ENERGY

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Wave-Particle Duality

In the last lecture we noted that light behaves both as waves and particles. Indeed, the appearance of interference patterns in the double slit experiment, is a clear manifestation of its wave-like properties while the photoelectric effect, illustrates its particle-like behaviour. This was the emergence of what we called the wave-particle duality for light quanta. Bohr later showed that the spectrum of radiating Hydrogen atom could be explained if the electron orbiting the nucleus is assumed to have quantized angular momentum. This further implied that only certain orbits were allowed. In 1924, De Broglie, raised the question, could matter particles like electrons be wavelike, have a duality similar to that of light? In particular, could the electron in Bohr’s atom be confined waves and therefore produce a discrete stationary pattern? For example, it could well be that the lowest atomic orbit is one in which one electron wavelength fits the circumference of the orbit, while the higher orbits fit two or more wavelengths.
Matter Waves

Let us review some salient features of photons. The energy of a photon, according to Einstein is:

\[ E = h \nu \]
\[ = \frac{hc}{\lambda} \]

where \( \nu \) is the frequency, \( \lambda \) the wavelength and \( c \) the speed of light.

On the other hand, from relativistic physics, Einstein also found an expression that connects the energy of a particle to its momentum:

\[ E^2 = p^2 c^2 + m^2 c^4 \]  \( (1) \)

where \( p \) is the momentum and \( m \) the mass of the particle. For photons, which are massless \( (m = 0) \), we have,

\[ E = pc. \]

Equating with \( E = \frac{hc}{\lambda} \), we have

\[ p = \frac{h}{\lambda} \quad \implies \quad \lambda = \frac{h}{p} \]
Electron Waves Observed

De Broglie, with a great amount of insight, suggested that all particles, not only the massless photons, obeyed this relation. In other words, the wavelength of an electron or any particle with mass is inversely proportional to its momentum. It is interesting to note that the experimental discovery of electron waves was reported in 1927 by Davidson & Germer. By appealing to de Broglie’s relation, they showed that a low energy beam of electrons, when directed towards a nickel crystal produced diffraction patterns. This was similar to diffraction patterns that were known to be produced by x-rays when reflected off crystals.
Bohr’s Quantization Condition Explained

De Broglie waves was able to provide a justification for Bohr’s quantization postulate:

\[ L = mvr = n\hbar. \]

Indeed, if one assumes that a Bohr orbit can only accommodate integral number of de Broglie’s waves:

\[ 2\pi r = n\lambda \quad n = 1, 2, 3, \ldots \]

then with

\[ \lambda = \frac{h}{p} = \frac{h}{mv} \]

one obtains

\[ 2\pi r = n\frac{h}{mv} \quad \implies \quad mvr = h\frac{h}{2\pi} = n\hbar. \]
Wave Equation

If matter is a wave, there should be a wave equation to describe matter waves. The wave equation for electromagnetic waves (light waves) was already known then and it took the form of

\[
\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0
\]

for an \( x \) propagating wave.

Before proceeding further, it is instructive to understand that the above equation describes any disturbance that is propagating at a constant velocity. Recall from a previous lecture, that if we want to propagate a profile \( y = f(x) \) with a constant velocity \( v \), then we replace \( x \) by \( x - vt \); i.e.

\[
y = f(x - vt).
\]

If we let \( z = x - vt \) then we have

\[
\frac{\partial y}{\partial x} = \frac{\partial f}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial f}{\partial z}
\]

(2)

since \( \frac{\partial z}{\partial x} = 1 \). Similarly, we have

\[
\frac{\partial y}{\partial t} = \frac{\partial f}{\partial z} \frac{\partial z}{\partial t} = -v \frac{\partial f}{\partial z}
\]

(3)
Wave Equation - cont’d

since $\frac{\partial z}{\partial t} = -v$. Combining equations (2) and (3) we obtain

$$\frac{\partial y}{\partial t} + v \frac{\partial y}{\partial x} = 0. \quad (4)$$

If we further differentiate this equation we respect to $t$, we have

$$\frac{\partial^2 y}{\partial t^2} + v \frac{\partial}{\partial t} \left( \frac{\partial y}{\partial x} \right) = 0.$$

The order of the partial derivatives in the second term can be interchanged, i.e.

$$\frac{\partial}{\partial t} \left( \frac{\partial y}{\partial x} \right) = \frac{\partial}{\partial x} \left( \frac{\partial y}{\partial t} \right)$$

so that equation (4) reads as

$$\frac{\partial^2 y}{\partial t^2} + v \frac{\partial}{\partial x} \left( \frac{\partial y}{\partial t} \right) = 0. \quad (5)$$

Substituting (4) into (5) we arrive at

$$\frac{\partial^2 y}{\partial t^2} - v^2 \frac{\partial^2 y}{\partial x^2} = 0 \quad (6)$$

called the classical wave equation.
Solutions to Wave Equation

It is clear from the derivation of the wave equation that any function of the form

\[ y = f(x - vt) \]

will be a solution to the wave equation. Now, let us see whether the usual waveform

\[ y = A \cos(k(x - vt)) = A \cos(kx - \omega t) \]

appropriately describes a free particle. If we use the relations

\[ k = \frac{p}{\hbar} \quad \text{and} \quad \omega = \frac{E}{\hbar} \]

we have a solution in terms of the momentum and energy of the particle:

\[ y = A \cos \left( \frac{px}{\hbar} - \frac{Et}{\hbar} \right) . \]  \hspace{1cm} (7)

On substituting into the wave equation (6), we obtain

\[ E = pv. \]

Now, this according to Einstein’s relativistic equation

\[ E^2 = p^2 c^2 + m^2 c^4 , \]
implies that
\[ p^2 (v^2 - c^2) = m^2 c^4 \]
Since \( v \) can never exceed \( c \) (velocity of light) the only plausible solution is that \( v = c \); otherwise mass \( m \) will be negative. Hence the wave equation above, only describes massless particles!. So the wave equation (6) is not what we are looking for. The solution to this problem was obtained by Schrodinger in in 1926. However, before, we proceed further we note that the energy-momentum relationship for a non-relativistic particle is

\[ E = \frac{p^2}{2m} \]

where the term on the right hand side is nothing but the expression for the kinetic energy of a particle with mass \( m \). We are assuming that the particle is free, in the sense that it is under no external forces. The potential energy term, in this case, is zero. Now, if we replace \( E \) by \( \hbar \omega \) and \( p \) by \( \hbar k \) we obtain

\[ \omega = \frac{\hbar}{2m} k^2. \]  
(8)
A Modified Wave Equation

This expression suggest that the wave-equation should be linear in the $t$-derivative term: $\frac{\partial y}{\partial t}$ but second order for the $x$-derivative: $\frac{\partial^2 y}{\partial x^2}$. We can thus try

$$\frac{\partial y}{\partial t} \propto \frac{\partial^2 y}{\partial x^2} \quad \text{or} \quad \frac{\partial y}{\partial t} = \alpha \frac{\partial^2 y}{\partial x^2}$$

where $\alpha$ is some constant of proportionality. If we try a solution of the form (7) then the left hand side gives

$$\frac{\partial y}{\partial t} = A\omega \sin(kx - \omega t)$$

while the right hand side yields

$$\alpha \frac{\partial^2 y}{\partial x^2} = -\alpha Ak^2 \cos(kx - \omega t).$$

We cannot match them as the left hand has a sine term while the right hand side has a cosine term. To rectify this, we note that a term of the type

$$y = Ae^{kx-\omega t}$$

will not have this problem but one loses the oscillatory nature of the wave function. This
prompts us to consider a function that is complex such as

\[ y = Ae^{i(kx-\omega t)} \]

where \( i \) has the property \( i^2 = -1 \). If we substitute this into \( () \), we obtain

\[ i\omega = \alpha k^2. \]

If we want equation \( (8) \) to be satisfied then we must choose \( \alpha \) to be

\[ \alpha = \frac{i\hbar}{2m}. \]

Hence the appropriate wave equation reads as

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \]

where we have replaced \( y \) with \( \psi \) and multiplied both sides by a factor of \( i\hbar \). Schrodinger proposed that a more general equation which involved external interaction could take the form of

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \]

where \( V(x) \) denotes a potential term. The above equation has been written with one spatial coordinate. This can be generalized to one which
includes all three spatial coordinates:

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V(x, y, z)\psi \]

This equation is called the Schrodinger Equation.

To summarize briefly, the classical wave-equation has been modified by replacing the second-order derivative with a first order one. This was motivated by a need to have \( \omega \) to be proportional to \( k^2 \). In doing this, we are forced to consider solutions that are complex. This seems to suggest that solutions of the Schrodinger equation are not real physical waves. This gives rise to the problem of interpretation: What does the wave function mean physically? The interpretation was furnished by Max Born.
Interpretation of the Wave function

The first interpretative problem taken up by Schrodinger and then Born was the physical meaning of the wave function \( \psi \). The concept that finally evolved was quite unexpected. Born concluded that that the Schrodinger equation gives probability waves. More precisely, he proposed that wavefunction provided the probability of finding an electron at a point \( x \) at time \( t \) through the prescription:

\[
P(x, t) = |\psi(x, t)|^2 \equiv \psi(x, t)^* \psi(x, t)
\]

where \( \psi(x, t)^* \) denotes the complex conjugate of \( \psi(x, t) \).\(^1\) Thus the wavefunction is a probability amplitude; its square gives the probability distribution. Moreover, since the particle must be somewhere, the probability integrated over all \( x \) (here we are considering only one spatial dimension) must be one:

\[
\int_{-\infty}^{\infty} P(x, t) dx = \int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1.
\]

\(^1\)The complex conjugate of a complex number \( z = x + iy \) is \( x - iy \).
This is referred to as the normalization condition.