CHAPTER 1

Introduction

We begin the book with a review of the basic physical problems that lead to the various equations we wish to solve.

1.1 HELMHOLTZ EQUATION

The *scalar* Helmholtz equation

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \qquad (1.1.1)$$

where $\psi(\mathbf{r})$ is a complex scalar function (potential) defined at a spatial point $\mathbf{r} = (x, y, z) \in \mathbb{R}^3$ and k is some real or complex constant, takes its name from Hermann von Helmholtz (1821–1894), the famous German scientist, whose impact on acoustics, hydrodynamics, and electromagnetics is hard to overestimate. This equation naturally appears from general conservation laws of physics and can be interpreted as a wave equation for monochromatic waves (wave equation in the frequency domain). The Helmholtz equation can also be derived from the heat conduction equation, Schrödinger equation, telegraph and other wave-type, or evolutionary, equations. From a mathematical point of view it appears also as an eigenvalue problem for the Laplace operator ∇^2. Below we show the derivation of this equation in several cases.

1.1.1 Acoustic waves

1.1.1.1 Barotropic fluids

The usual assumptions for acoustic problems are that acoustic waves are perturbations of the medium density $\rho(\mathbf{r}, t)$, pressure $p(\mathbf{r}, t)$, and velocity, $v(\mathbf{r}, t)$, where t is time. It is also assumed that the medium is inviscid, and that perturbations are small, so that:

$$\rho = \rho_0 + \rho', \qquad p = p_0 + p', \qquad \rho' \ll \rho_0, \qquad p' \ll p_0,$$
$$|\mathbf{v}'| \ll c \sim \sqrt{\frac{p_0}{\rho_0}}. \tag{1.1.2}$$

Here the perturbations are about an initial spatially uniform state (ρ_0, p_0) of the fluid at rest ($\mathbf{v}_0 = \mathbf{0}$) and are denoted by primes. The latter equation states that the velocity of the fluid is much smaller than the speed of sound c in that medium. In this case the linearized continuity (mass conservation) and momentum conservation equations can be written as:

$$\frac{\partial \rho'}{\partial t} + \nabla\cdot(\rho_0 \mathbf{v}') = 0, \qquad \rho_0 \frac{\partial \mathbf{v}'}{\partial t} + \nabla p' = 0, \tag{1.1.3}$$

where

$$\nabla = \mathbf{i}_x \frac{\partial}{\partial x} + \mathbf{i}_y \frac{\partial}{\partial y} + \mathbf{i}_z \frac{\partial}{\partial z}, \tag{1.1.4}$$

is the invariant "nabla" operator, represented by formula (1.1.4) in Cartesian coordinates, where $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$ are the Cartesian basis vectors.

Differentiating the former equation with respect to t and excluding from the obtained expression $\partial \mathbf{v}'/\partial t$ due to the latter equation, we obtain:

$$\frac{\partial^2 \rho'}{\partial t^2} = \nabla^2 p'. \tag{1.1.5}$$

Note now that system (1.1.3) is not closed since the number of variables (three components of velocity, pressure, and density) is larger than the number of equations. The relation needed to close the system is the equation of state, which relates perturbations of the pressure and density. The simplest form of this relation is provided by *barotropic* fluids, where the pressure is a function of density alone:

$$p = p(\rho). \tag{1.1.6}$$

We can expand this in the Taylor series near the unperturbed state:

$$p = p(\rho_0) + \left.\frac{dp}{d\rho}\right|_{\rho=\rho_0} (\rho - \rho_0) + O((\rho - \rho_0)^2). \tag{1.1.7}$$

Taking into account that $p(\rho_0) = p_0$ we, obtain, neglecting the second-order nonlinear term:

$$p' = c^2 \rho', \qquad c^2 = \left.\frac{dp}{d\rho}\right|_{\rho=\rho_0}, \tag{1.1.8}$$

where we used the definition of the speed of sound in the unperturbed fluid, which is a real positive constant (property of the fluid). Substitution of expression (1.1.8) into relation (1.1.5) yields the *wave equation* for pressure perturbations:

$$\frac{1}{c^2}\frac{\partial^2 p'}{\partial t^2} = \nabla^2 p'. \tag{1.1.9}$$

Obviously, the density perturbations satisfy the same equation. The velocity is a vector and satisfies the *vector* wave equation:

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{v}'}{\partial t^2} = \nabla^2 \mathbf{v}'. \tag{1.1.10}$$

This also means that each of the components of the velocity $\mathbf{v}' = (v'_x, v'_y, v'_z)$ satisfies the *scalar* wave equation (1.1.9). Note that these components are not independent. The momentum equation (1.1.3) shows that there exists some scalar function ϕ', which is called the *velocity potential*, such that

$$\mathbf{v}' = \nabla\phi, \qquad \frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} = \nabla^2\phi \qquad \left(\rho_0\frac{\partial\phi}{\partial t} = -p'\right). \tag{1.1.11}$$

So the problem can be solved for the potential and then the velocity field can be found as the gradient of this scalar field.

1.1.1.2 Fourier and Laplace transforms

The wave equation derived above is linear and has particular solutions that are periodic in time. In particular, if the time dependence is a harmonic function of *circular frequency* ω, we can write

$$\phi(\mathbf{r}, t) = \mathrm{Re}(e^{-i\omega t}\psi(\mathbf{r})), \qquad i^2 = -1, \tag{1.1.12}$$

where $\psi(\mathbf{r})$ is some complex valued scalar function and the real part is taken, since $\phi(\mathbf{r}, t)$ is real. Substituting expression (1.1.12) into the wave equation (1.1.11), we see that the latter is satisfied if $\psi(\mathbf{r})$ is a solution of the Helmholtz equation:

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = 0, \qquad k = \frac{\omega}{c}. \tag{1.1.13}$$

The constant k is called the *wavenumber* and is real for real ω. The name is related to the case of plane wave propagating in the fluid, where the *wavelength* is $\lambda = 2\pi/k$ and so k is the *number* of waves per 2π units of length.

The Helmholtz equation, therefore, stands for monochromatic waves, or waves of some given frequency ω. For *polychromatic* waves, or sums of waves of different frequencies, we can sum up solutions with different ω. More generally, we can perform the *inverse Fourier transform* of the potential $\phi(\mathbf{r}, t)$ with respect to the temporal variable:

$$\psi(\mathbf{r}, \omega) = \int_{-\infty}^{\infty} e^{i\omega t} \phi(\mathbf{r}, t) dt. \tag{1.1.14}$$

In this case $\psi(\mathbf{r}, \omega)$ satisfies the Helmholtz equation (1.1.13). Solving this equation we can determine the solution of the wave equation using the *forward Fourier transform*:

$$\phi(\mathbf{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \psi(\mathbf{r}, \omega) d\omega, \qquad \omega = ck. \tag{1.1.15}$$

We note that in the Fourier transform the frequency ω can either be negative or positive. This results in either negative or positive values of the wavenumber. However, the Helmholtz equation depends on k^2 and is *invariant* with respect to a change of sign in k. This phenomenon, in fact, has a deep physical and mathematical origin, and appears from the property that the wave equation is a *two-wave equation*. It describes solutions which are a superposition of two waves propagating with the same velocity in *opposite directions*. We will consider this property and rules for proper selection of sign in Section 1.2.

While monochromatic waves are important solutions with physical meaning, we note that mathematically we can also consider solutions of the wave equation of the type:

$$\phi(\mathbf{r}, t) = \mathrm{Re}(e^{st} \psi(\mathbf{r})), \qquad s \in \mathbb{C}, \tag{1.1.16}$$

where s is an arbitrary complex constant. In this case, as follows from the wave equation, $\psi(\mathbf{r})$ satisfies the following Helmholtz equation

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad k^2 = -\frac{s}{c}. \tag{1.1.17}$$

Here the constant k^2 can be an arbitrary complex number. This type of solution also has physical meaning and can be applied to solve initial value problems for the wave equation. Indeed, if we consider solutions of the wave equation, such that the fluid was unperturbed for $t \leq 0$ ($\phi(\mathbf{r}, t) = 0, t \leq 0$) while for $t > 0$ we have a non-trivial solution, then we can use the *Laplace transform*:

$$\psi(\mathbf{r}, s) = \int_{-\infty}^{\infty} e^{-st} \phi(\mathbf{r}, t) dt, \qquad \mathrm{Re}(s) > 0, \tag{1.1.18}$$

which converts the wave equation into the Helmholtz equation with complex k, (Eq. (1.1.17)). If an appropriate solution of the Helmholtz equation is available, then we can determine the solution of the wave equation using the *inverse* Laplace transform:

$$\phi(\mathbf{r}, t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^{st} \psi(\mathbf{r}, s) ds, \qquad \sigma > 0. \tag{1.1.19}$$

The above examples show that integral transforms with exponential kernels convert the wave equation into the Helmholtz equation. In the case of the Fourier transform we can state that the Helmholtz equation is the wave equation in the *frequency domain*. Since methods for fast Fourier transform are widely available, conversion from time to frequency domain and back are computationally efficient, and so the problem of the solution of the wave equation can be reduced to the solution of the Helmholtz equation, which is an equation of lower dimensionality (3 instead of 4) than the wave equation.

1.1.2 Scalar Helmholtz equations with complex k

1.1.2.1 Acoustic waves in complex media

Despite the fact that the barotropic fluid model is a good idealization for real fluids in certain frequency ranges, it may not be adequate for complex fluids, where internal processes occur under external action. Such processes may happen at very high frequencies due to molecular relaxation and chemical reactions or at lower frequencies if some inclusions in the form of solid particles or bubbles are present. One typical example of a medium with internal relaxation processes is plasma.

To model a medium with relaxation one can use the mass and momentum conservation equations (1.1.3) or a consequence of these. The difference between the models of barotropic fluid and relaxating medium occurs in the equation of state, which can sometimes be written in the form:

$$p = p(\rho, \dot{\rho}), \tag{1.1.20}$$

where the dot denotes the substantial derivative with respect to time. Being perturbed, the density of such a medium does not immediately follow the pressure perturbations, but rather returns to the equilibrium state with some dynamics. In the case of small perturbations, linearization of this equation yields:

$$p' = c^2 \left(\rho' + \tau_\rho \frac{\partial \rho'}{\partial t} \right). \tag{1.1.21}$$

Here τ_ρ is a constant having dimensions of time, and can be called the density relaxation time.

Equations (1.1.5) and (1.1.21) form a closed system, which has a particular solution oscillating with time so solutions of type Eq. (1.1.12) can be considered. To obtain corresponding Helmholtz equations for the wave equations considered, note that for a harmonic function we can simply replace the time derivative symbols:

$$\frac{\partial}{\partial t} \to -\mathrm{i}\omega. \tag{1.1.22}$$

This replacement of the time derivative with $-\mathrm{i}\omega$ can be interpreted as a transform of the equations from the time to the frequency domain. With this remark, we can derive from relations (1.1.5) and (1.1.21) a single equation for the density perturbation in the frequency domain (denoted by symbol ψ):

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = 0, \qquad k^2 = \frac{\omega^2}{c^2(1-\mathrm{i}\omega\tau_\rho)}. \tag{1.1.23}$$

Thus we obtained the Helmholtz equation with a complex wavenumber. At low frequencies, $\omega \ll \tau_\rho^{-1}$, the relaxation term is not important and we obtain the Helmholtz equation with real k. For high frequencies, the character of the dependency $k(\omega)$ is different, plus k appears to be complex.

A more general dependence of the pressure on the density and its derivatives can be considered for waves in complex media, e.g.

$$p = p(\rho, \dot{\rho}, \ddot{\rho}, \ldots). \tag{1.1.24}$$

Dependences of this type may also include integrals over time with kernels (media with memory). It is not difficult to see that various linearized equations of state result in equations of type:

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = 0, \qquad k^2 = k^2(\omega) \tag{1.1.25}$$

in the frequency domain. The function $k^2(\omega)$ depends on the particular medium considered and is related to its equation of state. The frequency dependence of the wavenumber is also called the *dispersion relationship*. If ω/k is characterized as the speed of sound, we can see that, in contrast to barotropic fluids in complex media, the speed of sound is now a function of frequency, and moreover, can be complex. In fact, the quantity

$$c_p = \frac{\omega}{\mathrm{Re}(k)} \tag{1.1.26}$$

is called the *phase velocity*, and characterizes the velocity of propagation of lines of constant phase, and the imaginary part of ω/k characterizes the attenuation of waves in the medium. The dependence of the real part on frequency is also known as the dispersion of the phase velocity (or simply, dispersion), which means that waves of different frequencies propagate with different velocities. There is a special case of the dispersion relationship, when $k(\omega)$ is real (e.g. this appears in some models of waves in plasma, and gravitation waves on a liquid free surface). In this case the medium is characterized as a medium with dispersion and without dissipation. As we can see from examples of medium with relaxation, the dispersion relationship (1.1.23) contains both real and imaginary parts, and so a medium with relaxation can also be characterized as a medium with dispersion and dissipation.

1.1.2.2 *Telegraph equation*

Another example of an equation that can be reduced to the Helmholtz equation is the telegraph equation. It is closely related to the equation for waves in a relaxating medium. The one-dimensional version of this equation first appeared in the description of signal transmission through a cable. It can be interpreted as a general wave equation with attenuation and extended to two and three dimensions, and is used by some researchers for modeling media with relaxation and dissipation, extremely low frequency electromagnetic wave propagation in the ionosphere, etc. This equation can be written in the time domain as:

$$\frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} + a\frac{\partial \Phi}{\partial t} + b\Phi = \nabla^2 \Phi, \tag{1.1.27}$$

where a, b, and c are some constants. In the frequency domain we obtain the following Helmholtz equation (see Eq. (1.1.22)):

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad k^2 = \frac{\omega^2}{c^2} + \mathrm{i}\omega a - b. \tag{1.1.28}$$

This is a special case of Eq. (1.1.25) where k is complex.

It is interesting to note that for $a = b = 0$ the telegraph equation turns into the usual wave equation, while for $c = \infty$, $b = 0$ it turns into the diffusion equation, discussed in Section 1.1.2.3, and for $c = \infty$, $a = 0$ it reduces to the Helmholtz equation in the time or frequency domains, with $k^2 = -b$. For real positive b both roots of the latter equation appear to be purely imaginary and this corresponds to two types of waves: exponentially growing and exponentially decaying. If there are no energy sources in the medium only decaying waves should be considered.

1.1.2.3 Diffusion

The heat conduction equation in solids can be written in the form:

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T, \tag{1.1.29}$$

where T is the perturbation of the temperature and κ is the thermal diffusivity. This equation also describes heat conduction in incompressible liquids if the convective term is negligibly small compared to the conductive term and is the case when the liquid is at rest or the temperature of the liquid changes much faster than the liquid flows.

The heat conduction equation is universal and appears in many other problems, e.g. for description of mass diffusion. In this case T should be interpreted as the perturbation of mass concentration and κ as the mass diffusivity. Another example interprets Eq. (1.1.29) as one describing diffusion of vorticity in viscous fluids. In this case T is a component of the vorticity vector and κ is a kinematic viscosity of the fluid.

In any case the heat conduction equation can be considered in the frequency domain using the Fourier transform. In that domain a corresponding equation can be easily found using rule (1.1.22):

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad k^2 = \frac{\mathrm{i}\omega}{\kappa}. \tag{1.1.30}$$

This is the Helmholtz equation with purely imaginary k^2. Therefore, the wavenumber in this case will have both real and imaginary parts. Since both k and $-k$ provide solutions of the Helmholtz equation then either two "thermal waves" can be considered or one solution can be set to zero, based on the problem. For example, for heat propagation from a body in an infinite medium, one should select solutions which decay at infinity.

It is also interesting to note that at high frequencies, $\omega \gg \tau_\rho^{-1}$, propagation of waves in media with relaxation is described by the same type of dispersion relationship as for the heat conduction equation (see Eq. (1.1.23)).

1.1.2.4 Schrödinger equation

Having its origin in quantum mechanics, the Schrödinger equation appears as a universal equation for modulations of quasi-monochromatic acoustic and electromagnetic waves in complex media, e.g. in plasma. Modulation waves in weakly nonlinear approximation are described by the nonlinear Schrödinger equation and in linear approximation by the linear Schrödinger equation:

$$-\mathrm{i}\frac{\partial \Psi}{\partial t} = \nabla^2 \Psi. \qquad (1.1.31)$$

Here Ψ is the wavefunction or the complex amplitude of a modulation wave. Transforming this equation into the frequency domain by using rule (1.1.22), we get:

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad k^2 = \omega. \qquad (1.1.32)$$

Therefore, as in the case of wave equation (1.1.13), we obtained the Helmholtz equation with real k^2. Despite a similarity to the Helmholtz equations, we note the following important differences from the physical view point. First, in the case of the Schrödinger equation we have a dispersion of the phase velocity (Eq. (1.1.26)), $c_p = c_p(\omega)$ while for the wave equation $c_p = c_0 =$ const. Second, since ω in the Fourier transform changes from $-\infty$ to ∞, k^2 appears to be negative for $\omega < 0$ and so k in this case is purely imaginary.

1.1.2.5 Klein–Gordan equation

The Schrödinger equation is a quantum mechanical equation for non-relativistic mechanics. For relativistic quantum mechanics the corresponding equation, which describes a free particle with zero spin, is called the Klein–Gordan equation and can be written in the form:

$$\frac{\partial^2 \Psi}{\partial t^2} = \nabla^2 \Psi - m^2 \Psi, \qquad (1.1.33)$$

where Ψ is the wavefunction and m is the normalized particle mass. In the frequency domain, this corresponds to the following Helmholtz equation:

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = 0, \qquad k^2 = -(m^2 - \omega^2). \qquad (1.1.34)$$

Let us look for time-independent solutions ($\partial \Psi / \partial t = 0$ or $\omega = 0$) of the Klein–Gordan equation. In this case it reduces to the Helmholtz equation with purely imaginary $k = \mathrm{i}m$. The spherically symmetrical solution of this equation decaying at infinity is

$$\Psi = \frac{C}{r} \mathrm{e}^{-mr}, \qquad r = |\mathbf{r}|, \qquad (1.1.35)$$

where C is some constant. The case $m = 0$ corresponds to non-relativistic approximation and in this case the potential is a fundamental solution of the Laplace equation $\sim r^{-1}$, which is known from electrostatics or gravitation theory. For non-zero m this potential is known as the *Yukawa potential*. The Yukawa potential can be used in the theory of relativistic gravitation or as an analog of the electrostatic potential for description of intermolecular forces and interactions.

1.1.3 Electromagnetic waves

1.1.3.1 Maxwell's equations

Consider now the appearance of the scalar Helmholtz equation in the context of Maxwell equations describing propagation of electromagnetic waves. For a medium free of charges and imposed currents, these equations can be written as:

$$\nabla\times\mathbf{E}=-\mu\frac{\partial\mathbf{H}}{\partial t},\quad \nabla\times\mathbf{H}=\varepsilon\frac{\partial\mathbf{E}}{\partial t},\quad \nabla\cdot\mathbf{E}=0,\quad \nabla\cdot\mathbf{H}=0, \tag{1.1.36}$$

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic field vectors, and μ and ε are the magnetic permeability and electric permittivity in the medium, respectively. In the case of a vacuum we have

$$\mu=\mu_0,\quad \varepsilon=\varepsilon_0,\quad c=(\mu_0\varepsilon_0)^{-1/2},$$

where c is the speed of light in a vacuum and $c\approx 3\times 10^8$ m/s.

Taking the curl of the first equation and using the second equation, we have

$$\nabla\times\nabla\times\mathbf{E}=-\mu\frac{\partial}{\partial t}\nabla\times\mathbf{H}=-\mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2}=-\frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2}, \tag{1.1.37}$$

Due to the following well-known identity for the ∇ operator and the third equation in Eq. (1.1.36):

$$\nabla^2\mathbf{E}=\nabla(\nabla\cdot\mathbf{E})-\nabla\times\nabla\times\mathbf{E}=-\nabla\times\nabla\times\mathbf{E}, \tag{1.1.38}$$

we obtain

$$\frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2}=\nabla^2\mathbf{E}. \tag{1.1.39}$$

Similarly,

$$\frac{1}{c^2}\frac{\partial^2\mathbf{H}}{\partial t^2}=\nabla^2\mathbf{H}. \tag{1.1.40}$$

Thus, both the electric and magnetic field vectors satisfy the vector wave equation. Transformation of this equation into the frequency domain yields

$$\begin{aligned}(\nabla^2+k^2)\hat{\mathbf{E}}&=0,\qquad k=\frac{\omega}{c}\\(\nabla^2+k^2)\hat{\mathbf{H}}&=0,\end{aligned} \tag{1.1.41}$$

where we use circumflex to denote that we are in the frequency domain and $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ are the complex amplitudes of $\mathbf{E}$ and $\mathbf{H}$ for harmonic oscillations with frequency ω. These complex functions are also known as *phasors*.[1]

Note that the number of scalar equations (1.1.41) in three dimensions is six (each Cartesian component of $\hat{\mathbf{E}}$ or $\hat{\mathbf{H}}$ satisfies the scalar Helmholtz equation), while the original formulation (1.1.36) provide eight relations for the same quantities. The missing relations are equations stating that the divergence of the electric and magnetic fields is zero. This imposes limitations on the components of the electric and magnetic field vectors, since they should be constrained to satisfy these additional equations. So any of these fields is described by the following system of equations:

$$(\nabla^2 + k^2)\hat{\mathbf{E}} = 0, \qquad \nabla\cdot\hat{\mathbf{E}} = 0, \tag{1.1.42}$$

where $\hat{\mathbf{E}}$ can be replaced by $\hat{\mathbf{H}}$. It is interesting to note that, in the equation describing propagation of acoustic waves (Eq. (1.1.10)), the velocity field also satisfies the vector wave equation (so its phasor satisfies the vector Helmholtz equation) with an additional condition $\nabla \times \mathbf{v}' = 0$. This is equivalent to the existence of a scalar potential which satisfies the scalar wave equation, $\mathbf{v}' = \nabla\phi$. Below we will show that the second equation in Eq. (1.1.42) enables the introduction of two scalar potentials, which satisfy the scalar equations, and both vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ can be expressed via these functions.

1.1.3.2 Scalar potentials

Since the components of $\hat{\mathbf{E}}$ are related via the divergence free condition, we can consider the representation of $\hat{\mathbf{E}}$ via two independent scalar functions ψ_1 and ψ_2, where each of these the functions satisfies the scalar Helmholtz equation:

$$(\nabla^2 + k^2)\psi_1 = 0, \qquad (\nabla^2 + k^2)\psi_2 = 0. \tag{1.1.43}$$

To do this we prove the following two theorems using vector algebra (these theorems can be found elsewhere).

THEOREM 1 *Let ψ be a scalar function that satisfies the Helmholtz equation (1.1.43). Then the function $\hat{\mathbf{E}} = \nabla\psi \times \mathbf{r}$ satisfies the constrained vector Helmholtz equations (1.1.42).*

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[1] In general we can define the phasor as a Fourier-image of the function. For example, in Eq. (1.1.14) function Ω is the phasor of ϕ'.

PROOF. First we note that this function is a curl of some vector:

$$\hat{\mathbf{E}} = \nabla\psi \times \mathbf{r} = \nabla \times (\mathbf{r}\psi) \tag{1.1.44}$$

So it is a solenoidal (or divergence free) field:

$$\nabla\cdot\hat{\mathbf{E}} = \nabla\cdot[\nabla \times (\mathbf{r}\psi)] = 0. \tag{1.1.45}$$

Thus the second equation in Eq. (1.1.42) is satisfied. Consider now the first equation in Eq. (1.1.42). We have

$$\begin{aligned}(\nabla^2 + k^2)\hat{\mathbf{E}} &= -\nabla \times \nabla \times \nabla \times (\mathbf{r}\psi) + k^2\nabla \times (\mathbf{r}\psi) \\ &= \nabla \times [-\nabla \times \nabla \times (\mathbf{r}\psi) + k^2\mathbf{r}\psi] = \nabla \times [\nabla^2(\mathbf{r}\psi) + k^2\mathbf{r}\psi]. \end{aligned} \tag{1.1.46}$$

The last equality holds due to:

$$-\nabla \times \nabla \times (\mathbf{r}\psi) = \nabla^2(\mathbf{r}\psi) - \nabla[\nabla\cdot(\mathbf{r}\psi)], \tag{1.1.47}$$

and the curl of of the last term in Eq. (1.1.47) is zero (the curl of gradient). Consider now:

$$\begin{aligned}\nabla^2(\mathbf{r}\psi) &= \nabla^2(\mathbf{i}_x x\psi) + \nabla^2(\mathbf{i}_y y\psi) + \nabla^2(\mathbf{i}_z z\psi) \\ &= \mathbf{i}_x\nabla^2(x\psi) + \mathbf{i}_y\nabla^2(y\psi) + \mathbf{i}_z\nabla^2(z\psi) \\ &= (\mathbf{i}_x x + \mathbf{i}_y y + \mathbf{i}_z y)\nabla^2\psi + 2(\mathbf{i}_x\nabla x\cdot\nabla\psi + \mathbf{i}_y\nabla y\cdot\nabla\psi + \mathbf{i}_z\nabla z\cdot\nabla\psi) \\ &= \mathbf{r}\nabla^2\psi + 2\nabla\psi. \end{aligned} \tag{1.1.48}$$

So from Eqs. (1.1.43) and (1.1.46) we have:

$$\begin{aligned}(\nabla^2 + k^2)\hat{\mathbf{E}} &= \nabla \times [\nabla^2(\mathbf{r}\psi) + k^2\mathbf{r}\psi] = \nabla \times [\mathbf{r}(\nabla^2 + k^2)\psi + 2\nabla\psi] \\ &= 2\nabla \times \nabla\psi = 0. \end{aligned} \tag{1.1.49}$$

This proves the theorem. □

COROLLARY 1 *Let ψ be a scalar function that satisfies the Helmholtz equation (1.1.43). Then the function $\hat{\mathbf{E}} = \nabla\psi \times \mathbf{r}_*$, where $\mathbf{r}_*$ is an arbitrary constant vector (also called a "pilot vector"), satisfies Eqs. (1.1.42).*

PROOF. To prove this statement it is sufficient to see that the Maxwell (or corresponding Helmholtz) equations are invariant with respect to selection of the origin of the reference frame. Therefore, the function $\hat{\mathbf{E}}_1 = \nabla\psi \times (\mathbf{r} - \mathbf{r}_*)$ satisfies Eqs. (1.1.42). Because of the linearity of equations the difference $\hat{\mathbf{E}} = \nabla\psi \times \mathbf{r} - \nabla\psi \times (\mathbf{r} - \mathbf{r}_*) = \nabla\psi \times \mathbf{r}_*$ also satisfies Eqs. (1.1.42). □

THEOREM 2 *Let ψ be a scalar function that satisfies the Helmholtz equation (1.1.43). Then $\hat{\mathbf{E}} = \nabla \times (\nabla\psi \times \mathbf{r})$ satisfies Eqs. (1.1.42).*

PROOF. Since $\hat{\mathbf{E}}$ is the curl of some vector we immediately have $\nabla \cdot \hat{\mathbf{E}} = 0$. We also have

$$(\nabla^2 + k^2)\hat{\mathbf{E}} = \nabla \times \nabla \times [\nabla^2(\mathbf{r}\psi) + k^2 \mathbf{r}\psi] = 0, \tag{1.1.50}$$

which follows from identities (1.1.46) and (1.1.49). This proves the theorem. □

COROLLARY 2 *Let ψ be a scalar function that satisfies the Helmholtz equation (1.1.43). Then the function $\hat{\mathbf{E}} = \nabla \times (\nabla\psi \times \mathbf{r}_*)$, where $\mathbf{r}_*$ is an arbitrary constant (pilot) vector, satisfies Eqs. (1.1.42).*

PROOF. The proof is similar to the proof of the corollary for Theorem 2. □

One can then think that, by application of the curl, more linearly independent solutions can be generated. This is not true since operator $\nabla \times \nabla \times$ can be expressed via the Laplacian as:

$$\nabla \times \nabla \times (\nabla\psi \times \mathbf{r}) = -\nabla^2(\nabla\psi \times \mathbf{r}) = k^2(\nabla\psi \times \mathbf{r}). \tag{1.1.51}$$

Thus the function $\hat{\mathbf{E}}^{(2)} = \nabla \times \nabla \times (\nabla\psi \times \mathbf{r}) = k^2 \hat{\mathbf{E}}^{(0)}$ linearly depends on $\hat{\mathbf{E}}^{(0)}$, where $\hat{\mathbf{E}}^{(0)} = \nabla\psi \times \mathbf{r}$ and is a solution of the Maxwell equations. This shows that all solutions produced by multiple application of the curl operator to $\nabla\psi \times \mathbf{r}$ can be expressed via the two basic solutions $\nabla\psi \times \mathbf{r}$ and $\nabla \times (\nabla\psi \times \mathbf{r})$ and, generally, we can represent solutions of the Maxwell equations in the form:

$$\hat{\mathbf{E}} = \nabla\psi_1 \times \mathbf{r} + \nabla \times (\nabla\psi_2 \times \mathbf{r}), \tag{1.1.52}$$

where ϕ and ψ are two arbitrary scalar functions that satisfy Eqs. (1.1.43). Owing to identity (1.1.44) this also can be rewritten as:

$$\hat{\mathbf{E}} = \nabla \times [\mathbf{r}\psi_1 + \nabla \times (\mathbf{r}\psi_2)]. \tag{1.1.53}$$

Note that the above decomposition is *centered* at $\mathbf{r} = \mathbf{0}$ ($\mathbf{r} = \mathbf{0}$ is a special point). Obviously the center can be selected at an arbitrary point $\mathbf{r} = \mathbf{r}_*$. For some problems it is more convenient to use a constant vector $\mathbf{r}_*$ instead of $\mathbf{r}$ for the decomposition we used above. More generally, one can use a decomposition in the form:

$$\hat{\mathbf{E}} = \nabla \times \{(a_1\mathbf{r} + \mathbf{r}_{*1})\psi_1 + \nabla \times [(a_2\mathbf{r} + \mathbf{r}_{*2})\psi_2]\}, \tag{1.1.54}$$

which is valid for arbitrary constants a_1 and a_2 (can be zero) and vectors $\mathbf{r}_{*1}$ and $\mathbf{r}_{*2}$, which can be selected as convenience dictates for the solution of a particular problem.

Consider now the phasor of the magnetic field vector. As follows from the first equation (1.1.36) it satisfies the equation:

$$\mathrm{i}\omega\mu\hat{\mathbf{H}} = \nabla \times \hat{\mathbf{E}}. \tag{1.1.55}$$

Substituting here decomposition (1.1.43) and using identities (1.1.44) and (1.1.51), we obtain

$$\mathrm{i}c\mu k\hat{\mathbf{H}} = \nabla \times (\nabla\psi_1 \times \mathbf{r}) + k^2(\nabla\psi_2 \times \mathbf{r}) = \nabla \times [k^2\mathbf{r}\psi_2 + \nabla \times (\mathbf{r}\psi_1)]. \tag{1.1.56}$$

This form is similar to the representation of the phasor of the electric field (1.1.53) where functions ψ_1 and ψ_2 exchange their roles and some coefficients appear. In the case of more general decomposition (1.1.54) we have:

$$\mathrm{i}c\mu k\hat{\mathbf{H}} = \nabla \times \{k^2(a_2\mathbf{r} + \mathbf{r}_{*2})\psi_2 + \nabla \times [(a_1\mathbf{r} + \mathbf{r}_{*1})\psi_1]\}. \tag{1.1.57}$$

This shows that solution of Maxwell equations in the frequency domain is equivalent to two scalar Helmholtz equations. These equations can be considered as independent, while their coupling occurs via the boundary conditions for particular problems.

Note that the wavenumber k in the scalar Helmholtz equations (1.1.43) is real. More complex models of the medium can be considered (say, owing to the presence of particles of sizes much smaller than the wavelength and for waves whose period is comparable with the periods of molecular relaxation or resonances once we consider waves in some media, not vacuum). In such a medium one can expect effects of dispersion and dissipation such as we considered for acoustic wave propagation in complex media. This will introduce a dispersion relationship $k = k(\omega)$ and complex k.

1.2 BOUNDARY CONDITIONS

The Helmholtz equation is an equation of the elliptic type, for which it is usual to consider boundary value problems. Boundary conditions follow from particular physical laws (conservation equations) formulated on the boundaries of the domain in which a solution is required. This domain can be finite (internal problems) or infinite (external problems). For infinite domains, the solutions should satisfy some conditions at the infinity. These conditions also have a physical origin. For the Helmholtz equation that arises as a transform of the wave equation into the frequency domain, the boundary conditions should be understood in the context of the original wave equation.

1.2.1 Conditions at infinity

1.2.1.1 Spherically symmetrical solutions

To understand the conditions which should be imposed on solutions of the Helmholtz equation in infinite domains, we start with the consideration of spherically symmetrical solutions of the scalar wave equation. In this case a function ϕ, which satisfies the wave equation (1.1.11), depends on the distance $r = |\mathbf{r}|$ only. It is well known that a solution of this equation can be written in the following D'Alembert form:

$$\phi(r,t) = \frac{1}{r}[f(t + r/c) + g(t - r/c)], \qquad (1.2.1)$$

where f and g are two arbitrary differentiable functions. The former function describes *incoming waves* towards the center $r = 0$ and the latter function describes *outgoing waves* from the center $r = 0$. Indeed the incoming wave phase can be characterized by some constant value of f, which is realized at $r = -ct + \text{const}$, and so the wavefronts converge towards the center as t is growing. Inversely, the outgoing wave phase is characterized by some constant value of g, which is realized at $r = ct + \text{const}$ and so the wavefronts for the outgoing waves diverge from the center as increasing t.

Therefore, a spherically symmetrical solution of the scalar wave equation can be characterized by specification of two functions of time $f(t)$ and $g(t)$. Assume that these functions satisfy the necessary conditions to perform the Fourier transform. Then, in the frequency domain we have images of these functions according to Eq. (1.1.11):

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} f(t)dt, \qquad \hat{g}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} g(t)dt. \qquad (1.2.2)$$

With these definitions and solution (1.2.1) we can determine the image, or phasor $\psi(r,\omega)$ of $\phi(r,t)$ in the frequency domain as:

$$\begin{aligned}\psi(r,\omega) &= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega t}\phi(r,t)\mathrm{d}t \\ &= \frac{1}{r}\left[\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega t} f(t+r/c)\mathrm{d}t + \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega t} g(t-r/c)\mathrm{d}t\right] \\ &= \frac{1}{r}\left[\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega(t'-r/c)} f(t')\mathrm{d}t' + \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega(t'+r/c)} g(t')\mathrm{d}t\right] \\ &= \frac{1}{r}\hat{f}(\omega)\mathrm{e}^{-\mathrm{i}kr} + \frac{1}{r}\hat{g}(\omega)\mathrm{e}^{\mathrm{i}kr}, \qquad k = \frac{\omega}{c}. \end{aligned} \tag{1.2.3}$$

Here we defined $k = \omega/c$ and so this quantity is negative for $\omega < 0$ and positive for $\omega > 0$. The function $\psi(r,\omega)$ is a solution of the spherically symmetrical Helmholtz equation (1.1.13). It is seen that solutions corresponding to the incoming waves are proportional to $\mathrm{e}^{-\mathrm{i}kr}$ while solutions corresponding to the outgoing waves are proportional to $e^{\mathrm{i}kr}$.

It is not difficult to see also that at large r we have:

$$r\left(\frac{\partial\psi}{\partial r} - \mathrm{i}k\psi\right) = -2\mathrm{i}k\hat{f}(\omega)\mathrm{e}^{-\mathrm{i}kr} + O\left(\frac{1}{r}\right), \tag{1.2.4}$$

$$r\left(\frac{\partial\psi}{\partial r} + \mathrm{i}k\psi\right) = 2\mathrm{i}k\hat{g}(\omega)\mathrm{e}^{\mathrm{i}kr} + O\left(\frac{1}{r}\right). \tag{1.2.5}$$

This means that if the condition

$$\lim_{r\to\infty}\left[r\left(\frac{\partial\psi}{\partial r} - \mathrm{i}k\psi\right)\right] = 0 \tag{1.2.6}$$

holds then $\hat{f}(\omega) \equiv 0$. This results in $f(t) \equiv 0$ and in this case $\phi(r,t)$ consists only of outgoing waves. Similarly, in the case if the condition

$$\lim_{r\to\infty}\left[r\left(\frac{\partial\psi}{\partial r} + \mathrm{i}k\psi\right)\right] = 0 \tag{1.2.7}$$

holds, the solution consists only of incoming waves and $g(t) \equiv 0$.

1.2.1.2 Sommerfeld radiation condition

The problems which are usually considered in relation to the wave equation in three-dimensional unbounded domains are scattering problems. In this case the wave function is specified as:

$$\phi(\mathbf{r},t) = \phi_{\text{in}}(\mathbf{r},t) + \phi_{\text{scat}}(\mathbf{r},t), \tag{1.2.8}$$

where both functions $\phi_{\text{in}}(\mathbf{r}, t)$ and $\phi_{\text{scat}}(\mathbf{r}, t)$ satisfy the wave equation. The function $\phi_{\text{in}}(\mathbf{r}, t)$ is the potential of the incident field, while $\phi_{\text{scat}}(\mathbf{r}, t)$ is the potential of the scattered field, which arises due to the presence of one or several scatterers. In the absence of scatterers $\phi(\mathbf{r}, t) = \phi_{\text{in}}(\mathbf{r}, t)$ is some given function (e.g. the potential of a plane wave propagating along the z-direction, $\phi_{\text{in}}(\mathbf{r}, t) = F(t - z/c)$).

To understand the scattered field we may turn our attention to the *Huygens principle*, which represents wave propagation as an emission of secondary wave from the points located on the current wavefront. When the primary wave described by $\phi_{\text{in}}(\mathbf{r}, t)$ reaches the scatterer boundary the secondary waves are generated from the boundary points located at the intersection of the boundary and the wavefront. Owing to the finite speed of wave propagation, spatial points far from the boundary "do not know" about these secondary waves, so these waves can be thought of as waves *outgoing* from the boundary points. For each point we can then write the secondary wave potential in the form (1.2.1), where $f \equiv 0$ and, therefore, in the frequency domain condition (1.2.6) holds. Since the total scattered field, $\phi_{\text{scat}}(\mathbf{r}, t)$, can now be seen as a superposition of outgoing waves, the corresponding potential in the frequency domain should satisfy the condition:

$$\lim_{r\to\infty}\left[r\left(\frac{\partial \psi_{\text{scat}}}{\partial r} - \mathrm{i}k\psi_{\text{scat}}\right)\right] = 0. \tag{1.2.9}$$

This condition is called the *Sommerfeld radiation condition* or just the *radiation condition*. It states that the scattered field consists of outgoing waves only. Solutions of the Helmholtz equation which satisfy the radiation condition are called *radiating solutions* or *radiating functions*.

In some wave problems considered in infinite domains all the wave sources and scatterers can be enclosed inside some sphere. Since in the absence of the wave sources the solution of the wave equation is trivial, $\phi(\mathbf{r}, t) \equiv 0$, then all perturbations for points located outside the sphere come only from some events inside the sphere. This means that in this case the total field in the frequency domain, $\psi(\mathbf{r}, \omega)$ is a radiating function.

We emphasize that the radiation condition (1.2.9) derived from consideration of point sources is applied to a set of sources, i.e. to the case $\psi_{\text{scat}} = \psi_{\text{scat}}(\mathbf{r}, k)$. Generally, the far-field asymptotics of ψ_{scat} is

$$\psi_{\text{scat}} \sim \frac{1}{r}\Psi(\theta, \varphi)\mathrm{e}^{ikr}, \tag{1.2.10}$$

where $\Psi(\theta, \varphi)$ is the angular dependence on spherical angles θ and φ, and so condition (1.2.9) holds. Indeed, from a very remote point, a set of sources or scatterers is seen as one point (like we see galaxies consisting of many stars as one "star"). While for different angles there will be different values of of ψ_{scat} (so it is not spherically symmetrical), for given, or fixed, angles θ and φ there is no difference between the asymptotic behavior of a set of sources and an equivalent single source.

1.2.1.3 Complex wavenumber

As we showed above, the Helmholtz equation with complex k can appear in some models:

$$k = k_r + \mathrm{i}k_i, \qquad k_i \neq 0. \tag{1.2.11}$$

For any $k \neq 0$, the solution of the spherically symmetrical Helmholtz equation can be written in the form:

$$\begin{aligned}\psi(r,k) &= \frac{1}{r}\hat{f}(k)\mathrm{e}^{-\mathrm{i}kr} + \frac{1}{r}\hat{g}(k)\mathrm{e}^{\mathrm{i}kr} \\ &= \frac{1}{r}\hat{f}(k)\mathrm{e}^{k_i r}\,\mathrm{e}^{-\mathrm{i}k_r r} + \frac{1}{r}\hat{g}(k)\mathrm{e}^{-k_i r}\,\mathrm{e}^{\mathrm{i}k_r r},\end{aligned} \tag{1.2.12}$$

where $\hat{f}(k)$ and $\hat{g}(k)$ are some integration constants.

In the case $k_r = 0$, which is realized, e.g. for the Klein–Gordan equation, we have a sum of exponentially growing and decaying solutions. The decaying solution is nothing but the Yukawa potential (1.1.35) and so it should be selected if we request that solutions are bounded outside a sphere which contains the point of singularity $r = 0$. Hence in this case the boundary condition is:

$$\lim_{r\to\infty} \psi = 0. \tag{1.2.13}$$

The case $k_r \neq 0$ deserves a more detailed consideration. Assume that solution (1.2.12) represents the complex amplitude of a monochromatic wave propagating in complex medium (1.1.12):

$$\phi(r,t) = \frac{1}{r}\mathrm{Re}(\hat{f}(k)\mathrm{e}^{k_i r}\,\mathrm{e}^{-\mathrm{i}k_r(r+c_p t)} + \hat{g}(k)\mathrm{e}^{-k_i r}\,\mathrm{e}^{\mathrm{i}k_r(r-c_p t)}), \tag{1.2.14}$$

where c_p is the phase velocity (1.1.26). Since k appears in the Helmholtz equation as k^2 and the definition of the sign of k depends on our choice, we can define its sign, as in the case of real k, in such a way that the phase velocity is positive at positive frequencies, i.e. $k_r > 0$ at $\omega > 0$. This means that the first term in expression (1.2.14) describes the incoming wave, while the second term corresponds to the outgoing wave. In the case of wave scattering or propagation outside of waves generated in a finite spatial domain we need to select only the solution corresponding to outgoing waves—in other words to set $\hat{f}(k) = 0$. Therefore, as in the case of real k, we impose the following condition for asymptotic behavior as $r \to \infty$ of solutions of the Helmholtz equation:

$$\psi(\mathbf{r}, k) \sim \frac{1}{r} e^{ikr}. \tag{1.2.15}$$

Now we note that if $k_i > 0$ this solution is decaying at $r \to \infty$, so it can be replaced with condition (1.2.12). This is the case for dissipative media, which means that small perturbations should not grow as they propagate in the medium. For example, for relaxating media with a dispersion relationship (1.1.23) the root corresponding to $k_r > 0$ at $\omega > 0$ is:

$$k = \frac{\omega}{c(1 + \tau_\rho^2 \omega^2)^{1/2}} (1 + i\omega\tau_\rho)^{1/2}, \qquad k_i > 0. \tag{1.2.16}$$

Therefore, condition (1.2.13) can be used in this case. The same holds for the diffusion equation, where for positive ω, k_r, and diffusivity κ, Eq. (1.1.30) yields:

$$k = (1 + i)\left(\frac{\omega}{2\kappa}\right)^{1/2}, \qquad k_i > 0. \tag{1.2.17}$$

Despite the situation where $k_i < 0$ at $\omega/k_r > 0$ being rather unusual, it is not impossible. In this case we can see that the outgoing wave should grow in amplitude as it propagates in the medium. The unperturbed state of such media should be characterized as *linearly unstable*, since any small perturbation will exponentially (explosively) grow as it propagates. The examples of media of such type can be found in the theory of superheated liquids, active media, which can release energy under perturbations (explosives), etc. We can see that condition (1.2.12) is not applicable in this case, since the physical meaning requires to select a solution not decaying at infinity, but a growing solution. Our reasoning here is based on the *causality principle*.

1.2.1.4 Silver–Müller radiation condition

The Silver–Müller radiation condition is a condition that is imposed on the scattered electromagnetic field when solving the Maxwell equations. It can be stated as:

$$\begin{aligned} &\lim_{r \to 0} (\mu^{1/2} \hat{\mathbf{H}}_{\text{scat}} \times \mathbf{r} - r\varepsilon^{1/2} \hat{\mathbf{E}}_{\text{scat}}) = \mathbf{0}, \\ &\lim_{r \to 0} (\varepsilon^{1/2} \hat{\mathbf{E}}_{\text{scat}} \times \mathbf{r} + r\mu^{1/2} \hat{\mathbf{H}}_{\text{scat}}) = \mathbf{0}, \end{aligned} \tag{1.2.18}$$

where $\hat{\mathbf{E}}_{\text{scat}}$ and $\hat{\mathbf{H}}_{\text{scat}}$ are the phasors of the scattered electric and magnetic fields arising from the decomposition of the total field in to the incident and scattered fields:

$$\hat{\mathbf{E}} = \hat{\mathbf{E}}_{\text{in}} + \hat{\mathbf{E}}_{\text{scat}}, \qquad \hat{\mathbf{H}} = \hat{\mathbf{H}}_{\text{in}} + \hat{\mathbf{H}}_{\text{scat}}.$$

The physical meaning of these conditions is similar to those for the scalar field—they simply state that the scattered field consists of outgoing waves only. Indeed, if we consider a point $\mathbf{r} = (r, \theta, \varphi)$ located on a very large sphere enclosing all the scatterers, we can see that quantities $\hat{\mathbf{E}}_{\text{scat}}$ and $\hat{\mathbf{H}}_{\text{scat}}$ represent plane waves propagating in the radial direction from the center of the sphere, whose amplitude decays as r^{-1} due to the sphericity.

Consider now a plane wave solution of Maxwell equations. Let unit vector $\mathbf{s}$, $|\mathbf{s}| = 1$, characterize the direction of the plane wave propagation. In this case

$$\hat{\mathbf{E}} = \mathbf{c}\, e^{ik\mathbf{s}\cdot\mathbf{r}}, \tag{1.2.19}$$

satisfies the vector Helmholtz equation (1.1.42) and vector $\mathbf{c}$ should be orthogonal to $\mathbf{s}$ to satisfy the divergence free condition, $\mathbf{c}\cdot\mathbf{s} = 0$. This condition can be enforced if we take $\mathbf{c} = \mathbf{s} \times \mathbf{q}$, where $\mathbf{q}$ is an arbitrary vector. So the plane wave solution of Maxwell equations can be written in the form:

$$\hat{\mathbf{E}} = (\mathbf{s} \times \mathbf{q})e^{ik\mathbf{s}\cdot\mathbf{r}}. \tag{1.2.20}$$

From relation (1.1.55) we can then determine the phasor of the magnetic field vector:

$$i\omega\mu\hat{\mathbf{H}} = \nabla \times [(\mathbf{s} \times \mathbf{q})e^{ik\mathbf{s}\cdot\mathbf{r}}] = ik[\mathbf{s} \times (\mathbf{s} \times \mathbf{q})]e^{ik\mathbf{s}\cdot\mathbf{r}} = ik\mathbf{s} \times \hat{\mathbf{E}}. \tag{1.2.21}$$

Due to the vector identity

$$[\mathbf{s} \times (\mathbf{s} \times \mathbf{q})] \times \mathbf{s} = [(\mathbf{s}\cdot\mathbf{q})\mathbf{s} - \mathbf{q}] \times \mathbf{s} = (\mathbf{s} \times \mathbf{q}), \tag{1.2.22}$$

we can see that

$$i\omega\mu\hat{\mathbf{H}} \times \mathbf{s} = ik\{[\mathbf{s} \times (\mathbf{s} \times \mathbf{q})] \times \mathbf{s}\}e^{ik\mathbf{s}\cdot\mathbf{r}} = ik(\mathbf{s} \times \mathbf{q})e^{ik\mathbf{s}\cdot\mathbf{r}} = ik\hat{\mathbf{E}}. \tag{1.2.23}$$

This shows that for plane waves propagating in direction $\mathbf{s}$ we have:

$$\mu^{1/2}\hat{\mathbf{H}} \times \mathbf{s} - \varepsilon^{1/2}\hat{\mathbf{E}} = \mathbf{0}, \qquad \varepsilon^{1/2}\hat{\mathbf{E}} \times \mathbf{s} + \mu^{1/2}\hat{\mathbf{H}} = \mathbf{0},$$
$$c = \frac{\omega}{k} = \frac{1}{\sqrt{\mu\varepsilon}}. \tag{1.2.24}$$

From the above arguments as $r \to \infty$, we can see that if we replace $\mathbf{s} = \mathbf{r}/r$ in relations (1.2.24) and take into account that for a given direction (θ, φ)

the principal term of the scattered field is proportional to r^{-1} then we obtain the Silver–Müller conditions (1.2.18).

Note that these conditions are not necessary when considering the reduction of Maxwell equations to the scalar Helmholtz equations. If the scalar potentials satisfy the Sommerfield radiation conditions, the Silver–Müller conditions hold automatically, since both state the same physical fact.

1.2.2 Transmission conditions

Real systems can be considered as a unity of domains occupied by relatively homogeneous media. While the physical properties of different substances can differ substantially (say, air and rigid particles), one should keep in mind that waves of different nature can propagate in any substance (e.g. acoustic waves) and, therefore, wave-type equations can be used for their description. Owing to the difference in properties, the speed of propagation of perturbations is different for different media. Therefore, for descriptions of waves in each domain we can apply the wave equation with the speed of sound or light corresponding to the medium that occupies that domain. The problem then is to provide sufficient conditions on the domain boundaries that enable us to match solutions in different domains and build solutions for the corresponding wave equation. These conditions are known as *transmission* conditions, which can also be interpreted as *jump conditions* or conditions for discontinuities, since the wave function and/or its derivatives may jump on the contact boundaries. In general, the jump conditions can be derived from the same conservation equations that lead to the governing equations. The form of these conservation laws should be written in integral form to allow discontinuities and then the conditions arise after shrinking the domain to the contact surfaces. Below we provide examples of transmission conditions for acoustic and electromagnetic waves.

1.2.2.1 Acoustic waves

In acoustics we usually consider problems when the boundaries of the domains are either immovable or move with velocities much smaller than the speed of sound. We also consider the case when the amplitude of pressure perturbations is small and perturbations of the mass velocity are small as well. In the linear approximation, this results in the following two conditions on a contact surface S with normal n separating two media marked as 1 and 2:

$$\mathbf{v}_1' \cdot \mathbf{n} = \mathbf{v}_2' \cdot \mathbf{n}, \qquad p_1' = p_2'. \tag{1.2.25}$$

The first condition states that the velocities normal to the surface are the same. In fluid mechanics this is known as kinematic condition. In fact, it follows from the mass conservation equation in its assumption that there is no mass transfer through the surface S. The second condition, sometimes called dynamic conditions, follows from the momentum conservation equation and is valid if there are no surface forces. As follows from this description, these conditions should be modified if mass is transferred through the surface (say, owing to phase transitions), and if there are some appreciable surface forces (for example, surface tension). These conditions are sufficient to match solutions of the wave or Helmholtz equation in two domains.

Depending on the problem to be solved (wave equation for pressure or for the velocity potential), conditions (1.2.25) can be written in terms of pressure or velocity potential and their derivatives only. Consider first the pressure equations. As follows from the momentum conservation equation (1.1.3) written in the frequency domain, the phasors of pressure and velocity perturbations, $\hat{p}'$ and $\hat{\mathbf{v}}'$, satisfy equations

$$-\mathrm{i}\omega\rho_1\hat{\mathbf{v}}'_1 + \nabla\hat{p}'_1 = \mathbf{0}, \qquad -\mathrm{i}\omega\rho_2\hat{\mathbf{v}}'_2 + \nabla\hat{p}'_2 = \mathbf{0}. \tag{1.2.26}$$

Taking the scalar product of these equations with normal $\mathbf{n}$, denoting the normal derivative $\partial/\partial n = \mathbf{n}\cdot\nabla$, and noticing that relations (1.2.25) also hold in the frequency domain (remember our assumption that the speed of the boundary is much smaller than the speed of sound!), we obtain the following transmission conditions for pressure perturbations applicable to matching solutions of the Helmholtz equation in domains 1 and 2:

$$\frac{1}{\rho_1}\frac{\partial\hat{p}'_1}{\partial n} = \frac{1}{\rho_2}\frac{\partial\hat{p}'_2}{\partial n}, \qquad \hat{p}'_1 = \hat{p}'_2. \tag{1.2.27}$$

Here ρ_1 and ρ_2 are the respective medium densities.

Now consider the problem formulation for the Helmholtz equation written in terms of the velocity potential (1.1.11). The integral of the momentum equation (the expression in parentheses in equation (1.1.11)) can be written in phasor space, where we use notation ψ for the phasor of ϕ (see Eq. (1.1.14)) as:

$$\mathrm{i}\omega\rho_1\psi_1 = p'_1, \qquad \mathrm{i}\omega\rho_2\psi_2 = p'_2. \tag{1.2.28}$$

Hence, relations (1.2.25) lead to the following transmission conditions:

$$\frac{\partial\psi_1}{\partial n} = \frac{\partial\psi_2}{\partial n}, \qquad \rho_1\psi_1 = \rho_2\psi_2. \tag{1.2.29}$$

Comparing these conditions with relation (1.2.27) we can see that, in the case of the pressure formulation, the function which satisfies Helmholtz equations in two different domains is continuous, while its normal derivatives have a discontinuity. The opposite situation, when the normal derivative is continuous while the wave function itself has a jump on the boundary, is the case in terms of the velocity potential.

Note that, for acoustic waves in complex media (dispersion, dissipation, relaxation), conditions (1.2.27) and (1.2.29) should be modified according to the model of the media. Proper transmission conditions in this case can be obtained from general mass and momentum conservation relations (1.2.25) and specific equations of state for the medium, such as Eq. (1.1.21), written in the frequency domain.

1.2.2.2 Electromagnetic waves

Here we consider transmission conditions in the case when two dielectrics with electric permittivities ε_1 and ε_2 and magnetic permeabilities μ_1 and μ_2 are in contact over a surface S with normal $\mathbf{n}$. To match two solutions of the Maxwell equation we require that the tangential components of the vectors of electric and magnetic fields are continuous. These components can be found by taking the cross product of the respective vectors with the normal, and therefore, can be written in the phasor space as:

$$\mathbf{n}\times\hat{\mathbf{E}}_1 = \mathbf{n}\times\hat{\mathbf{E}}_2, \qquad \mathbf{n}\times\hat{\mathbf{H}}_1 = \mathbf{n}\times\hat{\mathbf{H}}_2. \tag{1.2.30}$$

1.2.3 Conditions on the boundaries

Conditions on the boundaries of domain 1 are used when either the properties of the boundary material (medium 2) are very different from the properties of medium 1 or can be modeled or assumed. In the former case the transmission conditions can be simplified and provide sufficient conditions for solution of the Helmholtz equation. In the latter case, simplification of the general problem usually follows from consideration of some model problem by applying the results to a more general case. Since such modeling is outside the scope of this book, we mention here the following basic types of boundary conditions for scalar wave equation and Maxwell equations. Here we assume that the domain of consideration is medium 1 (we also call it the host, carrier, or just a medium with no index), and the material of the boundary has the properties of medium 2 (we will drop the indexing if it is clear from the context). The normal derivative in each case is taken inward in to the domain of the carrier medium (direction from medium 2 to medium 1).

1.2.3.1 Scalar Helmholtz equation

- The Dirichlet boundary condition

$$\psi|_S = 0 \tag{1.2.31}$$

  appears, e.g. for complex amplitude pressure in acoustics, when the surface material has a very low acoustic impedance compared to the acoustic impedance of the carrier medium ($\rho_2 c_2 \ll \rho_1 c_1$). In this case the surface is called *sound soft*.
- The Neumann boundary condition

$$\left.\frac{\partial \psi}{\partial n}\right|_S = 0 \tag{1.2.32}$$

  in acoustics holds for complex amplitude of pressure, when the surface material has a much higher acoustic impedance than the acoustic impedance of the host medium ($\rho_2 c_2 \gg \rho_1 c_1$). In this case the surface is called *sound hard*.
- The Robin (or mixed, or impedance) boundary condition

$$\left.\left(\frac{\partial \psi}{\partial n} + i\sigma\psi\right)\right|_S = 0 \tag{1.2.33}$$

  in acoustics is used to model the finite acoustic impedance of the boundary. In this case σ is the admittance of the surface. Solutions of the Helmholtz equation with the Robin boundary condition in limiting cases $\sigma \to 0$ and $\sigma \to \infty$ turn into solutions of the same equation with the Neumann and Dirichlet boundary conditions, respectively.

The boundary value problems with those conditions are called the Dirichlet, Neumann, and Robin problems, respectively.

1.2.3.2 Maxwell equations

We mention here two cases important for wave scattering problems:

- Perfect conductor boundary condition

$$\mathbf{n} \times \hat{\mathbf{E}}|_S = 0. \tag{1.2.34}$$

  When we express the electric field vector via scalar potentials (1.1.53), this condition turns into

$$\mathbf{n} \times \nabla \times [\mathbf{r}\psi_1 + \nabla \times (\mathbf{r}\psi_2)]|_S = 0. \tag{1.2.35}$$

  This can also be modified for the more general representation (1.1.54).

- The Leontovich (or impedance) boundary condition

$$[\mathbf{n}\times\hat{\mathbf{H}} - \lambda(\mathbf{n}\times\hat{\mathbf{E}})\times\mathbf{n}]|_S = 0. \tag{1.2.36}$$

  Here λ is a constant called boundary impedance. In terms of scalar potentials (1.1.53) and (1.1.56) this can be written as:

$$\begin{aligned} &\mathbf{n}\times\nabla\times[(\mathrm{i}\lambda' + \nabla\times)(\mathbf{r}\psi_1) + (k^2 + \mathrm{i}\lambda'\nabla\times)(\mathbf{r}\psi_2)]|_S = \mathbf{0}, \\ &\lambda' = \mu ck\lambda. \end{aligned} \tag{1.2.37}$$

  Modification for more general forms can be achieved by substituting equations (1.1.54) and (1.1.57) into relation (1.2.36). We can also see that, in limiting case $\lambda' \to \infty$, condition (1.2.37) transforms to condition (1.2.35).

1.3 INTEGRAL THEOREMS

Integral equation approaches are fundamental tools in the numerical solution of the Helmholtz equation and equations related to it. These approaches have significant advantages for solving both external and internal problems. They also have a few disadvantages and we discuss both below.

A major advantage of these methods is that they effectively reduce the dimensionality of the domain over which the problem has to be solved. The integral equation statement reduces the problem to one of an integral over the surface of the boundary. Thus, instead of the discretization of a volume (or a region in 2D), we need only discretize surfaces (or curves in 2D). The problem of creating discretizations ("meshing") is well known to be a difficult task—almost an art—and the simplicity achieved by a reduction in dimensionality must not be underestimated. Further, the number of variables required to resolve a solution is also significantly reduced.

Another major advantage of the integral equation representation for external problems is that these ensure that the far-field Sommerfeld (or Silver–Müller conditions) are automatically exactly satisfied. Often volumetric discretizations must be truncated artificially and effective boundary conditions imposed on the artificial boundaries. While considerable progress has been made in developing so-called perfectly matched layers to imitate the properties of the far-field, these are relatively difficult to implement.

Despite these advantages the integral equation approaches have some minor disadvantages. The first is that their formulation is usually more complex mathematically. However, this need not be an obstacle to their understanding and implementation since there are many clear expositions of the integral equation approaches.

A second disadvantage of the integral equation approach is that it leads to linear systems with dense matrices. These dense matrices are expensive with which to perform computations. Many modern calculations require characterization of the scattering off complex shaped objects. While integral equation methods may allow such calculations, they can be relatively slow. The fast multipole methods discussed in this book alleviate this difficulty. They allow extremely rapid computation of the product of a vector with a dense matrix of the kind that arises upon discretization of the integral equation and go a long way towards alleviating this disadvantage.

Below we provide a brief introduction to the integral theorems and identities which serve as a basis for methods using integral formulations.

1.3.1 Scalar Helmholtz equation

1.3.1.1 Green's identity and formulae

Green's function

The free-space Green's function G for the scalar Helmholtz equation in three dimensions is defined as:

$$G(\mathbf{x}, \mathbf{y}) = \frac{\exp(\mathrm{i}k|\mathbf{x}-\mathbf{y}|)}{4\pi|\mathbf{x}-\mathbf{y}|}, \qquad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3. \tag{1.3.1}$$

As follows from the definition, this is a symmetric function of two spatial points $\mathbf{x}$ and $\mathbf{y}$:

$$G(\mathbf{x}, \mathbf{y}) = G(\mathbf{y}, \mathbf{x}), \tag{1.3.2}$$

and is a distance function between points $\mathbf{x}$ and $\mathbf{y}$. This function satisfies the equation:

$$\nabla^2 G(\mathbf{x}, \mathbf{y}) + k^2 G(\mathbf{x}, \mathbf{y}) = -\delta(\mathbf{x}-\mathbf{y}), \tag{1.3.3}$$

where $\delta(x-y)$ refers to the Dirac delta function (distribution) which is defined as:

$$\int_{\mathbb{R}^3} f(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})\mathrm{d}V(\mathrm{x}) = \begin{cases} f(\mathbf{y}), & \text{for } \mathbf{y} \in \mathbb{R}^3, \\ 0, & \text{otherwise.} \end{cases} \tag{1.3.4}$$

Here $f(\mathbf{x})$ is an arbitrary function and integration is taken over the entire space. The Green's function is thus a solution of the Helmholtz equation in the domain $\mathbf{x} \in \mathbb{R}^3 \backslash \mathbf{y}$ or $\mathbf{y} \in \mathbb{R}^3 \backslash \mathbf{x}$. Note that, in the entire space $\mathbb{R}^3$, the Green's function does not satisfy the Helmholtz equation, since the right-hand side of this equation is not zero everywhere. The equation which it satisfies is a *non-uniform Helmholtz equation*. Generally written as

$$\nabla^2 \psi(\mathbf{r}) + k^2 \psi(\mathbf{r}) = -f(\mathbf{r}), \tag{1.3.5}$$

it is a wave analog (in the frequency domain) of the Poisson equation (the case $k = 0$), which has in the right-hand side some function $f(\mathbf{r})$ responsible for the spatial distribution of charges (or sources).

This "impulse response" of the Helmholtz equation is a fundamental tool for studying the Helmholtz equation. It is also referred to as the point source solution or the fundamental solution.

Divergence theorem

The following theorem from Gauss relates an integral over a domain $\Omega \subset \mathbb{R}^3$ to the surface integral over the boundary S of this domain:

$$\int_\Omega (\nabla \cdot \mathbf{u}) \mathrm{d}V = \int_S (\mathbf{n} \cdot \mathbf{u}) \mathrm{d}S, \tag{1.3.6}$$

where $\mathbf{n}$ is the normal vector on the surface S that is outward to the domain Ω. This theorem holds for finite or infinite domains assuming that the integrals converge. In generalized informal form for n-dimensional space, the divergence theorem can be written as:

$$\int_{\Omega^n} (\nabla \circ \mathbf{A}) \mathrm{d}V = \int_{\partial\Omega^n} (\mathbf{n} \circ \mathbf{A}) \mathrm{d}S, \qquad \Omega^n \subset \mathbb{R}^n, \tag{1.3.7}$$

where $\circ$ is any operator and $\mathbf{A}$ is a scalar or vector quantity for which $\circ$ is defined.

Green's integral theorems

These theorems play a role analogous to the familiar "integration by parts" in the case of integration over the line. Recall that, for integrals over a line, we can write:

$$\int_a^b u \, \mathrm{d}v = -\int_a^b v \, \mathrm{d}u + (uv)|_a^b. \tag{1.3.8}$$

Green's first integral theorem states that for a domain Ω with boundary S, given two functions $u(\mathbf{x})$ and $v(\mathbf{x})$, we can write:

$$\int_\Omega (u \nabla^2 v + \nabla u \cdot \nabla v) \mathrm{d}V = \int_\Omega \nabla \cdot (u \nabla v) \mathrm{d}V = \int_S \mathbf{n} \cdot (u \nabla v) \mathrm{d}S, \tag{1.3.9}$$

where we have used the divergence theorem on the quantity $u\nabla v$. This formula may be put into a form that is reminiscent of the formula of integration by parts by rearranging terms

$$\int_{\Omega} u\nabla\cdot(\nabla v)\mathrm{d}V = -\int_{\Omega} \nabla u\cdot\nabla v\,\mathrm{d}V + \int_{S} u(\mathbf{n}\cdot\nabla v)\mathrm{d}S, \tag{1.3.10}$$

where we observe that the derivative operator has been exchanged from the function v to the function u, and that the boundary term has appeared.

To derive *Green's second integral theorem*, we write Eq. (1.3.9) by exchanging the roles of u and v, as:

$$\int_{\Omega} (v\nabla^2 u + \nabla u\cdot\nabla v)\mathrm{d}V = \int_{S} v(\mathbf{n}\cdot\nabla u)\mathrm{d}S, \tag{1.3.11}$$

and subtract it from Eq. (1.3.9). This yields:

$$\int_{\Omega} (u\nabla^2 v - v\nabla^2 u)\mathrm{d}V = \int_{S} \mathbf{n}\cdot(u\nabla v - v\nabla u)\mathrm{d}S. \tag{1.3.12}$$

This equation can also be written as:

$$\int_{\Omega} u\nabla^2 v\,\mathrm{d}V = \int_{\Omega} v\nabla^2 u\,\mathrm{d}V + \int_{S} \mathbf{n}\cdot(u\nabla v - v\nabla u)\mathrm{d}S. \tag{1.3.13}$$

Green's formula

Let us consider a domain Ω with boundary S. Using the sifting property of the delta function (1.3.4) we may write for a given function ψ at a point $\mathbf{y} \in \Omega$:

$$\int_{\Omega} \psi(\mathbf{x})\delta(\mathbf{x} - \mathbf{y})\mathrm{d}V(\mathbf{x}) = \psi(\mathbf{y}), \qquad \mathbf{y} \in \Omega. \tag{1.3.14}$$

Using Eq. (1.3.3) the function may be written as:

$$\psi(\mathbf{y}) = -\int_{\Omega} \psi(\mathbf{x})[\nabla_{\mathbf{x}}^2 G(\mathbf{x},\mathbf{y}) + k^2 G(\mathbf{x},\mathbf{y})]\mathrm{d}V(\mathbf{x}), \tag{1.3.15}$$

where $\nabla_{\mathbf{x}}$ is the nabla operator with respect to variable $\mathbf{x}$. Using Green's second integral theorem (1.3.13), where we set $u = \psi$ and $v = G$, we can write the above as:

$$\psi(\mathbf{y}) = -\int_{\Omega} k^2\psi(\mathbf{x})G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x}) - \int_{\Omega} G(\mathbf{x},\mathbf{y})(\nabla_{\mathbf{x}}^2\psi)\mathrm{d}V(\mathbf{x})$$
$$- \int_S \mathbf{n}\cdot[\psi(\mathbf{x})\nabla_{\mathbf{x}}G(\mathbf{x},\mathbf{y}) - G(\mathbf{x},\mathbf{y})\nabla_{\mathbf{x}}\psi(\mathbf{x})]\mathrm{d}S(\mathbf{x})$$
$$= -\int_{\Omega} [\nabla_{\mathbf{x}}^2\psi(\mathbf{x}) + k^2\psi(\mathbf{x})]G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x})$$
$$- \int_S \mathbf{n}\cdot[\psi(\mathbf{x})\nabla_{\mathbf{x}}G(\mathbf{x},\mathbf{y}) - G(\mathbf{x},\mathbf{y})\nabla_{\mathbf{x}}\psi(\mathbf{x})]\mathrm{d}S(\mathbf{x}). \quad (1.3.16)$$

Let us assume now that the function $\psi(\mathbf{x})$ satisfies the non-uniform Helmholtz equation (1.3.5). Then we see that the solution to this equation can be written as:

$$\psi(\mathbf{y}) = \int_{\Omega} f(\mathbf{x})G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x}) - \int_S \mathbf{n}\cdot[\psi(\mathbf{x})\nabla_{\mathbf{x}}G(\mathbf{x},\mathbf{y})$$
$$- G(\mathbf{x},\mathbf{y})\nabla_{\mathbf{x}}\psi(\mathbf{x})]\mathrm{d}S(\mathbf{x}). \quad (1.3.17)$$

If the domain has no boundaries, we see that the solution to the problem is obtained as a convolution of the right-hand side with the impulse response:

$$\psi(\mathbf{y}) = \int_{\Omega} f(\mathbf{x})G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x}). \quad (1.3.18)$$

Let us consider the case when ψ in domain Ω satisfies the Helmholtz equation, or Eq. (1.3.5) with $f = 0$. Then relation (1.3.17) provides us with the solution for ψ in the domain from its boundary values:

$$\psi(\mathbf{y}) = \int_S \left[G(\mathbf{x},\mathbf{y})\frac{\partial\psi(\mathbf{x})}{\partial n(\mathbf{x})} - \psi(\mathbf{x})\frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})}\right]\mathrm{d}S(\mathbf{x}), \quad (1.3.19)$$
$$\mathbf{y} \in \Omega, \quad \mathbf{n} \text{ directed outside } \Omega,$$

where we denoted $\partial/\partial n(\mathbf{x}) = \mathbf{n}\cdot\nabla_{\mathbf{x}}$.

The obtained equation is valid for the case when $\mathbf{y}$ is in the domain (and not on the boundary). In the case of infinite domains, function $\psi(\mathbf{y})$ satisfies the Sommerfeld condition as $|\mathbf{y}| \to \infty$. This equation is also called the Helmholtz integral equation or the Kirchhoff integral equation. Note that we derived this equation assuming that $\mathbf{n}$ is the normal directed outward the domain Ω. In the case of infinite domains, when S is the surface of some body (scatterer), usually the opposite direction of $\mathbf{n}$ is used, since it is defined as a normal *outer to the body*. In the case of this definition of the normal, which we also accept for the solution of scattering problems, Green's formula is:

$$\psi(\mathbf{y}) = \int_S \left[\psi(\mathbf{x}) \frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})} - G(\mathbf{x},\mathbf{y}) \frac{\partial \psi(\mathbf{x})}{\partial n(\mathbf{x})} \right] \mathrm{d}S(\mathbf{x}), \tag{1.3.20}$$

$$\mathbf{y} \in \Omega, \quad \mathbf{n} \text{ directed inside } \Omega.$$

If ψ and $\partial\psi/\partial n$ vanish at the boundary, or more generally in a region, the above equation says that ψ vanishes identically.

1.3.1.2 Integral equation from Green's formula for ψ

In general a well-posed problem for ψ that satisfies Helmholtz equation will specify boundary conditions for ψ (Dirichlet boundary conditions (1.2.31)) or for its normal derivative $\partial\psi/\partial n$ (Neumann boundary conditions (1.2.32)) or for some combination of the two (Robin or "impedance" boundary condition (1.2.33)), but not both ψ and $\partial\psi/\partial n$. Thus at the outset we will only know either ψ or $\partial\psi/\partial n$ or a combination of them on the boundary, but not both. However, to compute ψ in the domain using Eq. (1.3.20), both ψ and $\partial\psi/\partial n$ are needed on the boundary.

To obtain both these quantities, we can take the ψ on the right-hand side to lie on the boundary. However, there are two issues with this. First, the Green's function G is singular when $\mathbf{x} \to \mathbf{y}$ so we need to consider the behavior of the integrals involving G and $\mathbf{n}\cdot\nabla G$ for $\mathbf{y}$ on the boundary and as $\mathbf{x} \to \mathbf{y}$. Second, we derived this formula using the definition of the δ function, where we assumed that the point $\mathbf{y}$ was in the domain.

Our intuition would be that, if the point $\mathbf{y}$ were on a smooth portion of the boundary, it would include half the effect of the δ function. If $\mathbf{y}$ were at a corner it would include a fraction of the local volume determined by the solid angle, γ, subtended in the domain by that point. In fact the analysis will mostly bear out this intuition, and the equation for ψ when $\mathbf{y}$ is on the boundary is:

$$\alpha\psi(\mathbf{y}) = \int_S \left(\psi(\mathbf{x}) \frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})} - G(\mathbf{x},\mathbf{y}) \frac{\partial \psi(\mathbf{x})}{\partial n(\mathbf{x})} \right) \mathrm{d}S(\mathbf{x}),$$

$$\alpha = \begin{cases} 1/2 & y \text{ on a smooth part of the boundary} \\ \gamma/4\pi & y \text{ at a corner on the boundary} \\ 1 & y \text{ inside the domain} \end{cases} \tag{1.3.21}$$

Using the boundary condition for ψ or $\partial\psi/\partial n$, we can solve for the unknown component on the boundary. Once the boundary values are known we can obtain ψ elsewhere in the domain. The only caveat is that, for a given boundary condition, there are some wavenumbers k at which the integral on the boundary vanishes, even though the solution exists.

The theory of layer potentials provides a way to study these integrals, identify the problems associated with them, and avoid these problems.

1.3.1.3 Solution of the Helmholtz equation as distribution of sources and dipoles

Distribution of sources

The Green's function $G(x, y)$ can be interpreted in acoustics as the potential or free space field measured at point $\mathbf{y}$ and generated by a point source of unit intensity located at $\mathbf{x}$. Due to symmetry of Green's function with respect to its arguments, the locations of the field point and the source can be exchanged. This gives rise to the so-called *reciprocity principle*, which can be written in more general terms, but we do not proceed with this issue here. If we are interested in solutions of the Helmholtz equation in some domain Ω to which $\mathbf{y}$ belongs, owing to the linearity of this equation we can decompose the solution to a sum of linearly independent functions, such that each function satisfies the Helmholtz equation in this domain. A set of Green's functions corresponding to sources located at various points *outside* Ω is a good candidate for this decomposition.

Some problems naturally provide a distribution of sources. For example, if one considers computation of a sound field generated by N speakers which emit sound in all directions more or less uniformly (omnidirectional speakers), and the size of the speakers is much smaller than the scale of the problem considered, then the field can be modeled as:

$$\psi(\mathbf{y}) = \sum_{j=1}^{N} Q_j G(\mathbf{x}_j, \mathbf{y}), \qquad \mathbf{y} \in \mathbb{R}^3 \backslash \{\mathbf{x}_j\}, \tag{1.3.22}$$

where Q_j and $\mathbf{x}_j$ are the intensity and location of the jth speaker, respectively.

In a more general case we can consider a continuous analog of these formulae and represent the solution in the form:

$$\psi(\mathbf{y}) = \int_{\bar{\Omega}} q(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) \mathrm{d}V(\mathbf{x}), \qquad \mathbf{y} \in \Omega, \ \ \bar{\Omega} \cap \Omega = \emptyset. \tag{1.3.23}$$

Here $q(\mathbf{x})$ is the distribution of source intensities, or *volume density* of sources and integration is taken over domain $\bar{\Omega}$, which is outer to Ω. In the case if $\bar{\Omega}$ is finite and Ω is infinite, the nice thing is that $\psi(\mathbf{y})$ satisfies the Sommerfield radiation conditions automatically. The problem then is to find an appropriate for particular problem distribution of sources $q(\mathbf{x})$. This can be done, say by solving appropriate integral equations.

Single layer potential

A particularly important case for construction of solutions of the Helmholtz equation is the case when all the sources are located on the surface S, which is the boundary of domain Ω. In this case, instead of integration over the volume, we can sum up all the sources over the surface:

$$\psi(\mathbf{y}) = \int_S q_\sigma(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) \mathrm{d}S(\mathbf{x}), \qquad \mathbf{y} \in \Omega, \quad S = \partial\Omega. \tag{1.3.24}$$

Function $q_\sigma(\mathbf{x})$ is defined on the surface points and is called the *surface density* of sources. Being represented in this form, function $\psi(\mathbf{y})$ is called the *single layer potential*. The term "single layer" is historical, and comes here to denote that we have only one "layer" of sources (one can imagine each source as a tiny ball and a surface covered by one layer of these balls).

Dipoles

Once we have two sources of intensities Q_1 and Q_2 located at $\mathbf{x}_1$ and $\mathbf{x}_2$, we can consider a field generated by this pair in the assumption that $\mathbf{x}_1$ and $\mathbf{x}_2$ are very close to each other. The field due to the pair is omnidirectional and we have:

$$\psi(\mathbf{y}) = \lim_{x_1 \to x_2} [Q_1 G(\mathbf{x}_1, \mathbf{y}) + Q_2 G(\mathbf{x}_2, \mathbf{y})] = (Q_1 + Q_2) G(\mathbf{x}_2, \mathbf{y}). \tag{1.3.25}$$

Assume now that $Q_1 = -Q_2 = 1$. The above equation shows that in this case $\psi(\mathbf{y}) \equiv 0$. Since $\psi(\mathbf{y})$ is not zero at $\mathbf{x}_1 \neq \mathbf{x}_2$ and zero otherwise, we can assume that it is proportional to the distance $|\mathbf{x}_1 - \mathbf{x}_2|$ (the validity of this assumption is clear from the further consideration):

$$\psi(\mathbf{y}) = |\mathbf{x}_2 - \mathbf{x}_1| M(\mathbf{x}_2, \mathbf{y}) + o(|\mathbf{x}_2 - \mathbf{x}_1|), \qquad |\mathbf{x}_2 - \mathbf{x}_1| \to 0 \tag{1.3.26}$$

Then we can determine the first order term as:

$$M^{(\mathbf{p})}(\mathbf{x}_2, \mathbf{y}) = \lim_{\mathbf{x}_1 \to \mathbf{x}_2} \frac{G(\mathbf{x}_1, \mathbf{y}) - G(\mathbf{x}_2, \mathbf{y})}{|\mathbf{x}_2 - \mathbf{x}_1|} = -\mathbf{p} \cdot \nabla_{\mathbf{x}} G(\mathbf{x}_2, \mathbf{y}),$$
$$\mathbf{p} = \frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_2 - \mathbf{x}_1|}. \tag{1.3.27}$$

The obtained solution is called *dipole* ("two poles"). While this function satisfies the Helmholtz equation at $\mathbf{x} \neq \mathbf{y}$, we can see that, in contrast to the source, the field of the dipole is not omnidirectional, but has one preferred direction specified by vector $\mathbf{p}$, which is called the *dipole moment*. As we can see, this direction is determined by the relative location of the positive and negative sources generating the multipole.

Distribution of dipoles and double layer potential

The field of the dipole is different from the field of the monopole, so the dipole $M^{(\mathbf{p})}(\mathbf{x}, \mathbf{y})$ presents another solution of the Helmholtz equation, singular at $\mathbf{x} = \mathbf{y}$. As earlier, we can then construct a solution of the Helmholtz equation as a sum of dipoles with different intensities and moments distributed in space. As in the case with omnidirectional speakers, some problems can be solved immediately if the singularity is modeled as a dipole. By the way, in modeling of speakers, dipoles are also used to model the fact that the sound from the speaker comes in a certain direction. So the sound field generated by a set of N-directional speakers with intensities Q_j and dipole moments p_j will be:

$$\psi(\mathbf{y}) = \sum_{j=1}^{N} Q_j M^{(\mathbf{p}_j)}(\mathbf{x}_j, \mathbf{y}), \qquad \mathbf{y} \in \mathbb{R}^3 \backslash \{\mathbf{x}_j\}. \tag{1.3.28}$$

This can be generalized for continuous distributions. The case of particular interest is the field generated by a set of dipoles which are distributed over the boundary of the domain whose moments are directed as the normal to the surface. The potential of the field in this case is called the *double layer potential* and can be written according to definition (1.3.27) as:

$$\psi(\mathbf{y}) = \int_S q_\mu(\mathbf{x}) \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{x})} \mathrm{d}S(\mathbf{x}), \qquad \mathbf{y} \in \Omega, \qquad S = \partial\Omega. \tag{1.3.29}$$

Here function $q_\mu(\mathbf{x})$ is a distributed strength of the dipoles or the surface density of dipoles. The term "double layer" is clear in the context of the representation of a dipole as a superposition of the fields due to negative and positive sources (so if one imagines each source as a tiny ball, then the surface should be covered by two layers, positive and negative, of these balls).

Connection to the Green's formula

Green's formula (1.3.20) provides an amazing finding that any solution $\psi(\mathbf{y})$ of the Helmholtz equation in an arbitrarily shaped domain can be represented as a sum of single and double layer potentials (1.3.24) and (1.3.29) with surface densities $q_\sigma(\mathbf{x}) = -\partial\psi/\partial n(\mathbf{x})$ and $q_\mu(\mathbf{x}) = \psi(\mathbf{x})$, respectively. The surface densities here are expressed via the values of the function itself.

1.3.2 Maxwell equations

In the case of Maxwell equations, which can be reduced to two vector Helmholtz equations for the phasors of the electric and magnetic field vectors with additional conditions that the fields should be solenoidal, the concept of Green's function can be generalized to handle the vector case and represent the field as a sum of corresponding vector (in fact, tensor) Green's functions.

To derive the Green's function for the Maxwell equation, we remind ourselves that the Green's function is not a solution of the Helmholtz or Maxwell equations in the entire space, since this function is singular at the location of a charge (or source). The Maxwell equations as written in form (1.1.36) do not have any terms which generate the electromagnetic field and describe the propagation of waves generated somewhere in the source/current free domain. These equations can be modified to include generators of the electromagnetic field. In fact, for homogeneous media ($\mu, \varepsilon = \text{const}$), we can modify only the second and the third equations in Eq. (1.1.36) as:

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}, \qquad \varepsilon \nabla \cdot \mathbf{E} = \rho, \tag{1.3.30}$$

where $\mathbf{J}$ is the current density and ρ is the charge density. These equations in the frequency domain take the form:

$$\nabla \times \hat{\mathbf{H}} = -\mathrm{i}\omega\varepsilon\hat{\mathbf{E}} + \hat{\mathbf{J}}, \qquad \varepsilon \nabla \cdot \hat{\mathbf{E}} = \hat{\rho}, \tag{1.3.31}$$

where $\hat{\mathbf{J}}$ and $\hat{\rho}$ are the phasors of $\mathbf{J}$ and ρ. Taking the divergence of the first equation and using the second equation, we can see that:

$$\mathbf{0} = -\mathrm{i}\omega\varepsilon\nabla \cdot \hat{\mathbf{E}} + \nabla \cdot \hat{\mathbf{J}} = -\mathrm{i}\omega\hat{\rho} + \nabla \cdot \hat{\mathbf{J}}. \tag{1.3.32}$$

To obtain a single equation for $\hat{\mathbf{E}}$ we substitute expression of the magnetic field phasor (1.1.55) via $\hat{\mathbf{E}}$ into the first equation (1.3.31). This yields

$$\nabla \times \nabla \times \hat{\mathbf{E}} - k^2\hat{\mathbf{E}} = \mathrm{i}\omega\mu\hat{\mathbf{J}}. \tag{1.3.33}$$

Owing to vector identity $\nabla \times \nabla \times = -\nabla^2 + \nabla(\nabla \cdot)$ we have from this equation and Eq. (1.3.32):

$$\begin{aligned} \nabla^2\hat{\mathbf{E}} + k^2\hat{\mathbf{E}} &= \frac{1}{\varepsilon}\nabla\hat{\rho} - \mathrm{i}\omega\mu\hat{\mathbf{J}} = -\mathrm{i}\omega\mu\left[\hat{\mathbf{J}} + \frac{1}{\varepsilon\mu\omega^2}\nabla(\nabla \cdot \hat{\mathbf{J}})\right] \\ &= -\mathrm{i}\omega\mu\left(\mathbf{I} + \frac{1}{k^2}\nabla\nabla\right) \cdot \hat{\mathbf{J}}. \end{aligned} \tag{1.3.34}$$

Here, assuming that the reader is familiar with elements of tensor analysis (otherwise we recommend reading definitions from appropriate handbooks), we introduced notation $\mathbf{I}$ and $\nabla\nabla$ for *second rank tensors*, or *dyadics*, which are represented in the three-dimensional case by the following 3×3 symmetric matrices in the basis of Cartesian coordinates:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \nabla\nabla = \begin{pmatrix} \dfrac{\partial^2}{\partial x^2} & \dfrac{\partial^2}{\partial x\,\partial y} & \dfrac{\partial^2}{\partial x\,\partial z} \\ \dfrac{\partial^2}{\partial x\,\partial y} & \dfrac{\partial^2}{\partial y^2} & \dfrac{\partial^2}{\partial y\,\partial z} \\ \dfrac{\partial^2}{\partial x\,\partial z} & \dfrac{\partial^2}{\partial y\,\partial z} & \dfrac{\partial^2}{\partial z^2} \end{pmatrix}. \tag{1.3.35}$$

There are two ways to proceed with the representation of solutions of the *non-uniform* Maxwell equations. In fact, they lead to the same result, and the difference is from a methodological point of view. The first way is based simply on a notice that the vector non-uniform Helmholtz equation (1.3.34) is nothing but a set of three scalar equations for each Cartesian component of the phasor of the electric field vector. For example, taking a scalar product with $\mathbf{i}_x$ of each term of Eq. (1.3.34), we obtain the following scalar equation for the x component:

$$\nabla^2 \hat{E}_x + k^2 \hat{E}_x = -\mathrm{i}\omega\mu\left[\left(\mathbf{I} + \frac{\nabla\nabla}{k^2}\right)\cdot\hat{\mathbf{J}}\right]\cdot\mathbf{i}_x = -\mathrm{i}\omega\mu\left[\hat{J}_x + \frac{\partial}{\partial x}(\nabla\cdot\hat{\mathbf{J}})\right], \tag{1.3.36}$$
$$\hat{E}_x = \hat{\mathbf{E}}\cdot\mathbf{i}_x, \qquad \hat{J}_x = \hat{\mathbf{J}}\cdot\mathbf{i}_x.$$

The solution of this equation for free space, which is Eq. (1.3.5), can be obtained using the scalar Green's function (1.3.18):

$$\hat{E}_x(\mathbf{y}) = \mathrm{i}\omega\mu \int_{\bar{\Omega}} \left[\hat{J}_x(\mathbf{x}) + \frac{\partial}{\partial x}(\nabla_{\mathbf{x}}\cdot\hat{\mathbf{J}}(\mathbf{x}))\right] G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x}). \tag{1.3.37}$$

Here we assumed that, in domain Ω, which is outside some domain $\bar{\Omega}$, there are no imposed currents, $\hat{\mathbf{J}}(\mathbf{x}) = \mathbf{0}$. Writing similar equations for the other two components of $\hat{\mathbf{E}}$, we can summarize the result in one vector formula:

$$\hat{\mathbf{E}}(\mathbf{y}) = \mathrm{i}\omega\mu \int_{\bar{\Omega}} \left[\hat{\mathbf{J}}(\mathbf{x}) + \nabla_{\mathbf{x}}(\nabla_{\mathbf{x}}\cdot\hat{\mathbf{J}}(\mathbf{x}))\right] G(\mathbf{x},\mathbf{y})\mathrm{d}V(\mathbf{x}). \tag{1.3.38}$$

If $\mathbf{y}$ is from a domain free of imposed currents, $\mathbf{y} \in \Omega$, $\bar{\Omega} \cap \Omega = \emptyset$, then, as follows from Eqs. (1.3.32) and (1.3.34), the phasor of the electric field vector satisfies uniform Maxwell equations (1.1.42). This is a situation, similar to the scalar case (1.3.23), where we constructed a solution of the Helmholtz equation by placing sources outside the domain. In the case of Maxwell equations, instead of some scalar field $q(\mathbf{x})$ characterizing the source density distribution, we have a vector field $\hat{\mathbf{J}}(\mathbf{x})$ or *current density distribution*. As in the scalar case, the problem is to determine this unknown distribution and this can be done by different methods, including boundary integral equations. Indeed, we can derive these equations in the same way as we derived Eq. (1.3.38) by considering scalar equations for each component of the electric field vector.

The second way is to introduce dyadic Green's function immediately as a solution of Maxwell equations (1.1.42) everywhere in free space except for one singular point, where the solution blows up. This is the way we introduced the scalar Green's function (1.3.3). The "impulse response" of Maxwell equations can be found by solving the following equation for dyadic Green's function:

$$-\nabla \times \nabla \times \mathbf{G}(\mathbf{x}, \mathbf{y}) + k^2 \mathbf{G}(\mathbf{x}, \mathbf{y}) = -\mathbf{I}\delta(\mathbf{x} - \mathbf{y}). \tag{1.3.39}$$

This form is dictated first by Eq. (1.3.33), where we should assume that the source term is due to currents in the domain, which can be contracted into one point. Second, representing $\hat{\mathbf{E}}(\mathbf{y})$ as a convolution of $\hat{\mathbf{J}}(\mathbf{x})$ with the impulse response function

$$\hat{\mathbf{E}}(\mathbf{y}) = -\mathrm{i}\omega\mu \int_{\bar{\Omega}} \mathbf{G}(\mathbf{x}, \mathbf{y}) \cdot \hat{\mathbf{J}}(\mathbf{x}) \mathrm{d}V(\mathbf{x}), \tag{1.3.40}$$

we can see, comparing this result with relation (1.3.38), that $\mathbf{G}(\mathbf{x}, \mathbf{y})$ should be a second rank tensor.

Function $\mathbf{G}(\mathbf{x}, \mathbf{y})$ defined by Eq. (1.3.39) can be related to scalar Green's function (1.3.1). The relation is:

$$\mathbf{G}(\mathbf{x}, \mathbf{y}) = \left(\mathbf{I} + \frac{1}{k^2} \nabla_{\mathbf{x}} \nabla_{\mathbf{x}}\right) G(\mathbf{x}, \mathbf{y}), \tag{1.3.41}$$

and can be checked by substitution into Eq. (1.3.40) followed by integration by parts to obtain form (1.3.38). It is interesting to note that the dyadic Green's function for Maxwell equations involves not only $G(\mathbf{x}, \mathbf{y})$, but also the second derivatives of this function. As will be shown in Chapter 2, the second derivatives of a *monopole* ($G(\mathbf{x}, \mathbf{y})$) can be expressed in terms of dipoles and *quadrupoles*.

However, if the statement of the problem allows determination of $\hat{\mathbf{E}}$, then $\hat{\mathbf{H}}$ can be found simply from relation (1.1.55) and the problems for $\hat{\mathbf{H}}$ can be considered in terms of this vector only. This is due to an obvious symmetry between $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ in the free space Maxwell equations (one can replace these vectors taking care with constants and signs).

Consideration of the solution for $\hat{\mathbf{E}}$ given above is physics based, since it operates with such terms as “charges” and “currents”. It is noteworthy that, despite there being no magnetic charges in the Maxwell equations, one can nonetheless introduce “fictitious” magnetic charges and currents *outside* the domain, where solution of the free-field Maxwell equations should be obtained, as a *mathematical* trick. Indeed, relation (1.3.38) provides integral representation for solenoidal solutions of the vector Helmholtz equation in the domain free of charges ($\mathbf{y} \in \Omega, \bar{\Omega} \cap \Omega = \emptyset$), which is the equation for solenoidal vector $\hat{\mathbf{H}}$.

1.4 WHAT IS COVERED IN THIS BOOK AND WHAT IS NOT

The research field of acoustics and electromagnetics is huge and every year hundreds of publications in the form of papers, technical reports, monographs, and text books extend the knowledge in this field. Thus the objective of the book is far from giving a review of all these materials or the state of art in the entire field. We also did not have as an objective to provide the basics of wave theory, for which we can refer the reader to several well-written books on the fundamentals of acoustics [FHLB99, LL75, MI68] and electromagnetics [Che90, Jac75, LL60]. The book is also not about the field of differential equations or pure mathematics dedicated to the theory of elliptic equations and, particularly, the Helmholtz equation.

Trying to present some mathematical theory which can be applied to a solution of the Helmholtz equation, we focus on some issues that are important from the computational point of view, and therefore, miss several cases of this equation. For example, in the book we consider only the three-dimensional case for the scalar Helmholtz equation. The two-dimensional Helmholtz equation has its own beauty and symmetries and, while the translation theory for this case appears to be simpler than in three dimensions, this case deserves separate consideration for fast computational methods.

Another item missed is the theory for Maxwell equations. While these equations can be reduced to a solution of scalar wave equations and solved with the methods described in this book, efficient application of multipole methods here seems to require a deeper study of operations with vector or tensor spherical harmonics. Despite the fact that the technique for fast operations with vector spherical harmonics and vector spherical basis functions is currently developed in many aspects, we considered that putting this technique in the present book will make it less transparent and, since it cannot be understood without the basics of translation theory for scalar spherical harmonics, that we should present this theory elsewhere.

As can be seen from the present chapter, the Helmholtz equation can appear in various physical problems with complex k. Most results from the translation theory described in this book are universal and can be applied for any $k \neq 0$. However, since our focus was on the case of real k, we do not provide results such as error bounds for the case when the imaginary part of k is not zero. It can be argued that, in the case of complex k due to exponential decay of solutions, these solutions should be "better" than in the case of real k, and the case of real k is, in fact, the more difficult case. In our view, this situation requires a separate study and again must be presented elsewhere.