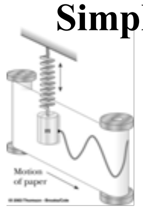
Wave function:
An equation associated with the electron (or, a property of the electron) that may be used to calculate the probability of finding the electron at a particular location.

To understand the concept of a wave function, it is useful to think of an analogous function that describes the behavior of particles undergoing simple harmonic motion

Simple Harmonic Motion



Total Energy:

Square of the amplitude of displacement function is . . .
proportional to total energy of particle

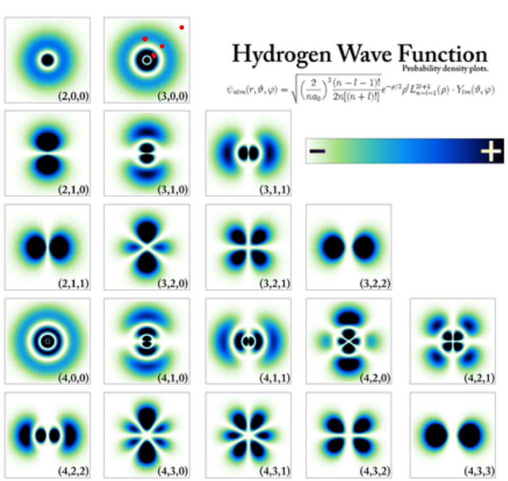
Displacement Function:

Quantum Mechanical Atom

Example of an Electron Wave

$$\Psi = A\sin\left(\frac{n\pi x}{L}\right)$$

Square of amplitude:
proportional to probability of finding the electron at a particular location.

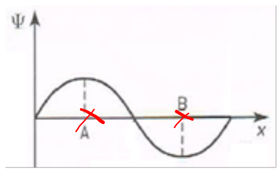


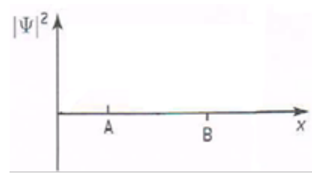
Total Energy:

$$\frac{d^2\Psi}{dx^2} = -\frac{8\pi^2 m}{h^2}(E - V)\Psi$$

(Schrödinger's wave equation)

1. A particle has a wave function shown by the graph at right. Where is the particle most likely to be found?





2. The wave functions of three different particles are shown below. Indicate on each graph where each particle is most likely to be found.

Probability Density Function

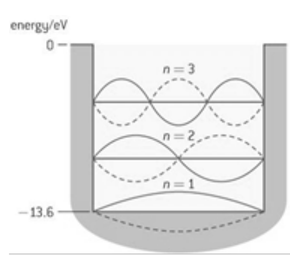
Where P (r) = probability of finding particle at distance r

$|\psi|^2$ = square of amplitude of wave function

ΔV = small volume

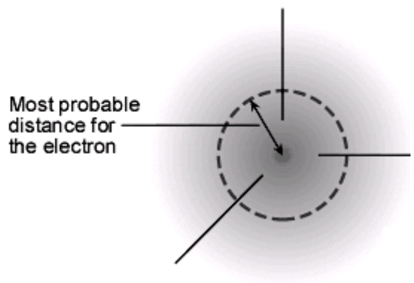
$P(r) = |\psi|^2 \Delta V$

In a simplified (one-dimensional) versions of the quantum mechanical hydrogen, the position of the electron is undefined but it would be detected somewhere between the nucleus and "outside edge" of the atom. These are shown as the boundaries of a standing wave – the electron's wave function for each energy level.



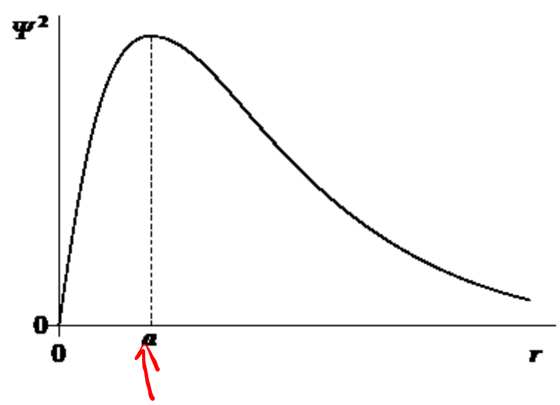
A plot of the probability density function (including square of the wavefunction) can show where the electron is most likely to be found.

"electron cloud" of probability for the first electron energy level



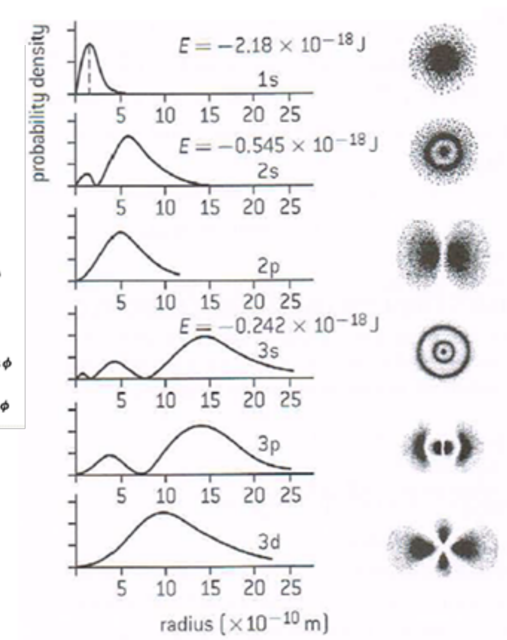
What is the significance of location $r = a$?

plot of the square of the wave function (probability) versus radial distance from the nucleus for the electron in its lowest energy state



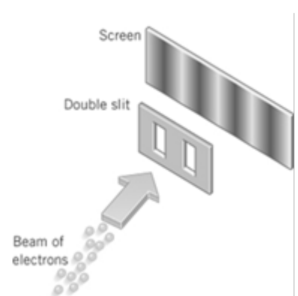
Wave functions for more complex versions of a quantum mechanical atom and the associated plots of the probability density functions are shown

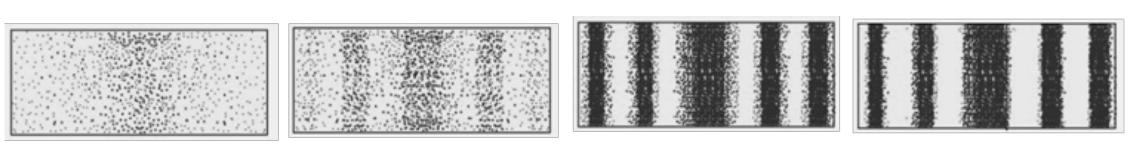
$$
\begin{array}{llll}
n=1, & l=0, & m=0 & \psi_{1s}=\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma} \\
n=2, & l=0, & m=0 & \psi_{2s}=\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2} \\
 & l=1, & m=0 & \psi_{2p_z}=\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta \\
 & l=1, & m=\pm 1 & \psi_{2p_x}=\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta\cos\phi \\
 & & & \psi_{2p_y}=\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta\sin\phi \\
n=3, & l=0, & m=0 & \psi_{3s}=\frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27-18\sigma+2\sigma^2)e^{-\sigma/3} \\
 & l=1, & m=0 & \psi_{3p_z}=\frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma(6-\sigma)e^{-\sigma/3}\cos\theta \\
 & l=1, & m=\pm 1 & \psi_{3p_x}=\frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma(6-\sigma)e^{-\sigma/3}\sin\theta\cos\phi \\
 & & & \psi_{3p_y}=\frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma(6-\sigma)e^{-\sigma/3}\sin\theta\sin\phi
\end{array}
$$



How can wave functions help to explain electron diffraction?

While it is not possible to specify in advance where a particular electron will hit the screen after passing through one or the other slit, one can predict the probability of it hitting at a certain location. Bright fringes correspond to places where electrons have a high probability of landing, and thus over time many electrons do hit there as shown below, and dark fringes correspond to places where electrons have a low probability of landing. The wave function associated with each electron can thus be seen as a probability wave.





Heisenberg's Uncertainty Principle

Werner Heisenberg (German physicist, 1901-1976) won a Nobel prize in 1932 for the development of his uncertainty principle which identifies a fundamental limit to the possible precision of any physical measurement.

Uncertainty Principle

1) Both the position and momentum of a particle cannot be precisely known at the same time.
2) Both the energy state of a particle and the amount of time it is in that energy state cannot be precisely known at the same time.

conjugate quantities: position/momentum or energy/time

Implications

a) The more you know about one of the conjugate quantities, the less you know about the other.
b) If one of the conjugate quantities is known precisely, all knowledge of the other is lost.

Mathematical Representations of the Uncertainty Principle

Position-Momentum Conjugates

$\Delta x \Delta p \geq \frac{h}{4\pi}$ $\qquad \frac{\hbar}{2}$

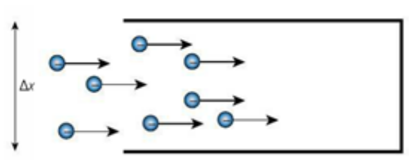
Note Δx = uncertianty in position

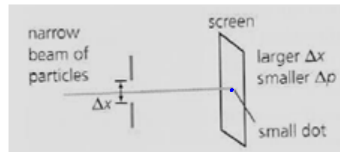
$\Delta E \Delta t \geq h/4\pi$

Energy-Time Conjugates

Electron Diffraction

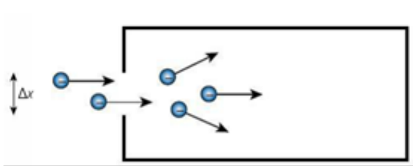
A beam of electrons is fired into an open box. If they are shot primarily horizontally then there will be very little uncertainty about their momentum Δp. But since the opening of the box is so large the electrons could be entering at any point, so the uncertainty in their position Δx is also very large.

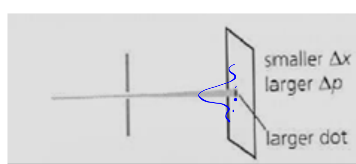


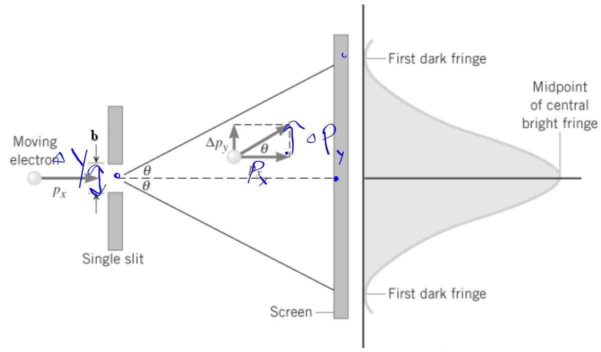


To reduce the uncertainty in position, the opening of the box is made smaller. As a result, however, some electrons are now deflected up or down vertically by the edges of the opening. (Alternatively, if the electrons are thought of as waves, one can say that they are now diffracted.) This increases the uncertainty in their momentum.

$\theta = \frac{\lambda}{b}$







$\frac{h}{4\pi} \le \Delta p_y \Delta y$

$\frac{\lambda}{b} = \frac{\lambda}{\Delta y} = \frac{\Delta p_y}{p_x} \leftarrow \frac{h}{\lambda}$

Electrons passing through a single slit can be diffracted up or down within the central maximum as far as the location of the first minimum (dark fringe) – neglecting the other bright fringes. This means that although the electron originally had no momentum in the vertical direction before entering the slit, now it may have a vertical momentum component as large as Δp_y. Thus, the uncertainty in its momentum is only in the vertical direction and is equal to Δp_y. Its horizontal momentum component remains constant at p_x and so $\Delta p_x = 0$.

NOTE: uncertainty in the momentum is perpendicular to its original momentum

1. If the width of the slit is $\underbrace{1.5 \times 10^{-11}}_{\Delta y}$ m, find the minimum uncertainty in the:

a) horizontal component of the momentum

b) vertical component of the momentum

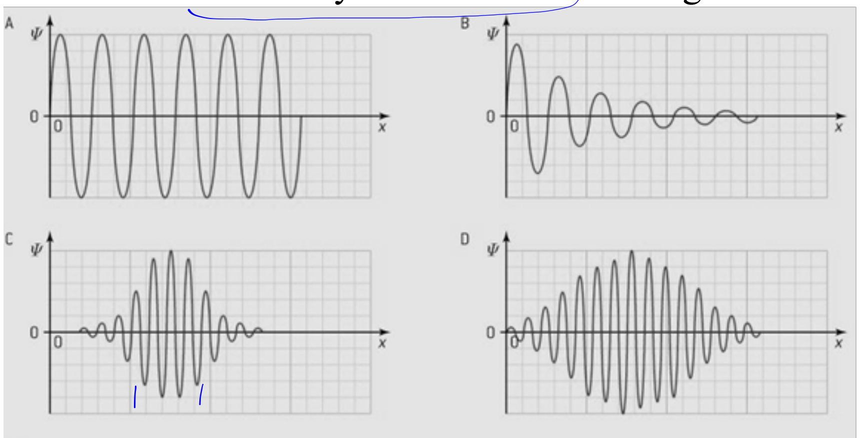
$\Delta y \Delta p \ge h/4\pi$

$\Delta p \ge \frac{h}{4\pi \Delta y} = \frac{6.63 \times 10^{-34}\ \mathrm{J/Hz}}{4\pi\ 1.5 \times 10^{-11}\ \mathrm{m}} \approx 3.5 \times 10^{-24}\ \mathrm{kg\,m/s}$

NOTE:

uncertainty in the momentum is perpendicular to its original momentum

2. The diagrams below show the variations with distance x of the wave functions ψ of four different electrons. For which electron is the uncertainty in momentum the largest?

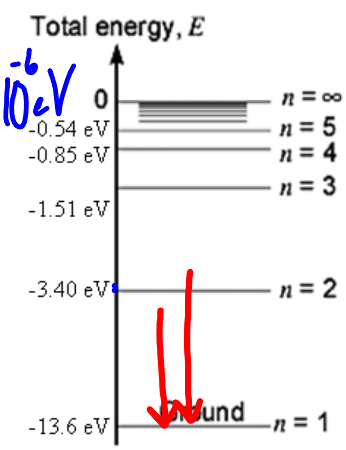


2. An electron stays in the first excited state of hydrogen for a time of approximately $\underbrace{1.0 \times 10^{-10}\ \text{s}}_{\Delta t}$.

a) Determine the uncertainty in the energy of the electron in the first excited state.

$$\Delta E\, \Delta t \geq \frac{h}{4\pi}$$

$$\Delta E \geq \frac{h}{4\pi \cdot \Delta t} = \frac{4.14 \times 10^{-15}\ \text{eV s}}{4\pi\ 10^{-10}\ \text{s}} \approx 3 \times 10^{-6}\ \text{eV}$$



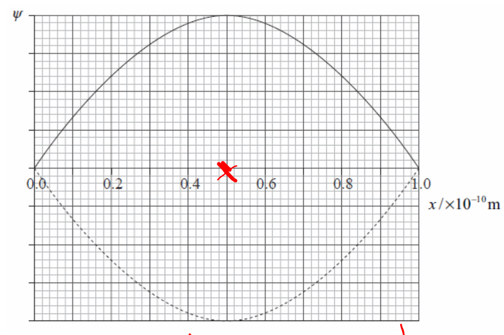
b) Discuss what implications this uncertainty will have for photons emitted as an electrons transition from the first excited state to the ground state.

$$E = h\frac{c}{\lambda}$$

range of wavelengths, predict thickness of spectrum lines

1. The wavefunction ψ for an electron confined to a "box" of linear size 1.0 x 10^{-10} m is shown in the graph as a standing wave.

Å



Δx

a) Where is the electron most likely to be found?

b) What is the electron's de Broglie wavelength?

2×10^{-10} m

c) What is the uncertainty in the electron's position?

d) What is the minimum uncertainty in the electron's momentum?

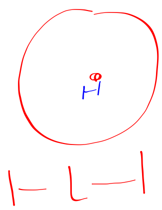
$p = \frac{h}{\lambda}$

$\Delta p \Delta x \geq h/4\pi$

$\Delta p = \frac{h}{4\pi \Delta x} = \frac{6.63 \times 10^{-34}\ J \cdot s}{4 \cdot \pi \cdot 10^{-10}\ m} = 5.3 \times 10^{-25}\ kg\,m/s$

Estimate:
a) the energy of the ground state of an atom

When an electron is known to be confined within an atom the uncertainty in its position must be less than the size of the atom L.



$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

$$\Delta p \geq \frac{h}{4\pi L}$$

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

$$= \frac{h^2}{4^2\pi^2 L^2 2m} \sim 1\ eV$$

L: 10^{-10} m

b) Estimate the impossibility of an electron existing within a nucleus

$$\Delta E \sim 10^{10}\ eV$$