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BASIC EQUATIONS OF DIFFRACTIVE NANOPHOTONICS

There are several books on modern nanophotonics [1–5]. The book [1] is devoted only to photonic crystals and does not address other important areas of nanophotonics. Calculation of band gaps in photonic crystals [1] is based on solving Maxwell's equations, rewritten in the form of a problem of the eigenvalues and eigenvectors.

The book [2] deals with almost all areas of nanophotonics, but does not consider the mathematical methods of modelling the diffraction of light. The book [3] focuses on the near-field microscopy for the observation of quantum structures, molecules and biological systems. Analysis of the interaction of light with matter [3] is based on the dipole approximation, which applies to particles of matter with dimensions much smaller than the wavelength of light. The book [4] deals with only one field of nanophotonics and one modelling method. In [4], the authors consider only the localized plasmons as resonance vibrations of metal nanoparticles excited by electromagnetic radiation. Localized plasmons are different from surface plasmons, which are discussed in chapter 4 of this book. Localized plasmons in [4] are analyzed by means of the eigenfunctions of plasmon oscillations, which are the eigenfunctions of the Laplace equation. The book [5] is closest to the present book. The book [5] addresses many aspects of nanophotonics: near-field microscopy, photonic crystals, surface plasmons, quantum emitters, optical capture. The mathematical modelling methods in nanophotonics problems are discussed: the method of moments, the method of coupled dipoles, the Green's function method. However, the book [5] does not address important areas of nanophotonics, such as as photonic–crystal waveguides and lenses, subwavelength gratings with magnetic and metal layers. Also, the book [5] does not consider the most universal methods for simulation of light diffraction – difference methods for solving Maxwell's equations: FDTD-method and the BPM-method.

Therefore, chapter 1 of this book presents the basic equations of diffractive nanophotonics, which are used in this book: Maxwell's equations in integral and differential forms, and other differential and integral equations derived from Maxwell's equations. Chapter 2 discusses the two main difference methods for solving Maxwell's equations: finite-difference time-domain method (FDTD-method) and the beam propagation method (BPM-method).

1.1. Maxwell equations

1.1.1. Mathematical concepts and notations

In the Cartesian coordinate system with unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ we determine the differential operators grad, div, rot and Δ with respect to the scalar f and vector $\mathbf{F}$ functions as follows:

$$\operatorname{grad} f \equiv \nabla f = \mathbf{e}_x \frac{\partial f}{\partial x} + \mathbf{e}_y \frac{\partial f}{\partial y} + \mathbf{e}_z \frac{\partial f}{\partial z},$$

$$\operatorname{div} \mathbf{F} \equiv \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z},$$

$$\operatorname{rot} \mathbf{F} \equiv \nabla \times \mathbf{F} = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) \mathbf{e}_x + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) \mathbf{e}_y + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \mathbf{e}_z,$$

$$\Delta f \equiv \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2},$$

$$\Delta \mathbf{F} \equiv \nabla^2 \mathbf{F} = \operatorname{grad} \operatorname{div} \mathbf{F} - \operatorname{rot} \operatorname{rot} \mathbf{F} \cdot$$

For a cylindrical coordinate system with unit vectors $\mathbf{e}_\rho$, $\mathbf{e}_\varphi$, $\mathbf{e}_z$:

$$\operatorname{grad} f = \mathbf{e}_\rho \frac{\partial f}{\partial \rho} + \mathbf{e}_\varphi \frac{1}{\rho} \frac{\partial f}{\partial \varphi} + \mathbf{e}_z \frac{\partial f}{\partial z},$$

$$\operatorname{div} \mathbf{F} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho F_\rho \right) + \frac{1}{\rho} \frac{\partial F_\varphi}{\partial \varphi} + \frac{\partial F_z}{\partial z},$$

$$\operatorname{rot} \mathbf{F} = \left(\frac{1}{\rho} \frac{\partial F_z}{\partial \varphi} - \frac{\partial F_\varphi}{\partial z} \right) \mathbf{e}_\rho + \left(\frac{\partial F_\rho}{\partial z} - \frac{\partial F_z}{\partial \rho} \right) \mathbf{e}_\varphi + \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho F_\varphi \right) - \frac{1}{\rho} \frac{\partial F_\rho}{\partial \varphi} \right) \mathbf{e}_z,$$

$$\Delta f = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 f}{\partial \varphi^2} + \frac{\partial^2 f}{\partial z^2}.$$

In a spherical coordinate system with unit vectors $\mathbf{e}_r$, $\mathbf{e}_\theta$, $\mathbf{e}_\varphi$ the following representations apply:

$$\operatorname{grad} f = \mathbf{e}_r \frac{\partial f}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial f}{\partial \theta} + \mathbf{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial f}{\partial \varphi},$$

$$\operatorname{div} \mathbf{F} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 F_r \right) + \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta F_\theta \right) + \frac{1}{r \sin\theta} \frac{\partial F_\varphi}{\partial \varphi},$$

$$\operatorname{rot}\mathbf{F} = \left(\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta F_\varphi\right) - \frac{1}{r\sin\theta}\frac{\partial F_\theta}{\partial\varphi}\right)\mathbf{e}_r$$
$$+\left(\frac{1}{r\sin\theta}\frac{\partial F_r}{\partial\varphi} - \frac{1}{r}\frac{\partial}{\partial r}\left(rF_\varphi\right)\right)\mathbf{e}_\theta$$
$$+\left(\frac{1}{r}\frac{\partial F_r}{\partial r}\left(rF_\theta\right) - \frac{1}{r}\frac{\partial F_r}{\partial\theta}\right)\mathbf{e}_\varphi,$$

$$\Delta f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2}.$$

The most important integral relationships of vector analysis are:

The Gauss–Ostrogradskii theorem:

$$\int_V div\mathbf{F}dv = \oint_S \left(\mathbf{F},\mathbf{n}\right)ds,$$

where $\mathbf{n}$ is the unit vector of the external normal; V is a region of space bounded by the surface S.

Stokes' theorem:

$$\int_S \operatorname{rot}\mathbf{F}ds = \oint_L \mathbf{F}dl,$$

where L is the contour bounding the surface S.

1.1.2 Maxwell's equations in differential form

The electromagnetic theory of light is based on a system of Maxwell's equations [1]:

$$\operatorname{rot}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{D}}{\partial t} + \frac{4\pi}{c}\mathbf{j} + \frac{4\pi}{c}\mathbf{j}_{cm}, \tag{1.1}$$

$$\operatorname{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}, \tag{1.2}$$

$$\operatorname{div}\mathbf{D} = 4\pi\rho, \tag{1.3}$$

$$\operatorname{div}\mathbf{B} = 0. \tag{1.4}$$

The names of the electromagnetic quantities appearing in (1.1)–(1.4) are given in Table 1.1.

Functions $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$, $\mathbf{H} = \mathbf{H}(\mathbf{r}, t)$, $\mathbf{D} = \mathbf{D}(\mathbf{r}, t)$, $\mathbf{B} = \mathbf{B}(\mathbf{r}, t)$ describe the electromagnetic field in an environment characterized by parameters $\varepsilon = \varepsilon(\mathbf{E}, \mathbf{r}, t)$, $\mu = \mu(\mathbf{H}, \mathbf{r}, t)$, $\rho = (\mathbf{r}, t)$, $\mathbf{j} = \mathbf{j}(\mathbf{E}, \mathbf{r}, t)$ ($\mathbf{r}$ are the spatial coordinates, t is time), and external current $\mathbf{j}_e$, the use of which will be stipulated separately.

Assuming that the processes are local and instantaneous (at each point the state is independent of neighbouring points and at each moment of time of 'prehistory'), we associate the characteristics of the field and the medium by material equations [1]

Table 1.1. Electromagnetic quantities in the Gaussian CGS system

Name	Designation
Charge	q
Current	I
Charge density	ρ
Current density	j
Conductivity	σ
Electric vector	E
Magnetic vector	H
Electric displacement	D
Magnetic induction	B
Permittivity	ε
Magnetic permeability	μ
Speed of light in vacuum	c

$$\mathbf{D} = \varepsilon \mathbf{E}, \tag{1.5}$$

$$\mathbf{B} = \mu \mathbf{H}, \tag{1.6}$$

$$\mathbf{j} = \sigma \mathbf{E}, \tag{1.7}$$

and the law of conservation of charge

$$\text{div}\mathbf{j} = -\frac{\partial \rho}{\partial t}. \tag{1.8}$$

It is also assumed that the paremeters of the medium are independent of the vectors of the field and do not change with time: $\varepsilon = \varepsilon(\mathbf{r}), \mu = \mu(\mathbf{r})$ (linear medium), are scalar (isotropic medium), the field does not cause polarization and magnetization of the medium. $\varepsilon\omega\ \rho$

If the electric and magnetic vectors can be expressed as $\mathbf{E}$ = Re ($\mathbf{E}$ exp($-i\omega t$)), $\mathbf{H}$ = Re ($\mathbf{H}$ exp($-i\omega t$)), where $\mathbf{E} = \mathbf{E}$ ($\mathbf{r}$), $\mathbf{H} = \mathbf{H}$ ($\mathbf{r}$) are the complex functions [1], ω is the cyclic frequency, i is the imaginary unit, we speak of a monochromatic field for which (1.1) and (1.2) take the form:

$$\text{rot}\mathbf{H} = -ik_0\dot{\varepsilon}\mathbf{E}, \tag{1.9}$$

$$\text{rot}\mathbf{E} = ik_0\mu\mathbf{H}, \tag{1.10}$$

where $\dot{\varepsilon} = \varepsilon - i\dfrac{\sigma}{\omega}$, $k_0 = \dfrac{\omega}{c} = \dfrac{2\pi}{\lambda}$ - the wave number.

1.1.3 Maxwell's equations in integral form

Integrating (1.1) (1.2) on the surface S, bounded by L, and applying the Stokes theorem, we obtain the equation:

$$\oint_L \mathbf{H} dl = \frac{1}{c}\frac{d}{dt}\int_S \mathbf{D} ds + \frac{4\pi}{c}\mathbf{I}, \tag{1.11}$$

$$\oint_L \mathbf{E} dl = -\frac{1}{c}\frac{\mathrm{d}}{\mathrm{d}t}\int_S \mathbf{B} ds. \tag{1.12}$$

Equations (1.3) (1.4) are integrated over the volume V, bounded by the surface S. Then, applying the Gauss–Ostrogradskii theorem, we obtain:

$$\oint_S (\mathbf{D}, \mathbf{n})\,\mathrm{d}s = 2\pi q, \tag{1.13}$$

$$\oint_S (\mathbf{B}, \mathbf{n})\,\mathrm{d}s = 0. \tag{1.14}$$

The system (1.11)–(1.14) is called the Maxwell equations in integral form.

1.1.4. Fields at interfaces

Applying Maxwell's equations in integral form for an infinitely small contours and volume at the interface between two media, we obtain the following boundary conditions [1] for the electromagnetic fields:

$$((\mathbf{D}_1 - \mathbf{D}_2), \mathbf{e}_y) = 4\pi\xi, \tag{1.15}$$
$$((\mathbf{E}_1 - \mathbf{E}_2), \mathbf{e}_z) = 0, \tag{1.16}$$
$$((\mathbf{B}_1 - \mathbf{B}_2), \mathbf{e}_y) = 0, \tag{1.17}$$
$$((\mathbf{H}_1 - \mathbf{H}_2), \mathbf{e}_z) = 4\pi(\boldsymbol{\eta}, \mathbf{i})c, \tag{1.18}$$

where $\xi = \lim\limits_{\Delta S \to 0} \dfrac{\Delta q}{\Delta S}$ is the surface charge density, $\eta = \lim\limits_{\Delta l \to 0} e_x \dfrac{\Delta \mathbf{I}}{\Delta l}$ is the density of the surface current (the plane separating media 1 and 2 perpendicular to the vector $\mathbf{e}_y$).

1.1.5. Poynting's theorem

Multiplying (1.1) by $\mathbf{E}$, and (1.2) by $\mathbf{H}$, we obtain:

$$(\mathbf{E}, \mathrm{rot}\,\mathbf{H}) = \frac{1}{c}\left(\mathbf{E}, \frac{\partial \mathbf{D}}{\partial t}\right) + \frac{4\pi}{c}(\mathbf{E}, \mathbf{j}),$$

$$(\mathbf{H}, \mathrm{rot}\,\mathbf{E}) = -\frac{1}{c}\left(\mathbf{H}, \frac{\partial \mathbf{B}}{\partial t}\right).$$

Subtracting the second equation from the first, we obtain the Poynting theorem [1], in which

$$\mathrm{div}[\mathbf{E}, \mathbf{H}] = -\frac{1}{c}\left(\left(\mathbf{H}, \frac{\partial \mathbf{B}}{\partial t}\right) - \left(\mathbf{E}, \frac{\partial \mathbf{D}}{\partial t}\right)\right) - \frac{4\pi}{c}(\mathbf{j}, \mathbf{E}). \tag{1.19}$$

In the integral form

$$\frac{c}{4\pi}\oint_S ([\mathbf{E}, \mathbf{H}], \mathbf{n})\,ds = -\frac{1}{4\pi}\int_V \left(\left(\mathbf{H}, \frac{\partial \mathbf{B}}{\partial t}\right) + \left(\mathbf{E}, \frac{\partial \mathbf{D}}{\partial t}\right)\right) dv - \int_V (\mathbf{j}, \mathbf{E})\,dv \tag{1.20}$$

we have the energy balance equation of the electromagnetic field in the volume V. The energy in the volume V is $W = \dfrac{1}{8\pi}\displaystyle\int_V ((\mathbf{H}, \mathbf{B}) + (\mathbf{E}, \mathbf{D}))\,dv$, the consumed power

$P = \int\limits_V (\mathbf{j}, \mathbf{E})\, dv$, and $\mathbf{\Pi} = \frac{c}{4\pi}[\mathbf{E}, \mathbf{H}]$ is the Umov–Poynting vector indicating the direction of energy movement and equal in magnitude to the density of its flux.

The monochromatic field is described using the complex Umov–Poynting vector $\mathbf{\Pi} = \frac{c}{8\pi}\left[\mathbf{E}, \mathbf{H}^*\right]$, where the asterisk denotes complex conjugation, and the average value of the Umov–Poynting is equal to the real part of the complex.

1.2. Differential equations of optics

1.2.1. The wave equation

In Maxwell‘s equations, we eliminate from consideration the currents and charges which usually absent in the problems of optics. Then, equations (1.1) and (1.2) take the form:

$$\operatorname{rot} \mathbf{H} = \frac{\varepsilon}{c} \frac{\partial \mathbf{E}}{\partial t}, \tag{1.21}$$

$$\operatorname{rot} \mathbf{E} = \frac{\mu}{c} \frac{\partial \mathbf{H}}{\partial t}. \tag{1.22}$$

Divide both sides of (1.22) by μ and apply the operator rot

$$\operatorname{rot}\left(\frac{1}{\mu} rot \mathbf{E}\right) + \frac{1}{c} \operatorname{rot} \frac{\partial \mathbf{H}}{\partial t} = 0. \tag{1.23}$$

Equation (1.21) is differentiable with respect to time in order to eliminate the second term of equation (1.23):

$$\operatorname{rot}\left(\frac{1}{\mu} \operatorname{rot} \mathbf{E}\right) + \frac{\varepsilon}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0.$$

Then, given that

$$\operatorname{rot} \alpha u = \alpha \operatorname{rot} u + \left[\operatorname{grad} \alpha, u\right] \text{ and}$$

we obtain:

$$\nabla^2 \mathbf{E} - \frac{\varepsilon\mu}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \left(\operatorname{grad}\left(\ln \mu\right)\right) \times \operatorname{rot} \mathbf{E} - \operatorname{grad} \operatorname{div} \mathbf{E} = 0 \tag{1.24}$$

To the equation div(ε**E**) = 0 we apply the identity div αu = α div u + (u, grad α),and obtain ε div **E** + (**E**, grad ε) = 0. Expressing from the last equation divE, we substitute it into (1.24), writing the wave equation [1] for the electric field in an inhomogeneous dielectric medium

$$\nabla^2 \mathbf{E} - \frac{\varepsilon\mu}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \left[\operatorname{grad}\left(\ln \mu\right), \operatorname{rot} \mathbf{E}\right] + \operatorname{grad}\left(\mathbf{E}, \operatorname{grad}\left(\ln \varepsilon\right)\right) = 0. \tag{1.25}$$

Similarly, we obtain the wave equation for the magnetic field vector **H**:

$$\nabla^2 \mathbf{H} - \frac{\varepsilon\mu}{c^2}\frac{\partial^2 \mathbf{H}}{\partial t^2} + \left[\operatorname{grad}\left(\ln\varepsilon\right),\ \operatorname{rot}\mathbf{H}\right] + \operatorname{grad}\left(\mathbf{H},\ \operatorname{grad}\left(\ln\mu\right)\right) = 0. \tag{1.26}$$

For a homogeneous medium, electric ε and magnetic μ permeability are constant and the wave equations take the form

$$\nabla^2 \mathbf{E} - \frac{\varepsilon\mu}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} = 0, \tag{1.27}$$

$$\nabla^2 \mathbf{H} - \frac{\varepsilon\mu}{c^2}\frac{\partial^2 \mathbf{H}}{\partial t^2} = 0. \tag{1.28}$$

1.2.2. Helmholtz equations

The wave equations written for the complex amplitudes (monochromatic waves), called the Helmholtz equation. For an inhomogeneous medium, they have the form:

$$\nabla^2 \mathbf{E} + k_0^2 \varepsilon\mu\mathbf{E} + \left[\operatorname{grad}\left(\ln\mu\right), \operatorname{rot}\mathbf{E}\right] + \operatorname{grad}\left(\mathbf{E},\ \operatorname{grad}\left(\ln\varepsilon\right)\right) = 0, \tag{1.29}$$

$$\nabla^2 \mathbf{H} + k_0^2 \varepsilon\mu\mathbf{H} + \left[\operatorname{grad}\left(\ln\varepsilon\right), \operatorname{rot}\mathbf{H}\right] + \operatorname{grad}\left(\mathbf{H}, \operatorname{grad}\left(\ln\mu\right)\right) = 0, \tag{1.30}$$

and for a homogeneous one

$$\nabla^2 \mathbf{E} + k_0^2 \varepsilon\mu\mathbf{E} = 0, \tag{1.31}$$

$$\nabla^2 \mathbf{H} + k_0^2 \varepsilon\mu\mathbf{H} = 0. \tag{1.32}$$

Equations (1.31) and (1.32) can be solved independently for each projection of the electric and magnetic vectors **E** and **H**, and these projections can be described by a single scalar function U:

$$\nabla^2 U + k_0^2 \varepsilon\mu U = 0. \tag{1.33}$$

1.2.3. The Fock–Leontovich equation

We represent the function U as $U = U \exp(ik_0 z)$ and substitute it into equation (1.33) for the vacuum. Assuming that $\left|\frac{\partial^2 U}{\partial z^2}\right| << k_0 \left|\frac{\partial U}{\partial z}\right|$, we obtain the Fock–Leontovich parabolic wave equation

$$2ik_0 \frac{\partial U}{\partial z} + \Delta_\perp U = 0, \tag{1.34}$$

where $\Delta_\perp U = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}$.

The parabolic equation (1.34) in the scalar optics is used to describe paraxial optical fields, which are distributed mainly along a certain direction in space in a small solid angle.

1.2.4. Eikonal and transport equations

We write the function U as $U = U_0 \exp(ik_0\psi)$, where $\psi = \psi(x, y, z)$ – eikonal, U_0 is the amplitude (real function). Substituting it into (1.33), we obtain:

$$\frac{\partial^2 U_0}{\partial x^2}+\frac{\partial U^2{}_0}{\partial y^2}+\frac{\partial^2 U_0}{\partial z^2}+2ik_0\left(\frac{\partial \psi}{\partial x}\frac{\partial U_0}{\partial x}+\frac{\partial \psi}{\partial y}\frac{\partial U_0}{\partial y}+\frac{\partial \psi}{\partial z}\frac{\partial U_0}{\partial z}\right)+$$
$$ik_0 U_0\left(\frac{\partial^2 \psi}{\partial x^2}+\frac{\partial^2 \psi}{\partial y^2}+\frac{\partial^2 \psi}{\partial z^2}\right)-$$
$$-k_0^2 U_0\left(\left(\frac{\partial \psi}{\partial x}\right)^2+\left(\frac{\partial \psi}{\partial y}\right)^2+\left(\frac{\partial \psi}{\partial z}\right)^2\right)+k_0^2\varepsilon\mu U_0=0.$$

Equating to zero the imaginary part, we obtain the transport equation:

$$2\left(\frac{\partial \psi}{\partial x}\frac{\partial U_0}{\partial x}+\frac{\partial \psi}{\partial y}\frac{\partial U_0}{\partial y}+\frac{\partial \psi}{\partial z}\frac{\partial U_0}{\partial z}\right)+U_0\left(\frac{\partial^2 \psi}{\partial x^2}+\frac{\partial^2 \psi}{\partial y^2}+\frac{\partial^2 \psi}{\partial z^2}\right)=0. \quad (1.35)$$

The remaining terms amount to the following equation:

$$\frac{1}{k_0^2}\left(\frac{\partial^2 U_0}{\partial x^2}+\frac{\partial U^2{}_0}{\partial y^2}+\frac{\partial^2 U_0}{\partial z^2}\right)-U_0\left(\left(\frac{\partial \psi}{\partial x}\right)^2+\left(\frac{\partial \psi}{\partial y}\right)^2+\left(\frac{\partial \psi}{\partial z}\right)^2\right)+\varepsilon\mu U_0=0,$$

from which, putting $\lambda \to 0$ (geometrical optics approximation), we obtain the eikonal equation,

$$\left(\frac{\partial \psi}{\partial x}\right)^2+\left(\frac{\partial \psi}{\partial y}\right)^2+\left(\frac{\partial \psi}{\partial z}\right)^2=n^2, \quad (1.36)$$

where $n=\sqrt{\varepsilon\mu}$ is the refractive index of the medium.

1.3. Integral theorems of optics

Analysis of the electromagnetic field can be carried out not only by means of differential equations of Maxwell, Helmholtz, and others, but also with the help of equivalent integral equations and transformations. In this case, the Maxwell equations for monochromatic light in a homogeneous region of space are equivalent to the Stratton–Chu vector integral equations. The solution of the differential Helmholtz equation is convenient to study with the help of the Kirchhoff–Helmholtz integral expression (third Green's formula), and the Fock–Leontovich paraxial equation is equivalent to the Fresnel integral transform.

1.3.1. Green's formulas

For two continuous functions unctions $u(x, y, z)$ and $v(x, y, z)$ together with their derivatives in region V, bounded by a piecewise smooth surface S, there is the second Green formula [1]:

$$\int_V (u\Delta v - v\Delta u)dV = \oint_S (u\frac{\partial v}{\partial \mathrm{n}} - v\frac{\partial u}{\partial \mathrm{n}})dS. \quad (1.37)$$

where n is the vector of the outer normal to surface S, $\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplace operator or Laplacian.

With the help of Green's formula (1.37) the solution of the Helmholtz equation at interior points of a homogeneous region V can be expressed in terms of values of the solution and its derivatives on the boundary S using the third Greens formula (Helmholtz–Kirchhoff integral [2])

$$u(x) = \frac{1}{4\pi}\oint_S \left\{ \frac{\partial u(x')}{\partial n}\frac{e^{ikR}}{R} - u(x')\frac{\partial}{\partial n}\left(\frac{e^{ikR}}{R}\right)\right\} dS, \quad (1.38)$$

where R is the distance between points $\mathbf{x} \in V$ and $\mathbf{x}'\in S$, $u\ (x, y, z)$ is the solution of the Helmholtz equation in a homogeneous space

$$(\Delta + k^2)u(x, y, z) = 0,$$

$k = 2\pi/\lambda$ is thewave number of light with wavelength λ

The function

$$G = \frac{e^{ikR}}{4\pi R} \quad (1.39)$$

describes a spherical wave, is the Green function of a homogeneous space and satisfies the inhomogeneous Helmholtz equation with a point source

$$(\Delta + k^2)G(x, x') = \delta(x - x'). \quad (1.40)$$

In regions of space with a constant refractive index and without sources, the integral representation (1.38) holds for any Cartesian component of the vector of the strength of the electric field

$$\mathbf{E}(\mathbf{x}) = \frac{1}{4\pi}\oint_S \left\{ \frac{\partial \mathbf{E}(\mathbf{x}')}{\partial \mathbf{n}}\frac{\mathrm{e}^{ikR}}{R} - \mathbf{E}(\mathbf{x}')\frac{\partial}{\partial \mathbf{n}}\left(\frac{\mathrm{e}^{ikR}}{R}\right)\right\} dS. \quad (1.41)$$

Diffraction of scalar waves on a dielectric object

For example, consider the scalar problem of diffraction of electromagnetic waves in a homogeneous dielectric object [3]. Let the function $E_1(x)$ and $E_2\ (x)$ satisfy the two Helmholtz equations inside the region V (inside the object) and on the outside:

$$\begin{aligned} &(\Delta + k_1^2)E_1(\mathbf{x}) = 0, \quad \mathbf{x} \in V, \\ &(\Delta + k_2^2)E_2(\mathbf{x}) = -g, \quad \mathbf{x} \notin V + S \end{aligned} \quad (1.42)$$

the boundary conditions

$$E_1(\mathbf{x})|_S = E_2(\mathbf{x})|_S, \quad (1.43)$$

$$\frac{\partial E_1(\mathbf{x})}{\partial \mathbf{n}}\Big|_S = \frac{\partial E_2(\mathbf{x})}{\partial \mathbf{n}}\Big|_S$$

and the Sommerfeld radiation conditions at infinity

$$\frac{\partial E_2(\mathbf{x})}{\partial \mathbf{n}} - ik_2 E_2(\mathbf{x}) = o\left(\frac{1}{r}\right), \quad r \to \infty. \tag{1.44}$$

where $o(x)$ is a function whose order of magnitude is larger than x when $x \to 0$.

In equations (1.42), the function g describes the density of light sources outside the region V, occupied by an object; there are no sources within the object. With the help of Green's theorem (1.37) and (1.38) the solution of (1.42) with the conditions taken into account (1.43) and (1.44) can be reduced to solving a Fredholm integral equation of the second kind

$$E_1(\mathbf{x}) = \frac{k_1^2 - k_2^2}{4\pi} \int_V E_1(\mathbf{x}') \frac{e^{ik_2 R}}{R} dV + \frac{1}{4\pi} \int_{V'} g(\mathbf{y}) \frac{e^{ik_2 R}}{R} dV, \quad \mathbf{x} \in V, \tag{1.45}$$

where $\mathbf{x}$ and $\mathbf{x}'$ belong to the object region V, and point $\mathbf{y}$ belongs to V', external to the region V. The second term in equation (1.45) describes the complex amplitude of the light incident on the object field, which in diffraction problems can be regarded as a known function:

$$E_0(\mathbf{x}) = \frac{1}{4\pi} \int_{V'} g(\mathbf{y}) \frac{e^{ik_2 R}}{R} dV. \tag{1.46}$$

Solving the equation (1.45), the diffraction field outside the object (in region V') we find, using the integral transform

$$E_2(\mathbf{x}) = \frac{k_1^2 - k_2^2}{4\pi} \int_V E_1(\mathbf{x}') \frac{e^{ik_2 R}}{R} dV + E_0(\mathbf{x}), \quad \mathbf{x} \in V'. \tag{1.47}$$

Equations (1.45) and (1.47) for the two-dimensional problem ($\partial/\partial z = 0$) have the form:

$$E_1(x,y) = \frac{i(k_1^2 - k_2^2)}{4} \int_V E_1(x',y') H_0^{(2)}(k_2 r) dV + E_0(x,y), \quad (x,y) \in V,$$
$$r = \left[(x-x')^2 + (y-y')^2\right]^{1/2}, \tag{1.48}$$

$$E_2(x,y) = \frac{i(k_1^2 - k_2^2)}{4} \int_V E_1(x',y') H_0^{(2)}(k_2 r) dV + E_0(x,y), \quad (x,y) \in V', \tag{1.49}$$

where $H_0^{(2)}(x)$ is the Hankel function of second kind of zeroth order, $G(x, y; x', y') = i/4 H_0^{(2)}(kr)$ is the Green function of a homogeneous space for a two-dimensional Helmholtz equation.

Equations (1.48) and (1.49) solve the problem of diffraction of a cylindrical (two-dimensional) electromagnetic wave with TE polarization (E_0, E_1 and E_2 are projections on the z-axis of the vectors of strength of the electric field) on a uniform cylindrical dielectric object. Similar formulas for TM polarization can be found in [3].

1.3.2. Stratton–Chu formula

Green vector formulas can be derived by the same procedure by Green's scalar formulas (1.37) and (1.38). The Gauss–Ostrogradskii equation is used:

$$\int_V \operatorname{div}\mathbf{F} dV = \oint_S \mathbf{F}\mathbf{n} dS. \tag{1.50}$$

If the vector field $\mathbf{F}$ as a vector product $\mathbf{F} = [\mathbf{P}, \operatorname{rot} \mathbf{Q}]$ is substituted into (1.50), we can obtain the vector analogue of Green's second formula:

$$\int_V \left(\mathbf{Q} \text{ rot rot } \mathbf{P} - \mathbf{P} \text{ rot rot } \mathbf{Q}\right) d = \oint_S \left\{\left[\mathbf{P}, \text{ rot } \mathbf{Q}\right] - \left[\mathbf{Q}, \text{rot } \mathbf{P}\right]\right\} \mathbf{n}\, dS. \tag{1.51}$$

Given the known vector relations

$$\begin{aligned}&\mathbf{Q} \text{ rot rot } \mathbf{P} - \mathbf{P} \text{ rot rot } \mathbf{Q} = \mathbf{P}\Delta Q - \mathbf{Q}\Delta\mathbf{P} + \mathbf{Q} \text{ grad div } \mathbf{P} - \mathbf{P} \text{ grad di} v\, \mathbf{Q} = \\ &= \mathbf{P}\Delta\mathbf{Q} - \mathbf{Q}\Delta\mathbf{P} + \operatorname{div}\left(\mathbf{Q} \operatorname{div} \mathbf{P} - \mathbf{P} \operatorname{div} \mathbf{Q}\right)\end{aligned}$$

equation (1.51) can be rewritten as:

$$\int_V \left(\mathbf{P}\Delta\mathbf{Q} - \mathbf{Q}\Delta\mathbf{P}\right) \mathrm{d}\, V = \oint_S \left\{\mathbf{n}\left[\mathbf{P}, \text{rot } \mathbf{Q}\right] - \mathbf{n}\left[\mathbf{Q}, \text{ rot } \mathbf{P}\right] + \mathbf{n}\mathbf{P} \operatorname{div} \mathbf{Q} - \mathbf{n}\mathbf{Q} \operatorname{div} \mathbf{P}\right\} \mathrm{d}\, S, \tag{1.52}$$

From (1.51) and (1.52) we can easily obtain the integral relations for the electromagnetic field in space. Suppose $\mathbf{P} = \mathbf{E}$, $\mathbf{Q} = \mathbf{a}G$. $G(\mathbf{x} - \mathbf{x}_0) = \exp(ikR)/R$, $\mathbf{a}$ is the unit vector of arbitrary direction, where $R = |\mathbf{x} - \mathbf{x}_0|$, $\mathbf{x}$ is the radius vector of the observation point, $\mathbf{x}_0$ is a point on the surface S. In this case, the function $\mathbf{Q}$ satisfies the vector Helmholtz equation with a point source:

$$\Delta\mathbf{Q} + k^2\mathbf{Q} = -4\pi\mathbf{a}\delta(\mathbf{x} - \mathbf{x}_0), \tag{1.53}$$

where $\operatorname{rot}\mathbf{Q} = \left[\text{grad } G, \ \mathbf{a}\right]$, $\operatorname{div}\mathbf{Q} = (\mathbf{a}, \text{ grad } G)$, $k^2 = \omega^2\varepsilon\mu/c^2$.

The vector of the strength of the electric and magnetic fields of the monochromatic light wave in a homogeneous and isotropic space satisfy the inhomogeneous Helmholtz equations:

$$\begin{aligned}&\Delta\mathbf{E} + \frac{\omega^2\varepsilon\mu}{c^2}\mathbf{E} = -4\pi\mathbf{J}_2, \\ &\mathbf{J}_2 = \frac{i\omega\mu}{c^2}\mathbf{j} + \frac{i \text{grad div } \mathbf{j}}{\omega\varepsilon}, \\ &\Delta\mathbf{H} + \frac{\omega^2\varepsilon\mu}{c^2}\mathbf{H} = -\text{rot}\,\mathbf{j},\end{aligned} \tag{1.54}$$

where $\mathbf{j}$ the density of secondary electric current, ω is the cyclic oscillation frequency of monochromatic light, ε, μ is the dielectric constant and magnetic permeability of the homogeneous medium, c is the speed of light in vacuum.

Using (1.52)–(1.54) and the formula $(\mathbf{n}, [\mathbf{E}, [\text{grad } G, \mathbf{a}]]) = (\mathbf{a}, [\text{grad } G, [\mathbf{E}, \mathbf{n}]])$, we obtain the expression:

$$\mathbf{E}(x)\mathbf{a} = \mathbf{a}\left\{ \int_{?} \mathbf{J}_2(\mathbf{x}_0)\, G(\mathbf{x}-\mathbf{x}_0)\, dV + \frac{1}{4\pi} \oint_S \left\{ \mathbf{n}\, G(\mathbf{x}-\mathbf{x}_0)\, \mathrm{div}_0\, \mathbf{E}(\mathbf{x}_0) \right\} dS + \right.$$

$$+ \frac{1}{4\pi} \oint_S \left\{ \left[\mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0), \left[\mathbf{n}, \mathbf{E}(\mathbf{x}_0)\right]\right] + \left[\mathrm{rot}_0\, \mathbf{E}(\mathbf{x}_0), \mathbf{n}\right] G(\mathbf{x}-\mathbf{x}_0) - \right.$$

$$\left. \left. - \mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0)\left(\mathbf{n}, \mathbf{E}(\mathbf{x}_0)\right) \right\} dS \right\}. \tag{1.55}$$

Given that div $\mathbf{E} = 0$, and the arbitrariness of the vector $\mathbf{a}$, we obtain the integral representation

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}) +$$

$$+ \frac{1}{4\pi} \oint_S \left\{ \left[\mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0), \left[\mathbf{n}, \mathbf{E}\right]\right] + \left[\mathrm{rot}_0\, \mathbf{E}, \mathbf{n}\right] G(\mathbf{x}-\mathbf{x}_0) - \mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0)\left(\mathbf{nE}\right) \right\} dS, \tag{1.56}$$

where

$$\mathbf{E}_0(\mathbf{x}) = \int_{?} \mathbf{J}_2(\mathbf{x}_0)\, G(\mathbf{x}-\mathbf{x}_0)\, dV.$$

By analogy with (1.56) we can obtain an integral representation for the magnetic field

$$\mathbf{H}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x}) + \frac{1}{4\pi} \times$$

$$\times \oint_S \left\{ \left[\mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0), \left[\mathbf{n}, \mathbf{H}(x_0)\right]\right] + \left[\mathrm{rot}_0\, \mathbf{H}(\mathbf{x}_0), \mathbf{n}\right] G(\mathbf{x}-\mathbf{x}_0) - \mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0)\left(\mathbf{nH}(\mathbf{x}_0)\right) \right\} \mathrm{d}S, \tag{1.57}$$

where $\mathbf{H}_0(\mathbf{x}) = \dfrac{1}{4\pi} \displaystyle\int_{?} \mathrm{rot}\ \mathbf{j}\ G(\mathbf{x}-\mathbf{x}_0)\, dV.$

In (1.56) and (1.57) $\mathbf{E}_0(\mathbf{x})$ and $\mathbf{H}_0(\mathbf{x})$ are the strengths of the electric and magnetic fields in the incident wave.

Equations (1.56) and (1.57) are called the Stratton–Chu formulas.

Diffraction on a perfectly reflecting object

For example, consider the solution of a problem of electromagnetic wave diffraction by an ideally reflecting object, which occupies a region of space V, with the surface S.

We introduce the notation for the surface density of electric and magnetic currents: $(4\pi/c)\mathbf{j}_e(\mathbf{x}_0) = [\mathbf{n}, \mathbf{H}(\mathbf{x}_0)]$, $(4\pi/c)\mathbf{j}_m(\mathbf{x}_0) = [\mathbf{n}, \mathbf{E}(\mathbf{x}_0)]$. We take into account that rot $(\Phi\mathbf{F}) = \Phi$ rot $\mathbf{F}$ +[grad Φ, $\mathbf{F}$], rot $j_m(\mathbf{x}_0) = 0$, rot $\mathbf{E} = ik\mathbf{H}$, where $k = \dfrac{\omega}{c}\sqrt{\varepsilon\mu}$,

$$\left[\mathrm{grad}_0\, G(\mathbf{x}-\mathbf{x}_0),\, \mathrm{j}_m(\mathbf{x}_0)\right] = -\left[\mathrm{grad}\ G(\mathbf{x}-\mathbf{x}_0),\, \mathrm{j}_m(\mathbf{x}_0)\right] =$$

$$= -\mathrm{rot}\left(G(\mathbf{x}-\mathbf{x}_0)\mathrm{j}_m(\mathbf{x}_0)\right) + G(\mathbf{x}-\mathbf{x}_0)\ \mathrm{rot}\ \mathrm{j}_m(\mathbf{x}_0).$$

As a result, instead of (1.56) we obtain the following representation for the electric field

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}) - \frac{1}{4\pi}\,\text{rot} \oint_S \mathrm{j}_m(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\;\mathrm{d}S - \\ - \frac{\mathrm{i}k}{4\pi} \oint_S \mathrm{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\;\mathrm{d}S + \frac{1}{4\pi}\,\text{grad} \oint_S G(\mathbf{x}-\mathbf{x}_0)\;(\mathbf{n},\mathbf{E}(\mathbf{x}_0))\,\mathrm{d}S. \tag{1.58}$$

Applying the operation rot to both sides of (1.58) and taking into account that rot (grad Φ) = 0, we obtain the following representation for the magnetic field:

$$\mathbf{H}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x}) - \frac{1}{4\pi ik}\,\text{rot rot} \oint_S \mathbf{j}_m(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\,dS - \frac{1}{4\pi}\,\text{rot} \oint_S \mathbf{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\; dS. \tag{1.59}$$

From equation (1.57) by analogy we obtain an integral representation for the electric field

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}) + \frac{1}{4\pi ik}\,\text{rot rot} \oint_S \mathbf{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\,dS - \frac{1}{4\pi}\,\text{rot} \oint_S \mathbf{j}_m(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\; dS. \tag{1.60}$$

Given the boundary conditions on the perfectly conducting surface $[\mathbf{n},\mathbf{E}] = 0$, $(\mathbf{n}, \mathbf{H}) = 0$, equations (1.59) and (1.60) can be rewritten as:

$$\mathbf{H}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x}) - \frac{1}{4\pi}\,\text{rot} \oint_S \mathbf{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\; dS, \tag{1.61}$$

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}) + \frac{1}{4\pi ik}\,\text{rot rot} \oint_S \mathbf{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\; dS. \tag{1.62}$$

To obtain an integral equation of the first kind for the electric current density on the surface of an ideal conductor, we assume that the vector **x** belongs to the surface. Multiplying (1.61) by the vector of the normal at point **x** and taking into account the boundary condition for a perfect conductor, we obtain the integral equation:

$$\left[\mathbf{E}_0(\mathbf{x}),\mathbf{n}(\mathbf{x})\right] = -\frac{1}{4\pi ik}\,\text{rot rot} \oint_S \left[\mathbf{j}_e(\mathbf{x}_0),\,\mathbf{n}(\mathbf{x})\right] G(\mathbf{x}-\mathbf{x}_0)\; dS. \tag{1.63}$$

Thus, the problem of finding the electromagnetic field is divided into two stages:

1) the solution of the integral equation (1.63) with respect $\mathbf{j}_e(\mathbf{x}_0)$;
2) the calculation of the field components from (1.61) and (1.62).

From equation (1.61) we can similarly obtain the Fredholm integral equation of the first kind for the unknown current density on the surface S in terms of known values of the magnetic field of the incident wave:

$$\mathbf{H}_0(\mathbf{x}) = \frac{1}{4\pi}\,\text{rot} \oint_S \mathbf{j}_e(\mathbf{x}_0)\; G(\mathbf{x}-\mathbf{x}_0)\; dS, \quad \mathbf{x} \in S. \tag{1.64}$$

Diffraction on a transmitting object

Consider the solution of the problem of diffraction of an electromagnetic monochromatic wave on a homogeneous dielectric object. For this we consider Maxwell's equations in a homogeneous area of the object V_1 with the characteristics ε_1 and μ and also in the outer region V_2 with the characteristics of the medium ε_2 and μ:

$$\begin{aligned} \mathrm{rot}\mathbf{H}_1 &= -i\frac{\omega\varepsilon_1}{c}\mathbf{E}_1 , \\ \mathrm{rot}\mathbf{E}_1 &= i\frac{\omega\mu}{c}\mathbf{H}_1 , \quad \mathbf{x}\in V_1 , \end{aligned} \tag{1.65}$$

$$\begin{aligned} \mathrm{rot}\mathbf{H}_2 &= -i\frac{\omega\varepsilon_2}{c}\mathbf{E}_2 + \frac{4\pi}{c}\mathbf{j} , \\ \mathrm{rot}\mathbf{E}_2 &= i\frac{\omega\mu}{c}\mathbf{H}_2 , \quad \mathbf{x}\in V_2 , \end{aligned} \tag{1.66}$$

with the boundary conditions on the surface S of the interface of the media V_1 and V_2

$$\begin{aligned} [\mathbf{n},\mathbf{E}_1] \,\big|_S &= [\mathbf{n},\mathbf{E}_2] \,\big|_S , \\ [\mathbf{n},\mathbf{H}_1] \,\big|_S &= [\mathbf{n},\mathbf{H}_2] \,\big|_S , \end{aligned} \tag{1.67}$$

and with the radiation condition at infinity

$$[\mathbf{n},\mathbf{E}_2]+[\mathbf{n}[\mathbf{n},\mathbf{H}_2]] = o\left(\frac{1}{r}\right), \quad r\to\infty \tag{1.68}$$

With the Green's vector formula (1.52) we can obtain a Fredholm integral equation of the second kind for the magnetic field strength

$$\begin{aligned} \mathbf{H}_1(\mathbf{x}) &= \frac{\varepsilon_2}{4\pi\,\varepsilon_1}\int\limits_{V_2} G(\mathbf{x}-\mathbf{x}_0)\mathrm{rot}\mathbf{j}\,dV + \frac{\omega^2\mu(\varepsilon_2-\varepsilon_1)}{4\pi\,c^2}\int\limits_{V_1} G(\mathbf{x}-\mathbf{x}_0)\,\mathbf{H}_1(\mathbf{x}_0)dV + \\ &+\frac{\varepsilon_2-\varepsilon_1}{4\pi\,\varepsilon_1}\oint\limits_S \left\{[\mathrm{grad}G(\mathbf{x}-\mathbf{x}_0)[\mathbf{n},\mathbf{H}_1]] - (\mathbf{n},\mathbf{H}_1)\mathrm{grad}G(\mathbf{x}-\mathbf{x}_0)\right\}dS, \quad \mathbf{x}\in V_1. \end{aligned} \tag{1.69}$$

The first term in equation (1.69) can be regarded as a known field incident on the object

$$\mathbf{H}_0(\mathbf{x}) = \frac{\varepsilon_2}{4\pi\varepsilon_1}\int\limits_{V_2} G(\mathbf{x}-\mathbf{x}_0)\mathrm{rot}\mathbf{j}\,dV,$$

and the impulse response function $G(\mathbf{x}–\mathbf{x}_0)$ satisfies the equation (1.53).

The magnetic field in the outer region V_2 after solving (1.69) is determined by the integral transform

$$\begin{aligned} \mathbf{H}_2(\mathbf{x}) &= \mathbf{H}_0(\mathbf{x}) + \frac{\omega^2\varepsilon_1\mu(\varepsilon_2-\varepsilon_1)}{4\pi\,c^2\varepsilon_2}\int\limits_{V_1} G(\mathbf{x}-\mathbf{x}_0)\,\mathbf{H}_1(\mathbf{x}_0)dV + \\ &+\frac{\varepsilon_2-\varepsilon_1}{4\pi\,\varepsilon_2}\oint\limits_S \left\{[\mathrm{grad}G(\mathbf{x}-\mathbf{x}_0)[\mathbf{n},\mathbf{H}_1]] - (\mathbf{n},\mathbf{H}_1)\mathrm{grad}G(\mathbf{x}-\mathbf{x}_0)\right\}dS, \quad \mathbf{x}\in V_2. \end{aligned} \tag{1.70}$$

The strengths of the electric field $\mathbf{E}_1$ and $\mathbf{E}_2$ are located across the known functions of $\mathbf{H}_1$ and $\mathbf{H}_2$ from the Maxwell equations (1.65) and (1.66).

Instead of (1.69) and (1.70), to find the magnetic field of diffraction we can use Green's vector formula (1.52) to obtain the Fredholm integral equation of the second kind to find the electric vector of the diffraction field

$$\begin{aligned}\mathbf{E}_1(\mathbf{x}) &= \frac{-\varepsilon_2}{4\pi\,\varepsilon_1}\int\limits_{V_2} G(\mathbf{x}-\mathbf{x}_0)\left\{\frac{i\omega\mu}{c^2}\mathbf{j}-\frac{i}{\omega\varepsilon_1}\operatorname{grad}\operatorname{div}\mathbf{j}\right\}dV - \\ &-\frac{\omega^2\mu(\varepsilon_2-\varepsilon_1)}{4\pi\,c^2}\int\limits_{V_1} G(\mathbf{x}-\mathbf{x}_0)\,\mathbf{E}_1(\mathbf{x}_0)dV + \\ &+\frac{\varepsilon_2-\varepsilon_1}{4\pi\,\varepsilon_1}\oint\limits_{S}\left\{[\operatorname{grad}G(\mathbf{x}-\mathbf{x}_0)[\mathbf{n},\mathbf{E}_1]]-(\mathbf{n},\mathbf{E}_1)\operatorname{grad}G(\mathbf{x}-\mathbf{x}_0)\right\}dS, \quad \mathbf{x}\in V_1,\end{aligned} \tag{1.71}$$

where the known vector of the strength of the electric field of the incident wave is expressed in terms of current density in the outer region:

$$\mathbf{E}_0(\mathbf{x}) = \frac{-\varepsilon_2}{4\pi\varepsilon_1}\int\limits_{V_2}\left\{\frac{i\omega\mu}{c^2}\mathbf{j}-\frac{i}{\omega\varepsilon_1}\operatorname{grad}\operatorname{div}\mathbf{j}\right\}G(\mathbf{x}-\mathbf{x}_0)dV. \tag{1.72}$$

The vector of the strength electric diffraction field in the outer region V_2 is found by solving (1.71) and the integral transformation

$$\begin{aligned}\mathbf{E}_2(\mathbf{x}) &= \mathbf{E}_0(\mathbf{x}) - \frac{\omega^2\varepsilon_1\mu(\varepsilon_2-\varepsilon_1)}{4\pi\,c^2\varepsilon_2}\int\limits_{V_1} G(\mathbf{x}-\mathbf{x}_0)\,\mathbf{E}_1(\mathbf{x}_0)dV + \\ &+\frac{\varepsilon_2-\varepsilon_1}{4\pi\,\varepsilon_2}\oint\limits_{S}\left\{[\operatorname{grad}G(\mathbf{x}-\mathbf{x}_0)[\mathbf{n},\mathbf{E}_1]]-(\mathbf{n},\mathbf{E}_1)\operatorname{grad}G(\mathbf{x}-\mathbf{x}_0)\right\}dS, \quad \mathbf{x}\in V_2.\end{aligned} \tag{1.73}$$

1.4. Integral transformations in optics

In the framework of the scalar theory of diffraction monochromatic light is described by the complex amplitude function $F(\mathbf{x}) = F(x, y, z)$, which satisfies the Helmholtz equation (1.33):

$$(\Delta + k^2)F(x,y,z) = 0, \tag{1.74}$$

where k is the wavenumber of the light. In a homogeneous and isotropic space without charges and currents the complex amplitude $F(\mathbf{x})$ can be represented by any projection of the vectors of the strength of electric $\mathbf{E}(\mathbf{x})$ and magnetic $\mathbf{H}(\mathbf{x})$ fields of the light wave.

Solving equation (1.74) by using the complex amplitude through the two-dimensional Fourier transform

$$F(x,y,z) = \int\int\limits_{-\infty}^{\infty} A(\alpha,\beta,z)\exp[-ik(x\alpha+y\beta)]d\alpha\, d\beta, \tag{1.75}$$

where $A(\alpha, \beta, z)$ is the amplitude of the spatial spectrum of plane waves, we can obtain the decomposition of the complex amplitude with respect to plane waves

$$F(x,y,z)=\int\int_{-\infty}^{\infty} A_0(\alpha\,,\beta)\exp[-ik(x\alpha+y\beta\pm z\sqrt{1-\alpha^2-\beta^2})]d\alpha\,d\beta, \quad (1.76)$$

where $A_0(\alpha, \beta) = A(\alpha, \beta, z = 0)$ is also the amplitude of the spatial spectrum of plane waves at $z = 0$. If we know the direction of light propagation, in the exponent in equation (1.76) we can leave only one sign (when the wave propagates along the z axis we select the plus sign).

We represent the function A0 (α,β) via the inverse Fourier transform

$$A_0(\alpha,\beta)=\frac{k^2}{2\pi}\int\int_{-\infty}^{\infty} F_0(x,y)\exp[ik(x\alpha+y\beta)dx\,dy. \quad (1.77)$$

From equations (1.76) and (1.77) follows the integral transformation of the complex amplitude of the light field [4]

$$F(x,y,z)=k^2\int\int_{-\infty}^{\infty} F_0(x',y')H(x-x',y-y',z)dx'dy', \quad (1.78)$$

where

$$H(x,y,z)=\frac{1}{2\pi}\int\int_{-\infty}^{\infty} \exp[-ik(x\alpha+y\beta\pm z\sqrt{1-\alpha^2-\beta^2})]d\alpha\,d\beta. \quad (1.79)$$

$H(x, y, z)$ is the pulse response function of the homogeneous space, $F_0(x,y)=F(x,y,z=0)$ is the complex amplitude of light at $z = 0$. If $\alpha^2+\beta^2>1$, then the integral exponential factor $\exp(-kz\sqrt{\alpha^2+\beta^2-1})$ appears to be described by the inhomogeneous surface waves that propagate in the plane $z = 0$ and at $z \gg \lambda$ not contributing to the light field. Therefore, if $z \gg \lambda$ the integral in (1.79) can be calculated not in infinite limits, and at $\alpha^2+\beta^2<1$.

1.4.1. Kirchhoff integral

Using the known expansion of the amplitude of a spherical wave in plane waves

$$\frac{e^{ikR}}{R}=ik\int\int_{-\infty}^{\infty} \frac{\exp\left[-ik(x\alpha+y\beta-z\sqrt{1-\alpha^2-\beta^2})\right]d\alpha\,d\beta}{\sqrt{1-\alpha^2-\beta^2}}. \quad (1.80)$$

where $R = (x^2 + y^2 + z^2)^{1/2}$ – the pulse response function, defined by equation (1.79) can be written as:

$$H(x,y,z)=-\frac{1}{2\pi k^2}\frac{\partial}{\partial z}\left(\frac{e^{ikR}}{R}\right)=\frac{e^{ikR}}{R}\frac{\partial R}{\partial z}\left(R^{-2}-ik\right). \quad (1.81)$$

If we assume that the distance from the plane $z = 0$ to the plane of observation z is much greater than the wavelength of $R \gg \lambda$, $z \gg \lambda$, then instead of (1.81) we can approximately assume that the following equality is satisfied

$$H(x,y,z) = -ik\frac{e^{ikR}}{R}\frac{z}{R}. \tag{1.82}$$

Then, instead of the integral transform (1.79) we obtain the Kirchhoff integral

$$F(x,y,z) = \frac{-ik}{2\pi}\int_{-\infty}^{\infty}\int F_0(x',y')\frac{e^{ikR}}{R}\frac{z}{R}dx'dy', \tag{1.83}$$

where $R = [(x-x')^2 + (y-y')^2 + z^2]^{1/2}$. Sometimes, given the fact that $R \approx z$ instead of (1.83) the Kirchhoff integral is written as:

$$F(x,y,z) = \frac{-ik}{2\pi}\int_{-\infty}^{\infty}\int F_0(x',y')\frac{e^{ikR}}{R}dx'dy'. \tag{1.84}$$

The physical meaning of the Kirchhoff integral (1.84) is associated with the Huygens–Fresnel wave principle and consists in the fact that the Kirchhoff integral is an expansion of the complex amplitude of the light field in spherical waves.

1.4.2. Fresnel transform

Integral transforms (1.78) and (1.83) describe the propagation of non-paraxial optical fields in a homogeneous space along the axis z. To describe the propagation of paraxial optical fields that propagate in a small solid angle, we use the Fresnel integral transform.

The complex amplitude of the paraxial light field is represented as:

$$U(x,y,z) = e^{ikz}F(x,y,z). \tag{1.85}$$

and the slowly varying complex amplitude $F(x, y, z)$ satisfies the Fock–Leontovich parabolic equation (1.34) [2]

$$\left(2ik\frac{\partial}{\partial z} + \nabla_{xy}^2\right)F(x,y,z) = 0, \tag{1.86}$$

where $\nabla_{xy}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is the transverse Laplacian. Any solution of equation (1.86) can be written in integral form:

$$F(x,y,z) = \frac{-ik}{2\pi z}\int_{-\infty}^{\infty}\int F_0(\xi,\eta)\exp\left\{\frac{ik}{z}\left[(x-\xi)^2 + (y-\eta)^2\right]\right\}d\xi\, d\eta, \tag{1.87}$$

where $F_0(x, y, z) = F(x, y, z = 0)$.

The Fresnel transform (1.87) is the expansion of the paraxial light field on the parabolic waves, and it is easily obtained from the Kirchhoff integral (1.84), using a Taylor series expansion to the second term of the distance R in the exponent:

$$R = \left[(x-\xi)^2 + (y-\eta)^2 + z^2\right]^{1/2} \approx z + \frac{1}{2z}\left[(x-\xi)^2 + (y-\eta)^2\right].$$

The transition from the Kirchhoff integral (1.84) for the Fresnel integrals (1.87) is possible under the condition:

$$\frac{kr^4}{8z^3} << \pi,$$

where r is the effective radius of the light field.

At a considerable distance from the initial plane $z = 0$, when the conditions of the far zone of diffraction (or Fraunhofer diffraction zone)

$$\frac{kr^2}{2z} << \pi, \tag{1.88}$$

instead of the Fresnel integral transform (1.87) we can use the Fourier transform of the parabolic wave multiplier in front of the integral:

$$F(x,y,z) = \frac{-ik}{2\pi z}\exp[\frac{ik}{2z}(x^2+y^2)]\int_{-\infty}^{\infty}\int F_0(\xi,\eta)\exp[\frac{-ik}{z}(x\xi+y\eta)]d\xi\, d\eta. \tag{1.89}$$

The Fourier transform (1.89) is the expansion of paraxial optical fields on plane waves. The integral on the right-hand side of (1.89), written with the help of the spatial frequencies $u = k\xi/z$, $v = k\eta/z$, has the form of the normal Fourier integral:

$$F(x,y) = \int_{-\infty}^{\infty}\int F_0(u,v)\exp[-i(xu+yv)]dudv. \tag{1.90}$$

The Fourier transforms (1.89) and (1.90) also describe the complex amplitude of the light field in the plane of spatial frequencies of a thin spherical lens.

Conclusion

This chapter introduces the basic differential and integral equations, which are necessary for solving problems of the diffraction of electromagnetic waves. Based on the general system of differential equations for the vectors of electric and magnetic fields of the electromagnetic wave, the wave equation, the Helmholtz equation for monochromatic light, the Fock–Leontovich equation for the paraxial optical fields, as well as the eikonal equation describing the propagation of rays in geometrical optics were derive. Similarly, using the scalar and Green vector theorems, we derived the basic integral relations for the monochromatic electromagnetic field: the Stratton–Chu and Kirchhoff–Helmholtz formulas. We presented the basic Fredholm integral equations of the first and second kind for solving problems of the diffraction of a monochromatic electromagnetic wave by perfectly reflecting and homogeneous dielectric (transmitting) objects. For the scalar complex amplitude, which can be regarded as any of the projections of the vectors of the strength of the electric and magnetic fields, we discussed the widely used integral representations: field expansion in plane waves, the expansion in spherical waves (the Kirchhoff integral), the expansion of the parabolic waves (Fresnel transform).

Many of the relationships in this chapter are used in subsequent chapters for solving direct and inverse problems of diffractive nanophotonics. Chapter 2 presents difference methods for solving Maxwell's equations (variants of the

FDTD method) and finite difference methods for solving the wave equation (BPM-method). Chapter 3 discusses the solution of the Helmholtz equation based on the Galerkin finite element method and the solution of the integral Fredholm equation of the second type, which describes the diffraction of light by dielectric objects. Chapter 4 deals with the solution of the Helmholtz equation on the basis of the Fourier modes method, or the expansion of plane waves for periodic objects (RCWA method).Chapter 5 uses the solution of Maxwell's equations based on the difference FDTD-method in cylindrical coordinates. In Chapter 6 the Helmholtz equation is solved by the method of matched sinusoidal modes. Chapter 7 deals with the paraxial equation of propagation and uses Fresnel and Fourier transform to describe the propagation of laser beams. In Chapter 8, to calculate the force of light pressure on the microparticle, we use an iterative solution of the integral equation of diffraction obtained on the basis of Green's theorem.

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