

Lecture 15 — February 23, 2016

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1 Outline

Agenda: Wave optics¹

1. The phenomenon of diffraction
2. History of diffraction²
3. Mathematical preliminaries
4. (Fresnel-Kirchhoff) Rayleigh-Sommerfeld theory

Last Time: We concluded our study of magnetic resonance imaging (MRI) by discussing imaging methods weighted by relaxation times, as well as the use of gradient fields to allow for selective excitation. These topics completed for us a high-level understanding of nuclear magnetic resonance (NMR), and how it is exploited (with the help of Fourier analysis via the signal equation) to produce a remarkable imaging modality.

2 Diffraction

Let us quickly dispel a common confusion: diffraction is not refraction. And perhaps less often confused, refraction is not reflection. For the sake of completeness, let us first briefly review these latter two concepts, which should be familiar to us. It is important to note that reflection and refraction are derived from **geometric optics**, in which light is modeled by straight-line rays.

Reflection occurs when a ray encounters a material surface, and as a consequence, it reflects off this surface (see Fig. 1a). We observe this very clearly when a mirror is placed in the trajectory of a light ray. The principle that describes reflection, properly named the **Law of Reflection**, establishes that

1. The incident ray, the reflected ray, and the direction normal to the surface (at the point of incidence), lie in a common plane.

¹An excellent text and resource is J. Goodman, *“Introduction to Fourier optics”*, 3rd edition, Roberts and Company Publishers, 2005.

²See, for instance, H.C. Hoerber, K. Klem-Musatov, T.J. Moser and M. Pelissier, *“Diffraction – A Historical Perspective”*, 72nd EAGE Conference & Exhibition, June 2010.

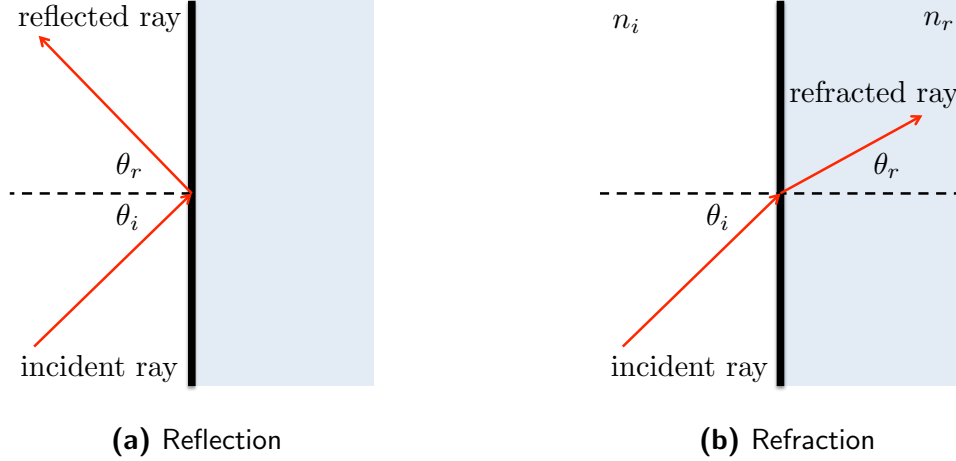


Figure 1: In geometric optics, the propagation of light is explained by three main effects: propagation along rectilinear paths, reflection on surfaces, and refraction at the interface between two translucent, homogeneous media. **(a) Reflection:** The angle that the incident ray forms with the normal direction to the surface is the same as that of the reflected ray and the normal direction. **(b) Refraction:** When light passes from one translucent, homogeneous medium to another, the difference of the angle θ_i , between the incident ray and the normal direction, to the angle θ_r , between the refracted ray and the normal direction, is determined by Snell's law (1).

2. The incident and the reflected ray form the same angle with the normal direction (at the point of incidence).

Refraction occurs when a ray encounters a surface that separates two different media through which light propagates at different speeds (see Fig. 1b). As a consequence, the ray bends. This effect is described by **Snell's law**. If we denote by θ_i and θ_r the angles that the incident and refracted ray, respectively, form with the normal direction, then

$$n_i \sin \theta_i = n_r \sin \theta_r, \quad (1)$$

where n_i and n_r are the ratios of the speed of light in a vacuum to the speed of light in the propagation medium of the incident and refracted rays, respectively. In particular, $n_i, n_r \geq 1$ (i.e. light travels most quickly in a vacuum).

These are simple rules that describe what happens when a ray encounters an **interface**. There are, however, many phenomena not explained by these principles. Historically, these have been identified from experiments in which light traverses an **aperture** (see Fig. 2). Roughly speaking, an aperture is an opening within an opaque surface, allowing light to pass through. For us, the opaque surface will be planar. If we place an aperture between a source and a screen parallel to the aperture, geometric optics would predict a solid bright shape on the screen, matching the shape of the aperture. But this is not the case, as we observe **interference patterns** on the screen.

To properly understand these phenomenon, then, we need a more accurate description of light. From physics, we have learned that the correct interpretation of light is as a *wave*. And generally speaking, waves can scatter. That is, their direction of propagation can be deflected due to inhomogeneities in the medium through which they propagate. Of particular interest to us will be the phenomenon of **diffraction**, which is caused by the confinement of the lateral extent of a light

wave. An aperture is precisely the type of inhomogeneity that causes this confinement (again, see Fig. 2).

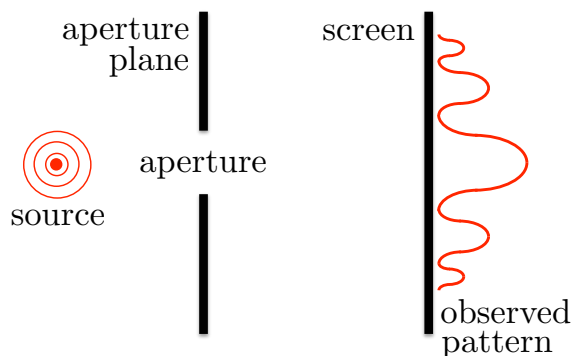
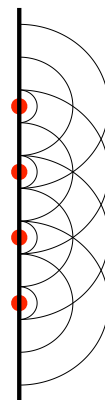


Figure 2: Generic setup for diffraction experiments.

3 History

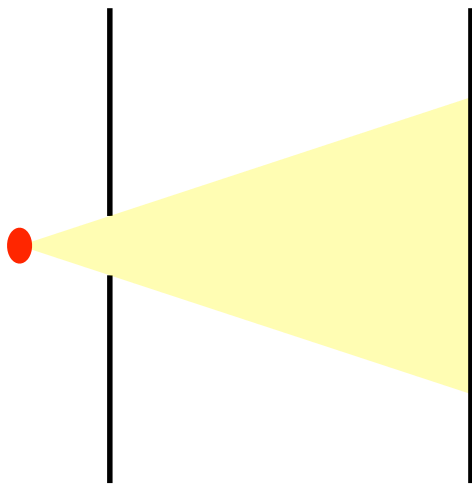
In 1665, Francesco Maria Grimaldi (1618-1663) performed several experiments with apertures that suggested light need not propagate along rectilinear paths. The images he witnessed on the observation plane did not match the shape of the apertures. The sharp boundaries one would expect from geometric optics were replaced by blurred patterns of light and dark regions. The patterns change with the size and shape of the aperture (see Fig. 3). He gave this unexpected behavior the name *diffraction*, which literally means “to break in different directions.”

Not long after, in 1678, Christiaan Huygens (1629-1695) submitted his thesis on a **wave theory** of light to the French Academy of Sciences. In his work, later published in 1690, Huygens introduced a construction now known as the **Huygens-Fresnel principle**. This principle proposes that every point in a wave front is the source of a spherical wave, acting as a secondary source of light to other points. The superposition of these secondary sources is supposed to determine the evolution of wave front (see right). This theory was able to at least partially explain the diffraction phenomena, as apertures are seen to remove some of the secondary sources. The remaining sources continue to propagate spherically, giving rise to an image distinct from the aperture.

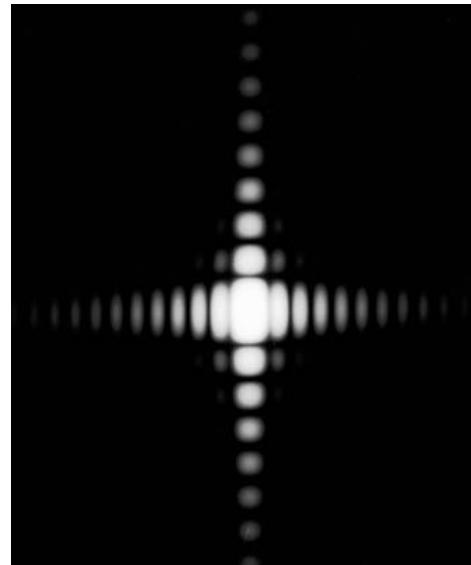


In 1704, Isaac Newton (1642-1727) published his book *Optiks*, in which he set forth his **corpuscular theory** of light. He rejected Huygen’s idea that light was composed of waves, arguing instead that it is composed of small, *discrete* particles called corpuscles. This allowed for a reasonable explanation of reflection and refraction, but failed to account for diffraction (and interference, which we discuss below).

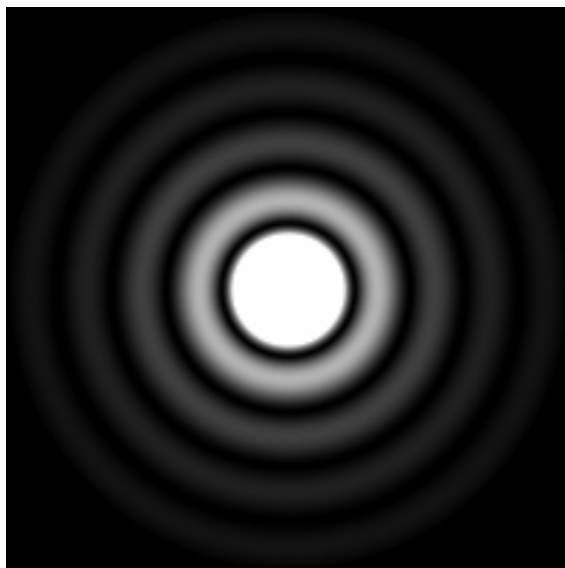
Almost a century later, in 1804, Thomas Young (1773-1829) published an article entitled “*The Bakerian Lecture: Experiments and calculations relative for physical optics.*” In it, he described his now famous **double-slit experiment**, performed a year earlier, which gave further evidence



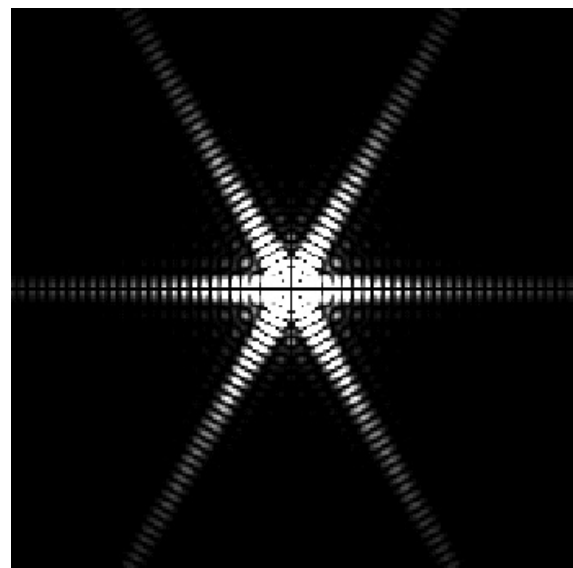
(a) geometric prediction



(b) rectangular aperture



(c) circular aperture



(d) triangular aperture

Figure 3: Diffraction patterns. A light source is placed behind a small aperture within a thin, opaque surface. **(a)** Profile of experiment. Geometric optics predicts a linear propagation of light, so that the pattern seen on the observational plane is just an illumination in the shape of aperture. **(b)**-**(d)** Observed diffraction patterns with different shapes of apertures. These results are far from the predictions of geometric optics.

of light behaving like a wave. In particular, light passing through two apertures produced diffraction patterns distinct from those seen when light passed through either individual aperture (see Fig. 4). These patterns are the consequence of **interference**, whereby waves superpose in either a constructive *or* destructive fashion, resulting in alternating light and dark regions. Part of what

made Young’s arguments particularly convincing is the fact that the double-slit experiment can be performed with water waves in a ripple tank, and the same interference and diffraction effects are observed.

Roughly at the same time, Augustin-Jean Fresnel (1788-1827) was working to develop a mathematical framework with which to calculate diffraction patterns. He modified Huygens’s principle and provided a construction that allowed him to explain diffraction. He also extended the wave theory of light to other optical phenomena. When submitted to the French Academy of Sciences, his work was initially rejected by Simeon Poisson (1781-1840) on the grounds that his constructions predicted an on-axis bright spot on the shadow of a circular obstacle blocking a point source of light. Then François Arago (1786-1853) actually performed the experiment and observed the predicted spot. This spot is now referred to as an **Arago spot**, or sometimes a **Fresnel spot**, or even (bizarrely) a **Poisson spot** (see Fig. 5). Fresnel is also credited with proposing, in 1827, that light only has a transverse component, as an explanation of the **polarization** of light (when waves vibrate along a *single* plane perpendicular to the direction of propagation). In 1845, Michael Faraday (1791-1867) discovered experimentally that the plane of polarization of polarized light rotates when an external magnetic field is present. This is called **Faraday rotation** or the **Faraday effect**, and its discovery was key in establishing a link between electromagnetism and light.

These ideas were unified in 1862, when James Clerk Maxwell (1831-1879) published “*On Physical Lines of Force*,” in which he established that electromagnetic radiation propagates in a vacuum at the speed of light, and concluded light is a form of electromagnetic radiation. He remarked, “*we can scarcely avoid the conclusion that light consists in the transverse undulations of the same medium which is the cause of electric and magnetic phenomena.*” Building on Maxwell’s work, and on advances in the theory of partial differential equations (PDEs) made by George Green (1793-1841) and Hermann von Helmholtz (1821-1894), Gustav Kirchhoff (1824-1887) showed that Young’s and Fresnel’s work could be deduced as a suitable approximation of the Fresnel-Kirchhoff integral formula. His deduction came to be known as **Kirchhoff’s theory of diffraction** or the **Fresnel-Kirchhoff theory of diffraction**. Finally, in 1896 Arnold Sommerfeld (1868-1951) published “*Mathematical Theory of Diffraction*.” He developed in the book a systematic study of diffraction of waves by formally reducing it to the study of a boundary value problem in mathematical physics. The next year John W. Strutt (Lord Rayleigh) (1842-1919) published “*On the passage of waves through apertures in plane screens*,” in which he examined the consequences of imposing different boundary conditions on the solutions to the Helmholtz equation.

4 Mathematical preliminaries

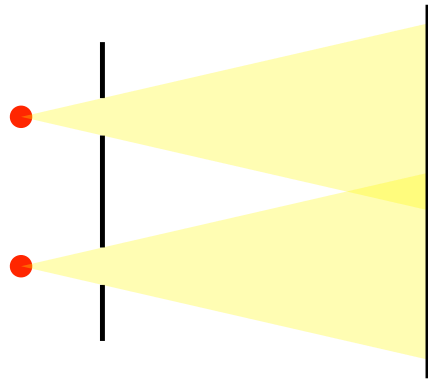
To describe light propagation, we use Maxwell’s equations. When there are no sources (i.e. charge density and current density equal to 0), they reduce to

$$\operatorname{div} \mathbf{B} = \nabla \cdot \mathbf{B} = 0 \quad (\text{Gauss’s flux theorem})$$

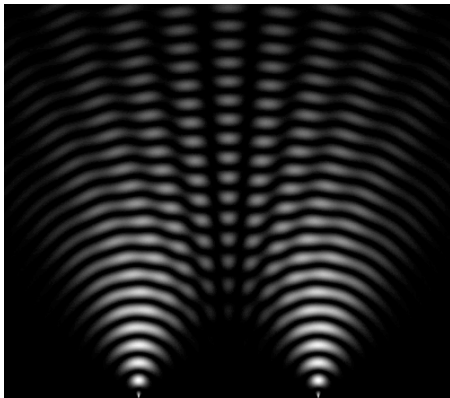
$$\operatorname{div} \mathbf{E} = \nabla \cdot \mathbf{E} = 0 \quad (\text{Gauss’s law for magnetism})$$

$$\operatorname{curl} \mathbf{E} = \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (\text{Faraday’s law})$$

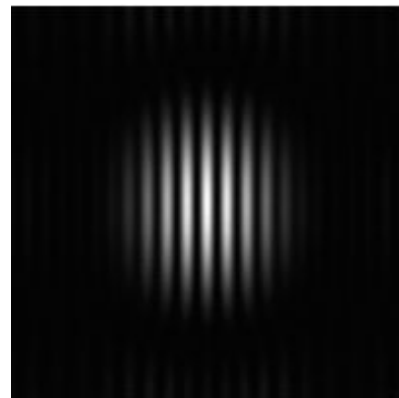
$$\operatorname{curl} \mathbf{B} = \nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}, \quad (\text{Ampère’s law})$$



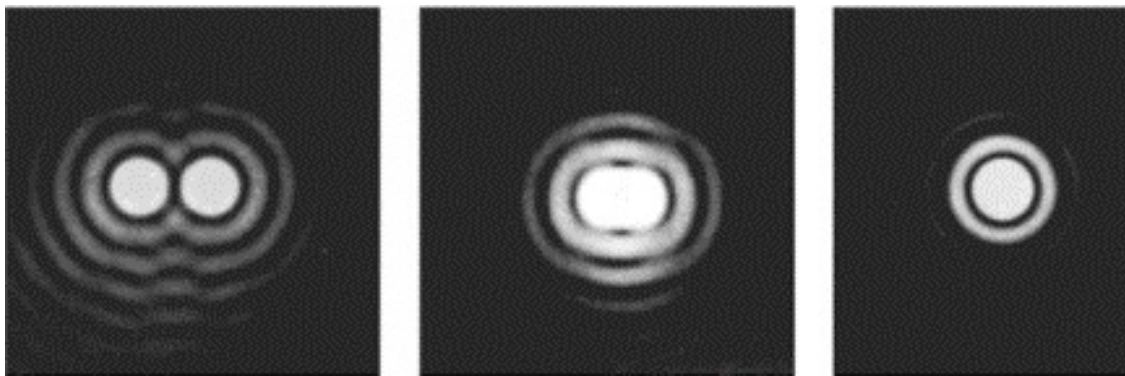
(a) geometric prediction



(b)

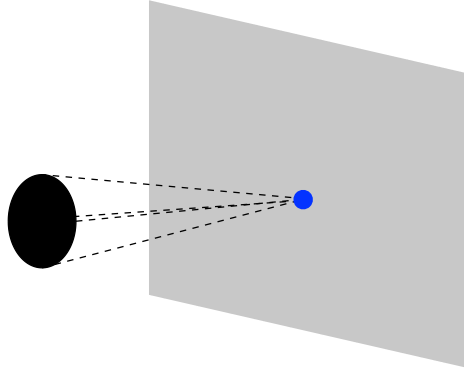


(c)

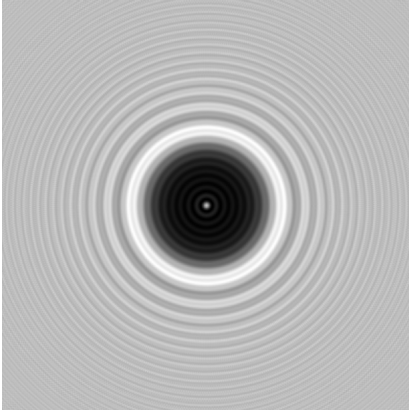


(d)

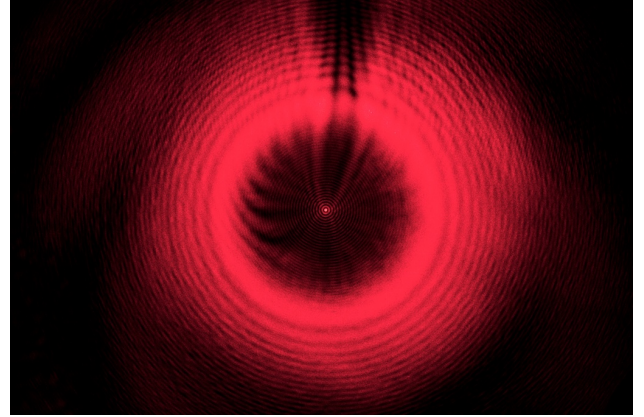
Figure 4: Interference patterns, first demonstrated by Young. **(a)** If apertures are close enough together, geometric optics predicts a central region of brightness. In reality, interference may produce a central region of *darkness*. **(b)-(c)** Experimentally observed interference patterns. **(d)** Evolution of interference pattern as two apertures are brought together.



(a) experimental setup



(b) numerical simulation



(c) experimental observation

Figure 5: The Arago spot. Its presence can be explained by Huygen's principle: All points on the boundary of the circular obstacle are equidistant from the circle's center, projected onto the observational plane. There is then constructive interference from the secondary sources on this boundary, from which light is suggested to propagate spherically.

where c is the speed of light in a vacuum. First note that

$$\text{curl curl } \mathbf{E} = -\frac{\partial}{\partial t} \text{curl } \mathbf{B} = -\frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}.$$

Then, using the identity

$$\text{curl curl } \mathbf{E} = \nabla \text{div } \mathbf{E} - \Delta \mathbf{E},$$

we conclude

$$\Delta \mathbf{E} = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0.$$

Since this equation decouples the evolution of the three components of the field, we can solve for each component independently. We will denote the chosen component by E , and we look to solve

the **scalar wave equation**:

$$\Delta E - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0.$$

In a general medium with refractive index c/n , the speed of propagation is n/c , and the scalar wave equation becomes

$$\Delta E - \frac{n^2}{c^2} \frac{\partial^2 E}{\partial t^2} = 0. \quad (2)$$

Solutions of particular interest to us are **monochromatic waves**, which are functions of the form

$$E(\mathbf{x}, t) = \operatorname{Re} u(\mathbf{x}) e^{-i2\pi\omega t}, \quad \omega \in \mathbb{R}$$

They are called “monochromatic” because oscillation occurs at single (angular) frequency ω . In this context, the envelope u of the wave is called the **wave field**. If (2) is to hold true for E , then a simple calculation shows that the **Helmholtz equation** must hold for u :

$$\Delta u + \frac{k^2}{c^2} u = 0, \quad (3)$$

where

$$k = \frac{2\pi\omega n}{c} = \frac{\omega_0}{c}$$

is the **wavenumber**. Alternatively,

$$k = \frac{2\pi}{\lambda}, \quad \text{where} \quad \lambda = \frac{c}{n\omega}$$

is the **wavelength**. It will be important that in optics, where we consider visible light, λ is between 400nm (blue) and 720nm (red).

So how do we solve the Helmholtz equation? Let us define

$$G(\mathbf{x}) = \frac{e^{ik\|\mathbf{x}\|}}{\|\mathbf{x}\|}, \quad (4)$$

and note it is smooth except at the origin. This function is called the **fundamental solution** or the **Green’s function** of the Helmholtz equation³. It is an outgoing spherical wave with source at the origin. By calling G a Green’s function, we are suggesting that (i) G is a solution, and (ii) other solutions are found by convolutions with G .

We first show G is a solution of Helmholtz equation away from the origin. If we write

$$G(\mathbf{x}) = \frac{1}{\|\mathbf{x}\|} + i \int_0^k e^{is\|\mathbf{x}\|} ds,$$

and we exchange integrals and derivatives with respect to the space variable, we can write

$$\Delta G(\mathbf{x}) = \sum_{\ell=1}^3 \left(\frac{\partial^2}{\partial x_\ell^2} \left(\frac{1}{\|\mathbf{x}\|} \right) + i \int_0^k \frac{\partial^2}{\partial x_\ell^2} e^{is\|\mathbf{x}\|} ds \right).$$

³That is, in dimension 3

A direct computation shows that

$$\frac{\partial^2}{\partial x_\ell^2} \left(\frac{1}{\|\mathbf{x}\|} \right) = \frac{\partial}{\partial x_\ell} \left(-\frac{x_\ell}{\|\mathbf{x}\|^3} \right) = -\frac{1}{\|\mathbf{x}\|^3} + 3\frac{x_\ell^2}{\|\mathbf{x}\|^5},$$

and

$$\frac{\partial^2}{\partial x_\ell^2} e^{is\|\mathbf{x}\|} = is \frac{\partial}{\partial x_\ell} \left(\frac{x_\ell}{\|\mathbf{x}\|} e^{is\|\mathbf{x}\|} \right) = -s^2 \frac{x_\ell^2}{\|\mathbf{x}\|^2} e^{is\|\mathbf{x}\|} + is \frac{\partial}{\partial x_\ell} \left(\frac{1}{\|\mathbf{x}\|} - \frac{x_\ell^2}{\|\mathbf{x}\|^3} \right) e^{is\|\mathbf{x}\|},$$

from which it follows that

$$\Delta \left(\frac{1}{\|\mathbf{x}\|} \right) = 0 \quad \text{and} \quad \Delta(e^{is\|\mathbf{x}\|}) = -s^2 e^{is\|\mathbf{x}\|} + 2is \frac{1}{\|\mathbf{x}\|} e^{is\|\mathbf{x}\|}.$$

Finally, since

$$\int_0^k s^2 e^{is\|\mathbf{x}\|} ds = k^2 \frac{1}{i\|\mathbf{x}\|} e^{ik\|\mathbf{x}\|} - \frac{2}{i\|\mathbf{x}\|} \int_0^k s e^{is\|\mathbf{x}\|} ds = -ik^2 G(\mathbf{x}) + \frac{2i}{\|\mathbf{x}\|} \int_0^k s e^{is\|\mathbf{x}\|} ds,$$

we conclude

$$\Delta G(\mathbf{x}) = i \int_0^k \left(-s^2 e^{is\|\mathbf{x}\|} + 2is \frac{1}{\|\mathbf{x}\|} e^{is\|\mathbf{x}\|} \right) ds = -k^2 G(\mathbf{x}),$$

as we wanted to show.

Using the Green's function for the Helmholtz equation we can, in fact, construct other solutions. To do this, we will make use **Green's theorem**, which can be thought of as a generalization of integration by parts.

Theorem 1 (Green). *For a domain $\Omega \subset \mathbb{R}^3$, and u, v sufficiently regular, we have*

$$\int_\Omega (u \Delta v - v \Delta u) d\mathbf{x} = \int_{\partial\Omega} \left(u \frac{\partial v}{\partial \mathbf{n}} - v \frac{\partial u}{\partial \mathbf{n}} \right) dS(\mathbf{x}),$$

where $\mathbf{n} = \mathbf{n}(\mathbf{x})$ is the outward-pointing unit normal to the boundary $\partial\Omega$ of Ω at \mathbf{x} , and

$$\frac{\partial}{\partial \mathbf{n}} = \langle \mathbf{n}, \nabla \rangle$$

is the normal derivative.

Now, suppose we have a region Ω and a point $\mathbf{x}_0 \in \Omega^\circ$, the interior of Ω . We would like to use Green's theorem with $v(\mathbf{x}) = G(\mathbf{x} - \mathbf{x}_0)$. However, the theorem requires regularity of v at the interior of Ω , and our choice of v has a singularity at \mathbf{x}_0 . In order to overcome this, we will “remove” a small ball around \mathbf{x}_0 , and use Green's theorem on this new domain. Let $\delta > 0$ and define $\Omega_\delta = \Omega \setminus B(\mathbf{x}_0, \delta)$, where $B(\mathbf{x}_0, \delta)$ is the Euclidean ball of radius δ centered at \mathbf{x}_0 . Assume that δ is small enough that $B(\mathbf{x}_0, \delta) \subset \Omega^\circ$, so that $\partial\Omega_\delta$ is the disjoint union $\partial\Omega \cup \partial B(\mathbf{x}_0, \delta)$.

Green's theorem states that

$$\begin{aligned} \int_{\Omega_\delta} (u \Delta v - v \Delta u) d\mathbf{x} &= \int_{\partial\Omega_\delta} \left(u \frac{\partial v}{\partial \mathbf{n}} - v \frac{\partial u}{\partial \mathbf{n}} \right) dS(\mathbf{x}) \\ &= \int_{\partial\Omega} \left(u \frac{\partial v}{\partial \mathbf{n}} - v \frac{\partial u}{\partial \mathbf{n}} \right) dS(\mathbf{x}) \\ &\quad - \int_{\partial B(\mathbf{x}_0, \delta)} \left(u \frac{\partial v}{\partial \mathbf{n}} - v \frac{\partial u}{\partial \mathbf{n}} \right) dS(\mathbf{x}), \end{aligned} \tag{5}$$

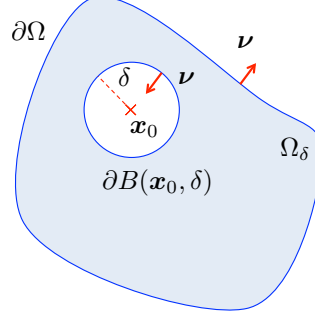


Figure 6: Description of the contour of integration, and the quantities used to deduce Fresnel-Kirchhoff integral formula (6). Note the relation between the outward pointing unit normals to $\partial\Omega_\delta$ and $\partial B(\mathbf{x}_0, \delta)$.

where the minus sign on the last term comes from the fact that the outward pointing unit normal to $\partial B(\mathbf{x}_0, \delta)$ is the negative of the outward pointing unit normal to $\partial\Omega_\delta$ at the same point. A direct computation shows that

$$\nabla G(\mathbf{x}) = \left(ik \frac{e^{ik\|\mathbf{x}\|}}{\|\mathbf{x}\|} - \frac{e^{ik\|\mathbf{x}\|}}{\|\mathbf{x}\|^2} \right) \nabla \|\mathbf{x}\| = \left(\frac{ik}{\|\mathbf{x}\|} - \frac{1}{\|\mathbf{x}\|^2} \right) G(\mathbf{x}) \mathbf{x},$$

and, since for $\mathbf{x} \in \partial B(\mathbf{x}_0, \delta)$ we have $\mathbf{n}(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_0)/\delta$, we deduce

$$\left. \frac{\partial v}{\partial \mathbf{n}} \right|_{\mathbf{x}} = \langle \mathbf{n}(\mathbf{x}), \nabla v(\mathbf{x}) \rangle = \frac{1}{\delta} \left(\frac{ik}{\|\mathbf{x} - \mathbf{x}_0\|} - \frac{1}{\|\mathbf{x} - \mathbf{x}_0\|^2} \right) G(\mathbf{x} - \mathbf{x}_0) \|\mathbf{x} - \mathbf{x}_0\|^2 = \left(ik - \frac{1}{\delta} \right) \frac{1}{\delta} e^{ik\delta}.$$

The last term in (5) becomes

$$\begin{aligned} \frac{1}{\delta} e^{ik\delta} \int_{\partial B(\mathbf{x}_0, \delta)} \left(\left(ik - \frac{1}{\delta} \right) u(\mathbf{x}) - \left. \frac{\partial u}{\partial \mathbf{n}} \right|_{\mathbf{x}} \right) dS(\mathbf{x}) = \\ e^{ik\delta} \int_{\partial B(0,1)} \left((ik\delta - 1) u(\mathbf{x}_0 + \delta \mathbf{x}) - \delta \left. \frac{\partial u}{\partial \mathbf{n}} \right|_{\mathbf{x}_0 + \delta \mathbf{x}} \right) dS(\mathbf{x}). \end{aligned}$$

If u is well-behaved so that, for instance, it has continuous gradient, then the above converges to

$$e^{ik\delta} \int_{\partial B(0,1)} \left((ik\delta - 1) u(\mathbf{x}_0 + \delta \mathbf{x}) - \delta \left. \frac{\partial u}{\partial \mathbf{n}} \right|_{\mathbf{x}_0 + \delta \mathbf{x}} \right) dS(\mathbf{x}) \longrightarrow -4\pi u(\mathbf{x}_0),$$

as $\delta \rightarrow 0$. Now, suppose u is another solution to (3) on Ω . Then

$$\int_{\Omega_\delta} (u \Delta v - v \Delta u) d\mathbf{x} = \int_{\Omega_\delta} (-k^2 uv + k^2 uv) d\mathbf{x} = 0$$

for all $\delta > 0$. We have arrived at the following conclusion: if u is a solution to the Helmholtz equation on a domain Ω , then

$$u(\mathbf{x}_0) = \frac{1}{4\pi} \int_{\partial\Omega} \left(u(\mathbf{x}) \left. \frac{\partial G}{\partial \mathbf{n}} \right|_{\mathbf{x} - \mathbf{x}_0} - G(\mathbf{x} - \mathbf{x}_0) \left. \frac{\partial u}{\partial \mathbf{n}} \right|_{\mathbf{x}} \right) dS(\mathbf{x}). \quad (6)$$

This is called the **Fresnel-Kirchhoff integral formula**. From this expression we see that the values of the wave field at any point within the domain can be obtained by knowing only the values of the field, and its normal derivative, at the boundary. Therefore, it establishes a connection between the local and global behavior of the solution. This mathematical identity will be our starting point for the study of diffraction. In particular, we will establish that G satisfies the second property of a Green's function, namely that other solutions are found by a convolution with G .