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Reference Book:
Garcia Narciso, Damask Arthur, Physics for Computer Science Students, Springer-Verlag

The Uncertainty Principle

An experiment cannot simultaneously determine a component of the momentum of a particle, p_x, and the exact value of the corresponding coordinate, x.

The best one can do is

$$\Delta p_x \Delta x \geq \hbar$$

1. The limitations imposed by the uncertainty principle have nothing to do with the quality of the experimental instrument.
2. The uncertainty principle does not say that one cannot determine the position or the momentum exactly. However, if $\Delta x = 0$, then the uncertainty in the momentum will be infinite, and vice versa.
3. The uncertainty principle is a direct consequence of de Broglie's hypothesis, which, as we have seen, is confirmed by experiment. Thus the uncertainty principle is based on experiment.

An Example of Moon
Mass of the moon = $6 \times 10^{22} kg$,
average orbital velocity = $10^3 m/sec$.

Suppose that we are able to determine the position of the moon with an uncertainty $\Delta x = 10^{-6} m$

Then,

$$\Delta p_x \geq \frac{\hbar}{\Delta x} = \frac{10^{-34}}{10^{-6}} = 10^{-28} kg\ m/sec$$

Because by definition $p_x = mv_x$ it follows that

$$\Delta v_x = \frac{\Delta p_x}{m} \geq \frac{10^{-28}}{6 \times 10^{22}} \approx 10^{-50} m/sec$$

This is an insignificant error when we compare it with the measured value of $v = 10^3 m/sec$.

An Example of Electron

- Consider an electron in the hydrogen atom.
- Smallest radius of a Bohr orbit is approximately $0.5 \times 10^{-10} m$.
- Let $\Delta x \approx 10^{-10} m$ (The electron can be anywhere in the orbit, and therefore x can take any value between $-0.5x10^{-10}m$ and $+0.5x10^{-10}m$)

$$\Delta p_x \geq \frac{\hbar}{\Delta x} = \frac{10^{-34}}{10^{-10}} = 10^{-24} kg\ m/sec$$

- The KE of electron is $13.6eV$ (Look at previous class-notes)

$$E_k = 13.6eV = 13.6 \times 1.6 \times 10^{-19} = 2.18 \times 10^{-18} J$$

$$p = \sqrt{2mE_k} = \sqrt{2 \times 9.1 \times 10^{-31} \times 2.18 \times 10^{-18}} = 2 \times 10^{-24} kg\ m/sec$$

$$\frac{\Delta p_x}{p_x} = \frac{10^{-24}}{2 \times 10^{-24}} = 0.5 = 50\%$$

Numerical Problems

1. A small particle of mass $10^{-6} g$ moves along the x axis; its speed is uncertain by $10^{-6} m/sec$. (a) What is the uncertainty in the x coordinate of the particle? (b) Repeat the calculation for an electron assuming that the uncertainty in its velocity is also $10^{-6} m/sec$.

2. The uncertainty in the position of a particle is equal to the de Broglie wavelength of the particle. Calculate the uncertainty in the velocity of the particle in terms of the velocity of the de Broglie wave associated with the particle.

Physical Origin of the Uncertainty Principle

$$\Delta p_x(photon) = 2p_{photon}\sin\phi$$

Conservation of linear momentum:

$$\Delta p_x(electron) = 2p_{photon}\sin\phi$$

$$\Delta p_x(electron) = 2\frac{h}{\lambda}\sin\phi$$

In the process of locating the electron, we have introduced an uncertainty in its momentum.

We could reduce the uncertainty in p_x of the electron in two ways.

- use photons of longer wavelength
- reduce ϕ, the angle subtended by the lens: make aperture of the lens small.

Both these factors that would reduce the uncertainty in p_x lead to an increase in the uncertainty of the position of the electron that we are trying to locate.

Longer wavelengths and smaller lens aperture will increase the uncertainty about the origin of the photon entering the microscope, that is, about the position of the scattering electron.

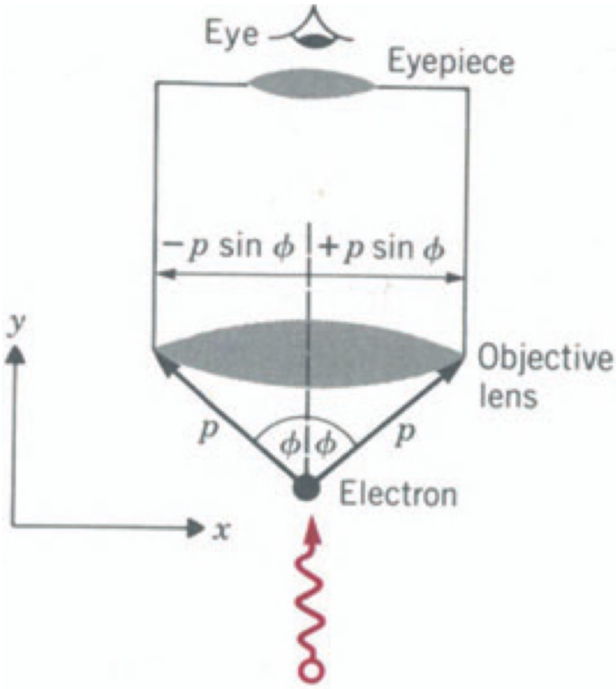

Figure 1: "Looking" at an electron with a hypothetical microscope in Bohr's thought experiment. The electron is illuminated with light (photons) The photons scattered by the electron that enter the objective lens of the microscope are detected by the eye of the observer.

Matter Waves and the Uncertainty Principle
Equation of a wave is given by

$$\psi(x,t) = A \sin(kx - \omega t)$$

Amplitude A ; Wavelength $\lambda = \frac{2\pi}{k}$; Frequency $\nu = \frac{\omega}{2\pi}$; Velocity $v = \lambda\nu = \frac{2\pi}{k}\frac{\omega}{2\pi}$

Can we associate this wave with a free particle? We have seen that to describe a localized particle we can use a wave packet according to de Broglie hypothesis. Because the wave packet accompanies the particle and tells us approximately where the particle may be found, it must travel with the same velocity as the particle.

Let us take two traveling waves that differ slightly in wavelength and frequency,

$$\psi_1 = A \sin[kx - \omega t] \cdots\cdots\cdots (1)$$

$$\psi_2 = A \sin[(k + \Delta k)x - (\omega + \Delta\omega)t] \cdots\cdots\cdots (2)$$

where $\Delta k << k$ and $\Delta\omega << \omega$

The resulting $\psi(x,t)$ will be

$$\psi(x,t) = \psi_1 + \psi_2$$

$$\psi(x,t) = A \sin[kx - \omega t] + A \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

If we use the trigonometric relation

$$\sin A + \sin B = 2 \sin \frac{A+B}{2} \cos \frac{A-B}{2}$$

we get

$$\psi(x,t) = 2A \cos\left(\frac{\Delta kx - \Delta\omega t}{2}\right) \sin(kx - \omega t) \cdots\cdots\cdots (3)$$

where we have used the approximation $2k + \Delta k \approx 0,\ 2\omega + \Delta\omega \approx 2\omega$.

The resulting wave is thus the product of two traveling waves. The second term of Eq. (3) represents a wave having roughly the same frequency and wavelength as the original waves. The first term represents a wave having a much larger wavelength and much smaller frequency.

We can consider ψ as a wave similar to the original ones except that its amplitude is modulated by the first term, giving rise to a periodically varying amplitude. A "snapshot" of ψ is shown in Figure. Such a ψ could be used to describe a beam of particles, with one particle in each wave packet. The velocity of the wave inside the envelopes is the same as the velocity of the individual waves. The envelops (that is, the wave packets) travel with velocity, called group

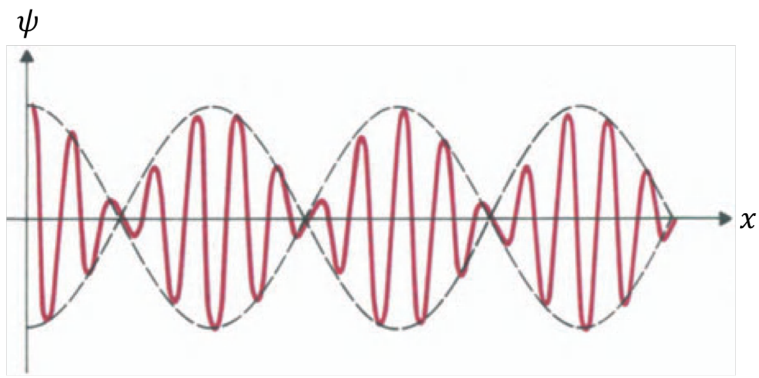

Figure 2: A "snapshot" of a wave with a periodically varying amplitude. Such a wave is obtained by adding two sinusoidal traveling waves of slightly different frequency and wavelength.

velocity, v_{group}, given by

$$v_{group} = \frac{\frac{\Delta\omega}{2}}{\frac{\Delta k}{2}} = \frac{\Delta\omega}{\Delta k} \approx \frac{d\omega}{dk} \cdots\cdots\cdots (4)$$

We can show that v_{group} is the same as the velocity of the particle, by using de Broglie's relations,

$$\lambda = \frac{h}{p} \text{ and } \lambda = \frac{2\pi}{k}; \ \Rightarrow k = \frac{p}{\hbar} \quad \Rightarrow \quad dk = \frac{dp}{\hbar}$$

And,

$$\nu = \frac{E}{h} \text{ and } \nu = \frac{\omega}{2\pi}; \ \Rightarrow \omega = \frac{E}{\hbar} \quad \Rightarrow \quad d\omega = \frac{dE}{\hbar}$$

Therefore, from equation (4),

$$v_{group} = \frac{dE}{dp} \cdots\cdots\cdots (5)$$

But we know that $E = \frac{1}{2}mv_{particle}^2 = \frac{p^2}{2m}$;

$$E = \frac{p^2}{2m} \quad \Rightarrow \frac{dE}{dp} = \frac{p}{m} = \frac{mv_{particle}}{m} = v_{particle} \cdots\cdots\cdots (6)$$

From equation (5) and (6) we get,

$$v_{group} = v_{particle}$$

The wave packet moves with the particle.

Numerical Problems to Practice

1. After being excited, the electron of a hydrogen atom eventually falls back to the ground state. This can take place in one jump or in a series of jumps, the electron falling into lower excited states before it ends up in the ground state. Consider a hydrogen atom that has been raised to the second excited state, that is, $n = 3$. Calculate the different photon energies that may be emitted as the atom returns to the ground state.
2. Calculate the shortest and the longest wavelength of the Balmer series of hydrogen.
3. What are (a) the energy, (b) the momentum, and (c) the wavelength of the photon that is emitted when a hydrogen atom undergoes a transition from the state $n = 3$ to $n = 1$? (The momentum of the photon is given by $h\nu/c$).
4. The shortest wavelength of the Paschen series from hydrogen is 8204Å. From this fact, calculate the Rydberg constant.
5. The ground-state and the first excited-state energies of potassium atoms are $-4.3eV$ and $-2.7eV$, respectively. If we use potassium vapor in the Franck-Hertz experiment, at what voltages would we see drops in the plot of current versus voltage?
6. A beam of monochromatic neutrons is incident on a KCl crystal with lattice spacing of 3.14Å. The first-order diffraction maximum is observed when the angle θ between the incident beam and the atomic planes is 37°. What is the kinetic energy of the neutrons?
7. The de Broglie wavelength of a proton is $10^{-13}m$. (a) What is the speed of the proton? (b) Through what potential difference must the proton be accelerated to acquire such a speed?
8. An α particle is emitted from a nucleus with an energy of $5MeV(5 \times 10^6 eV)$. Calculate the wavelength of an α particle with such energy and compare it with the size of the emitting nucleus that has a radius of $8 \times 10^{-15}m$.
9. In neutron spectroscopy a beam of monoenergetic neutrons is obtained by reflecting reactor neutrons from a beryllium crystal. If the separation between the atomic planes of the beryllium crystal is 0.732Å, what is the angle between the incident neutron beam and the atomic planes that will yield a monochromatic beam of neutrons of wavelength 0.1Å?
10. A small particle of mass $10^{-6}g$ moves along the x axis; its speed is uncertain by $10^{-6}m/sec$. (a) What is the uncertainty in the x coordinate of the particle? (b) Repeat the calculation for an electron assuming that the uncertainty in its velocity is also $10^{-6}m/sec$.
11. The uncertainty in the position of a particle is equal to the de Broglie wavelength of the particle. Calculate the uncertainty in the velocity of the particle in terms of the velocity of the de Broglie wave associated with the particle.

Schrodinger theory of quantum mechanics and its application

In trying to find the wave associated with the particle, de Broglie's postulates give us the first guideline. We have seen that if a particle has a well-defined momentum and energy, we can use a sinusoidal traveling wave, that is, either

$$\psi = A\sin(kx - wt) \quad \text{or} \quad \psi = A\cos(kx - wt)$$

or a linear combination of both. As we have seen, if we want to describe a free particle, which is partially localized, we could use a wave packet.

De Broglie's hypothesis does not tell us what type of wave one can associate with a particle that is not free and that is acted on by a force. If a particle is acted on by a force, its momentum and its energy will not be constant. Therefore, it is meaningless to talk about a λ and a ν, because these quantities are changing. The Schrodinger theory tells us how to obtain the wavefunction $\psi(x,t)$ associated with a particle, when we specify the forces acting on the particle, by giving the potential energy associated with the forces. (In quantum mechanics the potential energy is often referred to simply as the potential). The Schrodinger theory also tells us how to extract information about the particle from the associated wavefunction.

Schrodinger developed a differential equation whose solutions yield the possible wavefunctions that can be associated with a particle in a given physical situation. This equation, known as the *Schrodinger equation*, tells us how the wavefunction changes as a result of the forces acting on the particle. Because the wavefunction ψ is a function of space and time, the equation contains derivatives (remember that a derivative represents the rate of change) with respect to x, y, and z and with respect to t.

The total energy of a particle is equal to the kinetic energy plus the potential energy,

$$E = \frac{1}{2}mv^2 + E_p \quad = \frac{p^2}{2m} + E_p$$

Therefore,

$$E\psi = \frac{p^2}{2m}\psi + E_p\psi \cdots\cdots\cdots (1)$$

In quantum mechanics physical observables are generally expressed as operators. Operators for some of the observables are

Observable		Operator
$Energy(E)$	$\rightarrow$	$i\hbar\frac{\partial}{\partial t}$
$Momentum(p)$	$\rightarrow$	$-i\hbar\frac{\partial}{\partial x}$

Substituting the operators in equation (1), we get,

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi + E_p\psi$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + E_p\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + E_p\psi = i\hbar\frac{\partial\psi}{\partial t} \cdots\cdots\cdots (2)$$

Equation (2) is known as the one-dimensional time-dependent Schrodinger equation. If the potential energy E_p is known, this equation can be solved in principle, and the solution will yield the possible wavefunctions that we can associate with the particle. The Schrodinger equation is to quantum mechanics what Newton's second law is to classical physics.

The Schrodinger Equation for a Free Particle

Let us consider a free particle moving along the x axis with definite momentum $p = mv$ and definite energy $E = 1/2mv^2$. If no force acts on the particle, that is, $F = 0$, the potential energy is $E_p = constant$, which we can choose to be 0. Thus, the condition $F = 0$ requires that $E = constant$. The Schrodinger equation (Eq. 2) in this case may be written for $E_p = 0$ as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t} \cdots\cdots\cdots (3)$$

As mentioned at the beginning of Section 20.2a, because we are dealing with a particle of well-defined momentum and energy, we might expect that the solution would be in the form of a traveling wave, that is, either

$$\psi = A\sin(kx - wt) \quad \text{or} \quad \psi = A\cos(kx - wt)$$

or some linear combination of these two functions. If one tries either of these by substitution into Eq. 20.3, one finds that neither satisfies the Schrodinger equation. The reason is that when you differentiate a sine function twice with respect to x, you get the sine function back, but when you differentiate it with respect to time once, you get a cosine function. For example, let us consider I/J = A sin (kx - wt). Differentiating with respect to x, we first get

$$\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}\left[A\sin(kx - \omega t)\right] = kA\cos(kx - \omega t)$$

and the second differentiation yields

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial}{\partial x}\left[kA\cos(kx - \omega t)\right] = -k^2A\sin(kx - \omega t)$$

The derivative of ψ with respect to t yields

$$\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial t}\left[A\sin(kx - \omega t)\right] = -\omega A\cos(kx - \omega t)$$

Substituting these results for $\partial^2\psi/\partial x^2$ and $\partial\psi/\partial t$ in Eq. 3, we obtain

$$\frac{k^2\hbar^2}{2m}A\sin(kx - \omega t) = -i\hbar\omega\, A\cos(kx - \omega t)$$