Lecturer Two

2-1 The Wave-Particle Duality

The conclusion from the Planck (see (1-2) in chapter 1) , Einstein and Compton (see (1-3) and (1-4) in chapter 1) analyses was that light, which was thought to be a wave classically, could also behave like a particle at the quantum level. It was then natural to ask the question of whether this "particle wave duality" may apply to other objects that carry energy and momentum? For example, could a classical particle such as an electron behave like a wave at the quantum level? Indeed in 1923 DE Broglie postulated such a particle-wave duality and assigned the wavelength:

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

to any particle that has momentum p. This is consistent with the photon's electromagnetic wave momentum (p = E/c = hν/c = h/λ). But he proposed this momentum-wavelength relation to be true for the electron or other classical particles as well, even though the energy-momentum relation for these particles is quite different than the photon's (i.e. $E = p^2/2m$ or $E = (p^2c^2 + m^2c^4)^{1/2}$).

2-2 Diffraction and the Heisenberg uncertainty relation

The uncertainty principle states that the uncertainty in the measurement of the position of a particle (Δz) multiplied by the uncertainty in the measurement of its momentum along the same direction (Δp_z) is larger than the order of magnitude of h, Planck's constant. The Equation 1 shows a formulation used in most physical textbooks.

$$\Delta Z \times \Delta p_z \geq h \qquad (1)$$

Imagine that you send a laser beam (horizontally) toward a *z* screen. This is an ideal beam, so that the photons have no vertical component for their velocity vector. In other words, the momentum in the vertical direction (the vertical axis from here on is referred to as *z*) is also zero and so is the uncertainty associated with the value of the momentum along this axis. Since Δp_z is zero, one would expect that $\Delta p_z \times \Delta z$ = 0 (<*h*), thereby

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violating the uncertainty principle. Fortunately, this is not the case, because the lack of vertical motion also means that the impression the beam leaves on the screen is one (or zero) dimensional and not observable. The uncertainty in the measurement of the position is infinite and the uncertainty principle holds.

Suppose, however, that we decide to use a slit to define the vertical position of the laser beam. Let us say, a 1-mm slit. In that case, we may believe that we still have $\Delta p_z = 0$ and $\Delta z = 1$ mm, so that now we do have $\Delta p_z \times \Delta z = 0$. Our thought experiment does not succeed, however, because the act of introducing the slit results in a diffraction pattern. This means that the photons acquire a momentum in the vertical direction, and Δp_z is no longer equal to zero. The slit can be made as small as necessary (thereby decreasing Δz), but this increases the size of the diffraction pattern (i.e., it makes Δp larger). See below for a description of a real experiment.
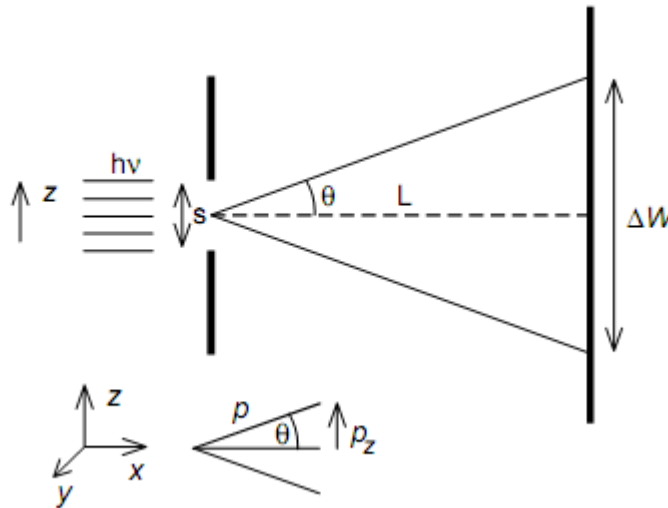

Figure 1. Schematics of the experiment: s is the slit size; L is the distance from the slit to the screen; ΔW is the distance between the two lines of destructive interference closest to the center of the laser beam; p_z is the z component of the momentum, p.

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Figure 1 represents a schematic of the experiment with the variables involved. The laser beam travels parallel to the xy plane. Therefore, the condition would hold (before a slit is introduced) that $2p_z = \Delta p = 0$. Once the slit (of width s) is introduced (see Fig. 2), a diffraction pattern is observed on the screen. The distance between the two lines of darkness closest to the center of the beam is labeled ΔW. ΔW is related to the value of p_z, because the width of the spot (ΔW), will be larger if p gets bigger. (ΔW is also related to the distance between the slit and the screen, L).

We will use the approximation that the uncertainty in the measurement of the momentum (in the z direction), Δp, is equal to twice the value of the z component of the momentum for the photons that reach the screen within the boundaries of the first two lines of darkness (Fig. 1, inset). Although this is just an approximation, we can rationalize choosing the photons within the two lines of darkness closest to the center with the following arguments.

The uncertainty in the measurement of any physical observable can be defined as the standard deviation, $\Delta \alpha = (\alpha 2 - \alpha 2)1/2$. The standard deviation of an observable, in turn, defines an interval where a majority of measurements are recorded (see, for instance, ref 3). In this experiment, the central spot is by far the most intense spot in the diffraction pattern. Since this spot contains the majority of the photons, it stands that it is a good approximation to use it to define the uncertainty in the momentum in the z direction. A second consideration is related to the fact that the uncertainty principle indicates that Δz × Δp is larger than ~h. By choosing to relate Δp$_z$ to ΔW (as defined in Fig. 1), we are ensuring that we do not overestimate Δp. We would rather have an underestimate, because if the uncertainty principle holds for an underestimated value of Δp$_z$, it must hold for the true Δp. In other words, by defining ΔW as the interval between the two lines of darkness closest to center to approximate the value of Δpz, we are choosing the minimum value for the uncertainty in the momentum. This ensures that when one establishes that Δz × Δp ≥h, this is

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due to a physical reason (i.e., the uncertainty principle) and not to the use of an excessive value for Δp. This allows us to relate Δp_z to ΔW using the common angle θ.

$$\Delta p_z \approx 2p_z, \text{ and } \sin \theta = \frac{p_z}{p} \rightarrow \Delta p_z \approx 2p \sin \theta$$

Also, since $\theta \approx 0$ (note that ΔW is of the order of centimeters when L is several meters, see below), $\sin \theta$ can be obtained from $\sin \theta \approx \tan \theta = \frac{(\frac{1}{2}\Delta W)}{L}$. Therefore,

$$\Delta p_z \approx 2p\frac{\Delta W}{2L} \approx \frac{p\Delta W}{L}$$

If we know the wavelength of the laser beam, we can get information about the total momentum, p: $p = h/\lambda$. Equation shows the final expression for p_z.

$$\Delta p_z \approx \frac{h\Delta W}{\lambda L}$$

Since $\Delta z = s$, we can write a formulation of the uncertainty principle related to the variables of our experiment:

$$\Delta p_z \times \Delta z \gtrsim h \rightarrow s\frac{h\Delta W}{\lambda L} \gtrsim h$$

$$\therefore \quad \frac{s\Delta W}{\lambda L} \gtrsim 1$$

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2-3 <u>Schrödinger Equation</u>

The deBrogli postulate does provide us with a complete theory for the behavior of a particle, and does not tell us the way in which the associate waves propagate. So, we must have an equation which will tell how the waves propagate under the difference of forces. The waves are represented by the mathematical function ψ (x,t) which is called the *wave function*. Schrödinger equation must satisfy the following requirements:

1- It must be consistent with the equation

- The deBrogli equation $\qquad \lambda = \frac{h}{p}$ $\qquad\qquad$ (1)

- The Einstein Equation $\qquad \upsilon = \frac{E}{h}$ $\qquad\qquad$ (2)

- The total energy $\qquad E = \frac{p^2}{2m} + V$ $\qquad$ (3)

2- It must be linear in ψ (x,t). That is if ψ₁ (x,t) and ψ₂ (x,t) are solutions to the equation, a linear combination of these functions:
ψ (x,t) =a₁ ψ₁ (x,t) +a₂ ψ₂ (x,t)   must also be a solution for any value of the constants a1 and a2 this requirement ensure that we should be able to add together wave functions to be product the interference phenomena and to permit the construction of wave packets.

3- The potential energy V is, in general, a function of x and t. The wave associated with the free-particle can be represented by the following forms:

ψ (x,t)=sin (kx-ωt) $\qquad\qquad$ (4)

ψ (x,t)=cos (kx-ωt) $\qquad\qquad$ (5)

or   ψ (x,t)=γ sin (kx-ωt) + cos (kx-ωt) $\qquad$ (6)

where γ is a constant to determined

we must find an equation consistent with equation 3, which can be written as:

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$$\frac{\hbar k^2}{2m} + V_0 = \hbar\omega \qquad\qquad (7)$$

To find an equation consistent with equation (6), we must take the derivative to the wave function from equation 6 twice w.r.t x, to bring a factory of k^2, and differentiating once w.r.t. time to bring a factor of ω.

So we try the equation:

$$\alpha\frac{\partial^2\psi}{\partial^2 x} + V_0\psi = \beta\frac{\partial\psi}{\partial t} \qquad\qquad (8)$$

where α and β are constants to be determined .
we may try to construct the differential equation by starting with a combination of two functions;

$$\frac{\partial\psi}{\partial x} = -k\sin(kx - \omega t) + k\gamma\cos(kx - \omega t) \qquad\qquad (9)$$

$$\frac{\partial\psi^2}{\partial x^2} = -k^2\cos(kx - \omega t) - k^2\gamma\cos(kx - \omega t) \qquad (10)$$

$$\frac{\partial\psi}{\partial t} = -\omega\sin(kx - \omega t) - \omega\gamma\cos(kx - \omega t) \qquad\qquad (11)$$

Substituted equations (9, 10,11) in equation 8, we can obtain:

$$[-\alpha k^2 + V_0 + \beta\omega\gamma]\cos(kx - \omega t) + [-\alpha k^2\gamma + V_0\gamma - \beta\omega](kx - \omega t) = 0 \quad (12)$$

If this is to be true for all value of x and t, the coefficient of both cosine and sine must vanish (linearly dependent).

- $\alpha k^2 + V_0 = -\beta\,\omega\,\gamma$ (13)
- $\alpha k^2 + V_0 = -\frac{\beta}{\gamma}\omega$ (14)

By subtracting 13 and 14 we can find that:

$$0 = -\beta\omega\gamma - \frac{\beta\omega}{\gamma} \quad\Rightarrow \gamma^2 = -1$$
$$\gamma = \pm i$$

If we take γ=+I and substitute it back into equation (13)

         - $\alpha k^2 + V_0 = -i\beta\,\gamma$ (15)

Comparing this with equation (7)

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$$\propto = -\frac{\hbar^2}{2m} \; ; \qquad -i\beta = \hbar \qquad \beta = i\,\hbar$$

The differential equation (8) becomes;

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial^2 x} + V_0 \Psi = i\hbar \frac{\partial \psi}{\partial t} \qquad (16)$$

The Solution of the above equation $\quad \psi(x,t) = e^{\,i(kx-\omega t)}$

Equation (16) has been obtained for the special case of a constant potential V(x,t)=V$_o$ for free particle.

For the general case in which V(x,t) is not a constant, the differential equation controlling the propagation of the wave function is of the same as equation 16:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial^2 x} + V(x,t)\Psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \qquad (17)$$

The above equation is One Dimension Time Dependence Schrödinger Equation (ODTDSE)

$$-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\Psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \qquad (18)$$

When comparing Schrödinger equation with the classical wave equation:

$$\frac{\partial^2 \cup}{\partial^2 x} = \frac{1}{u^2}\frac{\partial^2 \cup}{\partial^2 t} \qquad (19)$$

We notice that the difference appears with the time derivative. Also Schrodinger equation contain the imaginary number (i) which means that *the wave function ψ(x,t) is a complex function of real quantities x and t.*

3-3 **Interpretation of the wave function:**

The wave function ψ(x,t), which is a solution of the wave function of equation 18 is assumed to provide a quantum mechanical complete

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description of the behavior of a particle of mass m with the potential energy of V(x,t) and hence it is analogous to the classical trajectory x(t).

In order to obtain information we must have a quantitative connection between ψ(x,t) and the dynamical quantities describing the associated particle. It has been mentioned that these must be a relation between some measure of the intensity of ψ(x,t), in the region of the coordinate x at the time t, and the probabilities per unit length, or probability density P(x,t), of finding the associate particle in that region at that instant.

The probability density is a real quantity, whereas the wave function is complex, so ψ(x,t) cannot simple by set equal to P(x,t).

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