

## Matter Waves

### de Broglie's Hypothesis

Einstein proposed in his photon model of light that

$$E = hf, \quad (7.1)$$

where  $E$  is the energy of the photon and  $f$  is the frequency of the associated light wave.

This can be rewritten as

$$E = \frac{hc}{\lambda}, \quad (7.2)$$

where  $\lambda$  is the wavelength. Now from relativistic dynamics, we know that

$$\frac{u}{c} = \frac{pc}{E}, \quad (7.3)$$

where  $p$  is the momentum of the particle,  $E$  is its relativistic energy, and  $u$  its velocity. For a photon,  $u = c$ , so,  $pc = E$ . Using Eq. (7.2), one finds that

$$p = \frac{h}{\lambda}. \quad (7.4)$$

Thus, a photon carries momentum given by Eq. (7.4), a fact amply verified by Compton's theory and experiments.

Now, experiments such as Young's double-slit interference experiment indicate that light exhibits wavelike behavior. In contrast, the photoelectric effect and Compton scattering convincingly demonstrate the particle nature of light. Louis de Broglie, in his doctoral thesis, proposed that this dual behavior is not limited to light. He argued that every particle (electrons, atoms, etc.) that carries momentum and energy will exhibit wavelike behavior. The frequency and wavelength of the associated wave and the energy and momentum of the particle obey Eqns. (7.1) and (7.4). de Broglie's argument was based upon the fact that in relativity, matter and energy are equivalent. It follows that material particles (matter) and photons (energy) should exhibit the same fundamental behavior. Eq (7.4) is now called the de Broglie relation.

How would one verify such a hypothesis? One could show that a beam of material particles exhibits diffraction or interference. This is precisely what was done by C. Davisson and L. Germer with a beam of electrons.<sup>1</sup> Davisson and Germer bombarded a nickel crystal<sup>2</sup> with an electron beam. The scattered electrons exhibited a diffraction pattern identical to that predicted by the Bragg law!<sup>3</sup>

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<sup>1</sup> We know electrons exhibit particle-like behavior due to trajectories in bubble chambers. Picture: Pg. 58 Unit Q, Six Ideas

<sup>2</sup> Large Ni crystals were created by D&G accidentally when their vacuum system broke and the Ni sample was oxidized. In the process of removing the oxide layer, larger crystals were obtained. Diagram: Diffraction patterns. Krane p. 88-89.

<sup>3</sup> G. P. Thomson and A. Reid did similar experiments with thin foils.

An important point to note is that the wavelength of the electrons had to be comparable to the distance  $D$  between adjacent atoms (lattice parameter) in nickel. For nickel,  $D = 0.215 \text{ nm}$ .<sup>4</sup> In the Davisson-Germer experiment the kinetic energy of the electrons was 54 eV. What was the corresponding wavelength? For  $K = 54 \text{ eV}$ , the electrons are decidedly non-relativistic, so  $K = \frac{1}{2}mu^2$ . Now,  $p = mu$ , so that

$$p = \sqrt{2Km}. \quad (7.5)$$

Inserting the expression for  $p$  in Eq. (7.5) into Eq. (7.4) and solving for  $\lambda$  gives

$$\lambda = \frac{hc}{\sqrt{2Kmc^2}}. \quad (7.6)$$

Substituting values yields  $\lambda = 0.167 \text{ nm}$ .

The Bragg condition<sup>5</sup> for  $n = 1$  gives  $D \sin \phi = \lambda$ , where  $\phi$  is the angle between the incident and scattered beams. [Note that this is not the *standard* Bragg formula!] Solving for  $\phi$  yields

$$\phi = \sin^{-1}\left(\frac{\lambda}{D}\right) = \sin^{-1}\left(\frac{0.167 \text{ nm}}{0.215 \text{ nm}}\right) = 51^\circ.$$

A bright spot was seen at this angle by Davisson and Germer. [Show picture. Also PhET simulation.]

Note that for a given kinetic energy, a particle with a smaller mass will have a larger wavelength. Wavelike behavior cannot be observed for macroscopic objects because the large masses ( $\sim 1 \text{ kg}$ ) give rise to exceedingly small wavelengths, due to the extremely small value of Planck's constant. In the 1960s a double-slit interference experiment was done with electrons for the first time. The unmistakable double-slit pattern, known for centuries to be exhibited by light was now seen to be displayed by electrons as well.<sup>6</sup> [Show picture.]

So de Broglie's bold hypothesis about matter waves was verified by experiments. de Broglie even used his theory to explain the quantization of angular momentum in the Bohr model of the atom (incorrectly, as it turned out). Despite these successes, serious questions remained. What is the nature of the wave associated with a material particle? What is the physical meaning of the amplitude of this wave?<sup>7</sup>

### The Wave Function and Its Interpretation

To shed some light on these questions, we examine the double-slit interference experiment more carefully. It seems on the face of it that the wave and particle models of light are in conflict in this experiment. The wave model holds that light waves originating from each slit superpose to form an interference pattern. Let us use a detector array to detect the interference pattern.<sup>8</sup> Detectors in the regions of constructive interference will register high intensities, whereas detectors in regions of destructive interference will record low intensities. In the wave picture,

<sup>4</sup> See Tipler & Llewellyn, 4<sup>th</sup> ed.

<sup>5</sup> See Tipler & Llewellyn, 4th Ed. for a good discussion

<sup>6</sup> Interference effects have been seen for protons, neutrons, atoms, and molecules, including C-60

<sup>7</sup> See AJP 70, 200 (2002)

<sup>8</sup> Diagram, Double slit interference with individual photons detected, p. 76, Unit Q, Six Ideas

the intensity of the light is proportional to the square of the magnitude of the electric field. More precisely,

$$I = \epsilon_0 c \langle |\vec{E}|^2 \rangle, \quad (\text{in vacuum}) \quad (7.7)$$

where the angle brackets denote a time average. The electric field at every point in space beyond the slits is given by the superposition of the fields from each slit:

$$\vec{E} = \vec{E}_1 + \vec{E}_2. \quad (7.8)$$

Thus,

$$\begin{aligned} I &= \epsilon_0 c \langle |\vec{E}|^2 \rangle = \epsilon_0 c \langle |\vec{E}_1 + \vec{E}_2|^2 \rangle \\ &= \epsilon_0 c \langle (\vec{E}_1 + \vec{E}_2) \cdot (\vec{E}_1 + \vec{E}_2) \rangle \\ &= \epsilon_0 c \left( \langle |\vec{E}_1|^2 \rangle + \langle |\vec{E}_2|^2 \rangle + 2 \langle \vec{E}_1 \cdot \vec{E}_2 \rangle \right). \end{aligned}$$

The first two terms in parentheses in the equation above are constants. The third term depends on the phase difference between the two wave trains, which is a function of position. This term gives rise to interference.

A Newtonian particle model would predict no interference. There would be just two bright regions along straight-line paths from each slit, with overlap in the middle. However, if the intensity of the light used in the experiment is very low, the detectors do register discrete events, which indicate interaction of a single particle with the detector. If the experiment is done with low-intensity light, the same double-slit interference pattern is formed even though there may be only one photon going through the entire apparatus at a time. Therefore, one can rule out interaction between photons as a mechanism for transmitting information about the pattern. Clearly, the simple Newtonian prediction is incorrect. So how do the particles “know” where to go in order to form an interference pattern? [PhET simulation.]

We can get some insight into this seeming paradox by examining how the interference pattern evolves over time. Initially, the photons that are detected seem to be randomly distributed. However, after a statistically large number of photons have been detected, the double-slit pattern emerges. Thus, one cannot predict exactly where a given photon will strike the detector array. However, we can say that *on average*, more photons will strike the detectors located in the regions of the constructive interference than those detectors in the regions of destructive interference. In other words, the *probability that a given photon will strike a given detector is proportional to the intensity of the interference pattern at that detector predicted by the wave model of light*. The wave model describes **the statistical distribution of measured positions of a large number of identically prepared photons**. This interpretation must also be true for “material particles” such as electrons, which undergo double-slit interference. It is within this context that the de Broglie wave is interpreted.

The matter wave associated with each quantum particle is described by a wave function  $\Psi(\vec{r}, t)$ . This wave function is in general a complex quantity, with a real and an imaginary part:

$$\Psi(\vec{r}, t) = \Psi_{\text{real}}(\vec{r}, t) + i\Psi_{\text{imag}}(\vec{r}, t). \quad (7.9)$$

The imaginary number  $i = \sqrt{-1}$ . The probability that the particle will be found at position  $\vec{r}$  in a volume  $dV$  at time  $t$  is proportional to the intensity of the matter wave and the volume  $dV$ . Hence,

$$dP = |\Psi(\vec{r}, t)|^2 dV, \quad (7.10)$$

where

$$|\Psi(\vec{r}, t)|^2 = \Psi_{real}^2(\vec{r}, t) + \Psi_{imag}^2(\vec{r}, t). \quad (7.11)$$

The square of the modulus of a complex number (and the modulus itself) is a real number, which the probability has to be. From Eq. (7.10), we see that  $|\Psi(\vec{r}, t)|^2$  represents the probability density (i.e., probability per unit volume) for finding the particle at position  $\vec{r}$  at time  $t$ .

Let us cover up one slit in the double-slit experiment. We note that at the position of a given detector, there is a non-zero probability for a photon passing through the open slit to hit that detector. (We are ignoring single-slit diffraction minima here.) If we now cover the open slit and open the covered one, there is again a non-zero probability for a photon passing through the open slit to hit that the same detector. If both slits are open and the detector is at a position of destructive (double-slit) interference, *there is zero probability for a photon coming through the slits to hit that detector*. We see why the wave function has to be a complex number: Only two complex numbers with non-zero amplitudes can add together to give zero as required by interference. (Note that the wave function is not a vector.)

This probabilistic interpretation of the wave function is due to Max Born. It is the foundation of modern quantum mechanics as practiced by most physicists, and is known as the *Copenhagen Interpretation* (due to the influence of Bohr and co-workers in Copenhagen, Denmark).

### Double-slit Experiment Revisited

The statistical interpretation of matter waves leads us to the conclusion that the precise location of a quantum particle cannot be predicted. *One can only precisely predict the probability that the particle will be at a particular location*. The entire Newtonian concept of precise trajectories loses its meaning, since in Newtonian mechanics, trajectories are deterministic. Initial conditions and the equations of motion contain all the necessary information to accurately and precisely predict the position of a particle at all times. In the double-slit interference experiment, since the detectors do detect particles, it still may seem that each particle follows a definite trajectory, but perhaps the experimenter just does not have enough information. To try to get more information, we might try to determine exactly which slit a particle goes through on its way to the detector. To do this, one might place “which path” detectors<sup>9</sup> near each slit. If a particle passes through a particular slit, the associated path detector is triggered. Such experiments have actually been done, with the result that only one detector fires at a time. **[PhET simulation]** This supports the particle concept that holds that a particle can go through only one slit at a time. Now all one has to do is patiently wait for many particles to go through the slits and form the interference pattern. But, a funny thing happens. No interference pattern is formed! It is completely destroyed – the overlapping bright regions immediately behind the slits characteristic of ordinary particle

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<sup>9</sup> The detectors detect the presence of a particle e.g., by its electric or magnetic fields. The detectors are located behind the slits.

behavior is what emerges. The very act of determining which slit the “particle” goes through destroys the matter-wave interference pattern. This result is true regardless of the type of which-path detector used. Thus, one cannot measure the trajectory without drastically affecting the outcome of the experiment. Hence, in the double-slit experiment the question of “which slit does the electron go through?” is a futile one if you expect to get interference as well. If there are no which-path detectors at the slits, the electron goes through both slits. This gives rise to the interference pattern, i.e., "wavelike" behavior. If we determine which slit the electron goes through, the interference pattern is destroyed, leading to "particle-like" behavior. Thus, the electron (and all quantum particles) exhibit *complementary* behaviors. If you probe wavelike properties (no knowledge of path of the particle at the slits), you detect interference, which is wavelike behavior. If you probe particle-like properties (like the path of the particle), you will detect particle-like behavior, i.e., no interference. This behavior arises because the position of the quantum particle at the slits becomes "entangled" with the which-path detectors being used to detect it. The wave function of the particle must be modified to reflect the presence of the detectors. This new wave function gives no interference or interference depending on whether "which path" information is *available* or not; actual detection or measurement of the particle's position is not necessary. [See "Quantum Erasure" paper.]

We note that when a quantum particle is detected by one of the detectors in the array that detects the interference pattern (or lack of it), the particle's position has been measured by the detector. The position of the particle is now well-defined. Before the particle hits the detector, *it does not have a well-defined position*. The state before the measurement is a combination or superposition of all possible outcomes.

Summarizing, in the double-slit experiment, the wave function of a quantum particle at the slits is a combination or superposition of probability waves originating from both slits.

$|\Psi(\vec{r}, t)|^2$  exhibits the required interference pattern, with its value at a point in space being proportional to the probability of finding the particle at that point. If the path of the particle through a particular slit is established (or capable of being established), the interference pattern disappears. The particle does not have a well-defined position or trajectory before it is ultimately localized by a detector.

### Wave Packets

The matter wave description of quantum particles forces us to radically change our characterization and representation of a particle. One concept that has to be discarded is the idea of a “point particle.” We know that waves are not localized to a single point. Hence, with the wave description comes the fact that the particle's position cannot in general be precisely specified. To delve deeper into the description of matter waves, we look to the de Broglie and Einstein relations for insight. A matter wave has a frequency and wavelength given by  $E = hf$  and  $p = h/\lambda$ . A pure sinusoidal wave (or harmonic wave) also has a single frequency and wavelength: [Picture of harmonic wave]

$$F(x, t) = A \sin(kx - \omega t), \quad (7.12)$$

where  $F$  is the wave function (for waves on a string  $F$  is the displacement of particles from equilibrium),  $k = 2\pi / \lambda$  is the wave number, and  $\omega = 2\pi f$  is the angular frequency. Note that the Einstein relation can be rewritten as

$$E = hf = h \left( \frac{\omega}{2\pi} \right) = \hbar\omega. \quad (7.13)$$

The de Broglie relation can be similarly rewritten:

$$p = \frac{h}{\lambda} = h \left( \frac{k}{2\pi} \right) = \hbar k. \quad (7.14)$$

Eq. (7.12) represents a wave traveling to the right (positive  $x$ -axis) with phase velocity  $v_p = \omega/k$ . The phase velocity is the velocity of a fixed phase of the wave (e.g., a crest). Such a phase corresponds to a fixed value of the argument of the sinusoidal function:  $kx - \omega t = \text{constant}$ . Thus, taking differentials,  $kdx - \omega dt = 0$ , or  $v_p = dx/dt = \omega/k$ .

There are problems with the representation of a matter wave by a harmonic wave. First, the harmonic wave is completely unlocalized, i.e., it stretches from  $x = -\infty$  to  $+\infty$ . A particle is not everywhere at once! Related to this is the fact that  $|F(x,t)|^2$  (the probability density) has a finite non-negative value everywhere in space. The values oscillate with constant amplitude from  $x = -\infty$  to  $+\infty$ . Thus, when one finds the total probability by integrating  $|F(x,t)|^2$  over all space, the result is infinite. For a well-behaved and proper wave function, the result should be finite. A single harmonic wave is therefore inappropriate for use as a wave function that describes a physical particle, which must be localized in some finite region.

A clue to a more successful representation can be obtained from the results of the double-slit experiment. We saw that when two waves (one from each slit) were superposed, an interference pattern was obtained in which there were regions of high intensity (high probability for locating particle) and regions of very low intensity (low probability for locating particle). This represented *partial* localization, because there were some regions (low-intensity ones) where particles were unlikely to be found. Hence, perhaps a more localized wave function can be obtained by superposing many different harmonic waves. This is precisely what is indicated by the *Fourier Theorem*.

Joseph Fourier showed that any periodic wave function  $f(x)$  can be constructed by superposing a sufficiently large number of sinusoidal functions.<sup>10</sup>

We can write:

$$f(x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} \left\{ A_n \cos\left(\frac{2\pi nx}{\lambda}\right) + B_n \sin\left(\frac{2\pi nx}{\lambda}\right) \right\}. \quad (\text{Fourier series}) \quad (7.15)$$

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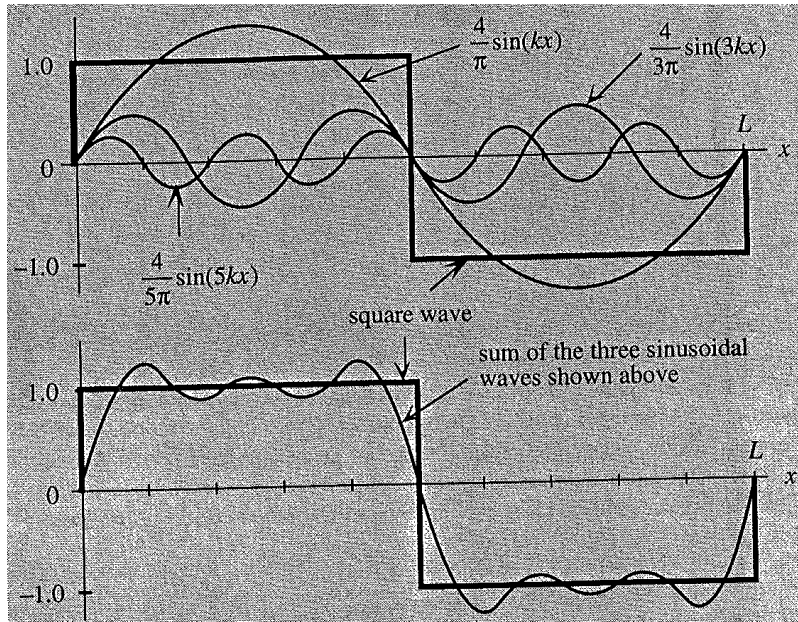
<sup>10</sup>  $f(x + \lambda) = f(x)$ ;  $f(x)$  defined on  $[-\lambda, \lambda]$ ; satisfies Dirichlet boundary conditions

Consider, e.g., a square wave  $f(x) = A$  ( $0 < x < L/2$ );  $f(x) = -A$  ( $L/2 < x < L$ ).<sup>11</sup>

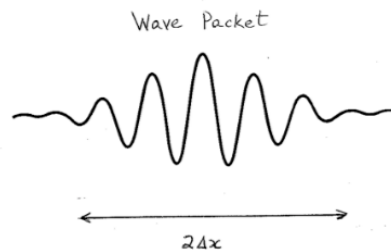
One can construct this function from the infinite sum

$$f(x) = A \left( \frac{4}{\pi} \right) \left[ \sin(kx) + \frac{1}{3} \sin(3kx) + \frac{1}{5} \sin(5kx) + \dots \right],$$

where  $k = 2\pi / \lambda$  is the wave number for the fundamental mode which  $n = 1$ .<sup>12</sup> [Note:  $\lambda = L$ .]



Let us now consider adding two sinusoidal waves with slightly different wave numbers. We are taking snapshots of the wave, i.e., the wave is “frozen” in time so we dispense with the time dependence. Adding the two waves together produces the phenomenon of beats. Note that localization has improved. [Show picture.] There are now distinct regions where the wave amplitude is diminished. One can continue adding more waves until a completely (or almost completely) localized wave or *wave packet* is produced. Note that better localization, i.e., more precise knowledge of the position comes at the expense of knowledge of the wavelength, which is now less precise (being a combination of many wavelengths.)



<sup>11</sup> Picture: p. 10 square wave; unit Q, Six Ideas

<sup>12</sup> Only sines because function is odd.

We note that a completely localized wave function is not periodic, or alternatively, has an infinite period. How can we use a Fourier series to represent a non-periodic function? Strictly speaking, we cannot. But a clue to obtaining a successful method of representing non-periodic functions is gleaned from the fact that in constructing our wave packet, we used a superposition of slightly different wave numbers (or wavelengths). If the differences between successive wave numbers are so small that the wave numbers essentially form a continuum, then the Fourier series becomes an integral:

$$f(x) = \frac{1}{\pi} \int_0^{\infty} dk \int_{-\infty}^{\infty} f(x') \cos k(x-x') dx'. \quad (7.16)$$

If we consider an even function,<sup>13</sup> the above relation becomes

$$f(x) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} F(k) \cos(kx) dk, \quad (7.17)$$

where

$$F(k) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(x) \cos(kx) dx \quad (7.18)$$

defines the amplitudes of the component waves.

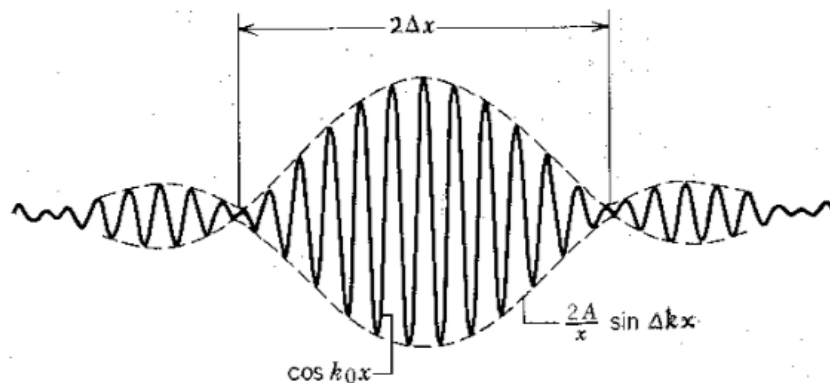
Let us consider an example.

Suppose that  $F(k) = A$  for  $k_0 - \Delta k < k < k_0 + \Delta k$   
 $= 0$  Otherwise

Then

$$\begin{aligned} f(x) &= \sqrt{\frac{2}{\pi}} \int_{k_0 - \Delta k}^{k_0 + \Delta k} A \cos kx dk = \sqrt{\frac{2}{\pi}} \frac{A}{x} \sin kx \Big|_{k_0 - \Delta k}^{k_0 + \Delta k} \\ &= \sqrt{\frac{2}{\pi}} \frac{A}{x} \{ \sin[(k_0 + \Delta k)x] - \sin[(k_0 - \Delta k)x] \} \\ &= \sqrt{\frac{2}{\pi}} \frac{2A}{x} \sin[(\Delta k)x] \cos(k_0 x). \end{aligned}$$

This function is plotted below. [Show plot with *Mathematica* or *MATLAB* in class.]



<sup>13</sup> Or one defined only for positive values of  $x$ .



We see that  $f(x)$  is quite highly localized. For different amplitude functions, even better localization can be achieved. [See PhET simulation.]

As was observed previously, we see that if  $\Delta k$  increases, i.e., if there are more wave number components in the packet,  $\Delta x$  decreases, i.e., the localization increases. It therefore seems that  $\Delta k$  and  $\Delta x$  have an inverse relationship to each other.

### Heisenberg Uncertainty Principle

In our discussion of wave packets in the previous section, we saw that the more localized a particle is, i.e., the smaller the uncertainty in its position, the larger the number of wave number components it contains, i.e., the greater the uncertainty in the wave number.

To be quantitative, we look more closely at the wave packet.<sup>14</sup> We see that  $2\Delta x$ , i.e., the spread of the packet is equal to half the spatial period  $x_{period}$  of the envelope function.

Now,  $\Delta k x_{period} = 2\pi$ , i.e.,  $x_{period} = 2\pi / \Delta k$ , so that  $\frac{1}{2} x_{period} = \pi / \Delta k$ . Therefore  $2\Delta x = \pi / \Delta k$ ,<sup>15</sup> or,

$$\Delta x \Delta k = \frac{\pi}{2}. \quad (7.19)$$

Now,  $\Delta p = \hbar \Delta k$ . Therefore, we find that

$$\Delta x \Delta p = \frac{\pi \hbar}{2}. \quad (7.20)$$

Note that Eq. (7.20) is only valid for the wave packet that we used to derive it. Eq. (7.20), though simple, is a profound statement about the nature of measurement. It says that if measurements of the positions of identically prepared quantum objects produce a small spread in values, then measurements of their momentum will produce a large spread, and vice versa.<sup>16</sup> This is true even if the experiment is done under ideal conditions so that there are no experimental or instrumental errors. For a certain packet, the uncertainty product is a minimum. Heisenberg proved that

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (\text{Heisenberg Uncertainty Relation}) \quad (7.21)$$

(Precisely,  $\Delta$  represents the standard deviation in repeated measurements on identically prepared systems.)

In three dimensions, we have

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}; \quad \Delta y \Delta p_y \geq \frac{\hbar}{2}; \quad \Delta z \Delta p_z \geq \frac{\hbar}{2}. \quad (7.22)$$

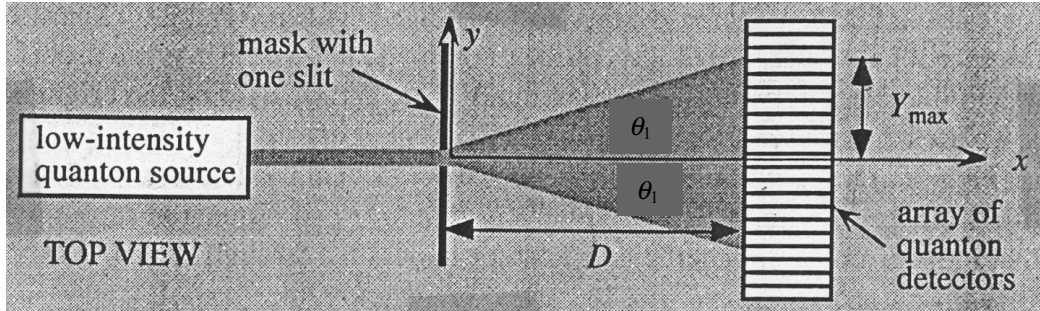
<sup>14</sup> See picture from Krane 105 or *Mathematica* output

<sup>15</sup>  $\Delta x$  taken as half-width

<sup>16</sup> A quantum particle's position and momentum cannot be simultaneously well-defined or precise.

These uncertainty relations and others comprise what is known as the Heisenberg Uncertainty Principle. Note that the Uncertainty Principle only applies to certain pairs of variables, e.g.,  $x$  and  $p_x$ , etc. (There is not such limitation on the measurement of  $x$  and  $p_y$ , for example.)<sup>17</sup>

Let us see the Heisenberg uncertainty principle (HUP) in action using single-slit diffraction. [Picture: p.92, Six Ideas; Also see Serway *et al.*]



A source produces particles, say electrons, with a precisely<sup>18</sup> defined momentum ( $p_x = p, p_y = 0$ ). We use a low-intensity source so that only one electron at a time goes through the slit. Due to diffraction, the electron wave function will broaden after the electron passes through the slit, producing a diffraction pattern at the detector after many electrons have passed through the slit. We focus on the central maximum of the diffraction pattern, where there is high intensity, i.e., there is a significant probability that an electron will strike a detector in the region [ $|\Psi|^2$  is large in this region]. The condition for the first minimum of the diffraction pattern is

$$w \sin \theta_1 = \lambda, \quad (7.23)$$

where  $w$  is the width of the slit and  $\theta_1$  is the angular position of the first minimum.

But, if an electron strikes a detector at a vertical position  $y \neq 0$ , then one could infer that the electron must have had a  $y$ -component of velocity and momentum. At the position of the first minimum, the  $y$ -component of momentum  $p_y$  can be approximated from

$$p_{y,\max} \approx p \sin \theta_1 = p \frac{\lambda}{w}. \quad (7.24)$$

But,  $p = h/\lambda$ , so Eq. (7.24) becomes

$$p_{y,\max} w \approx h. \quad (7.25)$$

Now,  $p_{y,\max} \approx \Delta p_y$ .<sup>19</sup> Further, the uncertainty in the  $y$ -position of the electron on passing through the slit is  $\Delta y \approx w/2$ . Thus, we find

$$\Delta y \Delta p_y \approx \frac{h}{2}. \quad (7.26)$$

<sup>17</sup> HUP limitation of little consequence in macroscopic cases, since  $h$  is so small. However, quantum experiments are now approaching the Heisenberg limit (see Quantum Measurement Heisenberg paper in Mod. Phys. Folder)

<sup>18</sup> As precise as possible

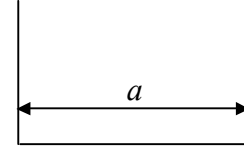
<sup>19</sup>  $p_y$  varies randomly between  $+p_{y,\max}$  and  $-p_{y,\max}$ , so  $\Delta p_y \approx p_{y,\max}$ .

This is consistent with the uncertainty principle. In this situation, the slit localizes the particle to a region of vertical dimension  $w$ . This causes the uncertainty in the  $y$ -component of the momentum to increase.

### Zero-Point Energy

A very significant result of the HUP is that a particle that is confined cannot have zero average momentum (magnitude) and therefore cannot have zero average kinetic energy. One can use the HUP to show this.

Consider a particle that is moving in one dimension and is confined to a region of width  $a$ . Thus, the minimum uncertainty in the particle's



position  $\Delta x = a/2$ .<sup>20</sup> By the HUP,  $\Delta p_x \geq \hbar/2\Delta x$ , i.e.,  $\Delta p_x \geq \hbar/a$ . The momentum of the particle must be at least of the order of  $\Delta p$ , i.e., the minimum average momentum magnitude  $\sim \Delta p$ .<sup>21</sup> Thus, the average KE associated with the momentum is  $K_{av} = (\Delta p_x)^2 / 2m$ . Using  $\Delta p_x \geq \hbar/a$ , we find

$$K_{av} \geq \frac{\hbar^2}{2ma^2}. \quad (\text{Zero-point Energy}) \quad (7.27)$$

### Energy-Time Uncertainty Relation

In investigating the Heisenberg uncertainty relations, we used a wave packet frozen in time. If we instead focus on the temporal behavior of the wave packet at a fixed point in space, the variation of the wave function has exactly the same shape. Our analysis follows in exactly the same way, except that we replace  $\Delta k$  by  $\Delta \omega$  and  $\Delta x$  by  $\Delta t$ . For the wave packet (temporal behavior), we therefore have  $\Delta \omega \Delta t = \pi/2$ . Since  $E = \hbar \omega$ , we find that

$$\Delta E \Delta t = \frac{\pi \hbar}{2}. \quad (7.28)$$

Heisenberg showed that

$$\Delta E \Delta t \geq \frac{\hbar}{2}. \quad (7.29)$$

If a particle remains in a state for a very short time, then the uncertainty in the energy of that state will be very large.<sup>22</sup> Another example is that states for which the energy of the particle is precisely specified (e.g., atomic states) are independent of time and are called *stationary states*. In general, the more precisely you wish to know the energy of a particle, the larger the time you have to take to measure the energy.

Example: The typical energy needed to ionize an atom is a few electron volts. Use the uncertainty principle to estimate the size of an atom.

Solution: Assume electron has KE = 1eV. This corresponds to a (non-relativistic) momentum

$$p = \sqrt{2mK} = 1 \text{ keV} / c. \text{ From the HUP, } \Delta x \geq \hbar/2\Delta p.$$

$$\text{Assume } \Delta p \approx p. \text{ So, } \Delta x \geq \hbar/2p = hc/2\pi pc = (1240 \text{ eV} \cdot \text{nm}) / (2\pi \times 1000 \text{ eV}) = 0.2 \text{ nm}.$$

<sup>20</sup> The formal result depends on this relation being precise.

<sup>21</sup> See Tipler & Llewellyn, Modern Physics (uses RMS deviation; use this method!)

<sup>22</sup> Short-lived elementary particles; Picture, pp. 156 and 157, Rohlf

Recall:  $a_B = 0.053$  nm for innermost shell of H atom, so our approximate method gives us the correct order of magnitude. The solution above is equivalent to using zero-point energy to do the calculation. Note that the atom is actually three-dimensional, which should be taken into account in the calculation.