OPTICAL TRANSFORMS

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The University of Manchester Institute of Science and Technology, Manchester, England

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Preface

Optics is one of the oldest branches of physics, and also one of the most persistent. In spite of repeated claims that its role is finished, because it does not directly lead to the study of the structure of the atom, optical apparatus and ideas continue to provide a necessary basis for many new concepts, which help both physics itself and the other branches of science of which physics is a necessary part. When microscopy was supposed to be a finished subject, Zernike invented the phase-contrast microscope, which has been of enormous use to the biologist; when light sources were thought to have reached their limit, Schawlow and Townes invented the laser, which now has applications in almost every branch of science; and when the theory of image formation was thought to be a closed subject, Leith and Upatnieks following up the much earlier work of Gabor, invented their improved version of holography, which is having a remarkable influence in technologies of all sorts.

This book deals with one particular part of optics—the production and use of optical transforms. Basically, optical transforms are Fraunhofer diffraction patterns, the study of which had been for a long time regarded as of only limited interest. Their application to X-ray diffraction problems, however, brought the realization that the diffraction pattern of an object sometimes provided information in a more direct form than an image of the object itself, and gradually it has become evident that this property can be useful in subjects other than X-ray diffraction.

I have therefore tried to gather together the experience of a number of workers who have made different uses of optical transforms. Each has presented his ideas in his own way in a separate chapter of the book. Although each author was given a brief outline of what all the others were writing, there is inevitably some overlapping, but I have thought it worthwhile not to eliminate this so that each chapter is complete in itself. For the same reason, references are collected at the end of each chapter, instead of being in a consolidated list at the end of the book.

The final chapter is different from the rest. Whereas in general my aim has been to include only those subjects that have, over the years, shown their value in established researches, in the last chapter some new and rather tentative projects are described. Most are still in embryonic form, but I hope that their inclusion will encourage the reader to think about the possibility of the application of diffraction methods to the solution of his own problems. In spite, therefore, of its rather unfinished appearance, it is possible that Chapter 11 will prove to be at least as important as the other chapters.

I hope, then, that the book will stimulate others who may find that optical ideas may have a place in their work that they had not previously suspected. The history of physics abounds in unexpected inter-relations between its various branches, and if this book induces any further instances of the applications of optics it will have served the purpose for which it was intended.

JANUARY 1972 H. LIPSON

Contents

9. Holography

J. SHAMIR

10. Optical Transforms in Teaching

S. G. LIPSON

11. Miscellaneous Applications

J. E. BERGER, C. A. TAYLOR, D. SHECHTMAN, AND H. LIPSON

CHAPTER 1

Basic Principles

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I. Historical Introduction

A. The Wavelength Problem

Many physical instruments have developed more or less accidentally, with little theoretical understanding of their basic principles. As the need for improvements has arisen, however, so theoretical investigations have become necessary, and from these more detailed designs have developed; ultimately quite complicated instruments have appeared, seeming perhaps almost completely unrelated to their humble origins. Theory may direct practice into unexpected channels, or may even indicate that limits may exist which preclude further practical developments.

Of no field is this more true than that of optics. From about 1600, when Leeuwenhoek's apprentice invented the first telescope, to the present day, with its gigantic astronomical telescopes, there has been tremendous progress, in which theory and practice have complemented each other. The microscope has taken even greater steps. From Hooke's early instruments to the electron microscope, which can show nearly atomic detail, there has been a series of steps forward which cover a range of resolution of about 10^5. Progress has not however been continuous; at certain stages, indeed, it has looked as if an impasse had been reached. In trying to find ways round these impasses, however, new ideas had been introduced and these have led to the remarkable progress in microscopy of which the electron microscope is the culmination.

This book is concerned with microscopy in its broadest sense. The first microscopes were simple lenses and it is amazing what discoveries were made with them—even with a drop of honey in a circular hole. But it was soon found that combinations of lenses were easier to use and gave better results, and even in the early days Huygens had worked out in detail the theory of the eyepiece that is still named after him. Ways to minimize or eliminate aberrations were discovered and with precise means for measuring the refractive indices and dispersive powers of glasses (in this study the name of Fraunhofer is particularly prominent) quite complicated lens systems of superb performance could be devised. With improved workmanship there appeared to be no limit to what could be accomplished.

In 1873, however, Abbe introduced his wave theory of image formation and showed that even with perfect lenses resolutions of less than about half the wavelength of light could not be achieved. It seemed, then, that Nature had set a limit of the order of 0·2 μm on what the microscopist could distinguish with his instrument. The only way round the limitation would be to see if some radiation with a shorter wavelength could be used in the image-forming process.

Ultra-violet radiation was an obvious suggestion; microscopes were built for the near ultra-violet, but difficulties of designing lenses for an invisible radiation and of using the instrument solely by photography made the relatively small gain in resolution hardly worth while. No other possibilities seemed to exist.

When, in 1912, came the discovery that X-rays—discovered by Röntgen in 1895—were a radiation with a wavelength of the order of 1 Å; Laue, Friedrich and Knipping diffracted the radiation by means of a crystal of copper sulphate and Bragg's interpretation of the diffraction pattern of rock salt enabled him to establish a scale of wavelength to an accuracy of about one per cent. Could a microscope be built to make use of this new radiation?

The answer was "No"; X-rays could not be appreciably refracted and so no lenses could be made, and, although they can be reflected from crystal planes, the task of making a mirror accurate enough to match the wavelength of the rays was out of the question. Although reflecting X-ray microscopes have been made, they cannot give resolution even as good as the light microscope.

In 1924 a more hopeful possibility emerged; de Broglie put forward his theory of the wave nature of moving particles, and it was soon verified experimentally for low-voltage electrons (Davisson and Germer, 1927) and for high-voltage electrons (Thomson, 1927). Electrons with energies of 50 KeV have a wavelength of about 0·05 Å and since they can be deflected by electric or magnetic fields, it should be possible, by designing suitably shaped electrodes or pole pieces, to produce focused beams and hence images of objects. The limit of resolution with such short wavelengths should be as much as any physicist could desire; the wavelength is a great deal smaller than atomic separations, which are round about 2 Å, and no detail smaller than this can be envisaged.

So electron microscopes were built and their limitations were explored. It was soon found—theoretically and practically—that corrected electron lenses could not be made and that to obtain a good image the lenses must be "stopped down" very considerably; beam angles θ of a fraction of a degree had to be used and the value of the limit of resolution, given by the expression $0{\cdot}6\lambda/\sin\theta$, was very much larger than $\lambda/2$. Soon however the resolution of light microscopes was reached and surpassed and it seemed likely that progress to 1Å would be reached. But in fact, resolutions have not reached this value. Below about 10 Å difficulties of design and electrical control mount up, and even the most sanguine claims do not reach atomic separations.

Moreover, the electron microscope is by no means a generally useful instrument like a light microscope; electron beams can be produced only in a vacuum and can pass only through extremely thin specimens. The electron microscope has produced results of immense importance, particularly in biology, but it has not reached the stage—nor is it likely to do so—of the general applicability of the light microscope.

Other suggestions based on de Broglie's theory have also been made. Protons, for example, can be used, but these heavy particles cannot compete with electrons and the proton microscope has not proved to be of great utility. We therefore seem to be in difficulties. X-rays would be usable, since they can pass through air, but they cannot be focused; electrons can produce images but only of specialized objects, and the ultimate resolution of electron waves cannot be exploited. What can we do?

B. Abbe's Theory

In order to answer this question, we must look into Abbe's theory more closely in order to see whether we can circumvent the problems that it raises. There are many ways of expressing this theory, but the most direct is that propounded by Zernike (1946), who states that the process of image formation in an optical instrument consists of two stages of diffraction: the incident light is diffracted by the object and the diffraction pattern formed when this diffracted light is brought to a focus in the image (Fig. 1). This statement of Abbe's theory emphasizes the importance of the illumination system: it is not merely required to throw light on to the object; it provides a necessary part

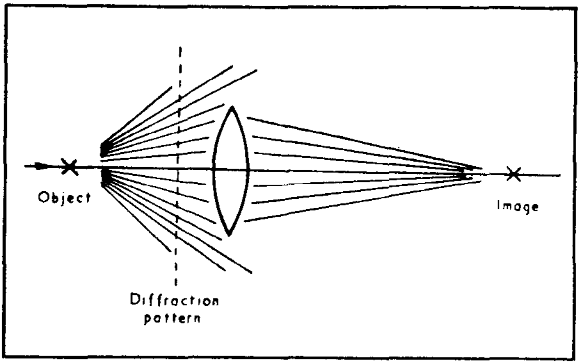

Fig. 1. Part of the light diffracted by an object is collected by a lens which refracts it to produce an interference pattern which is the image.

of the image-forming process and considerable care must be devoted to its construction if the highest possible resolution is to be obtained.

To understand these ideas it is simplest to assume that the object is illuminated by a plane parallel wave of wavelength λ, that is, by completely coherent light. (This concept will be discussed in more detail in Chapter 2.) The light will be scattered in all directions by the object (Fig. 1), the wave scattered in any particular direction being the sum of the waves scattered with different phase relations from different parts of the object. The amplitudes and phases of the scattered waves are functions of the direction of scattering; if we confine ourselves, to begin with, to a one-dimensional object, we may write for the wave ψ at an angle α (Fig. 2).

$$\psi = \int_{-\infty}^{\infty} f(x) \exp(-ikx \sin \alpha)\, dx \tag{1.1}$$

where $f(x)$ represents the amplitude of the wave scattered by a point distant x from the axis, and k is $2\pi/\lambda$ (Lipson and Lipson, 1969). This expression arises because the path difference between the wave scattered from 0 and that scattered from P (Fig. 2) in $x \sin\alpha$. It is convenient to put $k \sin\alpha = u$ and then

$$\psi(u) = \int_{-\infty}^{\infty} f(x) \exp(-iku) \, du. \tag{1.2}$$

$\psi(u)$ is said to be the *Fourier transform* of $f(x)$.

As we can see, ψ is in general a complex quantity, that is, it has both an amplitude and a phase. The amplitude is that of the light scattered in the direction θ, and the phase is the phase of the wave relative to that scattered by the point 0. Phases are, of course, always relative to some standard. Only

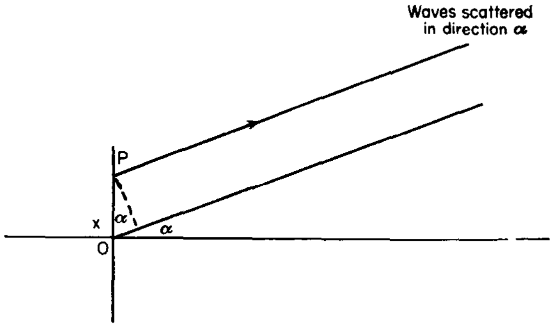

Fig. 2. Optical path difference between the waves scattered at an angle α by two points separated by a distance x.

the intensity is observable and this is equal to $|\psi|^2$ or to $\psi\psi^*$ where ψ^* is the complex conjugate of ψ.

In practice, the object will not be illuminated by a plane parallel wave; indeed, such illumination is quite undesirable and it is best to have incoherent illumination, that is, waves falling on the object from a large variety of directions. If we take one such wave falling at an angle β on the object, we then have that

$$\begin{aligned} \psi(u, \beta) &= \int_{-\infty}^{\infty} f(x) \exp\{-ikx(\sin\alpha + \sin\beta)\} \, dx \\ &= \psi(u) \exp\{-ikx \sin\beta\}. \end{aligned} \tag{1.3}$$

The wave scattered in a particular direction is now the sum of a large number of waves and the problem becomes too complicated to deal with unless $f(x)$

is an extremely simple function. It is for this reason we have considered only the simple case of plane parallel illumination.

To form an image, we need to bring all the waves scattered from one point x in the object to a single point in space, each point in the object space having a corresponding point in image space. This is the function of the optical instrument. Now the condition for an image point to exist is that all the waves should arrive at the point in the same phase, that is, that all the optical paths between the object point and image point should be equal. In the back focal plane F of the lens (Fig. 3) all the waves that are parallel to each other will come to a focus; therefore in this plane the function $|\psi|^2$ will be observed. Now since the relative phases between object points O and image points I' are the same and may be made zero, it is clear that the phase change between

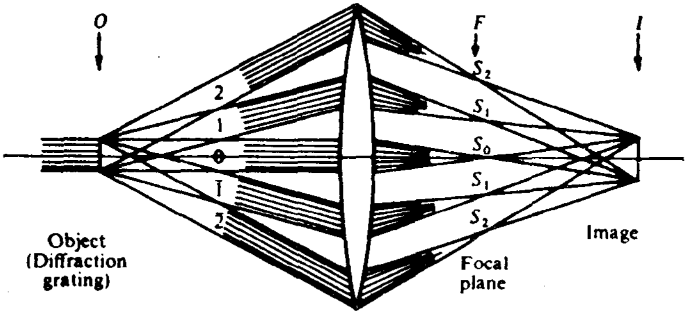

Fig. 3. Production of a diffraction pattern in the back focal plane of a lens. For clarity, the object is taken to be a diffraction grating, but the principle applies to any object.

O and F is equal and opposite to the phase change between F and I'. Thus the relation between the wave function in the focal plane of the lens to that in the image is the inverse of that between the wave function in the object and that in the focal plane of the lens. In other words, the image is the inverse Fourier transform of $\psi(u)$;

$$f'(x) = \int_{-\infty}^{\infty} \psi(u) \exp(iku)\, du, \tag{1.4}$$

the inverse nature of the transformation being indicated by the omission of the minus sign in the exponential.

This is the mathematical equivalent to Zernike's statement, quoted at the beginning of this chapter, that an image is the diffraction pattern of the diffraction pattern of the object.

The statement is perhaps easier to understand if we introduce the concept of interference, rather than diffraction, for the second stage. We may regard diffraction as a process that occurs naturally, when a light wave is limited in some way, and interference as the deliberate bringing together of a number of separate waves. The light wave diffracted by the object can be regarded as a large number of separate waves that are diverging from each other; these are brought together by a lens so that they interfere with each other, and in one plane—the image plane—the relative phases are such as to produce an image of the object.

C. *Optical Transforms*

The theory can be easily extended to two-dimensional plane objects, perpendicular to the axis of the lens system. Each point in the object now has to be specified by a vector **r**, the direction of the incident beam by a vector $\mathbf{s}_0$ and that of the diffracted beam by a vector **s**. If the diffracting object is represented by the function $f(\mathbf{r})$, we have that the total scattered wave is

$$\psi = \int_{-\infty}^{\infty} f(\mathbf{r}) \exp \frac{2\pi i|\mathbf{r}|}{\lambda} (\cos\alpha - \cos\beta)\, dA.$$

where dA is the element of area around the point **r**, and α and β are the angles of incidence and scattering respectively. If we give the vectors **s** and $\mathbf{s}_0$ moduli of $1/\lambda$, then Eq. (1.4) can be written as

$$\psi = \int_{-\infty}^{\infty} f(\mathbf{r}) \exp 2\pi i(\mathbf{r}.\mathbf{s} - \mathbf{r}.\mathbf{s}_0)\, dA \tag{1.5}$$

or

$$\psi = \int_{-\infty}^{\infty} f(\mathbf{r}) \exp (2\pi i\mathbf{r}.\mathbf{S})\, dA \tag{1.6}$$

where $\mathbf{S} = \mathbf{s} - \mathbf{s}_o$ (Lipson and Taylor, 1958).

This general expression is valid for all angles of incidence, a necessary condition when we come later to consider three-dimensional diffraction. For the moment, however, we need to deal only with normal incidence, and Eq. (1.6) becomes

$$\psi(\mathbf{S}) = \int_{-\infty}^{\infty} f(\mathbf{r}) \exp (2\pi i\mathbf{r}.\mathbf{S})\, dA \tag{1.7}$$

which is the *Fourier transform* of the diffracting object $f(\mathbf{r})$. The intensity observed is $|\psi|^2$ or $\psi\psi^*$ (Section I.B). This is the *optical transform*.

D. *X-ray Diffraction by Crystals*

As we saw in Section I.A, the problem raised in the use of X-rays to examine crystals is that there is no way of producing an image by means of lenses;

only the first stage of the image-forming process can be carried out—the observation of the diffraction pattern. It is therefore necessary to try to deduce the nature of the diffracting object purely from this diffraction pattern.

At first sight, the task would seem to be almost impossible. One can, of course, recognize simple objects, such as a circular or rectangular hole, from their diffraction patterns, or even simple combinations of these, but it is hardly to be expected that one could deduce the arrangements of large numbers of atoms in such an indirect way. In fact, considerable success *has* been achieved in this art, largely because of one basic fact—that most solid matter is crystalline and hence consists of a relatively small group of atoms regularly repeated in three dimensions. The periods of repetition in a crystal can be deduced quite simply from its diffraction pattern, and the basic problem then is to find the number (often quite small) of atoms in the repeating unit, which is called the *unit cell.*

A single crystal behaves as a diffraction grating. Because it is three-dimensional, the conditions for diffraction are more complicated than those for a one-dimensional grating (Lipson and Cochran, 1966), but they can be briefly summarized in the following way. First, each order of diffraction is specified by three integers, in place of the single integer for a one-dimensional grating; these integers are represented by the symbols *hkl*. W. L. Bragg (1913) showed that each order could be regarded as a reflexion from a set of lattice planes (*hkl*) and for this reason the orders of diffraction are commonly called reflexions. This nomenclature is acceptable so long as it is realized that ordinary specular reflexion is not taking place.

Secondly, because of the three-dimensional nature of the diffraction, three conditions, known as Laue's equations (Lipson and Cochran, 1966), have to be obeyed simultaneously. Since there are only two variables, represented by two independent direction cosines giving the direction of the incident beam with respect to the crystal, it is unlikely that any order of diffraction will be produced if a monochromatic beam of X-rays is allowed to fall on a stationary crystal. Thus another degree of freedom must be introduced. It may be a variation in wavelength, resulting in the now-obsolete Laue method which makes use of the white radiation from an X-ray tube. But more commonly it is a rotation, angular oscillation or some other form of angular motion. Details will not be discussed here, but the latest forms of apparatus, introducing also a movement of the film, result in X-ray diffraction photographs in which indices *hkl* can be assigned to each spot quickly and unambiguously. The most recent apparatus dispenses with photography, and uses electronic means to adjust the crystal and measure the intensities of the various orders of X-ray diffraction.

The ultimate result of any of these methods is to present a complete diffraction pattern of a crystal in the form of the intensity of each possible