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PHIL2011: Philosophy and Modern Physics.
Physics Lecture notes.
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Contents

1	Quantum theory.	5
1.1	The quantum principles.	5
1.2	From classical to quantum probability.	8
1.3	Quantum mechanics for free particles.	19
1.4	Quantum mechanics for oscillators.	24

Chapter 1

Quantum theory.

1.1 The quantum principles.

No useful description of the physical world can be given that does not account for chance and randomness. The quantum theory indicates that the universe is irreducibly random. If we are to exploit the quantum world to build a winning technology we need to understand the odds that nature is dealing us. Randomness is not a unique feature of the quantum world. All around us we see examples of apparently unpredictable and random behaviour. To appreciate what is special about the kind of randomness present at the quantum level we need to consider for a moment ordinary, everyday randomness.

No experiment is completely reproducible. In each trial, the results fluctuate a little. There is an 'experimental error', a small unpredictable variation in the results of the experiment caused by our inability to fully control the situation. Today when we introduce our students to the scientific method we devote a great deal of time to teaching them to correctly account for errors in their results. No one should accept an empirical result unless it is accompanied by some 'margin of error'.

Despite the unavoidable noise and error in any real measurement there is an instinctual belief that, were enough known about a physical system, the result of any measurement could be predicted with certainty. The triumph of physical science from the sixteenth century to the start of the twentieth century has certainly enforced a faith in the inherent predictability of the world. The primary source of this faith rests on the revelations of Newton's mechanics. Newton showed that precise mathematical relationships could be discovered behind the perplexing multiplicity of everyday phenomenon, from the fall of an apple to celestial motions. The scientific legacy of Newton is Newtonian mechanics, a clockwork

universe in which all matter followed a predetermined course, slowly unfolding a primordial configuration.

At the close of the nineteenth century, however, some disturbing hints began to emerge that this faith might be misplaced. The great French mathematician Henri Poincaré was the first to glimpse the jungle beyond the apparent simplicity of Newtonian mechanics. Poincaré was studying the motion of three objects undergoing mutual gravitational attractions, using powerful new geometrical tools which he had developed. He soon realised that the paths of motion must be exceedingly complex and twisted, with an infinite number of folding and stretching.

We now know that what Poincaré saw was but the tip of an iceberg. In all but the simplest and most exceptional systems, predictability is severely limited by the presence of chaos. If a system is chaotic, small errors in the initial conditions are amplified very rapidly, leading to apparently random behaviour, unrelated in any simple way to what we imagined were the starting points of the motion. But that is another story.

At about the time Poincaré was puzzling over the unimaginably complex motion of three gravitating objects, the first harbingers of a far more radical crisis for Newtonian mechanics had begun to appear. Hot objects emit energy as electromagnetic radiation. How hot they are determines the colour, or frequency, of the emitted radiation. The objective was to determine how changing the temperature changed the energy given off, and as a corollary, the frequencies emitted. The problem was the usual one; theory and experiment did not agree. This was known as 'the black-body problem'.

The two great triumphs of 19th century physics, electromagnetism and thermodynamics, were continuum theories; theories that regarded nature as continuous and not particulate. So strong was this belief, that doubts were even raised about the validity of atoms as the ultimate building blocks of the world. If pressed, I suspect a physicist of the time might have acknowledged that, at the bottom, all was atoms moving according to Newton's laws. However such a description might have been regarded as an unnecessary extravagance. Planck adopted a more cautious attitude to the atomic hypothesis. In 1895 he wrote[?];

I do not intend, at this point, to enter the arena [on behalf of] the mechanistic view of nature; for that purpose, one has to carry out far reaching and, to some extent, very difficult investigations.

It was left to Ludwig Boltzmann to attempt just these very difficult investigations by taking a radical step; Boltzmann supplemented mechanics with statistics, and in so doing laid the grounds for Planck's bold solution to the black body

problem and the beginning of the end for Newtonian physics. Boltzmann's attempt to found thermodynamics on mechanics, supplemented with statistics and probability, generated enormous opposition. That Boltzmann had recourse to the atomic hypothesis was bad enough, but to introduce statistical reasoning into mechanics, the most exact of sciences, was an anathema to many of his contemporaries. In the ensuing controversy Planck took the side of Boltzmann, if somewhat ambivalently.

On Sunday 7th October, the experimentalist Heinrich Rubens visited Planck at his home and told him of the latest results on black body radiation. Planck immediately sat down to incorporate these results into his thinking about the problem, with the result that he was able to write down a new formula. That same evening he communicated his result to Rubens on a postcard. Two days later Rubens returned to Planck. His formula agreed perfectly with the experimental observations.

Planck had the correct formula to describe black body radiation. Unfortunately he could not justify it on purely theoretical grounds. It did not take him long to find the crucial step needed to get the right result. To take that step Planck returned to Boltzmann's work, and made a decisive commitment to Boltzmann's probabilistic reasoning. If he used Boltzmann's statistical formulation of thermodynamics, he found he could derive the black body formula by making only one additional assumption; the energy of an oscillating particle is restricted to be an integer multiple of its frequency of oscillation times a new fundamental constant, now called Planck's constant. Planck had solved the problem of black body radiation.

Planck's bold hypothesis explained the experimental results, but the hypothesis itself remained unexplained. There is nothing in the physics of Newton which would require the motion of an oscillating particle to be restricted to certain energies.

We can imagine a very simple kind of oscillating particle as follows. Suppose we have a particle constrained to move only in a straight line, without friction, between two reflecting walls (see figure 1.1).

Between the walls, Newton's laws tell us that the particle will continue to move, in the same direction and at constant speed. When it hits the wall it experiences a force which reverses its motion. (To keep things simple we will assume that it loses no energy at each reflection). The particle can have any speed at all. However if Planck's hypothesis is correct, this cannot be true. If we restrict it to have only particular energies, it cannot move at an arbitrary speed. It is as if there were some strange road rule to the effect that, on the quantum highway, you can travel at 20 km/hour or 40km/hour or 60km/hour ... but never at any

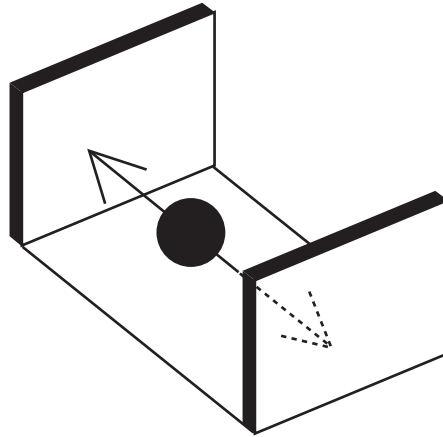


Figure 1.1:

other speed !

Twenty years would pass after Planck's address in Berlin, before a complete quantum theory, totally supplanting Newtonian mechanics, would arise to explain his hypothesis. The basic idea behind the quantum theory of an oscillating particle is simple enough, and I will explain it later in this chapter. The explanation turns on a new way to calculate the 'odds' for measurement results, a new probability calculus; a calculus so strange and unfamiliar that even today it generates heated debate among physicists (and others) as to exactly what it means. To get to this point however we need to reflect a little on how ordinary odds are calculated.

1.2 From classical to quantum probability.

Two-up has been described as Australia's very own way to part a fool and his money. As the name implies it is a game of chance played by throwing two coins. Two coins (pennies) are thrown into the air from a small wooden palette by the spinner, selected from the assembled crowd. The spinner aims to toss a pair of heads three times, before tossing a pair of tails or five consecutive odds (a tail and a head). If this is done the spinner is paid at 7:5, otherwise the bet is lost. Onlookers may place side bets, but here I will only discuss the game from the point of the spinner.

In one spin there are four possible outcomes, two heads (HH), two tails (TT), a head and a tail (HT) or a tail and a head (TH). How do we get from these simple facts to a calculation of the odds of a spinner tossing five consecutive odds? In

order to answer this question we need to know how to assign probabilities, or odds, to the elementary events which describe the outcome of each spin. Once we have these we then need to know how to combine these elementary events to get the odds for more complex events. The mathematical theory of probability arose precisely to answer such questions about games of chance, but has long since shrugged off its dubious genesis to become a respected branch of mathematics. Most people find probabilistic reasoning rather difficult, which is just as well for the continued viability of casinos and lotteries. Fortunately we only need a couple of simple results to understand two-up.

Games of chance are probably as old as humanity, but a mathematical theory of randomness did not arise until the Renaissance. It is rather puzzling that ancient Greek mathematics, which attained excellence in many areas, had little or nothing to contribute to the mathematics of chance. Perhaps studying games of chance was considered to be 'poor taste' in the intellectual circles of Aristotle or Archimedes. But more likely such questions didn't interest thinkers obsessed with geometry. A true mathematics of probability did not really get going until about 1660. About that time Antoine Gombault de Méré, a gifted nobleman with a penchant for gambling, asked his friend, the young Pascal, the following question. If two die are thrown, how many tosses are needed to have at least an even chance to get a double six? Pascal's answer is recorded in a letter he wrote to another great mathematician, Fermat, and represent the birth of mathematical probability in the western science. By the way, the answer to the Chevalier's question is 24 throws for a probability of 0.491 and 25 throws for a probability of 0.505.

Pascal's answer was arrived at through a novel counting argument supplemented with one essential assumption; each result, in a single roll of a dice is 'equally probable'. This came to be known as Laplace's rule of insufficient reason. Given this assumption, the rest is arithmetic. To see how it works let us look at the simpler case of a toss of two coins. Four results (TT, HH, TH, HT) are possible. If each is equally probable we 'assign' the probability of one quarter to each. Now we can calculate the probability for say an 'odd', that is a TH. Of the four possible outcomes this represents half of them, so the probability is one half. In other words we add the fundamental probabilities for each way an odd result can occur. Given the initial assignment of probabilities, the rules of arithmetic can be applied in an almost mechanical way to answer any number of questions, but is the original assignment reasonable?

When we ask this question we are going straight to the heart of what is so puzzling about probability. The assignment of the fundamental probabilities is based on our belief in what constitutes a fair dice or coin. Of course we can check

how reasonable this belief is by taking a particular coin and throwing it many times. If it always came down heads, we would soon begin to lose confidence in our original assignment of probability. As more knowledge becomes available we need to re-assign the fundamental probabilities. It seems that assigning probabilities is a curious mixture of belief and practice, of subjective and objective. It is this duality that makes probabilistic reasoning so difficult and gives philosophers endless cause for debate. It is especially disturbing then when probabilistic reasoning turns out to be useful in physics, which is supposed to be the objective science par excellence.

In some cases the rule of insufficient reason is itself rather insufficient. Common everyday usage of the word 'probability' seems to require more general rules. In some cities in Australia, the weather bureau adds to its daily forecast a statement of the 'probability of rain'. Just what does a 20% probability of rain actually mean and how is this number arrived at? It is far from clear how the rule of insufficient reason could be applied here. What are the equally likely alternatives? In some cases there are just too many alternatives. For example suppose you randomly select a number on the real line. What is the probability that the number selected is a rational number? There are an infinite number of rational numbers, but then there are infinitely many more non-rational numbers. In this case the probability of getting a rational number is zero, which does not mean it is impossible. Then there are special events. For example what is the probability that life will arise in a universe just like ours? Presumably this is 100%, but this doesn't quite answer the question. What we are really asking for is just how unlikely is life on earth. Was it a certainty or was it a one-in-a-million chance? Assigning probabilities is a far from straightforward matter.

Despite these misgivings the rule of insufficient reason does seem quite reasonable, at least for games of chance, and we can always check it against experience. Once the basic probabilities are assigned, the rest follows from arithmetic. Until the early years of the 20th century the probability calculus initiated by Pascal, was the only game in town. After awhile it begins to look as if it is the only possible way to calculate with probabilities. What a surprise then when experiments on matter at atomic scales suggested a new probability calculus — quantum mechanics.

In quantum mechanics the probabilities of elementary events are determined in an entirely new way, using a new set of numbers, complex numbers, unknown to Laplace or Pascal. As a result, some of the most obvious rules of classical probability theory do not apply under certain circumstances. One such rule is the sum rule used to calculate the probability for an odds in a two-up game. Knowing how such a simple rule can fail takes us to the heart of the quantum

theory.

Laplace's rule can be used when we have no idea what to expect for a given outcome. But in physics we know a lot about what to expect for a given arrangement of matter. If we know enough about the set up of a two-up game, for example we know the mass and shape of the pennies, their exact speed and orientation as they leave the skip, the effect of gravity and of the passing breeze, we might just be able to predict the outcome and clean up. On the other hand, even with the fastest super computer, we might die before we had finished the calculation for just one toss. In every experiment an exact description is impossible in practice and even unnecessary. If we want to get anywhere we include just the essential information and treat every thing else as a source of randomness or noise. However we can always console ourselves by continuing to think that a completely predictable description can be given.

In quantum theory however this classical ideal is forever abandoned. It is now known that at the atomic level nature is irreducibly random. Even if the entire experimental arrangement is completely specified, we cannot predict with certainty the results for all possible measurements we might care to make on the system. This is a deeply disturbing fact. The goal of physics has always been to provide explanations for observations. But quantum physics teaches us that this goal can be approached but not reached. Fortunately the theory does at least tell us how to calculate the probabilities for a particular observation even if in a particular run of the experiment we cannot predict with certainty what the result will be. We cannot avoid talking about probabilities if we are to describe the universe as it is.

Quantum theory is expressed in terms of probabilities for outcomes to measurements. That is not surprising. As we have seen, to get a realistic and practical description of the physical world we must put up with a certain amount of randomness. However, the rules for reckoning quantum odds are nothing like the obvious rules used in two-up. Quantum two-up is the fairest game in the land. I am going to describe a quantum two-up game played with light, but to begin we need to pause and ask; what is light? The answer to this question at the end of the 19th century, and the one you are likely to get today if you ask a high school physics student, is: light is a wave. This is not correct. Five years after Planck introduced the quantum hypothesis to explain observations on black body radiation, another exotic quantum bloom appeared in the garden. On 9 June 1905, a paper appeared in *Annalen der Physik* with the title, 'On a Heuristic point of view about the Creation and Conversion of Light'. The author was Albert Einstein. In a letter to a colleague he described the contents of this paper as 'very revolutionary'. A considerable understatement.

Consider for a moment the matter of air pollution monitoring. A standard method to monitor emissions of these substances is to continually sample a small amount of the gas going up a factory chimney. When oxides of nitrogen react with ozone, they emit light. By using the remarkable property of certain metals to develop a charge when exposed to light, the little bursts of light produced may be detected electrically. The explanation of this property was the subject of Einstein's paper.

If we take a metal plate and expose it to light it will acquire a positive charge. The explanation had been worked out six years before Einstein's paper of 1905. The light causes negatively charged electrons to be ejected from the surface. If the plate is electrically neutral to begin, losing a few electrons leaves it with an unbalanced positive charge. This seems straightforward enough until you examine things a little more closely. If you carefully control the wavelength of the light falling on the metal you find that above a certain wavelength, the light has no effect. The plate remains neutral. If you set up a little experiment to measure the speed of the ejected electrons you discover a very odd result. The maximum speed of ejected electrons, if any are ejected at all, does not depend on the intensity of the light. Increasing the intensity only increases the number of electrons ejected per second.

Both of these facts are inconsistent with the notion that light is a wave. Imagine a boat tied to a mooring, rocking up and down as waves pass by. If the height, or intensity, of the wave is big enough, the boat may break free of its moorings. If light were a wave, increasing its intensity should eventually supply sufficient energy to wrest the most tightly moored electron free of metal atoms in the surface. Yet that is not what happens. If the wavelength is not right, the electrons will remain bound to the surface of the metal, no matter how intense the light. Yet clearly, if the light supplies sufficient energy, the electrons must eventually break free. If increasing the frequency of the light causes the electrons to be emitted then there must be some relationship between the energy carried by light and its frequency. That was Einstein's insight (and the one that gained him the Nobel prize). He postulated that the energy carried by light was proportional to its frequency, and that the constant of proportionality was exactly the same constant that Planck used in his theory of black body radiators. Furthermore, according to Einstein's explanation, the best way to picture what is going on is to regard light as made up of little particles, photons, each with energy proportional to the frequency of the light. In this way we see why increasing the intensity increases the number of electrons ejected. For each photon of the right energy one electron can be ejected. Increasing the intensity increases the number of photons and thus increases the number of electrons emitted.

Thus began the quantum theory of light, which was not to achieve a full expression until the middle of the 20th century, long after a quantum theory of matter was accepted. (Why ? Light moves so fast that any theory of light must take into account the theory of relativity. A relativistic quantum theory was not so easy to come by). We don't usually need the quantum theory to describe light. But if we use light of very low intensity a quantum description is necessary. To describe light of different intensity, we use light of differing numbers of photons. To describe light of different colours we use photons of different energies. Before Einstein, all experiments with light were adequately explained by picturing light as a wave. Einstein used a particle picture to describe the observed effect of light on matter. So is light a particle ? No it is not. Neither is it a wave. However if we are to communicate with each other we must use familiar concepts, such as particle or wave, to describe the outcome of observation. So long as we only use our picture in the context of the observation we are trying to describe we won't get into trouble. That at least was the interpretation given to quantum theory by the Danish physicist Neils Bohr. It was an interpretation that was never accepted by Einstein. He continued to believe that it was possible to say just what light really was, without some intellectual tight-rope act in which properties depend on the act of observation.

To make a quantum two-up game with light we will use a device called a beam splitter. This is essentially a half-silvered mirror; half the light goes through and half gets reflected. What happens if we use light of such low intensity that it has only one photon ? When the photon encounters the beam splitter it can either be reflected or transmitted, see figure 1.2. In the figure we have two laser

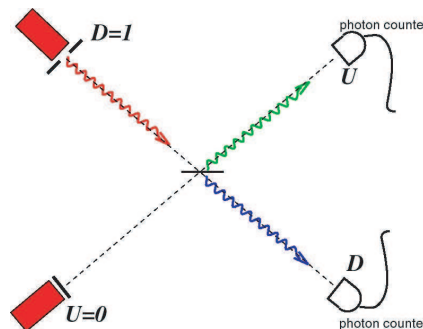


Figure 1.2:

sources labeled D (for downward directed) and U (for upward directed). For now we will assume that we only use the D source, so that all photons directed towards the beam splitter are traveling in the downward direction. If this photon

is transmitted it is still traveling downward and will be counted by the photon detector placed in the the path of this beam. We call this the D-detector. On the other hand, if a photon reflected it is now heading in an upward direction and will be detected by the photon counter placed in the path of the upward traveling photons, which we call the U-detector. If we repeat the experiment many times (many tosses of the coin) we see that roughly equal numbers are counted at either detector. If we insist on a physical picture to explain this we would say that any given photon is equally likely to be transmitted or reflected. The behaviour of any given photon is as random as a coin toss. Even if we know everything there is to know about the light we use, its intensity, colour, polarisation, we cannot predict whether any individual photon will be reflected or transmitted. The best we can do is give the odds (even in this case). This looks like a simple coin-toss.

However the situation is a bit more complicated. Suppose we 'toss' the photon again, see figure 1.3. After the first beam splitter we use two perfectly reflecting

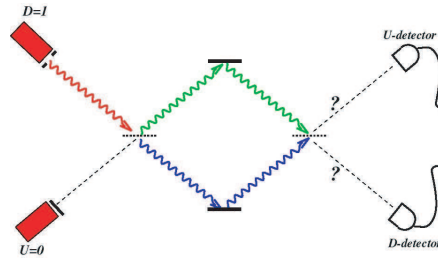


Figure 1.3:

mirrors, one in the downward path and one in the upward path to direct the photon back onto another, identical, beam splitter. The photon counters are now moved back to monitor the beams after the second beam splitter. What is the probability to detect a photon at, say, the upper detector, $P(U)$?

If the photon at a beam splitter really is a coin toss, we can argue like this. There are four possible *histories* for a photon: it can be reflected at the first beam-splitter and the second beam-splitter (RR), or it can be transmitted at both, (TT), or it be reflected at the first and transmitted at the second, (RT) or vice-versa (TR). Each case is equally likely, so we assign a probability of $1/4$ to each history, $P(RR) = P(TT) = P(RT) = P(TR)$. Detection at U can be achieved in two ways: RR and TT. Following the Bayes' rule the probability for detection at U is then

$$P(U) = P(RR) + P(TT) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} \quad (1.1)$$

When the experiment is done, the results are completely different: the photon is *always* detected at U . Detection at U is certain, so that $P(U) = 1$. See figure

1.4. In this experiment we see how quantum systems can exhibit both irreducible

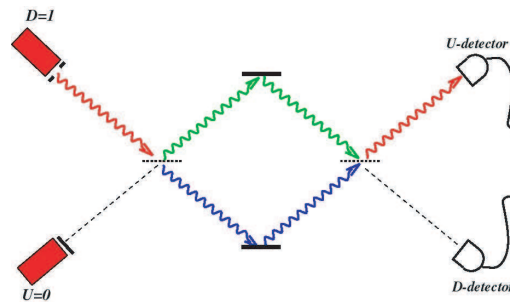


Figure 1.4:

uncertainty and certainty depending on how we interrogate the system. This is one of the keys features of quantum states. To help you remember them I will give them each a name.

The quantum principles:

- BOHR: Given complete knowledge of the state of a physical system, there is at least one measurement for which the results are completely random.
- HEISENBERG: Given complete knowledge of the state of a physical system, there is at least one measurement for which the results are completely certain.

The first of these represents a complete departure from the ideal of classical mechanics. In classical mechanics to have complete knowledge of a physical system means that we can predict the results of every measurement we may care to make upon it. The first principle suggests that, at heart, the world is a coin toss. Despite this it is nonetheless intelligible as the second principle makes clear.

How do we describe the experiment with beam splitters in the quantum formalism? The key feature of quantum mechanics is a new way to compute probabilities for experimental results. Probabilities are not the primary object, rather we first need to assign a *probability amplitude*. This is a number that is not necessarily positive (indeed it does not even need to be real, but we will not need that complication in this course). Given the probability amplitude for an event, the resulting probability is found by squaring the amplitude, which of course always yields a positive number.

Quantum theory has two distinct components. The first component is a calculus for dealing with probability amplitudes and turning them into probabilities. The second component tells us how to assign the probability amplitudes in the

first place. In the second component we find a number of mathematical tools, such as the Schrodinger equation, that tells us how to assign probability amplitudes given the physical description of a system. For the rest of this chapter we will assume the amplitudes are given and learn how to use them to compute the probability for measurement outcomes.

Perhaps one of the most surprising features of the quantum description is the following. Once we have a list of the probability amplitudes for the outcomes of the measurement of a *particular* physical quantity, we can compute the probability amplitudes for the outcomes of the measurement for *every* physical quantity. It is for this reason that we call the list of probability amplitudes the *quantum state* of a physical system.

We can now firm up what the quantum principles mean. To have complete knowledge of a quantum state means to have a complete list of all the probability amplitudes that describe the results of measurement of a particular physical quantity. If all the amplitudes have the same magnitude, for this particular measurement, the resulting probabilities will all be equal and for this measurement the results are totally random. Note, it follows that the sum of the squares of the probability amplitudes in the list must be unity.

However if this list really is complete, then the quantum formalism gives a way to transform this list of probability amplitudes to get the probability amplitudes for the measurement results of every other physical quantity. In particular there is a physical measurement for which the transformed list is made up of only one non zero element. For this physical quantity, only one result will be obtained and that will be obtained with certainty.

To see the calculus in action let us see how it works for the single photon with beam splitters. The first rule we need is the quantum version of Bayes' rule. To help you remember it, I will call it Feynman's rule.

Feynman's rule:

if an event can happen in two (or more) indistinguishable ways, first add the probability amplitudes, then square to get the probability.

In the case of the beam splitter experiment, there are only two possible measurement results: either the photon is counted at the U-detector or it is counted at the D-detector. The quantum state is then a list with just two elements, (t, r) , such that $P(D) = t^2$ and $P(U) = r^2$. Obviously we need to have $r^2 + t^2 = 1$. We can if we like refer to r as the probability amplitude for a photon to be reflected at the beam splitter and t is the probability amplitude for the photon to be transmitted.

We have explicitly introduced a particular notation for a quantum state as an ordered pair of probability amplitudes. We have chosen the order such that the

first entry represents the amplitude for a photon to be counted in the D -direction and the second entry corresponds to a photon being counted in the U -direction.

Using the notation of the previous paragraph, a single photon input in the D -direction can be described by the quantum state $(1, 0)$. The beam splitter then transforms the state according to $(1, 0) \rightarrow (t, r)$. In a self consistent way we could then describe the state of a photon input in the U direction as $(0, 1)$. It might seem at first sight that such a photon is transformed as $(0, 1) \rightarrow (r, t)$. There is a problem with this in the case of a 50/50 beam splitter, which highlights an important physical principle which we pause to consider.

In classical physics a beam splitter is an optical device described by Maxwell's equations. These equations describe the interaction of light and matter in a way which is completely reversible in time; no entropy can be generated in a system which is time reversal invariant. Put another way, no information can be lost. Among other things this implies that physically distinguishable input states cannot be transformed to the same output states. If that were to happen the information, on what distinguished the states originally, would be lost.

In the example we are considering, the two input states $(0, 1)$ and $(1, 0)$ are physically distinct but as it stands they are mapped to the same quantum state for a 50/50 beam splitter. The way to fix this is to note that we can get physical access only to the probability of transmission and reflection, which are equal to t^2 and r^2 . We can however change the sign of one of the components of the list of amplitudes without changing this. So we adopt the following transformation rule for beam splitters in general:

$$(1, 0) \rightarrow (t, r) \quad (1.2)$$

$$(0, 1) \rightarrow (-r, t) \quad (1.3)$$

A simple graphical representation can be used to keep track of where the minus sign should go, illustrated in figure 1.5 for a 50/50 beam splitter. We regard the ordered pair of probability amplitudes as a vector in a two dimensional space, with the horizontal component corresponding to the first entry (the D -direction amplitude) and the vertical component corresponding to the second entry (the U -directed entry). The general case is illustrated in figure 1.6

In the experiment indicated in figure 1.4, a photon must interact with two beam splitters, for example, to be reflected at the first and transmitted at the second beam splitter, and we need a new rule. In the case of a double coin toss, the probability to get a head AND a tail, $P(HT)$ is calculated by *multiplying* the probability for each event $P(HT) = P(H) \times P(T)$. The same rule applies for the quantum world but at the level of probability amplitudes. For example the list of probability amplitude for the histories RR, TT, TR, RT is $(r_1 r_2, t_1 t_2, t_1 r_2, r_1 t_2)$.

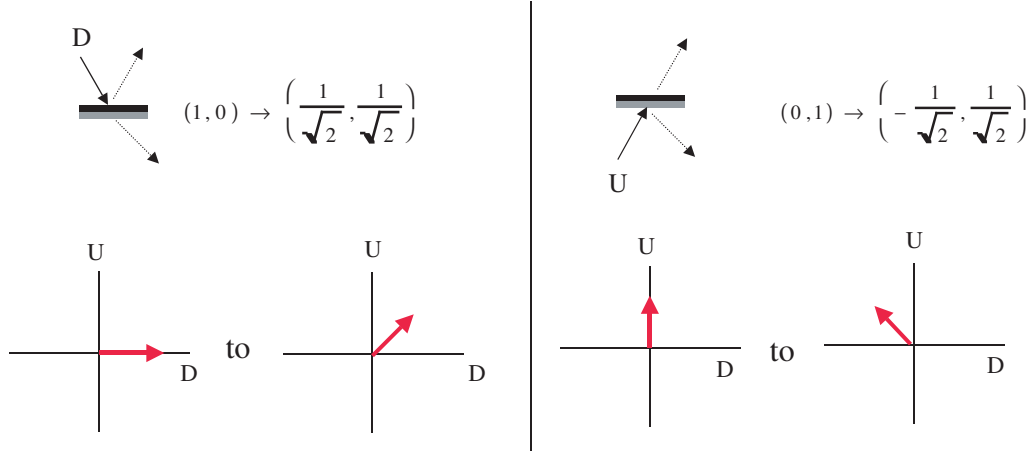


Figure 1.5: A graphical representation for how quantum states, considered as lists of probability amplitudes, are transformed by a beam splitter in the case of a 50/50 beam splitter.

The probability to detect a photon in the U -detector can now be calculated using Feynman's rule. This event can occur in two ways, either RR or TT , so the probability is

$$P(U) = (r_1 r_2 + t_1 t_2)^2 \quad (1.4)$$

Using the results in figure 1.5 we see that

$$\begin{aligned} P(U) &= \left(\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \right)^2 \\ &= 1 \end{aligned} \quad (1.5)$$

In a similar way,

$$P(D) = (r_1 t_2 + t_1 (-r_2))^2 \quad (1.6)$$

which for a 50/50 beam splitter gives, $P(D) = 0$.

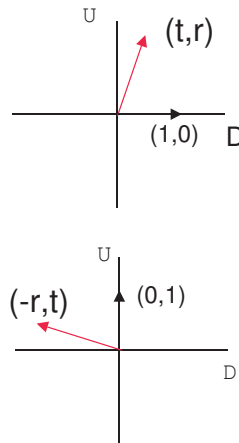


Figure 1.6: A graphical representation for how quantum states, considered as lists of probability amplitudes, are transformed by a beam splitter in the general case.

1.3 Quantum mechanics for free particles.

A free particle is one that is not acted on by a force. It can only have kinetic energy. In one dimension Newtonian physics gives the position as a function of time as

$$x(t) = x_0 + p_0 t / m \quad (1.7)$$

where x_0, p_0 are initial position and momentum.

In this case the possible outcome for a measurement of position is a point on the real line. The possible results are not only infinite but non denumerable. In the absence of any knowledge at all, such a particle could be found anywhere at all if the position is measured. How are we to fit a measurement such as this into the scheme of specifying a quantum state as a list of probability amplitudes for the outcomes of a measurement? If there are infinitely many possible outcomes, the list will need to be infinitely long!

And that is exactly how it is done. In a deeper treatment of quantum mechanics we need to be able to work with infinite lists. However for our purposes we will ignore this complication. For most situations of practical concern the probability distribution for position generally falls off outside of some region of interest, say the laboratory, and we can focus on this region. we will assign a single probability amplitude for each position, x . In general this is a complex number but at the level of this course we won't use complex numbers. Instead we will use another graphical trick. Traditionally the probability to find a particle at point x is denoted as $\psi(x)$.

The probability amplitude to find a particle in an infinitesimal region around position x is represented by a vector in a two dimensional space, figure 1.7. The length squared of the vector gives the probability for that position to be found upon measurement. It is important to remember that this vector does not “live” in real space but in an abstract space of probability amplitudes. The angle that the vector makes with the horizontal direction depends upon x . We will arbitrarily assign this angle to be $\pi/2$ for $x = 0$. We can do this as only *changes* in the angle as x is varied has a physical significance. So, how does this angle change with position?

The answer to this question was discovered by Schrödinger. In order to explain what it is, we need to revise some basic kinematics. You are probably quite familiar with kinematic concepts such as momentum, kinetic energy and angular momentum. You may be less familiar with *action*.

The *action* of a mechanical system is a rather special quantity that lies at the heart of the more sophisticated formulations of dynamics given by Lagrange and also by Hamiltonian. The action of a particle at point x which has momentum p at that point is $I(x, p) = xp$. As a particle moves the action will change. We usually solve Newton’s equations of motion to give the position and momentum as a function of time. However we can eliminate the time variable to specify the motion by giving the momentum as a function of position, $p(x)$. If we plot $p(x)$ versus x we get a curve that we will call an *orbit*. There is a remarkable fact about Newtonian mechanics: the particle will move such that the total action over the orbit is a *minimum*. This implies that if we were to plot $p(x)$ as a function of x , the area under the curve from the initial position to a final position is a minimum. This area is the total *action* of the orbit.

We can now state Schrödinger’s rule: the change in the angle of the probability amplitude vector as we change the position from the initial position x_i to the final position x_f , is proportional to the change in the action along that orbit.

As an example consider a free particle. In this case the momentum, $p = p_0$ is conserved and cannot change. Let us put the initial position at the origin, $x_i = 0$. The change in action of an orbit to an arbitrary position, x is then just, p_0x . The angle of the probability amplitude is, by Schrödinger’s rule is then

$$\theta = \pi/2 - \left(\frac{2\pi}{h}\right) p_0x \quad (1.8)$$

where we have used the assignment of an angle of $\pi/2$ for $x = 0$. The constant of proportionality is $2\pi/h$ where the constant h is new fundamental constant called *Planck’s constant* and in SI units has the value

$$6.067 \times 10^{-34} \text{Js} \quad (1.9)$$

which has units of action (which, by the way, are the same as the units of angular momentum).

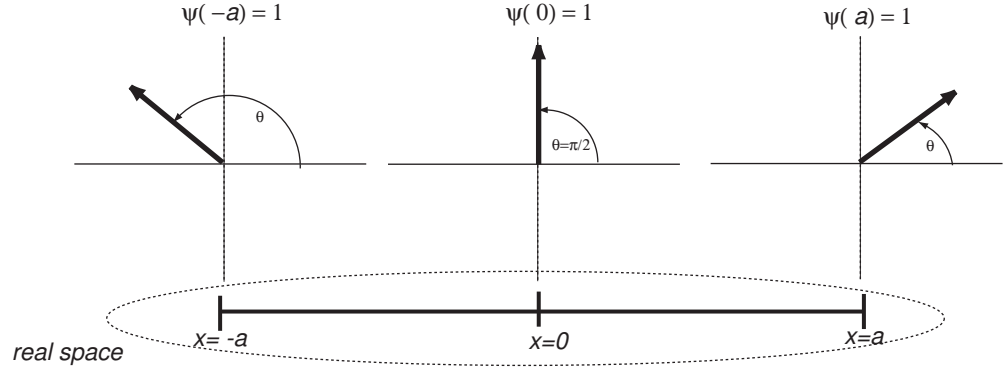


Figure 1.7: A representation of the probability amplitude for the outcome of a position measurement of a free particle with fixed momentum. The probability is given by the length squared of the arrow. The only way in which the arrow changes for different position outcomes is via a rotation: the length does not change. The rotation angle is given by Schrödinger's rule, Eq.(1.8)

In this example of constant momentum, the length of the vector has no dependence on position at all. This means that we are equally likely to find the particle at any position. In other words the position of the particle is very uncertain. As we discussed earlier, this must be an approximation. In reality the probability must eventually fall off for very large position measurements. Nonetheless the position uncertainty is going to be very large. This is a reflection of a very important principle, the *Heisenberg uncertainty principle*. If we specify a quantum state with a very well defined momentum, the position uncertainty will be very large, and conversely. If designate the uncertainty in position as Δx and the uncertainty in momentum, the Heisenberg principle says that there for all physical states we must have

$$\Delta x \Delta p \geq h/4\pi \quad (1.10)$$

In figure 1.8 we illustrate this for the example of figure 1.7

Let us look at an example with an uncertain momentum: a free particle with a definite *energy*. A free particle has only kinetic energy which is given by

$$E = \frac{p^2}{2m} \quad (1.11)$$

If E is fixed the magnitude of the momentum is fixed but not the sign. In other words a particle can have the same kinetic energy but could be either moving to

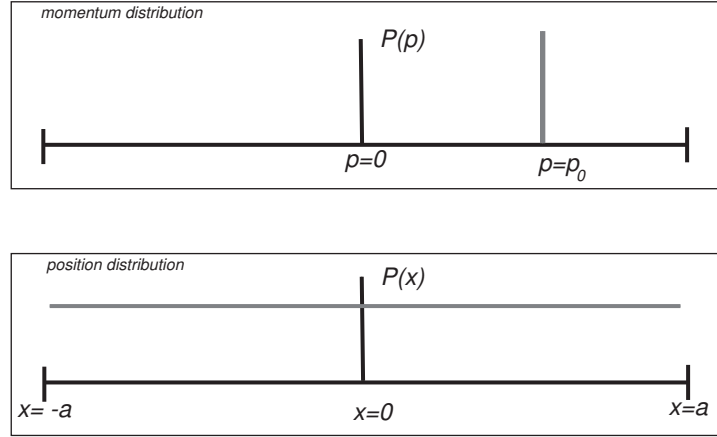


Figure 1.8: The momentum and position distributions for the state in figure 1.7. The momentum is definite and correspondingly the position is totally indefinite.

the left or moving to the right. The momentum is thus uncertain by an amount that scales as $\sqrt{E}$.

This is a situation where we can apply Feynman's rule, as a state of definite energy can be found at a position x with two values of momentum, $\pm\sqrt{2mE}$, which are indistinguishable if we only observe position. The graphical representation of this state must have *two arrows* each representing the particle being found at x with one or the other momentum.

As before, we will set the angle for both vectors to be $\pi/2$ for a particle to be found at $x = 0$. For results that are $x \neq 0$, the probability amplitude vectors rotate in opposite directions as the momenta have opposite sign. Some examples are depicted in figure 1.9. Applying Feynman's rule we need to add the two probability amplitudes, which in this case has to be vector addition. For $x = 0$ the two vectors are in the same direction and thus give a vector of twice the length of each. On the other hand there are some position measurement results for which the amplitude vectors point in opposite directions and cancel each other completely. The probability is zero and we will *never* find a particle at this position. A little geometry shows that the probability for position measurements will be given by

$$P(x) \propto \cos^2(2\pi px/h) \quad (1.12)$$

We do not put in the constant of proportionality here as we have chosen the lengths of the amplitude arrows to be arbitrarily set at unity. This is a reflection of the unphysical nature of such states in so far as the particle could be found at arbitrarily large distances. In such a situation we can really only look at the relative

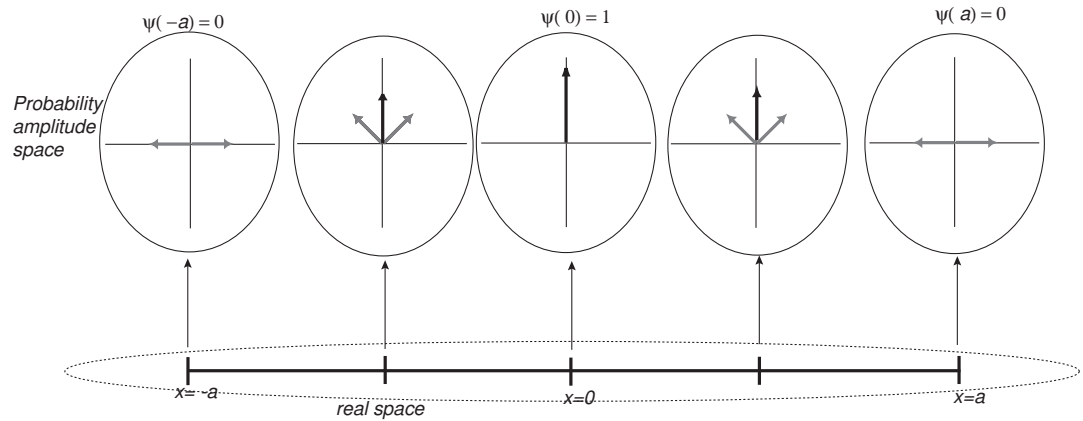


Figure 1.9: A representation of the probability amplitude for the outcome of a position measurement of a free particle with fixed energy. A definite value of energy can be realised in two indistinguishable ways corresponding to equal and opposite momentum. Thus at each position there are two probability amplitudes that need to be added first.

variation of probability with position, but the distributions cannot be normalised. In figure 1.10 we plot the position and momentum distribution for a free particle state of definite energy.

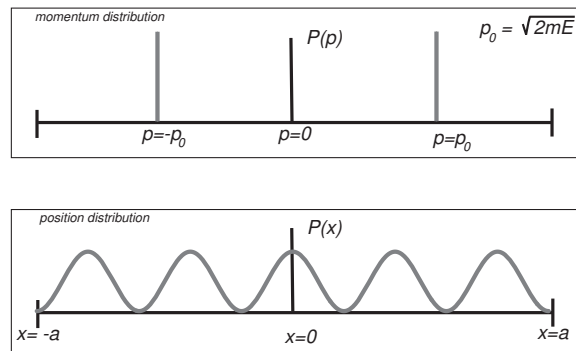


Figure 1.10: The momentum and position distribution for a free particle with a state of definite energy.

1.4 Quantum mechanics for oscillators.

We now consider the quantum description for dynamics of particles executing oscillatory motion in a confining potential. The most natural example is the simple harmonic oscillator; a single particle moving in a quadratic potential. This example was precisely the one that Planck considered when he ushered in his revolutionary proposal: the energy of oscillating systems are restricted.

The position, as a function of time, of a particle in a quadratic potential is

$$x(t) = x_0 \cos(2\pi t/T) \quad (1.13)$$

where T is the period of the motion. The momentum is

$$p(t) = -\frac{2\pi m x_0}{T} \sin(2\pi t/T) \quad (1.14)$$

The total energy of the particle is

$$E = \frac{p(t)^2}{2m} + \frac{2m\pi^2}{T^2} x(t)^2 \quad (1.15)$$

which is independent of time, and in fact determined by the initial position as

$$E = \frac{2m\pi^2}{T^2} x_0^2 \quad (1.16)$$

In this case one easily sees that the action of the orbit is simply the area of the ellipse in phase space defined by the curve in Eq.(1.15). This is shown in figure 1.11 One easily sees that the area is simply given by the product of the energy and the period as ET where the period, T , is the inverse of the frequency, f , and given by

$$T = \frac{1}{f} = 2\pi \sqrt{\frac{m}{k}} \quad (1.17)$$

Planck's rule now says that only those orbits are allowed for which the action is an integer multiple of Planck's constant. Thus we see that the allowed energies are given by

$$E_n = nhf \quad (1.18)$$

As another example we consider a not-so-simple oscillator: a particle bouncing elastically between two walls a distance L apart, see figure 1.12 The period of

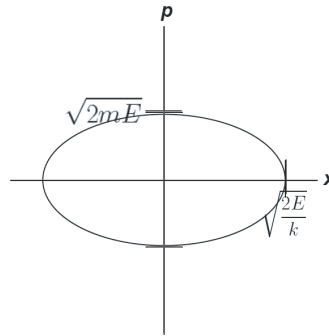


Figure 1.11: The phase space orbit for a simple harmonic oscillator with energy E

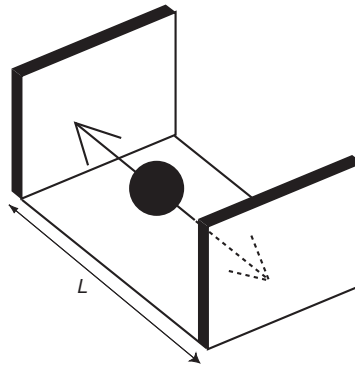


Figure 1.12: The square-well oscillator. Between the walls the energy is entirely kinetic, $E = p^2/2m$

motion obviously depends on energy, as the faster the particle moves the shorter time it takes to go from one side to the other. The period is in fact given by

$$T(E) = \frac{2mL}{p} = L\sqrt{\frac{2m}{E}} \quad (1.19)$$

The phase-space orbit is a rectangle, see figure 1.13 The area is given by $2L\sqrt{2mE}$ and applying Planck's rule to the area gives the allowed energies as

$$E_n = \frac{n^2 h^2}{8mL^2} \quad (1.20)$$

Planck's rule is a direct application of Schrödinger's rule and the way we sum probability amplitudes. The square-well oscillator is very much like the example

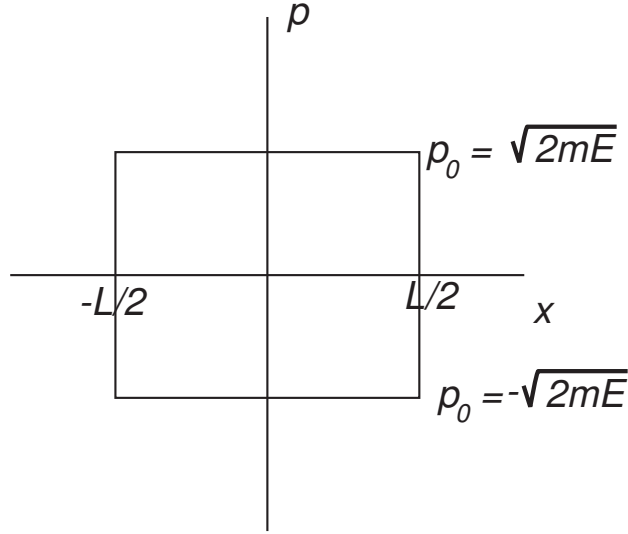


Figure 1.13: The phase-space orbit of the square-well oscillator square-well oscillator with kinetic energy, $E = p^2/2m$

of a free particle with fixed energy except that the probability to find the particle outside the box is zero. This means that we must set $P(x = L/2) = P(x = -L/2) = 0$. If you look back to the free-particle example you will see that this will necessarily restrict the momentum and thus the energy. For a free particle we saw that the position probability density was given by $P(x) \propto \cos^2(2\pi px/h)$. But if we set this to zero at $x = \pm L/2$ we see that the smallest momentum we can have consistent with this result is

$$p_{min} = \frac{h}{2L} \quad (1.21)$$

so that the minimum energy allowed is

$$E_{min} = \frac{h^2}{8mL^2} \quad (1.22)$$

which is the same result as that given by Planck's rule in Eq.(1.20).

This last result is curious when we compare it to what we would expect classically. In Newtonian mechanics of such a system the lowest energy is obviously zero for a particle that is not moving at all. In the quantum case, if we restrict the position of the particle it must have a minimum energy different from zero. This is in fact a reflection of the uncertainty principle as we now show.

The average energy for a particle in a square well is simply kinetic and given

by

$$E = \frac{\langle p^2 \rangle}{2m} \quad (1.23)$$

However the average of the momentum squared is related to the variance in momentum by

$$\langle p^2 \rangle = \Delta p^2 + \langle p \rangle^2 \quad (1.24)$$

However for a symmetric system such as this, a state of definite energy is a superposition of positive and negative momenta thus we expect the average momentum to be zero; $\langle p \rangle = 0$. We thus have that

$$E = \frac{\langle \Delta p^2 \rangle}{2m} \quad (1.25)$$

However by the uncertainty principle we must have

$$\Delta p^2 \geq \frac{h^2}{16\pi^2\Delta x^2} \quad (1.26)$$

We can crudely estimate that for a square-well, $\Delta x = L$, and thus we expect that

$$E \geq \frac{h^2}{32m\pi^2L^2} \quad (1.27)$$