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ABSTRACT

This monograph was written for the Conference on the New Instructional Materials in Physics, held at the University of Washington in summer, 1965. The measurement of very small distances and sizes, and the concept of models are discussed in the introduction. The optics of slits is dealt with in chapter 2. Chapter 3 presents the optics of holes. The phenomena of interference and diffraction are included in chapter 4. The author discusses the experimental determination of interatomic distances in a gas molecule for observation of interference effects in electron scattering in chapter 5. The monograph concludes with a number of references to physical optics. (LC)

Interference and Diffraction

MARC H. ROSS

University of Michigan

GENERAL PREFACE

This monograph was written for the Conference on the New Instructional Materials in Physics, held at the University of Washington in the summer of 1965. The general purpose of the conference was to create effective ways of presenting physics to college students who are not preparing to become professional physicists. Such an audience might include prospective secondary school physics teachers, prospective practitioners of other sciences, and those who wish to learn physics as one component of a liberal education.

At the Conference some 40 physicists and 12 filmmakers and designers worked for periods ranging from four to nine weeks. The central task, certainly the one in which most physicists participated, was the writing of monographs.

Although there was no consensus on a single approach, many writers felt that their presentations ought to put more than the customary emphasis on physical insight and synthesis. Moreover, the treatment was to be "multi-level" --- that is, each monograph would consist of several sections arranged in increasing order of sophistication. Such papers, it was hoped, could be readily introduced into existing courses or provide the basis for new kinds of courses.

Monographs were written in four content areas: Forces and Fields, Quantum Mechanics, Thermal and Statistical Physics, and the Structure and Properties of Matter. Topic selections and general outlines were only loosely coordinated within each area in order to leave authors free to invent new approaches. In point of fact, however, a number of monographs do relate to others in complementary ways, a result of their authors' close, informal interaction.

Because of stringent time limitations, few of the monographs have been completed, and none has been extensively rewritten. Indeed, most writers feel that they are barely more than clean first drafts. Yet, because of the highly experimental nature of the undertaking, it is essential that these manuscripts be made available for careful review by other physicists and for trial use with students. Much effort, therefore, has gone into publishing them in a readable format intended to facilitate serious consideration.

So many people have contributed to the project that complete acknowledgement is not possible. The National Science Foundation supported the Conference. The staff of the Commission on College Physics, led by E. Leonard Jossem, and that of the University of Washington physics department, led by Ronald Geballe and Ernest M. Henley, carried the heavy burden of organization. Walter C. Michels, Lyman G. Parratt, and George M. Volkoff read and criticized manuscripts at a critical stage in the writing. Judith Bregman, Edward Gerjuoy, Ernest M. Henley, and Lawrence Wilets read manuscripts editorially. Martha Ellis and Margery Lang did the technical editing; Ann Widditsch supervised the initial typing and assembled the final drafts. James Grunbaum designed the format and, assisted in Seattle by Roselyn Pape, directed the art preparation. Richard A. Mould has helped in all phases of readying manuscripts for the printer. Finally, and crucially, Jay F. Wilson, of the D. Van Nostrand Company, served as Managing Editor For the hard work and steadfast support of all these persons and many others, I am deeply grateful.

Edward D. Lambe
Chairman, Panel on the
New Instructional Materials
Commission on College Physics

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I would like to thank T. Goodrich, S. Sari, and C. Webb, students at the University of Washington, for listening to and criticizing this material. I would like to thank chemistry professors K. Hedberg, R. Bonham, and L. Brockway for advice about Chapter 5. These gentleman have not, however, read the material in advance of publication. I would like to thank Professor O. Bastiansen for permission to use material from Almenningen et al., *Journal of Chemical Physics*, 40, 3436 (1964) in Figs. 5.5 and 5.8.

1 INTRODUCTION

How are very small distances or sizes measured? I mean, for example, the "diameters" of "microscopic particles": atoms, atomic nuclei, and nucleons. Do very small distances even have meaning? Let us say we find a reasonable experimental technique. How can we know that the measurement should have a clear interpretation? Although it seems obvious that distances can take on any value, it is not certain that distance has the same properties when very small as it does in everyday experience. When physicists have attempted to extrapolate from established ideas to new realms of experience where measurements have not been made, there is often a breakdown or failure of their ideas. As a result of this failure we need to be open minded. It has been suggested, for example, (though never confirmed) that there is a very small fundamental length in nature, that distance is not a continuous variable. I can readily name some more concrete difficulties: (1) The object whose diameters we measure may be fuzzy like the earth's atmosphere (what is the diameter of the earth with its atmosphere?) (2) The object may not have a well-defined diameter in time, that is, it may be pulsating like a man's chest. (3) There is also the problem of the projectile used as a probe. The only objects fine enough to use as tools of measurement or probes are microscopic particles themselves. But the particle used as a probe may itself have a size or a fuzziness (Fig. 1.1).

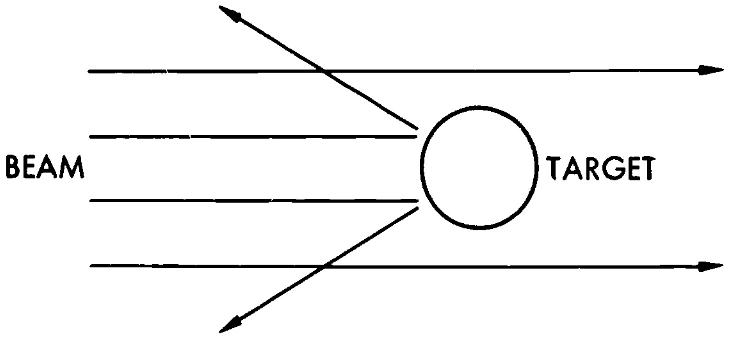

Fig. 1.1 A beam of small particles is shined on a target particle. We can imagine that the scattering gives us a measure of the diameter. It is hard to imagine that an accurate determination of the diameter could be made if the beam particles are larger than the target.

There are problems in defining diameter of objects too small to see, so it has to be done with care. Hopefully, different measurement procedures lead to about the same number for the diameter of a given object. If we can fit these different measurements into a theoretical framework and can calculate the small discrepancies between them, then we can be confident we know what we're talking about. There won't be time in this monograph for discussion of several different measurement procedures; but we will discuss one of the most widely used methods.

Let me give you a rough tabulation of the results of size measurements to set the scale, though I haven't as yet discussed how the measurements are made. Only in the case of interatomic distances is the meaning of the distance very clear. An atom looks as in Fig. 1.2. It is clear what we mean when we talk about the dis-

OBJECT	TYPICAL DISTANCE (IN CM)
Size of molecule	$\gtrsim 10^{-8}$
Spacing of neighboring atoms in a molecule	10^{-8}
Diameter of an atom	10^{-8}
Diameter of a nucleus	10^{-12}
Spacing of neighboring nucleons in a nucleus	10^{-13}
Diameter of a nucleon	10^{-13}

Table 1.1 SIZES OF MICROSCOPIC PARTICLES

Fig. 1.2 Model of an atom.

tance between atomic nuclei in, e.g., a diatomic molecule.

This table should not lead you to believe that the subject is closed and the questions I raised above merely pedagogical. In important cases the measurements have not been made or the interpretation is not yet clear. Some distance measurements, as we'll discuss, are current research problems. At 10^{-8} cm much of the research is now in the hands of the chemists. The techniques and interpretation at 10^{-12} cm are also becoming well established. Measurements at 10^{-13}-10^{-14} cm are, however, rather recent.

With ordinary mechanical means - the traveling microscope - we can measure distances to an accuracy of about 10^{-4} cm. This is done by placing cross hairs in the microscope view and attaching the stage of the microscope to a very finely machined screw drive. One can watch as the object is moved and thereby obtain a distance measurement. The distance 10^{-4} cm is about the size of one grain in fine-grain photographic film. There are several methods of extending distance measurements way down to the submicroscopic domain. These methods work more or less well in the case of different particles. I will discuss in detail two closely related methods, which I'll call interference and diffraction, which are probably the most widely used for measuring small distances. First, after some general notions are established, I will discuss the interference patterns obtained from electron scattering on gas molecules to determine the interatomic distances. We will see how chemists do these experiments and what problems they are currently interested in. In an extended version of this monograph, I will discuss the patterns obtained in diffraction scattering of high energy particles by a nucleus. We can obtain information about the diameter and shape of the nucleus. We will also discuss some details of the experimental techniques.

The theoretical basis of these techniques is the same as that of optics as taught in an introductory physics course. The same mathematics of wave motion, we can call it a wave model, works to describe what is observed in these scattering experiments in all their intricate detail. (See special topic: Models). We will not divert ourselves with questions why the wave model works. The experimental evidence for the model, some of which will be pointed out at the appropriate moment, is overwhelming. We begin then with a review of optics.

MODELS:[1] By "model" we mean "analog." It is a mechanical or electrical device or a system of mathematical expressions whose behavior we can take as an idealization of the behavior we want to describe. Consider a simple pendulum as a model. There are several input parameters such as a length of string, mass of bob, and the initial conditions. For given values of these inputs the pendulum has a definite behavior (i.e., its position as a function of time). Say I want to describe the rate of business activity in this country. After associating the various prop-

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[1] These special topics are to be used at the discretion of the reader.

erties of the pendulum with appropriate properties of the national product, I will have a model (albeit not a good one) which predicts business cycles. I use the simple pendulum as the analog of a system I don't understand as well. Other examples of models are collisions of billiard balls for collision of atoms or water in a pipe for direct current circuits. The wave model we are about to discuss is used, for example, to describe waves on a vibrating string, waves on the surface of water, alternating current, and light. I am going to talk in terms of the optical case because it is considered most thoroughly in introductory physics.

Most important models can be stated as systems of equations with several parameters. The strength of physics rests on the fact that a mathematical model can be used to describe many different physical systems. This enables physicists to go on as more and more experimental information is collected. The data would bury us if the description of every parcel of data had to be wholly different. Instead there are relatively few mathematical models which are used over and over.

2 OPTICS OF SLITS

(This may be a review - skip to the next section if you know the material.)

2.1 PROPERTIES OF THE WAVE MODEL

(1) The superposition principle: If a wave with amplitude A_1 describes a physical situation and so does a wave with amplitude A_2, then $A_1 + A_2$ also describes a physical situation. We will illustrate this directly with the double-slit example. Mathematically this property follows from the linearity of the wave equation and associated boundary conditions.

(2) Any amplitude A of "monochromatic" light, i.e., light of fixed frequency, has (at a fixed point in space), by definition the time dependence:

$$A = a \sin (\omega t + \phi).$$

Here a is the "magnitude" of the wave (a is positive),
ω is the "angular frequency",
$\nu = \omega/2\pi$ is the "frequency" and
$\tau = 1/\nu$ the "period,"
ϕ is the "phase."
See Fig. 2.1.

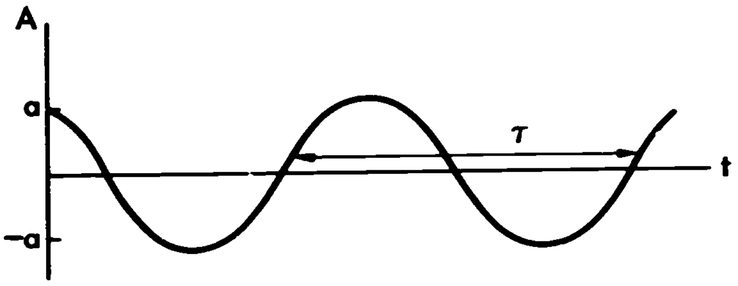

Fig. 2.1 Amplitude at a fixed point in space. In this figure the phase is just over 90°.

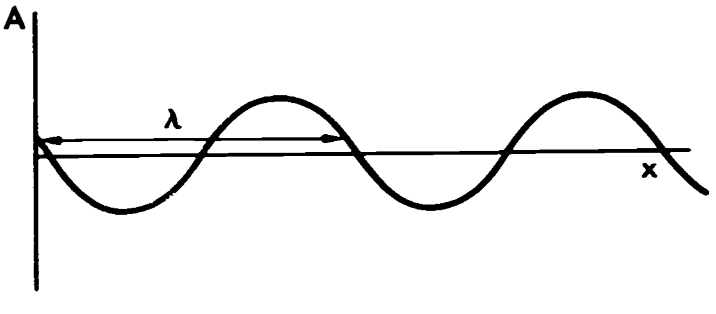

Fig. 2.2 The wavelength satisfies the relation $A(x + \lambda) = A(x)$. In this figure the phase is just under 180°.

(3) For monochromatic light moving in the x direction for all y, z (i.e., a plane wave) the amplitude has the form at fixed time:

$$A = a \sin (kx + \delta).$$

Here k is the "wave number,"
$\lambda = 2\pi/k$ is the "wavelength" (see Fig. 2.2),
δ is the phase.

We combine the space and time dependence so that the amplitude moving in the x direction has the form:

$$A = a \sin (kx - \omega t + \delta).$$

Here $v = \omega/k = \nu \cdot \lambda$, the "phase velocity," relates frequency and wavelength. In free space $v = c$, the velocity of the light (Fig. 2.3).

Any surface on which the amplitude has the same phase is called a "wavefront." That is, the time dependence at any point on a wavefront is $\sin (\omega t + \phi)$, the value of ϕ being the same everywhere on the surface.

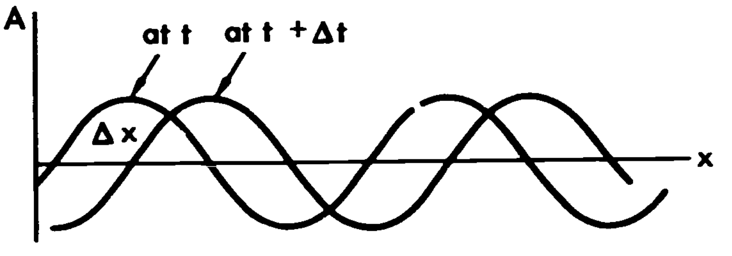

Fig. 2.3 Sine waves at t and $t + \Delta t$. In this illustration $\omega\Delta t \approx 90°$. The curve at $t + \Delta t$ is obtained from that at t by noting that as the ωt terms gets larger, if the kx term gets larger by the same amount the amplitude will be unchanged. Thus a shift Δx to the right satisfies

$$\sin \delta = \sin (k\Delta x - \omega\Delta t + \delta) \text{ so that}$$
$$v = \Delta x/\Delta t = \omega/k \quad \text{(constant)}.$$

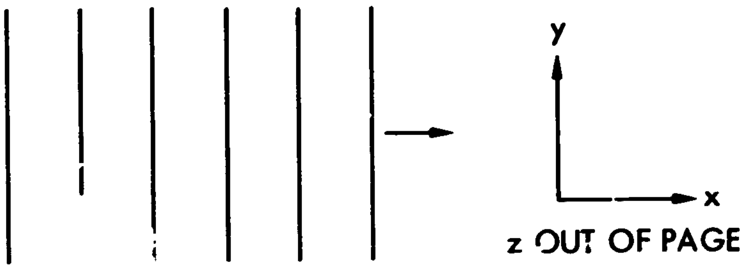

Fig. 2.4 Plane wave moving in the x direction. The lines indicate wavefronts which are planes parallel to the y, z plane. Formula:

$$A = a \sin (kx - \omega t + \delta)$$

Thus, in the example we are discussing, since A is completely independent of y and z, ϕ is certainly independent of y and z so that any plane parallel to the y, z plane is a wave front (see Figs. 2.4 and 2.5).

A completely general pattern of monochromatic waves is obtained by adding, with various magnitudes b and phases δ, sine waves, or plane waves moving in different directions:

$$A = \sum_{\vec{r}} b(\vec{r}) \sin (\vec{k}\cdot\vec{r} - \omega t + \delta (\vec{r}))$$

(4) The propagation of a wave amplitude in three dimensions is determined by the position of successive wavefronts in time. Successive wavefronts may be determined by Huygen's principle: Each point on a wavefront can be regarded as a new source of waves, which spread out spherically from the point. The new wavefronts are determined by adding these secondany waves (Fig. 2.6). (See special topic, Mathematical Statement of Huygen's principle.

(5) We observe, e.g., on a screen, the "intensity" which is defined as the time average of the square of the amplitude. The intensity can be considered to be energy/(area × time). The intensity does not satisfy superposition:

$$|A_1 + A_2|^2 \neq A_1^2 + A_2^2$$

MATHEMATICAL STATEMENT OF HUYGEN'S PRINCIPLE: Consider a wavefront. Let Q be a point on the front and the amplitude in the neighborhood of Q be

$$A(Q) = a(Q) \sin (kr_n - \omega t)$$

where r_n is distance normal to the wavefront (measured from the front). The amplitude at P a distance r and angle θ from Q due to an area ΔS of the wavefront at Q, is:

$$A(P) = \Delta S\, a(Q) \left[\frac{1 + \cos\theta}{2\lambda}\right] \frac{\sin\left(kr - \omega t - \frac{\pi}{2}\right)}{r}$$

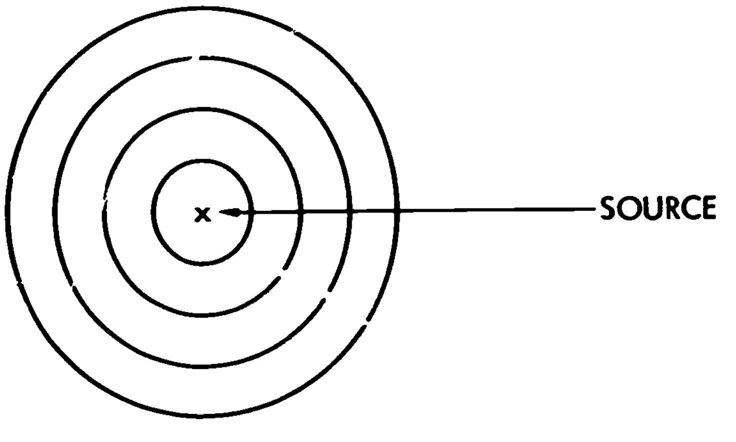

Fig. 2.5 Spherical waves. The circles indicate the wave fronts which are spheres centered on the source. Formula:

$$A = a(r) \sin (kr - \omega t + \delta).$$

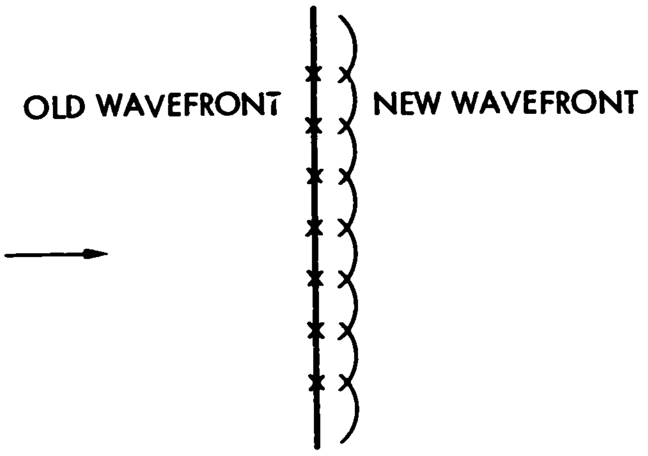

Fig. 2.6 The new wavefront a moment later can be obtained from the old by constructing the waves coming from each point and adding all these amplitudes.

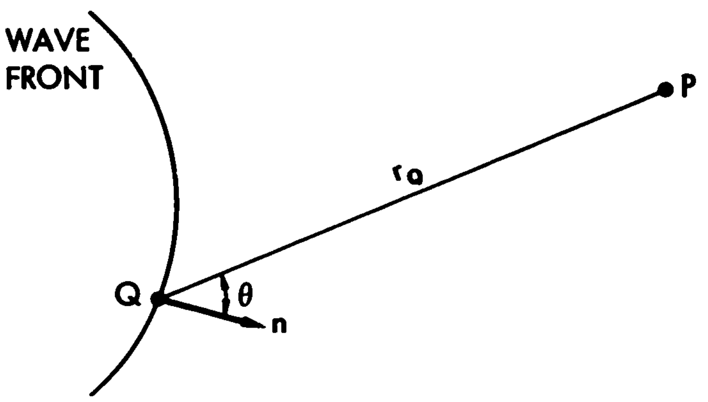

Fig. 2.7 Geometry for Huygen's principle.

Let's discuss this expression. The $\Delta S\ a(Q)$ factor in the magnitude is just what we would expect: proportionality to the magnitude at Q and to the area of wavefront we consider as a secondary source. The bracketed factor is largest when P is straight ahead of Q (in the direction r_n) and has a normalization factor we wouldn't guess. The $1/r$ factor is what we should expect for spherical waves, as discussed below. A sine wave $\sin(kr - \omega t)$ is what we might expect because $kr/2\pi = r/\lambda$ is number of waves which fit into the distance r. But the correct answer, as shown in the appendix, contains, in addition, the phase $-\pi/2$.

The net amplitude at P will then be

$$A(P) = \frac{1}{2\lambda} \int dS\ a(Q) \frac{\left(1+\cos\theta(Q)\right)\ \sin\left(kr_Q - \omega t - \frac{\pi}{2}\right)}{r_Q}.$$

The full derivation is given in the appendix.

2.2 THE DOUBLE SLIT

Consider the passage of monochromatic light from a distant source on the left through a double slit and onto an observing screen to the right (Fig. 2.8).

Parallel light arrives normally on the absorber with slits cut into it. Beyond the slits we place a lens so that parallel light is focused on the observing screen. In this way we in effect observe the <u>angle</u> θ of the light from the slits on the screen.

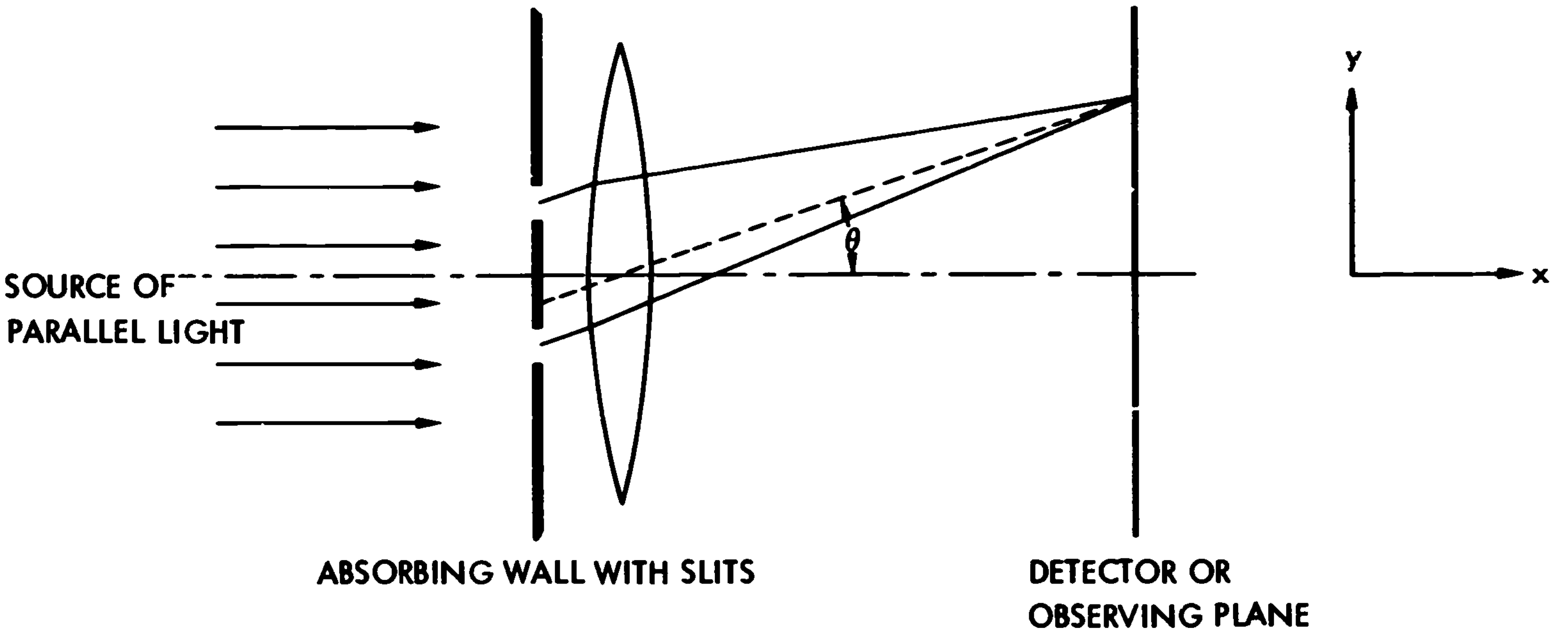

Fig. 2.8 The double slit: Light from the two slits emerging at the same angle θ is brought together by a lens at the same point on the observing screen.

Let the distance between slits be d. Let them be infinitely long out of the picture (z direction) for simplicity. Let their width, for later reference, be a. Let x be the initial direction of the light and y distance along the observing screen. The distance to the observing screen is D. (Fig. 2.9).

The wavefronts arrive parallel to the absorbing plane (y, z plane). At the first slit the amplitude of light is:

$$A_1 = a \sin(-\omega t).$$

At the second slit we have the identical amplitude

$$A_2 = a \sin(-\omega t).$$

Then amplitudes independently propagate from the slits, as if the slits were sources, over to the detector. At a given point P on the observing screen a distance r_1 from slit 1 and r_2 from slit 2,

$$\begin{aligned} A_1 &= b_1 \sin(kr_1 - \omega t) \\ &= b_1 \sin\left(\frac{r_1}{\lambda} 2\pi - \omega t\right) \\ A_2 &= b_2 \sin\left(\frac{r_2}{\lambda} 2\pi - \omega t\right). \end{aligned}$$

Here the coefficient b isn't too important. The phase kr, or $2\pi r/\lambda$ is just 2π times the number of cycles which fit into the path from the slit to the point of observation (Fig. 2.10).

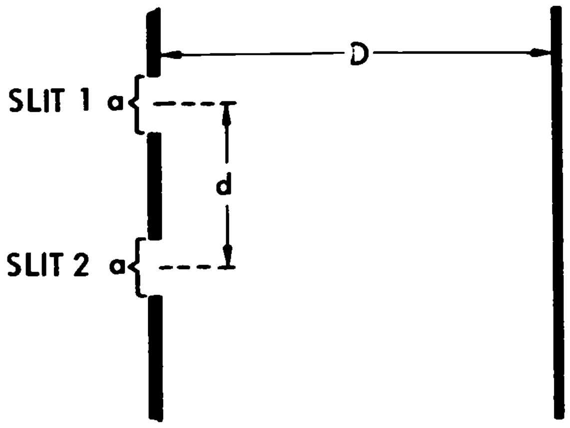

Fig. 2.9 Geometry for double slit.

Actually there are two minor facts hidden here. They are: (a) the mathematical form of Huygen's principle tells us that there is a phase loss of $-\pi/2$ or 1/4 cycle so we will think of r as the actual distance less $-\lambda/4$; (b) the distance r also needs to be modified because it is the "optical distance" including a little extra because the wave is squeezed in the lens. These refinements are unimportant, since both these aspects of the definition of r are exactly the same for r_1 and r_2, the difference $r_1 - r_2$ is unaffected.

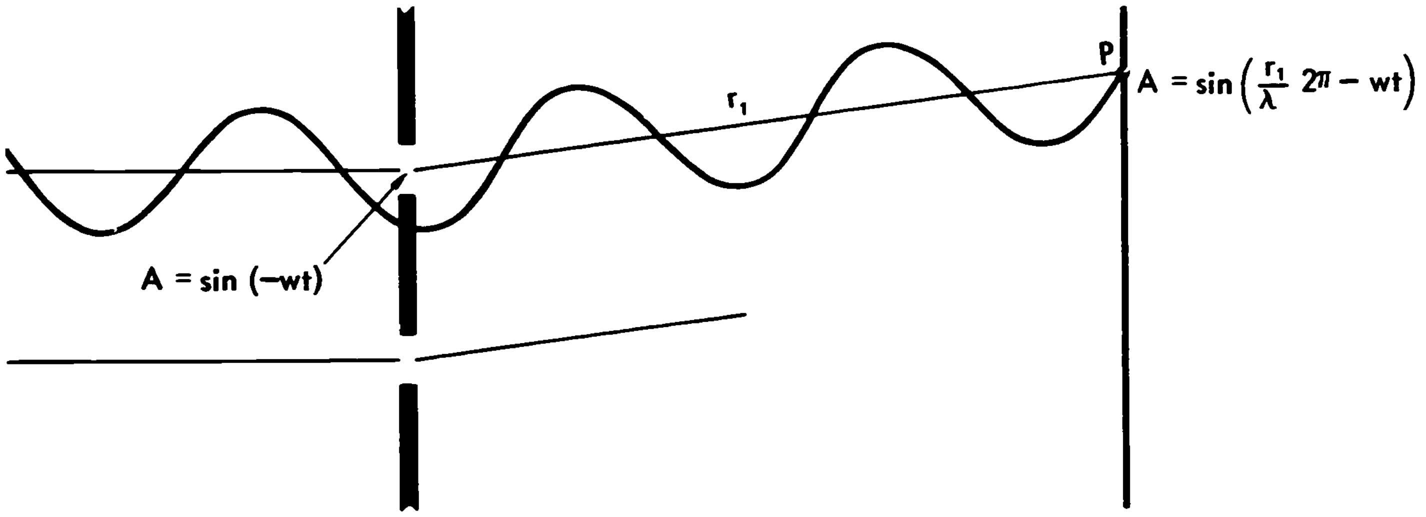

Fig 2.10 The change in the phase of the amplitude propagating from the slit to a point on the screen can be obtained by counting the number of waves (and fraction) along the path from slit to screen.

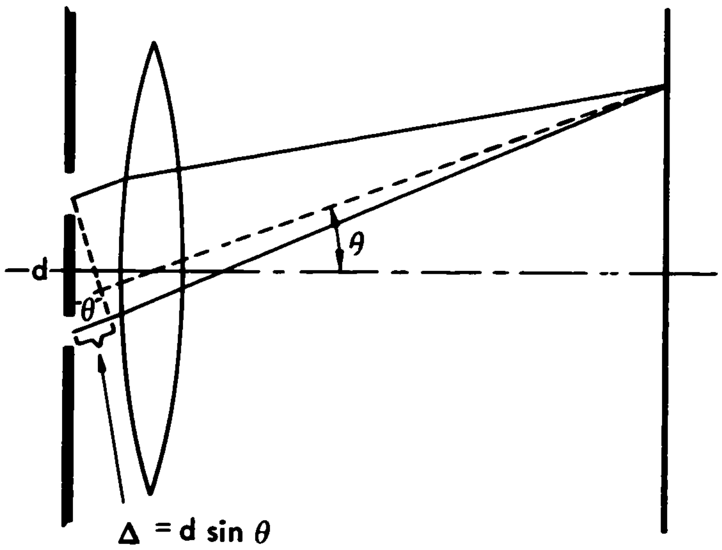

Fig. 2.11 Evaluation of the path difference.

Our results below only depend on this difference.

At the point P on the observing screen the amplitudes add constructively if $r_2 - r_1 \equiv \Delta = n\lambda$:

$$\Delta = r_2 - r_1 = n\lambda \quad \text{constructive}$$
$$\Delta = (n + 1/2)\lambda \quad \text{destructive}$$

where n is an integer. We are not satisfied with this incomplete result. Using trigonometric identities we can add the amplitudes in detail. The magnitudes b_i depend on angle and distance, but only slowly. We assume equal magnitudes $b_i = b$, which should be almost exactly true since from the two slits to P the angle is the same and distance almost the same. Omit the common factor b in the following:

$$A = \sin\left(\frac{r_1}{\lambda} 2\pi - \omega t\right) + \sin\left(\frac{r_1}{\lambda} 2\pi - \omega t + \frac{\Delta}{\lambda} 2\pi\right).$$

Fig. 2.12 Photograph of a double-slit interference pattern.

Let us write this as

$$A = \sin X + \sin (X + \phi)$$
$$= \sin X (1 + \cos \phi) + \cos X \sin \phi,$$

where $X = \frac{r_1}{\lambda} 2\pi - \omega t$ and $\phi = \frac{\Delta}{\lambda} 2\pi$.

If we square we obtain

$$A^2 = [\sin^2 X (1 + \cos \phi)^2 + \cos^2 X \sin^2 \phi] + \sin X \cos X (1 + \cos \phi) \sin \phi.$$

We take the time average to obtain the intensity using the facts that $\sin^2 (\omega t + \delta)$ and $\cos^2 (\omega t + \delta)$ average to 1/2 while $\sin (\omega t + \delta) \cos (\omega t + \delta)$ averages to zero. Thus

$$I \propto 1/2 \, [(1 + \cos \phi)^2 + \sin^2 \phi]$$
$$= 1 + \cos \phi = 2 \cos^2 \phi/2$$
$$I = 2b^2 \cos^2 \frac{\Delta\pi}{\lambda} = 2b^2 \cos^2 \left(\frac{\pi d \sin \theta}{\lambda}\right),$$

(which, is, at least, positive). The path difference Δ is found by geometrical construction (Fig. 2.11).

So $I = 2b^2 \cos^2 ((\pi/\lambda) \, d \sin \theta)$.

The observing screen will look as shown (Fig. 2.12). Graphically (output of photometer as a function of y), ignoring the variation of b, this result is shown in Fig. 2.13. The only approximation made in adding the amplitudes to find this intensity was to equate b_1 and b_2. If they are not equal we find

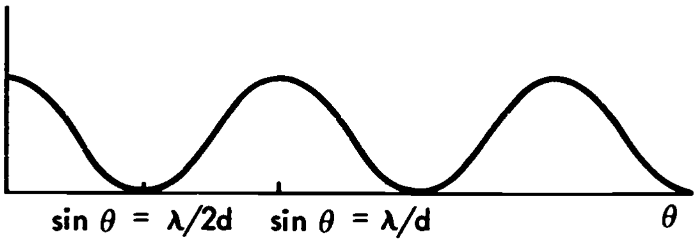

Fig. 2.13 The intensity $\cos^2 (\pi/\lambda \, d \sin \theta)$ as a function of θ (which is essentially y) on the screen.

$$I = \frac{b_1{}^2 + b_1{}^2}{2} + b_1 b_2 \cos\phi$$
$$= \frac{b_1{}^2 + b_2{}^2}{2} + b_1 b_2 \cos\frac{2\pi\ d \sin\theta}{\lambda}.$$

In this case the minima in intensity are not exactly zero since destructive interference can't be perfect when one magnitude is larger than the other. The position of maxima and minima are the same as before.

The intensity pattern we have found can be interpreted in terms of separation of the slits. The kind of thing I want to talk about when we get to molecules and nuclei is how we can determine the slit separation, d, by measuring the intensity as a function of distance. To do this, of course, I would have to be able to convert distance y on the screen to angle θ, which is easy if I know the large scale geometry, and I would have to know the wavelength.

THE INFORMATION CONTENT OF THE PATTERN: In order to obtain an accurate measure of the spacing in a pattern we want to have many maxima. If, for example, there was only one very broad maximum on the observing screen we would be hard pressed to obtain a quantitative measure of the pattern's structure. The more fringes we observe the greater the ease and accuracy of our measurement. This means that the angular interval of observation, $\Delta\theta$, should satisfy

$$\Delta\theta \gg \lambda/d,$$

and since the largest angular interval available to us is of the order of a radian:

$$\lambda \ll d.$$

This seems only reasonable; to obtain accurate information about d we should use a wavelength much smaller.

There is a limitation to this argument, which shows that there is nothing to gain by decreasing λ beyond a certain point. Consider the double slit. Let us superimpose on the same photograph the patterns from double slits of slightly different separations d. The patterns shift slightly with d. Consider double slits with separations d and $d(1+\epsilon)$ and that $\lambda \ll d$, $\epsilon \ll 1$. Since the argument in the expression for $I(\theta)$ is $\pi d \sin\theta/\lambda$, at and near angles which satisfy

$$d \sin\theta/\lambda = [d(1 + \epsilon) \sin\theta/\lambda] - 1/2$$

or

$$\sin\theta = \frac{\lambda}{2\ d\epsilon}$$

the maxima of one pattern fall on the other and the pattern disappears,

More generally if we have many double slits with separations distributed between $d(1-\epsilon)$ and $d(1+\epsilon)$, as in Fig. 2.14, then the pattern is blurred for all angles such that

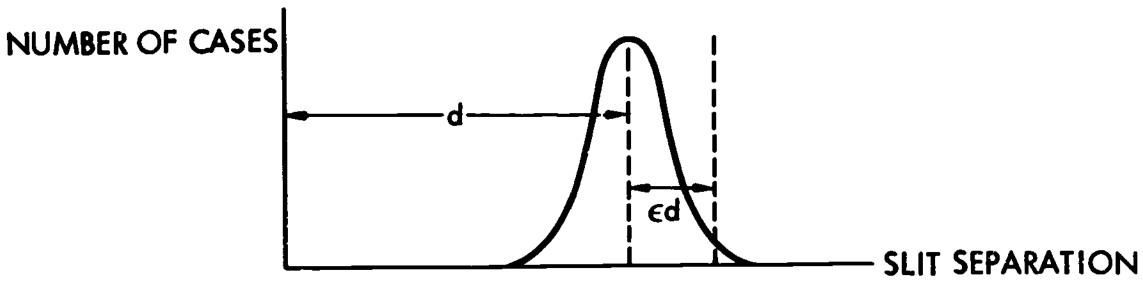

Fig. 2.14 Thought experiment where the intensity patterns for many different double-slit systems of slightly different d, as shown, are superimposed. The information content of the pattern is improved by decreasing λ until $\lambda \approx \epsilon d$, where ϵd is the width or spread of the distribution of slit separations as shown. You slowly lose information by decreasing the wavelength further.

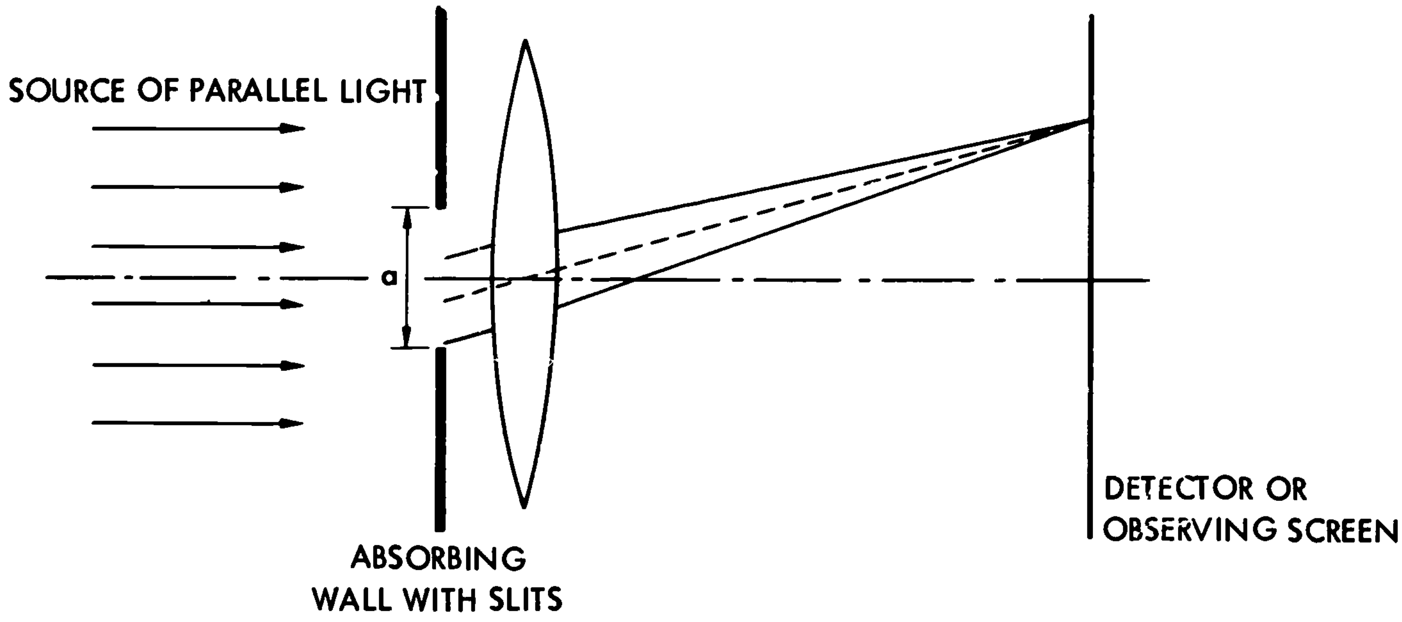

Fig. 2.15 Single-slit experiment.

$$\sin\theta \geq \frac{\lambda}{2\,d\epsilon}.$$

We conclude that the most suitable wavelength, from the standpoint of information in the pattern only, is roughly

$$\lambda \approx 2\,\epsilon d.$$

There is no advantage then in going to a wavelength smaller than the spread ϵd, in sizes of the object you wish to measure. Aside from technical difficulties you will eventually lose information because the useful part of the pattern will be squeezed into a smaller, more difficult to measure, angular interval.

2.3 THE SINGLE SLIT

I have sluffed over several questions. What about the individual slit width, a, and the wavelength λ? Will the simple formula we derived apply no matter what their values? The answer is no. To understand this look at the single-slit problem.

Divide the slit into many narrow strips of thickness Δy: At the slit let the amplitude be $A = \sin(-\omega t)$. The amplitude propagated from a particular strip centered at y is, at a point on the observing screen a distance r_y away,

$$A_y = b \sin(kr_y - \omega t)$$

$$= b \sin\left(\frac{r_y}{\lambda}\,2\pi - \omega t\right).$$

We have from the geometry that $r_y = r - y \sin\theta$.

To add up the contribution of all the narrow strips, we sum or integrate these amplitudes A_y over the slit from $y = -a/2$ to $y = +a/2$. Let X stand for

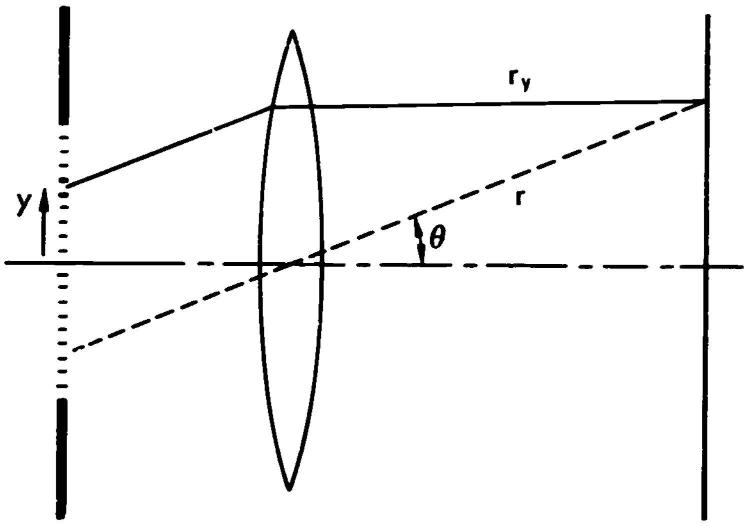

Fig. 2.16 Geometry of single slit. As in other figures, the lens must be considered close to the slit and the screen very far away.

the time dependent y independent term, $X = \omega t - 2\pi\ r/\lambda$

$$A \propto \int_{-a/2}^{a/2} dy \sin\left(X + \frac{2\pi y \sin\theta}{\lambda}\right)$$

$$= \frac{\cos\ (X - 2\pi\ a \sin\theta/\lambda)}{2\pi\ a \sin\theta/\lambda} - \frac{\cos\ (X + 2\pi\ a \sin\theta/\lambda)}{2\pi\ a \sin\theta/\lambda}$$

where $\propto$ means "is proportional to." Analogous to the double-slit case, trigonometric identities enable us to evaluate the intensity which comes out to be

$$I \propto \frac{\sin^2\left(\frac{\pi\ a \sin\theta}{\lambda}\right)}{\left(\frac{\pi\ a \sin\theta}{\lambda}\right)^2}$$

The intensity on the screen is a function of y or θ, so it is a series of parallel lines as in the double-slit case (Fig. 2.17).

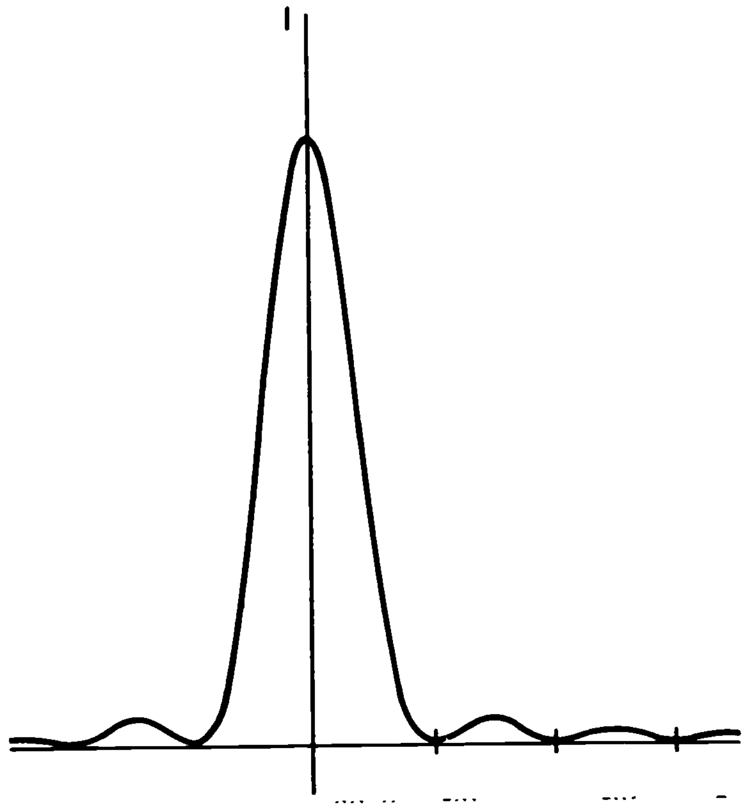

Fig. 2.17 The single-slit intensity $\sin^2\ (\pi\ a \sin\theta/\lambda)/(\pi\ a \sin\theta/\lambda)^2$. The function oscillates because of the numerator and decreases from the center of the pattern because of the denominator. The zeros occur at $\sin\ \theta = n\lambda/a$.

In introductory physics, instead of obtaining $I(\theta)$, the angles near which the maxima and minima occur are determined by a trick. Divide the slit into narrow stips and consider the contribution of only one strip at y position and one at $y - a/2$. For these two strips we have the double-slit problem with $d = a/2$. The result is

$$\frac{a}{2} \sin\theta = n\lambda \quad \text{constructive}$$

$$\frac{a}{2} \sin\theta = (n + 1/2)\lambda \quad \text{destructive}$$

This works for every pair and so for the entire slit. This condition for the minimum agrees with our formula. The result for the maximum is only approximately correct.

Let us look at two extreme cases. Any slit you can easily make is much wider than the wavelength of visible light. If a/λ is very large, $I \approx 0$ unless $\theta \approx 0$ (Fig. 2.18). So the illuminated region on the screen corresponds to the slit. We have almost perfectly sharp shadows beyond the slit. This is the kind of shadowing we observe in everyday life. Now consider $a \ll \lambda$. Since the argument $(\pi\ a \sin\theta/\lambda) \approx 0$ for all angles, the central maximum of the pattern is bigger than the screen. The entire screen is almost equally illuminated (Fig. 2.19).

We may conclude that at small enough angles the screen will be rather uniformly illuminated:

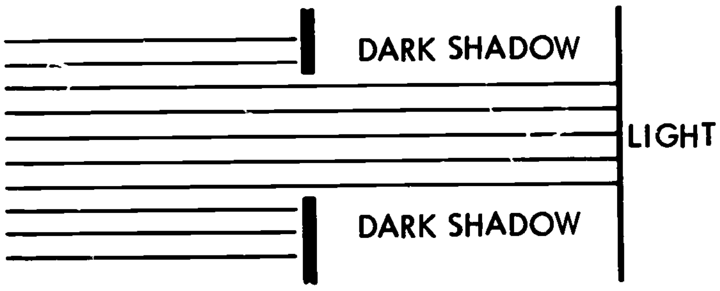

Fig. 2.18 Condition for sharp shadow: $a \gg \lambda$. There is illumination only if θ is essentially zero.

Fig. 2.19 Condition for no shadow: $a \ll \lambda$. The light passing through the narrow slit distributes faintly all over.

$$\theta \lesssim \frac{\lambda}{a} \text{ illuminated (uniformly),}$$

while at sufficiently large angles (if $\pi/2$ is large enough) there is darkness:

$$\theta \gg \frac{\lambda}{a} \text{ in shadow (if } \frac{\lambda}{a} < 1\text{).}$$

In deriving the double-slit formula we ignored the single-slit effect. We see that if we wish to neglect these effects we should work in the uniform region of the central maximum portion of the single-slit pattern. Thus we work at angles

$$\theta \ll \frac{\lambda}{a}.$$

We note however, that since $\theta < \pi/2$, there is no advantage in going to $a \ll \lambda$.

If we wish to obtain accurate measurements from a double-slit pattern we want the pattern to have many oscillations, so the angular integral over which we measure should satisfy $\Delta\theta \gg \lambda/d$ as discussed before under the special topic: <u>Information Content of the Pattern</u>. Combining this inequality with the one above, we obtain the condition

$$a \ll d$$

This is what we intuitively expect: If we want to measure the separation d between two slits, the width a of each slit should be much smaller than d.

COHERENCE. What pattern do we obtain if two slits of separation d are independently illuminated as in Fig. 2.20?

We say that these two amplitudes arriving at slits 1 and 2 are "incoherent" as contrasted with the "coherence" of amplitudes arriving from the same source. All the results up to this point are for the coherent case. If A_1 and A_2 are the amplitudes at the detector associated with slits 1 and 2 then in the coherent case we had:

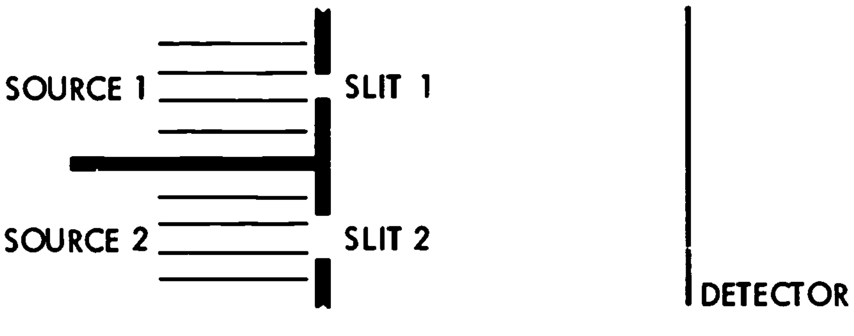

Fig. 2.20 Two distinct and independent sources provide the beams for slit 1 and slit 2. The intensity pattern will just be the sum of the two single-slit intensity patterns.

$$I = \overline{(A_1 + A_2)^2} = \overline{A_1^2} + \overline{A_2^2} + 2\,\overline{A_1 A_2}$$

Where the bar indicates time averaging. The 2 $\overline{A_1 A_2}$ term is called the "interference term" and is responsible for the double-slit pattern. Meanwhile for the incoherent case we have no interference:

$$I = \overline{A_1^2} + \overline{A_2^2} = I_1 + I_2.$$

The intensity pattern is simply the sum of the intensities for the two single slits separately.

The reason for this result is as follows: Coherent amplitudes have a definite relation between their time dependences: i.e., at any point $\vec{r}$ on the screen two coherent amplitudes A_1 and A_2 have time dependences of the form

$$A_1 = a_1 \sin(-\omega t + \delta_1)$$
$$A_2 = a_2 \sin(-\omega t + \delta_2).$$

Where the phase difference, $\delta_1 - \delta_2$ between the oscillations is independent of time. Two incoherent amplitudes have on the average no fixed phase difference. This is due to the nature of typical sources of light. You should imagine that a source emits a train of waves of time dependence

$$\sin(-\omega t + \delta)$$

only from time t_1 to t_2, where $t_2 - t_1$ is very long compared to the period $\tau = 2\pi/\omega$ but is still a short time. After t_2 a new wave with time dependence

$$\sin(-\omega t + \delta + \delta')$$

is emitted and so on. The various phases δ, δ', δ'', associated with the light emitted at closely spaced times by a single source, are unrelated to each other. They are random angles. As the value of δ changes to $\delta + \delta'$, a phase difference $\delta_1 - \delta_2$, associated with two coherent amplitudes goes to $(\delta_1 + \delta') - (\delta_2 + \delta') = \delta_1 - \delta_2$ and so remains undamaged. But the phase difference associated with two amplitudes arising from independent sources will go to $\delta_1 + \delta_1' - (\delta_2 + \delta_2')$ an angle unrelated to $\delta_1 - \delta_2$. We established above that two coherent amplitudes

$$A_1 = a_1 \sin(-\omega t + \delta_1)$$
$$A_2 = a_2 \sin(-\omega t + \delta_2)$$

give rise to an intensity

$$I = \frac{a_1^2 + a_2^2}{2} + a_1 a_2 \cos(\delta_1 - \delta_2).$$

For two incoherent amplitudes the period of time averaging is normally long enough to cover any random changes of phase so that

$$\overline{\cos(\delta_1 - \delta_2)} \rightarrow 0 \text{ (incoherent case)}$$

and

$$I = I_1 + I_2$$

3 OPTICS OF HOLES

3.1 SINGLE HOLE

Consider monochromatic light arriving normally on an absorbing plane into which has been cut a circular hole of diameter a (Fig. 3.1).

On the screen let's use, instead of y, z, coordinates ρ, ϕ. Here $\rho = r \sin \theta$ and ϕ is the azimuthal angle. The intensity pattern on the screen, which we do not derive, has of course, circular symmetry. That is, it does not depend on ϕ. The pattern will be a set of concentric circles about the $\rho = 0$ point. A photograph would appear as shown (Fig. 3.2) while the intensity plotted out from the center of the pattern along ρ is as shown in Fig. 3.3.

The formula for the intensity is

$$I = \text{constant} \cdot \frac{J_1^2 \ (\pi \ a \sin \theta/\lambda)}{(\pi \ a \sin \theta/\lambda)^2}$$

where J_1 is the "Bessel function" of first order. The initial coefficient is just

$$4 \frac{F}{\lambda^2 r^2} \left(\frac{\pi a^2}{4}\right)^2,$$

where F is the incident beam intensity.

You don't need to know any more about the Bessel function than I'll tell you. For the moment we are satisfied to know the rough inequalities:

$$\theta \ll \frac{\lambda}{a} \quad \text{illuminated (uniformly)}$$

$$\theta \gg \frac{\lambda}{a} \quad \text{shadow (for } \frac{\lambda}{a} < 1\text{)}.$$

The situation is analogous to the single slit of width a.

3.2 TWO HOLES

Let us now consider two holes in an absorbing plane (Fig. 3.4).

The two holes are arranged one above the other. For z = 0 on the screen (i.e., along the y axis) we find

$$A(y,\ z = 0) = {a_1}^2 \sin (kr_1 - \omega t) + {a_2}^2 \sin (kr_1 + kd \sin \theta - \omega t)$$

$$I(y,\ z = 0) = \frac{{a_1}^4 + {a_2}^4}{2} + {a_1}^2\ {a_2}^2 \cos \left(\frac{2\pi d \sin \theta}{\lambda}\right).$$

Here I have omitted a factor, approximately equal for the two slits. The derivation is the same as in the double-slit problem. Note that I do not assume the two holes to have the same diameter.

Now we generalize the problem so that the orientation of the holes

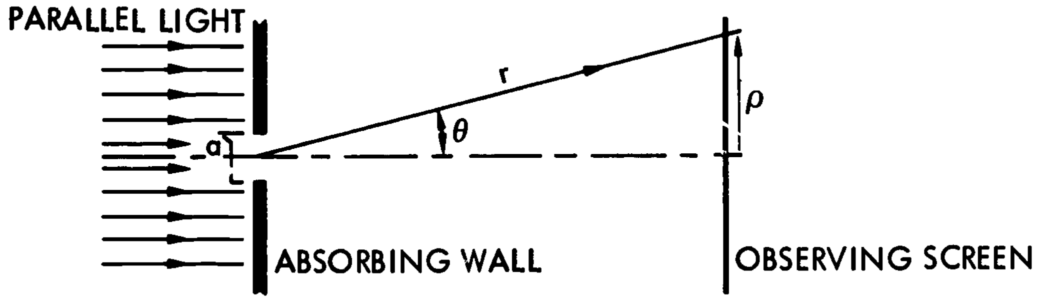

Fig. 3.1 Configuration for a single hole. We use coordinates $r = \sqrt{x^2+y^2+z^2}$ measured from an origin at the middle of the hole, $\rho = \sqrt{y^2+z^2}$, measured from the center of the screen, θ where $r \sin \theta = \rho$ as drawn, and ϕ the azimuthal angle on the screen.

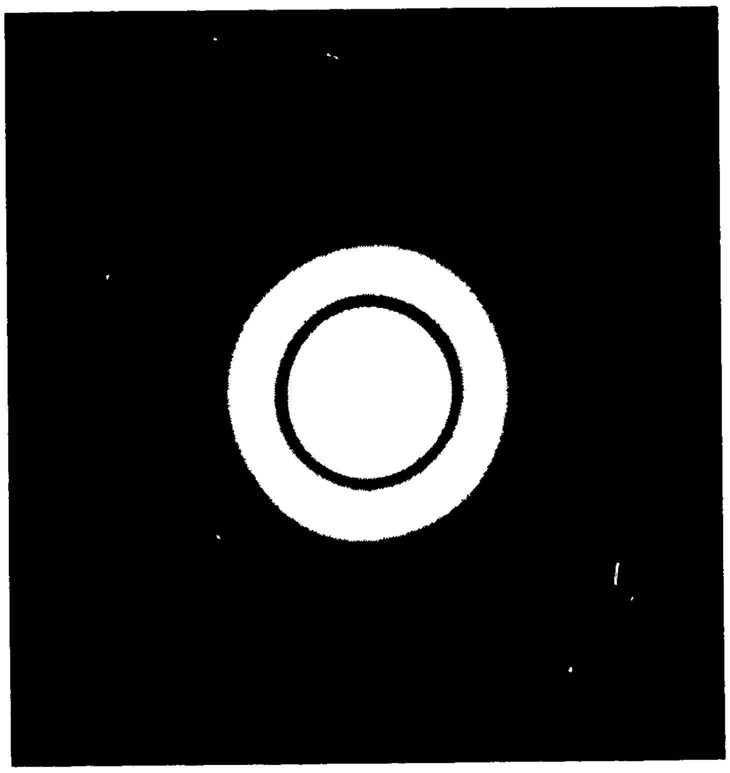

Fig. 3.2 Photograph of single-hole intensity pattern.

takes on any angle. That is, let the line joining the holes lie at angle α to the incident beam direction and at an azimuthal angle β (with respect, say, to the vertical). In the simple vertical arrangement discussed above $\alpha = 90^\circ$ and $\beta = 0$ (Fig. 3.5).

Looking at the geometry (Fig. 3.6) we find that

$$\Delta = d[\cos\alpha - \cos(\alpha + \theta)].$$

For general β one finds that

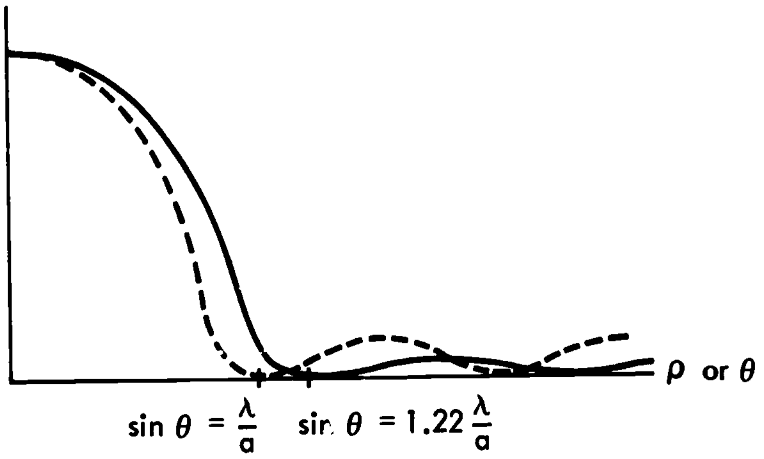

Fig. 3.3 Intensity as a function of distance from the center of a pattern, for a hole of diameter a. For reference the single-slit intensity $\sin^2 (\pi a \sin\theta/\lambda)/(\pi a \sin\theta/\lambda)^2$ for a slit width a is shown as a dashed curve. You note that the hole yields a pattern slightly broader and with smaller secondary maxima.

$$\Delta = d(\cos\alpha - \cos\alpha\cos\theta + \sin\alpha\sin\theta\cos\beta).$$

We will not go further to study the calculation of the intensity. What we want is the average of intensities over all α, β. Let me just state the result:

$$I = \frac{a_1^4 + a_2^4}{2} + a_1^2 a_2^2 \frac{\sin(2kd\sin\theta/2)}{(2kd\sin\theta/2)}$$

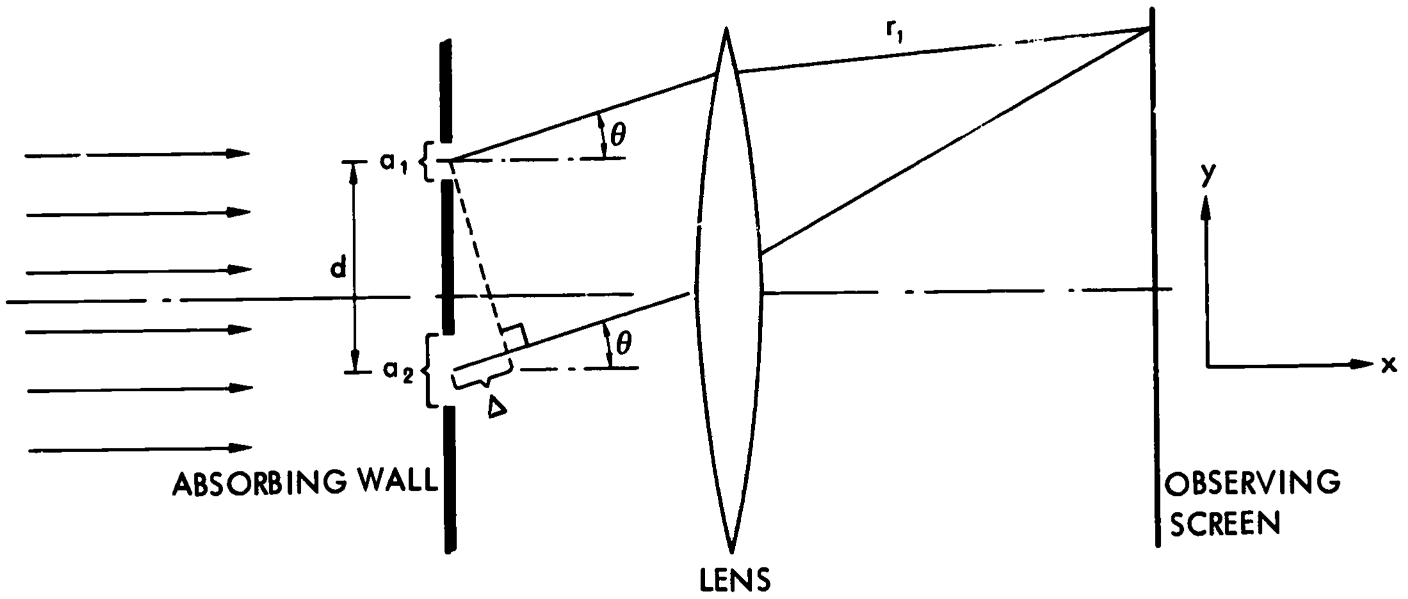

Fig. 3.4 Configuration for light incident on two holes of unequal diameter. Consider the vertical plane containing the holes ($z = 0$). At an angle θ the path difference is $\Delta = d\sin\theta$, just as for the double slit.

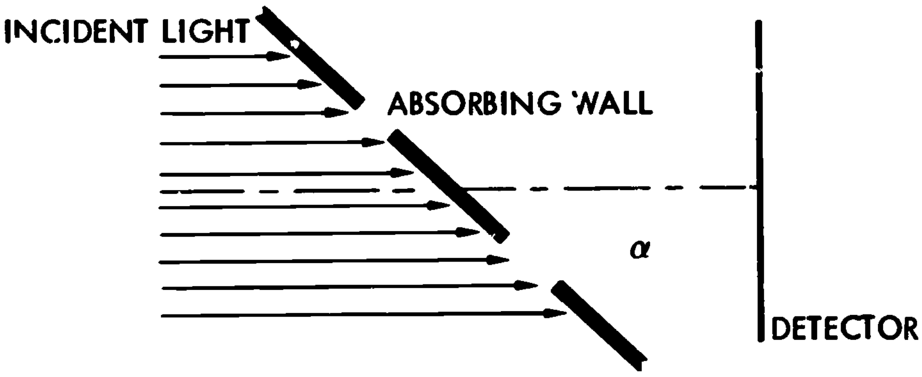

Fig. 3.5 Side view of two holes in a wall at angle α (with β = 0). By rotating the absorbing wall about the horizontal (x axis) keeping α fixed, we pass through different angles β.

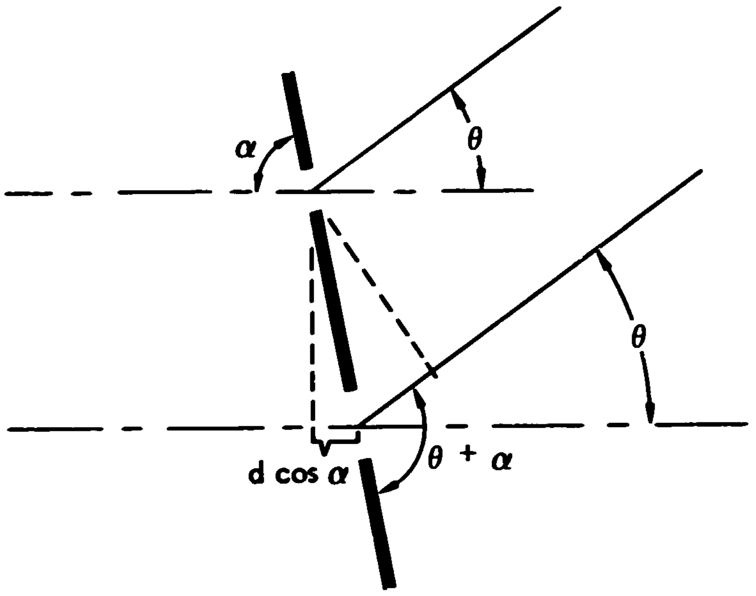

Fig. 3.6 Geometry for determination of Δ when β = 0. The path length difference is d cos α before the absorbing wall and −d cos (θ + α) which is a positive distance in the sketch, after the wall.

(recall $k = 2\pi/\lambda$). (See special topic: Mathematics of the Two-Hole Pattern). The pattern has circular symmetry around the center point $x = \theta = \rho = 0$ because the whole configuration is symmetric about the x axis. Thus, using our circular coordinates on the screen as in Fig. 3.1, it depends on radial distance ρ, not ϕ.

If the diameters of the two holes are rather different, then the difference between the intensities at maximum and minimum will be slight. The intensity will look as shown in Fig. 3.7.

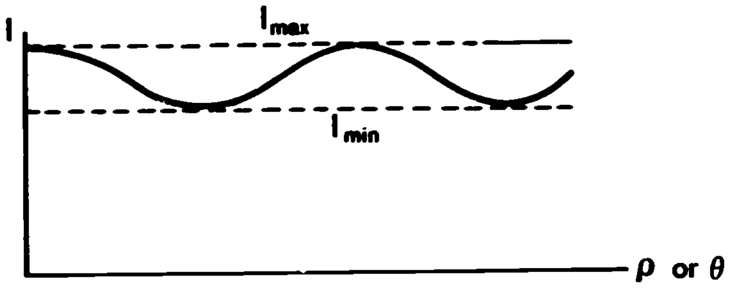

Fig. 3.7 Intensity pattern for holes of rather different diameter (e.g., $a_1 \gg a_2$) I_{max} is proportional to $(a_1 + a_2)^2$ and I_{min} is proportional to $(a_1 - a_2)^2$.

MATHEMATICS OF THE TWO-HOLE PATTERN: The two contributions to the amplitude at the screen have the form

$$A \propto a_1{}^2 \sin (kr - \omega t) + a_2{}^2 \sin (kr + k\Delta - \omega t).$$

The extra phase $k\Delta = 2\pi\Delta/\lambda$ for the second slit can be written

$$\vec{k}\cdot\vec{d} - \vec{k}'\cdot\vec{d}$$

where $\vec{d}$ is the vector from the

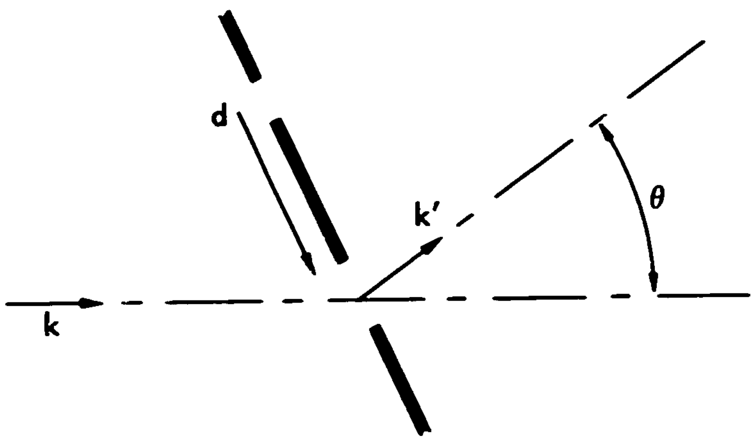

Fig. 3.8 Geometry for double-hole diffraction.

first to the second slit (oriented at angles α, β) and $\vec{k}$, $\vec{k}'$ are the "propagation vectors" before and after the absorbing wall. That is, $|\vec{k}| = |\vec{k}'| = k$ and the direction of $\vec{k}$ is the direction of motion of light: $\vec{k}$ is parallel to x and $\vec{k}'$ is at an angle θ.

The intensity for fixed orientation of the holes is the time average of the sum of the squares of the two terms in A plus the interference term. The latter, after time averaging, is

$$(a_1^2 \; a_2^2) \cos (\vec{d} \cdot (\vec{k} - \vec{k}')).$$

Now to average over the directions of $\vec{d}$ we take $\vec{k} - \vec{k}'$ to be the axis of a spherical coordinate system. The average of the interference term over all orientations of the absorbing wall is

$$(a_1^2 \; a_2^2)(1/2) \int_0^{\pi} \sin \gamma \, d\gamma$$

$$\cos (d \, |\vec{k} - \vec{k}'| \cos \gamma)$$

$$= a_1^2 \; a_2^2 \frac{\sin (d \, |\vec{k} - \vec{k}'|)}{d \, |\vec{k} - \vec{k}'|}.$$

We find $\vec{k} - \vec{k}'$ by geometrical construction:

$$|\vec{k}-\vec{k}'| = 2k \sin \theta/2.$$

Our final answer is then

$$I = \frac{a_1^4 + a_2^4}{2}$$

$$+ \; a_1^2 \; a_2^2 \frac{\sin (2 \, kd \sin \theta/2)}{(2 \, kd \sin \theta/2)}.$$

4 SCATTERING

4.1 OPTICAL SCATTERING FROM A BLACK DISK.

We want to consider the standard scattering experiment. An essentially parallel collimated beam arrives at a target and some of it is scattered on to a detector. Both the collimator opening and the distance to the detector are very large or macroscopic distances. The target is made up of microscopic particles or, in principle, a single microscopic particle. If the target is a single black disk, then we have the configuration shown in Fig. 4.1.

We need to know the amplitude, A_B, under the condition that the collimator diameter W is very, very large:

$$W \gg a$$

$$W \gg \lambda$$

When the black disk target is absent we just have the hole configuration considered before. We discussed how for $\theta \gg \lambda/W$ there is dark shadow at the detector. Let the amplitude when only the collimator is present be A_C. If we call A_H the amplitude for the configuration with only a small hole of diameter a, then to the right of the absorbing plane we have Fig. 4.2.

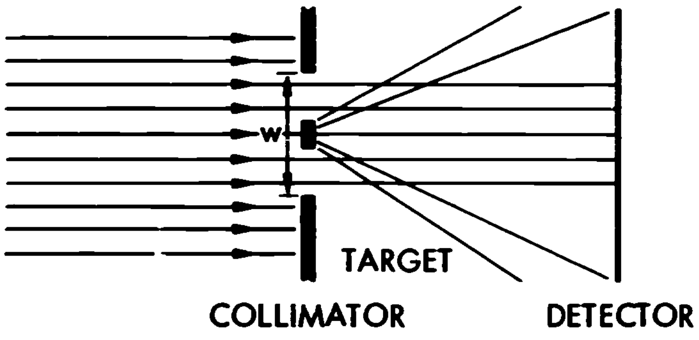

Fig. 4.1 Standard scattering experiment, with black disk target of diameter a, the collimator opening W is much larger than either λ or a. Both the collimator opening and the distance to the detector are very large or macroscopic distances.

$$A_B = A_C - A_H$$

Since A_C is essentially zero at the detector for $\theta \gg \lambda/W$ we find

$$A_B = -A_H,$$

and the intensity for black disk scattering is

$$I = \left[4\frac{F}{\lambda^2 r^2}\,\frac{\pi a^2}{4}\right]^2 \frac{J_1{}^2\left(\frac{\pi\ a \sin\theta}{\lambda}\right)}{\left(\frac{\pi\ a \sin\theta}{\lambda}\right)^2}$$

just as for transmission of light through a hole. Meanwhile at very small angles $\theta \lesssim \lambda/W$, the beam will overwhelm the light scattered from the disk so the pattern will not be easily discerned.

4.2 SCATTERING OF "MATTER" WAVES

We've seen how to calculate the scattering of light by a black disk (and by two black disks), and you

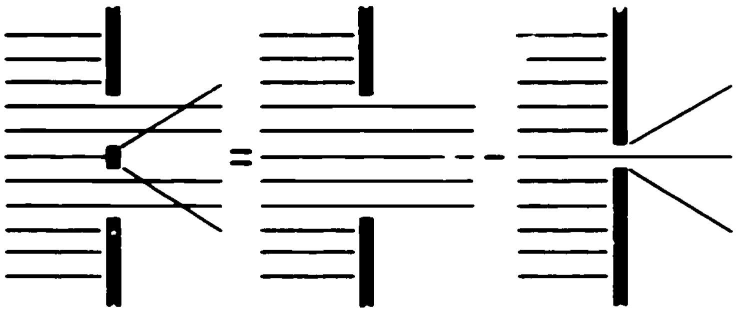

Fig. 4.2 The amplitude to the right of the absorbing plane for a black disk target is the difference between the collimated amplitude with no target and the amplitude for a small hole of the same diameter as the disk. This is because the amplitude must be zero just to the right of a black disk (by definition of "black").

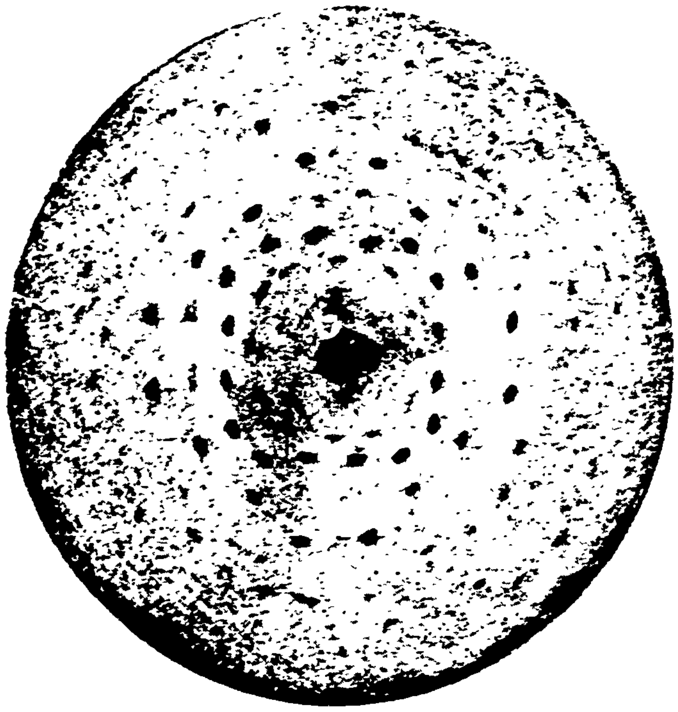

Fig. 4.3 A typical pattern of x-ray intensity on the observing screen with a crystalline target.

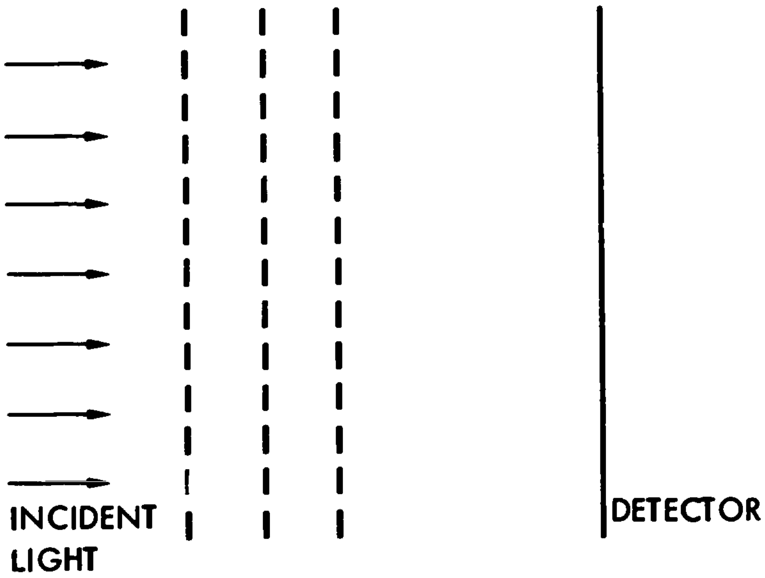

Fig. 4.4 If the wave fits in certain directions there will be a spot at the detector at that angle. The wave model predicts particular patterns of spots for different crystal targets.

can imagine how it would be done for other arrays of black disks (or for scatterers other than black disks). There are two essentially different types of arrays. There are crystals which consist of regularly aligned rows of atoms, and there are amorphous materials, gaseous, liquid or solid, which don't have such a regular structure between the molecules. The intensity pattern for scattering of light (in this case x rays to get small enough wavelengths) from a crystal is an arrangement of spots at certain angles (Fig. 4.3). It is the same as the pattern you obtain from light falling on a set of absorbing walls with regularly spaced holes in them (Fig. 4.4).

For an amorphous target the wave model predicts a pattern which is a series of concentric circles, as for the one and two black disk cases discussed. There may be some regularity as you go out in radius in such a pattern such as bright ring - not-so-bright ring, and so on.

In summary, we see that the wave model predicts complex patterns. Many of the features arise, however, from simple considerations.

If instead of directing a beam of light or x rays on a target, let us use an intense beam of "matter" particles of definite energy.[2] I mean particles such as electrons and protons. Under reasonable conditions it turns out that you observe the same kind of patterns as with light. If the target is a crystal you observe spots; if it is an amorphous material, rings.

We shall assume that the <u>wave model determines the intensity distribution for scattering of microscopic "matter" particles</u> as well as for scattering of electromagnetic radiation. We will use the same formula for the intensity. We will just need to know what to insert for the wavelength in the formula. I will discuss this later.

Let us digress from the main thread of our argument to point out that this assumption has two very pleasing aspects: (a) It can be shown that, in the case of particles larger and heavier than electrons and protons,

---

[2] Of course, more than the beam may have to be changed. The lens is inessential to any of these experiments and there is no known lens for x rays. If a lens would be helpful with the "matter" particles, a magnetic lens for charged particles can be used. The detector would probably be different although photographic film can be used in <u>all</u> cases.

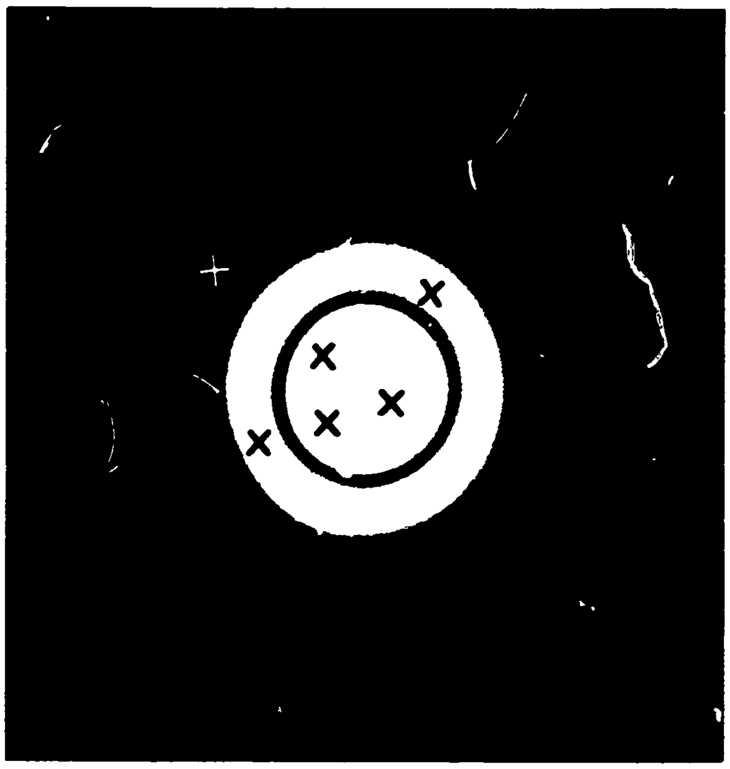

Fig. 4.5 Pattern obtained with intense beam (circles). Typical pattern obtained at very low intensity is made of individual dots, here denoted by crosses to make them stand out.

the wave model eventually goes over to classical mechanics. In the appropriate limit, it describes the scattering of billiard balls correctly. (Although the wave model has this consistency, the classical mechanics of large objects does not apply to microscopic particles.) (b) The wave model unifies some of our ideas about light and "matter" particles. Let us look at one aspect of this by discussing a thought experiment. Take a picture of the intensity pattern arising from scattering a beam of particles of definite energy and with a particular target. Say it is a ring pattern. Now reduce the beam intensity, leaving everything else the same. We may need to improve our detector. There is no problem, however, in obtaining very sensitive detection these days. As we decrease the intensity and reduce the exposure we will obtain a rather rough and vague pattern like a newspaper photograph rather than the smooth clear pattern obtained at high intensity. Reducing the intensity farther we will obtain just one or a few dots in a picture (Fig. 4.5). Reducing it further we will finally obtain nothing (i.e., no beam particle scattering into the detector). The least non-null result is one spot. Each spot is made by the arrival of a single scattered beam particle. Imagine obtaining many, many negatives, each with a few spots on it. Placing them one on top of the other and looking through you will see the same smooth pattern which would be obtained in a single high-intensity exposure. The same phenomenon occurs in the case of light. The light particles are called "photons." Normally an intense beam consists of so many of these units that it appears to be continuous.[3]

The wave model predicts the essentially continuous distributions which arise in cases of high intensity and long exposure. The wave model does not predict where any individual particle will arrive at the observing screen. But since a smooth intensity distribution is made up by adding the contributions of individual particles, the intensity distribution is a probability distribution for individual scatterings. We will not make use of this fact but will always consider the smooth pattern obtained with sufficiently intense beams and long exposures.

To complete this discussion let us state the wavelength relation for matter waves (and the energy relations for photons). For a matter particle (nonrelativistic):

$$E = \frac{mv^2}{2} = \frac{p^2}{2m}$$

---

[3] We do not usually have to worry that neighboring beam particles have any influence on each other. The density of beam particles in a beam is usually less than in the best vacuums man has made. For example, if the beam intensity is 10^{13}/sec $\times$ cm^2 (i.e., about one microampere on a cm^2 target - a typical order of magnitude), and the beam velocity is one-third the velocity of light then the beam density is $10^{13}/10^{10} = 10^3$ particles per cm^3. The beam particles are spaced 1 mm apart! They certainly do not influence each other during any atomic or subatomic scattering process.

where p is the momentum. The expression for the wavelength (in vacuum) to be used in the wave model is known as the de Broglie relation:

$$\lambda = \frac{h}{p} .$$

This relation, with the same value of the constant h has been found to be valid for all particles. Ordinarily h is stated in cgs. units as 6.63×10^{-27} erg x sec. We will not, however, use this unit system in our calculations. We will not here discuss the experiments which yield the best determinations of h. For photons, or any extreme relativistic particle, the relation between energy and momentum is

$$E = pc.$$

The de Broglie relation again applies so that

$$E = hc/\lambda \text{ (photons)}$$

$$E = h^2/2m\,\lambda^2 \text{ (nonrelativistic particles)}.$$

For completeness, although it doesn't enter into our intensity formula, I state the frequency relations. For light we saw that

$$\omega = kc \quad \text{or} \quad \nu = c/\lambda,$$

which implies,

$$E = h\nu.$$

This relation also applies to nonrelativistic particles.

Often you will see the constant

$$\hbar \equiv h/2\pi$$

used instead of h. If we also introduce the symbol

$$ƛ \equiv \lambda/2\pi$$

(the distance in which the amplitude's phase passes through one radian rather than one cycle), the above formulae become

$$ƛ = \hbar/p = 1/k \tag{4.1}$$

$$E = pc = \hbar c/ƛ = \hbar kc \quad \text{(photons)} \tag{4.2}$$

$$E = p^2/2m^2 = \hbar^2/2mƛ^2 = \hbar^2k^2/2m \quad \text{(nonrelativistic particles)} \tag{4.3}$$

and

$$E = \hbar\omega.$$

5 MOLECULAR STRUCTURE OF GASES BY ELECTRON DIFFRACTION

5.1 RIGID MOLECULES

We are going to discuss the experimental determination of interatomic distances in a gas molecule by observation of interference effects in electron scattering, commonly called "electron diffraction." Let us first assume that the various interatomic distances in a given molecule are fixed (i.e., the same at all times). The structure of the molecule is determined by listing the distances r_{ij} between all atoms i and j as indicated in Fig. 5.1.

The distances we are talking about, as you recall from Chapter 1, are the distances between the atomic nuclei. (The space between these nuclei is more or less fully occupied by atomic electrons.)

Imagine, then, a collimated beam of electrons of energy E scattered by a gas target (a well-defined jet of gas passing at right angles to the beam) onto a photographic plate (Fig. 5.2). A typical electron energy used is about 40 000 electron volts (40 kV). This is not much more than that delivered by the electron gun in the picture tube of a standard television receiver.

The reason for choosing this energy is discussed in the special topic, Information Content of a Pattern. Just for the moment, let us relax our assumption that the interatomic distances have fixed values and consider the realistic case where a typical interatomic distance r_{ij} is not exactly fixed, as a function of time, but takes on various values around its equilibrium value r_e, i.e., r takes on values from roughly $r_e + \Delta r$ to $r_e - \Delta r$. Then the best wavelength to use is

$$\lambda \approx \Delta r.$$

If you use a much smaller wavelength than this, the pattern smooths out to uniform illumination except at very small angles. A 40 kv electron has wavelength (Eq. (4.3)):

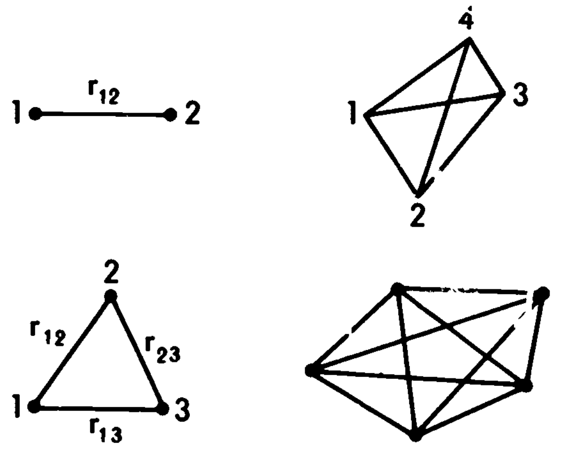

Fig. 5.1 If the distances between all atoms in a molecule are fixed, then the molecule has a definite rigid form as indicated by the examples. The 4 and 5 atom arrays may, of course, be three dimensional. Note that for a molecule with five or more atoms one or more of the distances r_{ij} can be found from the other r_{ij}'s.

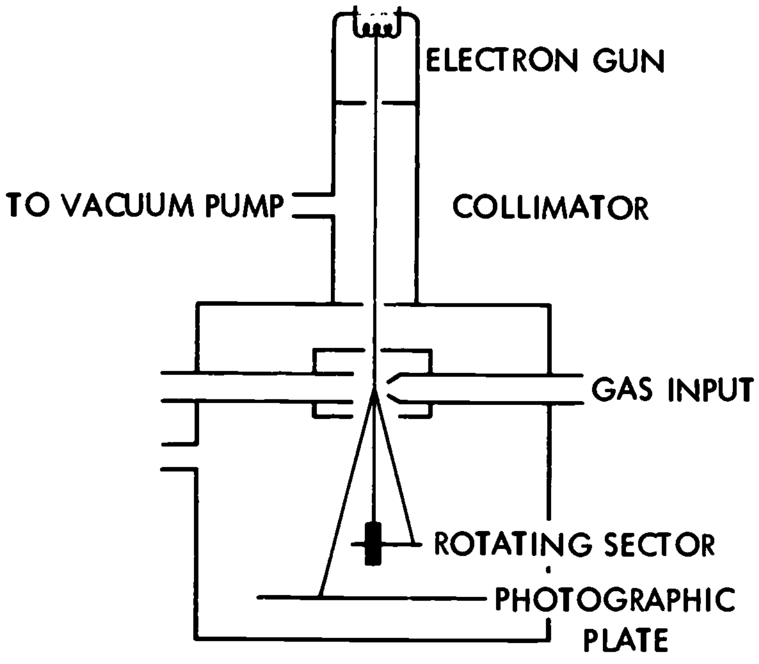

Fig. 5.2 Schematic drawing of the electron diffraction apparatus. The size from top to bottom is about one meter. The rotating sector is explained in Fig. 5.4.

$$\lambda = 2\pi\sqrt{\hbar^2/2mE}$$
$$\approx 0.06 \times 10^{-8} \text{ cm}$$

This wavelength is about equal to the spread Δr in the distribution of interatomic distances that is observed (see section 5.2). The wavelength is <u>much smaller</u> than the spread (effectively about 1 Å) in the distribution of positions of <u>atomic electrons</u>. The electron beam has sufficiently small wavelength that it is not strongly affected by the electrons in the target but only by the nuclei (Fig. 5.3).

In section 3.2 we established the intensity formula

$$I\ (s) \propto \frac{a_1{}^4 + a_2{}^4}{2} + a_1{}^2\ a_2{}^2\ \frac{\sin sr}{sr},$$

where instead of scattering angle θ, I have introduced s, the momentum transfer.[4] This notation is commonly used by physical chemists:

$$s \equiv 2\ k \sin \theta/2$$

and r is the separation of the two black disks (we saw in section 4.1 that this intensity formula applies to two black disks of diameter a_i as well as to two holes). To apply this intensity formula to scattering of electrons by atomic nuclei instead of black disk scattering, we need only one modification. For each atom substitute $f_i(s)$ for $a_i{}^2$. Here f_i is the Coulomb, or Rutherford, scattering amplitude for the scattering of one charged point particle by another. We don't derive this modification. The intensity is then

$$I = \frac{f_1{}^2 + f_2{}^2}{2} + f_1 f_2\ \frac{\sin sr}{sr}.$$

This is the formula for a rigid diatomic molecule.

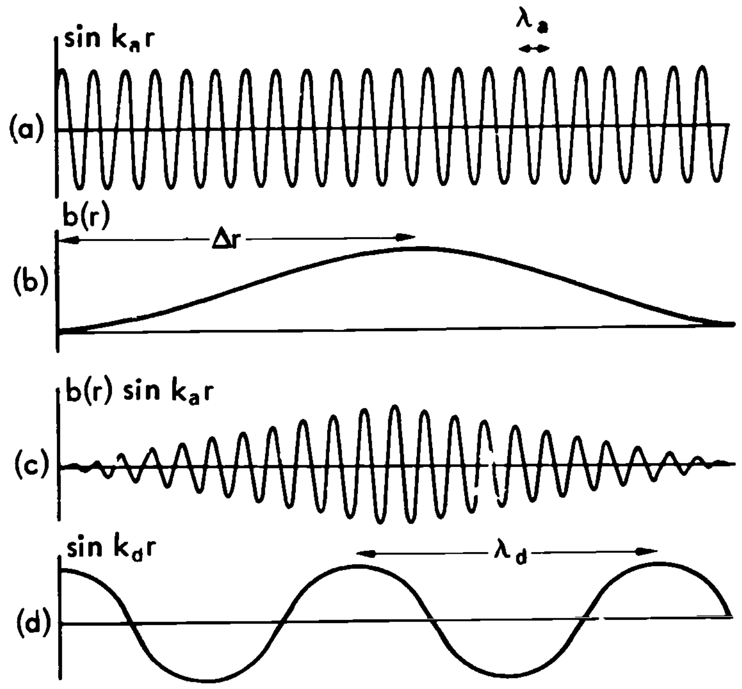

Fig. 5.3 We see that it is reasonable that a wave of short wavelength (a) doesn't notice a gradually changing (force) distribution (b), by multiplying the wave at every point by the distribution b. The result, $\sin k_a r \cdot b(r)$, is plotted in (c). The average value of (c) is very small, i.e., $\langle \sin k_a r \cdot b(r) \rangle_{ave} \approx 0$, since the positive and negative parts of the wave are almost equally affected by b. The criterion for a small effect is $\lambda \ll \Delta r$ where Δr is roughly the smallest distance in which there is a large relative change in b(r). Meanwhile the wave $\sin k_d r$ shown in (d), where $\lambda_d \approx \Delta r$, will be strongly influenced by b.

Just as for black disk scattering, the intensity pattern for a single atom, $I = f\ (s)^2$, is a much smoother function of angle than the interference term, $f_1 f_2 \sin (sr)/sr$ because of the sin (sr) factor (see section 2.3). The experimentalists subtract away the smooth background from I (s) and deal directly with the "molecular intensity":[5]

$$I_m\ (s) \propto f_1 f_2\ \frac{\sin sr}{sr}.$$

---

[4] Workers in x-ray and low energy electron scattering usually use notation such that 2θ is the scattering angle. You should check the definition of θ when reading an article by a chemist or an article on x-ray scattering.

[5] The photographic emulsion also records "inelastically" scattered electrons (to be covered in a future Chapter 6), which are distributed smoothly with s. If the total smooth background intensity $I_b = f_1{}^2 + I_{inelastic}$ then the molecular intensity is $I_m = \frac{\Sigma' f_i f_j \sin sr_{ij}/sr_{ij}}{I_b}$. This defines the constant of proportionality in Eq. (5.1).

For a polyatomic molecule the expression is

$$I_m(s) \propto \sum\nolimits' f_i f_j \frac{\sin sr_{ij}}{sr_{ij}}. \quad (5.1)$$

The primed sum means sum over i and j but with no i = j terms.

The intensity distribution for Coulomb scattering is strongly peaked at forward angles, falling off at large angles. For a single atom

$$I_C = f^2 \propto \frac{Z_{eff}{}^2}{\sin^4 \theta/2} \propto \frac{Z_{eff}{}^2}{s^4},$$

where Z_{eff} is the effective charge of the atomic nucleus. (We do not derive this formula here.) It is very inconvenient to handle this enormous range of intensities from small to large angles. A simple device which effectively multiplies I by s^3 or s^4, say, (whatever the experimentalist desires) is the rotating sector. This is a piece of metal which stops beam electrons which strike it but otherwise has no effect. It rotates about the same axis as the axis of the beam, and is shaped to cut out more of the forward scattered electrons than electrons scattered through a large angle (Fig. 5.4).

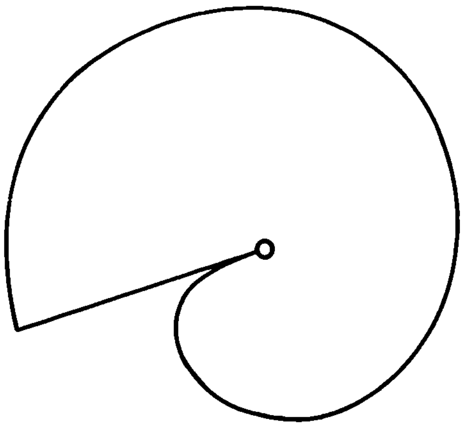

Fig. 5.4 Shape of metal sector rotated about the axis (into page) of the incident electron beam. This one effectively multiplies the scattered intensity by a factor proportional to s^3.

Now we can discuss results. A typical intensity curve for a complicated polyatomic molecule as a function of momentum transfers is shown in Fig. 5.5.

The particular distances r_{ij} in the intensity formula (5.1) which give a good fit to the data are found by various techniques. The most convenient procedure is discussed in Section 5.2. Typical results for r_{ij} are 1 to 5 Å with a reproduceability of up to 0.002 Å. The agreement with other techniques (analysis of spectroscopic data, neutron scattering and scattering of x rays) is well within 0.01 Å in favorable cases. Another check which is well satisfied is provided by the self consistency of the set of distances r_{ij} in a molecule of five or more atoms (see Fig. 5.1). So the results are quite convincing.

As a more concrete illustration of the technique, we show in Fig. 5.6 (a, b, c) three molecular intensity curves as a function of s as they might be obtained from an experiment. These curves are all for the molecule dichloroethylene ($C_2H_2Cl_2$) and they show the variation in the molecular intensity for three forms of the molecule. The molecules all lie in a plane but differ in the placing of the chlorine atoms with respect to the carbon as sketched in the figure next to the corresponding intensity curves. These forms of the molecule can be distinguished by measuring the distance between the two Cl atoms. In (a), called 1,1 dichloroethylene, the Cl atoms are close, in (b), called 1,2 cis dichloroethylene, they are further apart, and in (c) 1,2 trans-dichloroethylene, they are further apart.[6] The increasingly rapid oscillation of sin sr with increasing $r_{Cl-C'}$ is evident. The relative amounts c_i of these and other forms of dichloroethylene in a

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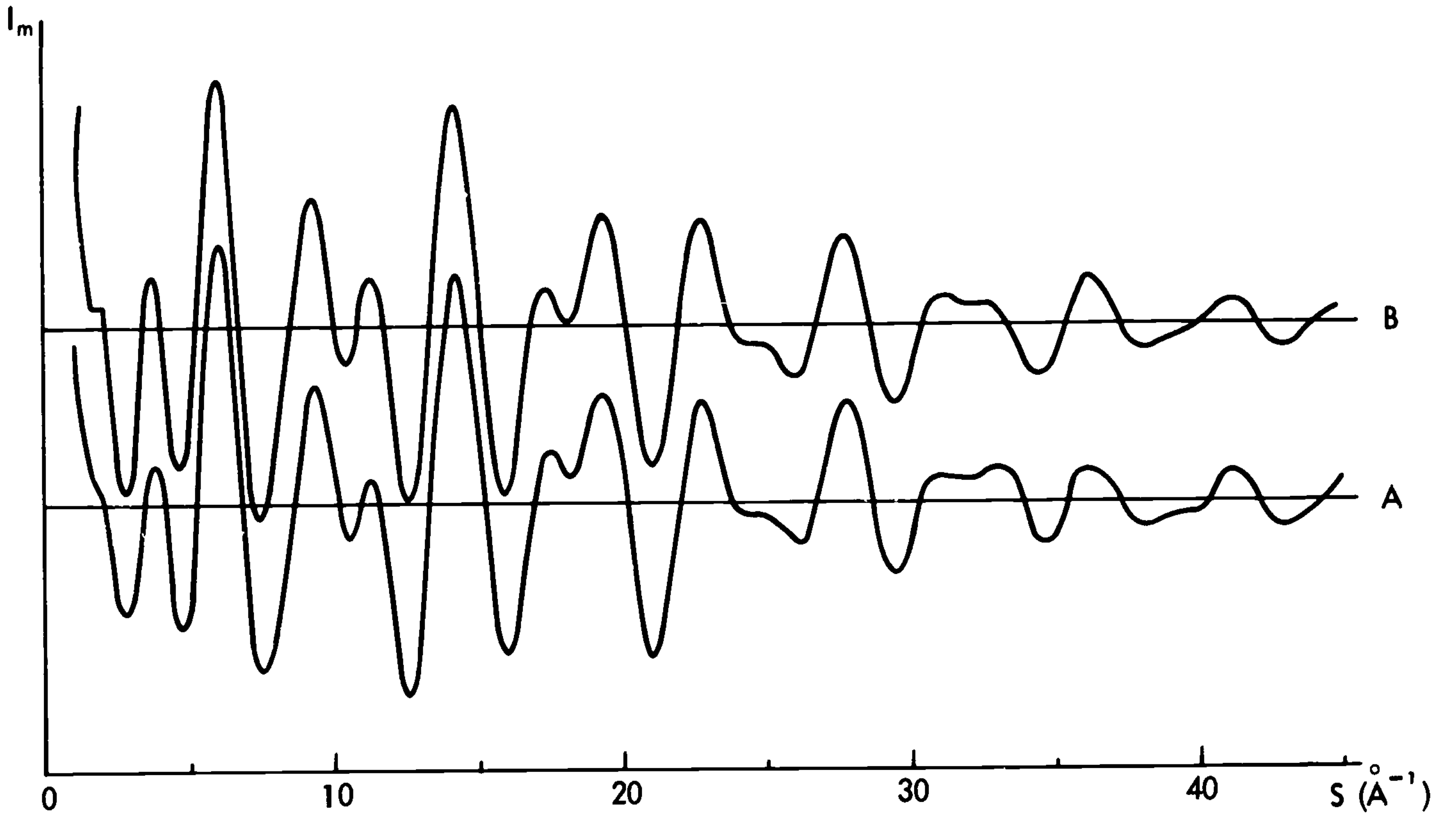
[6] The label 1,1 refers to the fact that both Cl atoms are attached to one carbon; and 1,2 refers to the fact that one Cl is attached to the first carbon and the other to the second.



C_1-H_1	1.070±0.005
C_1-C_2	1.424±0.002
C_1-C_3	2.304±0.004
C_1-H_2	2.230±0.010
C_1-H_3	3.340±0.010
Be-C	1.915±0.005
Be-C′	2.320±0.010
Be-H	2.720±0.020
Be-H′	3.020±0.020
C_1-C_1′	3.450±0.030

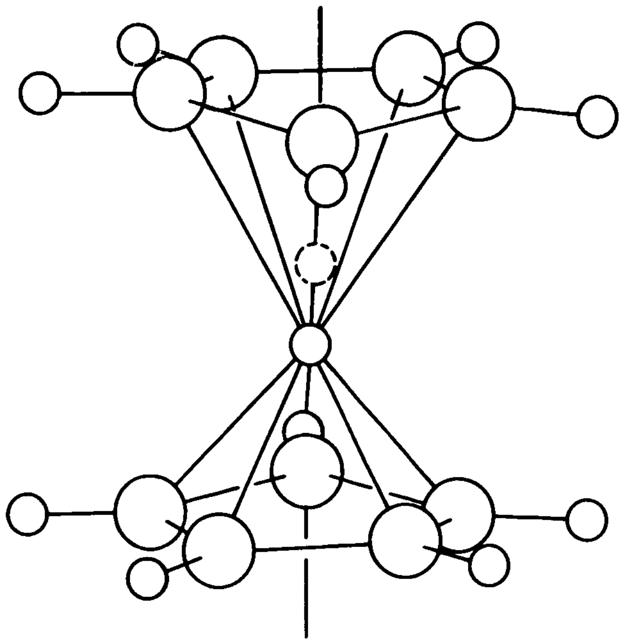
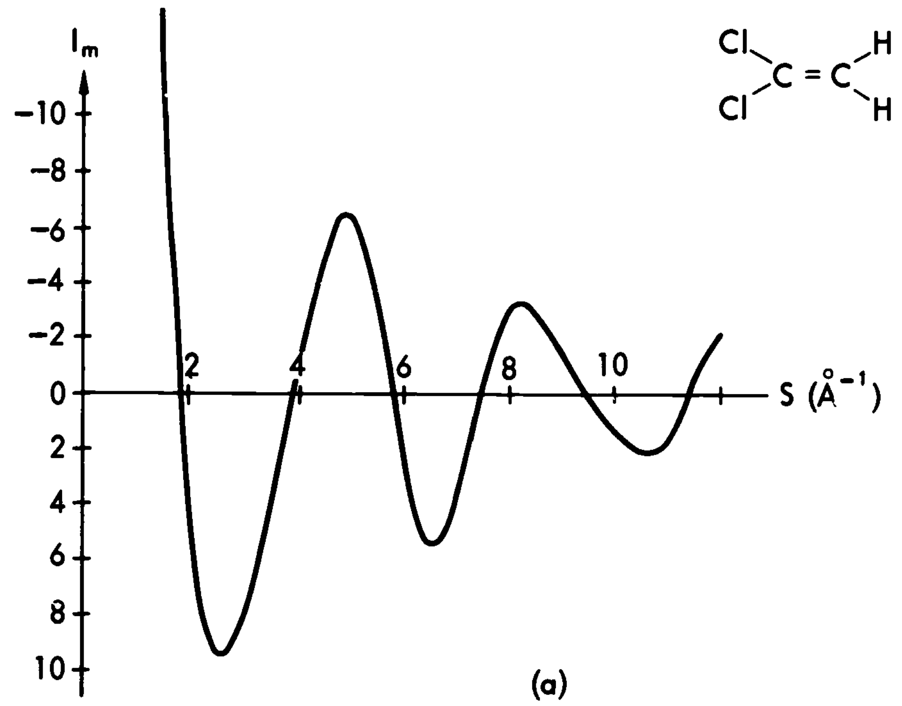


Fig. 5.5 Molecular intensity curves for $(C_5H_5)_2$ Be, dicyclopentadienylberyllium, are shown in the upper figure. Curve A is the experimental data and B is a theoretical fit to the data based essentially on Eq. (5.1). On the lower left are some of the distances determined with errors (representing the reproduceability of the results). On the lower right is a sketch of the structure of the molecule as deduced from this experiment.

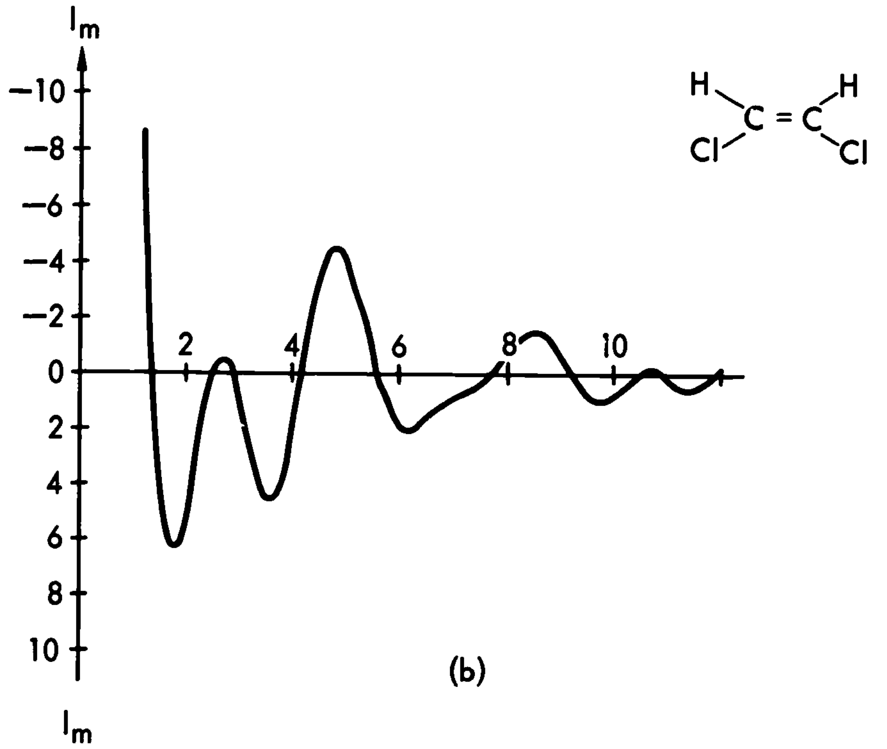
given sample of the gas can be determined by finding what linear combination

$$\Sigma c_i \, I_m^{(i)}(s)$$

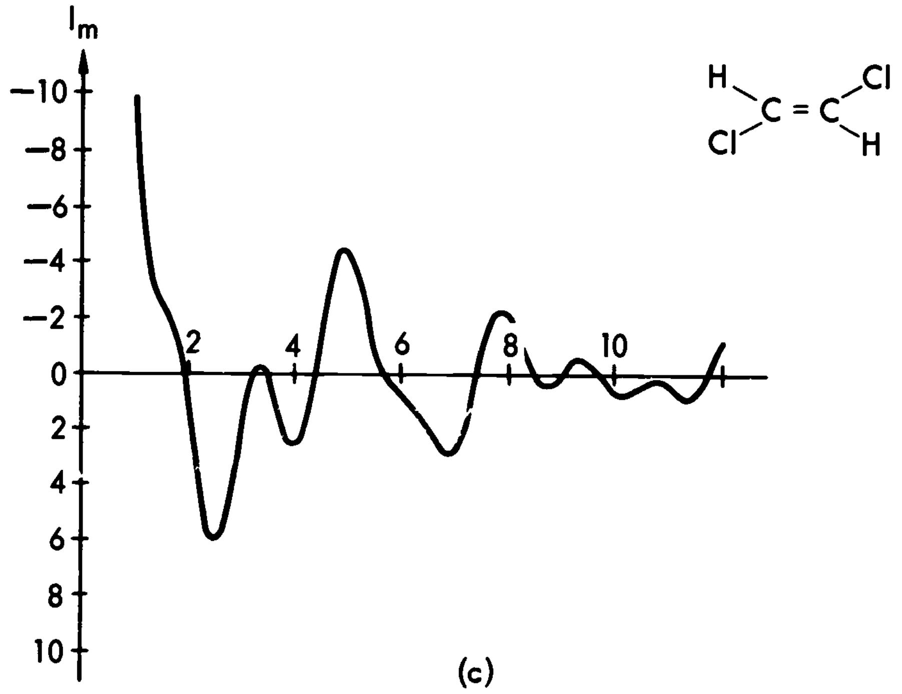
of the intensities $I^{(i)}$ for each form fits the electron scattering from that sample. (Usually there are better methods for making such a determination than electron scattering). An application of this type of experiment is that the concentrations c_i (T) measured at various temperatures enable calculation of some thermody-


I_m
-10
-8
-6
-4
-2
0
2
4
6
8
10
2
4
6
8
10
S (Å⁻¹)
Cl
Cl
C = C
H
H

(a)


I_m
-10
-8
-6
-4
-2
0
2
4
6
8
10
2
4
6
8
10
H
Cl
C = C
H
Cl

(b)


I_m
-10
-8
-6
-4
-2
0
2
4
6
8
10
2
4
6
8
10
H
Cl
C = C
Cl
H

(c)

namic properties of dichloroethylene.

An extensive discussion of the significance of the determination of interatomic distances in molecules is beyond the scope of the work, and is not understood by most physicists (including the author). I will just make a few general remarks. Theoretical models and accumulated experimental data on molecular structure indicate extensive regularities. For example, (a) various classes of molecules exhibit particular kinds of rotational symmetry such that the same angles occur in many molecules; (b) a bond such as the carbon-carbon bond is found to have a well-defined bond distance in a given general situation so that a given type of C-C bond has the same bond distance in many molecules. These relations for structure parameters, such as C-C bond distance as a function of the type of bond, are called semiempirical relations. An experimental determination of the structure of a particular molecule not only leads to a table of distances and angles for that molecule, but also influences the chemist's understanding of molecular structure in general, since the results may or may not agree with the semiempirical formulae.

There is considerable practical value in establishing semiempirical relations for structure parameters. For example, organic chemists are interested in designing and building new organic molecules. They can make good guesses about the constitution of new molecules with the help of the semiempirical relations. Another example is predicting the behavior of materials at very high temperatures where direct experimental tests are difficult. A theoretical prediction of the properties of a material via statistical mechanics can be made if the structure parameters are known.

5.2 VIBRATING MOLECULES

Two approximations are involved in the formula for the molecular intensity (e.g., for a diatomic molecule):

$$I_m \propto f_1 \; f_2 \sin sr/sr$$

(a) We assumed the interatomic distance r to be the same for all molecules of a given kind and the same at all times. (b) We assumed that scattering from one atom in the molecule is the same as scattering off the atom in isolation, e.g., such that the scattering amplitude f_1 is unaffected by the fact that atom 1 is very close to atom 2. We also assumed that the phases δ_i for each atomic scattering are the same since we omitted the $\cos(\delta_1 - \delta_2)$ factor. The assumption (a) is very poor but it is easy both to understand what is going on and how to do the problem without making the assumption. Assumption (b) is usually

Fig. 5.6 Molecular intensity curves for 1,1 dichloroethylene and cis and trans isomers of 1,2 dichloroethylene are shown in a, b, and c, along with sketches of the deduced molecular structure. The intensity curves look roughly like the experimental data for I_m. Since this type of experiment is now "ancient history" it was more convenient to calculate the curves using the expression:

$$I_m \propto Z_{Cl}{}^2 \frac{\sin sr_{Cl-Cl}}{sr_{Cl-Cl}} + 2Z_C Z_{Cl}\left[\frac{\sin sr_{C-Cl}}{sr_{C-Cl}} + \frac{\sin sr_{C-Cl'}}{sr_{C-Cl'}}\right] + Z_C{}^2 \frac{\sin sr_{C-C}}{sr_{C-C}}.$$

Here $Z_{Cl} = 17$ and $Z_C = 6$. The distance r_{Cl-Cl} is the chlorine-chlorine distance, with values 1.68, 3.06, and 4.23 Å in a, b, c, respectively. In each of the three cases there are two equal short distances from Cl to C atoms and two equal long ones and these two distances are the same for the three cases. These are $r_{Cl-C} = 1.68$ Å and $r_{Cl-C}{}' = 2.66$ Å. The electron scattering by hydrogen is neglected. The C-C distance is 1.38 Å.

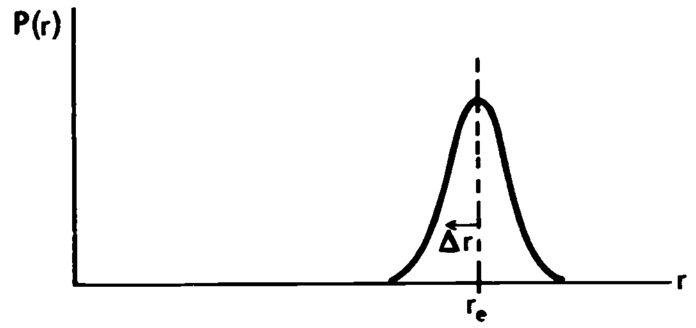


Fig. 5.7 Radial distribution for a diatomic molecule.

very well satisfied, so we need not go into the relatively sophisticated arguments needed to improve the intensity expression if this assumption is modified.

Instead of (a) we consider that a given kind of diatomic molecule has an interatomic distance which oscillates in time around an equilibrium value r_e. We assume that this vibration of the molecule is relatively slow so that a beam electron sees a fixed distance r as it passes a particular molecule. This approximation is excellent: since the mass of the electron is much smaller than the atomic mass, its velocity is much larger. Let the distribution of the r's be described by a function P (r). That is, imagine that we somehow examine a very large sample of molecules at one instant and plot the number of molecules observed to have interatomic distance r (say in each interval of r of width 0.001Å). We will obtain an essentially smooth curve (Fig. 5.7).

We would get the same curve from examination of a single molecule at many widely spaced times.[7] The equilibrium separation distance is r_e. The root mean square amplitude of vibration is indicated by Δr in the sketch. The shape of P(r) might be, for example,

$$P(r) \propto e^{-\frac{1}{2}\left(\frac{r-r_e}{\Delta r}\right)^2}.$$

The molecular intensity we observe is the result of many electrons independently scattering from a single type of molecule, and will be

$$I_m\ (s) \propto \int_0^\infty dr\ P(r)\ f_1\ f_2\ \frac{\sin sr}{sr} \quad (5.2)$$

We can obtain the fuction P(r) explicitly from $I_m(s)$ by transforming Eq. (5.2). We must assume in the following that the proportionality factor in Eq. (5.2), associated with the definition of I_m (see footnote 5) and with the rotating sector used, has an s dependence cancelling the s dependence of $f_1 f_2$. The Fourier integral theorem states that

$$g^{(x)} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[dke^{ikx}\ \int_{-\infty}^{\infty} dx' e^{ikx'}\ g^{(x')}\right]. \quad (5.3)$$

The important mathematical condition for the validity of (5.3) is that $\int |g(x)|^2\ dx$ is finite, which, you will see below, is true here. Now, in Eq. (5.2), omitting constant factors, and using $\sin sr = (e^{isr} - e^{-isr})/2isr$,

$$I_m\ (s) = \int_{-\infty}^{\infty} \frac{e^{isr}}{2isr}\ P(|r|)\ dr, \quad (5.4)$$

so that, rewriting (5.3), we find

$$\begin{aligned} \frac{P(r)}{r} &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dse^{-isr} \int_{-\infty}^{\infty} e^{isr'}\,\frac{P(|r'|)}{r'}\,dr' \\ &= -\frac{1}{i\pi}\int_{-\infty}^{\infty} se^{-isr}\ I_m(|s|)\ ds \\ &= \frac{2}{\pi}\int_0^\infty s\ \sin sr\ I_m(s)ds. \end{aligned}$$

The transform

$$\frac{P(r)}{r} = \frac{2}{\pi}\int_0^\infty ds\ s\ \sin\ (sr)\ I_m(s) \quad (5.5)$$

is called the "radial distribution function" and is just 1/r times the actual distribution of interatomic dis-

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[7] We would have to wait long enough to be sure that if we disturbed the molecule with one electron it would have time to settle down to its lowest state before the next electron arrived.

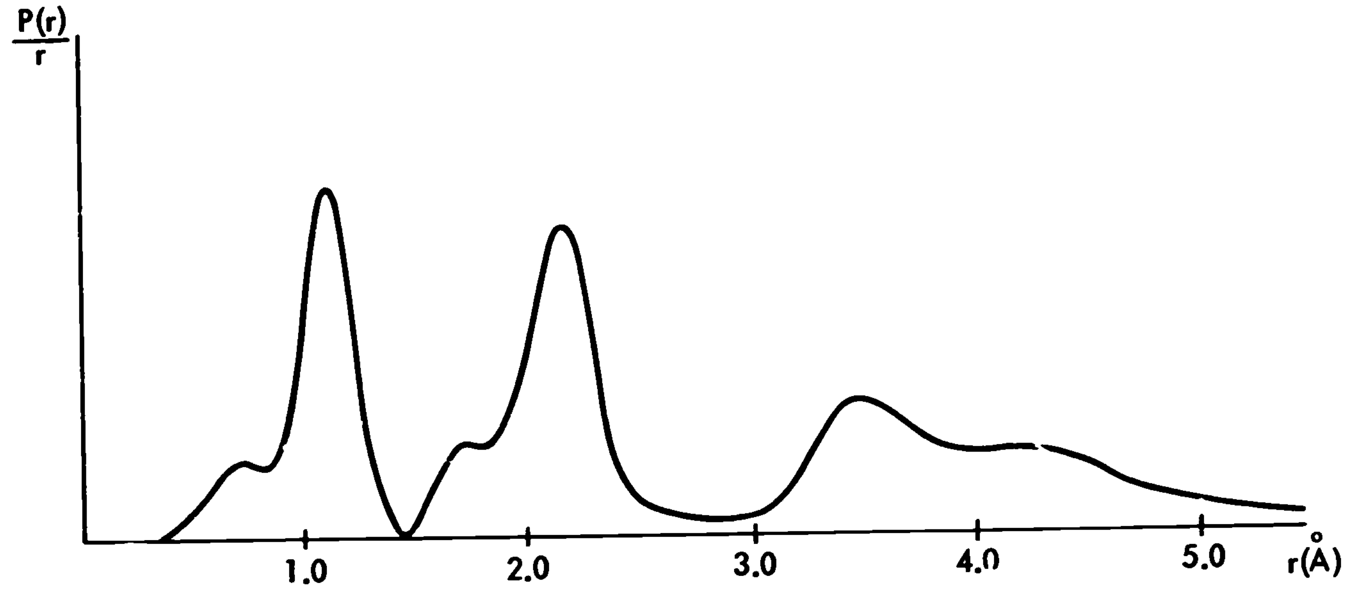

Fig. 5.8 Radial distribution curve corresponding to the polytomic molecule considered in Fig. 5.5.

tances. Exactly the same formula applies to polyatomic molecules.

A radial distribution function for a complex molecule is shown in Fig. 5.8. The central values of the peaks are essentially the equilibrium distances $(r_e)_{ij}$ between atoms. (Some study is of course necessary to make the proper assignment i j to each peak in P(r).)

The half width of any peak is related to the amplitude of vibration but, obviously, it is a complicated job to sort out the vibrations in a polyatomic molecule because the many vibrations are going on at the same time. They are not independent of each other.

Let us briefly discuss the vibrations of a diatomic molecule. The distribution of interatomic distances, P(r), will consist of a single peak as in Fig. 5.7. One can learn a lot about the vibration and the interatomic force from this information. It can be shown that the force between the two atoms has the form illustrated in Fig. 5.9.

Presumably, for small vibrations, the interatomic force is a restoring force about the equilibrium position r_e:

$$F(r) = -k(r - r_e).$$

In other words the potential energy near r_e has the form of an harmonic oscillator potential:

$$V(r) = \frac{1}{2} k (r - r_e)^2 + \text{const.}$$

This form will be valid roughly in the shaded region of Fig. 5.9. We haven't discussed enough quantum theory as yet to enable us to solve the harmonic oscillator problem, but this is one of the standard subjects of introductory quantum mechanics and perhaps you can

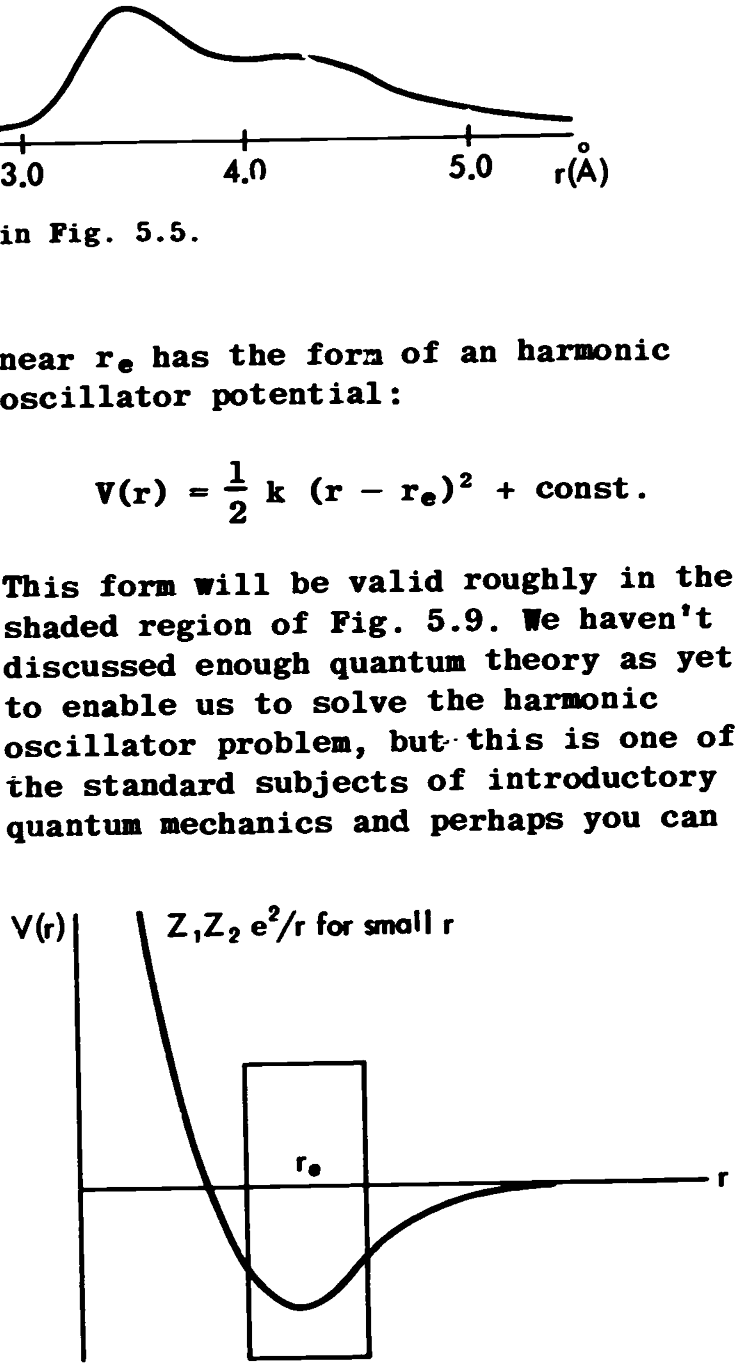

Fig. 5.9 A rough sketch of the potential energy as a function of the separation distance between the two atoms of a diatomic molecule. At small enough distances the coulomb repulsion is the dominant interaction. In the shaded region there is an attractive well which can trap the pair of atoms so that they form the molecule. The separation of the atoms in the molecule is approximately r_e.

come back to this molecular example when you take it up. Empirical knowledge of P(r) will enable you to deduce something about the force constant k and about the period of vibration. The latter can then, for example, be correlated with information about molecular spectra (i.e., the frequencies of electromagnetic radiation absorbed or emitted by the molecule).

Appendix A SOLUTION OF THE WAVE EQUATION

In this appendix we derive the integral formula for the amplitude at any point in terms of the amplitude on a wavefront, which was given in section 2.1.

The wave equation in three dimensions in a homogeneous nonabsorptive medium is:

$$\nabla^2 A(\vec{r},t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} A(\vec{r},t)$$

Here we assume that A is a scalar function. We will neglect polarization effects. $A(\vec{r},t)$ can represent the strength of either the electric or magnetic field. The wave equation can be derived from Maxwell's equations if one assumes a homogeneous isotropic medium, i.e., constant permeability and dielectric permittivity, and if one assumes zero conductivity and neglects polarization. Any intermediate or advanced text on electromagnetism will discuss this derivation of the wave equation from Maxwell's equations.

<u>We consider only monochromatic light, i.e., steady waves</u>. You can check that a particular plane wave solution moving in the direction k has the form:

$$A = a \sin (\vec{k}\cdot\vec{r} - \omega t + \phi), \qquad (A.1)$$

where $k = \omega/c$. The general solution of the wave equation for a monochromatic wave can be written as a general linear combination of these plane wave solutions:

$$A(\vec{r},t) = \int d\Omega\, a(\hat{\vec{k}}) \sin [\vec{k}\cdot\vec{r} - \omega t + \phi(\hat{\vec{k}})]. \qquad (A.2)$$

(You can check that you don't need to consider more than one plane wave along a given direction because two such waves are equivalent to a single wave moving in the same direction with appropriate magnitude and phase.)

Rather than seek solutions of the wave equation in terms of the coefficients $a(\vec{k})$ and phases $\phi(\vec{k})$, let us restate the problem. At any fixed point $\vec{r}$, a general monochromatic wave must have the form

$$A(\vec{r},t) = A(\vec{r}) \sin [-\omega t + \chi(\vec{r})]. \qquad (A.3)$$

This amplitude can be written:

$$A(\vec{r},t) = A_1(\vec{r}) \cos \omega t + A_2(\vec{r}) \sin \omega t, \qquad (A.4)$$

where according to (A.1) the A_i satisfy the "Helmholtz equation":

$$\nabla^2 A_i(\vec{r}) + k^2 A_i(\vec{r}) = 0 \qquad (A.5)$$

The intensity $I(\vec{r})$, which is the energy/(area × time) passing through a surface normal to the motion of the wave (thus the energy passing through the wave front at $\vec{r}$), is

$$I = \overline{A(r,t)^2} = \frac{1}{2} A(\vec{r})^2 \qquad (A.6)$$

where the bar indicates time averaging.

It is more convenient to deal with a single complex solution A_c than with the real solutions A_i even though electric and magnetic fields are real. We will use the complex amplitude in this appendix, but not in the main text. You can check that the results are the same for the two. Let $A_c(\vec{r},t)$ be a complex solution of the wave equation for monochromatic light. Instead of (A.3) we can write

$$A_c(\vec{r},t) = A_c(\vec{r})\, e^{-i\omega t} \qquad (A.7)$$

where $A_c(\vec{r})$ satisfies the "Helmholtz equation"

$$\nabla^2 A_c(\vec{r}) + k^2 A_c(\vec{r}) = 0 \qquad (A.8)$$

and

$$A_c(\vec{r}) = \frac{1}{\sqrt{2}} A(\vec{r}) e^{i\chi(\vec{r})} = \frac{1}{2} (A_1 + A_2). \qquad (A.9)$$

To go back and forth between the real and complex solutions we just remember that the phase in time of the real amplitude is the same as the complex phase of the complex spatial amplitude, and that the magnitude of the real time dependent amplitude, $A(r)$, is $\sqrt{2}$ times the magnitude of the complex amplitude. I have introduced the factor $1/\sqrt{2}$ to keep the prescription for the intensity simple. The intensity is the absolute value squared of the complex amplitude:

$$I = \frac{1}{2} A^2(\vec{r}) = |A_c(\vec{r})|^2 \qquad (A.10)$$

The solution of a differential equation such as (A.8) with boundary conditions is often more easily obtained by restating the differential equation and its boundary conditions as an integral equation (In our case the boundary conditions would be description of sources, absorbers, mirrors, etc.). Often, as is the case for us, a powerful approximation is suggested by the form of the integral equation: one approximates it by an integral over known functions.

To establish the integral equation we make use of an auxiliary function $G(\vec{r},\vec{r}_0)$ which is the amplitude corresponding to a point source at $\vec{r}_0$:

$$G = \frac{\exp(ik|\vec{r} - \vec{r}_0|)}{|\vec{r} - \vec{r}_0|}.$$

This is an outgoing sperical wave going out from the point $\vec{r}_0$. (Multiply as in Eq. (A.7) by $e^{-i\omega t}$ to see that the wave moves out radially from $\vec{r}_0$ with velocity c as time increases.) The intensity is

$$I = |G|^2 = 1/|\vec{r} - \vec{r}_0|^2,$$

inversely proportional to the square of the distance from $\vec{r}_0$. Through any cone with apex at $\vec{r}_0$ the energy flow is

$$I(\vec{r})\; a(\vec{r}) = \Delta\Omega,$$

where a is the cross-sectional area of cone and $\Delta\Omega$ is the solid angle subtended by the cone. The energy flow is independent of $|\vec{r} - \vec{r}_0|$ as expected. The total energy flow out from $\vec{r}_0$ is:

$$\int d\Omega = 4\pi.$$

The auxiliary function G is called a Green's function. Mathematically the statement is that G satisfies:

$$\nabla_r^2 G + k^2 G = -4\pi\, \delta\, (\vec{r} - \vec{r}_0) \qquad (A.12)$$

For those not familiar with the delta function, (A.12) is equivalent to the two relations

$$\nabla_r^2 G + k^2 G = 0 \qquad (A.13)$$

for $\vec{r} \neq \vec{r}_0$, and

$$\int_V d^3r (\nabla_r^2 G + k^2 G) = -4\pi \qquad (A.14)$$

for any volume V containing the point $\vec{r}_0$. To prove (A.13), note that in any neighborhood not containing the singular point $\vec{r}_0$ we can differentiate using the expression for ∇^2 in spherical coordinates

$$\left[\nabla_r^2 f = \frac{1}{r} \frac{\partial^2}{\partial r^2} (r\ f) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} f\right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\phi^2} f\right].$$

Thus

$$\nabla_r^2 \frac{\exp(ik|\vec{r} - \vec{r}_0|)}{|\vec{r} - \vec{r}_0|} = \frac{1}{R} \frac{d^2}{dR^2} e^{ikR} = -k^2 \frac{e^{ikR}}{R}$$

where $R = |\vec{r} - \vec{r}_0|$. To prove the relation (A.14) first observe that for a sphere of radius R_0 centered at $\vec{r}_0$

$$\int_V R^2 \, d\Omega \, dR \, \frac{e^{ikR}}{R} \to 0$$

as the radius of the sphere, R_0, goes to zero. The remaining term is

$$\int_V d^3R \, \nabla^2 G = \int_{\text{Surface}} d\vec{S}\cdot\vec{\nabla}G = 4\pi R^2 \left.\frac{dG}{dR}\right|_{R_0} \to -4\pi$$

since $\left.\frac{dG}{dR}\right|_{R_0} \to -\frac{1}{R_0}2$ as $R_0 \to 0$

To obtain our integral equation we form a standard combination: G times Eq. (A.8) for A minus A times Eq. (A.12) for G (we use the complex solution but will drop the subscript c). Integrating over a volume V containing $\vec{r}_0$ we have:

$$\int_V \left[G(\nabla^2 + k^2)\, A - A(\nabla^2 + k^2)G \right] d^3r = 4\pi \, A(\vec{r}_0). \qquad \text{(A.15)}$$

We manipulate the integrand to obtain

$$4\pi \, A(\vec{r}_0) = \int d^3r\,(G\nabla^2 A - A\nabla^2 G)$$
$$= \int d^3r\,\vec{\nabla} \cdot (G\vec{\nabla}A - A\vec{\nabla}G)$$

which, by Gauss' theorem becomes

$$4\pi \, A(\vec{r}_0) = \iint_S \left(A\frac{\partial}{\partial n}G - G\frac{\partial}{\partial n}A\right) dS \qquad \text{(A.16)}$$

where n is distance along the outward normal on the surface S which bounds the volume V.

We want to consider a particular configuration where there is a distant source to the left of an absorbing wall which has finite openings, connected in any way. To the right we can assume that space is empty. Equation (A.16) is an integral equation: we cannot in advance specify A and $\partial A/\partial n$ on some boundary and be consistent with the source and absorbers. The A and $\partial A/\partial n$ have to be solved for. The type of configuration we want to consider suggests the following approximation, however. Assume that we can take the amplitude arriving from the source to the left of the absorbing wall to be given. Just behind the absorbers we assume that A and $\partial A/\partial n$ vanish. Similarly on the distant boundary enclosing the volume to the right (we take the volume V to be large) we assume that A and $\partial A/\partial n$ vanish. The latter approximation may be justified by considering a slightly time-dependent wave rather than a steady wave and taking the right-hand surface to be far beyond the point $\vec{r}_0$. Then at times of interest there shouldn't be any contribution from the right surfaces to $A(\vec{r}_0)$.

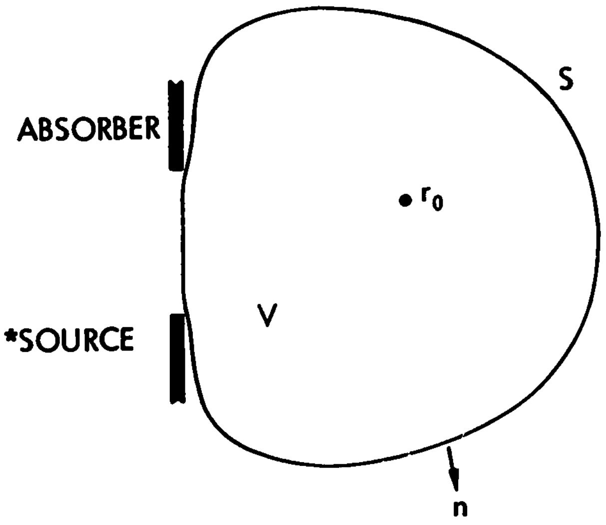

Fig. A.1 Typical geometry for expression (A.16).

At every opening in the absorber consider that the boundary surface is made up of a wavefront and necessary surfaces perpendicular to the front to complete covering the opening.

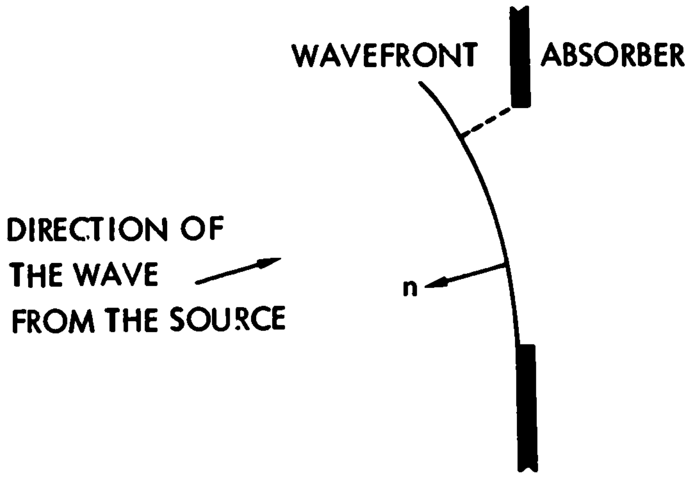

Fig. A.2 Sketch for evaluation of $\partial A/\partial n$.

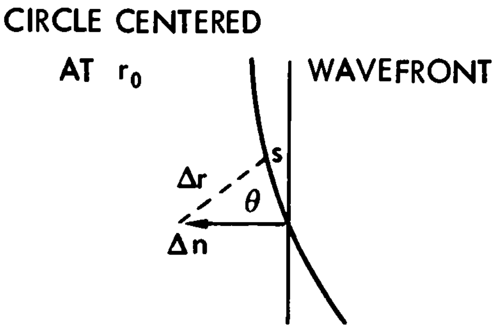

Fig. A.3 Sketch for evaluation of $\partial G/\partial n$. We see that $\Delta r = \Delta n \cos\theta$.

We neglect A and $\partial A/\partial n$ on the surfaces perpendicular to the front. Choose a front with zero phase, to be definite, so that

$$A(\vec{r},t) = a(\vec{r}) \exp(-ikn - i\omega t),$$

where $a(\vec{r})$ is a slowly varying function compared to the phase factor e^{-ikn} so that

$$\frac{\partial A}{\partial n} = -ikA.$$

Meanwhile, we see from Fig. A.3 that

$$\frac{\partial G}{\partial n} = ik \cos\theta\, G.$$

Again we have made use of the fact that the phase factor dominates the variation of the function.

With these approximations the integral equation becomes the integral:

$$A(\vec{r},t) = \frac{ik}{4\pi}\int A\, G(1 + \cos\theta)\, dS$$

$$= \frac{i}{2\lambda}\int dS\, a(\vec{r})\,(1 + \cos\theta)\,\frac{\exp(ik|\vec{r} - \vec{r}_0| - i\omega t)}{|\vec{r} - \vec{r}_0|}$$

Where the integration is over the wavefront arriving at the openings in the absorber. This is the expression we set out to derive, being just the complex version of the expression given in section 2.1.

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Text discussion can be found in physical chemistry texts.