1 Scattering at the plane interface between two media

Two kinds of features can be distinguished in the reflection and refraction of waves at the plane interface between two media:
i) Kinematical properties:
a) the angle of reflection coincides with the angle of incidence
b) the angle of refraction relates to the angle of incidence and the refractive indices of the media via Snel's law
ii) Dynamical properties:
a) the intensitities of reflected and refracted radiation
b) phase shifts and polarization

The kinematical properties follow from the wave nature of the phenomena and the existence of the boundary conditions. The dynamical properties depend fully on the characteristics of the waves and their boundary conditions.
The coordinate systems and symbols are defined in Fig. 1. The original plane wave (wave vector $\mathbf{k}$, angular frequency ω) is incident on the interface from the medium μ, ϵ (refractive index $m = \sqrt{\epsilon\mu/\epsilon_0\mu_0}$). The refracted plane wave propagates in the medium μ', ϵ' ($m' = \sqrt{\epsilon'\mu'/\epsilon_0\mu_0}$) with wave vector $\mathbf{k}_t$ and the reflected plane wave in the medium μ, ϵ with wave vector $\mathbf{k}_r$.
The kinematics are described by the angles of incidence θ_i, reflection θ_r, and refraction θ_t. Assume first that μ, ϵ, μ', ϵ' and therefor also m and m' are real-valued.
Based on what has already been described before, we can write the incident, reflected, and refracted fields as follows:

$$
\begin{aligned}
\mathbf{E}_i &= \mathbf{E}_{0i}e^{i\mathbf{k}_i\cdot\mathbf{x}-i\omega t} \\
\mathbf{B}_i &= \sqrt{\epsilon\mu}\frac{\mathbf{k}_i \times \mathbf{E}_i}{k_i}
\end{aligned}
\tag{1}
$$

$$
\begin{aligned}
\mathbf{E}_r &= \mathbf{E}_{0r}e^{i\mathbf{k}_r\cdot\mathbf{x}-i\omega t} \\
\mathbf{B}_r &= \sqrt{\epsilon\mu}\frac{\mathbf{k}_r \times \mathbf{E}_r}{k_r}
\end{aligned}
\tag{2}
$$

$$
\begin{aligned}
\mathbf{E}_t &= \mathbf{E}_{0t}e^{i\mathbf{k}_t\cdot\mathbf{x}-i\omega t} \\
\mathbf{B}_t &= \sqrt{\epsilon'\mu'}\frac{\mathbf{k}_t \times \mathbf{E}_t}{k_t}
\end{aligned}
\tag{3}
$$

The lengths of the wave vectors are

$$\begin{aligned}
|\mathbf{k}_i| &= |\mathbf{k}_r| = k_i = k_r = \omega\sqrt{\epsilon\mu} \\
|\mathbf{k}_t| &= k_t = \omega\sqrt{\epsilon'\mu'}
\end{aligned} \tag{4}$$

The boundary conditions are to be valid at the interface $z = 0$ at all times. Therefore, the spatial dependences of the fields need to coincide at the interface and, in particular, the arguments of the phase factors

$$(\mathbf{k}_i \cdot \mathbf{x})_{z=0} = (\mathbf{k}_r \cdot \mathbf{x})_{z=0} = (\mathbf{k}_t \cdot \mathbf{x})_{z=0} \tag{5}$$

independently of the detailed properties of the boundary conditions. It follows, first, that the wave vectors must be confined to a single plane. Second, it follows that $\theta_i = \theta_r$ and, third, we obtain Snel's law

$$\begin{aligned}
k_i \sin\theta_i &= k_t \sin\theta_t \\
\Leftrightarrow \quad m \sin\theta_i &= m' \sin\theta_t.
\end{aligned} \tag{6}$$

According to the boundary conditions of electromagnetic fields, the normal components of $\mathbf{D}$ and $\mathbf{B}$ and the tangential components of $\mathbf{E}$ and $\mathbf{H}$ must be continuous across the boundary. Then, at the interface $z = 0$, we have

$$\begin{aligned}
\hat{\mathbf{n}} &\cdot \quad [\epsilon(\mathbf{E}_{0i} + \mathbf{E}_{0r}) - \epsilon'\mathbf{E}_{0t}] = 0 \\
\hat{\mathbf{n}} &\cdot \quad [\mathbf{k}_i \times \mathbf{E}_{0i} + \mathbf{k}_r \times \mathbf{E}_{0r} - \mathbf{k}_t \times \mathbf{E}_{0t}] = 0 \\
\hat{\mathbf{n}} &\times \quad [\mathbf{E}_{0i} + \mathbf{E}_{0r} - \mathbf{E}_{0t}] = 0 \\
\hat{\mathbf{n}} &\times \quad [\frac{1}{\mu}(\mathbf{k}_i \times \mathbf{E}_{0i} + \mathbf{k}_r \times \mathbf{E}_{0r}) - \frac{1}{\mu'}(\mathbf{k}_t \times \mathbf{E}_{0t})] = 0
\end{aligned} \tag{7}$$

Let us divide the scattering problem into two cases: first, the incident field is linearly polarized so that the electric field is perpendicular to the plane defined by $\mathbf{k}_i$ and $\hat{\mathbf{n}}$; second, the electric field is within that plane. An arbitrary elliptic polarization can be treated as a linear sum of the results following for the two cases defined above.

First, let the electric field be perpendicular to the plane of incidence (see Fig. 2). The choice of $\mathbf{B}$-vectors guarantees a positive flow of energy in the direction of the wave vectors. With the help of the third and fourth boundary conditions above, we obtain

$$E_{0i} + E_{0r} - E_{0t} = 0$$

$$\sqrt{\frac{\epsilon}{\mu}}(E_{0i} - E_{0r})\cos\theta_i - \sqrt{\frac{\epsilon'}{\mu'}}E_{0t}\cos\theta_t = 0 \tag{8}$$

Denote the Fresnel coefficients by

$$r_\perp = \frac{E_{0r}}{E_{0i}}, \qquad t_\perp = \frac{E_{0t}}{E_{0i}}.$$

Then,

$$1 + r_\perp - t_\perp = 0$$

$$\sqrt{\frac{\epsilon}{\mu}}(1 - r_\perp)\cos\theta_i - \sqrt{\frac{\epsilon'}{\mu'}}t_\perp\cos\theta_t = 0 \tag{9}$$

and it follows that

$$t_\perp = 1 + r_\perp$$

$$\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i - \sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_t = \left(\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i + \sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_t\right)r_\perp \tag{10}$$

and, furthermore, we obtain, for the Fresnel coefficients,

$$r_\perp = \frac{\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i - \sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_t}{\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i + \sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_t}$$

$$t_\perp = \frac{2\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i}{\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i + \sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_t} \tag{11}$$

Second, let the electric field be within the plane of incidence (see Fig. 3). Again, based on the third and fourth boundary conditions above, we have

$$(E_{0i} - E_{0r})\cos\theta_i - E_{0t}\cos\theta_t = 0$$

$$\sqrt{\frac{\epsilon}{\mu}}(E_{0i} + E_{0r}) - \sqrt{\frac{\epsilon'}{\mu'}}E_{0t} = 0 \tag{12}$$

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Denote the Fresnel coefficients by

$$r_\| = \frac{E_{0r}}{E_{0i}}, \qquad t_\| = \frac{E_{0t}}{E_{0i}}.$$

Then,

$$
\begin{aligned}
(1 - r_\|)\cos\theta_i - t_\|\cos\theta_t &= 0 \\
\sqrt{\frac{\epsilon}{\mu}}(1 + r_\|) - \sqrt{\frac{\epsilon'}{\mu'}}t_\| &= 0
\end{aligned}
\tag{13}
$$

and we obtain the following pair of equations,

$$
\begin{aligned}
t_\| &= \frac{\cos\theta_i}{\cos\theta_t}(1 - r_\|) \\
\sqrt{\frac{\epsilon}{\mu}} - \sqrt{\frac{\epsilon'}{\mu'}}\frac{\cos\theta_i}{\cos\theta_t} &= -\left(\sqrt{\frac{\epsilon}{\mu}} + \sqrt{\frac{\epsilon'}{\mu'}}\frac{\cos\theta_i}{\cos\theta_t}\right)r_\|
\end{aligned}
\tag{14}
$$

allowing for the Fresnel coefficients to be explicitly solved for:

$$
\begin{aligned}
r_\| &= \frac{\sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_i - \sqrt{\frac{\epsilon}{\mu}}\cos\theta_t}{\sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_i + \sqrt{\frac{\epsilon}{\mu}}\cos\theta_t} \\
t_\| &= \frac{2\sqrt{\frac{\epsilon}{\mu}}\cos\theta_i}{\sqrt{\frac{\epsilon'}{\mu'}}\cos\theta_i + \sqrt{\frac{\epsilon}{\mu}}\cos\theta_t}
\end{aligned}
\tag{15}
$$

In the case of a plane wave normally incident on the interface ($\theta_i = 0$), we obtain

$$
\begin{aligned}
r_\| &= -r_\perp = \frac{\sqrt{\frac{\epsilon'}{\mu'}} - \sqrt{\frac{\epsilon}{\mu}}}{\sqrt{\frac{\epsilon'}{\mu'}} + \sqrt{\frac{\epsilon}{\mu}}} \to \frac{m' - m}{m' + m}, \mu = \mu' \\
t_\| &= t_\perp = \frac{2\sqrt{\frac{\epsilon}{\mu}}}{\sqrt{\frac{\epsilon'}{\mu'}} + \sqrt{\frac{\epsilon}{\mu}}} \to \frac{2m}{m' + m}, \mu = \mu'
\end{aligned}
\tag{16}
$$

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The Fresnel coefficients derived above are also valid for complex-valued ϵ, μ, ϵ', and μ'. Usually, for visible light, $\mu = \mu' = \mu_0$. The generalization of Snel's law for complex m' is left for an exercise. In addition, the derivation of the 4×4 reflection and refraction matrices relating the Stokes parameters of incident, reflected, and refracted light is left for an exercise. In the case of incident electric field polarized in the plane of incidence, we can find the so-called Brewster angle, at which there is no reflected wave. Let $\mu = \mu'$. At the Brewster angle,

$$
\begin{aligned}
m' \cos\theta_{iB} &= m\sqrt{1 - \frac{m^2}{m'^2}\sin^2\theta_{iB}} \\
(\frac{m'}{m})^2 \cos^2\theta_{iB} &= 1 - (\frac{m}{m'})^2 \sin^2\theta_{iB} \\
(\frac{m'}{m})^2 &= 1 + \tan^2\theta_{iB} - (\frac{m}{m'})^2 \tan^2\theta_{iB} \\
\tan^2\theta_{iB} &= \frac{(\frac{m'}{m})^2 - 1}{1 - (\frac{m}{m'})^2} = (\frac{m'}{m})^2
\end{aligned}
$$

The physical solution is

$$
\theta_{iB} = \arctan(\frac{m'}{m}) \tag{17}
$$

As a rule for other angles of incidence, too, the reflected light tends to be polarized perpendicular to the plane of incidence.

<u>Total internal reflection</u> can occur when $m > m'$ (the incident wave is "internal"). If $m > m'$, $\theta_t > \theta_{i0}$ according to Snel's law and

$$
\theta_{i0} = \arcsin\frac{m'}{m} \tag{18}
$$

When the angle of incidence is θ_{i0}, the refracted wave is propagating parallel to the interface and there is no energy flow across the interface. Thus, all the incident energy is reflected back. When $\theta_i > \theta_{i0}$, $\sin\theta_t > 1$ and θ_t must be a complex-valued angle that has a purely imaginary cosine,

$$
\cos\theta_t = i\sqrt{(\frac{\sin\theta_i}{\sin\theta_{i0}})^2 - 1} \tag{19}
$$

The refracted wave is of the form

$$
\begin{aligned}
e^{i\mathbf{k}_t \cdot \mathbf{x}} &= e^{ik_t(x\sin\theta_t - z\cos\theta_t)} \\
&= e^{-k_t\sqrt{(\frac{\sin\theta_i}{\sin\theta_{i0}})^2 - 1}|\mathbf{z}|} \, e^{ik_t(\frac{\sin\theta_i}{\sin\theta_{i0}})x}
\end{aligned}
\tag{20}
$$

and, thus, attenuates exponentially in the medium m' and propagates only in the direction of the interface.

1 Scattering at the short-wavelength limit. Scalar diffraction theory.

Traditionally, diffraction entails those deviations from geometric optics that derive from the finite wavelength of the waves. Thereby, diffraction is connected to objects (e.g., holes, obstacles) that are large compared to the wavelength. The possible geometries are described in the figure below (see Jackson). The sources of the radiation are located in region I and we want to derive the diffracted fields in the diffraction region II. The regions are bounded by the interfaces S_1 and S_2. Kirchhoff was the first one to treat this topic systematically.

For simplicity, we will first study scalar fields, whereafter we will extend the analysis to vector fields. Let $\psi(\mathbf{x}, t)$ be a scalar field, for which we assume a harmonic time dependence $e^{-i\omega t}$. In essence, ψ is one of the components of the $\mathbf{E}$ or $\mathbf{B}$ fields. We assume that ψ fulfils the scalar Helmholtz wave equation

$$(\nabla^2 + k^2)\psi(\mathbf{x}) = 0$$

in the volume V bounded by S_1 and S_2. We introduce the Green's function $G(\mathbf{x}, \mathbf{x}')$,

$$(\nabla^2 + k^2)G(\mathbf{x}, \mathbf{x}') = -\delta(\mathbf{x} - \mathbf{x}')$$

and start from Green's theorem

$$\int_V (\phi\nabla^2\psi - \psi\nabla^2\phi)d^3\mathbf{x}' = \oint_S [\phi\frac{\partial\psi}{\partial n} - \psi\frac{\partial\phi}{\partial n}]dA'$$

$$\frac{\partial\psi}{\partial n} \equiv \mathbf{n}' \cdot \nabla\psi$$

where $\mathbf{n}'$ is the unit inward normal vector of S. Let us now set $\psi = G$ and $\phi = \psi$ so that, with the help of the wave equations for ψ and G,

$$\psi(\mathbf{x}) = \oint_S dA'[\psi(\mathbf{x}')\mathbf{n}' \cdot \nabla'G(\mathbf{x}, \mathbf{x}') - G(\mathbf{x}, \mathbf{x}')\mathbf{n}' \cdot \nabla'\psi(\mathbf{x}')]$$

Kirchhoff's diffraction integral follows from this relation when G is chosen to be the free-space Green's function describing outgoing waves,

$$G(\mathbf{x}, \mathbf{x}') = \frac{e^{ikR}}{4\pi R}, \qquad \mathbf{R} = \mathbf{x} - \mathbf{x}', R = |\mathbf{R}|$$

Then

$$\psi(\mathbf{x}) = -\frac{1}{4\pi} \oint_S dA'\frac{e^{ikR}}{R}\mathbf{n}' \cdot [\nabla'\psi + ik(1 + \frac{i}{kR})\frac{\mathbf{R}}{R}\psi]$$

1

The surface S is composed of S_1 and S_2 and the integration can be divided into two parts. In the proximity of S_2, ψ is an outgoing wave and fulfils the so-called radiation condition

$$\psi \to f(\theta, \varphi)\frac{e^{ikr}}{r}, \qquad \frac{1}{\psi}\frac{\partial \psi}{\partial r} \to (ik - \frac{1}{r}).$$

By inserting these results into the integral above, it is possible to show that the integral over S_2 vanishes at least as the inverse of the radius of the sphere when the radius approaches infinity. There remains the integral over S_1, giving the final form of the Kirchhoff integral relation,

$$\psi(\mathbf{x}) = -\frac{1}{4\pi}\int_{S_1} dA' \frac{e^{ikR}}{R}\mathbf{n}' \cdot [\nabla'\psi + ik(1 + \frac{i}{kR})\frac{\mathbf{R}}{R}\psi]$$

In applying the integral relation, it is necessary to know both ψ and $\partial\psi/\partial n$ on the surface S_1. In general, these are not known, at least not precisely. Kirchhoff's approach was based on the idea that ψ and $\partial\psi/\partial n$ are approximated on S_1 for the computation of the diffracted wave. This so-called Kirchhoff's approximation consists of the following assumptions:

1. ψ and $\partial\psi/\partial n$ vanish everywhere else but the holes of S_1

2. ψ and $\partial\psi/\partial n$ in the holes are equal to the original field values when there are no diffracting elements in space.

These assumptions contain a serious mathemtical inconsistency: if ψ and $\partial\psi/\partial n$ are zero on a finite surface, then $\psi = 0$ everywhere. In spite of the inconsistency, the Kirchhoff approximation works in an excellent way in practical problems and constitutes the basis of all diffraction calculus in classical optics.

The mathematical inconsistencies can be removed by a proper choice of the Green's function. In the setup of the figure below (see Jackson), (both P and P' are located several wavelengths away from the hole) we obtain

$$\psi(P) = \frac{k}{2\pi i}\int_{S_1} dA' \frac{e^{ikr}}{r}\frac{e^{ikr'}}{r'}\mathcal{O}(\theta, \theta')$$

$$\mathcal{O}(\theta, \theta') = \begin{cases} \cos\theta, & ; \\ \cos\theta', & ; \\ \frac{1}{2}(\cos\theta + \cos\theta'), & \text{(Kirchhoffin approksimaatio)}. \end{cases}$$

The obliquity factor $\mathcal{O}(\theta, \theta')$ assumes less significance than the phase factors, which partly explains the success of the Kirchhoff approximation.

2

2 Vector Kirchhoff integral relation

The scalar Kirchhoff integral relation is an exact relation between the scalar fields on the surface and at infinity. In a corresponding way, the vector Kirchhoff integral relation is an exact relation between the $\mathbf{E}, \mathbf{B}$ fields on the surface S and the diffracted or scattered fields at infinity. Such a relation is interesting in itself and it is a correct guess that the relation carries practical significance, too.

In what follows, we derive the vector relation for the electric field $\mathbf{E}$, starting from the generalization of Green's theorem already appearing in the scalar case for all components of the $\mathbf{E}$-field,

$$\mathbf{E}(\mathbf{x}) = \oint_S dA' [\mathbf{E}(\mathbf{n}' \cdot \nabla' G) - G(\mathbf{n}' \cdot \nabla')\mathbf{E}],$$

when $\mathbf{x} \in V$ and V is the volume bounded by S. Again, $\mathbf{n}'$ is the unit normal vector pointing into the volume V. Since G is singular at $\mathbf{x}' = \mathbf{x}$ and we make use of vector calculus valid for smooth functions, we assume that S is composed of the outer surface S' and an infinitesimally small inner surface S'' so that the point $\mathbf{x}' = \mathbf{x}$ is left out from volume V (but the point is inside S''). In such a case, the left-hand side of the previous equation disappears, but the integration over S'' on the right-hand side returns $-\mathbf{E}(\mathbf{x})$ when the radius of S'' goes to zero.

The vector relation can now be written in the form

$$0 = \oint_S dA' [2\mathbf{E}(\mathbf{n}' \cdot \nabla' G) - \mathbf{n}' \cdot \nabla'(G\mathbf{E})]$$

and, with the help of the divergence theorem ja divergenssiteoreeman

$$\int_V dV' \nabla \cdot A = \oint_S dA' \mathbf{A} \cdot \mathbf{n},$$

the latter term can be transformed to a volume integral

$$0 = \oint_S dA' 2\mathbf{E}(\mathbf{n}' \cdot \nabla' G) + \int_V dV' \nabla'^2 (G\mathbf{E})$$

Now

$$\nabla^2 \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla \times (\nabla \times \mathbf{A})$$

$$\int_V dV \nabla \phi = \oint_S dA \mathbf{n} \phi, \qquad (\mathbf{n} \text{ ulkonormaali})$$

$$\int_V dV \nabla \times \mathbf{A} = \oint_S dA (\mathbf{n} \times \mathbf{A})$$

and the volume integral can be returned back to a surface integral

$$0 = \oint_S dA' [2\mathbf{E}(\mathbf{n}' \cdot \nabla' G) - \mathbf{n}'(\nabla' \cdot (G\mathbf{E})) + \mathbf{n}' \times (\nabla' \times (G\mathbf{E}))]$$

3

When the ∇-operations are carried out for $G\mathbf{E}$ and use is made of Maxwell's equations $\nabla' \cdot \mathbf{E} = 0, \nabla' \times \mathbf{E} = i\omega\mathbf{B}$, one obtains

$$0 = \oint_S dA'[i\omega(\mathbf{n}' \cdot \mathbf{B})G + (\mathbf{n}' \times \mathbf{E}) \times \nabla'G + (\mathbf{n}' \cdot \mathbf{E})\nabla'G]$$

and, furthermore,

$$\mathbf{E}(\mathbf{x}) = \oint_S dA'[i\omega(\mathbf{n}' \cdot \mathbf{B})G + (\mathbf{n}' \times \mathbf{E}) \times \nabla'G + (\mathbf{n}' \cdot \mathbf{E})\nabla'G]$$

where the volume bounded by S now again includes the point $\mathbf{x}$.

As in the case of the scalar relation, we can now derive the vector Kirchhoff integral relation

$$\mathbf{E}(\mathbf{x}) = \oint_{S_1} dA'[i\omega(\mathbf{n}' \cdot \mathbf{B})G + (\mathbf{n}' \times \mathbf{E}) \times \nabla'G + (\mathbf{n}' \cdot \mathbf{E})\nabla'G],$$

where the integration extends over S_1 only.

Finally, we derive a relation between the scattering amplitude and the near fields. For the fields in the vector Kirchhoff integral relation, we choose the scattered fields $\mathbf{E}_s, \mathbf{B}_s$, that is, the total fields $\mathbf{E}, \mathbf{B}$ minus the original fields $\mathbf{E}_i, \mathbf{B}_i$. If the observation point is far away from the scatterer, both the Green's function and the scattered electric field can be given in their asymptotic forms

$$G(\mathbf{x}, \mathbf{x}') = \rightarrow \frac{1}{4\pi}\frac{e^{ikr}}{r}e^{-i\mathbf{k}\cdot\mathbf{x}'}$$

$$\mathbf{E}_s(\mathbf{x}) \rightarrow \frac{e^{ikr}}{r}\mathbf{F}(\mathbf{k}, \mathbf{k}_0)$$

where $\mathbf{k}$ is a wave vector pointing in the direction of the observer, $\mathbf{k}_0$ is the wave vector of the original field, and $\mathbf{F}(\mathbf{k}, \mathbf{k}_0)$ is the vector scattering amplitude. In this limit, $\nabla'G = -i\mathbf{k}G$ and we obtain an integral relation for the scattering amplitude,

$$\mathbf{F}(\mathbf{k}, \mathbf{k}_0) = \frac{i}{4\pi}\oint_{S_1} dA' e^{-i\mathbf{k}\cdot\mathbf{x}'}[\omega(\mathbf{n}' \cdot \mathbf{B}_s) + \mathbf{k} \times (\mathbf{n}' \times \mathbf{E}_s) - \mathbf{k}(\mathbf{n}' \cdot \mathbf{E}_s)]$$

The relation depends explicitly on the direction of $\mathbf{k}$ and the dependence on $\mathbf{k}_0$ is implicit in $\mathbf{E}_s$ and $\mathbf{B}_s$. Since $\mathbf{k} \cdot \mathbf{F} = 0$, we can reduce the relation to

$$\mathbf{F}(\mathbf{k}, \mathbf{k}_0) = \frac{1}{4\pi i}\mathbf{k} \times \oint_{S_1} dA' e^{-i\mathbf{k}\cdot\mathbf{x}'}[\frac{c\mathbf{k} \times (\mathbf{n}' \times \mathbf{B}_s)}{k} - \mathbf{n}' \times \mathbf{E}_s]$$

Alternatively, one may want the scattering amplitude in direction $\mathbf{k}$ for a specific polarization state ϵ^*,

$$\epsilon^* \cdot \mathbf{F}(\mathbf{k}, \mathbf{k}_0) = \frac{i}{4\pi}\oint_{S_1} dA' e^{-i\mathbf{k}\cdot\mathbf{x}'}[\omega\epsilon^* \cdot (\mathbf{n}' \times \mathbf{B}_s) + \epsilon^* \cdot (\mathbf{k} \times (\mathbf{n}' \times \mathbf{E}_s))]$$

These integral relations are useful in scattering problems entailing short wavelengths and in the derivation of the optical theorem.

4

3 Diffraction by a circular aperture

Diffraction is divided into Fraunhofer and Fresnel diffraction depending on the geometry under consideration. There are three length scales involved: the size of the diffracting system d, the distance from the system to the observation point r and the wavelength λ. The diffraction pattern is generated when $r >> d$. In tht case, the slowly changing parts of the vector integral relation can be kept constant. Particular attention needs to be paid to the phase factor e^{ikR}. When $r >> d$, we obtain

$$kR = kr - k\mathbf{n} \cdot \mathbf{x}' + \frac{k}{2r}[r'^2 - (\mathbf{n} \cdot \mathbf{x}')^2] + \dots, \qquad \mathbf{n} = \frac{\mathbf{x}}{r}, \tag{1}$$

where $\mathbf{n}$ is a unit vector pointing in the direction of the observer. The magnitudes of the terms in the expansion are $kr, kd, (kd)^2/kr$. In Fraunhofer diffraction, the terms from the third one (inclusive) onwards are negligible. When the third term becomes significant (e.g., large diffracting systems), we enter the domain of Fresnel diffraction. Far enough from any diffracting system, we end up in the domain of Fraunhofer diffraction.

If the observation point is far away from the diffracting system, Kirchhoff's scalar integral relation assumes the form

$$\Psi(\mathbf{x}) = -\frac{e^{ikr}}{4\pi r} \int_{S_1} dA' e^{-i\mathbf{k} \cdot \mathbf{x}'} \left[\mathbf{n} \cdot \nabla'\Psi(\mathbf{x}') + i\mathbf{k} \cdot \mathbf{n}\Psi(\mathbf{x}'), \tag{2}$$

where $\mathbf{n}$ now is the unit normal vectoron, $\mathbf{x}'$ denotes the position of the element dA', and $r = |\mathbf{x}|, \mathbf{k} = k(\mathbf{x}/r)$. The so-called Smythe-Kirchhoff integral relation is an improved version of the pure Kirchhoff relation and, in the present limit, takes the form

$$\mathbf{E}(\mathbf{x}) = \frac{ie^{ikr}}{2\pi r}\mathbf{k} \times \int_{S_1} dA'\mathbf{n} \times \mathbf{E}(\mathbf{x}')e^{-i\mathbf{k} \cdot \mathbf{x}'} \tag{3}$$

Let us study next what the different diffraction formulae give for a circular hole (radius a) in an infinitesimally thin perfectly conducting slab.

Figure (see Jackson)

In the vector relation,

$$(\mathbf{n} \times \mathbf{E}_i)_{z=0} = E_0\epsilon_2 \cos \alpha e^{ik \sin \alpha x'} \tag{4}$$

and, in polar coordinates,

$$\mathbf{E}(\mathbf{x}) = \frac{ie^{ikr}E_0 \cos \alpha}{2\pi r}(\mathbf{k} \times \epsilon_2) \int_0^a d\zeta\zeta \int_0^{2\pi} d\beta e^{ik\zeta[\sin \alpha \cos \beta - \sin \theta \cos(\varphi - \beta)]} \tag{5}$$

Define

$$\xi \equiv \frac{1}{k}|\mathbf{k}_\perp - \mathbf{k}_{0,\perp}| = \sqrt{\sin^2 \theta + \sin^2 \alpha - 2\sin \theta \sin \alpha \cos \varphi}, \tag{6}$$

in which case the integral takes the form

$$\frac{1}{2\pi}\int_0^{2\pi}d\beta' e^{-ik\zeta\xi\cos\beta'} = J_0(k\zeta\xi) \tag{7}$$

that is, the result is the Bessel function J_0. Hereafter, the integration over the radial part can be calculated analytically, and

$$\mathbf{E}(\mathbf{x}) = \frac{ie^{ikr}}{r}a^2 E_0 \cos\alpha(\mathbf{k}\times\epsilon_2)\frac{J_1(ka\xi)}{ka\xi} \tag{8}$$

The time-averaged power as per unit solid angle is then

$$\frac{dP}{d\Omega} = P_i\cos\alpha\frac{(ka)^2}{4\pi}(\cos^2\theta + \cos^2\varphi\sin^2\theta)|\frac{2J_1(ka\xi)}{ka\xi}|^2 \tag{9}$$

$$P_i = (E_0^2/2z_0)\pi a^2\cos\alpha, \tag{10}$$

where P_i is the total power normally incident on the hole. If $ka >> 1$, the function $[(2J_1(ka\xi)/ka\xi)^2]$ peaks sharply at 1 with the argument $\xi = 0$ and falls down to zero at $\Delta\xi \approx 1/ka$. The main part of the wave propagates according to geometric optics and only modest diffraction effects show up. If, however, $ka \approx 1$, the Bessel function varies slowly as a function of the angles and the transmitted wave bends into directions considerably deviting from the propagation direction of the incident field. In the extreme limit $ka << 1$, the angular dependence derives from the polarization factor $\mathbf{k}\times\epsilon_2$, but the analysis fails because the field in the hole can no longer be the original undisturbed field as assumed earlier.

let us study the scalar solution assuming that Ψ corresponds the magnitude of the $\mathbf{E}$ field,

$$\Psi(\mathbf{x}) = -ik\frac{e^{ikr}}{r}a^2 E_0\frac{1}{2}(\cos\alpha + \cos\theta)\frac{J_1(ka\xi)}{ka\xi}$$

$$\frac{dP}{d\Omega} \cong P_i\frac{(ka)^2}{4\pi}\cos\alpha(\frac{\cos\alpha + \cos\theta}{2\cos\alpha})|\frac{2J_1(ka\xi)}{ka\xi}|^2 \tag{11}$$

Both the vector and scalar results include the Bessel part $[(2J_1(ka\xi)/ka\xi)^2]$ and the same wave number dependence. But whereas there is no azimuthal dependence in the scalar result, the vector result is significantly affected by the azimuthal dependence. The dependence derives from the polarization of the vector field. For an original field propagating in the direction of the normal vector, the polarization effects are not important, when additionally $ka >> 1$. Then, all the results reduce into the familiar expression

$$\frac{dP}{d\Omega} \cong P_i\frac{(ka)^2}{\pi}|\frac{J_i(ka\sin\theta)}{ka\sin\theta}|^2 \tag{12}$$

However, for oblique directions, there are large deviations and, for very small holes, the analysis fails completely.

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4   Scattering in detail

Let us now consider a small particle that is much larger than the wavelength and study what kind of tools the vector Kirchhoff integral relation offers, if the fields close to the surface can be estimated somehow.

For example, the surface of the scatterer is divided into the illuminated and shadowed parts. The boundary between the two parts is sharp only in the limit of geometric optics and, in the transition zone, the breadth of the boundary is of the order of $(2/kR)^{1/3} \cdot R$, where R is a typical radius of curvature on the surface of the particle.

On the shadow side, the scattered field must be equal to the original field but opposite in sign, in which case the total field vanishes. On the illuminated side, the field depends in a detailed way on the properties of the scattering particle. If the curvature radii are large compared to the wavelength, we can make use of Fresnel's coefficients and geometric optics in general. The analysis can be generalized into the case of a transparent particle and the method is known as the physical-optics approximation (or Kirchhoff approximation).

Let us write the scattering amplitude explicitly in two parts,

$$\epsilon^* \cdot \mathbf{F} = \epsilon^* \cdot \mathbf{F}_{sh} + \epsilon^* \cdot \mathbf{F}_{ill} \tag{13}$$

and assume that the incident fields is a plane wave

$$\mathbf{E}_i = E_0 \epsilon_0 e^{i\mathbf{k}_0 \cdot \mathbf{x}}$$
$$\mathbf{B}_i = \mathbf{k}_0 \times \mathbf{E}_i / kc$$

The shadow scattering amplitude is then ($\mathbf{E}_s \approx -\mathbf{E}_i, \mathbf{B}_s \approx -\mathbf{B}_i$)

$$\epsilon^* \cdot \mathbf{F}_{sh} = \frac{E_0}{4\pi i} \int_{sh} dA' \epsilon^* \cdot [\mathbf{n}' \times (\mathbf{k}_0 \times \epsilon_0) + \mathbf{k} \times (\mathbf{n}' \times \epsilon_0)] \cdot e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}'} \tag{14}$$

where the integration is over the shadowed region. The amplitude can be rearranged into the form

$$\epsilon^* \cdot \mathbf{F}_{sh} = \frac{E_0}{4\pi i} \int_{sh} dA' \epsilon^* \cdot [(\mathbf{k} + \mathbf{k}_0) \times (\mathbf{n}' \times \epsilon_0) + (\mathbf{n}' \cdot \epsilon_0)\mathbf{k}_0] \cdot e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}'} \tag{15}$$

In the short-wavelength limit, $\mathbf{k}_0 \cdot \mathbf{x}'$ and $\mathbf{k} \cdot \mathbf{x}'$ vary across a large regime and the exponential factor fluctuates rapidly and eliminates the integral everywhere else but the forward-scattering direction $\mathbf{k} \approx \mathbf{k}_0$. In that direction ($\theta \lesssim 1/kR$), the second factor is negligible compared to the first one since $(\epsilon^* \cdot \mathbf{k}_0)/k$ is of the order of $\sin\theta << 1, (\epsilon^* \cdot \mathbf{k} = 0, \mathbf{k}_0 \approx \mathbf{k})$. Thus,

$$\epsilon^* \cdot \mathbf{F}_{sh} = \frac{iE_0}{2\pi}(\epsilon^* \cdot \epsilon_0) \int_{sh} dA'(\mathbf{k}_0 \cdot \mathbf{n}')e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}'} \tag{16}$$

In this approximation, the integral over the shadow side only depends on the projected area against the propagation direction of the original field. This can be seen from the fact that

$\mathbf{k}_0 \cdot \mathbf{n}' dA' = k dx' dy' = k d^2 \mathbf{x}'_\perp$ ja $(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}' = k(1 - \cos\theta)z' - \mathbf{k}_\perp \cdot \mathbf{x}'_\perp \approx -\mathbf{k}_\perp \cdot \mathbf{x}'_\perp$. The final form of the shadow scattering amplitude is thus

$$\epsilon^* \cdot \mathbf{F}_{sh} = \frac{ik}{2\pi} E_0 (\epsilon^* \cdot \epsilon_0) \int_{sh} d^2 \mathbf{x}'_\perp e^{-i\mathbf{k}_\perp \cdot \mathbf{x}'_\perp} \tag{17}$$

In this limit, all scatterers producing the same prohjected area will have the same shadow scattering amplitude. For example, in the case of a circular cylindrical slab (radius a)

$$\int_{sh} d^2 \mathbf{x}'_\perp e^{-i\mathbf{k}_\perp \cdot \mathbf{x}'_\perp} = 2\pi a^2 \frac{J_1(ka\sin\theta)}{ka\sin\theta}, \tag{18}$$

$$\epsilon^* \cdot \mathbf{F}_{sh} \cong ika^2 E_0 (\epsilon^* \cdot \epsilon_0) \frac{J_1(ka\sin\theta)}{ka\sin\theta}. \tag{19}$$

This explains nicely the forward diffraction pattern in scattering by small particles.

The scattering amplitude due to the illuminated side of the scatterer cannot be calculated without defining the shape and optical properties of the particle. Let us assume in the following example that the illuminated region is perfectly conducting. Then, the tangential components of the fields $\mathbf{E}_s$ and $\mathbf{B}_s$ on S_1 are approximately opposite and similar to those of the original fields, respectively. The scattering amplitude due to the illuminated part is then

$$\epsilon^* \cdot \mathbf{F}_{ill} = \frac{E_0}{4\pi i} \int_{ill} dA' \epsilon^* \cdot [-\mathbf{n}' \times (\mathbf{k}_0 \times \epsilon_0) + \mathbf{k} \times (\mathbf{n}' \times \epsilon_0)] \cdot e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}'}$$

When this is compared with the shadow amplitude, the only notable difference is the sign in the first term. This sign difference results in a completely different scattering amplitude that can also be written in the form muodossa

$$\epsilon^* \cdot \mathbf{F}_{ill} = \frac{E_0}{4\pi i} \int_{ill} dA' \epsilon^* \cdot [(\mathbf{k} - \mathbf{k}_0) \times (\mathbf{n}' \times \epsilon_0) - (\mathbf{n}' \cdot \epsilon_0)\mathbf{k}_0] \cdot e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}'}$$

When again $kR >> 1$, the exponential factor fluctuates rapidly and one would expect a strong contribution in the forward direction; however, the first term goes to zero in the forward direction and no strong contribution can follow. The illuminated region contributes to scattering in the form of a reflected wave.

Assume next that the scattering particle is spherical (radius a). The predominating contribution to the scattering amplitude now derives from a region of integration where the phase of the exponential factor is stationary. If (θ, φ) are the coordinates of $\mathbf{k}$ and (α, β) those of $\mathbf{n}'$ (with respect to $\mathbf{k}_0$), the phase factor is

$$\phi(\alpha, \beta) = (\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{x}' = ka[(1 - \cos\theta)\cos\alpha - \sin\theta\sin\alpha\cos(\beta - \varphi)]$$

The stationary point can be found at angles α_0, β_0, where $\alpha_0 = \pi/2 + \theta/2$ and $\beta_0 = \varphi$. These angles correspond exactly to the angles of reflection on the surface of the sphere as dictated

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by geometric optics. At that point, the vector $\mathbf{n}'$ points in the direction of $(\mathbf{k} - \mathbf{k}_0)$. In the proximity of angles $\alpha = \alpha_0$ and $\beta = \beta_0$

$$\phi(\alpha, \beta) = -2ka \sin \frac{\theta}{2} [1 - \frac{1}{2}(x^2 + \cos^2 \frac{\theta}{2} y^2) + \ldots]$$

where $x = \alpha - \alpha_0$ and $y = \beta - \beta_0$. The integration can be carried out approximately:

$$\epsilon^* \cdot \mathbf{F}_{ill} \cong ka^2 E_0 \sin \theta e^{-2ika \sin \frac{\theta}{2}} (\epsilon^* \cdot \epsilon_r) \cdot \int dx e^{i[ka \sin \frac{\theta}{2}]x^2} \int dy e^{i[ka \sin \frac{\theta}{2} \cos^2 \frac{\theta}{2}]y^2}$$

$$\epsilon_r = -\epsilon_0 + 2(\mathbf{n}_r \cdot \epsilon_0)\mathbf{n}_r, \qquad \mathbf{n}_r = \frac{\mathbf{k} - \mathbf{k}_0}{|\mathbf{k} - \mathbf{k}_0|}$$

When $2ka \sin \frac{\theta}{2} >> 1$, the integrals can be calculated using the result $\int_{-\infty}^{\infty} dx e^{i\alpha x^2} = \sqrt{\pi i/\alpha}$,

$$\epsilon^* \cdot \mathbf{F}_{ill} \cong E_0 \frac{a}{2} e^{-2ika \sin \frac{\theta}{2}} \epsilon^* \cdot \epsilon_r$$

For large $2ka \sin \frac{\theta}{2}$, the intensity of the reflected part of the radiation is constant as a function of the angle, but the part has a rapidly varying phase. When $\theta \to 0$, the intensity vanishes as θ^2 (see the integral above).

Comparison of the amplitudes due to the shadowed and illuminated parts of the surface shows that, in the forward direction, the former amplitude predominates over the latter by a factor $ka >> 1$ whereas, at the scattering angles $2ka \sin \theta >> 1$, the ratio of the amplitudes is of the order of $1/(ka \sin^3 \theta)^{1/2}$. The differential scattering cross section (summed over the polarization states of the original and scattered waves) is

$$\frac{d\sigma}{d\Omega} \cong \begin{cases} a^2 (ka)^2 |\frac{J_1(ka \sin \theta)}{ka \sin \theta}|^2, & \theta \lesssim \frac{10}{ka} \\ \frac{a^2}{4}, & \theta >> \frac{1}{ka} \end{cases} ;$$

The total scattering cross section is twice the geometric cross section of the particle.

5   Optical theorem

The optical theorem is a fundamental relation that connects the extinction cross section to the imaginary part of the forward-scattering amplitude. Consider a plane wave with a wave vector $\mathbf{k}_0$ and field components $\mathbf{E}_i, \mathbf{B}_i$. The plane wave is incident on a finite-sized scatterer inside the surface S_1. The scattered field $\mathbf{E}_s, \mathbf{B}_s$ propagates away from the scatterer and is observed in the far zone in the direction $\mathbf{k}$. The total field outside the surface S_1 is, by definition,

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_i + \mathbf{E}_s \\ \mathbf{B} &= \mathbf{B}_i + \mathbf{B}_s. \end{aligned}$$

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In the general case, the scatterer absorbs energy from the original field. The absorbed power can be calculated by integrating the inward-directed Poynting-vector component of the total field over the surface S_1:

$$P_{abs} = -\frac{1}{2\mu_0} \oint_{S_1} dA' \text{Re}(\mathbf{E} \times \mathbf{B}^*) \cdot \mathbf{n}'$$

The scattered power is computed in the usual way from the asymptotic form of the Poynting vector for the scattered fields in the regime, where the fields are simple transverse spherical waves that attenuate as $1/r$. But since there are no sources between S_1 and infinity, the scattered power can as well be calculated as an integral of the outward-directed component of the Poynting vector for the scattered field over S_1:

$$P_{sca} = \frac{1}{2\mu_0} \oint_{S_1} dA' \text{Re}(\mathbf{E}_s \times \mathbf{B}_s^*) \cdot \mathbf{n}'$$

The total power is the sum of the absorbed and scattered power so that, after rearranging,

$$P = P_{abs} + P_{sca} = -\frac{1}{2\mu_0} \oint_{S_1} dA' \text{Re}(\mathbf{E}_s \times \mathbf{B}_i^* + \mathbf{E}_i^* \times \mathbf{B}_s) \cdot \mathbf{n}'$$

When the original field in written explicitly in the form

$$\begin{aligned} \mathbf{E}_i &= E_0 \epsilon_0 e^{i\mathbf{k}_0 \cdot \mathbf{x}} \\ c\mathbf{B}_i &= \frac{1}{k}\mathbf{k}_0 \times \mathbf{E}_i \end{aligned}$$

the total power can be transformed to the form

$$P = \frac{1}{2\mu_0} Re E_0^* \oint_{S_1} dA' e^{-i\mathbf{k}_0 \cdot \mathbf{x}} [\epsilon_0^* \cdot (\mathbf{n}' \times \mathbf{B}_s) + \epsilon_0^* \cdot \frac{\mathbf{k}_0 \times (\mathbf{n}' \times \mathbf{E}_s)}{kc}]$$

By comparing this with the scattering amplitude $\mathbf{F}(\mathbf{k}, \mathbf{k}_0)$ derived earlier, we can recognize that the total power is proportional to the value of $\mathbf{F}$ in the forward-scattering direction $\mathbf{k} = \mathbf{k}_0$ in the polarization state coinciding with that of the original field:

$$P = \frac{2\pi}{kZ_0} \text{Im}[E_0^* \epsilon_0^* \cdot \mathbf{F}(\mathbf{k} = \mathbf{k}_0)],$$

which is the basic form of the optical theorem.

The total or extinction cross section σ_e is defined as the ratio of the total and original flux densities ($|E_0|^2/2Z_0$, power as per unit surface area).

In a corresponding way, one can define a normalized scattering amplitude $\mathbf{f}$ (against the original field value at origin)

$$f(\mathbf{k} = \mathbf{k}_0) = \frac{\mathbf{F}(\mathbf{k}, \mathbf{k}_0)}{E_0}$$

The final form of the optical theorem is then

$$\sigma_e = \frac{4\pi}{k} \text{Im}[\epsilon_0^* \cdot \mathbf{f}(\mathbf{k} = \mathbf{k}_0)].$$

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1 Scattering by nonspherical particles (lecture 14)

Perfectly spherical particles constitute, practically, an exception in nature and even in industrial applications. In the recent past, numerical methods have been actively developed for light scattering by nonspherical particles. In practice, the methods require extensive computational capacity including supercomputers.

In what follows, one possible modeling of a nonspherical particle geometry is presented: the Gaussian random sphere. Thereafter, computation of scattering by Gaussian particles is discussed in various approxiamtions, whereafter a summary is given on essentially exact numerical methods and possibilities to apply these methods to scattering by Gaussian particles.

2 Gaussian random particle

Statistical modeling of nonspherical particle shapes seems reasonable, since nonspherical shapes usually show up as a wide spectrum of different-looking shapes. In the Gaussian-random-sphere model, the particle is assumed to be mathematically star-like so that there is an origin with respect to which the shape can be expressed as a function of the spherical coordinates. In the spherical geometry, the so-called lognormal statistics are being used so that the radial distance of the particle varies within $]0, \infty[$. The shape is unambiguously defined by the mean of the radial distance a and the covariance function of the logarithm of the radial distance Σ_s. Explicitly,

$$r(\theta, \varphi) = a e^{s(\theta, \varphi) - \frac{1}{2}\beta^2},$$

where s is the logarithmic radial distance and $\beta^2 = \Sigma_s(0)$ is the variance of s. Now

$$s(\theta, \varphi) = \sum_{lm} s_{lm} Y_{lm}(\theta, \varphi)$$

and, due to s being real-valued,

$$s_{l,-m} = (-1)^m s_{lm}^* \left\{ \begin{array}{l} l = 0, 1, 2, \ldots, \\ m = -l, \ldots, -1, 0, 1, \ldots, l, \end{array} \right. ;$$

$$Im(s_{l0}) = 0.$$

The spherical harmonics coefficients of the logarithmic radial distance $s_{lm}, m \geq 0$ are independent Gaussian random variables with zero means and with variances (l and m as above)

$$\mathrm{Var}[\Re(s_{lm})] = (1 + \delta_{m0})\frac{2\pi}{2l+1}c_l$$
$$\mathrm{Var}[\Im(s_{lm})] = (1 - \delta_{m0})\frac{2\pi}{2l+1}c_l$$

The coefficients $c_l \geq 0, l = 0, \ldots, \infty$ are the coefficients of the Legendre expansion for the covariance function Σ_s:

$$\Sigma_s(\gamma) = \beta^2 C_s(\gamma) = \sum_{l=0}^{\infty} c_l P_l(\cos \gamma), \qquad \sum_{l=0}^{\infty} c_l = \beta^2,$$

where γ is the angualr distance between two directions (θ_1, φ_1) and (θ_2, φ_2).

The two slopes on the Gaussian random particle (subscripts refering to partial derivatives)

$$s_\theta = \frac{r_\theta}{r}, \qquad \frac{1}{\sin\theta} s_\varphi = \frac{r_\varphi}{r\sin\theta}$$

are, again, independent Gaussian random variables with zero means and with standard deviations

$$\rho = \sqrt{-\Sigma_s^{(2)}(0)},$$

where $\Sigma_s^{(2)}$ is the second derivative of the covariance function with respect to γ. The correlation length l_c and correlation angle Γ_c are

$$l_c = 2\sin\frac{1}{2}\Gamma_c = \frac{1}{\sqrt{-c_s^{(2)}(0)}}.$$

Natural random shapes often exhibit covariance functions, for which the coefficients c_l follow the exponent form $c_l \propto l^{-\nu}, l \geq 2$. For $\nu = 4$, one obtains random shapes applicable, in the first place, to modeling Saharan sand particles, asteroids, as well as the shapes of terrestrial planets.

In the limiting case, the Gaussian random shape thus depends on a single free parameter insofar as the shape is concerned: the variance β^2 of the logarithmic radial distance. β^2 relates to the relative variance of the radius σ^2 via the simple relation

$$\sigma^2 = e^{\beta^2} - 1.$$

Increasing σ results in shapes, where the radial fluctuations are enhanced.

If, additionally, ν is treated as a free parameter, one obtains shorter correlation lengths with smaller values of ν (when the expansions are always truncated at a certain degree l_{max}) and thereby lrger numbers of hills and valleys as per unit solid angle.

For $\nu \geq 4$, non-fractal smooth shapes are obtained whereas, for $\nu < 4$, fractal shapes follow, in which case infinite expansions would yield non-differentiable surfaces rendering the discussion of slopes meaningless.

3 Scattering by Gaussian particles in different approximations

Light scattering by Gaussian random particles has been studied in the ray-optics, Rayleigh-volume, Rayleigh-Gans, anomalous-diffraction and perturbation-series approximations, as well as in the Rayleigh-ellipsoid approximation.

In the Rayleigh-volume approximation, the scattering by a small particle follows from its volume. In the case of the Gaussian particle, the (ensemble-averaged) absorption cross section

is proportional to the mean of the volume, whereas the scattering cross section is proportional to the mean of the squared volume. The angular characteristics of the scattering matrix are the same as in the Rayleigh approximation for spherical particles. The results are largely analytical.

In the Rayleigh-ellipsoid approximation, an ellipsoid is fitted to each realization of the Gaussian particle, the ellipsoid volume being equal to the volume of the realization. Scattering is then approximated with the existing electrostatics approximation for ellipsoidal scatterers. The most significant challenge in the Rayleigh-ellipsoid approximation is the numerical computation of the best-fit ellipsoid, whereafter the results follow in a straightforward way.

In the Rayleigh-Gans approximation (or the first Born approximation), the numerical computation of the form factor can be aided by analytical intermediate results. In practice, some numerical integrattion remains, preventing the treatment of arbitrarily large particles.

In anomalous diffraction, path lengths of rays inside the Gaussian sample particles are numerically computed in cases where the refractive index is close to unity. The absorption follows directly from the exponential attenuation and extinction is computed from the optical theorem. The angular dependence of scattering is obtained by averaging the square of the scattering amplitude. The most demanding task is the computation of the path lengths inside the particle, which is difficult for extremely nonspherical shapes.

In the second-order perturbation-series approach for the boundary conditions, analytical results follow for the cross sections and scattering matrices and the most challenging numerical part is the computation of the so-called $3j$-symbols. The unknown accuracy of the results is a problem. In practice, the perturbation-series method is applicable to wavelength-scale scatterers only, if the deviations from the spherical shape are small compared to the wavelength.

Approximations can be taken to be "the spice"that makes the scattering research "delicious", since, in practice, all so-called exact methods are based on approximation in some part. One can make the provocative statement that only approximations allow the computation of light scattering by realistic small particles. The applicability of the exact methods is usually limited to a narrow range of simple shapes. By the rapid development of computers and by the development of new analytical methods, the applicability of certain exact methods grows slowly but steadily.

4 Exact methods and their applicability to Gaussian particles

The numerical methods in light scattering can be divided into differential-equation and integral-equation methods. The traditional computational method is the separation-of-varaibles method that has been successful in the solution of the following scattering problems:

1. isotropic, homogeneous sphere

2. coated sphere consisting of the interior and coating (with common origin)

3. layered sphere that consists of several layers defined by concentric spherical cells

4. radially inhomogeneous sphere

5. optically active (chiral) sphere

6. homogeneous, istropic infinite circular cylinder

7. optically active infinite circular cylinder

8. isotropic infinite elliptic cylinder

9. isotropic, homogeneous spheroid

10. coated spheroid that consists of the interior and coating (with common origin)

11. optically active spheroid

The separation-of-variables method is not applicable to scattering by Gaussian particles.

The FEM-method (finite-element method) is a differenttial-equation method, where the scatterer is placed in a finite computational volume that is discretized into numerous small computational cells. Typically, there are 10-20 cells per wavelength and the electromagnetic field is solved for in the nodal points of the cells. The resulting linear group of equations consists of a sparse matrix. In the boundaries of the computational volume, an artifical absorbing boundary condition is invoked. Although FEM allows for the computations for arbitrary, even inhomogeneous particles, it has not yet been applied to Gaussian particles.

The FDTD-method (finite-difference time-domain method) is a differential-equation method that solves for the time dependence of the electromagnetic fields based on Maxwell's curl equations. Both time and spatial derivatives are expressed with finite differences and time elapses in finite steps. The scattering particle is again palced in a finite computational volume and an absorbing boundary condition is required in the boundary of the computational volume. The density of the discretization is as in the FEM-method. In FDTD, there is no need to solve a large group of equations. Recently, the method has yielded promising results in light scattering by Gaussian particles.

In the PM-method (point matching), the boundary conditions of the electromagnetic fields are required in a finite number of points on the surface of the particle. In the original method, there were as many points as unknown coefficients in the vector spherical harmonics expansion. It was concluded that the method was numerically instable. There is, however, nothing that prevents us from expanding the number of points and computing the coefficients using the least-squares method. This version of the method has been noticed to be stable and is one of the most popular numerical methods. The regime of application can be improved by expanding the fields with a number of suitably chosen origins within the particle. PM is promising also

for scattering by Gaussian particles. It is intriguing to ponder whether "an educated guess" can help speed up the solution of the coefficients.

The integral-equation methods are divided into a wide spectrum of different methods. In the VIEM method (volume-integral-equation), one considers the integral equation

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_i(\mathbf{r}) + k^2 \int_V d^3\mathbf{r}'[\mathbf{1} + \frac{1}{k^2}\nabla\nabla]\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} \cdot [m^2(\mathbf{r}') - 1]\mathbf{E}(\mathbf{r}').$$

By discretizing the integral on the right-hand side, one obtains a group of linear equations for the field values at the discretization points within the volume of the particle. Solving the equations results in the field inside the particle. Typically, again, 10-20 discretization points are required as per wavelength so that, after a straightforward calculation, it is clear that a group of equations with thousands of unknowns easily follows. In practice with current computers, up to 200 million unknowns can be treated (as of December 12, 2008). Various versions of the VIEM method have been successfully applied to Gaussian-particle scattering (foremost DDA, discrete-dipole approximation).

In the case of VIEM, the matrix of the group of linear equations is full, which makes the solution more difficult. When the internal field has been solved for, the same integral relation gives the scattered field outside the particle via straightforward integration (subtracting the original field).

DDA (discrete-dipole approximation) is a certain version of solution methods for the integral equation. DDA can be visualized in the following: the particle can be thought to be composed of dipole scatterers interacting with each other. In practice, the VIEM methods differ from one another in how they treat the singular self-term inside the integral, which is essential for the accuracy of the method.

The surface-integral-equation methods (SIEM) make use of two-dimensional integral equations that seem like a reasonable starting point, in particular, for homogeneous particles. However, the SIEM-methods are less stable than the VIEM-methods and usually require additional regularization.

The integral equation shown above in connection to the VIEM-method is Fredholm-type and the kernel has a singularity at $\mathbf{r} = \mathbf{r}'$. Via Fourier-transformation, handling of the singularity can be improved and the integral equation can be solved numerically in the wavenumber (or frequency) space. Surprisingly, the disadvantage of the method is the considerable analytical work needed for each different particle. These so-called FIEM-methods have not been very popular.

In the TMM method (transition matrix method), the analysis proceeds with the help of vector spherical harmonics functions and the word "transition" refers to the linear matrix relation between the original field and the scattered field. Compared to the direct vector spherical harmonics treatment of the boundary conditions, TMM has the advantage that a linear relation is obtained purely between the internal and original fields, reducing the number of unknowns in the group of linear equations. After solving the group of equations,

the scattered is computed from the vector Kirchhoff integral relation. The TMM method is an efficient method, in particular, for axially symmetric particles and useful results have been obtained, e.g., for spheroids to compare with the implications of the SVM method. However, TMM suffers from unpredictable convergence and instability problems and have not yet been extensively applied to scattering by Gaussian particles. As a tool the actual T-matrix is quite useful and, for a single particle, needs to be computed only once (independently of the orientation). Recently, an analytical version of the T-matrix method has been developed—this version is highly promising for studying scattering by Gaussian random particles.

In the superposition method for spheres and spheroids, scattering by particle clusters is computed using the translation and addition rules of vector spherical harmonics functions. The field scattered by the cluster is expressed as a superposition of the fields scattered by each constituent particle. The partial fields depend on each other due to the mutual electromagnetic interactions of the constituent particles. The scattering problem again manifests itself in a solution of a group of linear equations. Currently, precise solutions can be computed for clusters with several dozens of constituent particles, when constituent-particle size approaches the wavelength.

5   Applications of electromagnetic scattering

In his book, van de Hulst has presented an excellent review of the applications of light scattering in various fields of science. This is recommended reading bearing in mind, in particular, modern computational methods for nonspherical particles. Bohren and Huffman offer additional material on the applications, as well as Mishchenko et al. Finally, the publications from the meeting series entitled *Electromagnetic and Light Scattering by Nonspherical Particles: Theory, Measurements, and Applications* offer up-to-date information about the advances in light scattering by small particles.