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Applications of Quantum Mechanics

University of Cambridge Part II Mathematical Tripos

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Recommended Books and Resources

There are many good books on quantum mechanics. Here's a selection that I like:

- Griffiths, *Introduction to Quantum Mechanics*

An excellent way to ease yourself into quantum mechanics, with uniformly clear explanations. For this course, it covers both approximation methods and scattering.

- Shankar, *Principles of Quantum Mechanics*
- James Binney and David Skinner, *The Physics of Quantum Mechanics*
- Weinberg, *Lectures on Quantum Mechanics*

These are all good books, giving plenty of detail and covering more advanced topics. Shankar is expansive, Binney and Skinner clear and concise. Weinberg likes his own notation more than you will like his notation, but it's worth persevering.

This course also contains topics that cannot be found in traditional quantum textbooks. This is especially true for the condensed matter aspects of the course, covered in Sections 3, 4 and 5. Some good books include

- Ashcroft and Mermin, *Solid State Physics*
- Kittel, *Introduction to Solid State Physics*
- Steve Simon, *Solid State Physics Basics*

Ashcroft & Mermin and Kittel are the two standard introductions to condensed matter physics, both of which go substantially beyond the material covered in this course. I have a slight preference for the verbosity of Ashcroft and Mermin. The book by Steve Simon covers only the basics, but does so very well. (An earlier draft can be downloaded from his homepage; see below for a link.)

A number of lecture notes are available on the web. Links can be found on the course webpage: http://www.damtp.cam.ac.uk/user/tong/aqm.html

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0. Introduction

Without wishing to overstate the case, the discovery of quantum mechanics is the single greatest achievement in the history of human civilisation.

Quantum mechanics is an outrageous departure from our classical, comforting, common sense view of the world. It is more baffling and disturbing than anything dreamt up by science fiction writers. And yet it is undoubtably the correct description of the Universe we inhabit and has allowed us to understand Nature with unprecedented accuracy. In these lectures we will explore some of these developments.

The applications of quantum mechanics are many and various, and vast swathes of modern physics fall under this rubric. Here we tell only a few of the possible stories, laying the groundwork for future exploration. There are two major topics.

Much of these lectures is devoted to *condensed matter physics* or, more precisely, *solid state physics*. This is the study of "stuff", of how the wonderfully diverse properties of solids can emerge from the simple laws that govern electrons and atoms. We will develop the basics of the subject, learning how electrons glide through seemingly impenetrable solids, how their collective motion is described by a Fermi surface, and how the vibrations of the underlying atoms get tied into bundles of energy known as phonons. We will learn that electrons in magnetic fields can do strange things and start to explore some of the roles that geometry and topology play in quantum physics.

The second major topic is *scattering theory*. In the past century, physicists have developed a foolproof and powerful method to understand everything and anything: you take the object that you're interested in and you throw something at it. This technique was pioneered by Rutherford who used it to understand the structure of the atom. It was used by Franklin, Crick and Watson to understand the structure of DNA. And, more recently, it was used at the LHC to demonstrate the existence of the Higgs boson. In fact, throwing stuff at other stuff is the single most important experimental method known to science. It underlies much of what we know about condensed matter physics and all of what we know about high-energy physics.

In many ways, these lectures are where theoretical physics starts to fracture into separate sub-disciplines. Yet areas of physics which study systems separated by orders of magnitude — from the big bang, to stars, to materials, to information, to atoms and beyond — all rest on a common language and background. The purpose of these lectures is to build this shared base of knowledge.

1. Scattering Theory

The basic idea behind *scattering theory* is simple: there's an object that you want to understand. So you throw something at it. By analysing how that something bounces off, you can glean information about the object itself.

A very familiar example of scattering theory is called "looking at things". In this section we're going to explore what happens when you look at things by throwing a quantum particle at an object.

1.1 Scattering in One Dimension

We start by considering a quantum particle moving along a line. The maths here will be simple, but the physics is sufficiently interesting to exhibit many of the key ideas.

The object that we want to understand is some potential $V(x)$. Importantly, the potential is localised to some region of space which means that $V(x) \to 0$ as $x \to \pm\infty$. An example is shown to the right. We will need the potential to fall-off to be suitably fast in what follows although, for now, we won't be careful about what this means. A quantum particle moving along the line is governed by the Schrödinger equation,

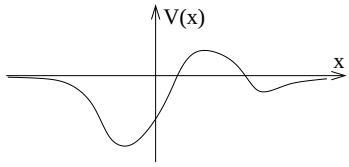


Figure 1:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{1.1}$$

Solutions to this equation are energy eigenstates. They evolve in time as $\psi(x,t) = e^{-iEt/\hbar}\psi(x)$. For any potential, there are essentially two different kinds of states that we're interested in.

- *Bound States* are states that are localised in some region of space. The wavefunctions are normalisable and have profiles that drop off exponentially far from the potential

  $$\psi(x) \sim e^{-\lambda|x|} \quad \text{as} \quad |x| \to \infty$$

  Because the potential vanishes in the asymptotic region, the Schrödinger equation (1.1) relates the asymptotic fall-off to the energy of the state,

  $$E = -\frac{\hbar^2\lambda^2}{2m} \tag{1.2}$$

  In particular, bound states have $E < 0$. Indeed, it is this property which ensures that the particle is trapped within the potential and cannot escape to infinity.

Bound states are rather special. In the absence of a potential, a solution which decays exponentially to the left will grow exponentially to the far right. But, for the state to be normalisable, the potential has to turn this behaviour around, so the wavefunction decreases at both $x \to -\infty$ and $x \to +\infty$. This will only happen for specific values of λ. Ultimately, this is why the spectrum of bound states is discrete, like in the hydrogen atom. It's where the name "quantum" comes from.

- *Scattering States* are not localised in space and, relatedly, the wavefunctions are not normalisable. Instead, asymptotically, far from the potential, scattering states take the form of plane waves. In one dimension, there are two possibilities

$$\begin{aligned} \text{Right moving:} \quad & \psi \sim e^{ikx} \\ \text{Left moving:} \quad & \psi \sim e^{-ikx} \end{aligned}$$

  where $k > 0$. To see why these are left or right moving, we need to put the time dependence back in. The wavefunctions then take the form $e^{\pm ikx - iEt/\hbar}$. The peaks and troughs of the wave move to the right with the plus sign, and to the left with the minus sign. Solving the Schrödinger equation in the asymptotic region with $V = 0$ gives the energy

$$E = \frac{\hbar^2 k^2}{2m}$$

  Scattering states have $E > 0$. Note that, in contrast, to bound states, nothing special has to happen to find scattering solutions. We expect to find solutions for any choice of k.

This simple classification of solutions already tells us something interesting. Suppose, for example, that the potential looks something like the one shown in the figure. You might think that we could find a localised solution that is trapped between the two peaks, with $E > 0$. But this can't happen because if the wavefunction is to be normalisable, it must have $E < 0$. The physical reason, of course, is quantum tunnelling which allows the would-be bound state to escape to infinity. We will learn more about this situation in Section 1.1.5.

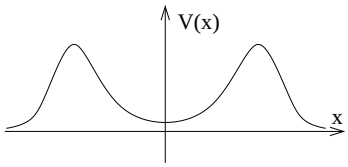


Figure 2:

1.1.1 Reflection and Transmission Amplitudes

Suppose that we stand a long way from the potential and throw particles in. What comes out? This is answered by solving the Schrödinger equation for the scattering

states. Because we have a second order differential equation, we expect that there are two independent solutions for each value of k. We can think of these solutions physically as what you get if you throw the particle in from the left or in from the right. Let's deal with each in turn.

Scattering from the Left

We throw the particle in from the left. When it hits the potential, one of two things can happen: it can bounce back, or it can pass straight through. Of course, this being quantum mechanics, it can quite happily do both at the same time. Mathematically, this means that we are looking for a solution which asymptotically takes the form

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to +\infty \end{cases} \tag{1.3}$$

We've labelled this state ψ_R because the ingoing wave is *right*-moving. This can be seen in the first term e^{ikx} which represents the particle we're throwing in from $x \to -\infty$. The second term re^{-ikx} represents the particle that is reflected back to $x \to -\infty$ after hitting the potential. The coefficient $r \in \mathbf{C}$ is called the *reflection amplitude*. Finally, the term te^{ikx} at $x \to +\infty$ represents the particle passing through the potential. The coefficient $t \in \mathbf{C}$ is called the *transmission coefficient*. (Note: in this formula t is a complex number that we have to determine; it is not time!) There is no term e^{-ikx} at $x \to +\infty$ because we're not throwing in any particles from that direction. Mathematically, we have chosen the solution in which this term vanishes.

Before we proceed, it's worth flagging up a conceptual point. Scattering is clearly a dynamical process: the particle goes in, and then comes out again. Yet there's no explicit time dependence in our ansatz (1.3); instead, we have a solution formed of plane waves, spread throughout all of space. It's best to think of these plane waves as describing a beam of particles, with the ansatz (1.3) giving us the steady-state solution in the presence of the potential.

The probability for reflection R and transmission T are given by the usual quantum mechanics rule:

$$R = |r|^2 \quad \text{and} \quad T = |t|^2$$

In general, both R and T will be functions of the wavenumber k. This is what we would like to calculate for a given potential and we will see an example shortly. But, before we do this, there are some observations that we can make using general statements about quantum mechanics.

Given a solution $\psi(x)$ to the Schrödinger equation, we can construct a conserved probability current

$$J(x) = -i\frac{\hbar}{2m}\left(\psi^\star\frac{d\psi}{dx} - \psi\frac{d\psi^\star}{dx}\right)$$

which obeys $dJ/dx = 0$. This means that $J(x)$ is constant. (Mathematically, this is the statement that the Wronskian is constant for the two solutions to the Schrödinger equation). For our scattering solution ψ_R, with asymptotic form (1.3), the probability current as $x \to -\infty$ is given by

$$\begin{aligned} J(x) &= \frac{\hbar k}{2m}\Big[\left(e^{-ikx} + r^\star e^{+ikx}\right)\left(e^{ikx} - re^{-ikx}\right) + \left(e^{ikx} + re^{-ikx}\right)\left(e^{-ikx} - r^\star e^{+ikx}\right)\Big] \\ &= \frac{\hbar k}{m}\left(1 - |r|^2\right) \qquad \text{as } \ x \to -\infty \end{aligned}$$

Meanwhile, as $x \to +\infty$, we have

$$J(x) = \frac{\hbar k}{2m}|t|^2 \qquad \text{as } \ x \to +\infty$$

Equating the two gives

$$1 - |r|^2 = |t|^2 \quad \Rightarrow \quad R + T = 1 \tag{1.4}$$

This should make us happy as it means that probabilities do what probabilities are supposed to do. The particle can only get reflected or transmitted and the sum of the probabilities to do these things equals one.

Scattering from the Right

This time, we throw the particle in from the right. Once again, it can bounce back off the potential or pass straight through. Mathematically, we're now looking for solutions which take the asymptotic form

$$\psi_L(x) \sim \begin{cases} t'e^{-ikx} & x \to -\infty \\ e^{-ikx} + r'e^{+ikx} & x \to +\infty \end{cases} \tag{1.5}$$

where we've now labelled this state ψ_L because the ingoing wave, at $x \to +\infty$, is *left*-moving. We've called the reflection and transmission amplitudes r' and t'.

There is a simple relation between the two solutions ψ_R in (1.3) and ψ_L in (1.5). This follows because the potential $V(x)$ in (1.1) is a real function, so if ψ_R is a solution then so is $\psi_R^\star$. And, by linearity, so is $\psi_R^\star - r^\star\psi_R$ which is given by

$$\psi_R^\star(x) - r^\star\psi_R(x) \sim \begin{cases} (1-|r|^2)e^{-ikx} & x \to -\infty \\ t^\star e^{-ikx} - r^\star t e^{ikx} & x \to +\infty \end{cases}$$

This takes the same functional form as (1.5) except we need to divide through by $t^\star$ to make the normalisations agree. (Recall that scattering states aren't normalised anyway so we're quite at liberty to do this.) Using $1-|r|^2 = |t|^2$, this tells us that there is a solution of the form (1.5) with

$$t' = t \quad \text{and} \quad r' = -\frac{r^\star t}{t^\star} \tag{1.6}$$

Notice that the transition amplitudes are always the same, but the reflection amplitudes can differ by a phase. Nonetheless, this is enough to ensure that the reflection probabilities are the same whether we throw the particle from the left or right: $R = |r|^2 = |r'|^2$.

An Example: A Pothole in the Road

Let's compute r and t for a simple potential, given by

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & \text{otherwise} \end{cases}$$

with $V_0 > 0$. This looks like a pothole in the middle of an, otherwise, flat potential.

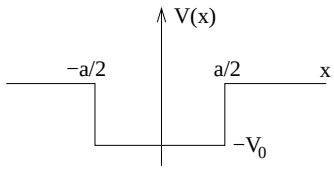


Figure 3:

Outside the potential, we have the usual plane waves $\psi \sim e^{\pm ikx}$. In the middle of the potential, the solutions to the Schrödinger equation (1.1) take the form

$$\psi(x) = Ae^{iqx} + Be^{-iqx} \qquad x \in [-a/2, a/2] \tag{1.7}$$

where

$$q^2 = \frac{2mV_0}{\hbar^2} + k^2$$

To compute the reflection and transmission amplitudes, r, r' and t, we need to patch the solution (1.7) with either (1.3) or (1.5) at the edges of the potential.

Let's start by scattering from the left, with the solution (1.3) outside the potential. Continuity of the wavefunction at $x = \pm a/2$ tells us that

$$e^{-ika/2} + re^{ika/2} = Ae^{-iqa/2} + Be^{iqa/2} \quad \text{and} \quad te^{ika/2} = Ae^{iqa/2} + Be^{-iqa/2}$$

Meanwhile, matching the derivatives of ψ at $x = \pm a$ gives

$$\frac{k}{q}\left(e^{-ika/2} - re^{ika/2}\right) = Ae^{-iqa/2} - Be^{iqa/2} \quad \text{and} \quad \frac{kt}{q}e^{ika/2} = Ae^{iqa/2} - Be^{-iqa/2}$$

These are four equations with four unknowns: A, B, r and t. One way to proceed is to add and subtract the two equations on the right, and then do the same for the two equations on the left. This allows us to eliminate A and B

$$A = t\left(1 + \frac{k}{q}\right)e^{i(k-q)a/2} = \left(1 + \frac{k}{q}\right)e^{-i(k-q)a/2} + r\left(1 - \frac{k}{q}\right)e^{i(k+q)a/2}$$

$$B = t\left(1 - \frac{k}{q}\right)e^{i(k+q)a/2} = \left(1 - \frac{k}{q}\right)e^{-i(k+q)a/2} + r\left(1 + \frac{k}{q}\right)e^{i(k-q)a/2}$$

We've still got some algebraic work ahead of us. It's grungy but straightforward. Solving these two remaining equations gives us the reflection and transmission coefficients that we want. They are

$$\begin{aligned} r &= \frac{(k^2 - q^2)\sin(qa)e^{-ika}}{(q^2 + k^2)\sin(qa) + 2iqk\cos(qa)} \\ t &= \frac{2iqke^{-ika}}{(q^2 + k^2)\sin(qa) + 2iqk\cos(qa)} \end{aligned} \tag{1.8}$$

Even for this simple potential, the amplitudes are far from trivial. Indeed, they contain a lot of information. Perhaps the simplest lesson we can extract comes from looking at the limit $k \to 0$, where $r \to -1$ and $t \to 0$. This means that if you throw the particle very softly ($k \to 0$), then it won't make it through the potential; it's guaranteed to bounce back.

Conversely, in the limit $k \to \infty$, we have $r = 0$. (Recall that $q^2 = k^2 + 2mV_0/\hbar^2$ so we also have $q \to \infty$ in this limit.) By conservation of probability, we must then have $|t| = 1$ and the particle is guaranteed to pass through. This is what you might expect; if you throw the particle hard enough, it barely notices that the potential is there.

There are also very specific values of the incoming momenta for which $r = 0$ and the particle is assured of passage through the potential. This occurs when $qa = n\pi$ with $n \in \mathbf{Z}$ for which $r = 0$. Notice that you have to fine tune the incoming momenta so that it depends on the details of the potential which, in this example, means V_0 and a.

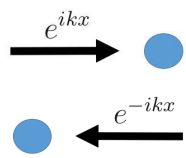
We can repeat the calculation above for scattering from the right. In fact, for our pothole potential, the result is exactly the same and we have $r = r'$. This arises because $V(x) = V(-x)$ so it's no surprise that scattering from the left and right are the same. We'll revisit this in Section 1.1.3.

1.1.2 Introducing the S-Matrix

The *S-matrix* is a convenient way of packaging the information about reflection and transmission coefficients. It is useful both because it highlights new features of the problem, and because it generalises to scattering in higher dimensions.

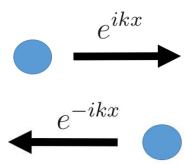
We will start by writing the above solutions in slightly different notation. We have two ingoing asymptotic wavefunctions, one from the left and one from the right

$$\text{Ingoing} \begin{cases} \text{right-moving:} & \mathcal{I}_R(x) = e^{+ikx} \quad x \to -\infty \\ \text{left-moving:} & \mathcal{I}_L(x) = e^{-ikx} \quad x \to +\infty \end{cases}$$



Similarly, there are two outgoing asymptotic wavefunctions,

$$\text{Outgoing} \begin{cases} \text{right-moving:} & \mathcal{O}_R(x) = e^{+ikx} \quad x \to +\infty \\ \text{left-moving:} & \mathcal{O}_L(x) = e^{-ikx} \quad x \to -\infty \end{cases}$$



The two asymptotic solutions (1.3) and (1.5) can then be written as

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} + \mathcal{S} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \tag{1.9}$$

where

$$\mathcal{S} = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix} \tag{1.10}$$

This is the *S-matrix*. As we've seen, for any given problem the entries of the matrix are rather complicated functions of k.

The S-matrix has many nice properties, some of which we will describe in these lectures. One of the simplest and most important is that $\mathcal{S}$ is unitary. To see this note that

$$\mathcal{S}\mathcal{S}^\dagger = \begin{pmatrix} |t'|^2 + |r|^2 & t'r'^\star + rt^\star \\ t'^\star r' + tr^\star & |t|^2 + |r'|^2 \end{pmatrix}$$

Unitarity then follows from the conservation of probability. The off-diagonal elements vanish by virtue of the relations $t' = t$ and $r' = -r^\star t/t^\star$ that we found in (1.6). Meanwhile, the diagonal elements are equal to one by (1.4) and so $\mathcal{S}\mathcal{S}^\dagger = \mathbf{1}$. The equivalence between conservation of probability and unitarity of the S-matrix is important, and will generalise to higher dimensions. Indeed, in quantum mechanics the word "unitarity" is often used synonymously with "conservation of probability".

One further property follows from the fact that the wavefunctions $\psi_R(x)$ and $\psi_L(x)$ do not change under complex conjugation if we simultaneously flip $k \to -k$. In other words $\psi(x;k) = \psi^\star(x;-k)$. This means that the S-matrix obeys

$$\mathcal{S}^\star(k) = \mathcal{S}(-k)$$

There are a number of other, more hidden properties of the S-matrix that we will uncover below.

1.1.3 A Parity Basis for Scattering

As we've seen above, for symmetric potentials, with $V(x) = V(-x)$, scattering from the left and right is the same. Let's first make this statement more formal.

We introduce the *parity* operator P which acts on functions $f(x)$ as

$$P : f(x) \to f(-x)$$

For symmetric potentials, we have $[P, H] = 0$ which means that eigenstates of the Hamiltonian can be chosen so that they are also eigenstates of P. The parity operator is Hermitian, $P^\dagger = P$, so its eigenvalues λ are real. But we also have $P^2 f(x) = f(x)$, which means that the eigenvalues must obey $\lambda^2 = 1$. Clearly there are only two possibilities: $\lambda = +1$ and $\lambda = -1$, This means that eigenstates of the Hamiltonian can be chosen to be either even functions ($\lambda = +1$) or odd functions ($\lambda = -1$).

Above we worked with scattering eigenstates ψ_R and ψ_L. These are neither odd nor even. Instead, for a symmetric potential, they are related by $\psi_L(x) = \psi_R(-x)$. This is the reason that symmetric potentials have $r = r'$. If we want to work with the parity eigenstates, we take

$$\begin{aligned}\psi_+(x) &= \psi_R(x) + \psi_L(x) = \psi_R(x) + \psi_R(-x)\\ \psi_-(x) &= -\psi_R(x) + \psi_L(x) = -\psi_R(x) + \psi_R(-x)\end{aligned}$$

which obey $P\psi_\pm(x) = \pm\psi_\pm(x)$.

Often, working with parity eigenstates makes the algebra a little easier. This is particularly true if our problem has a parity-invariant potential, $V(x) = V(-x)$.

The Pothole Example Revisited

Let's see how the use of parity eigenstates can make our calculations simpler. We'll redo the scattering calculation in the pothole, but now we'll take the asymptotic states to be ψ_+ and ψ_-. Physically, you can think of this experiment as throwing in particles from both the left and right at the same time, with appropriate choices of signs.

We start with the even parity wavefunction ψ_+. We want to patch this onto a solution in the middle, but this too must have even parity. This mean that the solution in the pothole takes the form

$$\psi_+(x) = A(e^{iqx} + e^{-iqx}) \qquad x \in [-a/2, a/2]$$

which now has only one unknown coefficient, A. As previously, $q^2 = k^2 + 2mV_0/\hbar^2$. We still need to make sure that both the wavefunction and its derivative are continuous at $x = \pm a/2$. But, because we're working with even functions, we only need to look at one of these points. At $x = a/2$ we get

$$\begin{aligned}e^{-ika/2} + (r+t)e^{ika/2} &= A(e^{iqa/2} + e^{-iqa/2})\\ \left(-e^{-ika/2} + (r+t)e^{ika/2}\right) &= \frac{q}{k}A(e^{iqa/2} - e^{-iqa/2})\end{aligned}$$

Notice that only the combination $(r+t)$ appears. We have two equations with two unknowns. If we divide the two equations and rearrange, we get

$$r + t = -e^{-ika}\,\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik} \tag{1.11}$$

which is all a lot easier than the messy manipulations we had to do when working with ψ_L and ψ_R. Of course, we've only got an expression for $(r+t)$. But we can play the

same game for the odd parity eigenstates to get a corresponding expression for $(r-t)$. Now, the solution in the pothole takes the form

$$\psi_-(x) = B(e^{iqx} - e^{-iqx}) \qquad x \in [-a/2, a/2]$$

Requiring continuity of the wavefunction and its derivative at $x = a/2$ we get

$$\begin{aligned} e^{-ika/2} + (r-t)e^{ika/2} &= B(e^{iqa/2} - e^{-iqa/2}) \\ \left(-e^{-ika/2} + (r-t)e^{ika/2}\right) &= \frac{q}{k}B(e^{iqa/2} + e^{-iqa/2}) \end{aligned}$$

Once again, dividing we find

$$r - t = e^{-ika}\frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)} \tag{1.12}$$

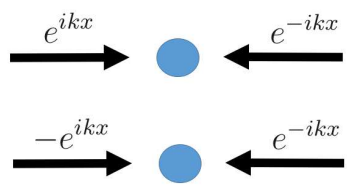
It's not immediately obvious that the expressions (1.11) and (1.12) are the same as those for r and t that we derived previously. But a little bit of algebra should convince you that they agree.

[A helping hand: this little bit of algebra is extremely fiddly if you don't go about it in the right way! Here's a reasonably a streamlined approach. First define the denominator of (1.8) as $D(k) = (q^2+k^2)\sin(qa) + 2iqk\cos(qa)$. Using the double-angle formula from trigonometry, we can write this as $D(k) = 2\cos^2(qa/2)(q\tan(qa/2) + ik)(q - ik\tan(qa/2))$. We can then add the two expressions in (1.8), and use the double-angle formula again, to get $r + t = 2e^{-ika}\cos^2(qa/2)(q\tan(qa/2) - ik)(ik\tan(qa/2) - q)/D(k)$ This coincides with our formula (1.11). Similar games give us the formula (1.12).]

The S-Matrix in the Parity Basis

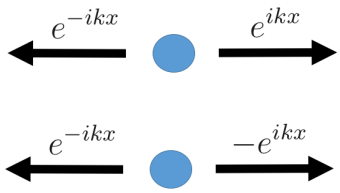
We can also think about the S-matrix using our new basis of states. The asymptotic ingoing modes are even and odd functions, given at $|x| \to \infty$ by

$$\text{Ingoing} \begin{cases} \text{parity-even:} & \mathcal{I}_+(x) = e^{-ik|x|} \\ \text{parity-odd:} & \mathcal{I}_-(x) = \text{sign}(x)\, e^{-ik|x|} \end{cases}$$



The two asymptotic outgoing modes are

$$\text{Outgoing} \begin{cases} \text{parity-even:} \qquad \mathcal{O}_+(x) = e^{+ik|x|} \\ \\ \text{parity-odd:} \qquad \mathcal{O}_-(x) = -\text{sign}(x)\, e^{+ik|x|} \end{cases}$$



These are related to our earlier modes by a simple change of basis,

$$\begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \quad \text{with} \quad \mathcal{M} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

We can define an S-matrix with respect to this parity basis. In analogy with (1.9), we write asymptotic solutions as

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} + \mathcal{S}^P \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} \tag{1.13}$$

where we use the notation $\mathcal{S}^P$ to denote the S-matrix with respect to the parity basis. We write

$$\mathcal{S}^P = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}$$

This is related to our earlier S-matrix by a change of basis. We have

$$\mathcal{S}^P = \mathcal{M} S \mathcal{M}^{-1} = \begin{pmatrix} t + (r+r')/2 & (r-r')/2 \\ (r'-r)/2 & t - (r+r')/2 \end{pmatrix}$$

As you may expect, this basis is particularly useful if the underlying potential is symmetric, so $V(x) = V(-x)$. In this case we have $r = r'$ and the S-matrix becomes diagonal. The diagonal components are simply

$$S_{++} = t + r \quad \text{and} \quad S_{--} = t - r$$

In fact, because $\mathcal{S}^p$ is unitary, each of these components must be a phase. This follows because r and t are not independent. First, they obey $|r|^2 + |t|^2 = 1$. Moreover, when $r' = r$, the relation (1.6) becomes

$$rt^\star + r^\star t = 0 \qquad \Rightarrow \qquad \text{Re}(rt\star) = 0$$

This is enough to ensure that both S_{++} and S_{--} are indeed phases. We write them as

$$S_{++} = e^{2i\delta_+(k)} \quad \text{and} \quad S_{--} = e^{2i\delta_-(k)}$$

We learn that for scattering off a symmetric potential, all the information is encoded in two momentum-dependent *phase shifts*, $\delta_\pm(k)$ which tell us how the phases of the outgoing waves $\mathcal{O}_\pm$ are changed with respect to the ingoing waves $\mathcal{I}_\pm$.

1.1.4 Bound States

So far we've focussed only on the scattering states of the problem. We now look at the bound states, which have energy $E < 0$ and are localised near inside the potential. Here, something rather magical happens. It turns out that the information about these bound states can be extracted from the S-matrix, which we constructed purely from knowledge of the scattering states.

To find the bound states, we need to do something clever. We take our scattering solutions, which depend on momentum $k \in \mathbf{R}$, and extend them to the complex momentum plane. This means that we analytically continue out solutions so that they depend on $k \in \mathbf{C}$.

First note that the solutions with $k \in \mathbf{C}$ still obey our original Schrödinger equation (1.1) since, at no point in any of our derivation did we assume that $k \in \mathbf{R}$. The only difficulty comes when we look at how the wavefunctions behave asymptotically. In particular, any putative solution will, in general, diverge exponentially as $x \to +\infty$ or $x \to -\infty$, rendering the wavefunction non-normalisable. However, as we will now show, there are certain solutions that survive.

For simplicity, let's assume that we have a symmetric potential $V(x) = V(-x)$. As we've seen above, this means that there's no mixing between the parity-even and parity-odd wavefunctions. We start by looking at the parity-even states. The general solution takes the form

$$\psi_+(x) = \mathcal{I}_+(x) + S_{++}\mathcal{O}_+(x) = \begin{cases} e^{+ikx} \ + \ S_{++}e^{-ikx} & x \to -\infty \\ e^{-ikx} \ + \ S_{++}e^{+ikx} & x \to +\infty \end{cases}$$

Suppose that we make k pure imaginary and write

$$k = i\lambda$$

with $\lambda > 0$. Then we get

$$\psi_+(x) = \begin{cases} e^{-\lambda x} \ + \ S_{++}e^{+\lambda x} & x \to -\infty \\ e^{+\lambda x} \ + \ S_{++}e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.14}$$

Both terms proportional to S_{++} decay asymptotically, but the other terms diverge. This is bad. However, there's a get-out. For any fixed k (whether real or complex), S_{++} is simply a number. That means that we're quite at liberty to divide by it. Indeed, the wavefunction above isn't normalised anyway, so dividing by a constant isn't going to change anything. We get

$$\psi_+(x) = \begin{cases} S_{++}^{-1}\, e^{-\lambda x} \;+\; e^{+\lambda x} & x \to -\infty \\ S_{++}^{-1}\, e^{+\lambda x} \;+\; e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.15}$$

Now we can see the loop-hole. The wavefunction above is normalisable whenever we can find a $\lambda > 0$ such that

$$S_{++}(k) \to \infty \qquad \text{as } k \to i\lambda$$

This, then, is the magic of the S-matrix. Poles in the complex momentum plane that lie on the positive imaginary axis (i.e. $k = i\lambda$ with $\lambda > 0$) correspond to bound states. This information also tells us the energy of the bound state since, as we saw in (1.2), it is given by

$$E = -\frac{\hbar^2\lambda^2}{2m}$$

We could also have set $k = -i\lambda$, with $\lambda > 0$. In this case, it is the terms proportional to S_{++} in (1.14) which diverge and the wavefunction is normalisable only if $S_{++}(k = -i\lambda) = 0$. However, since S_{++} is a phase, this is guaranteed to be true whenever $S_{++}(k = i\lambda)$ has a pole, and simply gives us back the solution above.

Finally, note that exactly the same arguments hold for parity-odd wavefunctions. There is a bound state whenever $S_{--}(k)$ has a pole at $k = i\lambda$ with $\lambda > 0$.

An Example: Stuck in the Pothole

We can illustrate this with our favourite example of the square well, of depth $-V_0$ and width a. We already computed the S-matrix in (1.11) and (1.12). We have,

$$S_{++}(k) = r + t = -e^{-ika}\,\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik}$$

where $q^2 = 2mV_0/\hbar^2 + k^2$. Setting $k = i\lambda$, we see that this has a pole when

$$\lambda = q\tan\left(\frac{qa}{2}\right) \qquad \text{with} \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

These are the usual equations that you have to solve when finding parity-even bound states in a square well. The form of the solutions is simplest to see if we plot these equations, as shown in the left-hand of Figure 4. There is always at least one bound state, with more appearing as the well gets deeper.

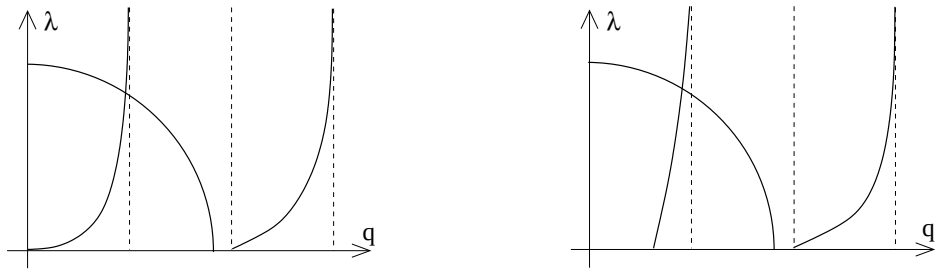


Figure 4: Bound state of even parity always exist, since the two equations shown on the left always have a solution with $\lambda, q > 0$. Bound states of odd parity, shown on the right, exist if the potential is deep enough.

Similarly, if we look at the parity-odd wavefunctions, we have

$$S_{--}(k) = t - r = e^{-ika}\frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)}$$

which has a pole at $k = i\lambda$ when

$$q = -\lambda \tan\left(\frac{qa}{2}\right) \qquad \text{with} \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2} \tag{1.16}$$

This too reproduces the equations that we found in earlier courses in quantum mechanics when searching for bound states in a square well. Now there is no guarantee that a bound state exists; this only happens if the potential is deep enough.

1.1.5 Resonances

We might wonder if there's any other information hidden in the analytic structure of the S-matrix. In this section, we will see that there is, although its interpretation is a little more subtle.

First, the physics. Let's think back again to the example shown on the right. One the one hand, we know that there can be no bound states in such a trap because they will have $E > 0$. Any particle that we place in the trap will ultimately tunnel out. On the other hand, if the walls of the trap are very large then we might expect that the particle stays there for a long time before it eventually escapes. In this situation, we talk of a *resonance*. These are also referred to as *unstable* or *metastable* states. Our goal is to show how such resonances are encoded in the S-matrix.

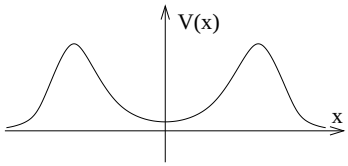


Figure 5:

Now, the maths. We'll restrict attention to parity-even functions. Suppose that the S-matrix S_{++} has a pole that lies on the complex momentum plane at position

$$k = k_0 - i\gamma$$

On general grounds, the wavefunction will have a second pole at $-k^\star = -k_0 - i\gamma$. We'd like to interpret these poles. First note that the energy is also imaginary

$$E = \frac{\hbar^2 k^2}{2m} \equiv E_0 - i\frac{\Gamma}{2} \tag{1.17}$$

with $E_0 = \hbar^2(k_0^2 - \gamma^2)/2m$ and $\Gamma = 2\hbar^2\gamma k_0/m$. An imaginary energy may sound strange, but it is has a very natural interpretation. Recall that the time dependence of the wavefunction is given by

$$e^{-iEt/\hbar} = e^{-iE_0 t/\hbar}\, e^{-\Gamma t/2\hbar} \tag{1.18}$$

This is the first clue that we need. We see that, for $\gamma > 0$, the overall form of the wavefunction decays exponentially with time. This is the characteristic behaviour of unstable states. A wavefunction that is initially supported inside the trap will be very small there at time much larger than $\tau = 1/\Gamma$. Here τ is called the *half-life* of the state, while Γ is usually referred to as the *width* of the state. (We'll see why in Section 1.2).

Where does the particle go? Including the time dependence (1.18), the same argument that led us to (1.15) now tells us that when $S_{++} \to \infty$, the solution takes the asymptotic form

$$\psi_+(x,t) = \begin{cases} e^{-iE_0 t/\hbar}\, e^{-ik_0 x}\, e^{-\gamma x - \Gamma t/2\hbar} & x \to -\infty \\ e^{-iE_0 t/\hbar}\, e^{+ik_0 x}\, e^{+\gamma x - \Gamma t/2\hbar} & x \to +\infty \end{cases} \tag{1.19}$$

The first two exponential factors oscillate. But the final factor varies as

$$e^{\pm\gamma(x \mp vt)} \quad \text{where} \quad v = \frac{\Gamma}{2\hbar\gamma} = \frac{\hbar k_0}{m}$$

This has the interpretation of a particle moving with momentum $\hbar k_0$. This, of course, is the particle which has escaped the trap.

Note that for fixed time t, these wavefunctions are not normalisable: they diverge at both $x \to \pm\infty$. This shouldn't concern us, because, although our wavefunctions are eigenstates of the Hamiltonian, they are not interpreted as stationary states. Indeed, it had to be the case. An unstable state has complex energy, but standard theorems in linear algebra tell us that a Hermitian operator like the Hamiltonian must have real eigenvalues. We have managed to evade this theorem only because these wavefunctions are non-normalisable and so do not, strictly speaking, live in the Hilbert space.

There's a lesson buried in all of this. If we were to take the standard axioms of quantum mechanics, we would simply throw away wavefunctions of the form (1.19) on the grounds that they do not lie in the Hilbert space and so are unphysical. But this would be a mistake: the wavefunctions do contain interesting physics, albeit of a slightly different variety than we are used to. Sometimes it's worth pushing our physical theories beyond our comfort zone to see what is lurking there.

The upshot of this discussion is that poles of the S-matrix in the lower-half complex plane correspond to resonances. It is often useful to write S_{++} as a function of energy rather than momentum. (They are related by (1.17)). Since S_{++} is a phase, close to a resonance it necessarily takes the form

$$S_{++} = \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}$$

An Example: A Pair of Delta-Functions

A pair of delta functions provide a simple and tractable example to illustrate the idea of resonances. The potential is given by

$$V(x) = V_0\Big[\delta(x-1) + \delta(x+1)\Big]$$

Recall that the effect of the delta-functions is simply to change the boundary conditions at $x = \pm 1$ when solving the Schrödinger equation. All wavefunctions should be continuous at $x = \pm 1$, but their derivatives are discontinuous. For example, at $x = +1$, solutions obey

$$\lim_{\epsilon \to 0} \Big[\psi'(1+\epsilon) - \psi'(1-\epsilon)\Big] = U_0\psi(1) \quad \text{with} \quad U_0 = \frac{2mV_0}{\hbar^2}$$

Working in the parity basis makes life simpler, not least because you only need to consider the matching at one of the delta-functions, with the other then guaranteed. The computation of the S-matrix is a problem on the exercise sheet. You will find

$$S_{++} = e^{-2ik}\left[\frac{(2k - iU_0)e^{ik} - iU_0 e^{-ik}}{(2k + iU_0)e^{-ik} + iU_0 e^{ik}}\right]$$

Note that the denominator is the complex conjugate of the numerator, ensuring that S_{++} is a phase, as expected. The poles of this S-matrix are given by solutions to the equation

$$e^{2ik} = -\left(1 - \frac{2ik}{U_0}\right) \tag{1.20}$$

To understand the physics behind this, let's first look at the situation where $U_0 \to \infty$, so that the weight of the delta-functions gets infinitely large. Then the poles sit at

$$e^{2ik} = -1 \quad \Rightarrow \quad k = k_n = \left(n + \frac{1}{2}\right)\pi$$

These correspond to bound states trapped between the two wavefunctions. For example, the $n = 0$ state is shown in the figure. Note that they're rather unusual because the poles sit on the real k-axis, rather than the imaginary k-axis. Correspondingly, these bound states have $E > 0$. This strange behaviour is only allowed because we have an infinitely large potential which forbids particles on one side of the barrier to cross to the other.

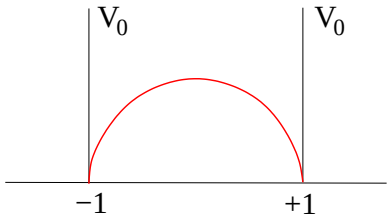


Figure 6:

As a side remark, we note that this same impenetrable behaviour is seen in scattering. When $U_0 \to \infty$, the S-matrix becomes $S_{++} \to -e^{2ik}$. This tells us that a particle coming from outside is completely reflected off the infinitely large barrier. The minus sign is the standard phase change after reflection. The factor of e^{2ik} is because the waves are forbidden from travelling through the region between the delta functions, which has width $x = 2$. As a result, the phase is shifted by e^{ikx} from what it would be if the barriers were removed.

Let's now look at what happens when U_0 is large, but finite? We'll focus on the lowest energy bound state with $n = 0$. We can expand (1.20) in $1/U_0$. (This too is left as a problem on the exercise sheet.) We find

$$k = \frac{\pi}{2} + \alpha - i\gamma$$

with

$$\alpha \approx -\frac{\pi}{2U_0} + \frac{\pi}{2U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right) \quad \text{and} \quad \gamma \approx \frac{\pi^2}{4U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right)$$

Note, in particular, that $\gamma > 0$, so the pole moves off the real axis and into the lower half-plane. This pole now has all the properties that we described at the beginning of this section. It describes a state, trapped between the two delta-functions, which decays with half-life

$$\tau = \frac{\hbar}{\Gamma} = \frac{4mU_0^2}{\hbar\pi^3}\left(1 + \mathcal{O}\left(\frac{1}{U_0}\right)\right)$$

This is the resonance.

1.2 Scattering in Three Dimensions

Our real interest in scattering is for particles moving in three spatial dimensions, with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$$

Recall that there are two distinct interpretations for such a Hamiltonian

- We could think of this as the motion of a single particle, moving in a fixed background potential $V(\mathbf{r})$. This would be appropriate, for example, in Rutherford's famous experiment where we fire an alpha particle at a gold nucleus.

- Alternatively, We could think of this as the relative motion of two particles, separated by distance $\mathbf{r}$, interacting through the force $\mathbf{F} = -\nabla V(\mathbf{r})$. We could take $V(r)$ to be the Coulomb force, to describe the scattering of electrons, or the Yukawa force to describe the scattering of neutrons.

In this section, we will use language appropriate to the first interpretation, but everything we say holds equally well in the second. Throughout this section, we will work with rotationally invariant (i.e. central) potentials, so that $V(\mathbf{r}) = V(|\mathbf{r}|)$.

1.2.1 The Cross-Section

Our first goal is to decide what we want to calculate. The simple reflection and transmission coefficients of the one-dimensional problem are no longer appropriate. We need to replace them by something a little more complicated. We start by thinking of the classical situation.

Classical Scattering

Suppose that we throw in a single particle with kinetic energy E. Its initial trajectory is characterised by the *impact parameter* b, defined as the closest the particle would get to the scattering centre at $r = 0$ if there were no potential. The particle emerges with *scattering angle* θ, which is the angle between the asymptotic incoming and outgoing trajectories, as shown in the figure. By solving the classical equations of motion, we can compute $\theta(b; E)$ or, equivalently, $b(\theta; E)$.

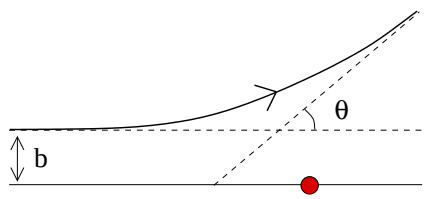


Figure 7:

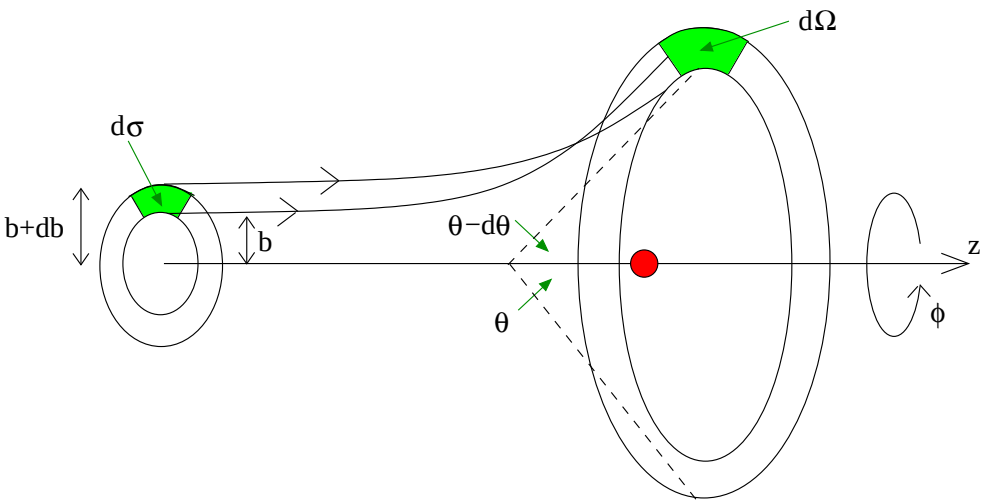


Figure 8: What becomes of an infinitesimal cross-sectional area after scattering.

Now consider a uniform beam of particles, each with kinetic energy E. We want to understand what becomes of this beam. Consider the cross-sectional area, denoted $d\sigma$ in Figure 8. We write this as

$$d\sigma = b\, d\phi\, db$$

The particles within $d\sigma$ will evolve to the lie in a cone of solid angle $d\Omega$, given by

$$d\Omega = \sin\theta\, d\phi\, d\theta$$

where, for central potentials, the infinitesimal angles $d\phi$ are the same in both these formulae. The *differential cross-section* is defined to be

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

The left-hand side should really be $|d\sigma/d\Omega|$, but we'll usually drop the modulus. The differential cross-section is a function of incoming momentum k, together with the outgoing angle θ.

More colloquially, the differential cross-section can be thought of as

$$\frac{d\sigma}{d\Omega}\, d\Omega = \frac{\text{Number of particles scattered into } d\Omega \text{ per unit time}}{\text{Number of incident particles per area } d\sigma \text{ per unit time}}$$

We write this in terms of *flux*, defined to be the number of particles per unit area per unit time. In this language, the differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{\text{Scattered flux}}{\text{Incident flux}}$$

6. Particles in a Magnetic Field

The purpose of this chapter is to understand how quantum particles react to magnetic fields. Before we get to describe quantum effects, we first need to highlight a few of the more subtle aspects that arise when discussing classical physics in the presence of a magnetic field.

6.1 Gauge Fields

Recall from our lectures on Electromagnetism that the electric field $\mathbf{E}(\mathbf{x},t)$ and magnetic field $\mathbf{B}(\mathbf{x},t)$ can be written in terms a scalar potential $\phi(\mathbf{x},t)$ and a vector potential $\mathbf{A}(\mathbf{x},t)$,

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A} \tag{6.1}$$

Both ϕ and $\mathbf{A}$ are referred to as *gauge fields*. When we first learn electromagnetism, they are introduced merely as handy tricks to help solve the Maxwell equations. However, as we proceed through theoretical physics, we learn that they play a more fundamental role. In particular, they are necessary if we want to discuss a Lagrangian or Hamiltonian approach to electromagnetism. We will soon see that these gauge fields are quite indispensable in quantum mechanics.

The Lagrangian for a particle of charge q and mass m moving in a background electromagnetic fields is

$$L = \frac{1}{2}m\dot{\mathbf{x}}^2 + q\dot{\mathbf{x}}\cdot\mathbf{A} - q\phi \tag{6.2}$$

The classical equation of motion arising from this Lagrangian is

$$m\ddot{\mathbf{x}} = q\left(\mathbf{E} + \dot{\mathbf{x}}\times\mathbf{B}\right)$$

This is the *Lorentz force law*.

Before we proceed I should warn you of a minus sign issue. We will work with a general charge q. However, many textbooks work with the charge of the electron, written as $q = -e$. If this minus sign leans to confusion, you should blame Benjamin Franklin.

An Example: Motion in a Constant Magnetic Field

We'll take a constant magnetic field, pointing in the z-direction: $\mathbf{B} = (0, 0, B)$. We'll take $\mathbf{E} = 0$. The particle is free in the z-direction, with the equation of motion $m\ddot{z} = 0$. The more interesting dynamics takes place in the (x, y)-plane where the equations of motion are

$$m\ddot{x} = qB\dot{y} \quad \text{and} \quad m\ddot{y} = -qB\dot{x} \tag{6.3}$$

which has general solution is

$$x(t) = X + R\sin(\omega_B(t - t_0)) \quad \text{and} \quad y(t) = Y + R\cos(\omega_B(t - t_0))$$

We see that the particle moves in a circle which, for $B > 0$ and $q > 0$, is in a clockwise direction. The *cyclotron frequency* is defined by

$$\omega_B = \frac{qB}{m} \tag{6.4}$$

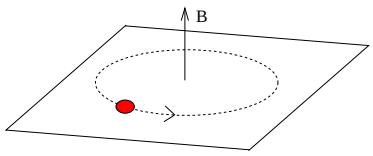


Figure 78:

The centre of the circle (X, Y), the radius of the circle R and the phase t_0 are all arbitrary. These are the four integration constants expected in the solution of two, second order differential equations.

6.1.1 The Hamiltonian

The *canonical momentum* in the presence of gauge fields is

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}} = m\dot{\mathbf{x}} + q\mathbf{A} \tag{6.5}$$

This clearly is not the same as what we naively call momentum, namely $m\dot{\mathbf{x}}$.

The Hamiltonian is given by

$$H = \dot{\mathbf{x}} \cdot \mathbf{p} - L = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi$$

Written in terms of the velocity of the particle, the Hamiltonian looks the same as it would in the absence of a magnetic field: $H = \frac{1}{2}m\dot{\mathbf{x}}^2 + q\phi$. This is the statement that a magnetic field does no work and so doesn't change the energy of the system. However, there's more to the Hamiltonian framework than just the value of H. We need to remember which variables are canonical. This information is encoded in the Poisson bracket structure of the theory (or, in fancy language, the symplectic structure on phase space). The fact that $\mathbf{x}$ and $\mathbf{p}$ are canonical means that

$$\{x_i, p_j\} = \delta_{ij} \quad \text{with} \quad \{x_i, x_j\} = \{p_i, p_j\} = 0$$

In the quantum theory, this structure transferred onto commutation relations between operators, which become

$$[x_i, p_j] = i\hbar\delta_{ij} \quad \text{with} \quad [x_i, x_j] = [p_i, p_j] = 0$$

6.1.2 Gauge Transformations

The gauge fields $\mathbf{A}$ and ϕ are not unique. We can change them as

$$\phi \to \phi - \frac{\partial \alpha}{\partial t} \quad \text{and} \quad \mathbf{A} \to \mathbf{A} + \nabla\alpha \tag{6.6}$$

for any function $\alpha(\mathbf{x}, t)$. Under these transformations, the electric and magnetic fields (6.1) remain unchanged, as does the Lagrangian (6.2) and the resulting equations of motion (6.3). Different choices of α are said to be different choices of *gauge*. We'll see some examples below.

The existence of gauge transformations is a redundancy in our description of the system: fields which differ by the transformation (6.6) describe physically identical configurations. Nothing that we can physically measure can depend on our choice of gauge. This, it turns out, is a beautifully subtle and powerful restriction. We will start to explore some of these subtleties in Sections 6.3 and 6.4

The canonical momentum $\mathbf{p}$ defined in (6.5) is not gauge invariant: it transforms as $\mathbf{p} \to \mathbf{p} + q\nabla\alpha$. This means that the numerical value of $\mathbf{p}$ can't have any physical meaning since it depends on our choice of gauge. In contrast, the velocity of the particle $\dot{\mathbf{x}}$ and the Hamiltonian H are both gauge invariant, and therefore physical.

The Schrödinger Equation

Finally, we can turn to the quantum theory. We'll look at the spectrum in the next section, but first we wish to understand how gauge transformations work. Following the usual quantisation procedure, we replace the canonical momentum with

$$\mathbf{p} \mapsto -i\hbar\nabla$$

The time-dependent Schrödinger equation for a particle in an electric and magnetic field then takes the form

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \frac{1}{2m}\Big(-i\hbar\nabla - q\mathbf{A}\Big)^2\psi + q\phi\psi \tag{6.7}$$

The shift of the kinetic term to incorporate the vector potential $\mathbf{A}$ is sometimes referred to as *minimal coupling*.

Before we solve for the spectrum, there are two lessons to take away. The first is that it is not possible to formulate the quantum mechanics of particles moving in electric and magnetic fields in terms of $\mathbf{E}$ and $\mathbf{B}$ alone. We're obliged to introduce the gauge fields $\mathbf{A}$ and ϕ. This might make you wonder if, perhaps, there is more to $\mathbf{A}$ and ϕ than we first thought. We'll see the answer to this question in Section 6.3. (Spoiler: the answer is yes.)

The second lesson follows from looking at how (6.7) fares under gauge transformations. It is simple to check that the Schrödinger equation transforms covariantly (i.e. in a nice way) only if the wavefunction itself also transforms with a position-dependent phase

$$\psi(\mathbf{x}, t) \to e^{iq\alpha(\mathbf{x},t)/\hbar}\psi(\mathbf{x}, t) \tag{6.8}$$

This is closely related to the fact that $\mathbf{p}$ is not gauge invariant in the presence of a magnetic field. Importantly, this gauge transformation does not affect physical probabilities which are given by $|\psi|^2$.

The simplest way to see that the Schrödinger equation transforms nicely under the gauge transformation (6.8) is to define the *covariant derivatives*

$$\mathcal{D}_t = \frac{\partial}{\partial t} + \frac{iq}{\hbar}\phi \quad \text{and} \quad \mathcal{D}_i = \frac{\partial}{\partial x^i} - \frac{iq}{\hbar}A_i$$

In terms of these covariant derivatives, the Schrödinger equation becomes

$$i\hbar\mathcal{D}_t\psi = -\frac{\hbar}{2m}\mathcal{D}^2\psi \tag{6.9}$$

But these covariant derivatives are designed to transform nicely under a gauge transformation (6.6) and (6.8). You can check that they pick up only a phase

$$\mathcal{D}_t\psi \to e^{iq\alpha/\hbar}\,\mathcal{D}_t\psi \quad \text{and} \quad \mathcal{D}_i\psi \to e^{iq\alpha/\hbar}\,\mathcal{D}_i\psi$$

This ensures that the Schrödinger equation (6.9) transforms covariantly.

6.2 Landau Levels

Our task now is to solve for the spectrum and wavefunctions of the Schrödinger equation. We are interested in the situation with vanishing electric field, $\mathbf{E} = 0$, and constant magnetic field. The quantum Hamiltonian is

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 \tag{6.10}$$

We take the magnetic field to lie in the z-direction, so that $\mathbf{B} = (0, 0, B)$. To proceed, we need to find a gauge potential $\mathbf{A}$ which obeys $\nabla \times \mathbf{A} = \mathbf{B}$. There is, of course, no unique choice. Here we pick

$$\mathbf{A} = (0, xB, 0) \tag{6.11}$$

This is called *Landau gauge*. Note that the magnetic field $\mathbf{B} = (0, 0, B)$ is invariant under both translational symmetry and rotational symmetry in the (x, y)-plane. However, the choice of $\mathbf{A}$ is not; it breaks translational symmetry in the x direction (but not in the y direction) and rotational symmetry. This means that, while the physics will be invariant under all symmetries, the intermediate calculations will not be manifestly invariant. This kind of compromise is typical when dealing with magnetic field.

The Hamiltonian (6.10) becomes

$$H = \frac{1}{2m}\left(p_x^2 + (p_y - qBx)^2 + p_z^2\right)$$

Because we have manifest translational invariance in the y and z directions, we have $[p_y, H] = [p_z, H] = 0$ and can look for energy eigenstates which are also eigenstates of p_y and p_z. This motivates the ansatz

$$\psi(\mathbf{x}) = e^{ik_y y + ik_z z}\,\chi(x) \tag{6.12}$$

Acting on this wavefunction with the momentum operators $p_y = -i\hbar\partial_y$ and $p_z = -i\hbar\partial_z$, we have

$$p_y\psi = \hbar k_y \psi \quad \text{and} \quad p_z\psi = \hbar k_z \psi$$

The time-independent Schrödinger equation is $H\psi = E\psi$. Substituting our ansatz (6.12) simply replaces p_y and p_z with their eigenvalues, and we have

$$H\psi(\mathbf{x}) = \frac{1}{2m}\Big[p_x^2 + (\hbar k_y - qBx)^2 + \hbar^2 k_z^2\Big]\psi(\mathbf{x}) = E\psi(\mathbf{x})$$

We can write this as an eigenvalue equation for the equation $\chi(x)$. We have

$$\tilde{H}\chi(x) = \left(E - \frac{\hbar^2 k_z^2}{2m}\right)\chi(x)$$

where $\tilde{H}$ is something very familiar: it's the Hamiltonian for a harmonic oscillator in the x direction, with the centre displaced from the origin,

$$\tilde{H} = \frac{1}{2m}p_x^2 + \frac{m\omega_B^2}{2}(x - k_y l_B^2)^2 \tag{6.13}$$

The frequency of the harmonic oscillator is again the cyloctron frequency $\omega_B = qB/m$, and we've also introduced a length scale l_B. This is a characteristic length scale which governs any quantum phenomena in a magnetic field. It is called the *magnetic length*.

$$l_B = \sqrt{\frac{\hbar}{qB}}$$

To give you some sense for this, in a magnetic field of $B = 1$ *Tesla*, the magnetic length for an electron is $l_B \approx 2.5 \times 10^{-8}$ m.

Something rather strange has happened in the Hamiltonian (6.13): the momentum in the y direction, $\hbar k_y$, has turned into the position of the harmonic oscillator in the x direction, which is now centred at $x = k_y l_B^2$.

We can immediately write down the energy eigenvalues of (6.13); they are simply those of the harmonic oscillator

$$E = \hbar\omega_B \left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m} \qquad n = 0, 1, 2, \ldots \tag{6.14}$$

The wavefunctions depend on three quantum numbers, $n \in \mathbf{N}$ and $k_y, k_z \in \mathbf{R}$. They are

$$\psi_{n,k}(x, y) \sim e^{ik_y y + ik_z z}\, H_n(x - k_y l_B^2) e^{-(x - k_y l_B^2)^2/2l_B^2} \tag{6.15}$$

with H_n the usual Hermite polynomial wavefunctions of the harmonic oscillator. The $\sim$ reflects the fact that we have made no attempt to normalise these these wavefunctions.

The wavefunctions look like strips, extended in the y direction but exponentially localised around $x = k_y l_B^2$ in the x direction. However, you shouldn't read too much into this. As we will see shortly, there is large degeneracy of wavefunctions and by taking linear combinations of these states we can cook up wavefunctions that have pretty much any shape you like.

6.2.1 Degeneracy

The dynamics of the particle in the z-direction is unaffected by the magnetic field $\mathbf{B} = (0, 0, B)$. To focus on the novel physics, let's restrict to particles with $k_z = 0$. The energy spectrum then coincides with that of a harmonic oscillator,

$$E_n = \hbar\omega_B \left(n + \frac{1}{2}\right) \tag{6.16}$$

In the present context, these are called *Landau levels*. We see that, in the presence of a magnetic field, the energy levels of a particle become equally spaced, with the gap between each level proportional to the magnetic field B. Note that the energy spectrum looks very different from a free particle moving in the (x, y)-plane.

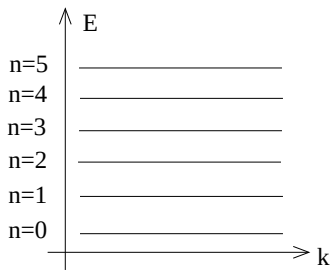


Figure 79: Landau Levels

The states in a given Landau level are not unique. Instead, there is a huge degeneracy, with many states having the same energy. We can see this in the form of the wavefunctions (6.15) which, when $k_z = 0$, depend on two quantum numbers, n and k_y. Yet the energy (6.16) is independent of k_y.

Let's determine how large this degeneracy of states is. To do so, we need to restrict ourselves to a finite region of the (x, y)-plane. We pick a rectangle with sides of lengths L_x and L_y. We want to know how many states fit inside this rectangle.

Having a finite size L_y is like putting the system in a box in the y-direction. The wavefunctions must obey

$$\psi(x, y + L_y, z) = \psi(x, y, z) \quad \Rightarrow \quad e^{ik_y L_y} = 1$$

This means that the momentum k_y is quantised in units of $2\pi/L_y$.

Having a finite size L_x is somewhat more subtle. The reason is that, as we mentioned above, the gauge choice (6.11) does not have manifest translational invariance in the x-direction. This means that our argument will be a little heuristic. Because the wavefunctions (6.15) are exponentially localised around $x = k_y l_B^2$, for a finite sample restricted to $0 \leq x \leq L_x$ we would expect the allowed k_y values to range between $0 \leq k_y \leq L_x/l_B^2$. The end result is that the number of states in each Landau level is given by

$$\mathcal{N} = \frac{L_y}{2\pi} \int_0^{L_x/l_B^2} dk = \frac{L_x L_y}{2\pi l_B^2} = \frac{qBA}{2\pi\hbar} \tag{6.17}$$

where $A = L_x L_y$ is the area of the sample. Strictly speaking, we should take the integer part of the answer above.

The degeneracy (6.17) is very very large. Throwing in some numbers, there are around 10^{10} degenerate states per Landau level for electrons in a region of area $A = 1\ cm^2$ in a magnetic field $B \sim 0.1\ T$. This large degeneracy ultimately, this leads to an array of dramatic and surprising physics.

6.2.2 Symmetric Gauge

It is worthwhile to repeat the calculations above using a different gauge choice. This will give us a slightly different perspective on the physics. A natural choice is *symmetric gauge*

$$\mathbf{A} = -\frac{1}{2}\mathbf{x} \times \mathbf{B} = \frac{B}{2}(-y, x, 0) \tag{6.18}$$

This choice of gauge breaks translational symmetry in both the x and the y directions. However, it does preserve rotational symmetry about the origin. This means that angular momentum is now a good quantum number to label states.

In this gauge, the Hamiltonian is given by

$$\begin{aligned} H &= \frac{1}{2m}\left[\left(p_x + \frac{qBy}{2}\right)^2 + \left(p_y - \frac{qBx}{2}\right)^2 + p_z^2\right] \\ &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{qB}{2m}L_z + \frac{q^2B^2}{8m}\left(x^2 + y^2\right) \end{aligned} \tag{6.19}$$

where we've introduced the angular momentum operator

$$L_z = xp_y - yp_x$$

We'll again restrict to motion in the (x, y)-plane, so we focus on states with $k_z = 0$. It turns out that complex variables are particularly well suited to describing states in symmetric gauge, in particular in the lowest Landau level with $n = 0$. We define

$$w = x + iy \quad \text{and} \quad \bar{w} = x - iy$$

Correspondingly, the complex derivatives are

$$\partial = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) \quad \text{and} \quad \bar{\partial} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)$$

which obey $\partial w = \bar{\partial}\bar{w} = 1$ and $\partial\bar{w} = \bar{\partial}w = 0$. The Hamiltonian, restricted to states with $k_z = 0$, is then given by

$$H = -\frac{2\hbar^2}{m}\partial\bar{\partial} - \frac{\omega_B}{2}L_z + \frac{m\omega_B^2}{8}w\bar{w}$$

where now

$$L_z = \hbar(w\partial - \bar{w}\bar{\partial})$$

It is simple to check that the states in the lowest Landau level take the form

$$\psi_0(w,\bar{w}) = f(w)e^{-|w|^2/4l_B^2}$$

for *any* holomorphic function $f(w)$. These all obey

$$H\psi_0(w,\bar{w}) = \frac{\hbar\omega_B}{2}\psi_0(w,\bar{w})$$

which is the statement that they lie in the lowest Landau level with $n = 0$. We can further distinguish these states by requiring that they are also eigenvalues of L_z. These are satisfied by the monomials,

$$\psi_0 = w^M e^{-|w|^2/4l_B^2} \quad \Rightarrow \quad L_z\psi_0 = \hbar M\psi_0 \tag{6.20}$$

for some positive integer M.

Degeneracy Revisited

In symmetric gauge, the profiles of the wavefunctions (6.20) form concentric rings around the origin. The higher the angular momentum M, the further out the ring. This, of course, is very different from the strip-like wavefunctions that we saw in Landau gauge (6.15). You shouldn't read too much into this other than the fact that the profile of the wavefunctions is not telling us anything physical as it is not gauge invariant.

However, it's worth revisiting the degeneracy of states in symmetric gauge. The wavefunction with angular momentum M is peaked on a ring of radius $r = \sqrt{2M}l_B$. This means that in a disc shaped region of area $A = \pi R^2$, the number of states is roughly (the integer part of)

$$\mathcal{N} = R^2/2l_B^2 = A/2\pi l_B^2 = \frac{qBA}{2\pi\hbar}$$

which agrees with our earlier result (6.17).

6.2.3 An Invitation to the Quantum Hall Effect

Take a system with some fixed number of electrons, which are restricted to move in the (x,y)-plane. The charge of the electron is $q = -e$. In the presence of a magnetic field, these will first fill up the $\mathcal{N} = eBA/2\pi\hbar$ states in the $n = 0$ lowest Landau level. If any are left over they will then start to fill up the $n = 1$ Landau level, and so on.

Now suppose that we increase the magnetic field B. The number of states $\mathcal{N}$ housed in each Landau level will increase, leading to a depletion of the higher Landau levels. At certain, very special values of B, we will find some number of Landau levels that are exactly filled. However, generically there will be a highest Landau level which is only partially filled.

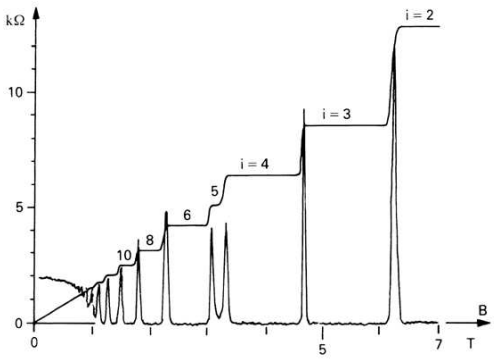


Figure 80: The integer quantum Hall effect.

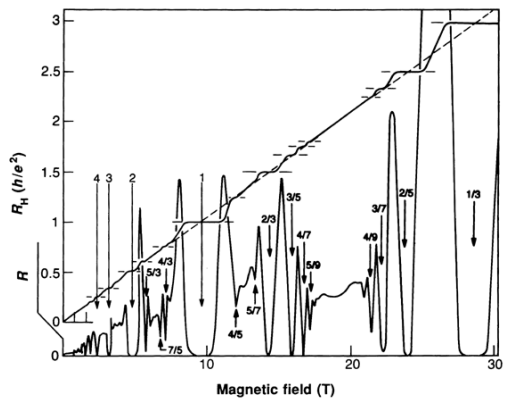


Figure 81: The fractional quantum Hall effect.

This successive depletion of Landau levels gives rise to a number of striking signatures in different physical quantities. Often these quantities oscillate, or jump discontinuously as the number of occupied Landau levels varies. One particular example is the de Haas van Alphen oscillations seen in the magnetic susceptibility which we describe in Section 4.3.4. Another example is the behaviour of the resistivity ρ. This relates the current density $\mathbf{J} = (J_x, J_y)$ to the applied electric field $\mathbf{E} = (E_x, E_y)$,

$$\mathbf{E} = \rho \mathbf{J}$$

In the presence of an applied magnetic field $\mathbf{B} = (0, 0, B)$, the electrons move in circles. This results in components of the current which are both parallel and perpendicular to the electric field. This is modelled straightforwardly by taking ρ to be a matrix

$$\rho = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix}$$

where the form of the matrix follows from rotational invariance. Here ρ_{xx} is called the *longitudinal resistivity* while ρ_{xy} is called the *Hall resistivity.*

In very clean samples, in strong magnetic fields, both components of the resistivity exhibit very surprising behaviour. This is shown in the left-hand figure above. The Hall resistivity ρ_{xy} increases with B by forming a series of plateaux, on which it takes values

$$\rho_{xy} = \frac{2\pi\hbar}{e^2}\frac{1}{\nu} \qquad \nu \in \mathbf{N}$$

The value of ν (which is labelled $i = 2, 3, \ldots$ in the data shown above) is measured to be an integer to extraordinary accuracy — around one part in 10^9. Meanwhile,

the longitudinal resistivity vanishes when ρ_{xy} lies on a plateaux, but spikes whenever there is a transition between different plateaux. This phenomenon, called the *integer Quantum Hall Effect*, was discovered by Klaus von Klitzing in 1980. For this, he was awarded the Nobel prize in 1985.

It turns out that the integer quantum Hall effect is a direct consequence of the existence of discrete Landau levels. The plateaux occur when precisely $\nu \in \mathbf{Z}^+$ Landau levels are filled. Of course, we're very used to seeing integers arising in quantum mechanics — this, after all, is what the "quantum" in quantum mechanics means. However, the quantisation of the resistivity ρ_{xy} is something of a surprise because this is a macroscopic quantity, involving the collective behaviour of many trillions of electrons, swarming through a hot and dirty system. A full understanding of the integer quantum Hall effect requires an appreciation of how the mathematics of topology fits in with quantum mechanics. David Thouless (and, to some extent, Duncan Haldane) were awarded the 2016 Nobel prize for understanding the underlying role of topology in this system.

Subsequently it was realised that similar behaviour also happens when Landau levels are partially filled. However, it doesn't occur for any filling, but only very special values. This is referred to as the *fractional quantum Hall effect*. The data is shown in the right-hand figure. You can see clear plateaux when the lowest Landau level has $\nu = \frac{1}{3}$ of its states filled. There is another plateaux when $\nu = \frac{2}{5}$ of the states are filled, followed by a bewildering pattern of further plateaux, all of which occur when ν is some rational number. This was discovered by Tsui and Störmer in 1982. It called the *Fractional Quantum Hall Effect*. The 1998 Nobel prize was awarded to Tsui and Stormer, together with Laughlin who pioneered the first theoretical ideas to explain this behaviour.

The fractional quantum Hall effect cannot be explained by treating the electrons as free. Instead, it requires us to take interactions into account. We have seen that each Landau level has a macroscopically large degeneracy. This degeneracy is lifted by interactions, resulting in a new form of quantum liquid which exhibits some magical properties. For example, in this state of matter the electron — which, of course, is an indivisible particle — can split into constituent parts! The $\nu = \frac{1}{3}$ state has excitations which carry 1/3 of the charge of an electron. In other quantum Hall states, the excitations have charge 1/5 or 1/4 of the electron. These particles also have a number of other, even stranger properties to do with their quantum statistics and there is hope that these may underly the construction of a quantum computer.

We will not delve into any further details of the quantum Hall effect. Suffice to say that it is one of the richest and most beautiful subjects in theoretical physics. You can find a fuller exploration of these ideas in the lecture notes devoted to the Quantum Hall Effect.

6.3 The Aharonov-Bohm Effect

In our course on Electromagnetism, we learned that the gauge potential A_μ is unphysical: the physical quantities that affect the motion of a particle are the electric and magnetic fields. Yet we've seen above that we cannot formulate quantum mechanics without introducing the gauge fields $\mathbf{A}$ and ϕ. This might lead us to wonder whether there is more to life than $\mathbf{E}$ and $\mathbf{B}$ alone. In this section we will see that things are, indeed, somewhat more subtle.

6.3.1 Particles Moving around a Flux Tube

Consider the set-up shown in the figure. We have a solenoid of area A, carrying magnetic field $\mathbf{B} = (0, 0, B)$ and therefore magnetic flux $\Phi = BA$. Outside the solenoid the magnetic field is zero. However, the vector potential is not. This follows from Stokes' theorem which tells us that the line integral outside the solenoid is given by

$$\oint \mathbf{A} \cdot d\mathbf{x} = \int \mathbf{B} \cdot d\mathbf{S} = \Phi$$

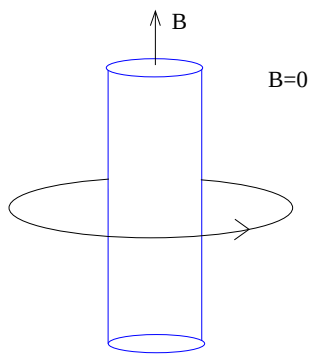


Figure 82:

This is simply solved in cylindrical polar coordinates by

$$A_\phi = \frac{\Phi}{2\pi r}$$

Now consider a charged quantum particle restricted to lie in a ring of radius r outside the solenoid. The only dynamical degree of freedom is the angular coordinate $\phi \in [0, 2\pi)$. The Hamiltonian is

$$H = \frac{1}{2m}\left(p_\phi - qA_\phi\right)^2 = \frac{1}{2mr^2}\left(-i\hbar\frac{\partial}{\partial\phi} - \frac{q\Phi}{2\pi}\right)^2$$

We'd like to see how the presence of this solenoid affects the particle. The energy eigenstates are simply

$$\psi = \frac{1}{\sqrt{2\pi r}}\, e^{in\phi} \qquad n \in \mathbf{Z} \tag{6.21}$$

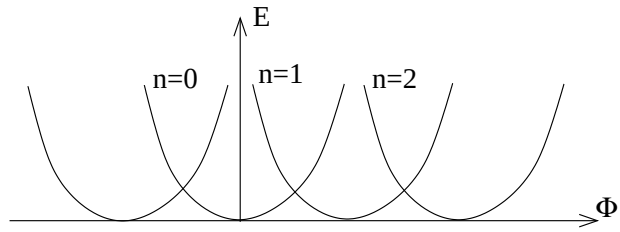


Figure 83: The energy spectrum for a particle moving around a solenoid.

where the requirement that ψ is single valued around the circle means that we must take $n \in \mathbf{Z}$. Plugging this into the time independent Schrödinger equation $H\psi = E\psi$, we find the spectrum

$$E = \frac{1}{2mr^2}\left(\hbar n - \frac{q\Phi}{2\pi}\right)^2 = \frac{\hbar^2}{2mr^2}\left(n - \frac{\Phi}{\Phi_0}\right)^2 \qquad n \in \mathbf{Z}$$

where we've defined the *quantum of flux* $\Phi_0 = 2\pi\hbar/q$. (Usually this quantum of flux is defined using the electron charge $q = -e$, with the minus signs massaged so that $\Phi_0 \equiv 2\pi\hbar/e > 0$.)

Note that if Φ is an integer multiple of Φ_0, then the spectrum is unaffected by the solenoid. But if the flux in the solenoid is not an integral multiple of Φ_0 — and there is no reason that it should be — then the spectrum gets shifted. We see that the energy of the particle knows about the flux Φ even though the particle never goes near the region with magnetic field. The resulting energy spectrum is shown in Figure 83.

There is a slightly different way of looking at this result. Away from the solenoid, the gauge field is a total divergence

$$\mathbf{A} = \nabla\alpha \quad \text{with} \quad \alpha = \frac{\Phi\phi}{2\pi}$$

This means that we can try to remove it by redefining the wavefunction to be

$$\psi \to \tilde{\psi} = \exp\left(\frac{-iq\alpha}{\hbar}\right)\psi = \exp\left(\frac{-iq\Phi}{2\pi\hbar}\phi\right)\psi$$

However, there is an issue: the wavefunction should be single-valued. This, after all, is how we got the quantisation condition $n \in \mathbf{Z}$ in (6.21). This means that the gauge transformation above is allowed only if Φ is an integer multiple of $\Phi_0 = 2\pi\hbar/q$. Only in this case is the particle unaffected by the solenoid. The obstacle arises from the fact that the wavefunction of the particle winds around the solenoid. We see here the first glimpses of how topology starts to feed into quantum mechanics.

There are a number of further lessons lurking in this simple quantum mechanical set-up. You can read about them in the lectures on the Quantum Hall Effect (see Section 1.5.3) and the lectures on Gauge Theory (see Section 3.6.1).

6.3.2 Aharonov-Bohm Scattering

The fact that a quantum particle can be affected by $\mathbf{A}$ even when restricted to regions where $\mathbf{B} = 0$ was first pointed out by Aharonov and Bohm in a context which is closely related to the story above. They revisited the famous double-slit experiment, but now with a twist: a solenoid carrying flux Φ is hidden behind the wall. This set-up is shown in the figure below. Once again, the particle is forbidden from going near the solenoid. Nonetheless, the presence of the magnetic flux affects the resulting interference pattern, shown as the dotted line in the figure.

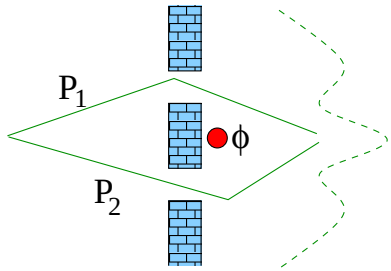


Figure 84:

Consider a particle that obeys the free Schrödinger equation,

$$\frac{1}{2m}\Big(-i\hbar\nabla - q\mathbf{A}\Big)^2\psi = E\psi$$

We can formally remove the gauge field by writing

$$\psi(\mathbf{x}) = \exp\left(\frac{iq}{\hbar}\int^{\mathbf{x}} \mathbf{A}(\mathbf{x}')\cdot d\mathbf{x}'\right)\phi(\mathbf{x})$$

where the integral is over any path. Crucially, however, in the double-slit experiment there are two paths, P_1 and P_2. The phase picked up by the particle due to the gauge field differs depending on which path is taken. The phase difference is given by

$$\Delta\theta = \frac{q}{\hbar}\int_{P_1}\mathbf{A}\cdot d\mathbf{x} - \frac{q}{\hbar}\int_{P_2}\mathbf{A}\cdot d\mathbf{x} = \frac{q}{\hbar}\oint\mathbf{A}\cdot d\mathbf{x} = \frac{q}{\hbar}\int\mathbf{B}\cdot d\mathbf{S}$$

Note that neither the phase arising from path P_1, nor the phase arising from path P_2, is gauge invariant. However, the difference between the two phases is gauge invariant. As we see above, it is given by the flux through the solenoid. This is the Aharonov-Bohm phase, $e^{iq\Phi/\hbar}$, an extra contribution that arises when charged particles move around magnetic fields.

The Aharonov-Bohm phase manifests in the interference pattern seen on the screen. As Φ is changed, the interference pattern shifts, an effect which has been experimentally observed. Only when Φ is an integer multiple of Φ_0 is the particle unaware of the presence of the solenoid.

6.4 Magnetic Monopoles

A *magnetic monopole* is a hypothetical object which emits a radial magnetic field of the form

$$\mathbf{B} = \frac{g\hat{\mathbf{r}}}{4\pi r^2} \quad \Rightarrow \quad \int d\mathbf{S} \cdot \mathbf{B} = g \tag{6.22}$$

Here g is called the *magnetic charge*.

We learned in our first course on Electromagnetism that magnetic monopoles don't exist. First, and most importantly, they have never been observed. Second there's a law of physics which insists that they can't exist. This is the Maxwell equation

$$\nabla \cdot \mathbf{B} = 0$$

Third, this particular Maxwell equation would appear to be non-negotiable. This is because it follows from the definition of the magnetic field in terms of the gauge field

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \Rightarrow \quad \nabla \cdot \mathbf{B} = 0$$

Moreover, as we've seen above, the gauge field $\mathbf{A}$ is necessary to describe the quantum physics of particles moving in magnetic fields. Indeed, the Aharonov-Bohm effect tells us that there is non-local information stored in $\mathbf{A}$ that can only be detected by particles undergoing closed loops. All of this points to the fact that we would be wasting our time discussing magnetic monopoles any further.

Happily, there is a glorious loophole in all of these arguments, first discovered by Dirac, and magnetic monopoles play a crucial role in our understanding of the more subtle effects in gauge theories. The essence of this loophole is that there is an ambiguity in how we define the gauge potentials. In this section, we will see how this arises.

6.4.1 Dirac Quantisation

It turns out that not any magnetic charge g is compatible with quantum mechanics. Here we present several different arguments for the allowed values of g.

We start with the simplest and most physical of these arguments. Suppose that a particle with charge q moves along some closed path C in the background of some gauge potential $\mathbf{A}(\mathbf{x})$. Then, upon returning to its initial starting position, the wavefunction of the particle picks up a phase

$$\psi \to e^{iq\alpha/\hbar}\psi \quad \text{with} \quad \alpha = \oint_C \mathbf{A} \cdot d\mathbf{x} \tag{6.23}$$

This is the Aharonov-Bohm phase described above.

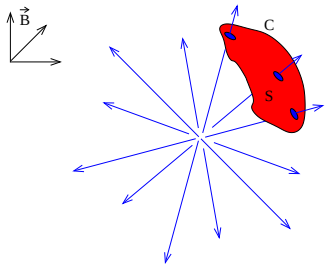


Figure 85: Integrating over S...

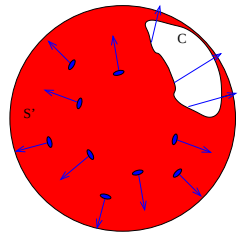


Figure 86: ...or over S'.

The phase of the wavefunction is not an observable quantity in quantum mechanics. However, as we described above, the phase in (6.23) is really a *phase difference*. We could, for example, place a particle in a superposition of two states, one of which stays still while the other travels around the loop C. The subsequent interference will depend on the phase $e^{iq\alpha/\hbar}$, just like in the Aharonov-Bohm effect.

Let's now see what this has to do with magnetic monopoles. We place our particle, with electric charge q, in the background of a magnetic monopole with magnetic charge g. We keep the magnetic monopole fixed, and let the electric particle undergo some journey along a path C. We will ask only that the path C avoids the origin where the magnetic monopole is sitting. This is shown in the left-hand panel of the figure. Upon returning, the particle picks up a phase $e^{iq\alpha/\hbar}$ with

$$\alpha = \oint_C \mathbf{A} \cdot d\mathbf{x} = \int_S \mathbf{B} \cdot d\mathbf{S}$$

where, as shown in the figure, S is the area enclosed by C. Using the fact that $\int_{\mathbf{S}^2} \mathbf{B} \cdot d\mathbf{S} = g$, if the surface S makes a solid angle Ω, this phase can be written as

$$\alpha = \frac{\Omega g}{4\pi}$$

However, there's an ambiguity in this computation. Instead of integrating over S, it is equally valid to calculate the phase by integrating over S', shown in the right-hand panel of the figure. The solid angle formed by S' is $\Omega' = 4\pi - \Omega$. The phase is then given by

$$\alpha' = -\frac{(4\pi - \Omega)g}{4\pi}$$

where the overall minus sign comes because the surface S' has the opposite orientation to S. As we mentioned above, the phase shift that we get in these calculations is

observable: we can't tolerate different answers from different calculations. This means that we must have $e^{iq\alpha/\hbar} = e^{iq\alpha'/\hbar}$. This gives the condition

$$qg = 2\pi\hbar n \quad \text{with } n \in \mathbf{Z} \tag{6.24}$$

This is the famous Dirac quantisation condition. The smallest such magnetic charge has $n = 1$. It coincides with the quantum of flux, $g = \Phi_0 = 2\pi\hbar/q$.

Above we worked with a single particle of charge q. Obviously, the same argument must hold for any other particle of charge q'. There are two possibilities. The first is that all particles carry charge that is an integer multiple of some smallest unit. In this case, it's sufficient to impose the Dirac quantisation condition (6.24) where q is the smallest unit of charge. For example, in our world we should take $q = \pm e$ to be the electron or proton charge (or, if we look more closely in the Standard Model, we might choose to take $q = -e/3$, the charge of the down quark).

The second possibility is that the particles carry electric charges which are irrational multiples of each other. For example, there may be a particle with charge q and another particle with charge $\sqrt{2}q$. In this case, no magnetic monopoles are allowed.

It's sometimes said that the existence of a magnetic monopole would imply the quantisation of electric charges. This, however, has it backwards. (It also misses the point that we have a wonderful explanation of the quantisation of charges from the story of anomaly cancellation in the Standard Model.) There are two possible groups that could underly gauge transformations in electromagnetism. The first is $U(1)$; this has integer valued charges and admits magnetic monopoles. The second possibility is $\mathbf{R}$; this has irrational electric charges and forbids monopoles. All the evidence in our world points to the fact that electromagnetism is governed by $U(1)$ and that magnetic monopoles should exist.

Above we looked at an electrically charged particle moving in the background of a magnetically charged particle. It is simple to generalise the discussion to particles that carry both electric and magnetic charges. These are called *dyons*. For two dyons, with charges (q_1, g_1) and (q_2, g_2), the generalisation of the Dirac quantisation condition requires

$$q_1 g_2 - q_2 g_1 \in 2\pi\hbar\mathbf{Z}$$

This is sometimes called the *Dirac-Zwanziger* condition.

6.4.2 A Patchwork of Gauge Fields

The discussion above shows how quantum mechanics constrains the allowed values of magnetic charge. It did not, however, address the main obstacle to constructing a magnetic monopole out of gauge fields $\mathbf{A}$ when the condition $\mathbf{B} = \nabla \times \mathbf{A}$ would seem to explicitly forbid such objects.

Let's see how to do this. Our goal is to write down a configuration of gauge fields which give rise to the magnetic field (6.22) of a monopole which we will place at the origin. However, we will need to be careful about what we want such a gauge field to look like.

The first point is that we won't insist that the gauge field is well defined at the origin. After all, the gauge fields arising from an electron are not well defined at the position of an electron and it would be churlish to require more from a monopole. This fact gives us our first bit of leeway, because now we need to write down gauge fields on $\mathbf{R}^3/\{0\}$, as opposed to $\mathbf{R}^3$ and the space with a point cut out enjoys some non-trivial topology that we will make use of.

Consider the following gauge connection, written in spherical polar coordinates

$$A_\phi^N = \frac{g}{4\pi r}\frac{1-\cos\theta}{\sin\theta} \tag{6.25}$$

The resulting magnetic field is

$$\mathbf{B} = \nabla \times \mathbf{A} = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(A_\phi^N \sin\theta)\,\hat{\mathbf{r}} - \frac{1}{r}\frac{\partial}{\partial r}(rA_\phi^N)\hat{\boldsymbol{\theta}}$$

Substituting in (6.25) gives

$$\mathbf{B} = \frac{g\hat{\mathbf{r}}}{4\pi r^2} \tag{6.26}$$

In other words, this gauge field results in the magnetic monopole. But how is this possible? Didn't we learn in kindergarten that if we can write $\mathbf{B} = \nabla \times \mathbf{A}$ then $\int d\mathbf{S}\cdot\mathbf{B} = 0$? How does the gauge potential (6.25) manage to avoid this conclusion?

The answer is that $\mathbf{A}^N$ in (6.25) is actually a singular gauge connection. It's not just singular at the origin, where we've agreed this is allowed, but it is singular along an entire half-line that extends from the origin to infinity. This is due to the $1/\sin\theta$ term which diverges at $\theta = 0$ and $\theta = \pi$. However, the numerator $1-\cos\theta$ has a zero when $\theta = 0$ and the gauge connection is fine there. But the singularity along the half-line $\theta = \pi$ remains. The upshot is that this gauge connection is not acceptable along the line of the south pole, but is fine elsewhere. This is what the superscript N is there to remind us: we can work with this gauge connection s long as we keep north.

Now consider a different gauge connection

$$A_\phi^S = -\frac{g}{4\pi r}\frac{1+\cos\theta}{\sin\theta} \tag{6.27}$$

This again gives rise to the magnetic field (6.26). This time it is well behaved at $\theta = \pi$, but singular at the north pole $\theta = 0$. The superscript S is there to remind us that this connection is fine as long as we keep south.

At this point, we make use of the ambiguity in the gauge connection. We are going to take $\mathbf{A}^N$ in the northern hemisphere and $\mathbf{A}^S$ in the southern hemisphere. This is allowed because the two gauge potentials are the same up to a gauge transformation, $\mathbf{A} \to \mathbf{A} + \nabla\alpha$. Recalling the expression for $\nabla\alpha$ in spherical polars, we find that for $\theta \neq 0, \pi$, we can indeed relate A_ϕ^N and A_ϕ^S by a gauge transformation,

$$A_\phi^N = A_\phi^S + \frac{1}{r\sin\theta}\,\partial_\phi\alpha \quad \text{where} \quad \alpha = \frac{g\phi}{2\pi} \tag{6.28}$$

However, there's still a question remaining: is this gauge transformation allowed? The problem is that the function α is not single valued: $\alpha(\phi = 2\pi) = \alpha(\phi = 0) + g$. And this should concern us because, as we've seen in (6.8), the gauge transformation also acts on the wavefunction of a quantum particle

$$\psi \to e^{iq\alpha/\hbar}\psi$$

There's no reason that we should require the gauge transformation ω to be single-valued, but we do want the wavefunction ψ to be single-valued. This holds for the gauge transformation (6.28) provided that we have

$$qg = 2\pi\hbar n \quad \text{with } n \in \mathbf{Z}$$

This, of course, is the Dirac quantisation condition (6.24).

Mathematically, we have constructed of a topologically non-trivial $U(1)$ bundle over the $\mathbf{S}^2$ surrounding the origin. In this context, the integer n is called the first Chern number.

6.4.3 Monopoles and Angular Momentum

Here we provide yet another derivation of the Dirac quantisation condition, this time due to Saha. The key idea is that the quantisation of magnetic charge actually follows from the more familiar quantisation of angular momentum. The twist is that, in the presence of a magnetic monopole, angular momentum isn't quite what you thought.

To set the scene, let's go back to the Lorentz force law

$$\frac{d\mathbf{p}}{dt} = q\,\dot{\mathbf{x}} \times \mathbf{B}$$

with $\mathbf{p} = m\dot{\mathbf{x}}$. Recall from our discussion in Section 6.1.1 that $\mathbf{p}$ defined here is not the canonical momentum, a fact which is hiding in the background in the following derivation. Now let's consider this equation in the presence of a magnetic monopole, with

$$\mathbf{B} = \frac{g}{4\pi}\frac{\mathbf{r}}{r^3}$$

The monopole has rotational symmetry so we would expect that the angular momentum, $\mathbf{x} \times \mathbf{p}$, is conserved. Let's check:

$$\begin{aligned}\frac{d(\mathbf{x}\times\mathbf{p})}{dt} &= \dot{\mathbf{x}}\times\mathbf{p} + \mathbf{x}\times\dot{\mathbf{p}} = \mathbf{x}\times\dot{\mathbf{p}} = q\mathbf{x}\times(\dot{\mathbf{x}}\times\mathbf{B}) \\ &= \frac{qg}{4\pi r^3}\mathbf{x}\times(\dot{\mathbf{x}}\times\mathbf{x}) = \frac{qg}{4\pi}\left(\frac{\dot{\mathbf{x}}}{r} - \frac{\dot{r}\mathbf{x}}{r^2}\right) \\ &= \frac{d}{dt}\left(\frac{qg}{4\pi}\hat{\mathbf{r}}\right)\end{aligned}$$

We see that in the presence of a magnetic monopole, the naive angular momentum $\mathbf{x} \times \mathbf{p}$ is not conserved! However, as we also noticed in the lectures on Classical Dynamics (see Section 4.3.2), we can easily write down a modified angular momentum that is conserved, namely

$$\mathbf{L} = \mathbf{x}\times\mathbf{p} - \frac{qg}{4\pi}\hat{\mathbf{r}}$$

The extra term can be thought of as the angular momentum stored in $\mathbf{E} \times \mathbf{B}$. The surprise is that the system has angular momentum even when the particle doesn't move.

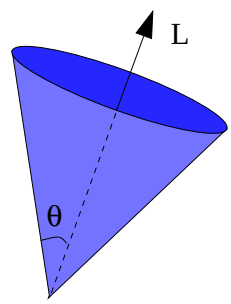


Figure 87:

Before we move on, there's a nice and quick corollary that we can draw from this. The angular momentum vector $\mathbf{L}$ does not change with time. But the angle that the particle makes with this vector is

$$\mathbf{L}\cdot\hat{\mathbf{r}} = -\frac{qg}{4\pi} = \text{constant}$$

This means that the particle moves on a cone, with axis $\mathbf{L}$ and angle $\cos\theta = -qg/4\pi L$.

So far, our discussion has been classical. Now we invoke some simple quantum mechanics: the angular momentum should be quantised. In particular, the angular momentum in the z-direction should be $L_z \in \frac{1}{2}\hbar\mathbf{Z}$. Using the result above, we have

$$\frac{qg}{4\pi} = \frac{1}{2}\hbar n \quad \Rightarrow \quad qg = 2\pi\hbar n \qquad \text{with } n \in \mathbf{Z}$$

Once again, we find the Dirac quantisation condition.

6.5 Spin in a Magnetic Field

As we've seen in previous courses, particles often carry an intrinsic angular momentum called *spin* $\mathbf{S}$. This spin is quantised in half-integer units. For examples, electrons have spin $\frac{1}{2}$ and their spin operator is written in terms of the Pauli matrices $\boldsymbol{\sigma}$,

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

Importantly, the spin of any particle couples to a background magnetic field $\mathbf{B}$. The key idea here is that the intrinsic spin acts like a magnetic moment $\mathbf{m}$ which couples to the magnetic field through the Hamiltonian

$$H = -\mathbf{m} \cdot \mathbf{B}$$

The question we would like to answer is: what magnetic moment $\mathbf{m}$ should we associate with spin?

A full answer to this question would require an extended detour into the Dirac equation. Here we provide only some basic motivation. First consider a particle of charge q moving with velocity $\mathbf{v}$ around a circle of radius $\mathbf{r}$ as shown in the figure. From our lectures on Electromagnetism, we know that the associated magnetic moment is given by

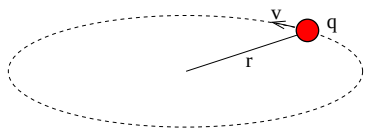


Figure 88:

$$\mathbf{m} = -\frac{q}{2}\mathbf{r} \times \mathbf{v} = \frac{q}{2m}\mathbf{L}$$

where $\mathbf{L} = m\mathbf{r} \times \mathbf{v}$ is the orbital angular momentum of the particle. Indeed, we already saw the resulting coupling $H = -(q/2m)\mathbf{L} \cdot \mathbf{B}$ in our derivation of the Hamiltonian in symmetric gauge (6.19).

Since the spin of a particle is another contribution to the angular momentum, we might anticipate that the associated magnetic moment takes the form

$$\mathbf{m} = g\frac{q}{2m}\mathbf{S}$$

where g is some dimensionless number. (Note: g is unrelated to the magnetic charge that we discussed in the previous section!) This, it turns out, is the right answer. However, the value of g depends on the particle under consideration. The upshot is that we should include a term in the Hamiltonian of the form

$$H = -g\frac{q}{2m}\mathbf{S}\cdot\mathbf{B} \tag{6.29}$$

The g-factor

For fundamental particles with spin $\frac{1}{2}$ — such as the electron — there is a long and interesting history associated to determining the value of g. For the electron, this was first measured experimentally to be

$$g_e = 2$$

Soon afterwards, Dirac wrote down his famous relativistic equation for the electron. One of its first successes was the theoretical prediction $g_e = 2$ for any spin $\frac{1}{2}$ particle. This means, for example, that the neutrinos and quarks also have $g = 2$.

This, however, was not the end of the story. With the development of quantum field theory, it was realised that there are corrections to the value $g_e = 2$. These can be calculated and take the form of a series expansion, starting with

$$g_e = 2\left(1 + \frac{\alpha}{2\pi} + \ldots\right) \approx 2.00232$$

where $\alpha = e^2/4\pi\epsilon_0\hbar c \approx 1/137$ is the dimensionless *fine structure constant* which characterises the strength of the Coulomb force. The most accurate experimental measurement of the electron magnetic moment now yields the result

$$g_e \approx 2.00231930436182 \pm 2.6 \times 10^{-13}$$

Theoretical calculations agree to the first ten significant figures or so. This is the most impressive agreement between theory and experiment in all of science! Beyond that, the value of α is not known accurately enough to make a comparison. Indeed, now the measurement of the electron magnetic moment is used to *define* the fine structure constant α.

While all fundamental spin $\frac{1}{2}$ particles have $g \approx 2$, this does not hold for more complicated objects. For example, the proton has

$$g_p \approx 5.588$$

while the neutron — which of course, is a neutral particle, but still carries a magnetic moment — has

$$g_n \approx -3.823$$

where, because the neutron is neutral, the charge $q = e$ is used in the formula (6.29). These measurements were one of the early hints that the proton and neutron are composite objects.

6.5.1 Spin Precession

Consider a constant magnetic field $\mathbf{B} = (0, 0, B)$. We would like to understand how this affects the spin of an electron. We'll take $g_e = 2$. We write the electric charge of the electron as $q = -e$ so the Hamiltonian is

$$H = \frac{e\hbar}{2m}\boldsymbol{\sigma} \cdot \mathbf{B}$$

The eigenstates are simply the spin-up $|\uparrow\rangle$ and spin-down $|\downarrow\rangle$ states in the z-direction. They have energies

$$H|\uparrow\rangle = \frac{\hbar\omega_B}{2}|\uparrow\rangle \quad \text{and} \quad H|\downarrow\rangle = -\frac{\hbar\omega_B}{2}|\downarrow\rangle$$

where $\omega_B = eB/m$ is the cyclotron frequency which appears throughout this chapter.

What happens if we do not sit in an energy eigenstate. A general spin state can be expressed in spherical polar coordinates as

$$|\psi(\theta, \phi)\rangle = \cos(\theta/2)|\uparrow\rangle + e^{i\phi}\sin(\theta/2)|\downarrow\rangle$$

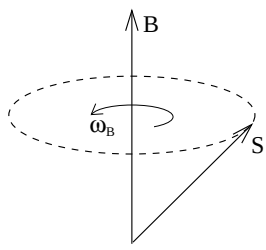


Figure 89:

As a check, note that $|\psi(\theta = \pi/2, \phi)\rangle$ is an eigenstate of σ^x when $\phi = 0, \pi$ and an eigenstate of σ^y when $\phi = \pi/2, 3\pi/2$ as it should be. The evolution of this state is determined by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

which is easily solved to give

$$|\psi(\theta,\phi;t)\rangle = e^{i\omega_B t/2}\Big[\cos(\theta/2)|\uparrow\rangle + e^{i(\phi-\omega_B t)}\sin(\theta/2)|\downarrow\rangle\Big]$$

We see that the effect of the magnetic field is to cause the spin to precess about the $\mathbf{B}$ axis, as shown in the figure.

6.5.2 A First Look at the Zeeman Effect

The Zeeman effect describes the splitting of atomic energy levels in the presence of a magnetic field. Consider, for example, the hydrogen atom with Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

The energy levels are given by

$$E_n = -\frac{\alpha^2 mc^2}{2}\frac{1}{n^2} \qquad n \in \mathbf{Z}$$

where α is the fine structure constant. Each energy level has a degeneracy of states. These are labelled by the angular momentum $l = 0, 1, \ldots, n-1$ and the z-component of angular momentum $m_l = -l, \ldots, +l$. Furthermore, each electron carries one of two spin states labelled by $m_s = \pm\frac{1}{2}$. This results in a degeneracy given by

$$\text{Degeneracy} = 2\sum_{l=0}^{n-1}(2l+1) = 2n^2$$

Now we add a magnetic field $\mathbf{B} = (0, 0, B)$. As we have seen, this results in perturbation to the Hamiltonian which, to leading order in B, is given by

$$\Delta H = \frac{e}{2m}(\mathbf{L} + g_e\mathbf{S})\cdot\mathbf{B}$$

In the presence of such a magnetic field, the degeneracy of the states is split. The energy levels now depend on the quantum numbers n, m_l and m_s and are given by

$$E_{n,m,s} = E_n + \frac{e}{2m}(m_l + 2m_s)B$$