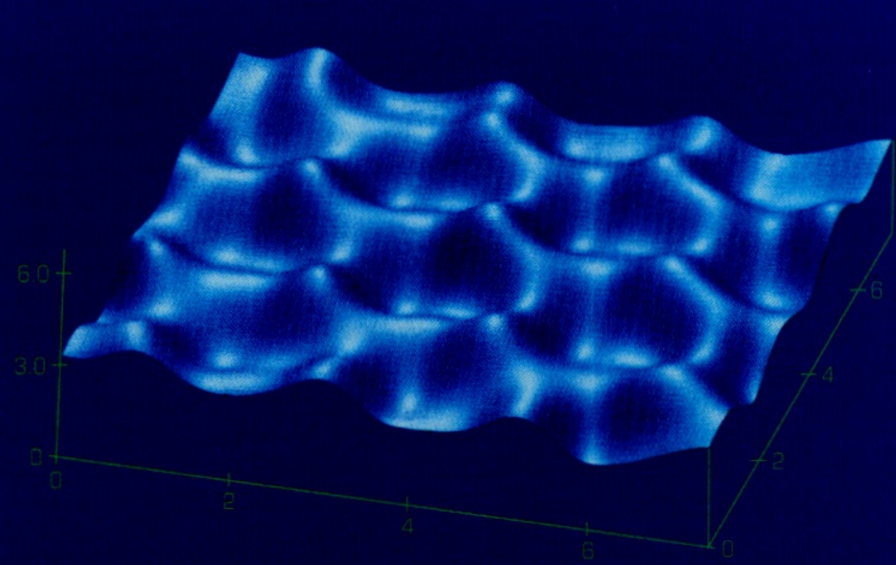
40 Wave Functions and Uncertainty



The surface of graphite, as imaged with atomic resolution by a scanning tunneling microscope. The hexagonal ridges show the most probable locations of the electrons.

▶ Looking Ahead

The goal of Chapter 40 is to introduce the wave-function description of matter and learn how it is interpreted. In this chapter you will learn to:

- Connect the particle and wave descriptions of matter.
- Use basic ideas about probability.
- Use the wave function to calculate the probabilities of detecting particles.
- Recognize the limitations on knowledge imposed by the Heisenberg uncertainty principle.

◀ Looking Back

The ideas developed in this chapter are highly dependent on understanding the double-slit interference experiment for both light and matter. Please review:

- Sections 21.8 and 22.2 Interference, beats, and the double-slit experiment.
- Sections 25.3 and 39.3 Photons.
- Sections 25.4 and 39.4 Matter waves, the de Broglie wavelength, and wave–particle duality.

You learned in the last two chapters that classical mechanics and electromagnetism were unable to explain the new phenomena associated with light, electrons, and atoms. Scientific theories that had triumphed during the 18th and 19th centuries stumbled over the smallest specks of matter. Many scientists refused to accept these limitations, thinking that it was only a question of time until someone discovered how to apply classical ideas to atoms. Their hopes were to go unfulfilled.

At the same time that classical physics was reaching its limits, the new ideas put forward by Einstein, Bohr, and de Broglie began pointing the way toward a new theory of light and matter. **Quantum mechanics,** as the theory came to be called, did not reach its completed form until the mid-1920s, but it has since proven to be the most successful physical theory ever devised.

This chapter and the next will introduce the essential ideas of quantum mechanics in one dimension. Although the full theory is beyond the scope of this textbook, we can delve far enough into quantum mechanics to learn how it solves the problems of atomic and nuclear structure. Our goal in this chapter is to introduce the concept of the *wave function.* The wave function, which reconciles the wave-like and particle-like aspects of matter, characterizes microscopic particles in terms of the *probability* of finding them at various points in space. The scanning tunneling microscope image of graphite seen above shows that the most probable place to find electrons is along the ring-like structures created by the carbon-carbon bonds.

Interference fringes in an optical double-slit interference experiment.

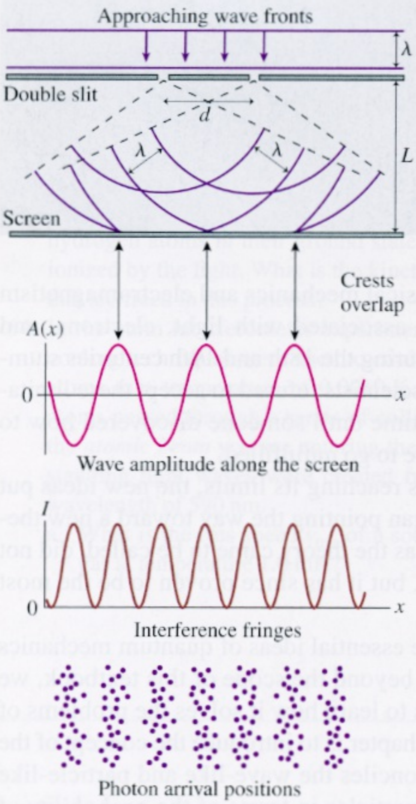
40.1 Waves, Particles, and the Double-Slit Experiment

You may feel surprise at how slowly we have been building up to quantum mechanics. Why not just write it down and start using it? There are two reasons. First, quantum mechanics explains microscopic phenomena that we cannot directly sense or experience. It was important to begin by learning how light and atoms behave. Otherwise, how would you know if quantum mechanics explains anything? Second, the concepts we'll need in quantum mechanics are rather abstract. Before launching into the mathematics, we need to establish a connection between theory and experiment.

We will make the connection by returning to the double-slit interference experiment, an experiment that goes right to the heart of wave–particle duality. The significance of the double-slit experiment arises from the fact that both light and matter exhibit the same interference pattern. Regardless of whether photons, electrons, or neutrons pass through the slits, their arrival at a detector is a particle-like event. That is, they make a collection of discrete dots on a detector. Yet our understanding of how interference "works" is based on the properties of waves. Our goal is to find the connection between the wave description and the particle description of interference.

A Wave Analysis of Interference

FIGURE 40.1 The double-slit experiment with light.



The interference of light can be analyzed from either a wave perspective or a photon perspective. Let's start with a wave analysis. FIGURE 40.1 shows light waves passing through a double slit with slit separation d. You should recall that the lines in a wave-front diagram represent wave crests, spaced one wavelength apart. The bright fringes of constructive interference occur where two crests or two troughs overlap. The graphs and picture below the detection screen (notice that they're aligned vertically) show the outcome of the experiment.

You studied interference and the double-slit experiment in Chapters 21 and 22. The two waves traveling from the slits to the viewing screen are traveling waves with displacements

$$D_1 = a\sin(kr_1 - \omega t)$$
$$D_2 = a\sin(kr_2 - \omega t)$$

where a is the amplitude of each wave, $k = 2\pi/\lambda$ is the wave number, and r_1 and r_2 are the distances from the two slits. The "displacement" of a light wave is not a physical displacement, as in a water wave, but a change in the electromagnetic field.

According to the principle of superposition, these two waves add together where they meet at a point on the screen to give a wave with net displacement $D = D_1 + D_2$. Previously (see Equation 22.12) we found that the amplitude of their superposition is

$$A(x) = 2a\cos\left(\frac{\pi d x}{\lambda L}\right) \tag{40.1}$$

where x is the horizontal coordinate on the screen, measured from $x = 0$ in the center.

The function $A(x)$, the top graph in Figure 40.1, is called the *amplitude function.* It describes the amplitude A of the light wave as a function of the position x on the viewing screen. The amplitude function has maxima where two crests from individual waves overlap and add constructively to make a larger wave with amplitude $2a$. $A(x)$ is zero at points where the two individual waves are out of phase and interfere destructively.

If you carry out a double-slit experiment in the lab, what you observe on the screen is the light's *intensity,* not its amplitude. A wave's intensity I is proportional to the *square* of the amplitude. That is, $I \propto A^2$, where $\propto$ is the "is proportional to" symbol.

Using Equation 40.1 for the amplitude at each point, we find the intensity $I(x)$ as a function of position x on the screen is

$$I(x) = C\cos^2\left(\frac{\pi d x}{\lambda L}\right) \tag{40.2}$$

where C is a proportionality constant.

The lower graph in Figure 40.1 shows the intensity as a function of position along the screen. This graph shows the alternating bright and dark interference fringes that you see in the laboratory. In other words, the intensity of the wave is the *experimental reality* that you observe and measure.

Probability

Before discussing photons, we need to introduce some ideas about probability. Imagine throwing darts at a dart board while blindfolded. **FIGURE 40.2** shows how the board might look after your first 100 throws. From this information, can you predict where your 101st throw is going to land? We'll assume that all darts hit the board.

No. The position of any individual dart is *unpredictable.* No matter how hard you try to reproduce the previous throw, a second dart will not land at the same place. Yet there is clearly an overall *pattern* to the where the darts strike the board. Even blindfolded, you had a general sense of where the center of the board was, so each dart was *more likely* to land near the center than at the edge.

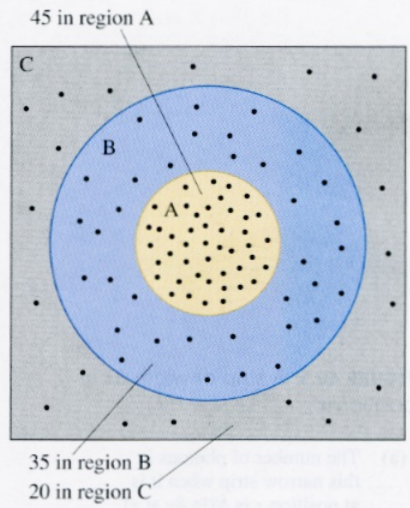


FIGURE 40.2 One hundred throws at a dart board.

Although we can't predict where any individual dart will land, we can use the information in Figure 40.2 to determine the *probability* that your next throw will land in region A or region B or region C. Because 45 out of 100 throws landed in region A, we could say that the *odds* of hitting region A are 45 out of 100, or 45%.

Now, 100 throws isn't all that many. If you throw another 100 darts, perhaps only 43 will land in region A. Then maybe 48 of the next 100 throws. Imagine that the total number of throws N_{tot} becomes extremely large. Then the **probability** that any particular throw lands in region A is defined to be

$$P_A = \lim_{N_{tot}\to\infty} \frac{N_A}{N_{tot}} \tag{40.3}$$

In other words, the probability that the outcome will be A is the fraction of outcomes that are A in an enormously large number of trials. Similarly, $P_B = N_B/N_{tot}$ and $P_C = N_C/N_{tot}$ as $N_{tot} \to \infty$. We can give probabilities as either a decimal fraction or a percentage. In this example, $P_A \approx 45\%$, $P_B \approx 35\%$, and $P_C \approx 20\%$. We've used $\approx$ rather than $=$ because 100 throws isn't enough to determine the probabilities with great precision.

What is the probability that a dart lands in either region A *or* region B? The number of darts landing in either A *or* B is $N_{A\text{ or }B} = N_A + N_B$, so we can use the definition of probability to learn that

$$\begin{aligned} P_{A\text{ or }B} &= \lim_{N_{tot}\to\infty} \frac{N_{A\text{ or }B}}{N_{tot}} = \lim_{N_{tot}\to\infty} \frac{N_A + N_B}{N_{tot}} \\ &= \lim_{N_{tot}\to\infty} \frac{N_A}{N_{tot}} + \lim_{N_{tot}\to\infty} \frac{N_B}{N_{tot}} = P_A + P_B \end{aligned} \tag{40.4}$$

That is, **the probability that the outcome will be A *or* B is the sum of P_A and P_B.** This important conclusion is a general property of probabilities.

Each dart lands *somewhere on* the board. Consequently, the probability that a dart lands in A *or* B *or* C must be 100%. And, in fact,

$$P_{somewhere} = P_{A\text{ or }B\text{ or }C} = P_A + P_B + P_C = 0.45 + 0.35 + 0.20 = 1.00$$

Thus another important property of probabilities is that **the sum of the probabilities of all possible outcomes must equal 1.**

Suppose exhaustive trials have established that the probability of a dart landing in region A is P_A. If you throw N darts, how many do you *expect* to land in A? This value, called the **expected value,** is

$$N_{A\,\text{expected}} = NP_A \tag{40.5}$$

The expected value is your best possible prediction of the outcome of an experiment. If $P_A = 0.45$, your *best prediction* is that 27 of 60 throws (45% of 60) will land in A. Of course, predicting 27 and actually getting 27 aren't the same thing. You would predict 30 heads in 60 flips of a coin, but you wouldn't be surprised if the actual number were 28 or 31. Similarly, the number of darts landing in region A might be 24 or 29 instead of 27. In general, the agreement between actual values and expected values improves as you throw more darts.

STOP TO THINK 40.1 Suppose you roll a die 30 times. What is the expected number of 1's *and* 6's?

A Photon Analysis of Interference

Now let's look at the double-slit results from a photon perspective. We know, from experimental evidence, that the interference pattern is built up photon by photon. The bottom portion of Figure 40.1 shows the pattern made on a detector after the arrival of the first few dozen photons. It is clearly a double-slit interference pattern, but it's made, rather like a newspaper photograph, by piling up dots in some places but not others.

The arrival position of any particular photon is *unpredictable*. That is, nothing about how the experiment is set up or conducted allows us to predict exactly where the dot of an individual photon will appear on the detector. Yet there is clearly an overall pattern. There are some positions at which a photon is *more likely* to be detected, other positions at which it is *less likely* to be found.

If we record the arrival positions of many thousands of photons, we will be able to determine the *probability* that a photon will be detected at any given location. If 50 out of 50,000 photons land in one small area of the screen, then each photon has a probability of $50/50{,}000 = 0.001 = 0.1\%$ of being detected there. The probability will be zero at the interference minima because no photons at all arrive at those points. Similarly, the probability will be a maximum at the interference maxima. The probability will have some in-between value on the sides of the interference fringes.

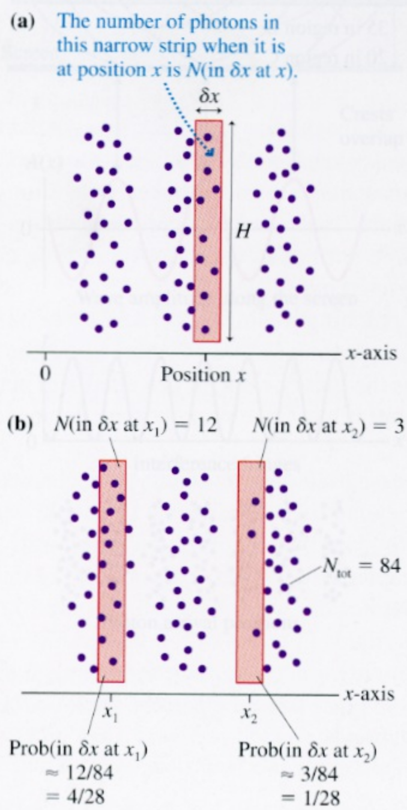
FIGURE 40.3a shows a narrow strip with width δx and height H. (We will assume that δx is very small in comparison with the fringe spacing, so the light's intensity over δx is very nearly constant.) Think of this strip as a very narrow detector that can detect and count the photons landing on it. Suppose we place the narrow strip at position x. We'll use the notation $N(\text{in } \delta x \text{ at } x)$ to indicate the number of photons that hit the detector at this position. The value of $N(\text{in } \delta x \text{ at } x)$ varies from point to point. $N(\text{in } \delta x \text{ at } x)$ is large if x happens to be near the center of a bright fringe; $N(\text{in } \delta x \text{ at } x)$ is small if x is in a dark fringe.

Suppose N_{tot} photons are fired at the slits. The *probability* that any one photon ends up in the strip at position x is

$$\text{Prob}(\text{in } \delta x \text{ at } x) = \lim_{N_{tot}\to\infty} \frac{N(\text{in } \delta x \text{ at } x)}{N_{tot}} \tag{40.6}$$

As **FIGURE 40.3b** shows, Equation 40.6 is an empirical method for determining the probability of the photons hitting a particular spot on the detector.

FIGURE 40.3 A strip of width δx at position x.



Alternatively, suppose we can calculate the probabilities from a theory. In that case, the *expected value* for the number of photons landing in the narrow strip when it is at position x is

$$N(\text{in } \delta x \text{ at } x) = N \times \text{Prob}(\text{in } \delta x \text{ at } x) \qquad (40.7)$$

We cannot predict what any individual photon will do, but we can predict the fraction of the photons that should land in this little region of space. Prob(in δx at x) is the probability that it will happen.

40.2 Connecting the Wave and Photon Views

The wave model of light describes the interference pattern in terms of the wave's intensity $I(x)$, a continuous-valued function. The photon model describes the interference pattern in terms of the probability Prob(in δx at x) of detecting a photon. These two models are very different, yet Figure 40.1 shows a clear correlation between the *intensity of the wave* and the *probability of detecting photons.* That is, photons are more likely to be detected at those points where the wave intensity is high and less likely to be detected at those points where the wave intensity is low.

The intensity of a wave is $I = P/A$, the ratio of light power P (joules per second) to the area A on which the light falls. The narrow strip in Figure 40.3a has area $A = H\delta x$. If the light intensity at position x is $I(x)$, the amount of light energy falling onto this narrow strip during each second is

$$E(\text{in } \delta x \text{ at } x) = I(x)A = I(x)H\delta x \qquad (40.8)$$

The notation E(in δx at x) refers to the energy landing on this narrow strip if you place it at position x.

From the photon perspective, energy E is due to the arrival of N photons, each of which has energy hf. The number of photons that arrive in the strip each second is

$$N(\text{in } \delta x \text{ at } x) = \frac{E(\text{in } \delta x \text{ at } x)}{hf} = \frac{H}{hf} I(x)\,\delta x \qquad (40.9)$$

We can then use the Equation 40.6 definition of probability to write the *probability* that a photon lands in the narrow strip δx at position x as

$$\text{Prob}(\text{in } \delta x \text{ at } x) = \frac{N(\text{in } \delta x \text{ at } x)}{N_{\text{tot}}} = \frac{H}{hfN_{\text{tot}}} I(x)\,\delta x \qquad (40.10)$$

Equation 40.10 is a critical link between the wave model and the photon model.

As a final step, recall that the light intensity $I(x)$ is proportional to $|A(x)|^2$, the square of the amplitude function. Consequently,

$$\text{Prob}(\text{in } \delta x \text{ at } x) \propto |A(x)|^2\,\delta x \qquad (40.11)$$

where the various constants in Equation 40.10 have all been incorporated into the unspecified proportionality constant of Equation 40.11.

In other words, **the probability of detecting a photon at a particular point is directly proportional to the square of the light-wave amplitude function at that point.** If the wave amplitude at point A is twice that at point B, then a photon is four times as likely to land in a narrow strip at A as it is to land in an equal-width strip at B.

NOTE ► Equation 40.11 is the connection between the particle perspective and the wave perspective. It relates the probability of observing a particle-like event—the arrival of a photon—to the amplitude of a continuous, classical wave. This connection will become the basis of how we interpret the results of quantum-physics calculations. ◄