1. The de Broglie Relations

1924   de Broglie proposed that a moving particle should exhibit wave-like
properties with a wavelength given by *

$$\lambda = \frac{h}{p} \qquad (h = \text{Planck's Constant}) \qquad (1)$$

1927   Davisson and Germer verified this by bombarding nickel crystal with
electrons. Regular lattice gives electron diffraction pattern.

1928   G.P.Thomson passed a beam of electrons through a metal foil. Random
arrangement of crystal surfaces in foil gives symmetric diffraction rings.

It is not possible rigorously to prove the Broglie relations from simpler
postulates. Some books may give the appearance of doing so, but there will always
be a carefully concealed assumption somewhere in their treatment. The best approach
is probably to regard the wavelength-momentum relation and the energy-frequency
relation

$$E = h\nu \qquad (2)$$

as experimental observations. Some plausibility can be given to the relations
however by the following lines of argument :
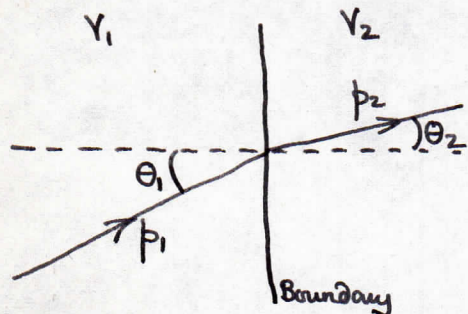
Consider a particle, initially with momentum
p_1, travelling in a region in which its
potential is V_1 at an angle θ_1 with the normal
to a plane boundary. On the other side of the
boundary the potential is V_2. If V_2 is less
than V_1, the particle is accelerated going
across the boundary, and comes off with a momentum p_2 at an angle θ_2. The total
energy of the particle must be unchanged by this process, and we can put :

$$E = T_1 + V_1 = T_2 + V_2 \qquad (3)$$

Also, as no force acts on the particle in the plane of the boundary, there is no
change of momentum in this plane, and we can write

$$p_1 . \sin\theta_1 = p_2 . \sin\theta_2 \qquad (4)$$

Now consider the refraction of a wave at the plane boundary between two regions
with refractive indices n_1 and n_2. We can say immediately that

$$\nu_1 = \nu_2 \quad (\text{i.e. the wave frequency is unaltered}) \qquad (5)$$

$$n_1/n_2 = \sin\theta_1/\sin\theta_2 \quad (\text{Snell's Law}) \qquad (6)$$

But $n_1/n_2 = \lambda_1/\lambda_2 = k_2/k_1$, where $k = 2\pi/\lambda$

Therefore (6) can be written in the form $k_1 . \sin\theta_1 = k_2 . \sin\theta_2$ $\qquad (7)$

By comparison of (4) and (7), it seems reasonable that if we are to associate
wave-like properties with particles, we should expect to link together the
quantities p and k between the particle and the wave, using a law $p = \beta k$, where β
is some constant. Note that this does not mean that we should expect β to be a
given number for all particles, so that β might be different for an electron, a
proton, a neutron, etc.

We cannot say anything quite so specific by considering (3) and (5) together. The
most we can expect to say is that E must be associated with some function of ν, the

form of the function being so far quite arbitrary. (Obviously, if $E = F(\nu)$, then E is constant if ν is constant, whatever the form of the function F) To decide what the function must be, we have to consider an experiment in which E (or ν) is allowed to change.
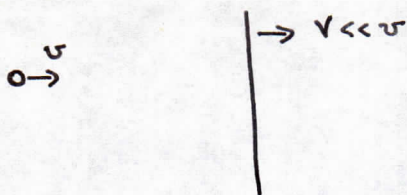
Consider a particle with initial velocity **v**, being reflected normally from a moving plate. The collision is perfectly elastic, and the velocity V of the plate is very much less than v. The particle rebounds with a velocity

$$v' = v - 2V$$

If the mass of the particle is m, then the change in its energy during the reflexion is

$$\Delta E = \Delta T = \Delta(\tfrac{1}{2}mv^2) = mv.\Delta v = mv.2V = 2pV \tag{8}$$

Writing $p = \beta k$ in accordance with the previous argument, $\Delta E = \beta.2kV \tag{9}$

Now consider a wave, with phase velocity c, incident on a mirror moving with velocity V. If the wave arrives normally, the reflected wave suffers a Doppler shift given by

$$\frac{\Delta\nu}{\nu} = \frac{2V}{c} \qquad \text{(you should be able to prove this)} \tag{10}$$

$$\text{Therefore } \Delta\nu = 2V.(1/\lambda) = 2V.(k/2\pi) = 2kV/2\pi \tag{11}$$

Substituting for 2kV in (9) from (11), we get

$$\Delta E = \beta.2\pi.\Delta\nu \text{ , or } \Delta E = \beta.\Delta\omega \tag{12}$$

Now (12) is the differential form of a law $E = \beta\omega + $ constant. This is the other de Broglie relation (when applied to material particles), and the constant arises because we do not define energies with respect to absolute zeroes. Thus, if we were trying to associate waves with particles in some way, it would be a sensible start to postulate the connexions

$$p = \beta k \text{ and } E = \beta\omega$$

Now in fact the constant $\beta = h/2\pi = \hbar$ was found to work for photons, and it turns out that de Broglie was right in anticipating that it should work for material particles also.

The above arguments do not of course PROVE the de Broglie relations, but they show that the relations are not really very surprising. If the Davisson and Germer experiment had failed to detect any wave properties, the above discussion would be dismissed as idle monkeying with symbols, no doubt!

2. Waves and Wave Equations

The equation $\psi = \psi_0.e^{i\omega t}$ may be thought of as representing a vector of length ψ_0 rotating in the complex plane.

The projection of the motion onto the real axis is an S.H.M. with period $T = 2\pi/\omega$. The complex exponential notation therefore provides us with a convenient shorthand for writing down S.H.M's if we understand that only the real part $R(\psi)$ is to be assigned meaning.

The expression $\psi = \psi_0.e^{i(kx + \omega t)}$ represents a travelling wave in one dimension, because $R(\psi)$ gives an S.H.M. whose phase depends on x with spatial periodicity $\lambda = 2\pi/k$ and temporal periodicity $T = 2\pi/\omega$. The equation governing the propagation of such a wave can be derived from this expression in the following way.

$$\frac{\partial\psi}{\partial x} = ik\psi \qquad \frac{\partial\psi}{\partial t} = i\omega\psi \tag{13}$$

Therefore the OPERATION of partially differentiating ψ w.r.t. x has the same result as the operation of multiplying by ik. Thus, as far as ψ is concerned, we can write the OPERATOR identity

$$\frac{\partial}{\partial x} = ik \ , \qquad k = \frac{1}{i} \cdot \frac{\partial}{\partial x} \tag{14}$$

Similarly, $\quad \dfrac{\partial}{\partial t} = i\omega \ , \qquad \omega = \dfrac{1}{i} \cdot \dfrac{\partial}{\partial t}$ (15)

(Those doing Whole Maths should recognise that ψ is an eigenfunction of the operator $\partial/\partial x$, with corresponding eigenvalue ik)

To get the equation of propagation of a wave from (14) and (15) all we have to do is to relate k to ω by the dispersion relation

$$k = \frac{\omega}{c} \tag{16}$$

This, taken with (14) and (15) gives the identity $\quad \dfrac{1}{i} \cdot \dfrac{\partial}{\partial x} = \dfrac{1}{c} \cdot \dfrac{1}{i} \cdot \dfrac{\partial}{\partial t}$, or the equation

$$\frac{\partial \psi}{\partial x} = \frac{1}{c} \cdot \frac{\partial \psi}{\partial t} \tag{17}$$

This is of course not the equation we usually call "the" wave equation. It represents the propagation of a wave all right, but only in the direction of negative x. This can be seen immediately from the dispersion relation (16), for as ω is necessarily positive, so must k be, and this implies that only one direction of propagation has been admitted. To include both directions of propagation we must use the relation

$$k^2 = \omega^2/c^2 \tag{18}$$

for then positive ω can imply positive or negative k. The equation obtained by using (14) and (15) in conjunction with this dispersion relation is then

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2} \cdot \frac{\partial^2 \psi}{\partial t^2} \tag{19}$$

This is "the" wave equation. It is the one most commonly met with in physics because we normally wish to consider both directions of propagation for our waves. The point to be made here is that there are many different "wave equations", and that (19) is merely a special case which happens to get most of our attention.

3. De Broglie Waves and Schrodinger's Equation

Now consider the equation which governs the propagation of de Broglie waves (or "matter waves"). This will be a very useful equation to have because it will enable us to work out how the de Broglie waves will spread themselves in a given situation, and therefore eventually to decide how particles will behave in experiments like the Davisson and Germer experiment. The equation will be derived in exactly the same way as (17) and (19) were derived above.

We write a de Broglie wave in the form $\quad \psi = \psi_0 \cdot \exp(ikx + i\omega t)$, then (14) and (15) are true. Using the de Broglie relations (1) and (2) in the form

$$p = \hbar k \quad \text{and} \quad E = \hbar \omega$$

we get $\qquad p = \dfrac{\hbar}{i} \cdot \dfrac{\partial}{\partial x} \quad \text{and} \quad E = \dfrac{\hbar}{i} \cdot \dfrac{\partial}{\partial t}$ (20)

What is to be the dispersion relation corresponding to (16) or (18) for the de Broglie waves ? We want a relation between k and ω, or equally well in this case between p and E. In the non-relativistic case (and the relativistic case is much too difficult to be considered for the present), we can put

$$E = T + V$$
$$= \frac{p^2}{2m} + V(x) \tag{21}$$

Here V(x) is the one-dimensional potential in which the particle moves with momentum p(x), the total energy E being constant. Using (21) as a dispersion relation, and the equations (20) as the operator identities, we reach the equation :

$$\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} - V(x)\psi = - i\hbar \cdot \frac{\partial \psi}{\partial t} \tag{22}$$

Note that $V(x)$ may be $V(x,t)$ also.

If we write $\psi(x,t) = \phi(x) \cdot \exp(-iEt/\hbar)$, in accordance with the expression for $\partial/\partial t$ in (20), then we can write the simpler time-independent equation

$$\frac{\hbar^2}{2m} \cdot \frac{d^2\phi}{dx^2} + (E - V(x))\phi = 0 \tag{23}$$

for the spatial part $\phi(x)$ alone. Equations (22) and (23) are known as the time-dependent and time-independent Schrodinger Equations. It is important to realise that they contain no more physics than the de Broglie relations and the dispersion law (21) from which they were derived. They express these facts in a more useful form, however, and enable the behaviour of particles to be predicted in a systematic way once an interpretation has been given for the functions $\psi(x,t)$ and $\phi(x)$.

4. The Interpretation of the Wave Function $\psi(x,t)$.

So far we have dealt entirely in experimental observations and mathematical deductions, but as soon as we try to explain what the quantity ψ really represents, we meet one of the deepest divisions of opinion in modern physics. There is no single interpretation which is clearly more acceptable than any of the others in all respects. If we regard the wave-function as being the "real" quantity in modern physics, we are sometimes led into awkward deductions, and equally well if we regard it merely as a "list of betting odds" on the outcome of a given experiment we must explain how apparently independent particles manage to co-operate with one another to show statistical behaviour.

Schrodinger attempted to represent the particles of modern physics as the maxima of wave functions. Obviously this cannot be done with a single monochromatic wave-function (definite p or λ), for this has an infinite number of maxima, and we cannot point to any particular one of these and say "there is the particle". We need to use a wave group, a combination of a number of monochromatic waves with different wavelengths (momenta), in order to produce a well-defined maximum in the ψ-function at one point. This point will be returned to later, as a mathematical analysis of this idea provides a method of demonstrating the Heisenberg Uncertainty Principle. For the moment we let it merely be remarked that a wave group constructed to represent a localised particle at one instant, if allowed to disperse according to the Schrodinger Equation, does not hold together, so that the localisation of the particle becomes more uncertain as time goes on. Thus, if we began by "synthesising" a number of particles in a system by constructing peaks in ψ-functions at a certain time, after a sufficiently large interval these peaks would become so smoothed out that the particles would be becoming indistinct and smeared out in space. This is clearly ridiculous, and so we are led straight away to the belief that ~~they~~ the wave-group peaks cannot actually <u>be</u> particles. It was pointed out by Born that we do not reach any such absurd conclusions if we regard the ψ-peaks as peaks in the <u>probability</u> of finding particles in the given positions. Then the smearing out of the wave groups predicted by Schrodinger's Equation only indicates the increasing statistical uncertainty in the probable positions of the particles as time goes on, arising from the fact that we could not be sure exactly where they were at the outset (because we only dealt with wave peaks, not infinitely sharp spikes in the ψ-function). Born proposed that the ψ-function should be regarded as generating the probability that a particle is in a given region at a given time, or as representing a particle density in systems where there were large numbers of similar particles.

It is immediately clear that ψ itself cannot be this probability or density however, for ψ is in general a complex number for given x and t. We cannot speak of $6 + 5i$ particles per cc.! Our statistical measure must be real, and so the simplest possible function which can be identified with it is $\psi*\psi$, where the $*$ denotes the complex conjugate.

Note that $\psi*\psi = \phi*(x) \cdot \exp(+iEt/\hbar) \cdot \phi(x) \cdot \exp(-iEt/\hbar) = \phi*\phi$

In general we must be prepared to accept a function of the form

$$a(\psi*\psi) + b(\psi*\psi)^2 + c(\psi*\psi)^3 + \ldots \text{ etc.}$$