 and J1 beyond the approximation implied in B0 and B1 has little effect on the results on account of the distance between the particle and the surface.[3] The results of our theory have the general shape of the results cited above but for the fact that the observed field do not vanish for grazing angle of observation.

For a last comparison we consider the ellipsometric experiment that was performed on small mercury spheres deposited on a dielectric substrate of carbon embedded into a liquid electrolyte.[23] In such an experiment the quantity of interest is the ratio

$$E_\theta / E_\phi = \tan\psi \exp(-i\Delta)$$

where the angles ψ and Δ are directly comparable with the results of the measurements. We remark that this experiment is not appropriate to show the differences between theory and experiment that are instead detectable through an angular analysis. For this reason we do not report a specific figure for this comparison but only state that, in the range of size parameter that was considered by Bobbert, Vlieger and Greef,[23] our results coincide fairly well with the ones of these authors with the same choice of l_{Max}.

Finally we come to discuss our specific results for the full scattering pattern from a sphere of radius $\rho = 126\,\mathrm{nm}$ and refractive index $n_0 = 3$ in contact with the surface. We already presented the scattering pattern from such a sphere on a perfectly reflecting surface[14] so that for the sake of comparison our present results are plotted in the same frame of reference that is depicted in Fig. 1 of ref. 14. In this respect we recall that the interface coincides with the x-z plane and that the plane of incidence is chosen to be the plane $\vartheta = 90°$; accordingly, the angle of incidence is denoted with φ_I and can range in the interval $180° \leq \varphi_I \leq 360°$ whereas the polar angles of the direction of observation can range in the intervals $0° \leq \vartheta_{Obs} \leq 180°$ and $0° \leq \varphi_{Obs} \leq 180°$. Even in the present case we chose $n' = 1$, $\lambda = 0.6283\,\mu\mathrm{m}$ and $\varphi_I = 225°$. In Fig. 5(a) $n'' = \infty$, in Fig. 5(b) $n'' = 9$ and in Fig. 5(c) $n'' = 1.3$; in all the figures we report $r^2 I_{\varphi\varphi}/I_{0\varphi}$, where $I_{0\varphi}$ is the intensity of the incident plane wave, i. e. both the incident and the observed field are polarized along $\hat{\varphi}$. We first notice that the plot in Fig. 5(a) is identical to the one in Fig. 2(a) of ref. 14. We stress, however, that in the present case we did not use image theory but calculated the scattered field by putting in Eq. (13) the elements of the multipole reflection matrix to the value that is obtained from Eq. (B4) when the Fresnel coefficients take on the values $F_\eta = (-)^{\eta-1}$ that are appropriate to a perfectly reflecting surface. The plots in Figs. 5(b) and 5(c) show the evolution of the scattering pattern when the refractive index n'' of the medium that fills the half-space $z > 0$ becomes smaller and smaller.

We notice that the present case of a non-perfectly reflecting surface shares in common with the case of a perfectly reflecting surface some features that do not depend on the refractive index but are due to the geometry only. In fact, when ϑ_{Obs} reaches its limiting values, $\vartheta_{Obs} = 0°$ and $\vartheta_{Obs} = 180°$, the angle φ_{Obs} is still well defined as this angle characterizes an observation with a well defined choice of the polarization along the parallels. Thus, the limiting curves of our patterns ($\vartheta_{Obs} = 0°$ and $\vartheta_{Obs} = 180°$) describe the observation of the scattered beam that propagates along the surface at right angles to the plane of incidence with a polarization that depends on φ_{Obs}: so, for the φ-polarized component of the observed wave, when $\varphi_{Obs} = 0°$ or $\varphi_{Obs} = 180°$, $\mathbf{E}^{Obs}$ is orthogonal to the surface, whereas, when $\varphi_{Obs} = 90°$, $\mathbf{E}^{Obs}$ is parallel to the surface. As a result, for any given polarization, the four extreme vertices of the pattern correspond to the same physical situation, so that the observed intensity must have the same value at all these extreme points; a further consequence is that e. g. $I_{\vartheta\varphi}(\vartheta_{Obs} = 0°, \varphi_{Obs} = 90°) = I_{\varphi\varphi}(\vartheta_{Obs} = 0°, \varphi_{Obs} = 0°)$. We do not report the patterns for the other possible choices of the incident and observed polarization because, at least for a single sphere, they do not show any significant new feature worth of a separate comment.

5. Conclusions

The exact theory that we described in this paper proved to yield reliable predictions for the scattering pattern from a sphere on a dielectric surface. On the contrary, on account of the comparisons that we presented in Section 4, it can be stated that the approximations that were assumed by other authors may affect the predicted spectrum not only quantitatively but also qualitatively. In this respect, a careful examination of Figs. 5(a), 5(b) and 5(c) shows that, when the refractive index of the medium beyond the surface is comparable with the refractive index of the sphere, the intensity of the field that propagates along the surface becomes so relevant that the pattern predicted by approximate approaches may be unacceptable.

Our approach may appear to be complicated by the introduction of the multipole reflection matrix $\mathcal{F}$: the calculation of the elements of this matrix proved, however, to add little to the computational effort. In this respect we stress that integrals that are involved in the calculation of $\mathcal{F}$ can be computed with high precision through the Gauss-Laguerre method.[12,24] On the other hand, according to our tests, Approximations B0 and J0 are computationally somewhat faster than our exact approach but, on account of the considerations that we made in Section 4, the reliability of the results that they yield need to be carefully checked. We are thus led to conclude that the approximations above do not present substantial computational advantages over our approach. On the other hand, the results of the simulation of Lee et al.[22] agree fairly well with our predictions but require a heavy computational effort. Therefore, both on the side of the computations and on the side of the reliability of the results our theory appears to be more expedient than the methods of the other authors.

Appendix A: Multipole expansion of the incident and reflected plane wave

The multipole expansion of a vector plane wave of wavevector $\mathbf{K} = K\hat{\mathbf{K}}$ and polarization vector $\hat{\mathbf{u}}$ is

$$\mathbf{E} = E_0\hat{\mathbf{u}} \exp[i\mathbf{K}\cdot\mathbf{r}] = E_0 \sum_{plm} W_{lm}^{(p)}(\hat{\mathbf{u}}, \hat{\mathbf{K}}) \mathbf{J}_{lm}^{(p)}(\mathbf{r}, K), \tag{A1}$$

where

$$\mathbf{J}_{lm}^{(1)}(\mathbf{r}, K) = j_l(Kr)\mathbf{X}_{lm}(\hat{\mathbf{r}}), \quad \mathbf{J}_{lm}^{(2)}(\mathbf{r}, K) = \frac{1}{K}\nabla \times j_l(Kr)\mathbf{X}_{lm}(\hat{\mathbf{r}}) \tag{A2}$$

are spherical vector multipoles and

$$W_{lm}^{(p)}(\hat{\mathbf{u}}, \hat{\mathbf{K}}) = 4\pi i^{p+l-1}(-)^{m+1}\mathbf{Z}_{l,-m}^{(p)}(\hat{\mathbf{K}}) \cdot \hat{\mathbf{u}} \tag{A3}$$

are their amplitudes. In Eq. (A2) the superscripts 1 and 2 are the values of a parity index p that distinguishes the magnetic multipoles ($p = 1$) from the electric ones ($p = 2$), the symbol $j_l(Kr)$ denotes the spherical Bessel functions and the functions $\mathbf{X}_{lm}$ are vector spherical harmonics. Using the notation and the phase conventions of Jackson,[15] the latter functions can be defined in terms of the spherical harmonics $Y_{lm}(\hat{\mathbf{r}})$ as

$$\mathbf{X}_{lm}(\hat{\mathbf{r}}) = [l(l+1)]^{-1/2}\mathsf{L}Y_{lm}(\hat{\mathbf{r}}),$$

where $\mathsf{L} = -i\mathbf{r} \times \nabla$ is the angular momentum operator. In Eq. (A3), in turn, the symbol $\mathbf{Z}_{lm}^{(p)}$ denotes the trasverse vector harmonics

$$\mathbf{Z}_{lm}^{(1)}(\hat{\mathbf{K}}) = \mathbf{X}_{lm}(\hat{\mathbf{K}}), \quad \mathbf{Z}_{lm}^{(2)}(\hat{\mathbf{K}}) = \mathbf{X}_{lm}(\hat{\mathbf{K}}) \times \hat{\mathbf{K}}. \tag{A4}$$

The vector spherical harmonics, and the transverse vector harmonics as well, have useful transformation properties both under rotation and under reflection of their argument across the x-y plane.[25] Using these properties it is an easy matter to show that

$$\hat{\mathbf{u}}_{R\eta} \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}_R) = (-)^{\eta+p+l+m}\,\hat{\mathbf{u}}_{I\eta} \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}_I) \tag{A5}$$

and thus also

$$W_{\eta lm}^{(p)}(\hat{\mathbf{u}}_{R\eta}, \hat{\mathbf{k}}_R) = (-)^{\eta+p+l+m}\,W_{\eta lm}^{(p)}(\hat{\mathbf{u}}_{I\eta}, \hat{\mathbf{k}}_I). \tag{A6}$$

Appendix B: Reflected scattered field

We expand each of the $\mathbf{H}$ multipole fields in Eq. (9) as a superposition of vector inhomogeneous plane waves as

$$\mathbf{H}_{lm}^{(p)}(\mathbf{r}', n'k) = \frac{(-i)^{p+l-1}}{2\pi}\int_{\mathcal{D}}\sum_{\eta}[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})]\,\hat{\mathbf{u}}_\eta \exp(i\mathbf{k}\cdot\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{R}')\,d\hat{\mathbf{k}}, \tag{B1}$$

where the domain of integration $\mathcal{D}$ is defined as $0 \le \varphi_k \le 2\pi$ and $0 \le \vartheta_k \le \pi/2 - i\infty$. Equation (B1) is the generalization to the vector case[12] of the integral expansion of Bobbert and Vlieger[2] for scalar multipole fields. All the vector plane waves in the integrand are polarized either parallel or perpendicular to the plane through the z axis and the integration wavevector $\mathbf{k}$ and can thus be reflected by the Fresnel reflection rule to yield the reflected field

$$\mathbf{H}_{Rlm}^{(p)} = \frac{(-i)^{p+l-1}}{2\pi}\int_{\mathcal{D}}\sum_{\eta}F_\eta(\vartheta_k)\left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right]\hat{\mathbf{u}}_{R\eta}\exp(i\mathbf{k}_R\cdot\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{R}')\,d\hat{\mathbf{k}}. \tag{B2}$$

By referring the integrand back to the origin O' by the phase factor $\exp(i\mathbf{k}_R \cdot \mathbf{R}')$ we get

$$\begin{aligned}\mathbf{H}_{Rlm}^{(p)} = {} & \frac{(-i)^{p+l-1}}{2\pi}\int_{\mathcal{D}}\sum_{\eta}F_\eta(\vartheta_k)\left[\hat{\mathbf{u}}_\eta \cdot \mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}})\right] \\ & \times\hat{\mathbf{u}}_{R\eta}\exp(i\mathbf{k}_R\cdot\mathbf{r}')\exp[i(\mathbf{k}_R - \mathbf{k})\cdot\mathbf{R}']\,d\hat{\mathbf{k}}.\end{aligned} \tag{B3}$$

Now, substituting into Eq. (B3) the multipole expansion of a vector plane wave, Eq. (A1), we are led to write the reflected field in the form reported in Eqs. (10) with

$$\mathcal{F}^{(p',p)}_{l'm'lm} = 2i^{p'-p+l'-l}(-)^{m+1}\int_{\mathcal{D}}\sum_{\eta} F_{\eta}(\vartheta_k)\left[\hat{\mathbf{u}}_{\eta}\cdot\mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{k}})\right]$$
$$\times\left[\hat{\mathbf{u}}_{R\eta}\cdot\mathbf{Z}^{(p')}_{l',-m'}(\hat{\mathbf{k}}_R)\right]\exp(2in'ka\cos\vartheta_k)\,d\hat{\mathbf{k}}. \tag{B4}$$

It is useful to notice that the quantities $\mathcal{F}$ have the properties

$$\mathcal{F}^{(p',p)}_{l'm'lm} = \mathcal{F}^{(p',p)}_{l',l;m}\delta_{mm'}, \tag{B5a}$$
$$\mathcal{F}^{(p',p)}_{l',l;-m} = \mathcal{F}^{(p,p')}_{l,l';m}, \tag{B5b}$$

that can be proved by performing the integration over φ_k with the help of the properties of the transverse vector harmonics.

Equation (10), in spite of its usefulness to impose the boundary conditions at the surface of the sphere, has the drawback that the **J** multipole fields do not satisfy the radiation condition at infinity. As a result, this equation cannot yield the reflected scattered field in the far region. Nevertheless, we remark that in Eq. (B3) the phase factor

$$\exp[i(\mathbf{k}_R-\mathbf{k})\cdot\mathbf{R}'] = \exp(2in'ka\cos\vartheta_k)$$

effects the translation of origin from the image point O'' to the actual center of the sphere O': with the help of Eq. (A5) we can write

$$\mathbf{H}^{(p)}_{Rlm} = \frac{(-i)^{p+l-1}(-)^{p+l+m-1}}{2\pi}\int_{\mathcal{D}}\sum_{\eta}(-)^{\eta+1}F_{\eta}(\vartheta_k)\left[\hat{\mathbf{u}}_{R\eta}\cdot\mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{k}}_R)\right]$$
$$\times\hat{\mathbf{u}}_{R\eta}\exp(i\mathbf{k}_R\cdot\mathbf{r}'')\,d\hat{\mathbf{k}}, \tag{B6}$$

so that the integrand contains only reflected plane waves that are referred to the origin O''. Now, in the limiting case of a perfectly reflecting interface, the Fresnel coefficients take on the value

$$F_{\eta} = (-)^{\eta-1},$$

so that, except for a sign, Eq. (B6) represents in the accessible half-space the multipole field $\mathbf{H}^{(p)}_{lm}(\mathbf{r}'',n'k)$ with origin at the image point O''. We are thus lead to assume that when the interface has general dielectric properties Eq. (B6) represents in the accessible half-space the linear combination of multipole fields with origin at O''

$$\mathbf{H}^{(p)}_{Rlm} = \sum_{p''l''m''}\mathbf{H}^{(p'')}_{l''m''}(\mathbf{r}'',n'k)a^{(p'',p)}_{l''m'',lm}. \tag{B7}$$

The amplitudes a can be determined by expressing the **H** multipole fields with origin at O'' as a combination of appropriate multipole fields with origin at O'. By defining $\mathbf{R}=\mathbf{R}'-\mathbf{R}''$ we get for the region inside the spherical surface with center at O' and radius R, i. e. for $r'<R$,

$$\mathbf{H}^{(p)}_{Rlm} = \sum_{p''l''m''}\sum_{p'l'm'}\mathbf{J}^{(p')}_{l'm'}(\mathbf{r}',n'k)\mathcal{H}^{(p',p'')}_{l'm',l''m''}(\mathbf{R},n'k)a^{(p'',p)}_{l''m'',lm}, \tag{B8}$$

where the quantities $\mathcal{H}$ are the elements of the matrix that effects the translation of origin of the vector multipole fields. The explicit expression of these quantities as well as of the quantities $\mathcal{J}$ was originally given, though in a different notation, in ref. 11, and in the present notation in ref. 14. When the translation takes place along the z axis the elements $\mathcal{H}$ do vanish unless $m'=m''$, as it was already stated for the elements $\mathcal{J}$. Therefore, by comparing Eq. (B8) and Eq. (10) and taking into account that both the origins O' and O'' lie on the z axis, we get for the coefficients a the expression

$$a^{(p'',p)}_{l''m'',lm} = \sum_{p'l'} (\mathcal{H}^{-1})^{(p'',p')}_{l'',l';m} \mathcal{F}^{(p',p)}_{l',l;m} = a^{(p'',p)}_{l'',l;m} \delta_{mm''}, \tag{B9}$$

so that, even these coefficients do vanish unless $m = m''$.

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Fig. 1. Sketch of the geometry that we adopted in the present study.

Fig. 2. Comparison of the results of our theory with those yielded by Approximations B0, B1, J0 and J1 (see text) for a sphere of radius $\rho = 0.27\,\mu$m, and refractive index $n_0 = 1.59$, in contact with the surface, illuminated by light of wavelength $\lambda = 0.6328\,\mu$m. The sphere is embedded in vacuo, $n' = 1$, and the refractive index of the medium beyond the surface is $n'' = 3.8$. We report, in μm^2 and for direction of incidence normal to the surface, the quantity $\mathcal{J}_{11} = r^2 I_{11}/I_{01}$ in (a) and $\mathcal{J}_{22} = r^2 I_{22}/I_{02}$ in (b), where $I_{0\eta}$ is the intensity of the incident wave; I_{11} and I_{22} are the intensities that would be observed for parallel and perpendicular polarization, respectively.

Fig. 3. Same as Fig 2 but for a sphere of radius $\rho = 0.38\,\mu$m.

Fig. 4. Comparison of the results of our theory with those of Approximations B0, B1, J0 and J1 for a small sphere, with polarizability α, whose distance a from the surface is such that $ka = \pi/2$. The quantity that is actually reported is $\mathcal{J} = (I_1 + I_2)/(2\alpha^2 k^4)$, where I_1 and I_2 are the intensities of the incident field for parallel and perpendicular polarization, respectively. The angle of incidence is held fixed at $\vartheta_I = -45°$.

Fig. 5. Full scattering pattern from a sphere of radius $\rho = 126.0$ nm and refractive index $n_0 = 3$ in contact with the surface. The quantity that is actually reported is $\mathcal{J} = r^2 I_{\varphi\varphi}/I_{0\varphi}$ in μm^2, where $I_{0\varphi}$ is the intensity of the incident light whose wavelength is $\lambda = 0.6283\,\mu$m and whose angle of incidence is $\varphi_I = 225°$. In (a) the surface is perfectly reflecting ($n'' = \infty$); the refractive index of the medium beyond the surface is $n'' = 9$ in (b) and $n'' = 1.3$ in (c). In all the figures $n' = 1$.

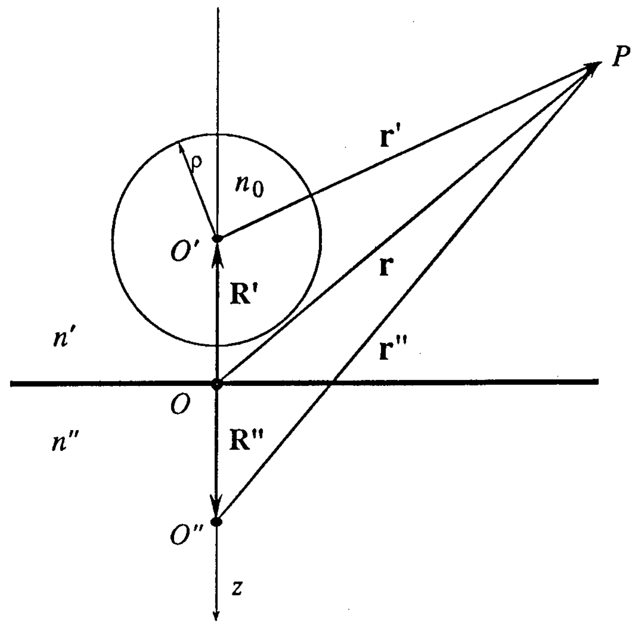
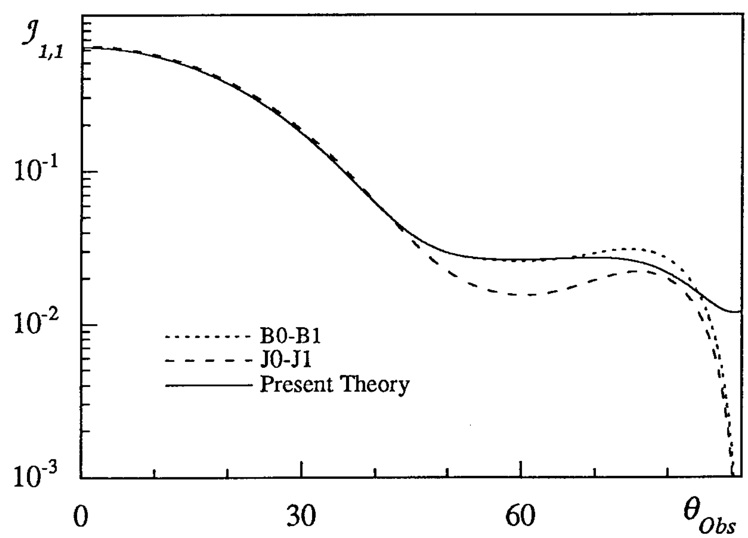


Fig 1



$\mathcal{J}_{1,1}$
10^{-1}
10^{-2}
10^{-3}
0
30
60
θ_{Obs}
B0-B1
J0-J1
Present Theory

Fig 2a

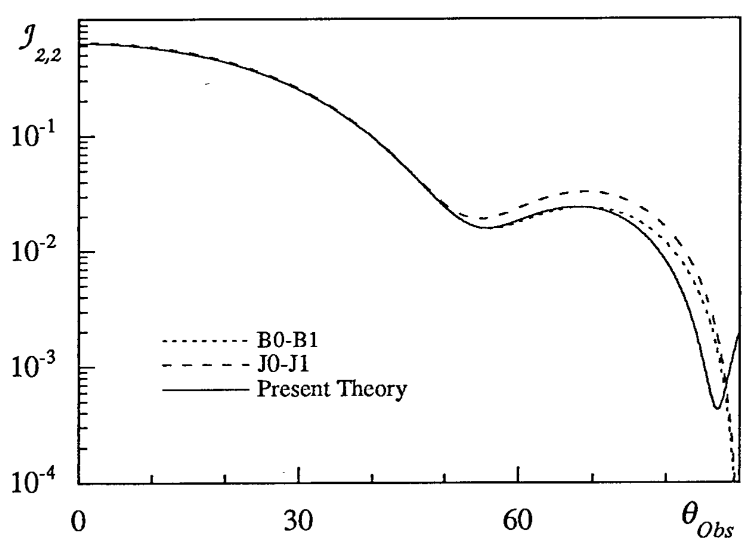
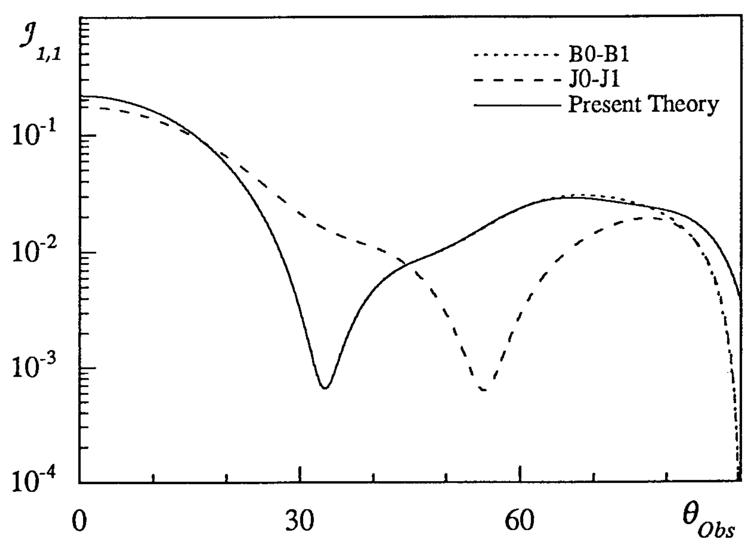

$\mathcal{J}_{2,2}$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
0
30
60
θ_{Obs}
B0-B1
J0-J1
Present Theory

Fig 2b



$\mathcal{I}_{1,1}$
B0-B1
J0-J1
Present Theory
10^{-1}
10^{-2}
10^{-3}
10^{-4}
0
30
60
θ_{Obs}

Fig 3a

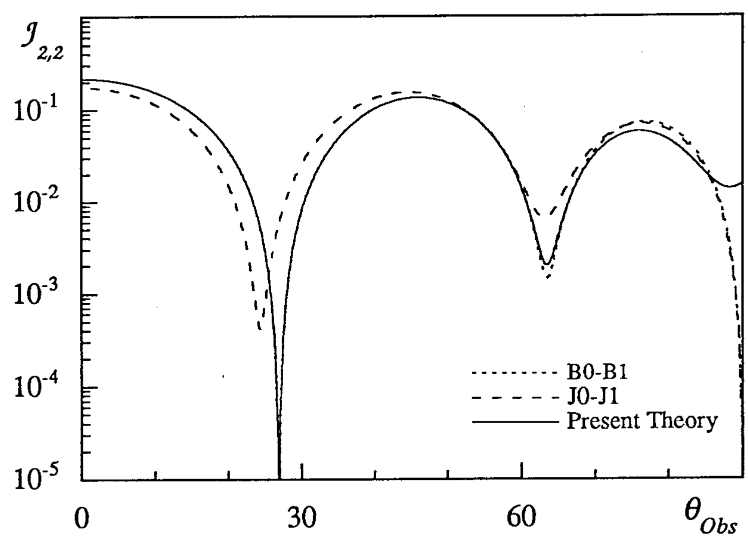
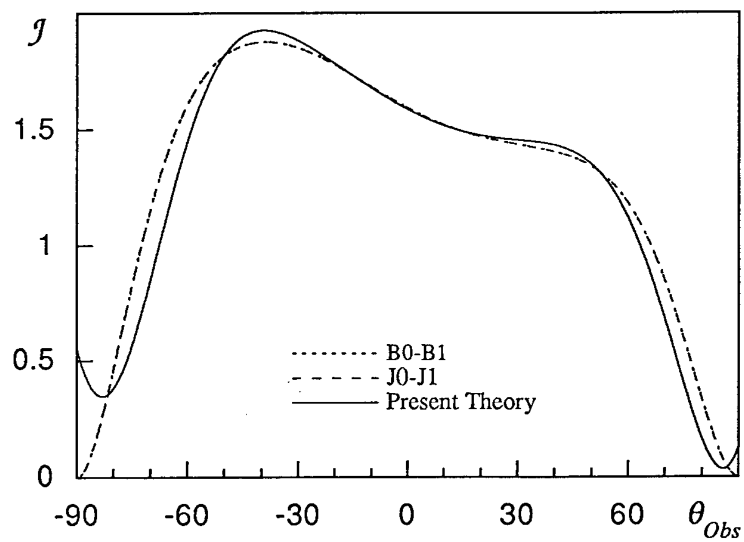

$\mathcal{J}_{2,2}$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
0
30
60
θ_{Obs}
B0-B1
J0-J1
Present Theory

Fig 3b



$\mathcal{J}$
1.5
1
0.5
0
-90
-60
-30
0
30
60
θ_{Obs}
B0-B1
J0-J1
Present Theory

Fig 4

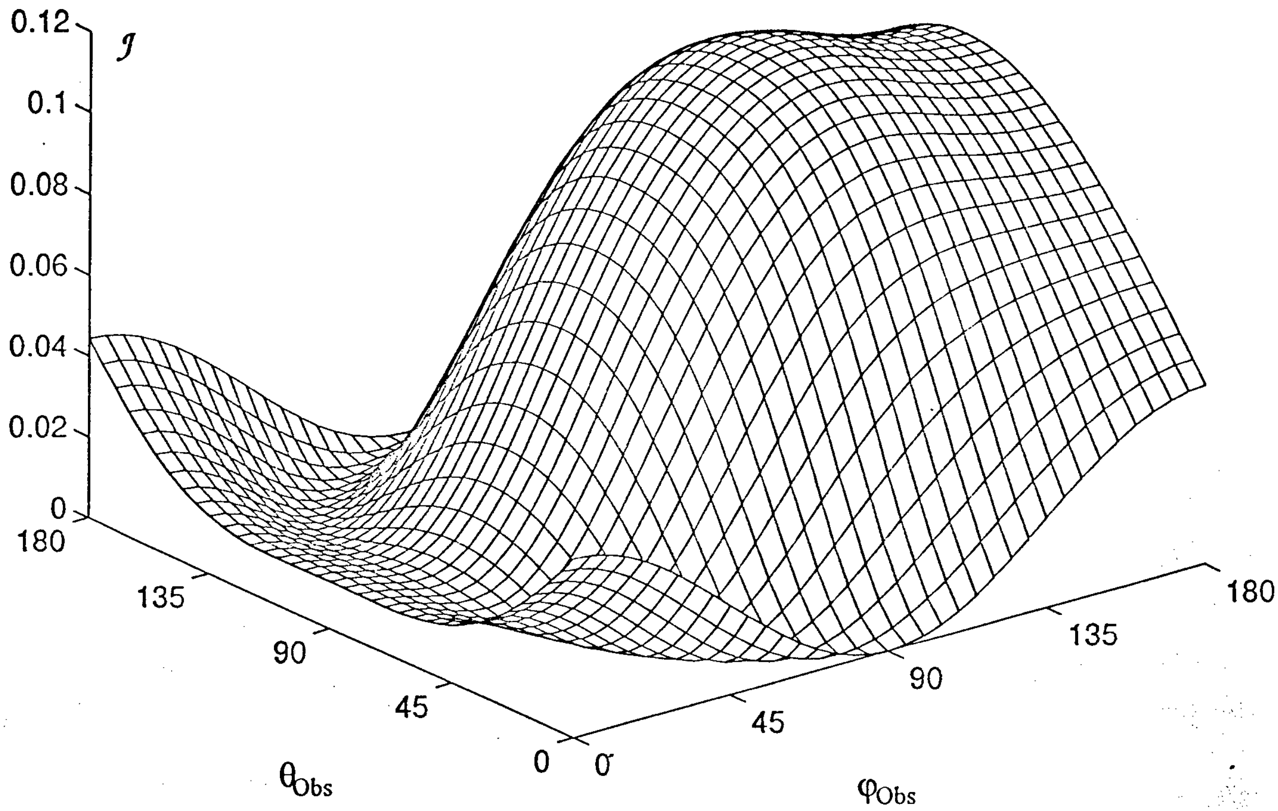
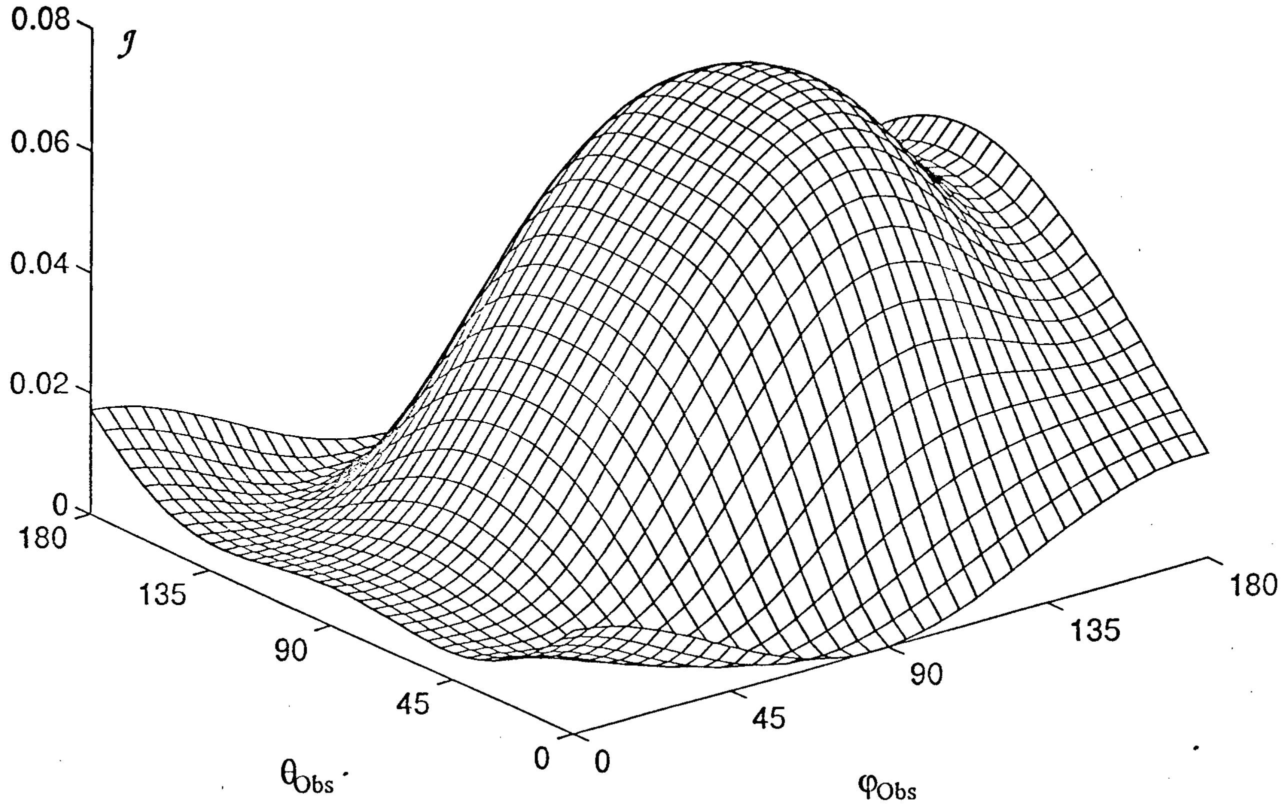
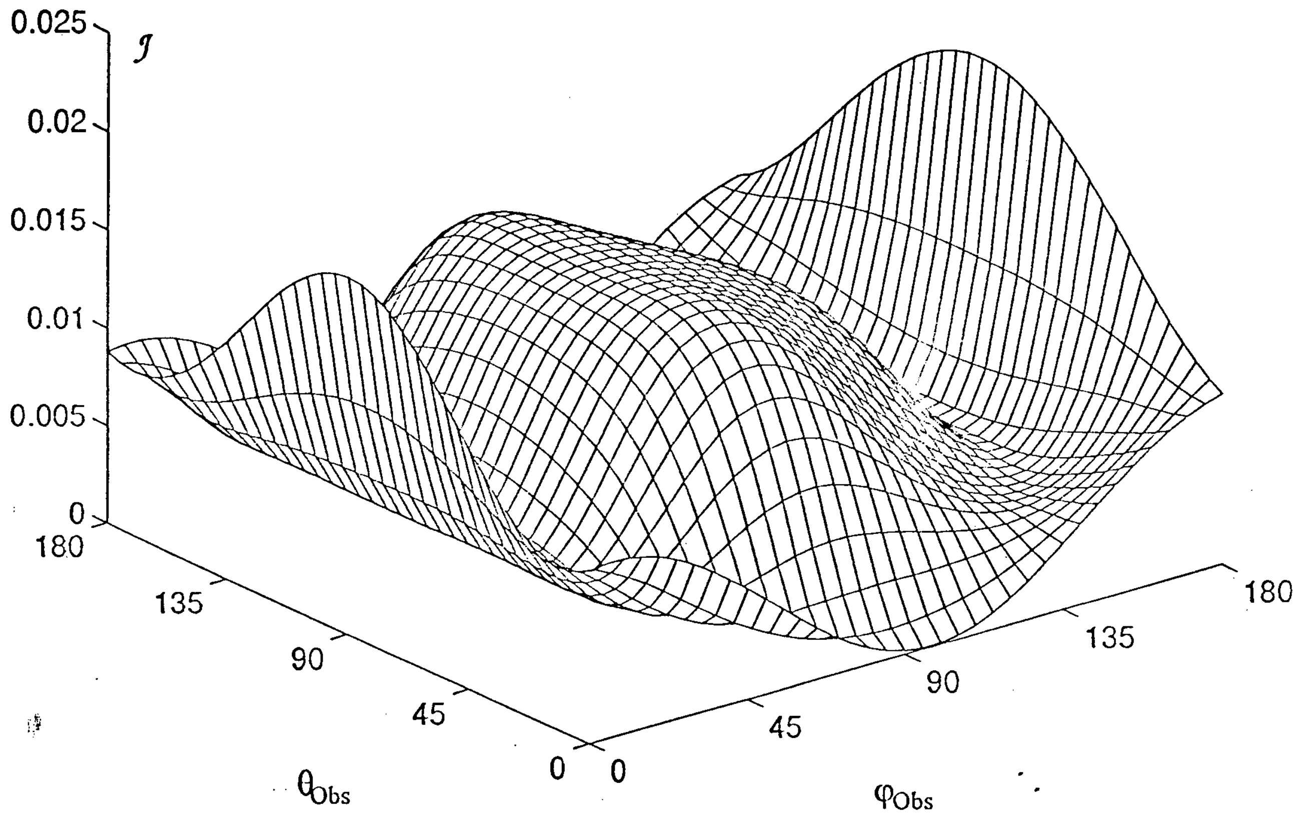


Fig. 5a



0.08
0.06
0.04
0.02
0
$\mathcal{J}$
180
135
90
45
0
θ_{Obs}
0
45
90
135
180
φ_{Obs}

Fig. 5b



0.025
0.02
0.015
0.01
0.005
0
J
180
135
90
45
0
θ_{Obs}
0
45
90
135
180
φ_{Obs}

Fig. 5C