

## “Wave-particle duality”: the basic experimental facts.

Let’s start with a potted history of the events which, historically, led to the development of quantum mechanics.

A problem which loomed large in the late nineteenth century was the thermal behavior of electromagnetic radiation in a box (the so-called “black-body” problem). According to (classical) electromagnetic theory, any wave is allowed in the box which fits the required conditions at the walls: roughly speaking, this condition is that the electric field is zero there, and so if  $\lambda$  is the wavelength of the wave we must have  $\lambda = 2L/n$  (i.e. an integral number of half-wavelengths in the box). Here  $n$  can be 1, 2 . . . in fact *any* integer, so there is an infinite number of allowed “modes” (waves) even in one dimension (and the infinity, as it were, gets worse in 3D). Now, according to (classical) thermodynamics, if the box is in thermal equilibrium at some temperature  $T$ , then each of these modes should possess an average energy  $k_B T$ , where  $k_B$  is Boltzmann’s constant (see lecture 24; the numerical value of  $k_B$  is about  $1.4 \times 10^{-23}$  Joules/degree). But this means that not only is the energy at any given temperature infinite, but that the specific heat (the energy necessary to *raise* the temperature by say 1 degree) is also infinite, in clear contradiction to the experimental facts. This paradox was known as the “ultraviolet catastrophe”.

In 1900 Max Planck put forward a revolutionary solution to this difficulty. He supposed energy is *quantized*, i.e. it comes in discrete “lumps” (Planck actually applied his argument to the energy of the “oscillators” which he assumed to exist in the walls of the cavity; it was Einstein, in 1905, who applied it directly to the electromagnetic radiation field itself). Specifically, he assumed that for a wave of frequency  $\nu$  ( $= c/\lambda$ ) the “quantum” of energy is given by the formula

$$E = h\nu$$

where  $h$  is a constant (now known as “Planck’s constant”) with dimensions of (energy  $\times$  time) and a numerical value of approximately  $6.6 \times 10^{-34}$  Joule seconds. Thus, we can associate with a wave of frequency  $\nu$  only the discrete energies zero,  $h\nu$ ,  $2h\nu$  . . . and so on. Notice that this postulate is completely alien to classical wave theory; in that theory the energy of the wave is simply proportional to  $A^2$ , the square of its “amplitude” (crest height) and for a wave of a given frequency the amplitude can take any value.

Why does Planck’s postulate help to solve the problem of the ultraviolet catastrophe? This requires us to know what statistical mechanics predicts when applied to this novel situation. Very crudely speaking\* the prescription is: Assign to each mode a number of quanta  $n$  such that the energy in the mode is as nearly as possible  $k_B T$ . That is,  $n$  is the integer which is closest to the ratio  $k_B T/h\nu$ . If  $h\nu \ll k_B T$ , this integer is large and the total energy  $nh\nu$  is very close to the classical value  $k_B T$ . However, if  $h\nu \gg k_B T$  the appropriate integer is zero and there is *no* energy in the mode! Although this argument is oversimplified, a more rigorous one shows that the qualitative conclusion is correct:

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\*In fact, as some of you will know, the average number of quanta in a mode is not integral and is given by the formula  $\langle n \rangle = [\exp h\nu/k_B T - 1]^{-1}$

the mean energy in a mode of frequency  $\nu$  is approximately  $k_B T$  if  $k_B T \gg h\nu$ , but much *smaller* than  $k_B T$  if  $k_B T \ll h\nu$ . An experimental study of the distribution of the energy in the different modes confirms this prediction; the mean energy indeed falls off sufficiently fast as  $\nu$  increases that the ultraviolet catastrophe is avoided.

An apparently unrelated problem that surfaced in the late nineteenth century was the discrete nature of atomic spectral lines. By passing the light from a given source through a prism we can deflect the different colors, i.e. different wavelengths, through different angles and thereby tell which wavelengths are represented. If we use a complex source such as a glowing piece of metal, then essentially all wavelengths will appear to one degree or another; if however, we use a gas of a single species of atom, say atomic sodium, then only certain special wavelengths (hence frequencies) appear - e.g. the well-known “yellow line” of sodium. The general pattern of these “special” lines seemed very complicated and puzzling, but in the case of hydrogen (which was already strongly suspected, on the basis of chemical evidence, to be the “simplest” atom, with one and only one unit of negative charge) then seemed to be a certain regularity: the frequency  $\nu$  of the line could always be represented in the form

$$\nu_{nm} = \text{const} \cdot \left( \frac{1}{m^2} - \frac{1}{n^2} \right) \quad (\text{“Ritz combination principle”})$$

where  $n$  and  $m$  were both integers. In the late nineteenth century, with no clear picture of what an atom was like available, this formula was a major mystery.

One piece of the puzzle was the discovery of the electron by Thomson in 1897; this confirmed what had been strongly suspected on chemical grounds, that negative charge comes in discrete units. But atoms are generally electrically neutral, and thus must have an equal amount of positive charge; because the size of a typical atom is  $\sim 1$  angstrom ( $10^{-10}$  m) it was the general belief that this positive charge was “smeared out” over a sphere of about this size. This belief was rudely shattered by the experiments of Rutherford around 1910, which demonstrated that the positive charge is also concentrated at a single point, in what we now call the atomic nucleus. Thus was born the so-called “planetary” model of the atom, in which the positively charged nucleus sits at the center immobile, like the Sun, while the negatively charged atomic electrons orbit it at various distances, like the planets.

The planetary model of the atom has a considerable intuitive appeal (as is shown by its persistence in the logos of various institutions which wish to stress their atomic associations!) and did in fact explain, at least qualitatively, quite a lot about the structure of matter. However, it had to face two major problems: it had no explanation for the discrete nature of spectral lines (let alone the Ritz formula for hydrogen), and, worse, because an accelerating electric charge is known to radiate and lose energy, it predicted that the atomic electrons would spiral down into the nucleus<sup>†</sup> within a time of  $\sim 10^{-9}$  secs!

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<sup>†</sup>The reason no such problem arises with the planets of the solar system is that they are electrically neutral and, while “gravitational” radiation is indeed believed to occur, its strength is about 40 orders of magnitude weaker than its electromagnetic counterpart.

A revolutionary breakthrough was made by Niels Bohr in 1913, when he postulated that the principle of “quantization” applies not only to the energy of the electromagnetic field as Einstein, following Planck, had proposed, *but also to the motion of the atomic electrons in their orbits*. In particular he postulated

- (a) that for any given type of atom, there exists a lowest or fundamental state, or set of orbits, of the atomic electrons (in German, “Grundzustand”, hence usually rendered “groundstate” in English); when in their groundstate, the electrons are forbidden to radiate further;
- (b) when the electrons of the atom make a transition from one quantized state to another, the energy of the quantum of light emitted is simply the difference in the energies of the two atomic states, i.e. for two states  $n, m$  we have

$$h\nu_{nm} = E_n - E_m$$

Combining this postulate with the Ritz combination principle for hydrogen, we immediately conclude that for the latter the allowed energies of the atomic states (“energy levels”) are given by the simple formula

$$E_n = -\text{const} \cdot \frac{h}{n^2}$$

Why should Nature impose this restriction on the energy levels? Bohr showed that it would follow from the assumption that *angular momentum* is quantized, in units of  $h/2\pi$  (this quantity is usually written  $\hbar$  and sometimes called Dirac’s constant). The argument, at least under the rather natural assumption of circular electron orbits, is sufficiently simple to be given here:

In a circular orbit of radius  $r$ , the centripetal acceleration is  $v^2/r$ , and since the force of attraction between the hydrogen nucleus (a single proton of charge  $+e$ ) and the single electron (charge  $-e$ ) is  $e^2/r^2$ , we have by Newton’s second law the relation

$$e^2/r^2 = mv^2/r$$

(and hence the kinetic energy  $\frac{1}{2}mv^2$ , is one half of minus the potential energy,  $e^2/r$ , and the total energy is thus  $-e^2/2r$ ). Suppose now we in addition impose the condition that the angular momentum is some integer  $n$  times  $\hbar$ , i.e.

$$mvr = n\hbar$$

We can then solve these two equations to obtain  $v$  and  $r$ . In particular we find that the radius of the orbit is also “quantized”:

$$r = na_0, \quad a_0 \equiv \hbar^2/me^2 \approx 0.5 \times 10^{-10} \text{ m}$$

But we already saw that the total energy of the electron in orbit was  $-e^2/2r$ , and hence the allowed values,  $E_n$  of the energy are given by

$$E_n = -\frac{e^2}{2n^2a_0} = -\frac{me^4}{2\hbar^2} \cdot \frac{1}{n^2} \quad n = 1, 2, \dots$$

What is amazing is that not only does this predict the  $1/n^2$  structure of the energy levels, but the constant comes out exactly right!

The success of Bohr’s ideas as applied to the hydrogen atom was so spectacular that it rapidly led to the development of a whole new theory (now usually known as the “old quantum theory”) which was essentially the usual mechanics and electromagnetic theory constrained by the quantization rules of Planck and Bohr, and other similar ones inferred later. This theory had some successes (though we now believe partly for the wrong reasons!), but the origin of the quantization rules remained a complete mystery. In particular, why should angular momentum always be quantized in units of  $n$ ? Meanwhile, more evidence was building up of the “particle-like” behavior of light—the photoelectric effect had shown that it exchanged energy with the electrons of a metal in “chunks” of  $h\nu$ , and the Compton effect (1923) showed that collisions of light with free electrons could be treated just as if the light was a particle (“photon”) with an energy  $E = h\nu$  and also a momentum<sup>‡</sup>  $p$  given by  $p = h/\lambda$  (where  $\lambda$  is the wavelength of the light). Thus, light appeared in more and more contexts to be behaving just like a mechanical particle!

The circle was closed in the early 20’s by a series of experiments by Davisson and Germer which showed that equally, under certain circumstances, electrons behaved like a wave! The phenomenon of *diffraction* of light by a regularly spaced array of slits, etc., had been well known since the early nineteenth century. For diffraction to occur at an observable level, the spacing and size of the diffracting slits must be comparable to the wavelength of the wave in question (hence, at the everyday level diffraction-type effects can occur with sound, but not with (visible) light). When X-rays were discovered at the end of the nineteenth century, the fact that they can be diffracted by a crystal lattice had been taken as irrefutable evidence that they were not “particles” but waves, in fact part of the electromagnetic spectrum. It was therefore a major shock when Davisson and Germer demonstrated that electrons—which quite clearly behave as *particles* in, for example, a cathode-ray tube, leaving discrete flashes on a screen - nevertheless can be diffracted by a crystal lattice in almost exactly the same way as X-rays!

The final, unifying step was taken by de Broglie in his thesis in 1924. He proposed, quite simply, that with every particle in nature there is associated a wave, and vice versa; just as light, usually thought of as a wave, behaves in some situations as “chunks” (particles), so an electron, traditionally thought of as a particle, can behave under certain circumstances as a wave. The quantitative correspondence (deduced by de Broglie from the original Planck formula  $E = h\nu$  by using considerations of relativistic invariance) is

$$\lambda = h/p$$

where  $\lambda$  is the wavelength of the “wave” and  $p$  ( $\equiv mv$  in the nonrelativistic limit) is the momentum of the “particle”. Note that for any reasonably “macroscopic” object the mass  $m$  is very large and hence  $\lambda$  is usually very small indeed; but for objects such as an electron, as we shall see,  $\lambda$  can be exactly of the order of an atomic size.

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<sup>‡</sup>Since  $E = cp$  for photons (light).

How does this help with the Bohr model of the atom? Imagine, first, a wave on say a string of length  $L$ . If it is to have a definite frequency (hence, according to the relation  $E = h\nu$ , a definite energy) it must also have a definite wavelength  $\lambda$ , and since the displacement must vanish at the (pegged) ends of the string the allowed values of  $\lambda$  are  $L/2n$ . Such a wave will be “standing”, i.e. it will change its overall amplitude in time but not its shape. (If we try to do anything more complicated, it will in general change its shape in time and hence not be associated with a definite frequency.) Next, go over to a water wave in a narrow annular trough. The situation is much the same, except that since the wave must “join on” to itself smoothly we must have

$$\lambda = 2\pi r/n, \quad n = 1, 2, \dots$$

where  $r$  is the radius of the trough.

Consider now an electron orbiting a nucleus in a circular orbit with radius  $r$ . If it is to be “represented” by a wave, and moreover is to be in a state of definite energy (so that the wave must have a definite single frequency), then we must, as above, satisfy the condition  $n\lambda = 2\pi r$ . But, according to de Broglie, the momentum  $p$  of the electron is  $h/\lambda$  and quite generally the angular momentum is defined (nonrelativistically) as  $mvr \equiv pr$ . Thus we finally obtain<sup>§</sup>

$$\text{angular momentum} = nh/2\pi \quad (\equiv n\hbar)$$

exactly as postulated by the Bohr model!

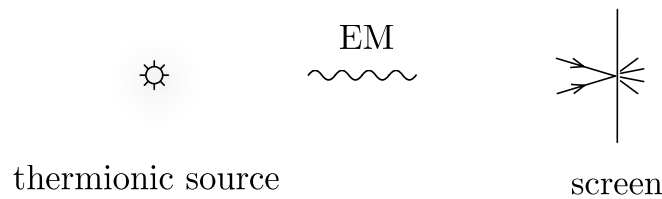
Once de Broglie’s idea (which is basically formulated for free motion) was in place, all that remained was to find the more general relation between the wave and particle aspects of matter. This was done within a few years by Schrodinger, Heisenberg, Dirac and others and is, of course, what is known as the “new quantum theory” or more briefly nowadays simply as quantum mechanics.

### The “2-slit” (“Young’s slits”) experiment.

From now on, I will proceed “logically” rather than historically, by discussing the conceptually simplest experiments rather than those which were actually done at an early stage in the development of QM. However, there is a grave danger here of going way beyond what we “know for a fact” (as in “quantum cosmology” etc.). So it is important to know that although the experiment to be discussed was widely discussed in textbooks before it was ever actually done, with extreme confidence that it would come out as QM says it should, in 2010 it *has actually been done* and indeed verified to work as advertised.

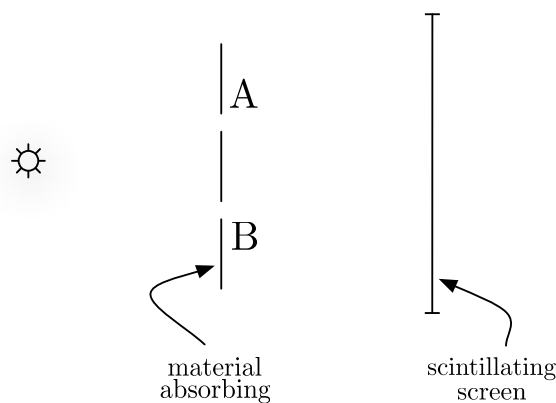
Let’s first consider the electron, the basic carrier of negative charge, and ask: How do we know that it is a “particle”? Essentially because we can detect the arrival of individual electrons, e.g. on a scintillating screen. It appears to be an experimental fact that in a

<sup>§</sup>Note also that the “inverse” of the de Broglie relation,  $p = h/\lambda$ , is when applied to *light* precisely what was required to explain the Compton effect.



setup like this, with adequate resolution at the screen, we see *individual flashes*, and if we count these and have a means of measuring the total charge emitted by the source, each flash indeed appears to correspond to a charge of exactly  $e$ . (Also (historically prior!) the Millikan oil-drop experiment). We *never* appear to see an amount of charge  $< e$ . Thus it appears that negative electric charge always moves in units of  $e$ , never smaller – and it most certainly is not spread out diffusely.

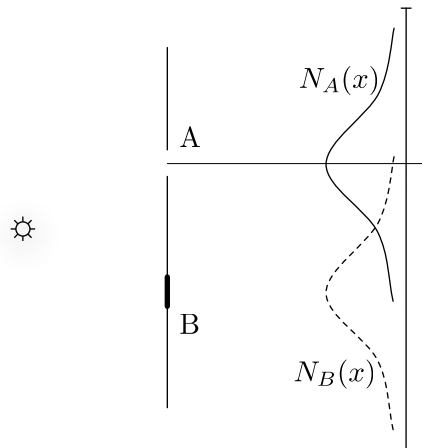
Now the crucial experiment:



We first do a series of crude experiments to show that it is possible to block one or both slits A and B, e.g. by sticking a bit of some absorbing material in them. Then we proceed as follows:

First, we block slit B and open slit A. What we see is a series of flashes on the further (scintillating) screen, just as in the “TV” experiment. At first these flashes appear random, but as time goes on and we build up a histogram, a pattern appears: typically, for the sort of apparatus shown, we would get a distribution of particles as a function of  $x$ ,  $N_A(x)$ ,<sup>¶</sup> of the unspectacular form of the solid line shown in the figure. Note: to get interesting effects at a later stage, the A-pattern should (preferably) overlap the point opposite slit B and vice versa. We now repeat the experiment blocking slit A but opening B. Again we get what at first seem random flashes, but a pattern is gradually built up: it is similar to the above, but shifted so that the maximum occurs roughly at the point opposite B. Call this pattern  $N_B(x)$  (shown by broken line in figure on the next page).

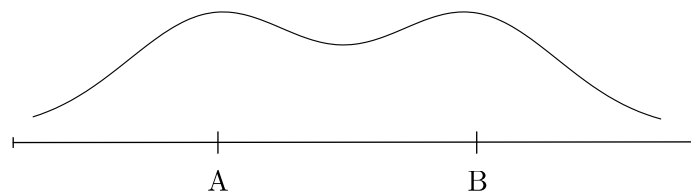
<sup>¶</sup>Technically, we want to keep the strength of the source fixed, and define  $N_A(x)$  as the number arriving per unit time and per unit area near  $x$ .



We now ask what will happen if we open both slits, A and B, simultaneously. In order to answer this question, we have to make some assumption about the physical effects of opening or shutting one slit on the propagation of electrons through the other. Since the slits are far apart, it seems reasonable to assume not such effect exists. (Note: We could envisage a theory where such an effect does exist and is just such as to reproduce the experimental results to be discussed below, but the result would be somewhat like the “ether” explanation of the Michelson-Marley experiment, with its physical length contractions, etc., indeed if anything it has to be even more contorted. So let us assume that the actual propagation of an electron through slit A is independent of whether slit B is open or shut, and vice versa.) Then, surely, we can argue:

- (1) The total number of electrons arriving at any point  $x$  in the final screen is the sum of the number arriving through slit A and the number arriving through slit B.
- (2) The number arriving at  $x$  through slit A is already measured to be  $N_A(x)$
- (3) The number arriving at  $x$  through slit B is already measured to be  $N_B(x)$

Conclusion: The number of electrons arriving at point  $x$  when both slits, A and B, are open (call it  $N_{A+B}(x)$ ) is simply given by

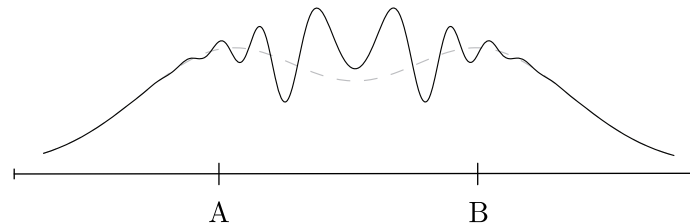


$$N_{A+B}(x) = N_A(x) + N_B(x)$$

Experimental observation:

THIS IS WRONG!

In fact, what we see (under appropriate experimental conditions) is something more like:



and in fact, with suitable arrangements, we can actually make  $N_{A+B}(x) = 0$  for some  $x$ , even though neither of  $N_A(x)$  and  $N_B(x)$  are individually zero! However, note that the *total* number arriving on the final screen is still simply the sum of the *total* numbers arriving through slits A and B separately. It is the numbers arriving *at a particular point* which do not “add up”!

These are the basic experimental facts, which by now no-one seriously doubts. (Actually the effect can be seen even more spectacularly in a neutron interferometer, where the “slits” can be  $\sim 10$  cm. apart). To clear up one red herring: is it possible that when both slits are open, the electrons coming through slit B somehow interact with those coming through slit A (e.g. repel them) in such a way as to produce the pattern seen? Answer: no, because we can turn down the strength of the source to the point where only one electron is in the apparatus at anyone time, and the pattern remains unchanged. (In the neutron interferometer version, the “next” neutron is still in the uranium nucleus in the reactor when detection takes place!)

The pattern of peaks and troughs seen experimentally is strongly reminiscent of what we get with ordinary visible light (or water waves). In fact, let us consider doing the corresponding experiment with a “high-school” (but monochromatized, etc.) light source. What would we see?

- When only slit A is open, we would see a pattern of *intensity* of light  $I_A(x)$  on the final screen which is similar to the distribution  $N_A(x)$ . But note that it is a *continuous* distribution: at this level of resolution we do *not* see anything which looks like discrete flashes.
- When only slit B is open, we similarly see an intensity distribution  $I_B(x)$  which is qualitatively similar to the pattern  $N_B(x)$ .
- When *both* slits A and B are open, we see an intensity pattern  $I_{A+B}(x)$  with peaks and troughs quite similar (qualitatively) to  $N_{A+B}(X)$

All this (i.e. the experiment with light) is quite easily understood in terms of a wave theory of light. Recall that the intensity is proportional to the total amplitude squared:



$I \propto A^2$  (averaged over time: note the period of visible light is  $\sim 10^{-16}$  seconds so we must in practice do this!). If only slit A is open, there is some amplitude  $A_A(x)$  at point  $x$ , and a corresponding intensity

$$I_A(x) = \overline{A_A^2(x, t)} \quad (\text{bar=average over time})$$

Similarly, if only slit B is open, then the amplitude at  $x$  is  $A_B(x)$  and the intensity correspondingly are

$$I_B(x) = \overline{A_B^2(x, t)}$$

Now suppose both slits are open. Then the amplitude at  $x$ ,  $A_{A+B}(x, t)$  is the algebraic sum of the amplitudes arriving through slits A and B:

$$A_{A+B}(x, t) = A_A(x, t) + A_B(x, t)$$

and the intensity is the square of this:

$$I_{A+B}(x) = \overline{[A_A(x, t) + A_B(x, t)]^2}$$

but this can be written

$$\begin{aligned} I_{A+B}(x) &= \overline{A_A^2(x, t)} + \overline{A_B^2(x, t)} + \overline{2A_A(x, t)A_B(x, t)} \\ &= I_A(x) + I_B(x) + \overline{2A_A(x, t)A_B(x, t)} \end{aligned}$$

Thus, the resultant intensity at  $x$  is the sum of  $I_A(x)$  and  $I_B(x)$  only if the last quantity vanishes. But in general this doesn't happen. In particular, consider a point (such do exist, at least approximately!) such that (a)  $I_A(x) = I_B(x)$ , and (b) the path lengths are such that waves arrive through the two slits exactly “out of phase”, i.e. a trough from A coincides with a peak from B and vice versa. Technically, this means  $A_B(x, t) = -A_A(x, t)$  (remember the amplitude can have either sign!).

Then we have:

- $I_A(x) + I_B(x) = 2I_A(x)$  (postulate (a))
- $\overline{2A_A(x, t)A_B(x, t)} = -\overline{2A_A^2(x, t)} = -2I_A(x)$  (postulate (b))
- and hence  $I_{A+B}(x) = 0$  – “total destructive interference”.

So in the case of water (and of high-school-level experiments with light), *prima facie* the experimental diffraction pattern is easy to explain – we are simply dealing with a wave. There is no question (yet!) of it having any kind of “particle” aspects (or at least, we have no evidence in this particular experiment).

How does quantum mechanics reconcile the “particle” aspects of the electron (as seen in the discrete flashes) with the “wave” aspect apparently revealed by the observed interference-like effects?

It first considers, not a *single* electron, but the “ensemble” (collection) of electrons emitted by the source under specific conditions. With this ensemble it then associates

a *wave function* or *probability amplitude*<sup>||</sup> which is a function of position and time<sup>\*\*</sup> conventionally denoted

$$\psi(x, t)$$

This wave function obeys a *linear* wave equation (Schrodinger’s equation) as a result of which, if  $\psi_1(x, t)$  is a solution and  $\psi_2(x, t)$  is also, then any combination of the form  $a\psi_1(x, t) + b\psi_2(x, t)$  is also a solution (cf. lecture 8). This principle is called the “principle of superposition” and is an absolutely fundamental and “nonnegotiable” aspect of the theory. The crucial point now is the interpretation of  $\psi(x, t)$ : the assumption is

$\psi^2(x, t)$  is is probability of finding an electron described by the wave function  $\psi(x, t)$  at point  $x$  at time  $t$ .

In particular, the probability of an electron arriving at point  $x$  on the final screen in the experiment discussed is proportional to  $\psi^2(x, t)$ , and hence so is the number of electrons, arriving (on average) per unit time:

$$N \propto \overline{\psi^2(x, t)}$$

How does this explain the observed interference effects? In exact analogy to the case of light (and leaving out the constant of proportionality, which is the same for all cases) we have:

- only slit A open:  $N_A(x) = \overline{\psi_A^2(x, t)}$  when  $\psi_A(x, t)$  is the “wave” propagated through slit A.
- only slit B open:  $N_B(x) = \overline{\psi_B^2(x, t)}$
- slits A and B both open  $\psi_{A+B}(x, t) = \psi_A(x, t) + \psi_B(x, t)$ , so

$$\begin{aligned} N_{A+B}(x) &= \overline{\psi_{A+B}^2(x, t)} = \overline{\psi_A^2(x, t) + \psi_B^2(x, t) + 2\psi_A(x, t)\psi_B(x, t)} \\ &= N_A(x) + N_B(x) + \overline{2\psi_A(x, t)\psi_B(x, t)} \end{aligned}$$

so that in general, just as in the case of light,  $N_{A+B}(x) \neq N_A(x) + N_B(x)$ . In particular, if it happens that we choose a point  $x$  such that  $N_B(x) = N_A(x)$  and  $\psi_B(x, t) = -\psi_A(x, t)$ , then  $N_{A+B}(x) = 0$ , i.e. no electrons whatever arrive there when both slits are open, even though when either alone was open a finite number were detected!

A crucial aspect here is the fundamental (?) interpretation of the wavefunction (or “state vector”, cf. lecture 18) in terms of *probability*. Thus, *prima facie* quantum mechanics is a fundamentally *indeterministic* theory – a violent break from classical physics. Actually, as we shall see, things are considerably worse than that!

<sup>||</sup>More precisely, a set of probability amplitudes: cf. lecture 18.

<sup>\*\*</sup>Actually,  $\psi(x, t)$  is a complex function in the mathematical sense. This means that in many cases of interest the quantity analogous to  $\psi^2(x, t)$  is actually independent of time and we can dispense with the time-averaging procedure.