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# FUNDAMENTALS OF THEORETICAL PHYSICS

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A BRIEF INTRODUCTION TO THE KEY TOPICS OF  
THEORETICAL PHYSICS

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# 1 Linear Dynamics

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## 1.1 Errors and Dimensions

Before we get started with our discussion of classical dynamics, it is worth taking the time to mention two small, but important concepts. The first is the concept of dimensions, which is fundamentally important in the process of connecting the mathematics that we use to describe the universe, to physical reality itself. Secondly, we shall discuss errors and uncertainties, which are crucially important when it comes to interpreting the results of experiment.

### 1.1.1 Dimensional Analysis

When we describe a physical quantity, it is always given as the product of both a numerical value, and some form of unit. It is this unit that assigns physical meaning to a value. For example, if we describe an object as having a length of 6 m, we are saying that the object is 6 times longer than some given reference length. As such, if our unit is to be useful, it has to be defined in such a way that, at least in principle, any experimenter could produce their own reference length, against which they could interpret physical values. There are a great many different systems of units in existence, with each having its own advantages and disadvantages. Throughout this text, we will use the international standard of SI units, which are based on the second, as defined below:

*One second is equal to the duration of precisely 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom.*

According to this definition, intervals of time are measured by counting the number of times a particular electromagnetic wave oscillates, and then dividing this value by 9 192 631 770, in order to obtain the time in seconds. In practice however, this is only done for the most precise of measurements, as it is usually sufficient to measure against some other frequency that has a known calibration relative to the caesium standard. This definition was chosen, because all caesium-133 atoms in the universe have exactly the same properties, with the only differences arising from their local environment. This makes the SI definition of the second completely unambiguous, and thus, highly reproducible.

From here, the SI system builds up a series of other base units by utilising certain physical laws, together with the definition of the second. For example, since we currently believe the speed of light in a vacuum to be a fundamental physical constant, we can use this to define a measure of distance. As such, the metre is defined by:

*One metre is equal to precisely  $\frac{1}{299\,792\,458}$  times the distance that light in a vacuum can travel in one second.*

A similar principle is applied to define a measure of mass, the kilogram. This is done by utilising both the Planck-Einstein relationship for the energy of a photon, and Einstein's principle of mass-energy equivalence.

*One kilogram is equal to the mass of particle, whose rest energy is equal to the smallest quantum of energy deliverable by electromagnetic radiation with a time period of precisely  $\frac{6.62\,607\,015 \times 10^{-34}}{(299\,792\,458)^2}$  seconds.*

There are 4 more base units corresponding to: electric current, thermodynamic temperature, amount of substance, and luminous intensity. However, since this chapter will only be dealing with masses, lengths, and times, we shall not examine their definitions in any detail. In addition to these base units, the SI is also equipped with a series of derived units, obtained by taking combinations of the existing base units. As an example, if we wished to state an object's velocity, we would have to use the unit of metres per second, which is defined such that an object moving at 1 metre per second would travel 1 metre in a single second. These derived units follow nicely from our idea that a physical quantity is the product of a number and a unit, as shown by (1.1) below, where the average velocity of an object that moved 8 m in 4 s is calculated.

$$v_{\text{avg}} = \frac{\Delta x}{\Delta t} \implies v_{\text{avg}} = \frac{8 \text{ m}}{4 \text{ s}} = 2 \frac{\text{m}}{\text{s}} = 2 \text{ m s}^{-1} \quad (1.1)$$

We can generalise this idea slightly by introducing the concept of dimensions. Any system of units introduces a set of basis dimensions, which have a one to one correspondence with that system's base units. The distinction is that the dimensions are not dependent on the actual sizes of the base units, only the quantities they represent. That is to say, the SI units of metres, kilograms, and seconds, share a dimensional basis with a unit system based on centimetres, grams and seconds. Just as with units, when we multiply or divide two physical quantities, we have to combine their dimensions accordingly. Given a system of  $n$  basis dimensions  $\pi_i$ , we can this express the dimensions of some arbitrary quantity  $Q$  in the form:

$$\dim Q = \prod_{i=1}^n \pi_i^{a_i} \quad (1.2)$$

The exponents  $a_i$  represent the dependence of  $Q$ 's numerical value on the scale of the  $i$ th base unit. That is to say that, if we decrease the magnitude of the  $i$ th base unit by a factor of  $\alpha$ , the numerical value of  $Q$  will increase by a factor of  $\alpha^{a_i}$ . Two quantities are described as being dimensionally consistent, if they possess all of the same  $a_i$  values. These quantities have the special property that, their ratio is invariant under any rescaling of the base units.

The useful thing about dimensions is that they place a lot of restrictions on what we can do with various physical quantities. The principle of dimensional homogeneity states that, only two quantities that are dimensionally consistent may be meaningfully compared or added to one another. This makes sense from since, if two quantities do not have the same dimensions, the ratio between them will change when the scale of the base units is changed. The laws of physics should be independent of the units we use to describe them, and as such, any comparison between dimensionally inconsistent quantities can not hold any physical meaning. Similarly, the sum of any two dimensionally inconsistent quantities can not have any physical meaning, since we could always rescale our units such that the contribution of one term was dominated by the other. It therefore follows that, functions, such as  $\sin x$  and  $e^x$ , which can be expressed as a power series, must have a dimensionless argument, otherwise the terms in the series would be dimensionally inconsistent.

Although we shall consistently use the SI units and dimensions throughout this text, it is worth being aware that vastly different systems do exist, and are frequently used within certain fields. In fact, there are even systems that possess only a single dimension, and hence only a single base unit; however, such systems are rarely useful in practical applications.

### 1.1.2 Error Propagation

When it comes to interpreting the results of an experiment, one of the most important things for us to be aware of is the uncertainty associated with every value. These uncertainties arise as a result of practical limitations on how accurately physical quantities can be measured. As such, if the same measurement is repeated multiple times, the measured values will not be the same, and will instead form some kind of distribution centred on the true value. Thus, when an experimental result is quoted, it also includes an estimate as to the standard deviation of that distribution, which we commonly call the error in that value. Errors are typically presented using either of the two notations shown below:

$$l = 1.07652 \text{ m} \pm 0.00017 \text{ m} = 1.07652(17) \text{ m} \quad (1.3)$$

When it comes to presenting errors, there are a few conventions that are worth being aware of. Firstly, since these errors are only estimates, they are typically only presented to one significant figure, although this requirement is often relaxed if the error has a 1 as its first significant digit. Secondly, measured values are never quoted to a greater precision than their errors, since it would be fairly meaningless to give a result to a greater precision than the precision of the experiment itself.

Often the results of an experiment are obtained by combining multiple different measurements, each of which has its own associated error. Thus, we need to be able to combine the errors, a process which is known as error propagation, because it allows us to follow how the errors move through a series of calculations. To begin with, we should consider exactly what we mean by the error in a value. Given a random variable  $X$ , its standard deviation  $\sigma_X$  is defined such that:

$$\sigma_X^2 = \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2 \quad (1.4)$$

Where the notation  $\langle \dots \rangle$  implies the expectation value of the quantity inside the brackets. Importantly, since an expectation value is simply generated by summing the product of every possible value that quantity could take multiplied by its probability (in the case of a continuous variable this becomes an integral of the quantity multiplied by the probability density function), the expectation is linear in its arguments. That is to say that:

$$\langle \alpha X + \beta Y \rangle = \alpha \langle X \rangle + \beta \langle Y \rangle \quad (1.5)$$

For constants  $\alpha$  and  $\beta$ . It is this property of the expectation value that allows us to derive the equivalence between the two expressions in (1.4). From here we can now calculate an expression for the standard deviation of the random variable  $X + Y$ . Simply substituting this in to equation (1.4) and then applying the linearity relation (1.5), we obtain:

$$\sigma_{X+Y}^2 = \sigma_X^2 + \sigma_Y^2 + 2[\langle XY \rangle - \langle X \rangle \langle Y \rangle] \quad (1.6)$$

The  $\langle XY \rangle - \langle X \rangle \langle Y \rangle$  term is known as the covariance of  $X$  and  $Y$ , and it measures how strongly the two variables depend on one another. In the special case that  $X$  and  $Y$  are independent, their covariance will be equal to zero, and thus, we obtain the relatively simple result:

$$\sigma_{X+Y}^2 = \sigma_X^2 + \sigma_Y^2 \quad (1.7)$$

Let us now consider the case of an arbitrary function  $F$ , which depends on  $n$  independent random variables  $X_i$ . In general finding the error in  $F$  is quite difficult; however, we can simplify things somewhat, if we assume that all of the  $X_i$  have fairly small standard deviations. In this case, we can use a Taylor series expansion of  $F$  in order to obtain:

$$F(X_i) \approx F(\langle X_i \rangle) + \sum_{i=1}^n \frac{\partial F}{\partial X_i} [X_i - \langle X_i \rangle] \quad (1.8)$$

Where the partial derivatives are evaluated with all of the variables equal to their expectation values. We can now use equation (1.5) to evaluate an approximate expectation value for  $F$  as shown below.

$$\langle F \rangle \approx F(\langle X_i \rangle) + \sum_{i=1}^n \frac{\partial F}{\partial X_i} \langle X_i - \langle X_i \rangle \rangle = F(\langle X_i \rangle) \quad (1.9)$$

Of course, this relationship is only approximate, after all, if the expectation of a function was always equal to that function evaluated at the expectations of its arguments, our definition of the standard deviation would be identically zero. Instead, we are saying that, deviations in the expectation of a function from the function applied to the expectations are of the order  $\sigma_{X_i}^2$ . We very rarely have to worry about these deviations, because any experiment that has errors large enough that terms of order  $\sigma_{X_i}^2$  become significant, is too imprecise for us to gain any useful information anyway.

We can also use equation (1.8) to evaluate the standard deviation in  $F$ . Since a constant is essentially just an independent random variable with zero standard deviation, we can apply equation (1.7), which yields:

$$\sigma_F^2 = \sum_{i=1}^n \left( \frac{\partial F}{\partial X_i} \sigma_{X_i} \right)^2 \quad (1.10)$$

Since the size of an error is fairly meaningless on its own (an error of the order 1 kg would be excellent for the mass of a star, but terrible for the mass of a subatomic particle), errors are often expressed as a fraction of the reported values.

$$\left( \frac{\sigma_F}{F} \right)^2 = \sum_{i=1}^n \left( \frac{\partial F}{\partial X_i} \frac{\sigma_{X_i}}{F} \right)^2 \quad (1.11)$$

Table 1.1 summarises some specific examples which occur fairly regularly, to show how different operations respond to errors.

Table 1.1: Different examples of error propagation.

$F$	$\sigma_F$	$F$	$\sigma_F$
$x + y$	$\sqrt{\sigma_x^2 + \sigma_y^2}$	$e^{ax}$	$a\sigma_x e^{ax}$
$xy$	$xy \sqrt{\frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2}}$	$\ln(ax)$	$\frac{\sigma_x}{x}$
$x^n$	$nx^{n-1}\sigma_x$	$\sin(ax)$	$a\sigma_x \cos(ax)$

## 1.2 Newton's Laws

One of the principle ideas behind all of classical dynamics is that of a force. Newton's three laws of motion introduce these ideas, and provide a definition of force in terms of an object's kinematics. This can then be coupled with other physical theories, which provide expressions to calculate the force a given object will experience, in order to evaluate how a system will evolve through time.

### 1.2.1 The 1st Law

Newton's first law states that an object in motion will stay in motion, moving with a constant velocity, unless some external, resultant force acts upon it. That is to say that the effect of a force on an object must be to change its velocity in some way. Importantly, Newton's first law refers to the resultant force acting on a body, which we interpret as the vector sum of all the individual forces it experiences. As an example, let us consider an object in equilibrium, that is to say, an object that is not accelerating, which is subjected to three external forces.

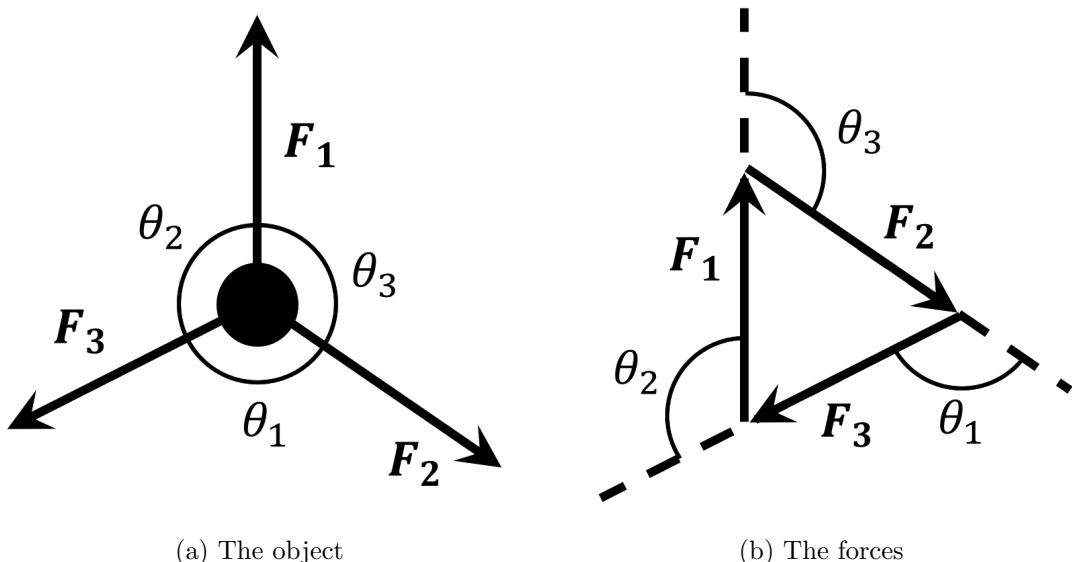


Figure 1.1: An object subjected to three external forces, whose vector sum is equal to zero.

In order to satisfy Newton's first law, the vector sum of the three forces must be equal to zero. By taking the vector product of this sum with each of the forces in turn, we arrive at the following relationships:

$$\mathbf{F}_1 \times \mathbf{F}_2 = \mathbf{F}_2 \times \mathbf{F}_3 = \mathbf{F}_3 \times \mathbf{F}_1 \quad (1.12)$$

We can rearrange this equation by dividing through by the product of the vector magnitudes  $|\mathbf{F}_1||\mathbf{F}_2||\mathbf{F}_3|$ , which leads us to Lami's theorem:

$$\frac{\sin \theta_1}{|\mathbf{F}_1|} = \frac{\sin \theta_2}{|\mathbf{F}_2|} = \frac{\sin \theta_3}{|\mathbf{F}_3|} \quad (1.13)$$

### 1.2.2 The 2nd Law

Newton's second law serves as a generalisation of his first, and quantifies the relationship between the resultant force felt by an object and its kinematics. The law states that the force applied to an object is directly proportional to its acceleration (the second time derivative of its position). The constant of proportionality in this relationship is the object's mass, which is fixed for any given object, leading to the conventional expression of the law:

$$\mathbf{F}_{\text{tot}} = m\ddot{\mathbf{r}} \quad (1.14)$$

We can then use other physical laws to express the force in terms of the object's position (and in some cases its velocity) to generate a differential equation for  $\mathbf{r}(t)$ . If we know the initial values of both the object's position and velocity, we can solve this equation for the object's subsequent motion. As an example, let us consider an object falling through a viscous fluid. We can model the force on the object as the combination of a constant gravitational acceleration and a viscous drag that is proportional to the velocity. This gives us an equation of motion of the form:

$$m\ddot{\mathbf{r}} = mg - b\dot{\mathbf{r}} \quad (1.15)$$

We can solve this equation by multiplying by the integrating factor  $e^{\frac{bt}{m}}$ . This allows us to rearrange the differential equation into:

$$\frac{d}{dt} \left[ e^{\frac{bt}{m}} \dot{\mathbf{r}} \right] = g e^{\frac{bt}{m}} \quad (1.16)$$

We can then integrate this result to obtain a solution for the velocity as a function of time. If we want to find the position as a function of time, we simply integrate this result again to obtain:

$$\dot{\mathbf{r}} = \left( \mathbf{v}_0 - \frac{mg}{b} \right) e^{-\frac{bt}{m}} + \frac{mg}{b} \quad \mathbf{r} = \mathbf{r}_0 + \frac{m}{b} \left( \mathbf{v}_0 - \frac{mg}{b} \right) \left( 1 - e^{-\frac{bt}{m}} \right) + \frac{mg t}{b} \quad (1.17)$$

Where  $\mathbf{r}_0$  and  $\mathbf{v}_0$  are the initial values of the object's position and velocity respectively.

### 1.2.3 The 3rd Law

Finally, Newton's third law connects the forces that two bodies can apply to one another. It states that, if an object  $A$  exerts a force  $\mathbf{F}_{AB}$  on a second object  $B$ , the object  $B$  will also exert a force  $\mathbf{F}_{BA}$  on object  $A$ , such that the two forces satisfy:

$$\mathbf{F}_{AB} = -\mathbf{F}_{BA} \quad (1.18)$$

An important consequence of this law is that, in an isolated system, all of the internal forces cancel out, meaning that any system can not exert a resultant force on itself. Furthermore, this law allows us to understand how forces are transmitted through a solid body. For example, when a string is placed under tension, the string element nearest to the applied force will move in the direction of the force until it is balanced by a tensile force from the element behind it. By Newton's third law, this element must therefore be feeling a tensile force equal to the original applied force, and so on down the length of the string.

## 1.3 Momentum and Energy

When it comes to dynamics, and indeed all of physics, two of the most important quantities for us to consider are energy and momentum. Throughout the course of this text, we will find that we use different expressions for both, depending on precisely what physical theory we are using. As such, we should take some time to clarify the fundamental definitions of these quantities. In short, the most important property of both is that they are conserved through time. Thus, the exact expression will change depending on what the physical model in question states will be conserved. Furthermore, as we shall see in section 1.5, energy and momentum are intimately connected to the symmetry of the laws of physics, in time and space respectively. It is this that forms the basis of their fundamental definitions.

### 1.3.1 Conservation of Momentum

Within classical mechanics, an object's momentum is equal to the product of its mass and its velocity. Since the mass of any given object always remains constant, we can reformulate the definition of a force in terms of the momentum:

$$\mathbf{p} = m\dot{\mathbf{r}} \implies \mathbf{F} = \dot{\mathbf{p}} \quad (1.19)$$

As it turns out, this definition is more useful than our previous formulation of Newton's second law, when considering more complicated models, and as such, we will take this as the definition of a force from now on. Furthermore, this definition of momentum also gives us a way to understand what the mass of an object actually represents. We start with the empirical observation that, in any collision we can multiply every object's velocity by some constant, to obtain a conserved quantity. In principle, we can then measure the mass of an object by colliding it with some standard unit mass, and then determining the constant that its velocity needs to be multiplied by in order for momentum to be conserved.

If we wish to calculate the momentum of a composite system, which contains  $n$  bodies, each of mass  $m_i$  and position  $\mathbf{r}_i$ , we simply sum all of the individual momenta:

$$\mathbf{p}_{\text{tot}} = \sum_{i=1}^n \mathbf{p}_i = \sum_{i=1}^n m_i \dot{\mathbf{r}}_i = M_{\text{tot}} \dot{\mathbf{r}}_{\text{CM}} \quad (1.20)$$

Where  $M_{\text{tot}}$  and  $\mathbf{r}_{\text{CM}}$  represent the total mass of the system and the position of its centre of mass respectively.

$$M_{\text{tot}} = \sum_{i=1}^n m_i \quad \mathbf{r}_{\text{CM}} = \frac{1}{M_{\text{tot}}} \sum_{i=1}^n m_i \mathbf{r}_i \quad (1.21)$$

We can then differentiate this expression and substitute in Newton's second law, to obtain the relationship between the total force experienced by the system and its momentum:

$$\dot{\mathbf{p}}_{\text{tot}} = M_{\text{tot}} \ddot{\mathbf{r}}_{\text{CM}} = \sum_{i=1}^n \dot{\mathbf{p}}_i = \sum_{i=1}^n \mathbf{F}_i = \mathbf{F}_{\text{tot}} \quad (1.22)$$

It follows from Newton's third law, that if the system is isolated, all of the internal forces must cancel, meaning that  $\dot{\mathbf{p}}_{\text{tot}}$  must be equal to zero. Thus, the total momentum of the system must be a conserved quantity.

### 1.3.2 Conservation of Energy

To understand the concept of energy, which is reasonably abstract, we should first consider the idea of work. In colloquial terms, we can think of the work done during a process as the effort that we had to expend during that process. Formally, we define the work done by a force  $\mathbf{F}$ , when it acts on an object that moves through an infinitesimal displacement  $d\mathbf{r}$ , to be given by:

$$dW = \mathbf{F} \cdot d\mathbf{r} \quad (1.23)$$

We can then calculate the total work done in any process, by simply integrating (1.23). This definition can be traced back to simple physical processes, for example, when lifting blocks of stone, it would take the same amount of work to lift one block through a given height, as it would to lift two blocks through half the height.

The energy of a system, which is measured relative to some given reference state, is equal to the amount of work that could be extracted from that system, when bringing it back to that reference state. As such, it follows from time symmetry that, the energy of a system is equal to the work that must be done, in order to bring it from the reference state to its current state. Using this definition, we can calculate the energy of a moving object, referred to as its kinetic energy. To do this we shall substitute equation (1.19) for the force into (1.23), which gives us:

$$dW = \dot{\mathbf{p}} \cdot d\mathbf{r} = (\dot{\mathbf{p}} \cdot \dot{\mathbf{r}})dt = \dot{\mathbf{r}} \cdot d\mathbf{p} \quad (1.24)$$

If we choose our reference state to be the object in question at rest, we can calculate the kinetic energy  $T$  by integrating the differential in (1.24). The exact result of this integration will depend on the definition of momentum being used; however, if we use the classical result from section 1.3.1, we obtain the formula:

$$T = \int dW = \int_0^{\mathbf{p}} \dot{\mathbf{r}}' \cdot d\mathbf{p}' = \frac{\mathbf{p} \cdot \mathbf{p}}{2m} = \frac{m}{2} \dot{\mathbf{r}} \cdot \dot{\mathbf{r}} = \frac{\mathbf{p} \cdot \dot{\mathbf{r}}}{2} \quad (1.25)$$

In addition to kinetic energy, an object might have potential energy, which represents the work that must be done in order to move that object from some reference point to its current position, without changing its momentum. If an object moves through a force field  $\mathbf{F}(\mathbf{r})$ , an external force of  $-\mathbf{F}(\mathbf{r})$  will be required to prevent it from accelerating. The potential energy  $U$  is thus given by integrating the work done by this force:

$$U = \int dW = - \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r} \quad (1.26)$$

This potential energy can only be well defined if  $\mathbf{F}(\mathbf{r})$  is conservative, that is to say that  $\nabla \times \mathbf{F} = \mathbf{0}$ . In non-conservative fields, the work done depends on the path taken between two points, and as such, it is impossible to assign an energy to any given position. This is because, such fields dissipate energy into other forms, such as heat. However, if the field is conservative we can introduce the potential energy function, such that  $\mathbf{F}(\mathbf{r}) = -\nabla U$ . It therefore follows that, for an object experiencing no external forces in such a field, the quantity  $E$ , representing its total energy, will be conserved through time.

$$E = T + U \implies dE = (\dot{\mathbf{p}} + \nabla U) \cdot d\mathbf{r} = \mathbf{F}_{\text{ext}} \cdot d\mathbf{r} \quad (1.27)$$

We can extend this concept to deal with systems of  $n$  bodies just as we did for momentum. Since an object's kinetic energy can not depend on its surroundings, it follows that the total kinetic energy of the system is obtained by simply summing together the kinetic energies of each of the bodies. Thus we obtain:

$$T_{\text{tot}} = \frac{1}{2} \sum_{i=1}^n m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i \quad (1.28)$$

The potential energy is calculated in much the same way as it was previously, only it can not be separated into a contribution from each body. This is because the work required to move one of the objects into position will depend on the positions of all the other objects (assuming that in general there is some interaction between them). As such, the interactions between the objects are considered to be conservative, if there exists some function  $U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n)$  of all of the positions, such that the force on the  $i$ th body is given by:

$$\mathbf{F}_i(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) = -\nabla^{(i)} U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) \quad (1.29)$$

We can put these two results together, in order to obtain the following expression for the total energy of the system. It follows, just as it did for a single body system, that if no external forces are acting on the system, this total energy will remain constant.

$$E_{\text{tot}} = T_{\text{tot}} + U = \frac{1}{2} \sum_{i=1}^n m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i + U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) \quad (1.30)$$

If the system is isolated, then it follows that the potential energy function should depend only on the relative positions of the different bodies, and not on their absolute position relative to the origin. In this case, changing all of the positions by some constant displacement  $\delta$  should have no effect on  $U$ , and thus we must have:

$$\sum_{i=1}^n \nabla^{(i)} U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) = \mathbf{0} \quad (1.31)$$

This is equivalent to the result we obtained from Newton's third law, that all of the internal forces in the system should cancel out. As such, we can say that the momentum of a system is conserved, if the potential is unchanged by a translation of the entire system relative to the origin. In cases where this symmetry only exists in certain directions, only the components of the momentum in those directions will be conserved. There is a similar symmetry that relates to the conservation of energy; the total energy is conserved, because the potential energy function is invariant with translations through time.

In the case of non-conservative interactions, it is impossible to describe all the forces acting on the bodies with a potential function. This is because these interactions are influenced by the microscopic scale of the objects in question. That is to say that non-conservative forces like friction, appear to remove kinetic energy from the system because they are actually converting the macroscopic kinetic energy associated with an object's centre of mass motion, into the internal kinetic energy of the atoms and molecules that make up that body. Since classical mechanics is typically concerned with much greater length scales than this, we simply describe the process as dissipating the system's kinetic energy. Thus, if we consider thermal energy, which accounts for this internal motion, the total energy of a system will still be conserved.

### 1.3.3 Frames of Reference

An appropriate choice of reference frame can often greatly simplify mechanics problems, so it is worth us taking the time to discuss how one converts between different frames. Broadly speaking, there are two different types of reference frame; inertial frames, within which Newton's laws of motion are valid, and non-inertial frames, within which every object experiences a set of additional, fictitious forces. In this chapter we shall be dealing with exclusively inertial frames; however, a discussion of non-inertial frames is included in chapter 5, in the context of rotational dynamics.

Inertial frames, which correspond to the rest frames of objects experiencing no net force, differ from one another only by the position and velocity of their origins. The coordinates of two inertial frames  $S$  and  $S'$ , which share a common origin at  $t = 0$  and have a relative velocity of  $\mathbf{v}$ , are related via the Galilean transformations:

$$t' = t \quad \mathbf{r}' = \mathbf{r} - \mathbf{v}t \quad (1.32)$$

Applying these transformations to the total momentum of a system, as calculated in section 1.3.1, we obtain the following result:

$$\mathbf{p}'_{\text{tot}} = \mathbf{p}_{\text{tot}} - M_{\text{tot}}\mathbf{v} = M_{\text{tot}}(\dot{\mathbf{r}}_{\text{CM}} - \mathbf{v}) \quad (1.33)$$

From this, we can see that, if the system does not experience any external forces, it will always be possible to adopt an inertial frame of reference, such that the system has zero momentum. This is often referred to as the system's centre of mass frame, since in this frame the centre of mass is at rest. Importantly, since the momentum differs between frames by an additive constant, any change in the system's momentum will be the same in all inertial frames.

We can follow a similar line of analysis for the total kinetic energy of a system, in order to obtain:

$$T'_{\text{tot}} = T_{\text{tot}} - \mathbf{p}_{\text{tot}} \cdot \mathbf{v} + \frac{M_{\text{tot}}}{2}\mathbf{v} \cdot \mathbf{v} = \frac{M_{\text{tot}}}{2}(\dot{\mathbf{r}}_{\text{CM}} - \mathbf{v}) \cdot (\dot{\mathbf{r}}_{\text{CM}} - \mathbf{v}) \quad (1.34)$$

It follows that, any change in the kinetic energy of the system shall be the same in all inertial frames, provided that the system's momentum remains constant. In cases where the system's total momentum does not remain constant, this difference is accounted for by the fact that, in one of the frames, the force that is causing the change in momentum moves through a greater distance, thus doing more work.

It can sometimes be useful to express these quantities purely in terms of the system's centre of mass, which yields the following expressions:

$$\mathbf{p}_{\text{tot}} = M_{\text{tot}}\dot{\mathbf{r}}_{\text{CM}} \quad T_{\text{tot}} = T^* + \frac{\mathbf{p}_{\text{tot}} \cdot \dot{\mathbf{r}}_{\text{CM}}}{2} \quad (1.35)$$

Where  $T^*$  represents the kinetic energy of the system, evaluated about its centre of mass. It is worth noting that, as per our discussion in section 1.3.2, this kinetic energy typically neglects the contributions of the microscopic motion within a solid body. That is to say that, we define  $T^*$  to be the macroscopic kinetic energy, which is zero when all of the macroscopic bodies are at rest, while the offset due to the internal, microscopic kinetic energy of the bodies is labelled as the system's thermal energy.

### 1.3.4 Collisions

We can model a collision between two bodies as an instantaneous interaction between them. That is to say that, each of the bodies moves at a constant velocity until they meet, before immediately leaving the collision at a different constant velocity. As such, the fundamental principles that govern a collision are ensuring that the momentum, and where appropriate the kinetic energy, remains the same before and after the interaction.

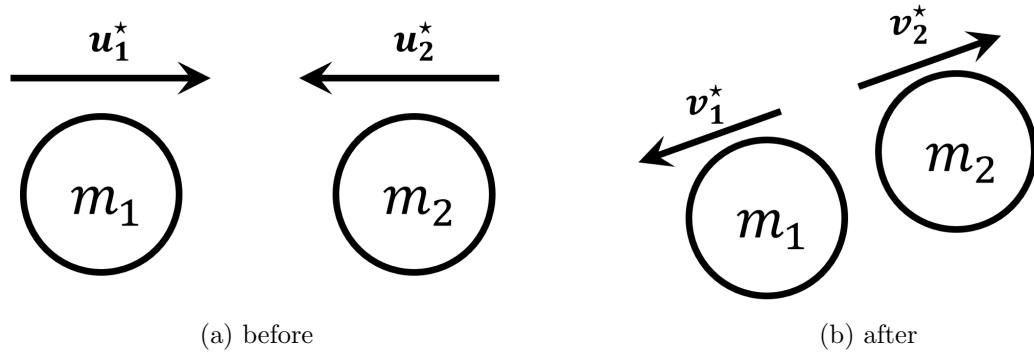


Figure 1.2: A collision, viewed in the centre of mass frame.

It turns out that, in general, collisions are best analysed in the centre of mass frame of the system. To demonstrate this, let us consider a collision between two masses  $m_1$  and  $m_2$ , with initial velocities  $\mathbf{u}_1$  and  $\mathbf{u}_2$ , such that their initial velocities in the centre of mass frame are given by:

$$\mathbf{u}_1^* = \mathbf{u}_1 - \frac{m_1 \mathbf{u}_1 + m_2 \mathbf{u}_2}{m_1 + m_2} \quad \mathbf{u}_2^* = \mathbf{u}_2 - \frac{m_1 \mathbf{u}_1 + m_2 \mathbf{u}_2}{m_1 + m_2} \quad (1.36)$$

As we would expect, the total momentum in this frame  $\mathbf{p}_{\text{tot}}^* = m_1 \mathbf{u}_1^* + m_2 \mathbf{u}_2^*$  is equal to zero. Thus it follows that, the final velocities in this frame must also satisfy the condition that  $m_1 \mathbf{v}_1^* + m_2 \mathbf{v}_2^* = \mathbf{0}$ , in order to conserve momentum. The only way that this can be the case is if, the two velocities are in opposite directions, and their magnitudes are related by:

$$|\mathbf{v}_1^*| = \eta |\mathbf{u}_1^*| \quad |\mathbf{v}_2^*| = \eta |\mathbf{u}_2^*| \quad (1.37)$$

Where  $\eta$  is a positive constant, known as the coefficient of restitution for the collision. As such, if we let  $\hat{\mathbf{e}}^*$  be a unit vector in the direction of  $\mathbf{v}_1^*$  we can express the final velocities in the original frame of reference as:

$$\mathbf{v}_1 = \frac{m_1 \mathbf{u}_1 + m_2 \mathbf{u}_2}{m_1 + m_2} + \eta |\mathbf{u}_1^*| \hat{\mathbf{e}}^* \quad \mathbf{v}_2 = \frac{m_1 \mathbf{u}_1 + m_2 \mathbf{u}_2}{m_1 + m_2} - \eta |\mathbf{u}_2^*| \hat{\mathbf{e}}^* \quad (1.38)$$

This also allows us to find a frame invariant expression for the coefficient of restitution by expressing it in terms of the relative velocities between the two masses:

$$\eta = \frac{|\mathbf{v}_1 - \mathbf{v}_2|}{|\mathbf{u}_1 - \mathbf{u}_2|} \quad (1.39)$$

The coefficient of restitution has an important interpretation as a measure of how much kinetic energy is conserved in the collision. In general,  $\eta^2$  represents the fraction of the system's internal kinetic energy (its kinetic energy in the centre of mass frame) is conserved in the collision. If  $\eta = 1$ , the collision is referred to as elastic, and kinetic energy is clearly conserved. Whereas, if  $\eta = 0$ , the collision is referred to as being perfectly inelastic and the maximum amount of kinetic energy possible is dissipated. A coefficient of restitution greater than 1, indicates that kinetic energy has been produced, which is characteristic of some form of explosion. The exact value of the coefficient of restitution can not be easily calculated and will depend on a lot of factors about the objects involved. However, most simple collisions can be reasonably well approximated as either elastic or perfectly inelastic.

Similarly, there is no easy method to calculate the direction of  $\hat{\mathbf{e}}^*$ , since this will depend on the exact nature of the contact surface between the two bodies. The exception to this rule occurs in the case of a perfectly elastic collision. Since such a collision conserves kinetic energy, there can be no frictional forces between the two objects, and as such, the only interaction between them is the normal contact force, which must act perpendicularly to the contact surface between them. This means that, if we know which surfaces of the bodies come into contact, we know the direction of the impulse (change in momentum) on each of them, which allows us to determine the directions of their outgoing velocities.

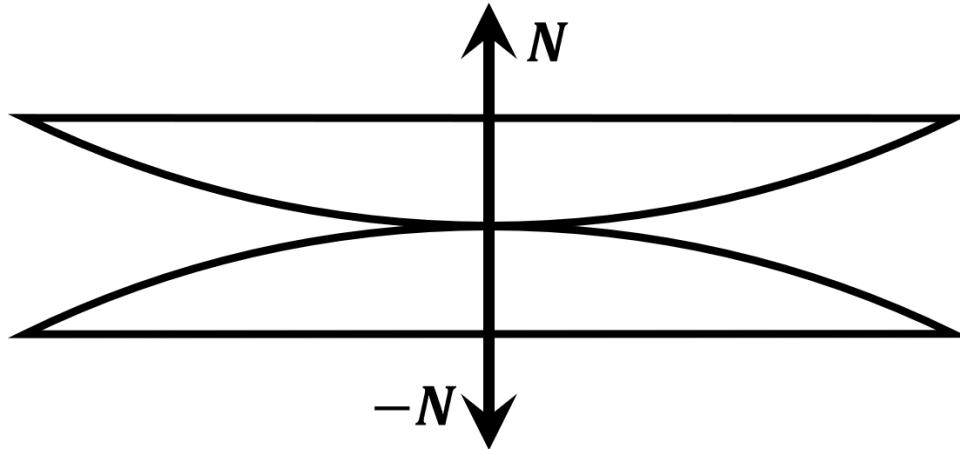


Figure 1.3: The normal reaction forces at a surface of contact.

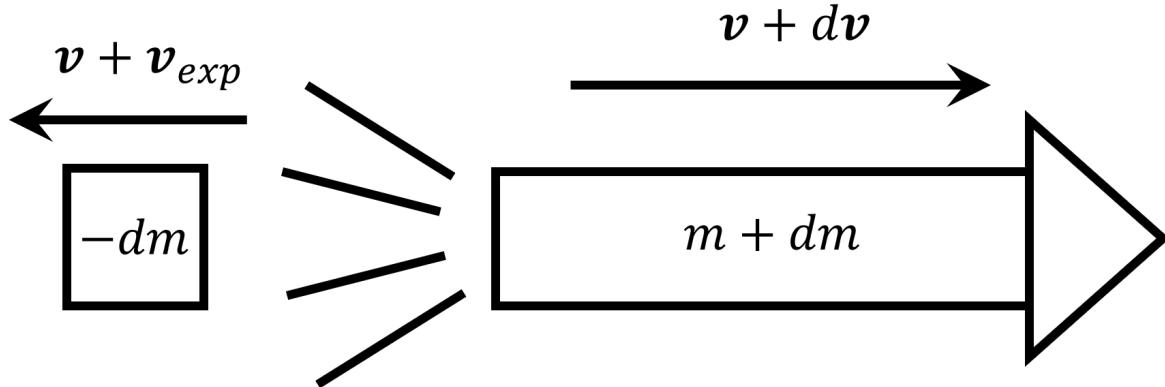
As an example, let us consider the elastic collision between two objects of equal mass, such that one of them is initially at rest. Parallel to the surface of contact, there is no impulse and so those components of the velocities remain unchanged. Perpendicular to the surface, the only way for to conserve both momentum and kinetic energy, is for all of the velocity of the moving body to be transferred to the stationary body. As such, following the collision, the two bodies will move with their velocities perpendicular to one another. We can see why this must be the case by noting that, since both objects have the same mass, the conservation laws can be written as:

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{u}_1 \quad \mathbf{v}_1 \cdot \mathbf{v}_1 + \mathbf{v}_2 \cdot \mathbf{v}_2 = \mathbf{u}_1 \cdot \mathbf{u}_1 \quad (1.40)$$

Taking the dot product of the first equation with itself, and then comparing this result to the second equation, we can immediately see that the two velocities are perpendicular:

$$\mathbf{v}_1 \cdot \mathbf{v}_1 + 2\mathbf{v}_1 \cdot \mathbf{v}_2 + \mathbf{v}_2 \cdot \mathbf{v}_2 = \mathbf{u}_1 \cdot \mathbf{u}_1 \implies \mathbf{v}_1 \cdot \mathbf{v}_2 = 0 \quad (1.41)$$

### 1.3.5 Rockets



$$d\mathbf{p} = \mathbf{v}dm + md\mathbf{v} - dm(\mathbf{v} + \mathbf{v}_{exp}) = \mathbf{F}dt$$

Figure 1.4: An infinitesimal time interval over which a rocket expels a mass  $-dm$  of fuel.

Unlike most conventional engines, which utilise the energy released by the combustion of fuel to turn a turbine of some description, a rocket generates thrust by expelling exhaust gases behind it. This has the consequence of changing the mass of the rocket significantly over the course of its flight, which we have to account for when analysing its dynamics. If we consider a rocket of mass  $m$  and velocity  $\mathbf{v}$ , the total external force acting on it is:

$$\mathbf{F} = m\dot{\mathbf{v}} - \dot{m}\mathbf{v}_{exp} \quad (1.42)$$

Although this result is reminiscent of the product rule for differentiation, we should note that  $\mathbf{v}_{exp}$  is not the velocity of the rocket, but instead the relative velocity with which the exhaust gases are expelled. This term arises due to the fact that as the exhaust gas is expelled, it is accelerated to a velocity of  $\mathbf{v}_{exp}$  relative to the rocket. As such, the exhaust exerts a thrust force of  $\dot{m}\mathbf{v}$  on the rocket, which is must be removed from  $m\dot{\mathbf{v}}$  to leave the external force. Equating (1.42) to the gravitational force on the rocket we obtain:

$$m\dot{\mathbf{v}} = \dot{m}\mathbf{v}_{exp} + mg \quad (1.43)$$

If we assume that the rocket moves over a sufficiently small height that  $\mathbf{g}$  remains constant, we can solve this equation by simply dividing through by  $m$  and integrating, which yields:

$$\mathbf{v}(t) = \mathbf{v}(0) + \mathbf{v}_{exp} \ln \left( \frac{m(t)}{m(0)} \right) + \mathbf{g}t \quad (1.44)$$

Once the rocket has burnt all of its fuel, it only moves under the influence of gravity, and as such, will either escape the Earth's gravitational field, or fall back to the ground. In order to minimize the time that the rocket spends decelerating in the Earth's gravitational field, rockets tend to launch by burning through all their fuel fairly quickly. As such, a rocket can be well approximated by a projectile launched with an initial velocity of  $\mathbf{v}_{exp} \ln(M_R)$ , where  $M_R$  is the fraction of the rocket's mass that will remain after all the fuel has been burnt.

## 1.4 Kinematics

Once we have utilised the principles outlined in the previous sections to determine a system's equation of motion, we then have to solve it for the system's time evolution. In general, this is quite a difficult thing to do; however, there are several useful cases for us to consider. This section shall focus on some of these cases, and we shall derive a few helpful results.

### 1.4.1 Constant Acceleration

The simplest example of an equation of motion is that of an object experiencing a constant force. In this case we can solve the equation of motion by simply integrating it twice, yielding the following results for the objects velocity  $\mathbf{v}$  and position  $\mathbf{r}$ :

$$\mathbf{v} = \mathbf{v}_0 + \mathbf{a}t \quad \mathbf{r} = \mathbf{r}_0 + \mathbf{v}_0 t + \frac{\mathbf{a}t^2}{2} \quad (1.45)$$

Where  $\mathbf{r}_0, \mathbf{v}_0$ , and  $\mathbf{a}$  are the initial values of the position, velocity, and acceleration respectively (the 0 subscript is omitted from the acceleration since this is the acceleration throughout the motion). By rearranging these equations somewhat, we can obtain two slightly different expressions for the object's position:

$$\mathbf{r} = \mathbf{r}_0 + \mathbf{v}t - \frac{\mathbf{a}t^2}{2} \quad \mathbf{r} = \mathbf{r}_0 + \frac{(\mathbf{v} + \mathbf{v}_0)t}{2} \quad (1.46)$$

In addition to this, there is one final result that we can obtain from (1.45). If we take the dot product of the first equation with itself, and then substitute in the second, we are left with:

$$\mathbf{v} \cdot \mathbf{v} = \mathbf{v}_0 \cdot \mathbf{v}_0 + 2\mathbf{a} \cdot (\mathbf{r} - \mathbf{r}_0) \quad (1.47)$$

This is actually nothing more than a statement of the relationship between the work done on an object and its kinetic energy, as outlined by equation (1.25) in section 1.3.2. These five results are known as the constant acceleration equations, and together they allow us to solve any problem featuring uniformly accelerated motion.

Let us now return to the expression for the object's position in equation (1.45). As the object moves along this trajectory, it traces out a parabolic path in space. To see this, let us adopt a set of coordinate axes  $x, y, z$ , such that:

$$\hat{\mathbf{x}} \parallel \mathbf{a} \times (\mathbf{v}_0 \times \mathbf{a}) \quad \hat{\mathbf{y}} \parallel \mathbf{a} \quad \hat{\mathbf{z}} \parallel \mathbf{v}_0 \times \mathbf{a} \quad (1.48)$$

Where  $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ , and  $\hat{\mathbf{z}}$  are unit vectors in each of the coordinate directions respectively. Using this coordinate system, we can represent the displacement of the object from its initial position as follows:

$$\mathbf{r} - \mathbf{r}_0 = \frac{|\mathbf{v}_0 \times \mathbf{a}|^2 t}{|\mathbf{a} \times (\mathbf{v}_0 \times \mathbf{a})|} \hat{\mathbf{x}} + \frac{|\mathbf{a}|^2 t^2 + 2\mathbf{a} \cdot \mathbf{v}_0 t}{2|\mathbf{a}|} \hat{\mathbf{y}} \quad (1.49)$$

Since the  $x$  coordinate is linear in  $t$ , while the  $y$  coordinate is quadratic in  $t$ , we can always eliminate the parameter to find that the trajectory is described by  $y$  as a quadratic function of  $x$ . Thus, the trajectory of the object must be parabolic.

One of the most common examples of uniform acceleration is projectile motion. A projectile is any object that moves solely under the influence of gravity, and as such, projectiles in the vicinity of the Earth's surface can be very well approximated as having a constant acceleration of  $g = 9.81 \text{ m s}^{-2}$  vertically downwards. Thus, if consider a projectile that leaves the origin with a velocity of magnitude  $v$ , making an angle  $\theta$  to the horizontal, we can use the constant acceleration equations to express the projectile's coordinates as functions of time:

$$x = vt \cos \theta \quad y = vt \sin \theta - \frac{gt^2}{2} \quad (1.50)$$

Where the  $x$  axis is oriented in the direction of the projectile's horizontal motion, and the  $y$  axis is oriented vertically upwards. By rearranging the first of these equations, and then substituting it into the second, we can obtain the following equation to describe the projectile's parabolic trajectory:

$$y = x \tan \theta - \frac{gx^2}{2v^2} \sec^2 \theta \quad (1.51)$$

When working with projectiles, one of the more useful results we could derive would be a formula for the necessary launching angle, in order to hit a specific target. To achieve this, we simply note that the trigonometric identity  $\sec^2 \theta = 1 + \tan^2 \theta$  turns (1.51) into a quadratic equation for  $\tan \theta$ . Since the general solution of a quadratic equation is well known, we can then immediately obtain the result:

$$\frac{gx^2}{2v^2} \tan^2 \theta - x \tan \theta + y + \frac{gx^2}{2v^2} = 0 \implies \tan \theta = \frac{v^2}{gx} \left( 1 \pm \sqrt{1 - \frac{2gy}{v^2} - \frac{g^2x^2}{v^4}} \right) \quad (1.52)$$

Thus, if we wish to hit a target located at a position  $(x, y)$  with respect to the origin, we can calculate the angle of projection from equation (1.52). This also allows us to determine the target area of the projectile, the region of all targets it is possible to hit with some choice of the angle  $\theta$ . We can simply note that (1.52) will have real solutions of  $\theta$  for any values of  $x$  and  $y$ , provided that  $\tan \theta$  is real. As such, the target area is described by:

$$y \leq \frac{v^2}{2g} \left( 1 - \frac{gx}{v^2} \right) \left( 1 + \frac{gx}{v^2} \right) \quad (1.53)$$

This target area can be quite helpful when determining the maximum range of a projectile, since its bounding parabola represents the extremes of all possible trajectories. For example, let us consider the maximum distance that a projectile, launched from a height  $h$ , can travel, before it hits the ground. To do this, we need only find the intersection between the parabola in (1.53) and the horizontal line  $y = -h$ . This is nothing more than solving a quadratic equation, which trivially leads to the result in (1.54). This value can then be substituted back into (1.52), to find the optimal angle of projection:

$$x_{\max} = \frac{v\sqrt{v^2 + 2gh}}{g} \quad \theta_{\max} = \arctan \left( \frac{v}{\sqrt{v^2 + 2gh}} \right) \quad (1.54)$$

### 1.4.2 The Virial Theorem

We are now going to move away from constant acceleration, in order to briefly discuss oscillatory motion. That is to say, we shall be considering systems that return to their original configuration after some fixed time period  $\tau$ . Let us consider the time averaged kinetic energy of a particle undergoing some form of periodic motion. Since the kinetic energy will vary continuously in time, this average is calculated by evaluating the following integral:

$$\langle T \rangle = \frac{1}{\tau} \int_0^\tau \frac{\mathbf{p} \cdot \dot{\mathbf{r}}}{2} dt \quad (1.55)$$

Since the particle's position and momentum must be the same at both  $t = 0$  and  $t = \tau$ , we can use integration by parts to convert this integral into the form:

$$\langle T \rangle = -\frac{1}{2\tau} \int_0^\tau \dot{\mathbf{p}} \cdot \mathbf{r} dt \quad (1.56)$$

If we substitute in Newton's second law that  $\mathbf{F} = \dot{\mathbf{p}}$ , and replace the integral in (1.56) with the time average of the integrand, we obtain the virial theorem:

$$\langle T \rangle = -\frac{\langle \mathbf{F} \cdot \mathbf{r} \rangle}{2} \quad (1.57)$$

We can generalise this result somewhat by considering what would happen if the particle's motion was not in fact periodic. In this case, there is no natural interval over which the time averaging should be carried out, and furthermore, there will be no interval over which the boundary terms will vanish. Thus, for non-periodic motion, averaged over some interval  $\tau$ , the equivalent to the virial theorem becomes:

$$2\langle T \rangle_\tau + \langle \mathbf{F} \cdot \mathbf{r} \rangle_\tau = \frac{\mathbf{p}(\tau) \cdot \mathbf{r}(\tau) - \mathbf{p}(0) \cdot \mathbf{r}(0)}{\tau} \quad (1.58)$$

Where we have added the subscript  $\tau$  to the averages to show that their values are dependent on the interval chosen. If the particle is stably bound in some potential well, then both its position and momentum will vary within some finite region. As such, in the limit that  $\tau \rightarrow \infty$ , the right hand side of (1.58) will tend towards zero, and thus the virial theorem will be restored. We can also extend the virial theorem to a system of  $n$  particles, by considering the time average of the total kinetic energy in the system:

$$\langle T \rangle = \frac{1}{\tau} \int_0^\tau \sum_{i=1}^n \frac{\mathbf{p}_i \cdot \dot{\mathbf{r}}_i}{2} dt \quad (1.59)$$

If we evaluate this integral by parts in the same way that we did for the one particle case, and use a similar argument to remove the boundary terms, we obtain the result:

$$\langle T \rangle = -\frac{1}{2} \sum_{i=1}^n \langle \mathbf{F}_i \cdot \mathbf{r}_i \rangle \quad (1.60)$$

Where  $\mathbf{F}_i$  and  $\mathbf{r}_i$  are the force experienced by and the position of the  $i$ th particle, respectively.

### 1.4.3 Continuous Systems

So far, all of our considerations have been limited to systems that are composed of discrete particles. Luckily, this is not actually a problem, since on an atomic scale, everything is made of particles. However, it is often convenient for us to model systems that exist on much larger length scales, as being continuous. As such, we are going to need to redevelop our ideas from the previous sections, for the context of a continuous system. Firstly, we can calculate the position of a continuous body's centre of mass using the following formulae, adapted from (1.21) in section 1.3.1.

$$M_{\text{tot}} = \int_V \rho dV \quad \mathbf{r}_{\text{CM}} = \frac{1}{M_{\text{tot}}} \int_V \rho \mathbf{r} dV \quad (1.61)$$

Where  $\rho$  is the density of the body at that point and the region of integration  $V$  is a volume of space, which contains all of the body's mass. If we wish to calculate the momentum of a continuous body, we have to use an adaptation of (1.20) from section 1.3.1:

$$\mathbf{p}_{\text{tot}} = \int_V \rho \mathbf{v} dV = M_{\text{tot}} \dot{\mathbf{r}}_{\text{CM}} \quad (1.62)$$

Where  $\mathbf{v}$  represents the velocity of the material at a given point. When proving the equivalence of the two expressions in (1.62), we have to be careful that it is  $\rho$  not  $\mathbf{r}$  in (1.61) that changes with time. The first step is to note that, since  $\rho \mathbf{v}$  is the mass flux of the system, it must obey the continuity equation below. Substituting this expression for  $\dot{\rho}$  into  $\dot{\mathbf{r}}_{\text{CM}}$  yields:

$$\dot{\rho} + \nabla \cdot (\rho \mathbf{v}) = 0 \implies M_{\text{tot}} \dot{\mathbf{r}}_{\text{CM}} = - \int_V \mathbf{r} \nabla \cdot (\rho \mathbf{v}) dV \quad (1.63)$$

Since the mass of the body is localised,  $\rho$  must be zero everywhere outside a finite region. This allows us to evaluate the integral in (1.63) by parts, using the vector calculus identity:

$$\oint_{\partial V} \mathbf{F}(\mathbf{G} \cdot d\mathbf{S}) = \int_V \mathbf{F} \nabla \cdot \mathbf{G} + (\mathbf{G} \cdot \nabla) \mathbf{F} dV \quad (1.64)$$

Since  $(\mathbf{F} \cdot \nabla) \mathbf{r} = \mathbf{F}$ , for all vector fields  $\mathbf{F}$ , this leads us to the required result. In addition to this, we may also require an expression for the total kinetic energy of a continuous body. This is given by the modified form of equation (1.28) in section 1.3.2:

$$T_{\text{tot}} = \frac{1}{2} \int_V \rho \mathbf{v} \cdot \mathbf{v} dV \quad (1.65)$$

Finally, we need to extend the concept of a force to a continuous system. To do this we introduce the force density  $\mathbf{f}$ , which represents the force per unit volume at a specific point within the body. It follows from Newton's second law that, if we divide  $\mathbf{f}$  by  $\rho$ , we will obtain the force per unit mass, which is equivalent to the rate of change of a mass element's velocity. However, since each mass element is also moving through space, this time derivative has to be evaluated as shown in equation (1.66):

$$\frac{\mathbf{f}(\mathbf{r}, t)}{\rho(\mathbf{r}, t)} = \lim_{\delta t \rightarrow 0} \frac{\mathbf{v}(\mathbf{r} + \mathbf{v}\delta t, t + \delta t) - \mathbf{v}(\mathbf{r}, t)}{\delta t} \implies \mathbf{f} = \rho(\dot{\mathbf{v}} + (\mathbf{v} \cdot \nabla) \mathbf{v}) \quad (1.66)$$

This result is known as Euler's equation for fluid flow and it serves as the equivalent for Newton's second law. The unusual  $(\mathbf{v} \cdot \nabla) \mathbf{v}$  term arises, because  $\mathbf{v}$  represents the velocity of the material at a specific point, and not the velocity of a specific element of material.

### 1.4.4 Rigid Bodies

A rigid body is a special case of a continuous system, that possesses the property that, the distance between any two elements of the body must remain constant, throughout its motion. While in practice, there is no such thing as a truly rigid body, they offer a very good approximation for a lot of solid systems, and as such, they are certainly worth discussing. Requiring that a body behaves rigidly places a lot of restrictions on how it can move, which will be the main focus of this section.

We shall begin by considering the mapping  $\mathbf{R}_t(\mathbf{r}) \mapsto \mathbf{r}'$ , which maps the position of some element in a rigid body at some initial time  $t_0$ , onto its position after a time interval  $t$ . We can summarise the rigidity condition by stating that this mapping must obey:

$$|\mathbf{R}_t(\mathbf{r}_1) - \mathbf{R}_t(\mathbf{r}_2)| = |\mathbf{r}_1 - \mathbf{r}_2| \quad \forall \mathbf{r}_1, \mathbf{r}_2 \quad (1.67)$$

We can put this result to use, by considering the mapping of  $\mathbf{R}_t(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM})$ . In order to determine this position, we will need to know the magnitude of its displacement from at least three distinct points in space. In fact, it turns out that, in general, even three points is not enough to uniquely determine the position; however, for our purposes it is sufficient. As such, we shall also be considering the displacements of this element from the mappings:  $\mathbf{R}_t(\mathbf{r}_1)$ ,  $\mathbf{R}_t(\mathbf{r}_2)$ , and  $\mathbf{R}_t(\mathbf{r}_{CM})$ . It follows from (1.67) that we must have:

$$\begin{aligned} |\mathbf{R}_t(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM}) - \mathbf{R}_t(\mathbf{r}_{CM})| &= |\mathbf{r}_1 - \mathbf{r}_{CM} + \mathbf{r}_2 - \mathbf{r}_{CM}| \\ |\mathbf{R}_t(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM}) - \mathbf{R}_t(\mathbf{r}_1)| &= |\mathbf{r}_2 - \mathbf{r}_{CM}| \\ |\mathbf{R}_t(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM}) - \mathbf{R}_t(\mathbf{r}_2)| &= |\mathbf{r}_1 - \mathbf{r}_{CM}| \end{aligned} \quad (1.68)$$

Geometrically, these equations describe three spheres in space, with the solution being represented by their intersection. In general, three spheres with non collinear centres, can intersect at a maximum of two distinct points, one on either side of the plane defined by their centres. However, if this intersection occurs in the plane containing all three centres, both points become the same, and thus there will only be a single solution. Similarly, if the centres are collinear, but not concentric, there will be a single solution, if the intersection occurs on the line defined by the centres. Either way, this is the case here, as we can see that  $\mathbf{R}_t(\mathbf{r}_1) + \mathbf{R}_t(\mathbf{r}_2) - \mathbf{R}_t(\mathbf{r}_{CM})$  will solve the equations in (1.68)<sup>1</sup>, and clearly lies in the plane defined by the centres  $\mathbf{R}_t(\mathbf{r}_1)$ ,  $\mathbf{R}_t(\mathbf{r}_2)$ , and  $\mathbf{R}_t(\mathbf{r}_{CM})$ . Thus, we can conclude that:

$$\mathbf{R}_t(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM}) = \mathbf{R}_t(\mathbf{r}_1) + \mathbf{R}_t(\mathbf{r}_2) - \mathbf{R}_t(\mathbf{r}_{CM}) \quad (1.69)$$

If we now wish to find the velocity of the body at a given point, we simply need to consider the limit of  $\mathbf{R}_{\delta t}(\mathbf{r})$  in the limit as  $\delta t$  tends towards zero. This then allows us to obtain a result for the velocity that is analogous to (1.69):

$$\mathbf{v}(\mathbf{r}) = \lim_{\delta t \rightarrow 0} \frac{\mathbf{R}_{\delta t}(\mathbf{r}) - \mathbf{r}}{\delta t} \implies \mathbf{v}(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{CM}) = \mathbf{v}(\mathbf{r}_1) + \mathbf{v}(\mathbf{r}_2) - \dot{\mathbf{r}}_{CM} \quad (1.70)$$

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<sup>1</sup>To verify that this solves the first equation we can use the geometrical identity that, for any two vectors  $\mathbf{u}$  and  $\mathbf{v}$  we must have:  $|\mathbf{u} + \mathbf{v}|^2 = 2|\mathbf{u}|^2 + 2|\mathbf{v}|^2 - |\mathbf{u} - \mathbf{v}|^2$ , together with (1.67). The other two follow immediately from (1.67).

We now introduce the mapping  $\mathbf{L}(\mathbf{r} - \mathbf{r}_{\text{CM}}) \mapsto \mathbf{v}(\mathbf{r}) - \dot{\mathbf{r}}_{\text{CM}}$ , which maps the displacement of an element from the body's centre of mass onto its relative velocity to the centre of mass. Using equation (1.70), we can verify that this must be a linear mapping:

$$\mathbf{L}(\mathbf{r}_1 - \mathbf{r}_{\text{CM}} + \mathbf{r}_2 - \mathbf{r}_{\text{CM}}) = \mathbf{v}(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_{\text{CM}}) - \dot{\mathbf{r}}_{\text{CM}} = \mathbf{L}(\mathbf{r}_1 - \mathbf{r}_{\text{CM}}) + \mathbf{L}(\mathbf{r}_2 - \mathbf{r}_{\text{CM}}) \quad (1.71)$$

Furthermore, in order to satisfy the rigidity condition between a point at  $\mathbf{r}$  and the centre of mass, we must find that  $|\mathbf{r} - \mathbf{r}_{\text{CM}} + (\mathbf{v}(\mathbf{r}) - \dot{\mathbf{r}}_{\text{CM}})dt| \approx |\mathbf{r} - \mathbf{r}_{\text{CM}}|$  to first order in  $dt$ . The only way that this can be true is for the relative velocity to be perpendicular to the displacement<sup>2</sup>. In other words, the mapping  $\mathbf{L}$  must satisfy the condition:

$$(\mathbf{r} - \mathbf{r}_{\text{CM}}) \cdot \mathbf{L}(\mathbf{r} - \mathbf{r}_{\text{CM}}) = 0 \quad (1.72)$$

Since an arbitrary linear mapping can always be represented by a matrix, we should be able to express (1.72) in matrix form. If we denote the elements of  $\mathbf{L}$  as  $L_{ij}$ , then we can say that, for all values of the coordinates  $x, y$  and  $z$ , we must have:

$$(x \ y \ z) \begin{pmatrix} L_{xx} & L_{xy} & L_{xz} \\ L_{yx} & L_{yy} & L_{yz} \\ L_{zx} & L_{zy} & L_{zz} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0 \quad (1.73)$$

We can see from this expression that all of the diagonal elements in the matrix must be equal to zero, otherwise it would always be possible to generate a non-zero result, by setting all but one of the coordinates to zero. Furthermore, by setting only one of the coordinates to zero at a time, we can deduce that the off diagonal elements must be skew symmetric, that is to say that  $L_{ij} = -L_{ji}$ , for each of the three pairs in the matrix. If we now construct the vector  $\boldsymbol{\omega}$  from these elements, as shown below, we can say, without loss of generality, that:

$$\boldsymbol{\omega} = \begin{pmatrix} L_{zy} \\ L_{xz} \\ L_{yx} \end{pmatrix} \implies \mathbf{L}(\mathbf{r} - \mathbf{r}_{\text{CM}}) = \boldsymbol{\omega} \times (\mathbf{r} - \mathbf{r}_{\text{CM}}) \quad (1.74)$$

Using this result, we can completely describe the motion of a rigid body by specifying two vectors: the velocity of the centre of mass  $\dot{\mathbf{r}}_{\text{CM}}$ , and the body's angular velocity  $\boldsymbol{\omega}$ . The velocity of the body at an arbitrary point is then given by:

$$\mathbf{v}(\mathbf{r}) = \dot{\mathbf{r}}_{\text{CM}} + \boldsymbol{\omega} \times (\mathbf{r} - \mathbf{r}_{\text{CM}}) \quad (1.75)$$

As we shall see in chapter 5, this is equivalent to saying that a rigid body can always be described by its centre of mass motion, combined with a rotation about its centre of mass. It is worth noting that, both  $\dot{\mathbf{r}}_{\text{CM}}$  and  $\boldsymbol{\omega}$  are in general time dependent, with an analysis of all the forces acting on the body throughout its motion being necessary to determine how they change with time.

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<sup>2</sup>To see this, we should note that since  $|\mathbf{a} + \mathbf{b}|^2 = |\mathbf{a}|^2 + |\mathbf{b}|^2 + 2\mathbf{a} \cdot \mathbf{b}$ ,  $|\mathbf{a} + \mathbf{b}| = \sqrt{|\mathbf{a}|^2 + |\mathbf{b}|^2 + 2\mathbf{a} \cdot \mathbf{b}}$ , which can be approximated to first order by  $|\mathbf{a}| + \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}|}$ , if  $|\mathbf{b}| \ll |\mathbf{a}|$

## 1.5 Variational Principles

We are going to conclude our discussion of classical dynamics with a brief overview of some of the different formalisms that can be used to derive a system's equations of motion. In particular, we will be looking at formulations that involve variational principles, that is to say that, these formulations are based on either maximising or minimising some quantity.

### 1.5.1 Lagrangian Dynamics

In Lagrangian mechanics, we consider a system whose state can be described by  $n$  coordinates  $x_i$ , and their time derivatives  $\dot{x}_i$ . If the system then evolves through time from some state  $A$  at time  $t_1$ , to another state  $B$  at time  $t_2$ , we define the action of this evolution  $S$  to be:

$$S = \int_{t_1}^{t_2} L(x_1, x_2, \dots, x_n, \dot{x}_1, \dot{x}_2, \dots, \dot{x}_n, t) dt \quad (1.76)$$

Where the Lagrangian  $L$  is some function of the system's coordinates and their derivatives, with a form specified by the physical theory in question. We can then apply the principle of stationary action, which states that the trajectory the system will take, as it evolves from  $A$  to  $B$ , is such that small perturbations in the path taken leave the action unchanged. To find this path, let us consider the change to the action, when each coordinate  $x_i$  is given a small perturbation  $\varepsilon_i(t)$ . It follows that, to first order, the change in the action is given by:

$$\delta S = \int_{t_1}^{t_2} \sum_{i=1}^n \frac{\partial L}{\partial x_i} \varepsilon_i(t) + \frac{\partial L}{\partial \dot{x}_i} \dot{\varepsilon}_i(t) dt \quad (1.77)$$

Now since the state of the system, and hence its coordinates, is fixed at both ends of the region of integration, we must find that  $\varepsilon_i(t_1) = \varepsilon_i(t_2) = 0$ . We can use this fact to integrate  $\dot{\varepsilon}_i(t)$  terms in (1.77) by parts, yielding:

$$\delta S = \int_{t_1}^{t_2} \sum_{i=1}^n \left[ \frac{\partial L}{\partial x_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) \right] \varepsilon_i(t) dt \quad (1.78)$$

If we now enforce the requirement that  $\delta S$  is equal to zero, for all possible perturbations  $\varepsilon_i(t)$ , we can see that the Euler-Lagrange equation below must be satisfied.

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0 \quad (1.79)$$

In deriving this result, we utilised the assumption that both the system's initial and final configurations had already been specified. However, this can seem to be circular reasoning, after all the reason why we wish to derive a system's equation of motion is to enable us to determine the end point from the starting point. We can deal with this issue by noting that, for any given state  $A$  at  $t_1$ , there will only be one possible state  $B$  at  $t_2$ , which can be reached by a trajectory obeying the Euler-Lagrange equation. As such, if we attempt to fix the end point to the wrong state, we will find that there is no path of stationary action from  $A$  to  $B$ , and thus, the system is not physically allowed to evolve from  $A$  to  $B$  over the specified time interval. Therefore, when we solve (1.79), subject to the initial conditions of being in a state  $A$  at time  $t_1$ , we are not only finding the trajectory of the system, we are also determining the only possible state  $B$  that can be reached at time  $t_2$ , by a path of stationary action.

Whilst in our previous formulation of mechanics, momentum was simply defined as something that was conserved, with the exact form of the momentum then being specified by the physical theory in question, the Lagrangian formulation provides a natural definition of the momentum in terms of the Lagrangian itself. We define a conjugate momentum  $p_i$  for each of the coordinates  $x_i$ , as shown in (1.80), which allows us to rewrite the Euler-Lagrange equation as:

$$p_i = \frac{\partial L}{\partial \dot{x}_i} \implies \frac{dp_i}{dt} = \frac{\partial L}{\partial x_i} \quad (1.80)$$

The Lagrangian used to describe classical dynamics takes a relatively simple form, and can be expressed neatly in terms of the kinetic and potential energies of a system as:

$$L = T - U \quad (1.81)$$

If we substitute into this equation the relevant expressions for a system of particles and evaluate all the necessary derivatives, we will arrive at all the standard results presented in section 1.3. One thing that we should be aware of is that, while the Lagrangian formulation naturally lends itself towards working in a component form, it is fairly typical to group together components into the vector notation we are more familiar with. For example, in the case of a single particle, both the component form that comes directly from the Euler-Lagrange equation, and the vector form of Newton's second law are presented below:

$$p_i = m\dot{x}_i \quad \frac{dp_i}{dt} = -\frac{\partial U}{\partial x_i} \iff \mathbf{p} = m\dot{\mathbf{x}} \quad \frac{d\mathbf{p}}{dt} = -\nabla U \quad (1.82)$$

When dealing with discrete systems, this Lagrangian approach can be a particularly powerful way to find the equations of motion. However, if we wish to extend these ideas to model continuous systems, we need to make a slight adjustment to our formulation. A continuous system can not generally be described by a finite number of coordinates, but instead a finite number of fields  $\phi_i$ , which are defined over the entire region of space and time that we are considering. As such, we define the action of a continuous system to be:

$$S = \int_{t_1}^{t_2} \int_V \mathcal{L}(\phi_i, \partial_t \phi_i, \partial_x \phi_i, \partial_y \phi_i, \partial_z \phi_i, t, x, y, z) dV dt \quad (1.83)$$

Where  $V$  is some volume which contains the system in question,  $\mathcal{L}$  is called the Lagrangian density of the system, and  $\partial_j \phi_i$  represents the partial derivative of the field  $\phi_i$ , with respect to the coordinate  $j$ . Using the same argument as we did before, we perturb each  $\phi_i$  by the small field  $\varepsilon_i$ , to find that the change in the action is:

$$\delta S = \int_{t_1}^{t_2} \int_V \sum_{i=1}^n \sum_{j=t,x,y,z} \left[ \frac{\partial \mathcal{L}}{\partial \phi_i} - \partial_j \left( \frac{\partial \mathcal{L}}{\partial (\partial_j \phi_i)} \right) \right] \varepsilon_i dV dt \quad (1.84)$$

By applying the principle of stationary action, and requiring that  $\delta S$  is equal to zero for arbitrary perturbations, we obtain the generalised form of the Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial \phi_i} = \sum_{j=t,x,y,z} \partial_j \left( \frac{\partial \mathcal{L}}{\partial (\partial_j \phi_i)} \right) \quad (1.85)$$

### 1.5.2 Hamiltonian Dynamics

While in Lagrangian mechanics, the fundamental variables that describe a system are the coordinates and their derivatives, it can sometimes be useful for us to reformulate our expressions in terms of the coordinates and their conjugate momenta. To do this, let us consider the differential of the Lagrangian:

$$dL = \frac{\partial L}{\partial t} dt + \sum_{i=1}^n \left( \frac{\partial L}{\partial x_i} dx_i + \frac{\partial L}{\partial \dot{x}_i} d\dot{x}_i \right) = \frac{\partial L}{\partial t} dt + \sum_{i=1}^n \left( \dot{p}_i dx_i + p_i d\dot{x}_i \right) \quad (1.86)$$

We can now use a Legendre transformation to remove the  $p_i d\dot{x}_i$  terms from the differential, by introducing a new function  $H$ , known as the Hamiltonian. We define this function to be given by:

$$H = \sum_{i=1}^n p_i \dot{x}_i - L \implies dH = -\frac{\partial L}{\partial t} dt + \sum_{i=1}^n \left( \dot{x}_i dp_i - \dot{p}_i dx_i \right) \quad (1.87)$$

As such, the fundamental equations of Hamiltonian mechanics can be expressed in terms of the derivatives of the Hamiltonian:

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} \quad \dot{x}_i = \frac{\partial H}{\partial p_i} \quad (1.88)$$

An interesting consequence of this reformulation can be seen if the Lagrangian does not explicitly depend on time. That is to say that, if a physical theory is invariant under translations through time, the partial derivatives of both the Lagrangian and the Hamiltonian, with respect to time, must be equal to zero. In this case, the total time derivative of the Hamiltonian is given by:

$$\frac{dH}{dt} = \sum_{i=1}^n \left( \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial x_i} \dot{x}_i \right) = \sum_{i=1}^n \left( \dot{x}_i \dot{p}_i - \dot{p}_i \dot{x}_i \right) = 0 \quad (1.89)$$

Thus, we can see that, if the Lagrangian, and hence the whole physical theory, is symmetric with respect to translations through time, the Hamiltonian will be a conserved quantity of a system. Furthermore, if we substitute in the equation (1.81) for the Lagrangian, the Hamiltonian becomes equal to the total energy of the system. In fact, this serves as a fairly general definition for the energy of a system, provided that its Lagrangian is known.

Just as we did before, we can extend these ideas to continuous systems by introducing a Hamiltonian density. In addition to this, if we want an equivalent of (1.89) for the conservation of the Hamiltonian, we must also introduce a Hamiltonian flux  $\mathcal{S}$  defined by:

$$\mathcal{H} = \sum_{i=1}^n \partial_t \phi_i \frac{\partial \mathcal{L}}{\partial (\partial_t \phi_i)} - \mathcal{L} \quad \mathcal{S}_j = \sum_{i=1}^n \partial_t \phi_i \frac{\partial \mathcal{L}}{\partial (\partial_j \phi_i)} \quad (1.90)$$

The equivalent of the conservation law in (1.89) is the continuity equation for  $\mathcal{H}$  below, which is derived under the same assumption of translational time symmetry. If a continuous system is localised,  $\mathcal{L}$  should tend towards zero at infinity, and thus so should  $\mathcal{S}$ , which implies that the integral of the Hamiltonian density over all space must be conserved.

$$\frac{\partial \mathcal{H}}{\partial t} + \nabla \cdot \mathcal{S} = 0 \quad (1.91)$$

### 1.5.3 Noether's Theorem

One of the most elegant results on all of physics is Noether's theorem, which states that, every differentiable symmetry in a physical system's action corresponds to a conserved quantity of that system. This means that, if a physical theory has an inherent symmetry, such as being invariant under translations through space and time, then certain quantities within that theory will be conserved. Formally, let us consider the coordinate transformation:

$$t \rightarrow t' = t + \varepsilon T \quad x_i \rightarrow x'_i = x_i + \varepsilon X_i \quad (1.92)$$

Where  $T$  is some constant, the  $X_i$  are functions of the coordinates, and  $\varepsilon \ll 1$ . In order for this transformation to be a symmetry of the system's action, it must leave the Lagrangian unchanged. As such, we can say that  $L(x'_i, \dot{x}'_i, t') = L(x_i, \dot{x}_i, t)$ , and thus, by expanding this equation to first order in  $\varepsilon$ , we obtain the result that:

$$\sum_{i=1}^n \left( \frac{\partial L}{\partial x_i} X_i + \frac{\partial L}{\partial \dot{x}_i} \dot{X}_i \right) + \frac{\partial L}{\partial t} T = 0 \quad (1.93)$$

It follows from the Euler-Lagrange equation that, when the system is evolving along the physically allowed trajectory, the term within the summation will be a perfect derivative:

$$\frac{\partial L}{\partial x_i} X_i + \frac{\partial L}{\partial \dot{x}_i} \dot{X}_i = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) X_i + \frac{\partial L}{\partial \dot{x}_i} \dot{X}_i = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} X_i \right) \quad (1.94)$$

Let us now consider the complete time derivative of the Lagrangian. We can expand this derivative using the chain rule of partial differentiation, which leads us to obtain the following expression:

$$\frac{dL}{dt} = \frac{\partial L}{\partial t} + \sum_{i=1}^n \left( \frac{\partial L}{\partial x_i} \dot{x}_i + \frac{\partial L}{\partial \dot{x}_i} \ddot{x}_i \right) \quad (1.95)$$

Using the same trick as we did to produce (1.94), we can express the term inside the summation as a perfect derivative. This then allows us to express the partial derivative of the Lagrangian with time as the total time derivative:

$$\frac{\partial L}{\partial t} = \frac{d}{dt} \left[ L - \sum_{i=1}^n \frac{\partial L}{\partial \dot{x}_i} \dot{x}_i \right] \quad (1.96)$$

By substituting (1.96) and (1.94) into equation (1.93), we can determine that, the time derivative of the following quantity must be equal to zero:

$$\frac{d}{dt} \left[ \left( \sum_{i=1}^n \frac{\partial L}{\partial \dot{x}_i} \dot{x}_i - L \right) T - \frac{\partial L}{\partial \dot{x}_i} X_i \right] = 0 \quad (1.97)$$

If we consider a Lagrangian that is invariant under translations in time, we can set  $T = 1$  and  $Q_i = 0$ , in which case the conserved quantity is precisely the same as the Hamiltonian from section 1.5.2. Similarly, if we consider a Lagrangian that is invariant under translation in any spatial direction, we obtain three conserved quantities (one for each dimension in space), which correspond to the components of the system's total momentum.

# 2 Oscillating Systems

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## 2.1 Simple Harmonic Motion

Simple harmonic motion is practically synonymous with oscillation, and indeed, it shall form the basis for everything that we discuss in this chapter. As we shall see later, simple harmonic motion is actually a very general approximation for a system's behaviour in the neighbourhood of a stable equilibrium, and as such, is applicable to some degree in the vast majority of situations. One of the most important properties of harmonic motion is that, the period of an oscillation is independent of its amplitude. It is this property, which is indicative of the more fundamental observation that the equation of motion is linear, that sets simple harmonic motion in a league of its own in terms of computational ease.

### 2.1.1 The Simple Harmonic Oscillator

A system can be described as a simple harmonic oscillator, if it has a potential energy that grows quadratically with displacement from the equilibrium position. It is most convenient for us to represent such a parabolic potential in the form of equation (2.1) below. Common examples of this include any system based around elastic strain, such as a mass on a spring, which has a potential energy of  $\frac{1}{2}kx^2$ , where  $k$  is the force constant of the spring.

$$U(x) = U_0 + \frac{m\omega_0^2}{2}x^2 \quad (2.1)$$

If  $x$  represents the displacement of a particle with mass  $m$ , then it follows that the system will have a kinetic energy of  $T = \frac{1}{2}m\dot{x}^2$ . From here, we can simply combine these results to obtain an expression for the total energy of the system in the form  $E = U_0 + \frac{1}{2}[m\dot{x}^2 + m\omega_0^2x^2]$ . Assuming that there are no external dissipative forces acting on our system, we must have:

$$\dot{E} = 0 \implies \ddot{x} + \omega_0^2x = 0 \quad (2.2)$$

This is known as the fundamental equation of simple harmonic motion, and is often taken to be the definition of harmonic motion. Equation (2.2) is actually a special case of a more general class of ordinary differential equation, which we shall cover in far greater detail later on. For now, we are going to use a fairly simple method to solve the equation. If we first multiply by  $\dot{x}$  and then integrate, we regain our statement of conservation of energy in the form of the first order differential equation:

$$\dot{x} = \pm\omega_0\sqrt{a_0^2 - x^2} \quad (2.3)$$

Where  $a_0$  is a new parameter, introduced to simplify our algebra later down the line, which is defined by the relationship  $E - U_0 = \frac{1}{2}m\omega_0^2a_0^2$ . Equation (2.3) is separable and so can be trivially solved to give:

$$x(t) = a_0 \cos(\omega_0 t + \phi) \quad (2.4)$$

Where  $\phi$  is a constant of integration. As is typical for an equation of motion, which is nearly always a second order differential equation, we have two arbitrary constants in our solution. These constants represent the freedom in the initial values of both  $x$  and  $\dot{x}$ .

### 2.1.2 The Phasor Representation

While there is nothing inherently wrong with expressing our solutions in terms of sine and cosine functions, as we did in section (2.1.1), physicists often prefer to use a slightly different notation. Although this can be unintuitive at first, it really does help to reduce the amount of algebra involved in manipulating these solutions. Since the fundamental equation of harmonic motion is linear with real coefficients, it follows that if any complex number  $\mathcal{X}(t)$  is a solution, both its real and imaginary parts must independently be solutions. We can now choose to represent our manifestly real and physical solution  $x(t)$  as nothing more than the real part of the complex number:

$$\mathcal{X}(t) = \mathcal{A}e^{i\omega_0 t} \quad (2.5)$$

We can express this complex amplitude in terms of our two previous constants through the equation  $\mathcal{A} = a_0 e^{i\phi}$ . The advantage of this representation becomes immediately apparent when taking derivatives. Since  $x$  is the real part of  $\mathcal{X}$ , we can conclude that  $\dot{x}$  must be the real part of  $\dot{\mathcal{X}}$ . It is trivial to see that  $\dot{\mathcal{X}}(t) = i\omega_0 \mathcal{X}(t)$  and thus, we must have:

$$x(t) = \Re \mathcal{X}(t) \implies \dot{x}(t) = -\omega_0 \Im \mathcal{X}(t) \quad (2.6)$$

Another advantage of this method comes when we consider the superposition of different solutions. Since the fundamental equation is linear, we can take any linear combination or superposition of solutions to obtain a new solution. The phasor representation gives us a nice geometric way of visualising the way in which these solutions can interfere with each other, by adding their amplitudes on the complex plane.

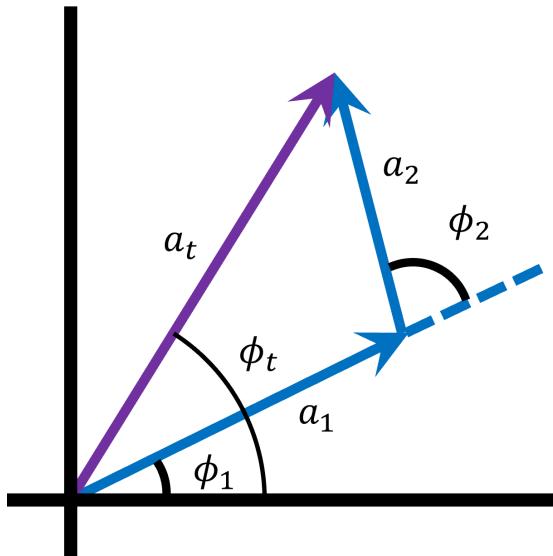


Figure 2.1: Two complex amplitudes being added on the complex plane to form a larger oscillation.

The one thing to watch out for, when using complex numbers in this way, is non-linearity. As soon we try to use some non-linear combination of complex variables, such as in the expressions of the kinetic and potential energies, the complex notation breaks down and we have to use the original sinusoidal functions.

### 2.1.3 Approximating General Potentials

Unfortunately, most real world systems have potential energy functions that are far more complicated than the simple quadratics we have been considering so far. One such potential is the Morse potential, which expresses the potential energy as  $U = D(1 - e^{-ax})^2$ . As we can see from figure 2.2, this function describes an asymmetric potential well, which grows very rapidly with displacement in one direction, whilst asymptotically approaching a constant in the other. This potential is normally used to describe a covalent bond between two atoms, where at long ranges the dominant interaction is the favourable sharing of electrons between both nuclei, which is eventually overwhelmed by the unfavourable repulsion of core electrons as the two nuclei get closer.

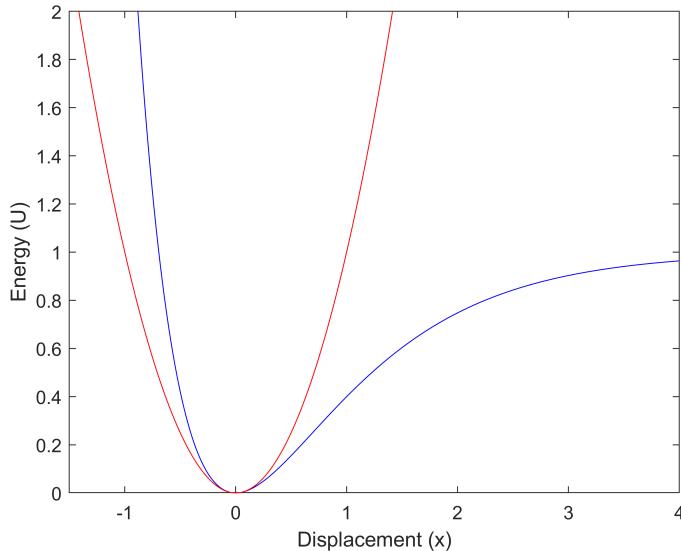


Figure 2.2: A typical Morse potential (blue) together with the best quadratic fit to the potential (red).

Although, in this case the equation of motion is significantly more complicated than equation (2.2), one significant benefit to the Morse potential is that there is still an analytic solution for  $x(t)$ . To find it, we use the same trick as we did in section (2.1.1), and turn our statement of energy conservation into a separable, first order differential equation in  $x$ :

$$\dot{x} = \sqrt{\frac{2E}{m} - \frac{2D}{m} (1 - e^{-ax})^2} \quad (2.7)$$

This equation can be solved, albeit with a bit of effort, by the standard technique of separating the variables and then integrating. After some rearrangement, this will give us the solution below, where we have introduced the substitutions  $\omega^2 = \frac{2a^2D}{m}(1 - \rho)$  and  $\rho = \frac{E}{D}$  for simplicity. Just as before we are able to vary the parameters  $\rho$  and  $\phi$  to obtain any initial conditions that we require.

$$x = \frac{1}{a} \ln \left( \frac{1 - \sqrt{\rho} \cos(\omega t + \phi)}{1 - \rho} \right) \quad (2.8)$$

As we can see, this solution is quite awkward to manipulate and so where possible, we would like to approximate it with something simpler.

As it turns out, there is a very general approximation, that we can apply in the neighbourhood of a stable equilibrium position. To see this, let us consider an arbitrary potential  $U(x)$ , which has such an equilibrium at  $x = x_0$ . If we take a Taylor series expansion about this point, we obtain:

$$U(x) = U(x_0) + U'(x_0)(x - x_0) + \frac{1}{2}U''(x_0)(x - x_0)^2 + \frac{1}{3!}U'''(x_0)(x - x_0)^3 + \dots \quad (2.9)$$

By definition, an equilibrium position represents a stationary point of the potential energy, and thus, we must find that the first derivative of  $U$  vanishes at  $x = x_0$ . Furthermore, in order for this equilibrium to be stable, it must correspond to a minimum in the potential energy and so the second derivative of  $U$  must be positive at  $x = x_0$ . If we now take the limit as  $|x - x_0| \rightarrow 0$ , we obtain:

$$U(x) \approx U(x_0) + \frac{U''(x_0)}{2}(x - x_0)^2 \quad (2.10)$$

If we were to now re-express the potential in terms of the new variable  $\xi = (x - x_0)$ , we would find that in the neighbourhood of the equilibrium position, the potential is approximately of the form required in equation (2.1) with  $m\omega_0^2 = U''(x_0)$ . Thus, it follows that for small amplitude oscillations about an equilibrium position, any system (with a non zero second derivative of the potential) will undergo simple harmonic motion.

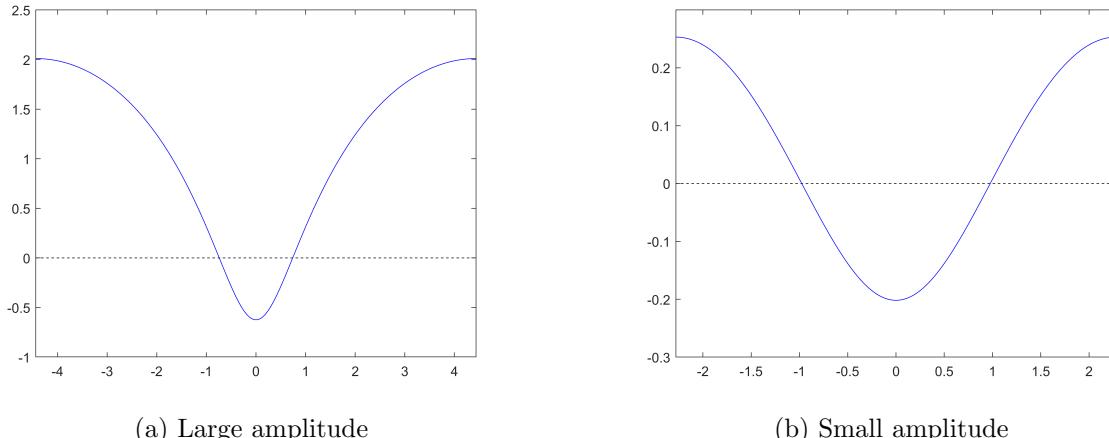


Figure 2.3: Morse oscillations at different amplitudes.

Figure 2.3 shows this principle in action for the Morse potential. At large amplitudes, we can see the high degree of asymmetry in  $U(x)$  leads to an oscillation that spends the vast majority of its time on one side of the equilibrium position. However, as the amplitude of the oscillations is reduced, this asymmetry becomes less significant and the motion approaches the sinusoidal shape that we would expect for simple harmonic motion.

## 2.2 General Oscillatory Motion

We are now going to adapt the work we have already done on simple harmonic motion, in order to account for a variety of less idealised systems. For simplicity, we shall still be neglecting any non-linear effects, such as turbulent drag, which varies with  $v^2$ . As we shall see, the introduction of even a linear friction term can vastly increase the complexity of the solutions, giving rise to several distinct cases that we must consider.

### 2.2.1 Damped Harmonic Motion

So far, all of the systems that we have considered will, once started, continue to oscillate indefinitely. Obviously this is unrealistic, because we have not yet taken into account non-conservative resistive forces. The simplest way that we can account for these resistive forces is by modifying our fundamental equation to dissipate energy at a rate proportional to  $\dot{x}^2$ , which is equivalent to having a resistive force proportional to  $\dot{x}$ , which would be the case for an object experiencing viscous drag.

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0 \quad (2.11)$$

The constant  $\gamma$  is called the coefficient of damping, and its value determines the nature of the subsequent motion. Trivially, if  $\gamma = 0$  then the system is undamped and will oscillate freely, as we have already discussed. If  $0 < \gamma < \omega_0$ , then the system is described as being lightly damped, and will undergo oscillations of exponentially decaying amplitude. If  $\gamma > \omega_0$ , the system is referred to as over damped, and will fail to oscillate, instead simply returning to its equilibrium position. If  $\gamma = \omega_0$ , we would describe the system as being critically damped, and it would return to equilibrium very quickly, without oscillating (although it may overshoot). If  $\gamma$  was positive, the displacement of the system would grow rapidly with time, and thus, this case is unphysical.

Equation (2.11) is the most general example of a second order ordinary differential equation, with constant coefficients. The solutions to equations of this form are well known; however, it is instructive for us to go through a full derivation of the results at least once. The most elegant method of obtaining the solutions to this equation is to first rewrite it in terms of the new constants  $\alpha$  and  $\beta$ , such that:

$$\ddot{x} - (\alpha + \beta)\dot{x} + \alpha\beta x = 0 \quad (2.12)$$

We can determine the values of  $\alpha$  and  $\beta$  in terms of  $\gamma$  and  $\omega_0$ , by noting that they must be the roots of the quadratic equation:

$$(\lambda - \alpha)(\lambda - \beta) = \lambda^2 + 2\gamma\lambda + \omega_0^2 = 0 \quad (2.13)$$

It directly follows from the fundamental theorem of algebra that,  $\alpha$  and  $\beta$  will always exist; however,, in general, they may be complex numbers. When this is the case, there are two different options on how to proceed. The first is to employ the method discussed in section 2.1.2, and regard the real and imaginary parts of the complex number as separate solutions to the equation, and then take linear combinations as appropriate. The second is to make a suitable choice of constants, in order to express the solution in a manifestly real form.

The first step in the solution of equation (2.12) is to multiply through by  $e^{-\alpha t}$ , and then integrate. For now, let us assume that  $(\alpha \neq \beta)$ , which is equivalent to assuming that  $\gamma \neq \omega_0$ , so that we can write our constant of integration in a more convenient form. Multiplying this result by  $e^{\alpha t}$  then yields the first order equation:

$$\dot{x} - \beta x = (\alpha - \beta)Ae^{\alpha t} \quad (2.14)$$

We can perform the same trick by multiplying through by  $e^{-\beta t}$ , and integrating, to obtain:

$$x(t) = Ae^{\alpha t} + Be^{\beta t} = Ae^{-(\gamma + \sqrt{\gamma^2 - \omega_0^2})t} + Be^{-(\gamma - \sqrt{\gamma^2 - \omega_0^2})t} \quad (2.15)$$

There are two distinct cases that arise from this solution. These correspond to the two cases either side of the discontinuity in our solution's support for the parameters  $\gamma$  and  $\omega_0$ . It is precisely because  $\gamma = \omega_0$  is the boundary between two distinct regimes, that it forms a special case in the solution of equation (2.11).

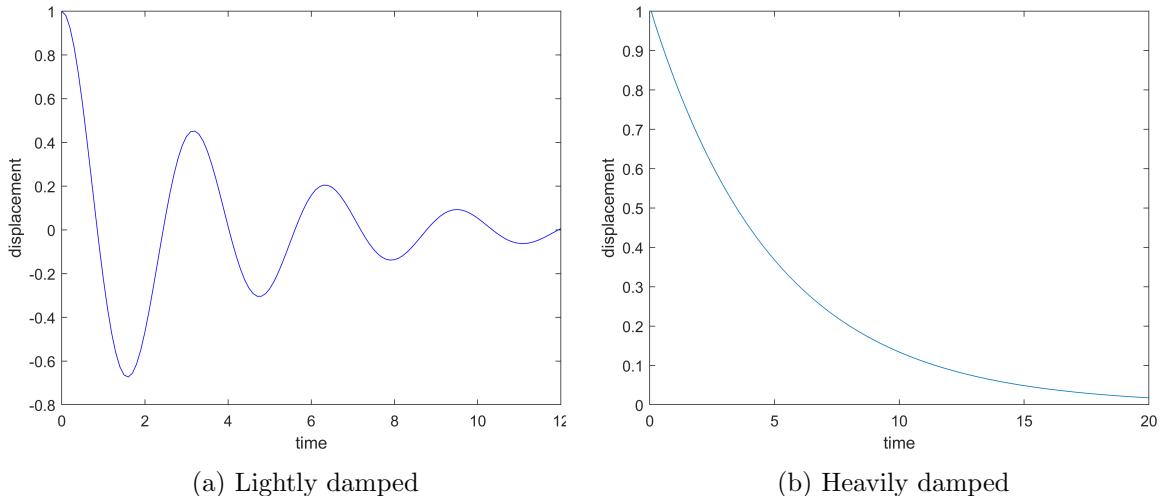


Figure 2.4: Examples of the solutions described in equation (2.15).

The first case, which corresponds to light damping, occurs when  $\gamma < \omega_0$  and the exponentials become complex. In this case, we can employ either of the two methods discussed earlier to convert this into the real solution:

$$x = a_0 e^{-\gamma t} \cos(\omega t + \phi) \quad (2.16)$$

Where  $\omega = \sqrt{\omega_0^2 - \gamma^2}$  is the new frequency of the oscillations. As we can see in figure 2.4 (a), this function simply represents a sinusoidal oscillation of exponentially decaying amplitude. Interestingly as the system becomes more heavily damped, the period of the oscillations increases until at the critical threshold  $\gamma = \omega_0$ , when the period is infinite and the system isn't really oscillating at all.

The second case, which is referred to as heavy damping, occurs when  $\gamma > \omega_0$ . In this case we find that the solutions appear exactly as they do in (2.15), simply decaying away with time. There isn't an awful lot more that can be gained from looking at these solutions directly; however, it is worth briefly examining what happens in the limit as  $\gamma \gg \omega_0$ . To do this we are going to use the Taylor series expansion of  $\sqrt{1+x}$ :

$$\sqrt{1+x} = 1 + \frac{x}{2} + \mathcal{O}(x^2) \quad (2.17)$$

We can substitute this into our solution, to obtain the approximate behaviour of  $x$  with time. We can further simplify this equation, by noting that, since  $\gamma \gg \omega_0$ , for all but the smallest values of  $t$ , the second term in the expression will be much larger than the first. This gives us:

$$x \approx a_0 e^{-\frac{\omega^2}{2\gamma} t} \quad (2.18)$$

Where  $a_0$  now represents the initial displacement of the particle. The interesting thing about this equation is that it has essentially removed the dependence of  $x$  on the initial velocity of the particle, which makes sense, because any initial velocity will be very rapidly dissipated by the large resistive forces.

Finally, we shall consider the case where  $\gamma = \omega$ , which implies that  $\alpha = \beta = -\gamma$ . In this case, we can return to our initial differential equation, and multiply by  $e^{\gamma t}$ , to find that:

$$e^{\gamma t} \ddot{x} + 2\gamma e^{\gamma t} \dot{x} + \gamma^2 e^{\gamma t} x = 0 \quad (2.19)$$

This equation can then be immediately integrated twice, and multiplied by  $e^{-\gamma t}$ , to obtain the solution:

$$x(t) = (At + B)e^{-\gamma t} \quad (2.20)$$

Critical damping gains its name from the fact that, it balances having enough of a resistive force that it can damp out any oscillations, without slowing the system down so much that, it takes a long time to return to equilibrium. As such, critical damping is of particular interest to engineers, since most structures tend to stop working if components are displaced from their equilibrium positions for too long. An interesting phenomenon occurs, when the initial conditions are chosen such that,  $A$  and  $B$  have opposite signs. In this case, we can clearly see that, at some point in time, the system will pass through, and then overshoot, its equilibrium position.

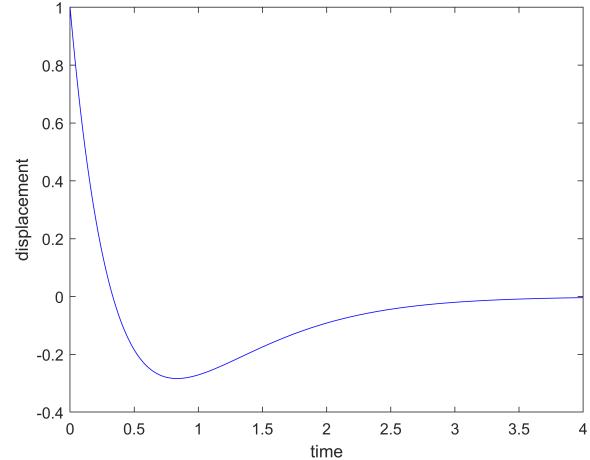


Figure 2.5: Critically damped motion

## 2.2.2 Driven Oscillations

So far, we have only been considering free oscillations, that is to say that, once our systems have been set in motion, there is no external intervention to alter their motion. While these models are useful for understanding the nature of oscillations, real examples of free oscillation are few and far between. It is far more common for a system to experience some kind of driving force, which causes it to oscillate in a specific way.

Accounting for this requires yet another modification to our fundamental equation, in order to allow for the extra force. If the system experiences a driving force  $F(t)$ , then the fundamental equation becomes:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = f(t) \quad (2.21)$$

Where  $f(t) = \frac{F(t)}{m}$  is the driving acceleration that is effecting the system. This modification transforms our homogeneous differential equation into an inhomogeneous one. As such, solving this equation is, in principle, no harder than what we have already done, when we solved the homogeneous equation. If we repeat the same process that we employed in section 2.2.1, we obtain the result:

$$x(t) = \tilde{f}(t) + x_h(t) \quad (2.22)$$

Where  $x_h(t)$  is called the complementary function, and takes the form of the appropriate solution to the homogeneous equation, from section 2.2.1, with the constants chosen to achieve the desired initial conditions. The function  $\tilde{f}(t)$  is known as the particular integral, and can be expressed in the form:

$$\tilde{f}(t) = e^{\beta t} \int \left[ e^{(\alpha - \beta)t} \int e^{-\alpha t} f(t) dt \right] dt \quad (2.23)$$

Now, since for all values of  $\gamma > 0$ ,  $x_h(t) \rightarrow 0$  as  $t \rightarrow \infty$ , we can say that the complementary function is nothing more than a transient response, which will, given sufficient time, always decay to zero. For this reason, we describe  $\tilde{f}(t)$  as the steady state solution, since if we leave a system long enough, it will always tend towards the behaviour  $x = \tilde{f}(t)$ , irrespective of the initial conditions.

We are particularly interested in driving forces which vary sinusoidally with time. That is to say that,  $f(t)$  is of the form  $f_0 \cos(\omega t)$ . In fact, any periodic driving force can be expressed as a linear combination of different sinusoids, making them essential in describing any kind of driven oscillations. To simplify the manipulation, we are going to describe our driving forces using the complex number representation we discussed earlier. Let  $f(t)$  be given by the real part of the complex number  $\mathcal{F}(t) = \mathcal{F}_0 e^{i\omega t}$ , and  $\tilde{f}(t)$  be given by the real part of the complex number  $\tilde{\mathcal{F}}(t)$ . Substituting this into equation 2.23, and evaluating the integrals, we find that:

$$\tilde{\mathcal{F}}(t) = \frac{\mathcal{F}_0 e^{i\omega t}}{\omega_0^2 - \omega^2 + 2i\gamma\omega} \quad (2.24)$$

It follows therefore, that the steady state behaviour of the system is to oscillate at the applied frequency  $\omega$ , with a complex amplitude given by  $\mathcal{A}(\omega)\mathcal{F}_0$ , where  $\mathcal{A}(\omega)$  is the normalised response function:

$$\mathcal{A}(\omega) = a(\omega) e^{i\phi(\omega)} = \frac{1}{\omega_0^2 - \omega^2 + 2i\gamma\omega} \quad (2.25)$$

There are two components to the response function: the amplitude  $a(\omega)$ , and the phase difference  $\phi(\omega)$ . The amplitude dictates how strongly the system will respond to a driving force of a given frequency, and is given by:

$$a(\omega) = \frac{1}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2}} \quad (2.26)$$

We are particularly interested in the driving frequency which elicits the highest amplitude response from the system, referred to as the system's resonant frequency  $\omega_r$ . To find the resonant frequency, we can complete the square on the denominator to obtain:

$$a(\omega) = \frac{1}{\sqrt{(\omega^2 + 2\gamma^2 - \omega_0^2)^2 + 4\gamma^2(\omega_0^2 - \gamma^2)}} \quad (2.27)$$

It immediately follows from this result that, provided the system is not too heavily damped, and  $\omega_0 > \sqrt{2}\gamma$ , the resonant frequency and amplitude are given by:

$$\omega_r^2 = \omega_0^2 - 2\gamma^2 \quad a(\omega_r) = \frac{1}{2\gamma\sqrt{\omega_0^2 - \gamma^2}} \quad (2.28)$$

If the coefficient of damping is too large for a resonant frequency to exist, then the maximum amplitude simply occurs at  $\omega = 0$ . In addition to the position of the resonant frequency, it is also worth noting what happens at both extremes of  $\omega$ . We can trivially see from equation (2.26) that, as  $\omega \rightarrow 0$ ,  $a(\omega) \rightarrow \frac{1}{\omega_0^2}$ , and as  $\omega \rightarrow \infty$ ,  $a(\omega) \rightarrow 0$ . All of this information is shown in figure 2.6 below.

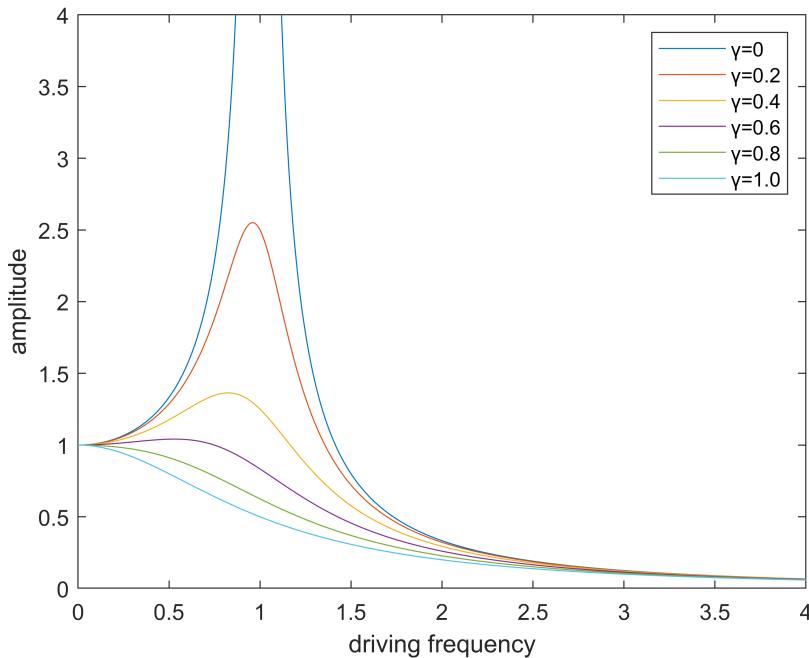


Figure 2.6: The resonances of different oscillators.

The other component of the response function, the phase difference, tells us by how much the system's response either lags or leads the driving force. The phase difference is given by the inverse tangent:

$$\phi(\omega) = \begin{cases} \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_0^2}\right) & \omega < \omega_0 \\ \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_0^2}\right) - \pi & \omega > \omega_0 \end{cases} \quad (2.29)$$

We can see that, when the driving frequency is much less than the natural frequency, the response will be in phase with the driver. However, for much higher frequencies, the response will be in anti-phase with the driver. Finally, when being driven at its natural frequency, the system provides a response which is precisely  $\frac{\pi}{2}$  radians behind the driver. This, in particular, is significant, because it means that the driving force is exactly in phase with the particle's velocity, which will allow the oscillator to dissipate a lot of power. As we can see in figure 2.7 below, the lighter the damping of an oscillator the faster it transitions from in phase to anti-phase.

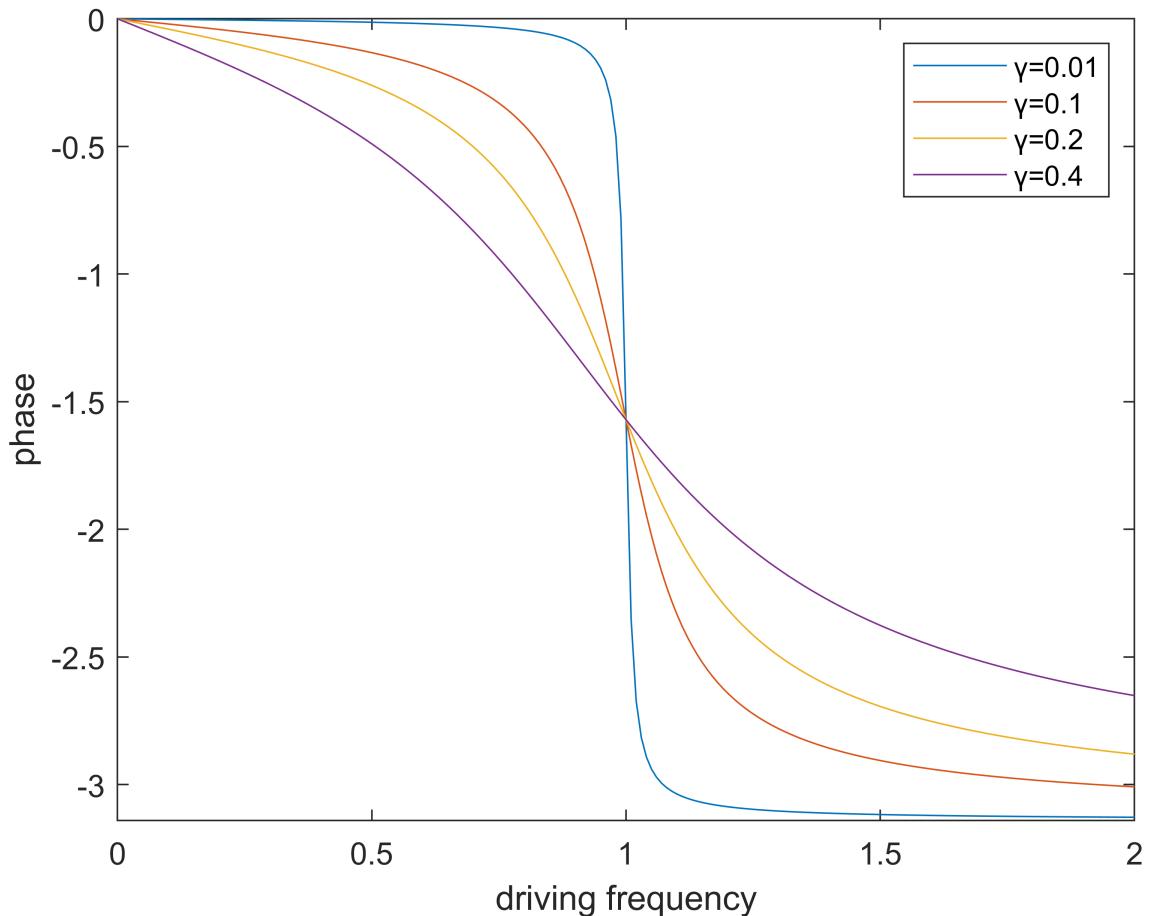


Figure 2.7: The phase differences of different oscillators.

One quantity that may be of interest to us is the power dissipated during forced oscillations. Now since the work done by the external force when it moves the mass through a distance  $dx$  is given by  $dW = Fdx$ , it follows that the power is given by  $P = F\dot{x}$ . We have to be careful here, because the power is not a linear function in our oscillating variables, and so we cannot simply multiply our complex force by our complex velocity. However, we can adapt this slightly by noting that:

$$A = \Re \mathcal{A}_0 e^{i\omega t} \quad B = \Re \mathcal{B}_0 e^{i\omega t} \implies \langle AB \rangle = \frac{\Re(\mathcal{A}_0 \overline{\mathcal{B}_0})}{2} \quad (2.30)$$

Where the notation  $\langle \dots \rangle$  implies time averaging, and the notation  $\overline{\mathcal{A}}$  implies complex conjugation. To obtain this result, we have used the fact that  $\langle \sin^2 \omega t \rangle = \frac{1}{2}$ , which can be trivially proven by noting that, by symmetry,  $\langle \sin^2 \omega t \rangle = \langle \cos^2 \omega t \rangle$ , and since  $\sin^2 \omega t + \cos^2 \omega t = 1$ , they must both be equal to  $\frac{1}{2}$ . If we now substitute in  $\dot{\mathcal{X}} = i\omega \mathcal{A}(\omega) \mathcal{F}$ , we obtain an expression for the average power dissipated by the oscillator:

$$\langle P \rangle = \frac{m\gamma\omega^2 |\mathcal{F}_0|^2}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2} \quad (2.31)$$

By dividing both the numerator and the denominator of this fraction by  $\omega^2$ , we can immediately deduce that the maximum power is dissipated, when  $\omega = \omega_0$ . Furthermore, we can tell that this maximum power is given by:

$$\langle P \rangle_{\max} = \frac{m|\mathcal{F}_0|^2}{4\gamma} \quad (2.32)$$

It is also quite useful for us to define the bandwidth of the oscillator  $\Delta\omega$  to be the difference between the two angular frequencies at which  $\langle P \rangle = \frac{1}{2}\langle P \rangle_{\max}$ . To find the frequencies of the half power points,  $\omega_+$  and  $\omega_-$ , we simply set:

$$\omega_{\pm}^2 - \omega_0^2 = \pm 2\gamma\omega_{\pm} \implies \omega_{\pm} = \sqrt{\omega_0^2 + \gamma^2} \pm \gamma \quad (2.33)$$

From this result, we can quickly see that the bandwidth is given by  $\Delta\omega = 2\gamma$ , and so, more lightly damped oscillators give a narrower resonance peak. If we are using our oscillator to pick up a certain frequency, then we want as narrow a bandwidth as possible, which leads us to define the quality factor of an oscillator:

$$Q = \frac{\omega_0}{\Delta\omega} = \frac{\omega_0}{2\gamma} \quad (2.34)$$

As it turns out, expressing some of our previous results in terms of the quality factor can often give some fairly easy to remember results. One such example is from the amplitude response function:

$$\frac{a(\omega_r)}{a(0)} = \frac{\omega_0^2}{2\gamma\sqrt{\omega_0^2 - \gamma^2}} = Q \left[ 1 + \mathcal{O} \left( \frac{\gamma^2}{\omega_0^2} \right) \right] \quad (2.35)$$

## 2.3 Oscillators with Multiple Dimensions

So far, we have only been considering systems that can oscillate in one dimension. Thus, in this section we shall be considering the process of extending these ideas to systems with multiple dimensions. Importantly, when we talk about higher numbers of dimensions, we are not necessarily referring to the dimensions of physical space, instead we are referring to the number of parameters needed to describe the state of the system, although the two are closely related. Since one dimensional systems are really rather uncommon, after all even a single particle has three spatial dimensions to move in, understanding these more complicated systems is of crucial importance.

### 2.3.1 A Particle in Three Dimensions

The simplest way to add extra dimensions to an oscillator is to consider the motion of a particle in a three dimensional potential  $U(\mathbf{x})$ . Just as we did in section 2.1.3, we can expand take a Taylor series expansion of  $U(\mathbf{x})$  about a stable equilibrium point  $\mathbf{x}_0$  to obtain:

$$U(\mathbf{x}) = U(\mathbf{x}_0) + \nabla U(\mathbf{x}_0) \cdot \boldsymbol{\xi} + \frac{1}{2} \left( (\boldsymbol{\xi} \cdot \nabla) \nabla U(\mathbf{x}_0) \right) \cdot \boldsymbol{\xi} + \mathcal{O}(|\boldsymbol{\xi}|^3) \quad (2.36)$$

Where  $\boldsymbol{\xi} = \mathbf{x} - \mathbf{x}_0$  is the displacement of the particle from equilibrium. By definition of an equilibrium position, we must have  $\nabla U(\mathbf{x}_0) = \mathbf{0}$ , and thus, the second term vanishes. From here, dealing with the third term in the expansion is a bit more troublesome. To understand what is going on we need to expand the derivatives out with respect to our axes  $x, y, z$ .

$$U(\mathbf{x}) \approx U(\mathbf{x}_0) + \frac{1}{2} \left[ U_{xx} \xi_x^2 + U_{yy} \xi_y^2 + U_{zz} \xi_z^2 \right] + U_{xy} \xi_x \xi_y + U_{yz} \xi_y \xi_z + U_{zx} \xi_z \xi_x \quad (2.37)$$

Where the notation  $U_{xx} = \frac{\partial^2 U}{\partial x^2}$  for all the pairs of variables, whilst  $\xi_x, \xi_y$  and  $\xi_z$  are simply the components of  $\boldsymbol{\xi}$  along each of the axes. Importantly, we can see that, due to the symmetry of mixed partial derivatives, which implies that  $U_{xy} = U_{yx}$ , the expansion only consists of six terms, as opposed to the nine we might expect. If we now consider rotating our axes in space to change each of the terms, it would require three angles (the three Euler angles being one example) to fully specify a rotation. As such, it follows that, within reason, it should be possible to impose three conditions on the terms of equation (2.37), by rotating our axes. This is not to say that it is possible to impose any set of three conditions, since, for example, it is impossible to make any one of the squared terms vanish; however, as it turns out, it is possible to choose our axes in such a way that all of the mixed terms vanish. Relative to this set of axes, the equations of motion for the particle become:

$$m \ddot{\xi}_x + U_{xx} \xi_x = m \ddot{\xi}_y + U_{yy} \xi_y = m \ddot{\xi}_z + U_{zz} \xi_z = 0 \quad (2.38)$$

This is nothing more than three independent equations of simple harmonic motion, and so, the particle oscillates along each of the coordinate directions simultaneously. If we so desired, we could always add a damping term into these equations to obtain the decaying solutions that we have previously encountered.

A special case arises, if the potential is locally isotropic at  $\mathbf{x}_0$ , meaning that  $U_{xx} = U_{yy} = U_{zz}$ . In this case, we can combine all three equations of motion into a single vector equation, which is directly analogous to equation (2.11) from section 2.2.1.

$$\ddot{\mathbf{x}} + 2\gamma\dot{\mathbf{x}} + \omega_0^2\mathbf{x} = \mathbf{0} \quad (2.39)$$

Since this equation essentially says that each of the components of  $\mathbf{x}$  must separately satisfy the damped oscillator equation, the only real difference between the solutions here, and those in section 2.2.1, is that this time, the constants of integration become vectors as well. The solutions, which are obtained by precisely the same method that we used before, are as follows:

$$\mathbf{x}(t) = \begin{cases} e^{-\gamma t} [\mathbf{A} \cos \omega_0 t + \mathbf{B} \sin \omega_0 t] & \gamma < \omega_0 \\ e^{-\gamma t} [\mathbf{A}t + \mathbf{B}] & \gamma = \omega_0 \\ \mathbf{A}e^{-[\gamma+\sqrt{\gamma^2-\omega_0^2}]t} + \mathbf{B}e^{-[\gamma-\sqrt{\gamma^2-\omega_0^2}]t} & \gamma > \omega_0 \end{cases} \quad (2.40)$$

The only part of this solution which is sufficiently different to merit discussion is the oscillations of the lightly damped case. As it happens, combining oscillations of the same frequency in three dimensional space, gives rise to an ellipse centred on the origin. To see this, let us consider the undamped case:

$$\mathbf{x}(t) = \mathbf{A} \cos \omega_0 t + \mathbf{B} \sin \omega_0 t \quad (2.41)$$

Since  $\mathbf{x}$  is oscillating with period  $\frac{2\pi}{\omega_0}$ , the particle's trajectory must form a closed loop in space. From this, it follows that  $|\mathbf{x}|$  must have at least four extremal points, at each of which the particle's motion must satisfy  $\dot{\mathbf{x}} \cdot \mathbf{x} = 0$ . If we set  $t = 0$  at one of these points, then we must have  $\mathbf{A} \cdot \mathbf{B} = 0$ , which makes equation (2.41) precisely the parametric form of an ellipse in the  $\mathbf{A}$ - $\mathbf{B}$  plane.

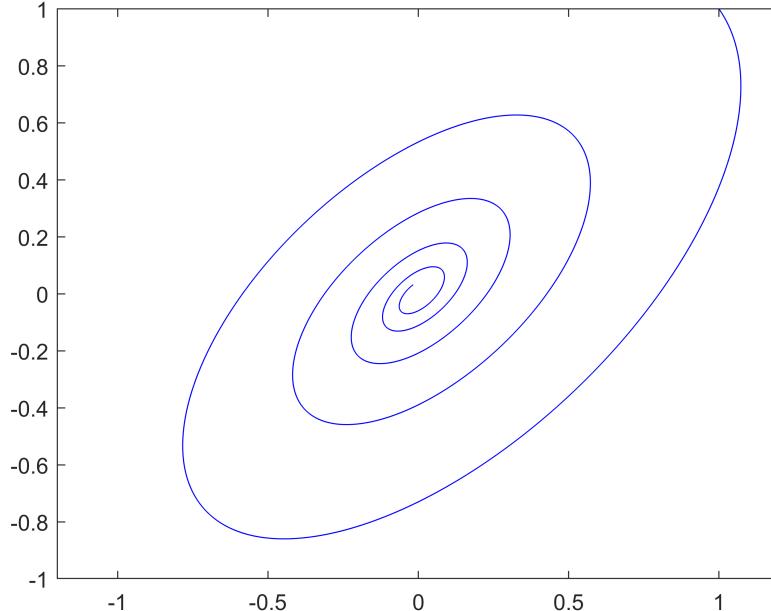


Figure 2.8: The trajectory of a lightly damped particle.

### 2.3.2 Normal Modes

Let us now consider an arbitrary system, which can be described by  $n$  coordinates. Taking a Taylor series expansion tells us that, in the neighbourhood of an equilibrium position, the potential energy is given by the generalised quadratic form:

$$U = U_0 + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n k_{ij} x_i x_j \quad (2.42)$$

Where  $x_i$  represents the displacement of the  $i$ th coordinate from its equilibrium value, and  $k_{ij}$  is a constant determined by the physical parameters of the system. Furthermore, we shall impose the restriction that  $k_{ij} = k_{ji}$ , in order to make the coefficients unique. Similarly, the kinetic energy of the system can be expressed as a generalised quadratic form of the coordinate velocities:

$$T = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n m_{ij} \dot{x}_i \dot{x}_j \quad (2.43)$$

With the same constraint that  $m_{ij} = m_{ji}$ . We can now combine these two equations to express the total energy of the system with the matrix equation:

$$E = \frac{1}{2} \dot{\mathbf{x}}^T \mathbf{M} \dot{\mathbf{x}} + \frac{1}{2} \mathbf{x}^T \mathbf{K} \mathbf{x} \quad (2.44)$$

Where  $\mathbf{x}$  is a  $n \times 1$  column vector formed from each of the coordinate displacements. Furthermore,  $\mathbf{M}$  and  $\mathbf{K}$  are  $n \times n$ , symmetric matrices, which are formed from the elements  $m_{ij}$  and  $k_{ij}$  respectively. Differentiating this equation, and then setting  $\dot{E} = 0$ , gives us the equation of motion:

$$\ddot{\mathbf{x}} + \mathbf{M}^{-1} \mathbf{K} \mathbf{x} = \mathbf{0} \quad (2.45)$$

Now since both  $\mathbf{M}$  and  $\mathbf{K}$  are real symmetric matrices, so too is  $\mathbf{M}^{-1} \mathbf{K}$ , and thus, it can be written as the matrix product  $\mathbf{O}^T \mathbf{D} \mathbf{O}$ , where  $\mathbf{O}$  is an orthogonal matrix, such that  $\mathbf{O}^T \mathbf{O} = \mathbf{O} \mathbf{O}^T = \mathbf{I}$ , and  $\mathbf{D}$  is diagonalised. If we now rewrite equation (2.45) in terms of the vector  $\mathbf{u} = \mathbf{O} \mathbf{x}$ , we obtain:

$$\ddot{\mathbf{u}} + \mathbf{D} \mathbf{u} = \mathbf{0} \quad (2.46)$$

Since  $\mathbf{D}$  is diagonal, this implies that each component of  $\mathbf{u}$  obeys its own form of the simple harmonic oscillator equation from section 2.1.1. Each of these components is referred to as a normal mode of the system because it can oscillate completely independently of all the others.

Accounting for generalised resistive forces is a highly non trivial exercise, and so shall not be covered here. If one needs to add some light damping to the system, then the simplest approximation is to just try and develop an average coefficient of damping for the system and apply it across each of the modes. A slightly more sophisticated approach would be to average the damping coefficients separately for each mode, to generate  $n$  oscillators, each with its own distinct values of  $\omega_0$  and  $\gamma$ . Unfortunately, this is as good an approximation as we can get, without significantly complicating the mathematics.

We are now going to demonstrate the fundamental principles of normal mode analysis with a simple mass spring system. Let us consider three identical masses arranged in a line and connected by two identical springs, as shown in figure 2.9.

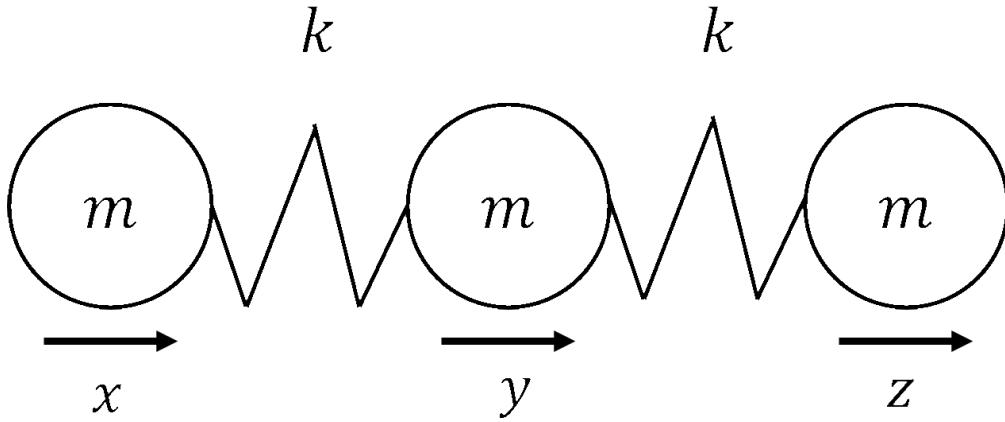


Figure 2.9: A simple mass spring system.

If we choose the displacements of the three masses ( $x$ ,  $y$  and  $z$  as shown in figure 2.9) to be our basis coordinates, then the matrices  $\mathbf{M}$  and  $\mathbf{K}$  take the form:

$$\mathbf{M} = \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{pmatrix} \quad \mathbf{K} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} \quad (2.47)$$

Inverting  $\mathbf{M}$ , and then multiplying in by  $\mathbf{K}$ , yields the symmetric matrix needed to form equation (2.45). We can then diagonalise this matrix to yield the following result:

$$\mathbf{M}^{-1}\mathbf{K} = \frac{k}{m} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \quad (2.48)$$

Not only does this imply that the frequencies of the normal modes are given by  $\omega_1^2 = 0$ ,  $\omega_2^2 = \frac{k}{m}$  and  $\omega_3^2 = \frac{3k}{m}$ , we can also use equation (2.48) to determine the behaviour of the masses in each mode. In the first mode, all of the masses move together, and the entire system simply translates through space without any internal motion. This is simply the centre of mass motion of the system, and can always be removed with an appropriate choice of reference frame. The second mode corresponds to a symmetric stretch of the outer masses, which leaves the central mass stationary. Finally, the third mode consists of an antisymmetric stretch, with the outer masses moving in one direction and the central mass moving in the other.

Since the number of normal modes is always exactly equal to the number of coordinates, it will always be possible to express the motion of the system as a superposition of the different normal modes. As such, normal mode analysis is actually the most efficient method of obtaining the general solution to a system's equation of motion, in the vicinity of an equilibrium position.

## 2.4 Electrical Oscillations

We are now going to discuss oscillating circuits, arguably the most important of all the oscillating systems we have discussed so far. Electrical oscillations differ from those that we have encountered so far, because unlike masses on springs or pendulum bobs, an electric circuit does not have a kinetic energy associated with it. Instead electrical oscillations occur, when energy is transferred between electric and magnetic fields within the different components that are present. However, before we can discuss these components in depth, we need to introduce Kirchhoff's laws, the fundamental equations which govern the behaviour of an electric circuit.

Kirchhoff's first law, also known as Kirchhoff's current law, states that, at any junction in a circuit:

$$\sum_{i=1}^n I_i = 0 \quad (2.49)$$

That is to say that the sum of the currents flowing in to the junction must always equal the sum of currents flowing out of that junction. If Kirchhoff's first law was violated, there would very quickly be a build up of substantial electric charge at the junction, which would naturally try and disperse due to the repulsion of like charges.

Kirchhoff's second law, or equivalently Kirchoff's voltage law, states that around any closed loop in a circuit:

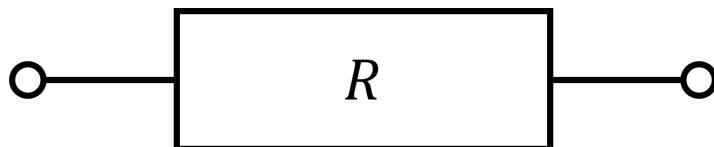
$$\sum_{i=1}^n V_i = 0 \quad (2.50)$$

Which is to say that, when a charged particle moves around any closed loop in a circuit, it gains as much energy as it loses. Kirchoff's second law is really nothing more than a statement of energy conservation.

### 2.4.1 Components

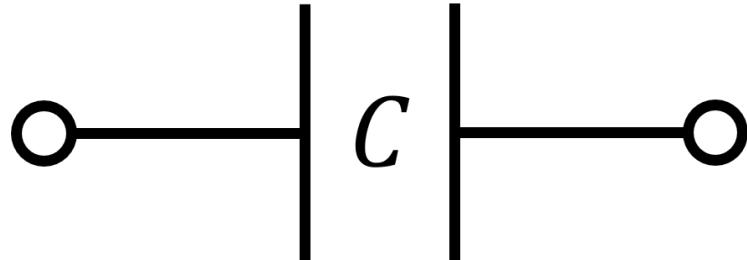
When we come to consider electrical oscillations, there are three key components that form the basis of most oscillating circuits. These are: the ideal resistor, the ideal inductor, and the ideal capacitor. In reality, such components do not exist, but most real components can be modelled to a good approximation by one or more of these fundamental ones.

#### 2.4.1.1 The Resistor



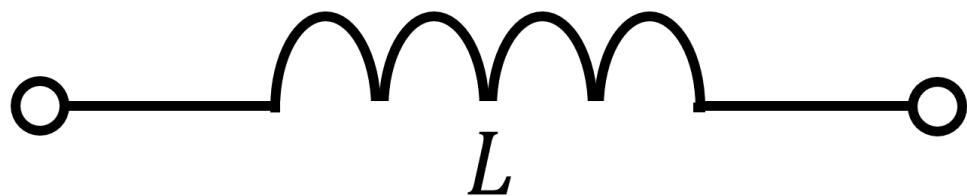
A resistor is a component that allows current to flow through it, whilst dissipating its energy. The defining feature of a resistor is that it obeys Ohm's law,  $V = IR$ . This means that the potential difference across a resistor is directly proportional to the current flowing through it, and that the constant of proportionality is defined to be the resistance  $R$ .

### 2.4.1.2 The Capacitor



A capacitor is a component that does not allow current to flow through it, and instead builds up two equal and opposite charges within itself. This means that we can think of current flowing through the capacitor, since it does flow into and out of the capacitor, although we should remember that the current does not really flow through the dielectric, and instead the capacitor plates act as current sources and sinks respectively. The defining equation of a capacitor is  $Q = CV$ , which is to say that the charge stored in the capacitor is proportional to the voltage across it, with the capacitance  $C$  as the constant of proportionality. The other important fact about a capacitor is that, since no charge can flow through the dielectric, all of the charge arriving in the form of current must go into the charge stored by the capacitor. Therefore we can also say that  $I = \dot{Q}$ .

### 2.4.1.3 The Inductor



An inductor is a component that resists changes to the current flowing through it. It does this by using the current to build up a strong magnetic field, such that, when the current changes, the changing magnetic field induces an electromotive force in the inductor. As per Lenz's law this electromotive force will act to oppose the change that created it, and as such, the current will have to expend energy doing work against this force, as it travels through the inductor. This requires the application of an external voltage across the inductor in order to maintain the acceleration of the current. The defining equation of an inductor is  $V = LI$ , meaning that the voltage applied across the inductor is proportional to the rate of change of the current through it. The inductance  $L$  then acts as the constant of proportionality for this relationship.

### 2.4.2 LCR Series Circuit

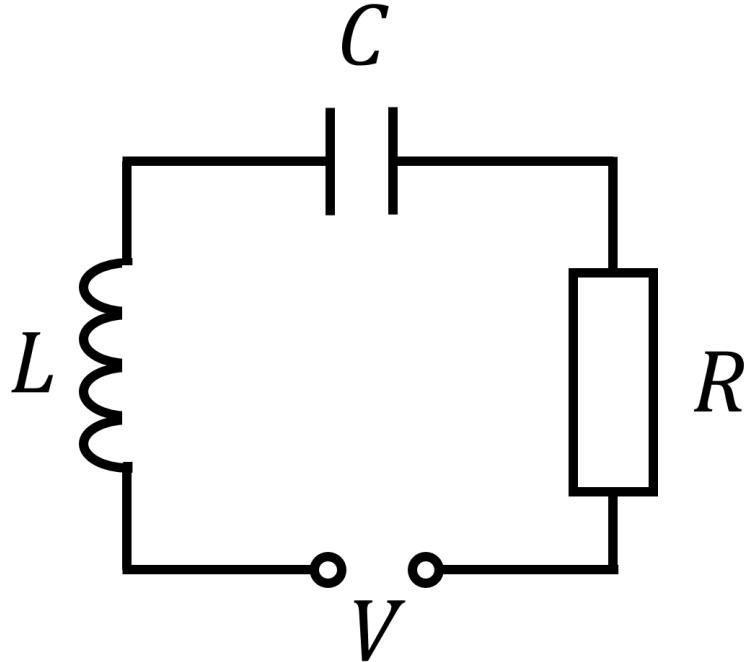


Figure 2.10: A resonant LCR circuit.

Consider the LCR series circuit shown in figure 2.10. By applying Kirchhoff's second law, we can obtain the following equation relating the applied voltage to the properties of each of the components, where  $Q$  is the charge stored in the capacitor, and  $I$  is the current throughout the circuit, defined such that, the positive direction of current increases the charge on the capacitor. The positive plate of the capacitor is defined to be the one connected to the positive terminal of the power supply.

$$L\dot{I} + IR + \frac{1}{C}Q = V \quad (2.51)$$

If we now substitute  $I = \dot{Q}$  into this equation, we obtain a second order differential equation, relating the applied voltage to the charge on the capacitor. Dividing through by the inductance  $L$  then gives us:

$$\ddot{Q} + \frac{R}{L}\dot{Q} + \frac{1}{LC}Q = \frac{V}{L} \quad (2.52)$$

This is precisely the driven oscillator equation (2.21), from section 2.2.2, if we identify the parameters  $\omega_0^2 = \frac{1}{LC}$ ,  $\gamma = \frac{R}{2L}$ , and  $f(t) = \frac{V}{L}$ . Since we have already studied the solutions to this equation in depth, there is no need to look any further.

Circuits of this nature can be very useful for filtering out specific frequencies from electrical noise, by tuning the values of  $R, C$  and  $L$  to obtain the correct resonant frequency and bandwidth.

### 2.4.3 Complex Impedance

In principle, any network of inductors, capacitors and resistors could be analysed in this manner, by using Kirchhoff's laws to generate a differential equation, or system of differential equations, which could then be solved; however, there is a much easier way. First, we need to consider the concept of a complex current or a voltage. This is essentially just an extension of the notation we already developed for representing oscillations with complex numbers. As such, we can represent sinusoidal voltage and current  $V$  and  $I$  with the real parts of the complex numbers  $\mathcal{V} = \mathcal{V}_0 e^{i\omega t}$  and  $\mathcal{I} = \mathcal{I}_0 e^{i\omega t}$ .

If we consider an LCR circuit, with an applied sinusoidal voltage, that has been allowed to reach a steady state, then each component will have an oscillating voltage across it, and an oscillating current through it. We define the impedance  $\mathcal{Z}$  of a component to be given by:

$$\mathcal{Z} = \frac{\mathcal{V}}{\mathcal{I}} \quad (2.53)$$

Where  $\mathcal{V}$  and  $\mathcal{I}$  are the complex voltage and current of that component. This is to draw a direct parallel to Ohm's law, as we can now say that  $\mathcal{V} = \mathcal{I}\mathcal{Z}$ . Importantly, since Kirchhoff's laws are linear in  $I$  and  $V$ , both the real and imaginary parts of complex voltages and currents also obey them. This means that the impedances of component networks can be calculated directly from Kirchhoff's laws. There are two fundamental rules for combining impedances: impedances in series can simply be summed together, whilst impedances in parallel sum in reciprocal:

$$\mathcal{Z}_s = \mathcal{Z}_1 + \mathcal{Z}_2 \quad \frac{1}{\mathcal{Z}_p} = \frac{1}{\mathcal{Z}_1} + \frac{1}{\mathcal{Z}_2} \quad (2.54)$$

If we wish to determine the impedances of the three fundamental components from section 2.4.1, then we simply need to consider their defining equations. In the case of a resistor it immediately follows that  $V = IR \implies \mathcal{V} = \mathcal{I}R$ . For a capacitor, we need to differentiate the fundamental equation to obtain  $Q = CV \implies \mathcal{I} = C\dot{\mathcal{V}}$ . With an inductor, we can simply obtain  $V = L\dot{I} \implies \mathcal{V} = L\dot{\mathcal{I}}$ . Evaluating the derivatives, and then rearranging these expressions, gives us:

$$\mathcal{Z}_R = R \quad \mathcal{Z}_C = -\frac{i}{\omega C} \quad \mathcal{Z}_L = iL\omega \quad (2.55)$$

To demonstrate the usefulness of impedances, let us consider once again the series circuit from section 2.4.2. We can calculate the total impedance of the circuit, and substitute this into the complex form of Ohm's law, to immediately determine that, for an applied voltage  $\mathcal{V} = \mathcal{V}_0 e^{i\omega t}$ , the complex current flowing through the circuit is:

$$\mathcal{I} = \frac{\mathcal{V}}{R + i(L\omega - \frac{1}{\omega C})} \quad (2.56)$$

Even in such a simple example, we can already see how much quicker the impedance is to use as opposed to setting up a differential equation and then solving it.

# 3 Waves and Optics

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## 3.1 Waves

In its most general sense, a wave is nothing more than a perturbation of some field, that can propagate through space in some manner. As a consequence of this very general definition, waves can be used to describe a wide range of different phenomena, with varying degrees of complexity. However, throughout this chapter we will be focusing primarily on the simplest examples of linear, non-dispersive waves, which obey particularly simple dynamics.

### 3.1.1 The Wave Equation

The simplest example of a wave is both linear, meaning that when two waves interfere by superposition, the result is a linear combination of the two original waves, and non-dispersive, which means that all the perturbations propagate throughout space with the same velocity. These properties are embodied in the so called wave equation, a second order partial differential equation, with the general form:

$$\frac{\partial^2 \psi}{\partial t^2} - c^2 \nabla^2 \psi = 0 \quad (3.1)$$

Where  $\psi(\mathbf{x}, t)$  is the function describing the wave itself, and  $c$  is the phase velocity of the wave, the speed at which perturbations can propagate through space. One feature of the wave equation that can be particularly useful is that, if  $\psi(\mathbf{x}, t)$  satisfies (3.1), so too must any derivative of  $\psi(\mathbf{x}, t)$ , by the symmetry of mixed partial derivatives. Of course, equation (3.1) only describes a specific type of wave; however, as we shall see later, it arises in a variety of different physical settings, and as such, is certainly worthy of our study.

#### 3.1.1.1 In One Dimension

In one dimension, the wave equation is a hyperbolic differential equation taking the form of equation (3.2) below. As is typical for partial differential equations of this type, it can be helpful to introduce a change of variables. In this case we choose  $u = x - ct$  and  $v = x + ct$ , which gives us:

$$\frac{\partial^2 \psi}{\partial t^2} - c^2 \frac{\partial^2 \psi}{\partial x^2} = 0 \iff \frac{\partial^2 \psi}{\partial u \partial v} = 0 \quad (3.2)$$

We can solve equation (3.2) by simply integrating it twice, once with respect to  $u$  and then again with respect to  $v$ . Remembering that, in a two dimensional system, constants of integration become functions of a single variable, we obtain general form of the solution in terms of the arbitrary functions  $f$  and  $g$ :

$$\psi(x, t) = f(x - ct) + g(x + ct) \quad (3.3)$$

If we consider one of these components in isolation, we can see that it describes some curve moving to either the left or to the right, depending on the sign of the  $ct$  term, with a velocity of  $c$ . These are referred to as travelling waves, and as we have shown, all solutions of the one dimensional wave equation can be represented as a superposition of two travelling waves. Typically, we are most interested in solving the wave equation for some set of boundary conditions, which will usually specify both  $\psi(x, 0)$  and  $\frac{\partial \psi(x, 0)}{\partial t}$ , in order to give a unique solution.

Let us consider some function  $\psi(x, t)$ , which satisfies the one dimensional wave equation, and obeys the boundary conditions:

$$\psi(x, 0) = \phi(x) \quad \frac{\partial\psi(x, 0)}{\partial t} = \xi(x) \quad (3.4)$$

If we wish to find the general expression for  $\psi(x, t)$ , we can substitute equation (3.3) into these boundary conditions, and then differentiate the first with respect to  $x$ , in order to obtain two simultaneous equations for  $f'(x)$  and  $g'(x)$ . These can then be solved, which yields:

$$f'(x) = \frac{\phi'(x)}{2} - \frac{\xi(x)}{2c} \quad g'(x) = \frac{\phi'(x)}{2} + \frac{\xi(x)}{2c} \quad (3.5)$$

It directly follows from the fundamental theorem of calculus that,  $\psi(x, t)$  can be expressed in integral form, as shown below:

$$\psi(x, t) = \phi(x) + \int_x^{x-ct} f'(u)du + \int_x^{x+ct} g'(u)du \quad (3.6)$$

If we now substitute (3.5) into (3.6), and evaluate the integrals where possible, we obtain d'Alembert's formula for the solution of the wave equation:

$$\psi(x, t) = \frac{\phi(x - ct) + \phi(x + ct)}{2} + \frac{1}{2c} \int_{x-ct}^{x+ct} \xi(u)du \quad (3.7)$$

We can see an interesting property of this solution by noting that, if  $\psi$  is a solution of the wave equation, so too is  $\psi_t$  (where the notation  $\psi_t = \frac{\partial\psi}{\partial t}$ ). Furthermore, the wave equation also implies that if  $\psi(x, 0) = 0$ , we must also have  $\psi_{tt}(x, 0) = 0$ . As such, if  $\eta(x, t)$  solves the wave equation for the initial conditions  $\eta(x, 0) = 0$  and  $\eta_t(x, 0) = \phi(x)$ ,  $\zeta(x, t) = \eta_t(x, t)$  must solve the wave equation with the initial conditions  $\zeta(x, 0) = \phi(x)$  and  $\zeta_t(x, 0) = 0$ . We can then use the linearity of the wave equation to obtain equation (3.8), which is equivalent to d'Alembert's formula.

$$\psi(x, t) = \frac{\partial}{\partial t} \left[ \frac{1}{2c} \int_{x-ct}^{x+ct} \phi(u)du \right] + \frac{1}{2c} \int_{x-ct}^{x+ct} \xi(u)du \quad (3.8)$$

This concept will be particularly useful, when we come to look at waves in three dimensions.

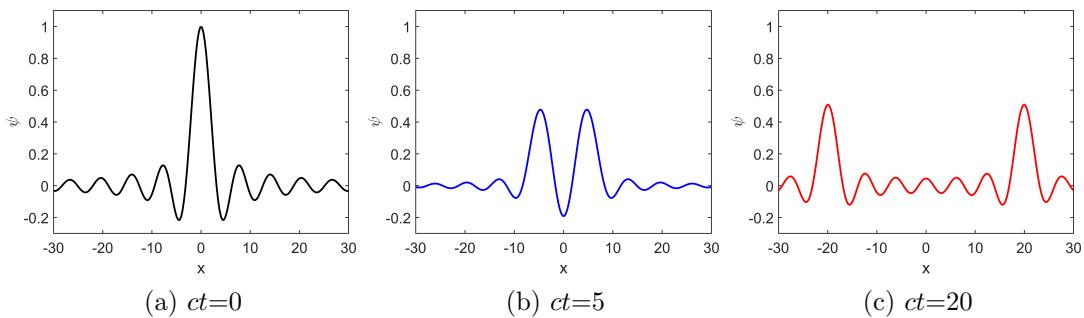


Figure 3.1: A pulse spreading out over time, as described by the wave equation.

### 3.1.1.2 In Three Dimensions

Unfortunately, the majority of waves are not confined to a single spatial dimension, and so can not be described by equation (3.2). Instead, we have to use the general wave equation (3.1), which, in three dimensional space, becomes:

$$\frac{\partial^2 \psi}{\partial t^2} - c^2 \left[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] = 0 \quad (3.9)$$

Alternatively, we might find it helpful to express the wave equation in polar coordinates, which gives us:

$$\frac{\partial^2 \psi}{\partial t^2} - c^2 \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] = 0 \quad (3.10)$$

A special case of this occurs when  $\psi$  is spherically symmetric, meaning that it is a function of  $r$  only, and thus, all of the angular terms vanish. If we then multiply the equation by  $r$ , it can be rearranged to give us the one-dimensional wave equation:

$$\frac{\partial^2 r\psi}{\partial t^2} - c^2 \frac{\partial^2 r\psi}{\partial r^2} = 0 \quad (3.11)$$

Formally speaking, (3.11) is not quite the same as the one dimensional wave equation that we were considering in section 3.1.1.1, because the radial coordinate can only take values of  $r \geq 0$ . We can avoid this difficulty by, first expanding our initial conditions for  $\psi$  into the region  $r < 0$ , by setting  $\psi(-r, 0) = \psi(r, 0)$  and  $\psi_t(-r, 0) = \psi_t(r, 0)$ , and then using d'Alembert's formula on  $r\psi(r, t)$ . The resulting function will satisfy the wave equation for  $r \geq 0$  (it will actually satisfy the wave equation everywhere, but the only physical part of the solution is  $r \geq 0$ ), whilst also obeying the necessary condition that  $r\psi(0, t) = 0$ , which is precisely what we need it to do.

Let us now consider the initial conditions:

$$\psi(r, 0) = 0 \quad \psi_t(r, 0) = \frac{e^{-\frac{r^2}{k^2}}}{(\pi k^2)^{\frac{3}{2}}} \quad (3.12)$$

It immediately follows from d'Alembert's formula that the wave is given by:

$$\psi(r, t) = \frac{1}{r} \left[ \frac{1}{2c} \int_{r-ct}^{r+ct} \frac{ue^{-\frac{u^2}{k^2}}}{(\pi k^2)^{\frac{3}{2}}} du \right] = \frac{1}{4\pi cr} \left[ \frac{e^{-\frac{(r-ct)^2}{k^2}}}{\sqrt{\pi k^2}} - \frac{e^{-\frac{(r+ct)^2}{k^2}}}{\sqrt{\pi k^2}} \right] \quad (3.13)$$

We can obtain a useful result by considering the limit as  $k \rightarrow 0$ , in which case, the initial conditions tend towards:

$$\psi(r, 0) \rightarrow 0 \quad \psi_t(r, 0) \rightarrow \delta(\mathbf{x}) = \delta(x)\delta(y)\delta(z) \quad (3.14)$$

Where  $\delta(x)$  and  $\delta(\mathbf{x})$  are the Dirac delta function in one and three dimensions respectively. We can also see that, for positive  $r$  and  $t$ , the wave itself tends towards:

$$\psi(r, t) \rightarrow \frac{\delta(r - ct)}{4\pi cr} \quad (3.15)$$

Since the wave equation is linear, we are free to superpose as many solutions of this type as we require, in order to satisfy any given initial conditions. As such, if we now consider the more general initial conditions that  $\psi(\mathbf{x}, 0) = 0$  and  $\psi_t(\mathbf{x}, 0) = \xi(\mathbf{x})$ , we obtain the following solution for  $t > 0$ :

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} \frac{\delta(|\mathbf{x} - \mathbf{x}'| - ct)}{4\pi c |\mathbf{x} - \mathbf{x}'|} \xi(\mathbf{x}') d^3 x' \quad (3.16)$$

While this solution looks fairly complicated, it actually has a relatively simple interpretation. To see this, let us consider the mean value of  $\xi$  on a spherical surface of radius  $r$  and centre  $\mathbf{x}$ , which we shall denote as  $M_{\mathbf{x},r}[\xi]$ . This mean value could be calculated by evaluating the integral:

$$M_{\mathbf{x},r}[\xi] = \int_{\mathbb{R}^3} \frac{\delta(|\mathbf{x} - \mathbf{x}'| - r)}{4\pi |\mathbf{x} - \mathbf{x}'|^2} \xi(\mathbf{x}') d^3 x' \quad (3.17)$$

By comparing (3.16) and (3.17), we can conclude that  $\psi(\mathbf{x}, t) = t M_{\mathbf{x},ct}[\xi]$ . If we wish to solve the more general initial value problem, we simply recognise that if  $t M_{\mathbf{x},ct}[\phi]$  satisfies the wave equation, then so too does  $\frac{\partial}{\partial t}(t M_{\mathbf{x},ct}[\phi])$ . It follows that this solution must obey the initial conditions  $\psi(\mathbf{x}, 0) = \phi(\mathbf{x})$  and  $\psi_t(\mathbf{x}, 0) = 0$ , and thus, by superposing the two solutions, we obtain:

$$\psi(\mathbf{x}, t) = \frac{\partial}{\partial t} \left( t M_{\mathbf{x},ct}[\phi] \right) + t M_{\mathbf{x},ct}[\xi] \quad (3.18)$$

Which solves the general initial value problem of  $\psi(\mathbf{x}, 0) = \phi(\mathbf{x})$  and  $\psi_t(\mathbf{x}, 0) = \xi(\mathbf{x})$ . If we explicitly evaluate the time derivative in equation (3.18), we obtain the equivalent formula:

$$\psi(\mathbf{x}, t) = M_{\mathbf{x},ct}[\phi] + ct M_{\mathbf{x},ct}[\nabla \phi \cdot \hat{\mathbf{n}}] + t M_{\mathbf{x},ct}[\xi] \quad (3.19)$$

Where  $\hat{\mathbf{n}}$  is the unit normal to the sphere over which the averaging is carried out. Another equivalent representation of (3.19) can be obtained, by utilising Gauss' theorem to rewrite the second term as a volume average, instead of a surface average.

$$\psi(\mathbf{x}, t) = M_{\mathbf{x},ct}[\phi] + \frac{c^2 t^2}{3} V_{\mathbf{x},ct}[\nabla^2 \phi] + t M_{\mathbf{x},ct}[\xi] \quad (3.20)$$

The volume average  $V_{\mathbf{x},r}[\eta]$  represents the mean value of  $\eta$  inside a sphere of radius  $r$ , centred on the point  $\mathbf{x}$ , and is given by:

$$V_{\mathbf{x},r}[\eta] = \frac{3}{r^3} \int_0^r u^2 M_{\mathbf{x},u}[\eta] du \quad (3.21)$$

Once again, we can see from this solution that the wave equation obeys causality, since all the information in the wave is propagating through space at speed  $c$ . That is to say that, observing any point on the wave for some period of time  $t$ , does not allow you to make any conclusions about the initial conditions of the wave outside a sphere of radius  $ct$ , centred on the point of observation.

It is also worth noting that, we can derive d'Alembert's formula from equation (3.18). If the initial conditions have no dependence on  $y$  and  $z$ , then we obtain a plane wave solution, which is essentially equivalent to the one dimensional waves we considered in section 3.1.1.1. d'Alembert's formula follows directly from substituting such a plane wave into equation (3.18). A similar process can also be used to solve the wave equation in two dimensions.

### 3.1.2 Sinusoidal Waves

There is one family of solutions to the wave equation that is of particular interest to us, sinusoidal plane waves. These waves are characterised by a wave vector  $\mathbf{k}$ , and an angular frequency  $\omega$ , which are related by the fact that  $\omega = c|\mathbf{k}|$ . The general form of one such wave is:

$$\psi(x, t) = A \cos(\omega t - \mathbf{k} \cdot \mathbf{x} + \phi) \quad (3.22)$$

It is also common to represent a wave of this nature by a complex number, with the implicit assumption that only the real part is physical. This notation has several advantages, not least of which is the fact that it helps to draw parallels between classical wave behaviour and quantum mechanics. As an example, the wave in equation (3.22) above would be represented by:

$$\psi(\mathbf{x}, t) = \mathcal{A} e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} \quad (3.23)$$

Where the complex amplitude  $\mathcal{A}$  is given by  $\mathcal{A} = Ae^{i\phi}$ . The similarities to simple harmonic motion arise, because in a wave of this nature, each individual point in space is oscillating sinusoidally, slightly out of phase with each of its neighbours. It is this connection that makes waves of this type so useful to consider. As we saw in chapter 2, the response of an oscillator to an external force can be analysed by decomposing that force into sinusoids via a Fourier transform. For this reason, the interactions of waves with other physical systems are typically best understood in terms of sinusoidal waves of different frequencies, in superposition with each other. A familiar example of this phenomenon is the dispersion of light through a prism; since the different frequencies (which are equivalent to colours in the case of light waves) interact differently with the atoms in the glass, they have different refractive indices, and so spread out in space, as they pass through the prism. It is worth noting that, this dispersion only occurs because within the prism the light no longer obeys the wave equation.

It is also possible for us to represent a general solution to the wave equation using sinusoidal waves. Since any wave of the form in (3.23) satisfies the wave equation, any arbitrary superposition of sinusoidal waves must also satisfy the wave equation. If we impose the same initial conditions as we did in section 3.1.1,  $\Re\psi(\mathbf{x}, 0) = \phi(\mathbf{x})$  and  $\Im\psi_t(\mathbf{x}, 0) = \xi(\mathbf{x})$ , then we can write our solution as the real part of:

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} \mathcal{A}(\mathbf{k}) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} d^3 k \quad (3.24)$$

The amplitude function  $\mathcal{A}(\mathbf{k})$ , which represents both the relative intensities and phases of the different frequencies present in the overall wave, can be calculated from the initial conditions by evaluating the Fourier transform:

$$\mathcal{A}(\mathbf{k}) = \frac{1}{2\pi} \int_{\mathbb{R}^3} \left( \phi(\mathbf{x}) - \frac{i\xi(\mathbf{x})}{c|\mathbf{k}|} \right) e^{i\mathbf{k} \cdot \mathbf{x}} d^3 x \quad (3.25)$$

This result highlights one of the major benefits of the complex representation, both  $\psi$  and  $\psi_t$  are encoded in the real and imaginary parts of the function respectively. As such, we can represent the initial conditions with a single complex valued function, instead of two separate real valued functions.

### 3.1.3 Boundary Conditions and Stationary Waves

Since physical systems are typically of finite size, we are often less interested in solving the wave equation over all space, which has been the subject of the previous sections, and more interested in applying it to some given region, with appropriate restrictions applied to its boundary. As an example, let us consider a violin string, which is both finite in length and fixed in place at both ends. When analysing this system, we wish to find solutions that obey the wave equation everywhere along the string, whilst also satisfying the condition that the string must always have zero displacement at its ends. In principle, there are two ways to do this, although in practice only one is commonly encountered. The first method is to extend any set of initial conditions, which will be defined along the length of the string, over all space, in such a way that the boundary conditions are always maintained, and then apply the solutions from section 3.1.1 to determine the subsequent evolution of the wave. Alternatively, we can solve the wave equation over a finite interval, using the Fourier method of separating the variables. We shall demonstrate this principle by solving the one dimensional wave equation, with the boundary conditions:

$$\psi(0, t) = \psi(L, t) = 0 \quad \psi(x, 0) = \phi(x) \quad \psi_t(x, 0) = \xi(x) \quad (3.26)$$

We start by looking for a separable solution of the form  $\psi(x, t) = X(x)T(t)$ , and substituting it into the wave equation. Rearranging, and then dividing through by  $\psi(x, t)$ , gives us the following equation:

$$\frac{X''(x)}{X(x)} = \frac{1}{c^2} \frac{T''(t)}{T(t)} \quad (3.27)$$

Since each side of the equation is a function of a different variable, they must both be equal to a constant, which for convenience we shall represent by  $-k^2$ . Equating each term separately to this constant, and then rearranging, gives us the two ordinary differential equations:

$$X''(x) + k^2 X(x) = 0 \quad T''(t) + \omega^2 T(t) = 0 \quad (3.28)$$

Where  $\omega = ck$ , just as it did in section 3.2. The solutions of these equations were explored in great depth in the previous chapter, so we can immediately express our separable solution to the wave equation in terms of the four constants  $\alpha_k, \beta_k, a_k$  and  $b_k$ , to obtain:

$$\psi(x, t) = (\alpha_k \sin kx + \beta_k \cos kx)(a_k \sin \omega t + b_k \cos \omega t) \quad (3.29)$$

Since the wave equation is linear, any linear combination of solutions in the form of (3.29) will also be a solution, and so we represent our general solution as:

$$\psi(x, t) = \sum_k (\alpha_k \cos kx + \beta_k \sin kx)(a_k \cos \omega t + b_k \sin \omega t) \quad (3.30)$$

We are now in a position to apply our boundary conditions. If we first require that the string remains fixed in place at both ends, we can conclude that  $\alpha_k = 0$  and that  $k = \frac{n\pi}{L}$  for some positive integer  $n$  (there is no reason why  $n$  can't be negative, it is simply redundant, because  $\sin x$  is an odd function). For simplicity, we shall introduce the new constants  $A_n = \beta_k a_k$  and  $B_n = \beta_k b_k$ , which gives us:

$$\psi(x, t) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \left[ A_n \cos\left(\frac{n\pi c t}{L}\right) + B_n \sin\left(\frac{n\pi c t}{L}\right) \right] \quad (3.31)$$

Substituting (3.31) into the initial conditions from (3.26), gives us the following restrictions on the constants  $A_n$  and  $B_n$ :

$$\phi(x) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) \quad \xi(x) = \sum_{n=1}^{\infty} \frac{n\pi c B_n}{L} \sin\left(\frac{n\pi x}{L}\right) \quad (3.32)$$

We can then solve for the individual coefficients, using the trigonometric orthogonality relation that, for integers  $n$  and  $m$ :

$$\frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = L\delta_{nm} \quad (3.33)$$

Multiplying each of the equations in (3.32) by  $\frac{2}{L} \sin\left(\frac{m\pi x}{L}\right)$ , and integrating over the whole length of the string, yields the following formulae for the coefficients:

$$A_n = \frac{2}{L} \int_0^L \phi(x) \sin\left(\frac{n\pi x}{L}\right) dx \quad B_n = \frac{2}{n\pi c} \int_0^L \xi(x) \sin\left(\frac{n\pi x}{L}\right) dx \quad (3.34)$$

Since the sinusoidal functions form a complete basis, we can replicate any set of initial conditions using solutions of this type. As such, we have successfully solved the wave equation for a finite string with fixed endpoints. We can see that the string is only able to carry waves of certain, discrete frequencies, given by:

$$\omega_n = \frac{n\pi c}{L} \quad n \in \mathbb{Z}^+ \quad (3.35)$$

These solutions are known as stationary waves, because they simply oscillate in place, without propagating along the string. A one dimensional stationary wave can be considered to be the superposition of two waves travelling in opposite directions, as shown below:

$$\psi(x, t) = \sin kx \cos \omega t = \frac{\sin(kx - \omega t) + \sin(kx + \omega t)}{2} \quad (3.36)$$

All of the same principles apply to systems of more than one spatial dimension. As an example, we could consider a sound wave in a cuboidal room, of dimensions  $a, b$  and  $c$  respectively. The boundary conditions are very similar, only in this instance it is the normal derivative of the pressure that must vanish at the walls. Applying Fourier's method to this problem to find a solution of the form  $\psi(x, y, z, t) = X(x)Y(y)Z(z)T(t)$ , we obtain:

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = \frac{1}{c^2} \frac{T''(t)}{T(t)} \quad (3.37)$$

Just as before, since each term in this equation is a function of a different variable, each term must be equal to a constant. If we go through the same process as we did for the one dimensional case we arrive at stationary waves given by (3.38) below. These solutions represent a superposition of 8 separate travelling waves, each of the form  $\cos\left(\frac{n\pi x}{a} \pm \frac{m\pi y}{b} \pm \frac{l\pi z}{c} \pm \omega t\right)$ .

$$\psi(\mathbf{x}, t) = A_{n,m,l} \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi y}{b}\right) \cos\left(\frac{l\pi z}{c}\right) \cos(\omega t + \phi) \quad (3.38)$$

Where the angular frequency is given by:

$$\omega = c\pi \sqrt{\frac{n^2}{a^2} + \frac{m^2}{b^2} + \frac{l^2}{c^2}} \quad n, m, l \in \mathbb{Z}^+ \quad (3.39)$$

## 3.2 Physical Systems

We are now going to spend some time looking at specific examples of physical systems, and deriving the relevant dynamics for each case. As we shall see, such systems can often be approximated by the relatively simple wave equation that we discussed at great length in section 3.1. We will also see that, in all of these cases, the deviations of the real system from the ideal assumptions give rise to various non-linear phenomena, such as attenuation and dispersion.

### 3.2.1 A String Under Tension

The first system for us to examine is an elastic string under tension. If we consider an infinitesimal string element  $\delta x$ , as shown in figure 3.2, we can see that, in order for the string to be in horizontal equilibrium, the horizontal component of the tension must remain constant along the length of the string. As such, if  $\psi(x, t)$  represents the transverse displacement of the string, the vertical component of the tension is given by  $T \frac{\partial \psi}{\partial x}$ . Thus, the resultant force acting on the string element is equal to the change in  $T \frac{\partial \psi}{\partial x}$  over a distance  $\delta x$ , which is proportional to the second derivative of  $\psi$ . Assuming that the string has a mass per unit length  $\mu$ , which will be constant as long as  $|\frac{\partial \psi}{\partial x}| \ll 1$ , we can substitute this into Newton's second law to obtain:

$$\mu \frac{\partial^2 \psi}{\partial t^2} \delta x = T \frac{\partial^2 \psi}{\partial x^2} \delta x \implies \frac{\partial^2 \psi}{\partial t^2} - \frac{T}{\mu} \frac{\partial^2 \psi}{\partial x^2} = 0 \quad (3.40)$$

This is simply the one dimensional wave equation, with a wave speed of  $c = \sqrt{\frac{T}{\mu}}$ . If the condition on the magnitude of the gradient is not met, the mass per unit length will vary significantly and thus any waves will change shape as they propagate along the string. Furthermore, if  $\frac{\partial \psi}{\partial x}$  is large enough, the string will be deformed plastically, dissipating energy in the process, which will lead to attenuation of waves as they travel.

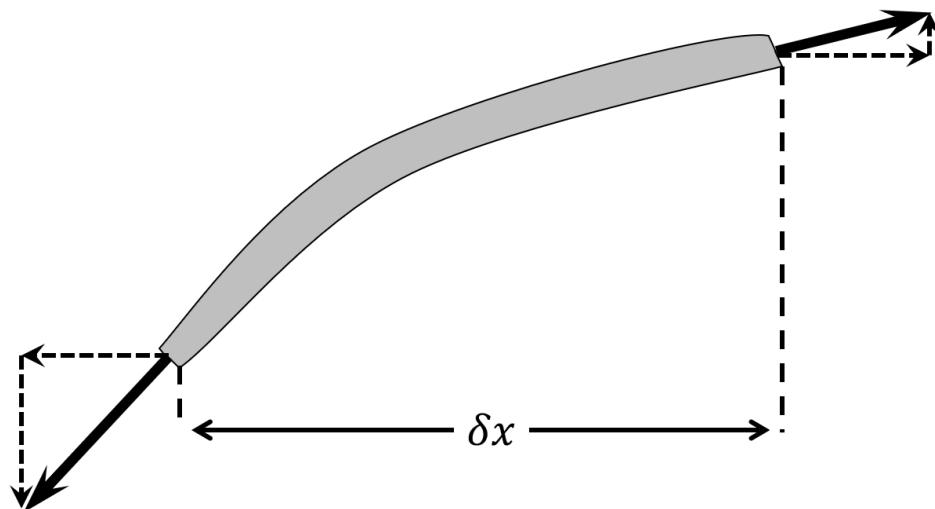


Figure 3.2: An infinitesimal string element.

It can also be useful to consider the energy carried by a wave in any given system. In the case of a stretched string, there are two forms of energy: the kinetic energy of the string's transverse motion, and the potential energy due to the string's elastic strain. In order to calculate the potential energy, we simply evaluate the work done in extending a string element:

$$\delta W = \int_0^{\frac{\partial\psi}{\partial x}} T\sqrt{1+u^2} d(\delta x\sqrt{1+u^2}) = T\delta x \int_0^{\frac{\partial\psi}{\partial x}} u du = \frac{T\delta x}{2} \left(\frac{\partial\psi}{\partial x}\right)^2 \quad (3.41)$$

Combining this with the standard result for the kinetic energy of a string element, we obtain the following expression for the total energy per unit length:

$$\mathcal{E} = \frac{1}{2} \left[ \mu \left( \frac{\partial\psi}{\partial t} \right)^2 + T \left( \frac{\partial\psi}{\partial x} \right)^2 \right] \quad (3.42)$$

Since waves are often used to transfer energy from a source to a receiver, it makes sense for us to consider the rate at which this energy flows, which is known as the energy flux  $J$ . If we consider the energy of a single string element, it follows from the conservation of energy that, we must have the continuity equation:  $\frac{\partial\mathcal{E}}{\partial t} + \frac{\partial J}{\partial x} = 0$ . Substituting in (3.42), and then utilising the wave equation (3.40) itself, yields:

$$J = T \left( \frac{\partial\psi}{\partial x} \right) \left( \frac{\partial\psi}{\partial t} \right) \quad (3.43)$$

In the special case of a travelling wave, we find that  $\psi_t = \pm c\psi_x$  and so the energy flux simplifies to  $J = \mathcal{E}c$ , just as we would expect.

### 3.2.2 A Stretched Membrane

A stretched membrane is simply an extension of a string into two spatial dimensions, and as such, many of the results we shall discuss are essentially the same as those in section 3.2.1. If the membrane has a surface tension<sup>3</sup>  $\gamma$ , and a mass per unit area  $\sigma$ , we can use exactly the same argument as we did for a string to arrive at the wave equation:

$$\frac{\partial^2\psi}{\partial t^2} - \frac{\gamma}{\sigma} \left[ \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} \right] = 0 \quad (3.44)$$

Furthermore, we can calculate the energy per unit area and the energy flux, which, in this case, is a vector pointing in the direction of greatest energy transfer, to obtain:

$$\mathcal{E} = \frac{1}{2} \left[ \sigma \left( \frac{\partial\psi}{\partial t} \right)^2 + \gamma |\nabla\psi|^2 \right] \quad \mathbf{J} = \gamma \frac{\partial\psi}{\partial t} \nabla\psi \quad (3.45)$$

Once again, we can see that in the case of a travelling wave,  $|\mathbf{J}| = \mathcal{E}c$ , as expected. Another interesting case to note is a sinusoidal wave of the form  $A \sin(\mathbf{k} \cdot \mathbf{x} - \omega t)$ , which has an average energy flux of  $\langle \mathbf{J} \rangle = \frac{\gamma A^2 \omega \mathbf{k}}{2}$ .

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<sup>3</sup>Surface tension is the force per unit length that acts on the boundary of an area element.

### 3.2.3 Shallow Water Waves

Although water waves are some of the best known examples of wave phenomena, they are actually reasonably complicated. Luckily, the dynamics of water waves can be significantly simplified, if we restrict our considerations to water of negligible depth compared to the scale of the waves along the surface. On top of this, we shall also assume that the amplitude of the waves is much smaller than the depth of the water, and as such, the velocity of any given fluid element is essentially parallel to the surface of the water. Furthermore, because the water is shallow, we can consider an entire column of water as having the same velocity. If we let  $h(x, y, t)$  and  $\mathbf{v}(x, y, t)$  be the height and velocity of the water column at position  $(x, y)$ , we obtain the two continuity equations:

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{v}) = 0 \quad \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} + g\nabla h = 0 \quad (3.46)$$

Which correspond to the conservation of mass and momentum respectively. We can simplify the second equation somewhat, by noting that, if the amplitude of the perturbations is significantly smaller than their typical length scale,  $|(\mathbf{v} \cdot \nabla)\mathbf{v}| \ll |\frac{\partial \mathbf{v}}{\partial t}|$ . We can now introduce the displacement of the water  $\psi(x, y, t) = h(x, y, t) - h_0$ , where  $h_0$  is the unperturbed depth of the water. So long as  $h_0$  is constant everywhere, and  $\psi \ll h_0$ , we can say that  $\nabla \cdot (h\mathbf{v}) \approx h_0 \nabla \cdot \mathbf{v}$ . Applying these approximations to (3.46):

$$\frac{\partial \psi}{\partial t} + h_0 \nabla \cdot \mathbf{v} = 0 \quad \frac{\partial \mathbf{v}}{\partial t} + g\nabla\psi = 0 \quad (3.47)$$

If we now take the time derivative of the first, and substitute in the second, we obtain the wave equation:

$$\frac{\partial^2 \psi}{\partial t^2} - gh_0 \nabla^2 \psi = 0 \quad (3.48)$$

This dependence of wave speed on depth is responsible for ocean waves always reaching the shore travelling perpendicularly to the coastline. As we shall see later, when waves move from faster media to slower media, their direction of travel bends towards the normal of the boundary. As such, the reduction in sea depth near the shore causes ocean waves to bend towards the normal in the way that we observe.

If we were to consider more general gravity waves on a water surface, with an arbitrary depth, they would be dispersive. This means that they do not obey a wave equation of the form in (3.48), and are instead best thought of as a superposition of sinusoidal waves, each travelling at a different velocity. With some effort, one can use the principles of mass and momentum continuity to determine that, for gravity waves of negligible amplitude, the dispersion relation (which connects  $\omega$  and  $k$ ) is:

$$\omega^2 = gk \tanh(kh_0) \quad (3.49)$$

If we define the phase velocity  $v_p$  of a sinusoidal plane wave to be the ratio of its angular frequency to its wave vector, we obtain the following expression:

$$v_p^2 = \frac{g}{k} \tanh(kh_0) \quad (3.50)$$

We can see that, in the shallow water limit ( $kh_0 \rightarrow 0$ ), this tends towards the simple non-dispersive result that we derived earlier.

### 3.2.4 Pressure Waves

Sound waves occur when the regions of either high pressure (known as compressions) or low pressure (known as rarefactions) propagate through a medium. The nature of sound waves is thus highly dependent on the medium through which they propagate. We shall only be considering idealised fluids, which have zero viscosity, and only posses a hydrostatic pressure  $P$ . As it turns out, this is a reasonably good approximation for most fluids we encounter, such as air and water. We can start our analysis with the two continuity equations (analogous to those in (3.47)), which represent mass and momentum conservation respectively.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad \frac{\partial \mathbf{j}}{\partial t} + \nabla P = 0 \quad (3.51)$$

Here  $\rho$  represents the density,  $\mathbf{j}$  the mass flux, and  $P$  the hydrostatic pressure of the fluid. Just as in section 3.2.3, there should also be a term proportional to  $(\mathbf{j} \cdot \nabla)\mathbf{j}$  in the second equation; however, it can be neglected as long as the amplitude of the pressure waves is small. If we now introduce  $\psi(\mathbf{x}, t)$  to represent the displacement of the pressure from its equilibrium value, we can express  $P$  and  $\rho$  as:

$$P = P_0 + \psi \quad \rho = \rho_0 + \left( \frac{\partial \rho}{\partial P} \right)_S \psi \quad (3.52)$$

Assuming that  $\psi$  is always small compared to  $P_0$ . The partial derivative is evaluated isentropically, since an ideal sound wave will not dissipate energy as it travels, and thus, must propagate in a reversible manner. Importantly, when we say that the partial derivative is evaluated at constant entropy, we mean that the entropy of any given fluid element remains constant, and not the entropy in any given volume. Of course, in a real fluid there will always be some heat flow, which will dissipate energy from the wave, and lead to attenuation as it propagates; however, this is often a fairly small effect. We can now substitute (3.52) into (3.51), and combine the two continuity equations, to obtain the wave equation:

$$\frac{\partial^2 \psi}{\partial t^2} - \left( \frac{\partial P}{\partial \rho} \right)_S \nabla^2 \psi = 0 \quad (3.53)$$

If we evaluate this derivative in the case of an ideal gas, we obtain equation (3.54) for the speed of sound. The heat capacity ratio  $\gamma$  shall be explored in much greater detail in chapter 9, but for now we can simply note that in the atmosphere it takes a value of about 1.4.

$$c = \sqrt{\frac{\gamma P_0}{\rho_0}} \quad (3.54)$$

### 3.2.5 Light Waves

Although it is probably the most prominent example of wave behaviour, we shall not be discussing electromagnetic radiation in any great detail here. Instead, we shall revisit the topic in chapter 8, once we have established the necessary laws of electrodynamics. For now, all we need to know is that the phase velocity of light in a vacuum ( $c \approx 3.0 \times 10^8 \text{ m s}^{-1}$ ) is a constant, that the refractive index of a medium gives the ratio between this constant and the phase velocity of light in that medium, and that the energy density of a light wave is proportional to its amplitude squared.

## 3.3 Geometric Optics

In principle, the dynamics of any wave could be analysed by determining the appropriate partial differential equation, and then solving it for the required initial conditions. However, in general this is going to be rather complicated, and thus, it is worth developing some techniques to help us approximate the behaviour of waves in general. To this end, we shall discuss the basic principles of geometric optics, which although primarily concerned with light, applies equally to any other type of wave. In geometric optics, we are primarily concerned with rays, waves which can be well approximated by a sinusoidal plane wave, within a region whose size is much larger than its wavelength. As such, geometric optics can be considered as the limit as the wavelength tends to zero, which for visible light ( $\lambda < 1 \mu\text{m}$ ) is a fairly good approximation.

### 3.3.1 Huygen's Principle

One of the ways in which we can understand geometric optics is through Huygen's principle, which states that every point on a wavefront acts as a source for secondary wavelets. That is to say that, every point on a wavefront scatters infinitesimal rays in all directions, and the subsequent wave is formed by the superposition of these rays. As we shall see, this idea will be particularly useful when we come to look at diffraction in section 3.4.

### 3.3.2 Fermat's Principle

Fermat's principle states that a ray will travel from point  $A$  to point  $B$ , via the path that it takes the wave the least time to traverse. We can understand this as follows; according to Huygen's principle, rays will travel from  $A$  to  $B$  along all available paths. Thus, for any given path, there is another, almost identical path which takes slightly longer to traverse. Since we are considering the limit as the frequency tends to infinity, even these small time differences will be enough for the rays to acquire a significant phase difference, leading to destructive interference between all of the different rays. Only on an extremal path, where the time taken is at a maximum or a minimum, and is hence unchanged by first order perturbations to the path, will the light rays be able to interfere constructively. As such, if this extremal path is blocked, all of the available paths will interfere destructively and the total amplitude of the wave at  $B$  will be zero. Thus, we can say that the ray travels along the extremal path.

To find this path in a medium with variable refractive index  $n$ , we can parametrise the path  $\mathbf{x}(\tau)$ , such that the path leaves  $A$  at  $\tau = 0$ , and reaches  $B$  at  $\tau = 1$ . It is also convenient for us to choose a parametrisation where  $n|\mathbf{x}'(\tau)|$  is constant, so that the parameter  $\tau$  relates linearly to the physical time. Under these circumstances, the time taken is given by:

$$T = \frac{1}{c} \int_0^1 n \left| \frac{d\mathbf{x}}{d\tau} \right| d\tau \quad (3.55)$$

Using the calculus of variations, as we did in chapter 1, this integral will have an extremal value, if the path  $\mathbf{x}(\tau)$  obeys the differential equation:

$$\frac{d^2\mathbf{x}}{d\tau^2} + \frac{2}{n} \left( \nabla n \cdot \frac{d\mathbf{x}}{d\tau} \right) \frac{d\mathbf{x}}{d\tau} - \frac{1}{n} \left( \frac{d\mathbf{x}}{d\tau} \cdot \frac{d\mathbf{x}}{d\tau} \right) \nabla n = \mathbf{0} \quad (3.56)$$

### 3.3.3 Reflection and Refraction

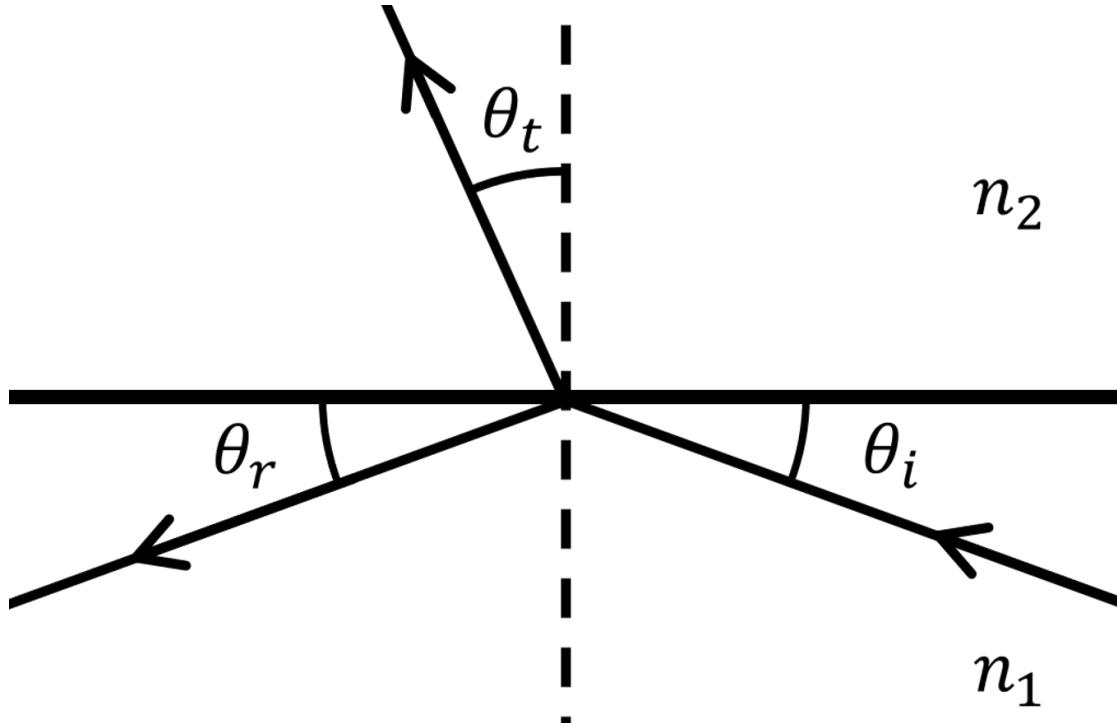


Figure 3.3: A boundary between two different refractive media.

When a ray encounters the boundary between two different media, each with its own refractive index, it can either be reflected, meaning it remains in the original medium but moves away from the boundary, or it can be refracted, which involves the ray propagating through the second medium. In general, the ray will do some combination of the two, by splitting into two new rays. To see this, let us consider a boundary between two media located at the plane  $z = 0$ . The refractive indices shall be  $n_1$  and  $n_2$  for the regions  $z < 0$  and  $z > 0$  respectively. Let us also choose our axes such that, the incident ray meets the boundary at the origin. We can now say that, in the neighbourhood of the origin, all three of the incident, reflected, and refracted rays can be well approximated by sinusoidal plane waves. Thus, we can represent the overall wave as:

$$\psi(\mathbf{x}, t) = \begin{cases} \mathcal{A}_i e^{i(\omega_i t - \mathbf{k}_i \cdot \mathbf{x})} + \mathcal{A}_r e^{i(\omega_r t - \mathbf{k}_r \cdot \mathbf{x})} & z < 0 \\ \mathcal{A}_t e^{i(\omega_t t - \mathbf{k}_t \cdot \mathbf{x})} & z > 0 \end{cases} \quad |\mathbf{x}| \approx 0 \quad (3.57)$$

Since these waves are governed by a second order partial differential equation, both the wave and its first derivatives must be continuous at the boundary, such that its second derivative always remains finite. We can immediately see from (3.57) that, if this continuity is to hold true for all time, all of the waves must have the same frequency. By a similar argument, we can also say that all the components of the wave vectors, parallel to the plane  $z = 0$ , must be the same. This gives us the relations:

$$\omega_i = \omega_r = \omega_t \quad \mathbf{k}_i \times \hat{\mathbf{z}} = \mathbf{k}_r \times \hat{\mathbf{z}} = \mathbf{k}_t \times \hat{\mathbf{z}} \quad (3.58)$$

Since the frequencies are the same, the magnitudes of the wave vectors must be proportional to their respective refractive indices. If we use this to expand the cross products in equation (3.58), we arrive at Snell's law, which relates the angles between each wave vector and the normal to the plane:

$$n_1 \sin \theta_i = n_1 \sin \theta_r = n_2 \sin \theta_t \quad (3.59)$$

Finally, we can utilise the continuity in  $\psi$  and  $\frac{\partial \psi}{\partial z}$  at the origin to determine the amplitudes of the reflected and refracted waves:

$$\mathcal{A}_r = \frac{1 - \zeta}{1 + \zeta} \mathcal{A}_i \quad \mathcal{A}_t = \frac{2}{1 + \zeta} \mathcal{A}_i \quad (3.60)$$

Where  $\zeta = \frac{n_2 \cos \theta_t}{n_1 \cos \theta_i}$ . Interestingly, if  $n_1 > n_2$ , there exists a critical angle beyond which  $\zeta$  becomes imaginary. If this is the case, we find that  $|\mathcal{A}_r| = |\mathcal{A}_i|$ , meaning that all of the energy from the incident wave is carried away by the reflected ray. For this reason, this phenomenon is referred to as total internal reflection. The refracted wave then acquires an imaginary component in its wave vector, which results in an evanescent wave of exponentially decaying amplitude, extending out into the  $z > 0$  region. If there is another boundary, to a medium of higher refractive index, beyond the  $z = 0$  plane, this evanescent wave can bridge the gap and allow some of the incident ray's energy to continue propagating forwards, in a process known as frustrated total internal reflection. As we shall see in chapter 4, this is the classical analogue of quantum tunnelling, the phenomenon where particles have a small probability of being found in a classically forbidden region.

### 3.3.4 Lenses

A lens is an optical device that uses refraction to bring different rays to a focus. To understand how a lens works, let us consider a spherical boundary between two media, of refractive indices  $n_1$  and  $n_2$  respectively, with a point source placed a distance  $u$  from the interface, as shown in figure 3.4. We shall now consider the path of a ray, that leaves the object at  $u$  and is then brought back onto the axis at a distance  $v$  from the interface.

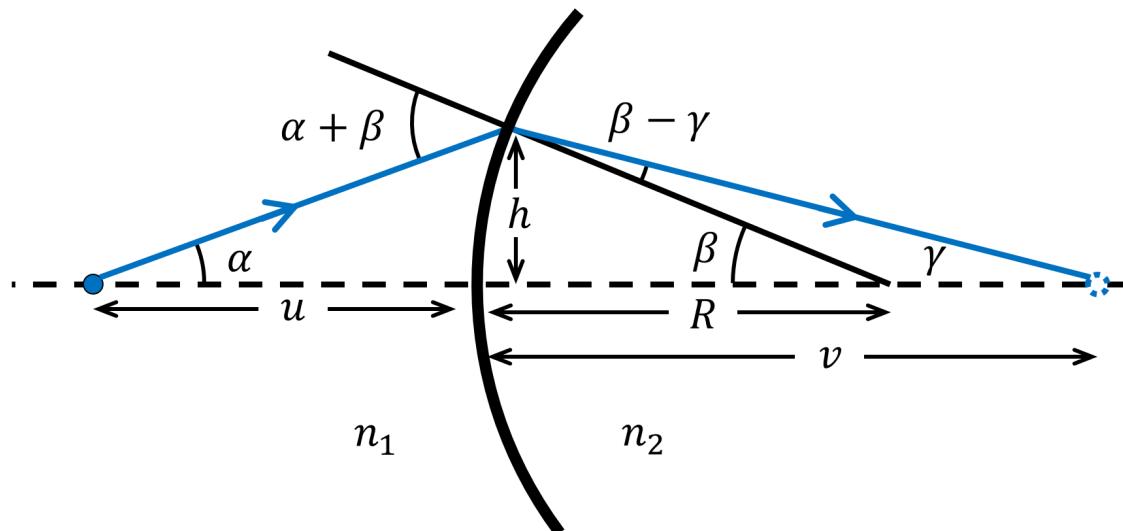


Figure 3.4: A spherical interface between two different refractive media.

When analysing optical components such as this, we often invoke the para-axial approximation, that is to say that we consider only those rays that are sufficiently close to the optical axis that we can use small angle approximations for  $\alpha$ ,  $\beta$  and  $\gamma$ . In this regime, we can use simple geometry to determine that the angles are given by:

$$\alpha = \frac{h}{u} \quad \beta = \frac{h}{R} \quad \gamma = \frac{h}{v} \quad (3.61)$$

If we apply the small angle approximation to Snell's law ,and substitute in for the angles, we find that  $h$  cancels and thus, all rays leaving the object must be brought to focus at the same point  $v$ , given by:

$$\frac{n_1}{u} + \frac{n_2}{v} = \frac{n_2 - n_1}{R} \quad (3.62)$$

A true lens combines two such spherical surfaces, and so the rays leaving the first are refracted again, as they travel through the second interface and back into the original medium. If the lens is biconvex, with radii of curvature  $R_1$  and  $R_2$  respectively, we can apply (3.62) twice, to obtain the lens maker's equation:

$$\frac{1}{u} + \frac{1}{v} = \frac{n_2 - n_1}{n_1} \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \quad (3.63)$$

Care must be taken with the signs of the various terms in the lens maker's equation, as they can all be negative whilst still maintaining some physical meaning. The distance  $u$  is positive, if the incident rays are emerging from a real object, and are thus, diverging from one another when they reach the lens. If instead we have a virtual object, that is to say that the incident rays were on course to converge into a single point behind the lens, then  $u$  is negative. Similarly, if a real image is formed, meaning that all of the refracted rays are brought to a focus behind the lens,  $v$  is positive, while if a virtual object is formed, meaning that all of the refracted rays appear to be diverging from a point in front of the lens,  $v$  is negative. The radii of curvature are then signed such that, in a biconvex lens they are both positive, while in a biconcave lens they would both be negative.

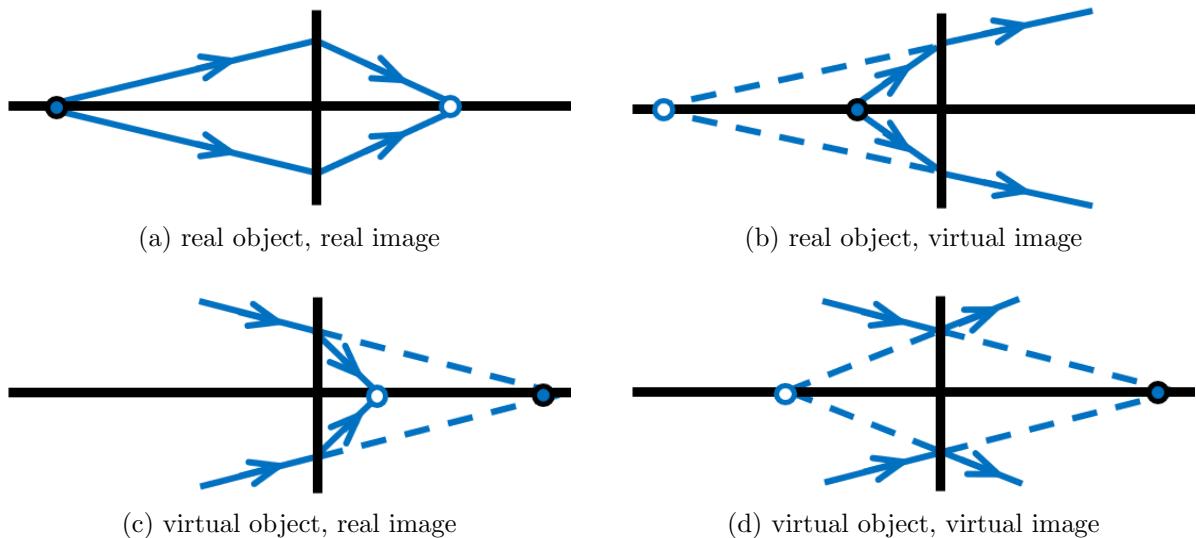


Figure 3.5: Different configurations of real/virtual objects and images.

So far we have only been considering objects that are on axis; however, as it happens, the lens maker's equation applies equally well to off axis objects (provided that they are close enough to the axis that the para-axial approximation holds). To see this, let us consider an off axis object at position  $u$  and a ray leaving the object, which meets the optical axis at position  $a$ . After passing through the lens, the refracted ray shall meet the optical axis at  $b$ , such that  $a$  and  $b$  satisfy the lens maker's equation. We shall also consider a second ray, travelling through the centre of the lens, with the intersection between the two rays occurring at position  $v$ .

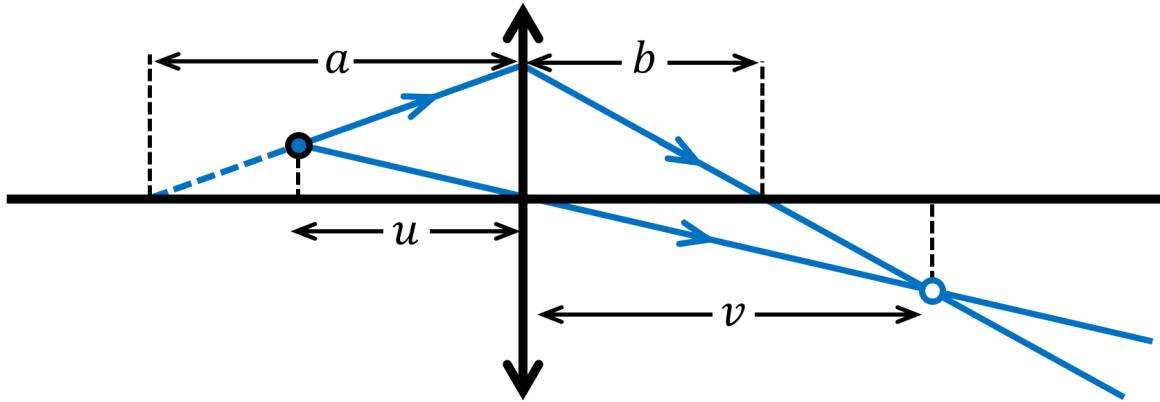


Figure 3.6: An off axis object being focused by a converging lens.

If we wish to determine the height of the focused image below the optical axis, we can use two different methods. The first is to simply note that, since the central ray subtends the same angle on either side of the lens, the height of the image must be  $\frac{v}{u}$  times the height of the object. Alternatively, we could use two sets of similar triangles in figure 3.6; the first to relate the object's height to the height at which the ray meets the lens, and the second to relate this height to the height of the image. Comparing these two results:

$$\frac{a}{a-u} \frac{v-b}{b} = \frac{v}{u} \quad (3.64)$$

If we rearrange equation (3.64), and substitute in the lens maker's equation for  $a$  and  $b$ , we find that all of the rays leaving the object are brought to a focus at the same point, which is also governed by the lens maker's equation:

$$\frac{1}{a} + \frac{1}{b} = \frac{1}{u} + \frac{1}{v} = \frac{n_2 - n_1}{n_1} \left( \frac{1}{R_1} - \frac{1}{R_2} \right) \quad (3.65)$$

It is often convenient for us to introduce a new parameter, the focal length  $f$ , which is defined as the distance at which an infinitely distant point source is brought to a focus. As such,  $f$  is equal to  $\lim_{u \rightarrow \infty} v$ , which is simply the reciprocal of the right hand side in (3.65). We may also be interested in the magnification of an image  $M$ , which as discussed earlier is equal to  $-\frac{v}{u}$  (the minus sign accounts for the fact that the image is inverted). Combining these ideas, we obtain the two equations:

$$v = \frac{uf}{u-f} \quad M = \frac{f}{f-u} \quad (3.66)$$

### 3.3.5 Mirrors

A mirror can be considered as a perfectly reflective surface, that is to say its refractive index is so large that, according to (3.60) in section 3.3.3, any incident wave is completely reflected (with a  $\pi$  phase shift), without penetrating the surface. In the case of a plane mirror, this simply results in the formation of a virtual object behind the mirror, as shown in figure 3.7. We can also see from 3.7 (b) that the image is inverted with respect to the object. However, this inversion is not the same as the inversion we saw earlier with a lens. In the case of a lens, the object is inverted in both directions (which is equivalent to rotating it  $\pi$  radians about the optical axis), whereas in the case of the mirror, the object is only inverted in one direction.

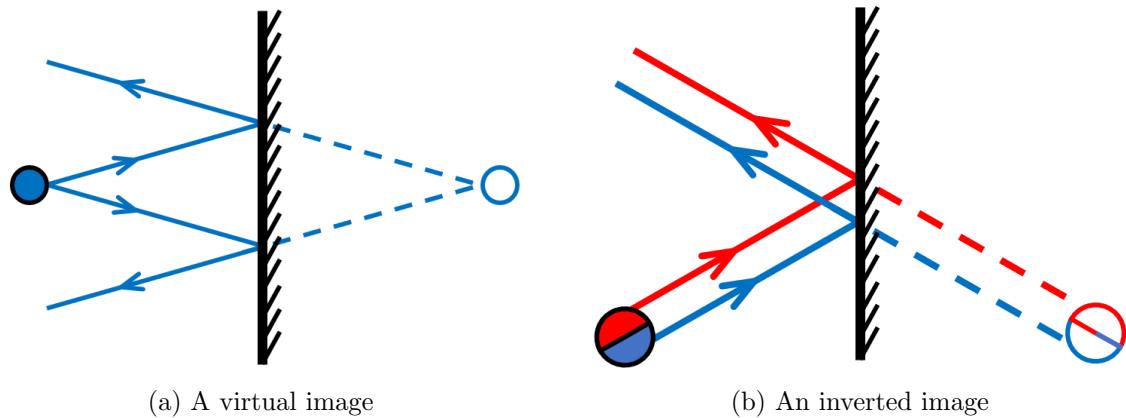


Figure 3.7: The formation of a virtual, inverted image in a plane mirror.

Another interesting case is that of a spherical mirror. Let us consider a point source, located a distance  $u$ , along the optical axis, from a mirrored surface with radius of curvature  $R$ . We shall now focus on a ray, which emanates from the point source at  $u$ , before meeting the mirror at a height  $h$  and being reflected back onto the axis at a position  $v$ .

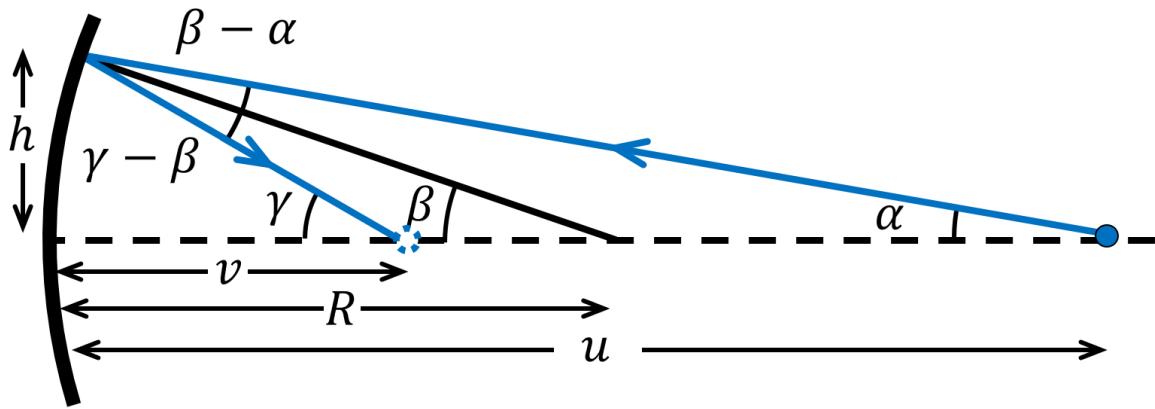


Figure 3.8: A ray being focused by a spherical mirror.

We can see from figure 3.8 that, if we apply the para-axial approximation, we obtain the following analogue to the lens maker's equation:

$$\frac{1}{u} + \frac{1}{v} = \frac{2}{R} \quad (3.67)$$

## 3.4 Diffraction

In section 3.3, we considered geometric optics in the limiting case that the wavelength of our rays tended towards zero. As such, the results we derived are valid, when the physical size of the rays is much larger than their wavelength. If however, we wish to consider phenomena that occur at the wavelength scale, we will require slightly more sophisticated tools to analyse them. One important consequence of this is diffraction, the phenomenon of waves being able to bend around obstacles of a size comparable to their wavelength.

### 3.4.1 Fraunhofer Diffraction

Let us consider a monochromatic light source in the  $x - y$  plane, such that the complex amplitude of the wave is given by the pupil function  $\mathcal{F}(x, y)$ . If we wish to find the amplitude of the wave on the surface of the plane  $z = l$ , then we simply need to sum the amplitudes of all of the rays leaving the source. Thus we obtain the expression:

$$\mathcal{A}(x, y) = \int_{\mathbb{R}^2} \frac{k\mathcal{F}(x', y')e^{-ik\sqrt{l^2+(x-x')^2+(y-y')^2}}}{2\pi\sqrt{l^2 + (x - x')^2 + (y - y')^2}} dx' dy' \quad (3.68)$$

The factor of  $k/2\pi\sqrt{l^2 + (x - x')^2 + (y - y')^2}$  arises as a consequence of the rays spreading out in space, and thus, decaying in amplitude. In fact, we have already seen this behaviour in section 3.1.1, when we considered spherical waves in three dimensions. Equation (3.68) is rather difficult to manipulate, so it is often convenient for us to consider the far field approximation. That is to say, if  $\mathcal{F}(x, y)$  is constrained to some region around the origin, we are interested in the case when  $l$  is much larger than the linear size of this region. In this limit, we can take a Taylor series expansion of the square root, to yield:

$$\mathcal{A}(x, y) \approx \int_{\mathbb{R}^2} \frac{k\mathcal{F}(x', y')e^{ik(\xi x' + \eta y')}}{2\pi\sqrt{l^2 + x^2 + y^2}} dx' dy' \quad (3.69)$$

Where we have discarded the constant factor of  $e^{-ik\sqrt{x^2+y^2+l^2}}$ , since we are typically only interested in the magnitude of  $\mathcal{A}$ . In addition, we have introduced the new coordinates  $\xi$  and  $\eta$  are equal to the sines of the angles subtended by the point  $(x, y, l)$ :

$$\xi = \frac{x}{\sqrt{x^2 + y^2 + l^2}} \quad \eta = \frac{y}{\sqrt{x^2 + y^2 + l^2}} \quad (3.70)$$

If we are only considering the region of the diffraction pattern in the neighbourhood of the origin, we can apply small angle approximations to  $\xi$  and  $\eta$ , to obtain the fairly simple expression:

$$\mathcal{A}(x, y) \approx \frac{k}{2\pi l} \int_{\mathbb{R}^2} \mathcal{F}(x', y') e^{\frac{ik}{l}(xx' + yy')} dx' dy' \quad |x|, |y| \ll l \quad (3.71)$$

Thus,  $\mathcal{A}$  is simply the Fourier transform of  $\mathcal{F}$ , albeit with a bit of scaling along the axes. This is particularly useful, since it allows us to invoke Parseval's theorem, which in this case, corresponds to the conservation of energy.

$$\int_{\mathbb{R}^2} \overline{\mathcal{A}}(x, y)\mathcal{A}(x, y) dx dy = \int_{\mathbb{R}^2} \overline{\mathcal{F}}(x, y)\mathcal{F}(x, y) dx dy \quad (3.72)$$

### 3.4.2 Infinitesimal Slits

One of the most well known example of diffraction is Young's double slit experiment. In this experiment, an opaque barrier, containing two thin slits, is illuminated by a uniform, monochromatic beam, and the resulting diffraction pattern is formed on a distant screen. Although, in practice, these slits will always have finite dimensions, the simplest model for this experiment is to describe the slits as infinitesimal point sources. If the two slits have a separation of  $s$ , we can represent the pupil function as:

$$\mathcal{F}(x, y) = \left[ \delta\left(x - \frac{s}{2}\right) + \delta\left(x + \frac{s}{2}\right) \right] h(y) \quad (3.73)$$

Where  $\delta(x)$  is the Dirac delta function, and  $h(y)$  describes the variation in amplitude with the height of the slit. Substituting this result into equation (3.71) gives us the diffraction pattern:

$$\mathcal{A}(x, y) \approx \frac{k}{\pi l} \cos\left(\frac{ksx}{2l}\right) \int_{\mathbb{R}} h(y') e^{\frac{ik}{l} yy'} dy' \quad (3.74)$$

Since the intensity of light is proportional to its amplitude squared, it follows that along any horizontal path, the intensity will oscillate between some maximum value and zero (which will appear visually in the form of bright and dark fringes on the screen), as described by equation (3.75):

$$I(x) = I_0 \cos^2\left(\frac{ksx}{2l}\right) \quad (3.75)$$

One of the key points to note about the two slit diffraction pattern is that all of the peaks have the same separation, given by  $\frac{2\pi l}{ks}$ . Furthermore, each of the bright fringes has the same intensity, a feature that is particularly characteristic of the two slit pattern. Obviously, these fringes can not continue on indefinitely, since this would require an infinite amount of energy; however, this is to be expected, given that our expression is only valid for small  $x$ .

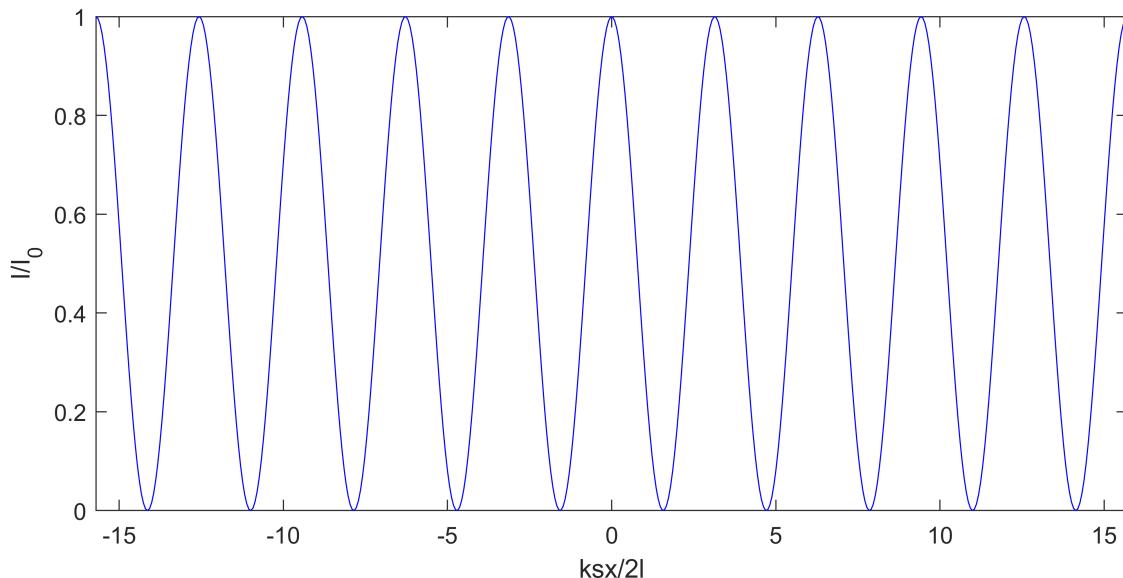


Figure 3.9: The diffraction pattern produced by two narrow slits.

It is an interesting exercise to generalise this result for  $n$  equally spaced narrow slits, instead of simply two. If we, once again, consider infinitesimally thin slits, with separation  $s$ , then the pupil function can be given by:

$$\mathcal{F}(x, y) = h(y) \sum_{m=0}^{n-1} \delta(x - x_0 + ms) \quad x_0 = \begin{cases} \frac{ns}{2} & n \in \text{even} \\ \frac{(n-1)s}{2} & n \in \text{odd} \end{cases} \quad (3.76)$$

If we substitute this pupil function back into equation (3.71), and evaluate the integral over  $x'$ , we obtain the following expression:

$$\mathcal{A}(x, y) = \frac{k}{2\pi l} \left[ e^{\frac{ikxx_0}{l}} \sum_{m=0}^{n-1} e^{\frac{ikmsx}{l}} \right] \int_{\mathbb{R}} h(y') e^{\frac{ik}{l}yy'} dy' \quad (3.77)$$

We can evaluate the sum in equation (3.77) fairly easily, by using the general formula for the sum of a geometric progression. We can then take the modulus squared of this result to find the variation in the intensity along a horizontal contour. After some rearrangement, this becomes:

$$I(x) = \frac{I_0 \sin^2 \left( \frac{knsx}{2l} \right)}{n^2 \sin^2 \left( \frac{ksx}{2l} \right)} \quad (3.78)$$

As shown in figure 3.10, this will give rise to evenly spaced principle maxima, separated from one another by a distance of  $\frac{2\pi l}{ks}$ , just as we saw in the two slit case. However, in general there will be  $n - 1$  minima, and thus  $4(n - 2)$  subsidiary maxima between each pair of principle maxima. These minima occur at evenly spaced intervals of  $\frac{2\pi l}{kns}$ , with the exception  $n$ th point, which is a principal maximum instead.

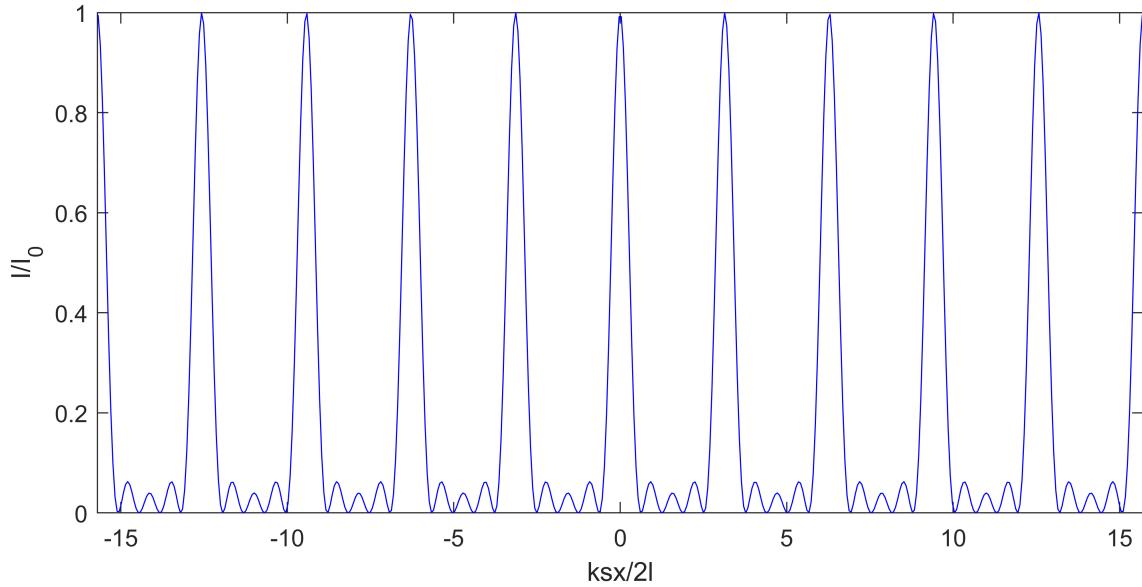


Figure 3.10: The diffraction pattern produced by five narrow slits.

A diffraction grating is composed of a very large number of such slits, all arranged next to one another in the manner we have been describing. As such, it can be thought of as the limiting case when  $n$  tends towards infinity, which results in all of the intensity being concentrated at the principal maxima.

### 3.4.3 Finite Slits

Unfortunately, it is impossible for us to ever produce a truly infinitesimal slit, and so we need to be able to model diffraction through apertures of a finite width  $w$ . To start with, we shall consider the interference pattern formed by only a single slit, which as we shall see, will form the basis for our analysis of the many slit systems we considered in section 3.4.2. For a single slit of width  $w$ , the pupil function is given by:

$$\mathcal{F}(x, y) = \begin{cases} h(y) & x \in [-\frac{w}{2}, \frac{w}{2}] \\ 0 & \text{elsewhere} \end{cases} \quad (3.79)$$

Just as we did before, we can substitute this result into equation (3.71), and then evaluate the integral to obtain an expression for the amplitude of the diffraction pattern. We can then square the amplitude to find the variation in intensity along a horizontal contour. This leads us to the result that:

$$\mathcal{A}(x, y) = \frac{\sin(\frac{kwx}{2l})}{\pi x} \int_{\mathbb{R}} h(y') e^{\frac{ik}{l}yy'} dy' \implies I(x) = I_0 \operatorname{sinc}^2\left(\frac{kwx}{2l}\right) \quad (3.80)$$

Where  $\operatorname{sinc}(x) = \frac{\sin(x)}{x}$ . We can see from figure 3.11 that, this will lead to a series of bright fringes, all of width  $\frac{2\pi l}{kw}$ , surrounding a large central maximum, which is twice as wide. Another important point is that, since energy is conserved, when a longer wavelength of light spreads out over a greater area, its intensity falls to compensate.

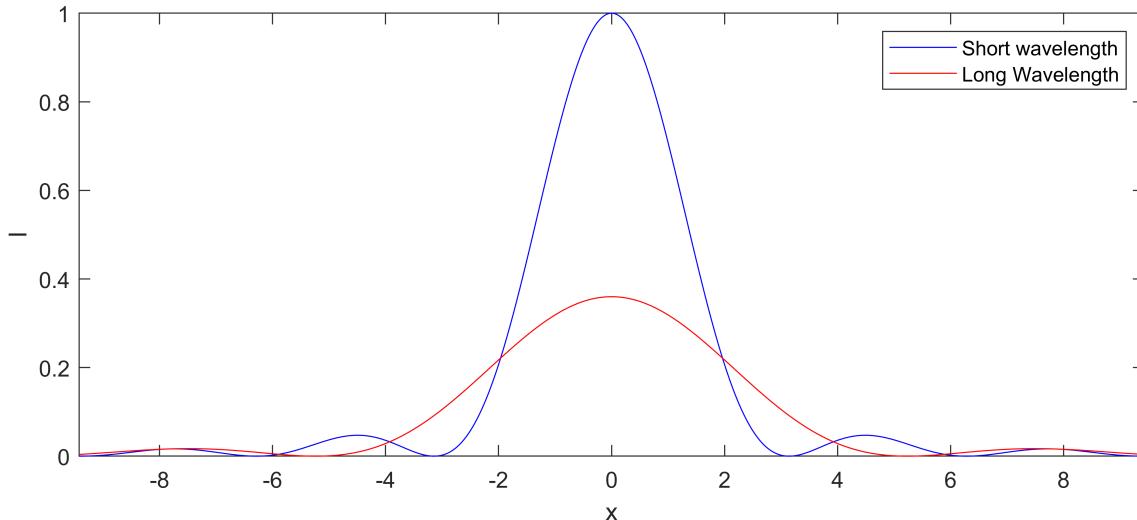


Figure 3.11: The diffraction pattern produced by two different wavelengths of light, when they pass through a single slit.

Diffraction in this manner often limits the resolution of optical devices, such as microscopes and telescopes. This is because the spreading out of light, in the manner that we have just been describing, makes it difficult to distinguish light rays that originate from different objects. Since shorter wavelengths spread out less, the resolution of these devices can be increased by switching to a higher frequency band of the electromagnetic spectrum.

We are now going to discuss the diffraction patterns produced by multiple slits of width  $w$ ; however, before we do, we should spend some time looking at the properties of the Fourier transform. Let us consider two functions  $f(x)$  and  $g(x)$ . We define their convolution to be given by:

$$(f * g)(x) = \int_{\mathbb{R}} f(u)g(x - u)du \quad (3.81)$$

A simple change of variables allows us to see that  $f * g = g * f$ . We can now compute the Fourier transform of this convolution using a similar change of variables:

$$\int_{\mathbb{R}} (f * g)(x)e^{ikx}dx = \int_{\mathbb{R}^2} f(u)g(x - u)e^{ikx}dudx = \int_{\mathbb{R}^2} f(u)e^{iku}g(v)e^{ikv}dudv \quad (3.82)$$

Since the new integral is separable in form, we arrive at the Fourier convolution theorem, which states that the Fourier transform of a convolution is equal to the product of the individual functions' Fourier transforms:

$$\int_{\mathbb{R}} (f * g)(x)e^{ikx}dx = \left[ \int_{\mathbb{R}} f(x)e^{ikx}dx \right] \left[ \int_{\mathbb{R}} g(x)e^{ikx}dx \right] \quad (3.83)$$

This is particularly relevant, because the pupil function for  $n$  finite slits can be expressed as the convolution of the single slit pupil function with the array of delta functions we used in equation (3.76). As such, the general  $n$  slit diffraction pattern consists of the uniform peaks described in section 3.4.2, multiplied by a  $\text{sinc}^2$  envelope function. This gives us the relationship that:

$$I(x) = I_0 \text{sinc}^2\left(\frac{kwx}{2l}\right) \frac{\sin^2\left(\frac{knsx}{2l}\right)}{n^2 \sin^2\left(\frac{ksx}{2l}\right)} \quad (3.84)$$

An example of such a diffraction pattern is shown in figure 3.12 below.

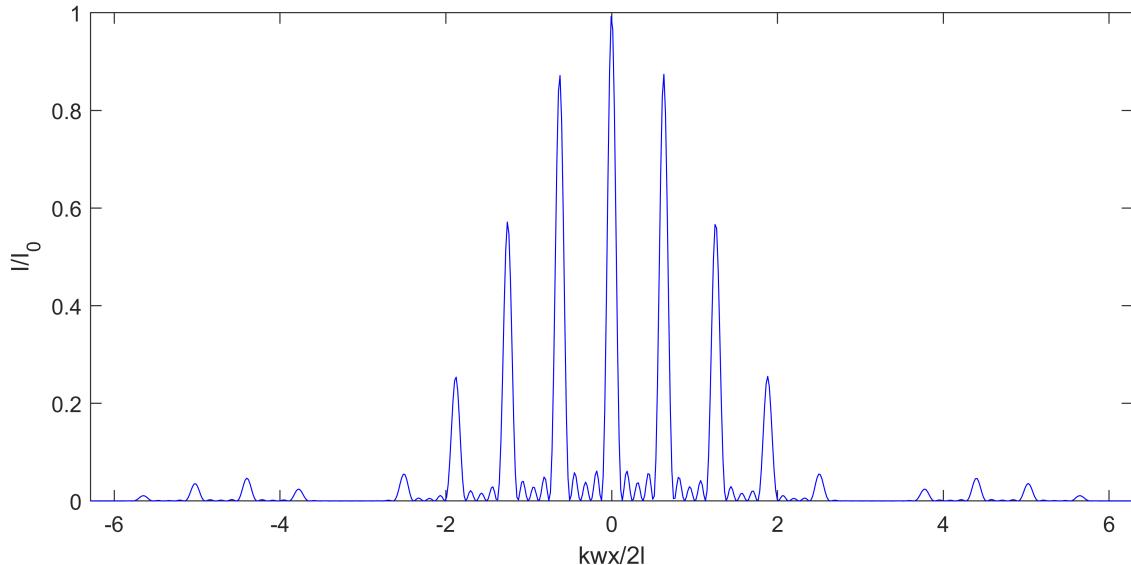


Figure 3.12: The diffraction pattern produced by five slits, which have a width of one fifth their separation.

### 3.4.4 Bragg Diffraction

One of the most important practical applications of diffraction is in x-ray crystallography, which utilises the fact that x-rays have wavelengths on the order of inter atomic spacings (usually a few Angstroms), to map out the atomic structure of a crystal. The crystal in this experiment can be thought of as a three dimensional diffraction grating, with each atom behaving like an aperture as they scatter the incident x-ray beam. To understand the diffraction patterns these crystals produce, we are going to start by analysing a very general case. Let us consider a region of space  $V$ , that is irradiated by a plane wave of wave vector  $\mathbf{k}_1$ . Every point in  $V$  has a scattering factor  $f(\mathbf{x})$ , which determines how much of the incident plane wave is scattered in all directions. If we now consider some distant point  $P$ , the only waves that will be detected are those that have a wave vector pointing from  $V$  towards  $P$ . Since this scattering is elastic (the modulus of the wave vector is conserved), there is only one possible wave vector  $\mathbf{k}_2$  that meets this requirement. The amplitude of the wave at  $P$  is thus proportional to the Fourier transform:

$$\tilde{f}(\mathbf{k}_2) = \int_V f(\mathbf{x}) e^{i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{x}} d^3x \quad (3.85)$$

Which accounts for the phase differences arising from both the different positions of each point with respect to  $P$ , and the different positions of each point within the incident plane wave. In the case of x-ray crystallography, the scattering factor is proportional to the electron density at that point, and since most of the electron density of an atom is concentrated in a tight shell around the nucleus,  $f(\mathbf{x})$  is essentially an array of delta functions at each of the atomic positions. For any real crystal,  $V$  will be so much larger than the atomic separations, that  $\tilde{f}(\mathbf{k}_2)$  will also become an array of delta functions, in a manner analogous to the behaviour of a diffraction grating from section 3.4.2. In this limit, the only values of  $\mathbf{k}_2$  with non-zero amplitude will be those for which all of the atomic sources are in phase at  $P$ .

A simple lattice, which is a typical crystal structure adopted by metallic elements, can be characterised by three lattice vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$ . Atoms are then located on the vertices of the parallelepipeds defined by these vectors, stacked one on top of the other. That is to say that:

$$\mathbf{x}_{\text{atom}} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \quad u, v, w \in \mathbb{Z} \quad (3.86)$$

The only way in which all of these sources can be in phase, is if the Laue conditions on the change in wave vector are met.

$$\Delta\mathbf{k} \cdot \mathbf{a} = 2\pi h \quad \Delta\mathbf{k} \cdot \mathbf{b} = 2\pi k \quad \Delta\mathbf{k} \cdot \mathbf{c} = 2\pi l \quad h, k, l \in \mathbb{Z} \quad (3.87)$$

By measuring the different values of  $\Delta\mathbf{k}$  that occur as a crystal is rotated through an x-ray beam, it is possible to determine the lattice vectors  $\mathbf{a}, \mathbf{b}$  and  $\mathbf{c}$  from the Laue equations, thus measuring the structure of the crystal. The analysis of more complicated crystals can be carried out in a similar manner, since it turns out that all crystal structures can be represented as a convolution of a simple lattice with a repeating motif. Finally, it is worth mentioning that, as a consequence of typical x-ray wavelengths, it is usually impossible to produce more than one diffraction peak at a time. For this reason x-ray diffraction is sometimes carried out on powder samples, which allows the incident beam to encounter the crystal in a variety of orientations, thus producing a full diffraction pattern.

# 4 Quantum Mechanics

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## 4.1 The Formulation of Quantum Mechanics

When it comes to quantum mechanics, there are two principle ways in which we can formulate our ideas. The more common of the two is Schrödinger's wave mechanics, and indeed this is the approach adopted in this chapter. However, an equally valid way to tackle the subject is through Heisenberg's matrix mechanics, although this does come at the disadvantage of being more difficult to visualise physically. The two formulations are, of course entirely equivalent, as was shown by Dirac when he developed his Bra-Ket notation.

In this chapter we will exclusively use the Schrödinger representation, and thus we will be expressing everything in terms of wave functions and partial differential equations. While arguably, this is not the most natural way for us to present all of the following ideas, it is certainly the easiest to visualise. Furthermore, by writing the laws of quantum mechanics in this form, we are drawing parallels to the material covered in chapter 3, in the form of the so called wave-particle duality.

## 4.2 The Wave Function

In quantum mechanics the wave function represents the most complete description of a system possible. This takes the form of some function, which allows us to calculate the probability that, upon measurement the physical parameters of the system will take a certain set of values. It is important to note here that we are not suggesting that the parameters have some fixed value that we just don't know, remember the wave function is the most complete description possible, instead we are saying that, at the moment of measurement, the parameters collapse into single values at random, with the probabilities determined by the quantum state of the system. It is this very unintuitive notion that a variable has no defined value until it is measured, that gives rise to much of the well known quantum weirdness.

Formally, the wave function  $\psi$  can be expressed as a complex valued function, such that, if the system can be characterised by an  $n$  dimensional vector  $\mathbf{X}$ , the probability of finding that vector in a space  $V$  is given by:

$$P(\mathbf{X} \in V) = \int_V \psi(\mathbf{x}, t)\bar{\psi}(\mathbf{x}, t)d^n x \quad (4.1)$$

Where the notation  $\bar{\psi}$  implies complex conjugation. This is equivalent to stating that,  $\psi\bar{\psi}$  is the probability density function of the system. Although in general, wave functions are multidimensional, this chapter is really only a brief introduction to quantum mechanics, and so we shall restrict ourselves to considering one-dimensional wave functions.

Wave functions are not completely arbitrary, and as we shall see there are very good reasons why they must have certain properties. In particular, both a wave function, and its first derivative must be continuous (except at certain singular points such as an infinite potential barrier). Furthermore, in order to obey the law of total probability, wave functions must be normalised such that, the integral of  $\psi\bar{\psi}$  over all possible values of its arguments is unity.

### 4.2.1 A Particle In One Dimension

We are now going to discuss the representation of a quantum mechanical particle in one dimension. Even for such a simple system, there are still a multitude of ways in which the wave function could be expressed; however, we are going to focus on just two: position basis and momentum basis. As we shall see, both representations are equivalent and one can always convert between them, although for most purposes it is easier to visualise what is going on in position basis.

#### 4.2.1.1 Position Basis

In position basis, the wave function is perhaps unsurprisingly a function of the particle's position. One example of such a wave function is shown below in figure 4.1. There are a few key features that are worth mentioning. Firstly, we should note that the wave function tends towards 0 at the extremes of  $x$ . This is a necessary condition for the wave function to be normalizable, and in fact, we can impose the stronger condition that it must decay to 0 faster than  $\mathcal{O}\left(\frac{1}{\sqrt{x}}\right)$ . In addition to this, we can note the point at which  $\psi = 0$ , this is called a node, and as we shall see, they can be a fairly useful indicator of a particle's energy. In very general terms, a wave function with more nodes tends to imply a higher energy state.

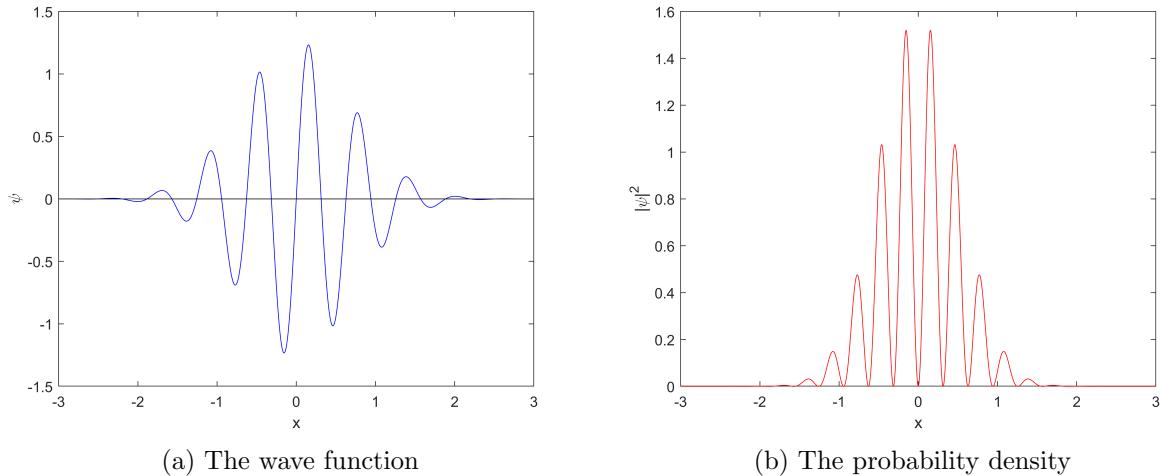


Figure 4.1: An example of a wave function  $\psi$  and the probability density  $\psi\bar{\psi}$ .

Since we tend to think of particles as being localised to a single point, it might be worth briefly discussing how such a particle could be constructed in quantum mechanics. We obviously need to construct a probability density function that is zero everywhere, except for one point, whilst still fulfilling the normalisation condition. Clearly, there is no sufficiently smooth and continuous function that satisfies this description, and so a true particle can only exist in the limiting case, as the probability density tends towards this description. The properties of this limit are identical to those of the Dirac delta function, which is defined by:

$$\delta(x) = 0 \quad \forall x \neq 0 \quad \int_{\mathbb{R}} \delta(x) dx = 1 \quad (4.2)$$

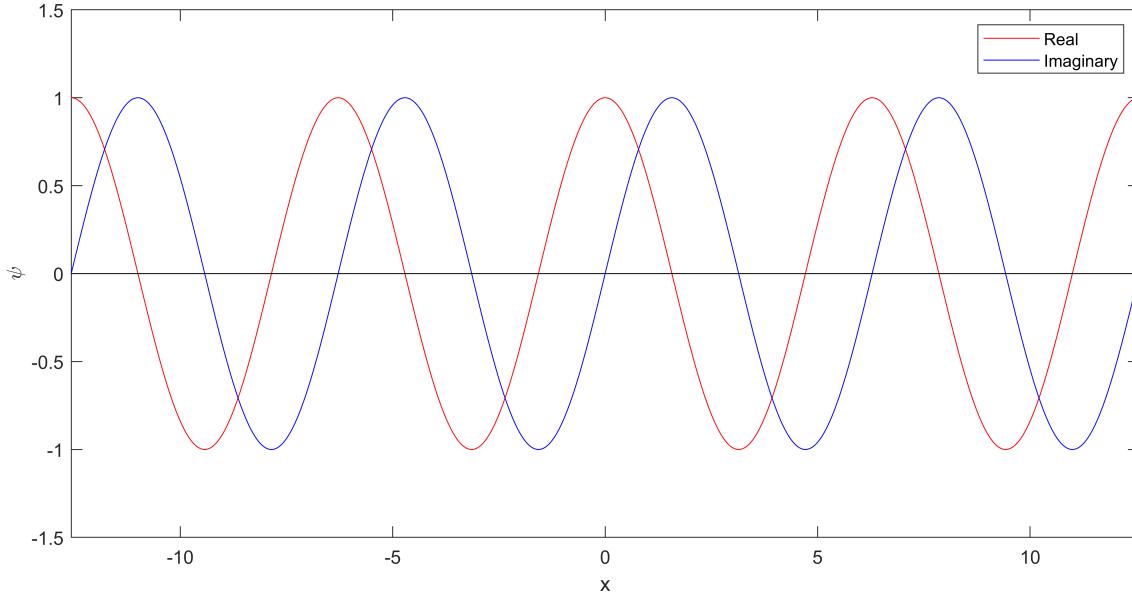


Figure 4.2: The wave function of a particle with fixed momentum.

We encounter a similar problem, if we try to describe a particle with fixed momentum. If we wish to find this wave function, we need to note two pieces of information. Firstly, since momentum is invariant under translations of the origin, the probability density of a definite momentum state must be uniform over all  $x$ . Secondly, in order to maintain consistency with the observed phenomenon that particle beams of momentum  $p$  behave like waves with wave vector  $k = \hbar p$ , our wave function must be of the form:

$$\psi(x) = A e^{\frac{ipx}{\hbar}} \quad (4.3)$$

Where  $\hbar$  is the reduced Planck's constant, equal to Planck's constant divided by  $2\pi$ . The problem here is obvious, since the wave function does not decay with  $x$  it is impossible to normalise for any finite value of the constant  $A$ . This is an example of the Heisenberg uncertainty principle, in order for us to know a particle's momentum exactly, we must lose all information about its position. Of course, definite momentum states never occur in reality, because it would be impossible for the particle's wave function to spread out over all space, without interacting with something that disturbs its momentum.

In order to deal with the difficulties normalising these wave functions, we can introduce the concept of normalising to the delta function. This means that, if  $\psi_u(x)$  is a wave function corresponding to an exact value  $u$  of some continuous variable, we normalise it such that:

$$\int_{\mathbb{R}} \psi_u(x) \overline{\psi_{u'}(x)} dx = \delta(u - u') \quad (4.4)$$

This is not to say that these would make acceptable wave functions for a physical particle, but this is not really important, since real particles can not take exact values of continuous variables. Instead, these wave functions are set up to allow for conversion between different representations of the wave function, as we shall see in section 4.2.1.2.

#### 4.2.1.2 Momentum Basis

In momentum basis, the wave function  $\phi(p)$  is related to the probability density of the particle's momentum, not its position. To convert between position and momentum basis, we utilise a fundamental postulate of quantum mechanics, which states that if  $\psi_p(x)$  is a wave function of momentum  $p$ , normalised according to equation (4.4), the probability density must be given by:

$$\phi(p)\bar{\phi}(p) = \left[ \int_{\mathbb{R}} \bar{\psi}_p(x)\psi(x)dx \right] \left[ \int_{\mathbb{R}} \psi_p(x)\bar{\psi}(x)dx \right] \quad (4.5)$$

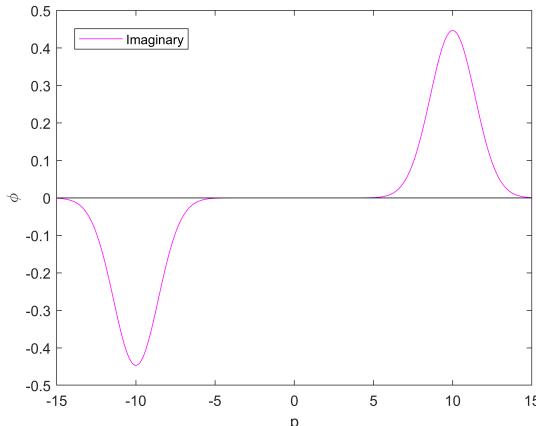
We already know that,  $\psi_p(x)$  takes the form of equation (4.3) from earlier, and it turns out that the correct normalisation constant is  $A = [2\pi\hbar]^{-\frac{1}{2}}$ . When it comes to the wave function, there is always a slight ambiguity, because if the whole thing is multiplied by  $e^{i\theta}$ , it has no physical effect. Furthermore, the complex conjugate of any given wave function will also produce all the same physical results. As such, it is simply a matter of convention, and thus, in accordance with (4.5), we let  $\phi(p)$  be given by:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \psi(x)e^{-\frac{ipx}{\hbar}} dx \quad (4.6)$$

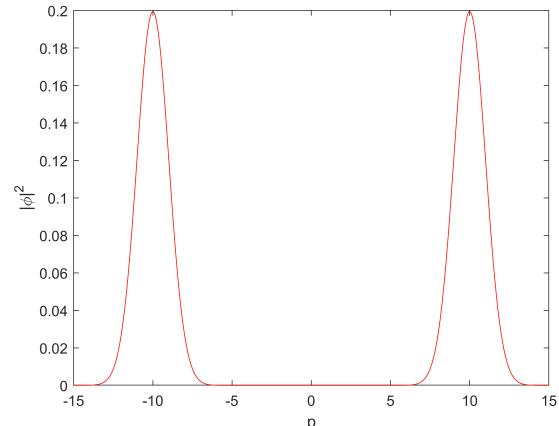
This is nothing more than a Fourier transform, and as such it can always be inverted, yielding equation (4.7) below. If we apply Parseval's theorem to this transformation, we can see that, normalising  $\psi$  guarantees the normalisation of  $\phi$  and vice versa, which is why we needed the extra normalisation constant in  $\psi_p(x)$ .

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \phi(p)e^{\frac{ipx}{\hbar}} dp \quad (4.7)$$

Figure 4.3 shows a plot of the momentum basis wave function for the particle in figure 4.1. We can see that, in this case, the particle is equally likely to be moving forwards or backwards, which is why the spatial wave function has no imaginary component.



(a) The wavefunction



(b) The probability density

Figure 4.3: The same plots as figure 4.1, except expressed in momentum basis.

### 4.2.2 A Particle Beam

Sometimes, it can be helpful to, instead of imagining a single particle, imagine a beam of non-interacting particles. This is essentially a way to get around the non-normalisability of definite momentum states. When describing a particle beam, we can use a wave function in the same way as before, only now  $\bar{\psi}\psi$  is equal to the particle density, instead of the probability density, as it was for a single particle. This is equivalent to multiplying the wave function by  $\sqrt{n}$ , where  $n$  is the total number of particles in the beam. Thus, we can have a finite valued wave function, representing a beam of an infinite number of particles.

When describing a beam in this way, a useful quantity to calculate is the particle flux, which represents the flow rate of particles through a given point. Let us consider a beam, whose wave function takes the form:

$$\psi = Ae^{ikx} \quad (4.8)$$

Since all of the particles are moving in the same direction, the particle flux at a given point is simply the product of the particle density and their velocity. For a beam of the form (4.8), the particle velocity is simply equal to  $\frac{\hbar k}{m}$ , a particle's momentum divided by its mass.

$$j_\psi = \frac{\hbar k \bar{A} A}{m} \quad (4.9)$$

In section 4.4.2, we will discuss the Schrödinger equation, which governs how a wave function evolves through time, and using it, we will derive a more general expression for the flux. For now, we shall simply make do with (4.9), although our derivation was far from rigorous.

Interestingly, we have already met this particle beam description before, although at the time it was not obvious that this was what we were describing. A monochromatic light ray produces a wave that is really very similar to what we have been describing here; it can undergo interference and superposition in exactly the same way that quantum wave functions can, and most importantly, the energy density of an electromagnetic wave is proportional to its amplitude squared, in much the same way as the particle density of our quantum beam. This is because, a light ray is really nothing more than a beam of photons, whose wave function is given by the electric field strength of the wave. It is for this reason that, much of the intuition we have developed about light, with regards to phenomena such as diffraction, actually translates directly into quantum mechanics. In fact, some of the most bizarre quantum phenomena have classical wave analogues. For example, the quantisation of energy levels in a potential well is essentially equivalent to the formation of stationary waves in a confined space. Furthermore, even quantum tunnelling, where a particle passes through a barrier it has insufficient energy to overcome, is analogous to frustrated internal reflection.

This realisation that, the quantum description of a particle is so similar to the classical wave behaviour, colloquially referred to as the wave-particle duality, is fundamental in explaining the outcome of a great many experiments. Two of the most famous examples are; electron diffraction, which showed that classical particles can exhibit wave-like behaviour, and the photoelectric effect, which demonstrated that the energy of electromagnetic radiation is delivered in discrete quanta, known as photons.

### 4.2.3 Superposition and Collapse

One of the most important consequences of the wave function description of quantum mechanics is the idea of superposition. That is to say that, given any two quantum states described by appropriate wave functions, we can create a new, equally valid state by taking linear combinations of the wave functions. If we have some particle that can exist in one of two states, for example two of the orbitals in a hydrogen atom, with wave functions  $\psi_1$  and  $\psi_2$  respectively, then we can write a general wave function in the form:

$$\psi = A\psi_1 + B\psi_2 \quad (4.10)$$

Where  $A$  and  $B$  are complex numbers. We can interpret this superposition using a fundamental postulate of quantum mechanics; the Born rule, which states that the probability of the particle being measured in state 1 is given by:

$$P(1) = \left[ \int_{\mathbb{R}} \bar{\psi}(x)\psi_1(x)dx \right] \left[ \int_{\mathbb{R}} \bar{\psi_1}(x)\psi(x)dx \right] \quad (4.11)$$

If states  $\psi_1$  and  $\psi_2$  are orthogonal, that is to say that  $\int_{\mathbb{R}} \bar{\psi_1}(x)\psi_2(x)dx = 0$ , which is normally the case for sensible states one can choose, such as different energy levels, this simplifies to give:

$$P(1) = \bar{A}A = |A|^2 \quad (4.12)$$

When the particle is measured a phenomenon known as wave function collapse occurs, where the wave function will spontaneously transition from its original superposition into one of  $\psi_1$  or  $\psi_2$  depending on the outcome of the measurement. What happens following a wave function collapse depends on the exact nature of the measured variable. If the energy of the particle was measured then it will collapse into a state of definite energy, known as an energy eigenstate or stationary state, which will remain essentially unchanged until it is disturbed by an interaction with some other particle. If instead, we were to measure the position of a particle, then it would collapse into a state of fairly well defined position (as previously mentioned states with exact position are not physically allowed, but since we can't measure the position to an arbitrary precision, this is not an issue), which would then immediately begin to spread out over space again.

We can also use the idea of superposition to gain a qualitative insight into the origins of the Heisenberg uncertainty principle. We can begin by considering what happens, when we take a superposition of several different momentum states. In general terms, as we move through space, the phase difference between the different states will change, and thus, we will alternate between interfering constructively and destructively. This will create localised regions of high probability density, surrounded by regions where the wave function is mostly cancelled out. If we wish to create a state of reasonably well defined position, we need to use a range of different momentum states, such that the regions where they are all in phase become fairly small. Since this state is formed from the superposition of many different momentum states, it must necessarily have a large uncertainty in its momentum. Conversely, if we wish for our state to have a fairly well defined momentum, we can only use a few different momentum states, which will cause the regions of constructive interference to be reasonably broad, giving a large uncertainty in the particle's position.

## 4.3 Operators and Eigenvalues

We are now going to look at some of the most important mathematical ideas that underpin all of quantum mechanics, in the form of linear operators. Quantum mechanics is very much written in the language of linear algebra, and so a firm understanding of the basic concepts is essential, if one wishes to study the subject in any great depth. It is at this point that we will start to understand how it is that the different formulations of quantum mechanics came to be. Indeed, the ideas that we shall discuss in this section, would conventionally be more at home in a chapter about matrices and vector spaces. Nonetheless, we can still grasp the basic principles from our wave mechanics representation.

### 4.3.1 Operators

For our purposes, we can consider an operator to be an algebraic entity that acts on a function to produce another function, through some kind of rule. That is to say that, the operator  $\hat{A}$  (throughout this chapter operators shall be identified by hats) provides a way of assigning some function  $g(x)$  to every function  $f(x)$ , which we would write as:

$$g(x) = \hat{A}f(x) \quad (4.13)$$

In particular we are concerned with linear operators, those operators which have the following useful property:

$$\hat{A}(\alpha f_1(x) + \beta f_2(x)) = \alpha \hat{A}f_1(x) + \beta \hat{A}f_2(x) \quad \forall f_1, f_2 \quad (4.14)$$

In fact, there is a fairly common example of a linear operator that we are already well acquainted with, the differential operator  $\frac{d}{dx}$ , which acts on a function to produce its derivative. The differential operator also highlights a very important property of linear operators. A linear transformation has an inverse if and only if there is no non-zero function that is mapped to 0 by transformation. In more mathematical terms we could say that:

$$\hat{A}^{-1} \text{ exists } \iff \nexists f(x) \neq 0 \text{ such that } \hat{A}f(x) = 0 \quad (4.15)$$

In the case of  $\frac{d}{dx}$ , the derivative of any constant term is 0 and so it is impossible to invert the transformation to recover a function from its derivative. This is not exactly new information to us, since we already know that when evaluating an indefinite integral we must always add an arbitrary constant for precisely this reason. Conversely however, if we were to restrict our considerations to only functions which satisfy  $f(0) = 0$ , we would no longer have any constants that map to zero and so the inverse must exist. This makes sense as specifying the value of a function at a single point is sufficient to uniquely determine the constant of integration.

One particularly useful thing for us to define is the adjoint of an operator. We denote the adjoint of the operator  $\hat{A}$  by  $\hat{A}^\dagger$ , which is defined such that:

$$\int_{\mathbb{R}} \bar{g}(x) \hat{A}f(x) dx = \int_{\mathbb{R}} f(x) \overline{\hat{A}^\dagger g(x)} dx \quad \forall f, g \quad (4.16)$$

A special case arises when an operator is self-adjoint, meaning that  $\hat{A} = \hat{A}^\dagger$ . Such an operator is referred to as being Hermitian.

### 4.3.2 Eigenvalue Equations

For every linear operator, there are certain functions which behave in a very special way, under the associated transformation. These are functions which remain unchanged by the action of the operator, except for being multiplied by some constant. These are referred to as the eigenfunctions of  $\hat{A}$ , and they are the solutions to the equation:

$$\hat{A}f(x) = \lambda f(x) \quad (4.17)$$

Where the constant  $\lambda$  is called an eigenvalue of  $\hat{A}$ . Finding the eigenfunctions, and their associated eigenvalues, of a given turns out to be incredibly useful in quantum mechanics and is referred to as solving the eigenvalue problem for that operator. Some operators will have a continuous spectrum of eigenvalues, whereas others will only have specific discrete values. Furthermore, it turns out that imposing certain restrictions on the available functions (for example requiring that they are normalisable or setting them equal to 0 at specific points etc.) can dramatically reduce the number of eigenvalues an operator possesses. For example, the second derivative operator  $\frac{d^2}{dx^2}$  has a continuous spectrum of eigenvalues:

$$\frac{d^2}{dx^2} e^{ax} = a^2 e^{ax} \quad (4.18)$$

However, if we impose the boundary conditions that  $f(0) = f(\pi) = 0$ , we find that the available eigenvalues are reduced to the discrete set of negative square numbers:

$$\frac{d^2}{dx^2} \sin(nx) = -n^2 \sin(nx) \quad n \in \mathbb{Z} \quad (4.19)$$

This phenomenon is one of the hallmarks of quantum theory, and is even the origin of its name, since within this framework the eigenvalues may only vary in discrete quanta.

### 4.3.3 Quantum Operators

In quantum mechanics, the role of operators is as follows. Every observable quantity, such as energy, position, and momentum, can be represented by a Hermitian operator. The eigenvalues of that operator then represent the allowed values of that observable when it is measured and the corresponding eigenfunctions are the wave functions with fixed, definite values of that observable. This is often expressed in terms of the eigenvalue equation:

$$\hat{A}\psi = a\psi \quad (4.20)$$

As a result, finding the correct quantum mechanical description for any given system is usually a matter of determining the forms of the appropriate operators, and then solving the eigenvalue problems. It is this principle which is responsible for many of the familiar quantum phenomena, such as the quantisation of an electron's energy in a hydrogen atom. One of the conveniences of the Schrödinger wave mechanics point of view is that, when expressed in position basis, these eigenvalue problems typically become differential equations, which are fairly familiar ways to describe physical systems. In addition, it turns out that, the differential equations in question are often very similar to those we encountered in chapter 3 to describe classical wave behaviour, further solidifying the connections between quantum particles and waves.

### 4.3.4 Hermitian Operators

Since we are specifically concerned with Hermitian operators, it makes sense for us to consider some general properties that they possess. Firstly, we should recall from section 4.3.1 that, by definition, a Hermitian operator must satisfy equation (4.21) below:

$$\int_{\mathbb{R}} \bar{\xi}(x) \hat{A}\psi(x) dx = \int_{\mathbb{R}} \psi(x) \overline{\hat{A}\xi(x)} dx \quad \forall \psi, \xi \quad (4.21)$$

It follows from this that, if  $\psi$  is an eigenfunction of  $\hat{A}$ , such that  $\hat{A}\psi(x) = a\psi(x)$ , then we must have:

$$\int_{\mathbb{R}} \bar{\psi}(x) a\psi(x) dx = \int_{\mathbb{R}} \psi(x) \overline{a\psi(x)} dx \quad (4.22)$$

If we now factor the constants out of the integrals, we find that the eigenvalue must satisfy  $a = \bar{a}$ , and thus,  $a$  must be a real number. It makes sense that the eigenvalues of Hermitian operators must be real, since they represent physical quantities which can not meaningfully take a complex value. Let us now consider the case when both  $\psi$  and  $\xi$  are eigenfunctions of  $\hat{A}$  with different eigenvalues, such that  $\hat{A}\psi(x) = a_1\psi(x)$  and  $\hat{A}\xi(x) = a_2\xi(x)$ , with  $a_1 \neq a_2$ . We must now have:

$$\int_{\mathbb{R}} \bar{\xi}(x) a_1 \psi(x) dx = \int_{\mathbb{R}} \psi(x) a_2 \bar{\xi}(x) dx \quad (4.23)$$

Where we have used our previous result to determine that,  $\bar{a_2} = a_2$ . Factoring the constants out of the integrals then tells us that as long as  $a_1 \neq a_2$  we must have:

$$\int_{\mathbb{R}} \bar{\xi}(x) \psi(x) dx = 0 \quad (4.24)$$

Therefore, distinct eigenfunctions of a Hermitian operator must all be mutually orthogonal. In the degenerate case, when multiple eigenfunctions share the same eigenvalue, any linear combination of those functions will also have that eigenvalue, because the transformation is linear. As such, we can then always pick a set of basis functions, which are mutually orthogonal, and span the space of those eigenfunctions.

### 4.3.5 Position and Momentum

Obviously, the exact form of any given operator will be dependent on the basis in which the wave function is expressed. For the sake of simplicity, we shall be exclusively working in position basis from this point forward, since it is often the easiest to understand. The simplest operator for us to consider is the position operator,  $\hat{X}$ . To understand the form of this operator, we need only consider its eigenfunctions, which, as per our discussion in section 4.2.1, must be delta functions. Since  $\delta(x - u)$  must be an eigenfunction of  $\hat{X}$ , with an eigenvalue of  $u$ , and any function can be represented as a convolution of itself with the delta function, it follows from the linearity of  $\hat{X}$  that, we must have:

$$\psi(x) = \int_{\mathbb{R}} \psi(u) \delta(x - u) du \implies \hat{X}\psi(x) = \int_{\mathbb{R}} u\psi(u) \delta(x - u) du = x\psi(x) \quad (4.25)$$

We can take our analysis of these operators even further by noting that the Born rule, which we used to interpret a quantum superposition in section 3.2.3, together with the orthogonality relation (4.24) in section 4.3.4, implies that the expected value of an observable, with operator  $\hat{A}$ , should be given by:

$$\langle A \rangle = \int_{\mathbb{R}} \bar{\psi}(x) \hat{A} \psi(x) dx \quad (4.26)$$

Applying this principle to the position operator, we obtain:

$$\langle X \rangle = \int_{\mathbb{R}} x \bar{\psi}(x) \psi(x) dx \quad (4.27)$$

Which is precisely what we would expect, given that probability density function of the position is  $\bar{\psi}\psi$  by definition of the wave function.

The next operator that we wish to consider is  $\hat{P}$ , the momentum operator. We can find the form of this operator by using a very similar argument based on its eigenfunctions, and the principle of linearity. In this case, the eigenfunctions must be plane waves of the form  $e^{\frac{ipx}{\hbar}}$ , with eigenvalues of  $p$ . As such, we can say that:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \phi(p) e^{\frac{ipx}{\hbar}} dp \implies \hat{P}\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} p \phi(p) e^{\frac{ipx}{\hbar}} dp = -i\hbar \frac{\partial\psi}{\partial x} \quad (4.28)$$

The partial derivative here is to remind ourselves that, technically the wave function is also dependent on time, although for convenience, we have not been including this as an argument. This brings us on to one of the most fundamental and most important results in quantum mechanics, the commutation relation between position and momentum. We can define the commutator of two operators (denoted by square brackets) as follows:

$$[\hat{X}, \hat{P}] = \hat{X}\hat{P} - \hat{P}\hat{X} \quad (4.29)$$

If we substitute in our expressions for the position and momentum operators and then apply the product rule, we can deduce that the commutator of  $\hat{X}$  and  $\hat{P}$  is:

$$[\hat{X}, \hat{P}] = i\hbar \quad (4.30)$$

The fact that the position and momentum operators do not commute has a profound impact on their properties. For example, one can fairly easily see that, given any pair of operators that do not commute, it would be impossible for any wave function to be an eigenstate of both observables. This is the origin of the Heisenberg uncertainty principle, which can be derived as follows. Firstly, we start with a direct statement of the commutation relation:

$$\hat{X}\hat{P}\psi(x) - \hat{P}\hat{X}\psi(x) = i\hbar\psi(x) \quad (4.31)$$

We can now multiply both sides of (4.31) by  $\bar{\psi}$  and integrate over all space, in order to obtain the result that:

$$\int_{\mathbb{R}} \bar{\psi}(x) \hat{X}\hat{P}\psi(x) dx - \int_{\mathbb{R}} \bar{\psi}(x) \hat{P}\hat{X}\psi(x) dx = i\hbar \quad (4.32)$$

It follows that, since  $\hat{X}$  and  $\hat{P}$  are both Hermitian, the two integrals must be complex conjugates of one another.

As such, we can re-express (4.32) in terms of the imaginary component of the first integral, and in doing so we obtain the inequality:

$$\left| \int_{\mathbb{R}} \bar{\psi}(x) \hat{X} \hat{P} \psi(x) dx \right| \geq \Im \int_{\mathbb{R}} \bar{\psi}(x) \hat{X} \hat{P} \psi(x) dx = \frac{\hbar}{2} \quad (4.33)$$

From here, we can use Schwartz's inequality, together with the definition of a Hermitian operator, to rearrange this inequality into the form of (4.34) below.

$$\left[ \int_{\mathbb{R}} \bar{\psi}(x) \hat{X}^2 \psi(x) dx \right] \left[ \int_{\mathbb{R}} \bar{\psi}(x) \hat{P}^2 \psi(x) dx \right] \geq \frac{\hbar^2}{4} \quad (4.34)$$

It follows from equation (4.26) that we can interpret these integrals as the expected values of the appropriate squared observables. Furthermore, since the two operators  $\hat{X} - \langle X \rangle \hat{I}$  and  $\hat{P} - \langle P \rangle$ , where  $\hat{I}$  is the identity operator, obey the same commutation relation as the position and momentum operators, it follows that variances  $\sigma_x^2$  and  $\sigma_p^2$  must be subject to the same restriction. Then by taking the square root of the inequality, we obtain the famous representation of the Heisenberg uncertainty principle:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \quad (4.35)$$

It is worth just briefly discussing how changes to the frame of reference can effect quantum mechanics. All of the laws of physics should be the same in all inertial reference frames, and quantum mechanics is no exception. We can shift our origin fairly easily by just translating the wave function in space, without affecting its momentum since this depends upon a derivative. Similarly, we can switch to a reference frame with velocity  $v$  by multiplying the wave function by  $e^{-\frac{imv}{\hbar}}$ . This will reduce the momentum by  $mv$ , but will not affect the position because it will always cancel out in  $\bar{\psi}\psi$ . Since the variances of the observables should be invariant, if we simply shift all of the values by a constant, it follows that if the uncertainty principle applies in one reference frame it applies in all reference frames.

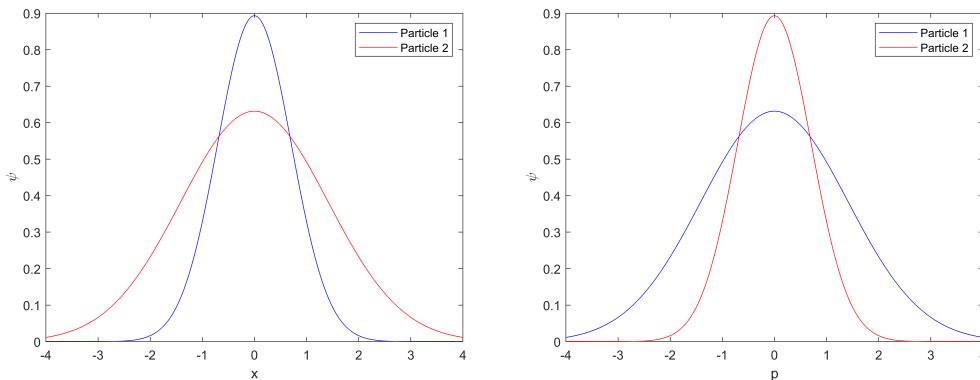


Figure 4.4: The wave functions of two different particles, in position basis (left) and momentum basis (right).

### 4.3.6 The Hamiltonian

We now come to arguably the most important operator we will encounter, the energy operator, which is called the Hamiltonian due to its similarities with the energy function in classical Hamiltonian mechanics. As such, the Hamiltonian is represented by  $\hat{H}$  and has the eigenvalue equation (4.36) below. This eigenvalue equation is sometimes referred to as the time independent Schrödinger equation, although really it is just the definition of  $\hat{H}$ .

$$\hat{H}\psi(x) = E\psi(x) \quad (4.36)$$

The form of the Hamiltonian is not as different to the classical expression as one might expect. There is a kinetic energy term, which is calculated using the formula  $T = \frac{p^2}{2m}$ , with the appropriate momentum operator instead of an actual value, and a potential energy term which simply consists of multiplying the wave function by the potential energy as a function of  $x$ . Thus we obtain:

$$\hat{H}\psi(x) = \frac{1}{2m}\hat{P}^2\psi(x) + V(x)\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x) \quad (4.37)$$

For a particle in free space,  $V(x) = 0$  and so, the eigenvalue equation simplifies down to the simple harmonic motion equation, which has sinusoidal solutions such as the  $Ae^{ikx}$  wave functions we encountered in section 4.2.1. One key difference here is that, while states of definite momentum always give a completely uniform probability distribution, states of definite energy can give a distribution that varies sinusoidally across space. This is because, both states with momenta  $p$  and  $-p$  have the same energy, and as such, it is possible to construct superpositions where the two momentum states interfere with one another.

## 4.4 The Schrödinger Equation

We are now ready to consider arguably the most important equation in all of quantum theory, the time dependent Schrödinger equation. This equation is often viewed as the quantum mechanical equivalent of Newton's second law since it is what allows us to determine the time evolution of a quantum system. The Schrödinger equation is as follows:

$$i\hbar\frac{\partial}{\partial t}\psi(x, t) = \hat{H}\psi(x, t) \quad (4.38)$$

Formally, if the Hamiltonian is itself time independent, one can solve this equation through the use of the operator exponential function, which gives us:

$$\psi(x, t) = e^{-\frac{it\hat{H}}{\hbar}}\psi(x, 0) \quad (4.39)$$

Where the exponential of an operator is defined in terms of its power series expansion, that is to say that:

$$e^{\hat{A}} = 1 + \hat{A} + \frac{1}{2}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \dots + \frac{1}{n!}\hat{A}^n + \dots \quad (4.40)$$

The operator  $e^{-\frac{it\hat{H}}{\hbar}}$  is called the time evolution operator because it allows us to determine how the wave function of the system changes with time.

### 4.4.1 Stationary States

A special case of the Schrödinger equation arises, when the wave function is an energy eigenstate. In this case, we must have  $\hat{H}\psi(x, 0) = E\psi(x, 0)$ , and so, when we expand out the operator exponential we obtain:

$$\psi(x, t) = e^{-i\omega t}\psi(x, 0) \quad (4.41)$$

Where  $E = \hbar\omega$ . Since the only thing which is changing in time is the phase of  $\psi$ , the actual probability density  $\bar{\psi}\psi$  remains invariant in time. For this reason, energy eigenstates are often referred to as stationary states of the Schrödinger equation. Since the Schrödinger equation is linear, we can generate a general solution by taking linear combinations of these stationary states. That is to say that, if the initial wave function can be expressed as a superposition of energy states:

$$\psi(x, 0) = \sum_{n=1}^{\infty} a_n \xi_n(x) \quad (4.42)$$

Where  $\xi_n(x)$  is the  $n$ th eigenfunction of the Hamiltonian, with an associated energy  $E_n$ . Then the resulting solution is given by:

$$\psi(x, t) = \sum_{n=1}^{\infty} a_n e^{-i\omega_n t} \xi_n(x) \quad (4.43)$$

With  $E_n = \hbar\omega_n$  for all values of  $n$ . It is worth noting that, just as in classical physics, the zero point of potential energy is ultimately arbitrary, since if all of the energies are changed by some constant  $V_0$ , then the wave function will just pick up a factor of  $e^{-\frac{iV_0 t}{\hbar}}$ , which will cancel from  $\bar{\psi}\psi$  thus having no physical effect.

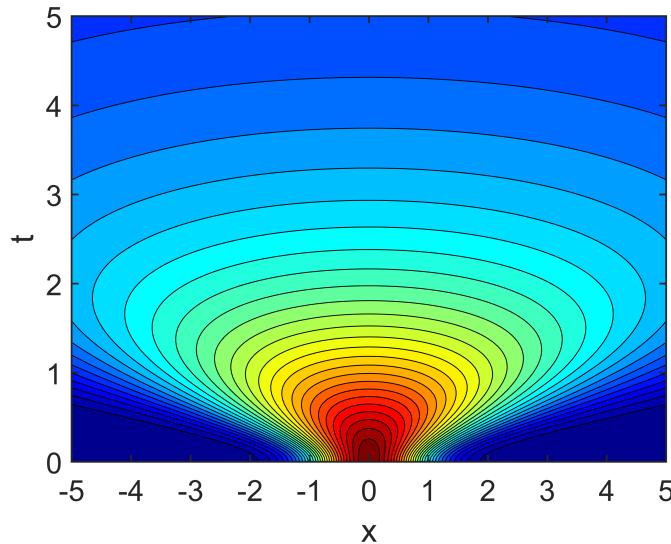


Figure 4.5: A free particle's probability density spreading out over time as predicted by the Schrödinger equation.

### 4.4.2 Particle Flux

We can use the Schrödinger equation to calculate the particle or probability flux of a general wave function. First we know that the probability of finding a particle in the region  $a \leq x \leq b$  at time  $t$  is given by:

$$P(a \leq x \leq b) = \int_a^b \bar{\psi}(x, t)\psi(x, t)dx \quad (4.44)$$

The time derivative of this probability should be equal to the flux flowing in at point  $a$  minus the flux flowing out at point  $b$ , and taking the time derivative into the integral we obtain:

$$j_b - j_a = \int_a^b \frac{\partial \bar{\psi}}{\partial t}\psi + \bar{\psi} \frac{\partial \psi}{\partial t} dx \quad (4.45)$$

Substituting in the Schrödinger equation gives us:

$$j_b - j_a = \frac{i}{\hbar} \int_a^b \psi \hat{H} \bar{\psi} - \bar{\psi} \hat{H} \psi = -\frac{2}{\hbar} \Im \int_a^b \bar{\psi}(x, t) \hat{H} \psi(x, t) dx \quad (4.46)$$

The first thing that we can see from equation (4.46) is that, if  $\psi(x, t)$  is a stationary state, the integral will be purely real, and thus, the change in probability density will be 0, just as we would expect. If we now consider that  $V(x)$  is always real, we can isolate the kinetic energy term in  $\hat{H}$  to obtain:

$$j_b - j_a = \frac{\hbar}{m} \Im \int_a^b \bar{\psi} \frac{\partial^2 \psi}{\partial x^2} dx \quad (4.47)$$

We can evaluate this integral by parts in order to obtain the result that:

$$j_b - j_a = \frac{\hbar}{2m} \left[ \bar{\psi} \frac{\partial \psi}{\partial x} - \psi \frac{\partial \bar{\psi}}{\partial x} \right]_a^b \quad (4.48)$$

Thus we obtain the general expression for the particle flux as being:

$$j = \frac{\hbar}{2m} \left[ \bar{\psi} \frac{\partial \psi}{\partial x} - \psi \frac{\partial \bar{\psi}}{\partial x} \right] \quad (4.49)$$

Now with something like the particle flux, there is always a slight ambiguity with regards to an additive constant, since this would have no impact on any measurable changes in probability density. However, since we would expect the flux to be 0, when the particle's momentum is equal to zero, it seems reasonable to use (4.9) as our expression for flux. Luckily, we can see that this is entirely consistent with equation (4.9) in section 2.2, which we derived for the special case of a definite momentum state.

Importantly, we can note that the expression for the flux is non-linear in  $\psi$ . That is to say that, if  $\psi$  can be represented as some linear combination of  $\xi$  and  $\chi$ , this does not imply that the resultant flux is given by the linear combination of the two fluxes.

$$\psi = a\xi + b\chi \Rightarrow j_\psi = aj_\xi + bj_\chi \quad (4.50)$$

## 4.5 Potential Wells

We are now going to apply the ideas we have been developing to a few simple examples. In each case, we shall start by introducing the potential energy function  $V(x)$ , and then solving the Hamiltonian eigenvalue problem for the stationary states. Importantly, we shall see that, confining a particle to a potential well restricts it to a set of quantised energy levels.

### 4.5.1 The Infinite Square Well

The first potential well we shall look at is the infinite square well, sometimes referred to as a particle in a box. This potential well represents a particle confined, such that it can only be found within a certain finite region. The potential energy function is given by:

$$V(x) = \begin{cases} 0 & x \in [-\frac{L}{2}, \frac{L}{2}] \\ \infty & \text{elsewhere} \end{cases} \quad (4.51)$$

Obviously, the infinite potential energy is not something that can actually be well defined, and strictly speaking, we should consider this as a limiting case of the finite potential well, that we shall consider in the next section. For now, we shall simply use this potential as given, whilst remembering that strictly speaking we are only considering the limiting behaviour of the wave function. This brings us to our eigenvalue equation:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x) = E\psi(x) \quad (4.52)$$

In order for this to be possible with a finite value of  $E$ , we must have  $\psi(x) = 0$  for all  $x$  where  $V(x) = \infty$ . In physical terms, what we are saying is that, the particle can not be found in a region of infinite potential energy, without itself having infinite energy. Furthermore, if we want the Hamiltonian to have a finite eigenvalue,  $\frac{\partial^2 \psi}{\partial x^2}$  must be finite everywhere, which implies that both the wave function and its first derivative must be continuous. As such, in order to maintain continuity, the wave function must go to zero at  $x = \pm \frac{L}{2}$ . There is however a slight subtlety here, since the discontinuity in the potential is itself infinite, we are allowed to have a discontinuity in  $\frac{\partial \psi}{\partial x}$  at the boundary, a fact that can only be verified by taking the limit of the case described in section 4.5.2. Within the well our eigenvalue equation reduces to:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi(x) = 0 \quad (4.53)$$

This is nothing more than the simple harmonic motion equation and can be fairly easily solved, subject to the boundary conditions, in order to give the appropriately normalised wave functions:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & x \in [-\frac{L}{2}, \frac{L}{2}] \quad n \text{ odd} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & x \in [-\frac{L}{2}, \frac{L}{2}] \quad n \text{ even} \\ 0 & \text{elsewhere} \end{cases} \quad (4.54)$$

Where  $n$  is a positive integer, often called a quantum number, because it identifies the quantum state of the particle. We can see from this result that the only possible energies for the particle to possess are given by the general form:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad n \in \mathbb{Z}^+ \quad (4.55)$$

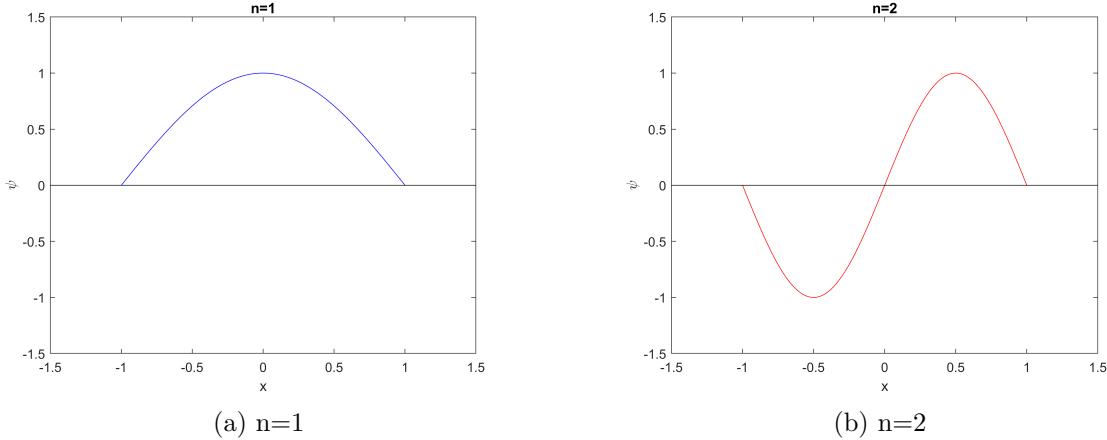


Figure 4.6: The ground and first excited states of a particle in an infinite square well.

As we can see in figure 4.6, which shows the first two energy eigenstates, the wave functions we have derived can all be classed as even or odd functions. This turns out to be a general principle that, if the potential is symmetric, then, assuming non degenerate eigenvalues, all of the stationary states will be either symmetric or antisymmetric with respect to the origin. Mathematically, this can be fairly simply proven by noting that, if  $V(x) = V(-x)$ , the entire Hamiltonian is unchanged by the inversion of  $x$ . As such, if  $\psi(x)$  is a solution with energy  $E$ ,  $\psi(-x)$  must be as well. If each energy level is non degenerate, then this must mean that  $\psi(x)$  and  $\psi(-x)$  differ only by a constant factor, and since  $\psi(-(-x)) = \psi(x)$  this factor can only be either 1 or -1. Physically speaking, this makes sense, since in both cases,  $\bar{\psi}\psi$  will have the same symmetry as its bounding potential, which is precisely what we would expect. In the case of a degenerate energy level, this will not hold true of all possible eigenstates; however, we will always be able to construct a basis of symmetric and antisymmetric eigenstates within that energy level.

The final thing worth noting about these solutions is that, in the limit as the energy (and hence  $n$ ) goes to infinity, the probability density fluctuates so quickly across the length of the well, that for all intents and purposes it simply averages out into a uniform distribution. This is exactly what we would predict classically, if we simply confined a particle with non-zero momentum to a box, and indeed, it is a general trend in quantum mechanics that the classical result is simply a limiting case of the quantum one.

### 4.5.2 The Finite Square Well

This now brings us on to the finite square well, which is essentially just a generalisation of the previous potential. In this case, a particle is still confined within a box; however, this time, the walls of the box only offer a finite potential barrier. For simplicity, we shall only consider the symmetric case, where:

$$V(x) = \begin{cases} 0 & x \in [-\frac{L}{2}, \frac{L}{2}] \\ V_0 & \text{elsewhere} \end{cases} \quad (4.56)$$

Furthermore, we shall only look for bound states with  $E < V_0$ , since the unbound states form a continuous spectrum, and are essentially just free particle states. As such, our Hamiltonian eigenvalue equation becomes:

$$\frac{\partial^2 \psi}{\partial x^2} = \begin{cases} -\frac{2mE}{\hbar^2} \psi(x) & x \in [-\frac{L}{2}, \frac{L}{2}] \\ \frac{2m[V_0-E]}{\hbar^2} \psi(x) & \text{elsewhere} \end{cases} \quad (4.57)$$

If we use the results about the parity from section 5.1, we can make life a bit easier for ourselves by looking specifically for even and odd solutions. If we first consider even solutions, we obtain:

$$\psi_+(x) = \begin{cases} A \cos kx & x \in [-\frac{L}{2}, \frac{L}{2}] \\ Be^{-\kappa x} & x > \frac{L}{2} \\ Be^{\kappa x} & x < -\frac{L}{2} \end{cases} \quad (4.58)$$

Where  $\kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}$ , and the constants  $A$  and  $B$  are determined by imposing the normalisation and continuity conditions on the wave function. We have discarded any exponentially growing solutions, since they would be impossible to normalise. The energy of this state is given by:

$$E = \frac{\hbar^2 k^2}{2m} \quad (4.59)$$

If we now require that both the wave function and its derivative are continuous at both boundaries we obtain the restriction that:

$$\kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2} = k \tan\left(\frac{kL}{2}\right) \quad (4.60)$$

Unfortunately this equation has no analytic solution for  $k$ ; however, we can see graphically in figure 4.7 that there will only be a finite number of solutions, and hence, only a finite number of bound states, and thus quantised energy levels. However we can see that, no matter what the value of  $V_0$  is, there will always be at least one bound state. This ground state is shown in figure 4.8 (a).

We can now repeat this analysis for odd solutions. In this case we obtain a solution with the general form:

$$\psi_-(x) = \begin{cases} A \sin kx & x \in [-\frac{L}{2}, \frac{L}{2}] \\ Be^{-\kappa x} & x > \frac{L}{2} \\ -Be^{\kappa x} & x < -\frac{L}{2} \end{cases} \quad (4.61)$$

Applying the continuity conditions to this solution then yields the restriction that:

$$\kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2} = -k \cot\left(\frac{kL}{2}\right) \quad (4.62)$$

Just as before, no analytic solution exists to equation (4.62), and so we have to resort to the graphical method in figure 4.7. We can see that, once again, only very specific values of  $k$  (and hence  $E$ ) are allowed. However, unlike the even states, if  $V_0$  is brought low enough, all of the odd states disappear. The critical value of  $V_0$  above which multiple bound states exist can be easily deduced from figure 4.7 and is given by:

$$V_{\text{crit}} = \frac{\hbar^2 \pi^2}{2mL^2} \quad (4.63)$$

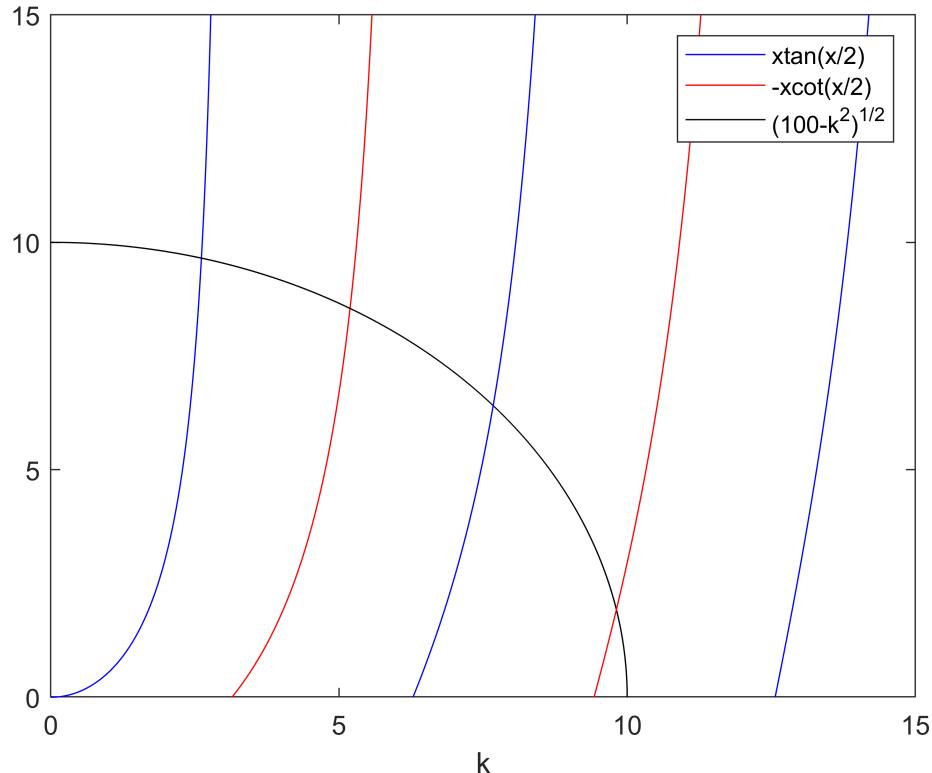


Figure 4.7: Plots of the functions from equations (4.60) and (4.62).

The ground state, and the first excited state are shown below in figure 4.8. We can see that the solutions of the finite well have a lot in common with those of the infinite well, with one key difference. In the finite well solutions, there is a non zero probability of finding the particle in the classically forbidden region, where it has more potential energy than total energy. This phenomenon is known as quantum tunnelling, and is the quantum analogue to a classical evanescent wave. Another interesting point to note is that, as the energy increases, the spacing between the energy levels decreases relative to the spacing in the infinite well. It turns out to be a fairly general trend for particles in finite wells that as they get closer to escaping and being able to access a full continuum of energies, the energy levels get closer together.

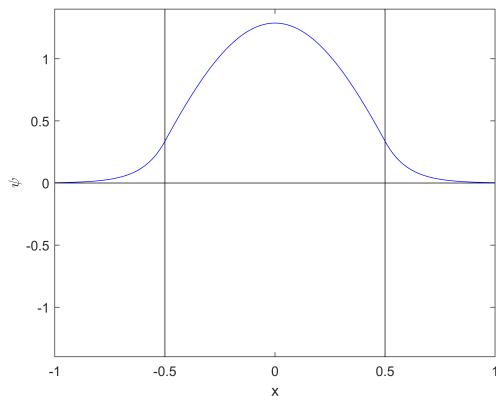
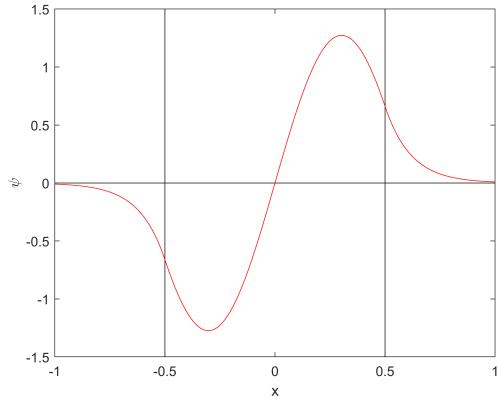
(a)  $n=1$ (b)  $n=2$ 

Figure 4.8: The ground and first excited states of a particle in a finite square well.

We may now notice a few general trends in the form of the wave functions we have seen so far. Firstly, we notice that as the energy increases the number of nodes (points for which  $\psi = 0$ ) increases as well. Qualitatively we can say that, this is because, the more nodes a wave function has, the more it has to change ‘direction’ and thus the larger its second derivative must be. This will result in the particle having more kinetic energy, as per the form of our Hamiltonian operator. A direct result of this is that in a symmetric potential, the ground state will normally be an even wave function, since the odd wave functions must always have at least one node.

Finally, it would be worth our time to check that in the limiting case of  $V_0 \rightarrow \infty$ , the behaviour of the finite well tends to that of the infinite well. This is indeed the case, since in this limit  $\kappa \rightarrow \infty$ , regardless of the value of  $k$ , and so all of the solutions occur at the vertical asymptotes on figure 4.7. This generates the regularly spaced sinusoidal solutions we saw in section 5.1. Furthermore, as  $\kappa \rightarrow \infty$ , the derivative of  $\psi$  outside the box itself becomes infinite. Thus, if continuity is to be maintained,  $\psi \rightarrow 0$  everywhere outside the box. This is precisely the behaviour that we saw in section 4.5.1.

### 4.5.3 The Step Barrier

This next potential is a little different, since it is not strictly speaking a potential well, and instead is simply a single barrier. For this reason, we shall not be considering a single particle, but instead a particle beam, directed towards the barrier. The potential takes the fairly simple form:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases} \quad (4.64)$$

Unlike the previous potentials, since we have not confined the particle to a well, it has a full spectrum of energies available to it. There are two distinct cases that we must consider in the analysis of this system. Firstly, let us consider the case when  $E > V_0$ . In this case, we would expect the particle beam to at least partially penetrate the barrier and it seems likely that some of the incident particle flux will be reflected. If we set up our eigenvalue problem it becomes:

$$\frac{\partial^2 \psi}{\partial x^2} = \begin{cases} -\frac{2mE}{\hbar^2} & x < 0 \\ -\frac{2m[E-V_0]}{\hbar^2} & x \geq 0 \end{cases} \quad (4.65)$$

Solving this gives us the following piecewise solution:

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x < 0 \\ Ce^{ik_2 x} & x \geq 0 \end{cases} \quad (4.66)$$

Where  $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$  and  $k_2 = \sqrt{k_1^2 - \frac{2mV_0}{\hbar^2}}$ . We have not included a left travelling beam in the second region, because we are assuming that after the barrier, the particles can continue on without being reflected backwards at some later point. This is a physical restriction imposed upon the solution rather than a mathematical one. Since we are considering a particle beam, the incident flux can be varied, and so there is no way to solve for all three constants  $A$ ,  $B$  and  $C$ . The best we can do is express  $B$  and  $C$  in terms of  $A$ . If we impose continuity of the wave function and its first derivative at  $x = 0$  we obtain:

$$\begin{aligned} A + B &= C & B &= \frac{k_1 - k_2}{k_1 + k_2} A \\ ik_1 A - ik_1 B &= ik_2 C & C &= \frac{2k_1}{k_1 + k_2} A \end{aligned} \quad (4.67)$$

We can use these relations, along with equation (4.49) in section 4.4.2 to calculate the fluxes on each side of the barrier. It is worth noting that, the left hand side is a special case, where the resultant flux is simply the sum of the fluxes of each constituent wave. As such, we can split it into an incident flux (corresponding to the right moving beam) and a reflected flux (corresponding to the left moving beam). If we let  $j_i$ ,  $j_r$ ,  $j_t$  represent the incident, reflected and transmitted fluxes respectively, we obtain:

$$j_r = -\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 j_i \quad j_t = \left(\frac{2k_1}{k_1 + k_2}\right)^2 j_i \quad (4.68)$$

We can see from these results that the total flux impinging on the barrier is equal to the total flux leaving the barrier, which is certainly a good thing, as otherwise we would somehow be either creating or destroying particles.

The second and arguably more interesting case arises when  $V_0 > E$ . In this case, we would not classically expect the beam to be able to penetrate the barrier. However, just as we saw with the finite square well, there will be a tunnelling effect, leading to some particle density collecting in the classically forbidden region. The eigenvalue problem and the solutions are more or less the same as before with:

$$\frac{\partial^2 \psi}{\partial x^2} = \begin{cases} -\frac{2mE}{\hbar^2} & x < 0 \\ \frac{2m[V_0-E]}{\hbar^2} & x \geq 0 \end{cases} \quad (4.69)$$

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x < 0 \\ Ce^{-\kappa x} & x \geq 0 \end{cases} \quad (4.70)$$

Where  $k_1$  is the same as before and  $\kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k_1^2}$ . We have discarded the exponentially growing solution, since it does not make sense physically for an essentially infinite particle density to collect in the classically forbidden region. We then perform the same analysis as before to determine  $B$  and  $C$  in terms of  $A$ , and find that:

$$\begin{aligned} A + B &= C \\ ik_1 A - ik_1 B &= -\kappa C \end{aligned} \implies \begin{aligned} B &= \frac{ik_1 + \kappa}{ik_1 - \kappa} A \\ C &= \frac{-2ik_1}{ik_1 + \kappa} A \end{aligned} \quad (4.71)$$

If we now calculate the fluxes, we find that the total flux is everywhere 0, that is to say that, although some particle density manages to penetrate the potential barrier, there is no flux of particles through the barrier. If we wished to tunnel a particle beam through such a barrier we would have to make the classically forbidden region of finite thickness, and then the evanescent wave could allow particles to travel to the other side of the barrier. This is the idea behind the phenomenon of frustrated total internal reflection, where a light ray passes through a glass surface despite being incident at an angle greater than the critical angle for that surface.

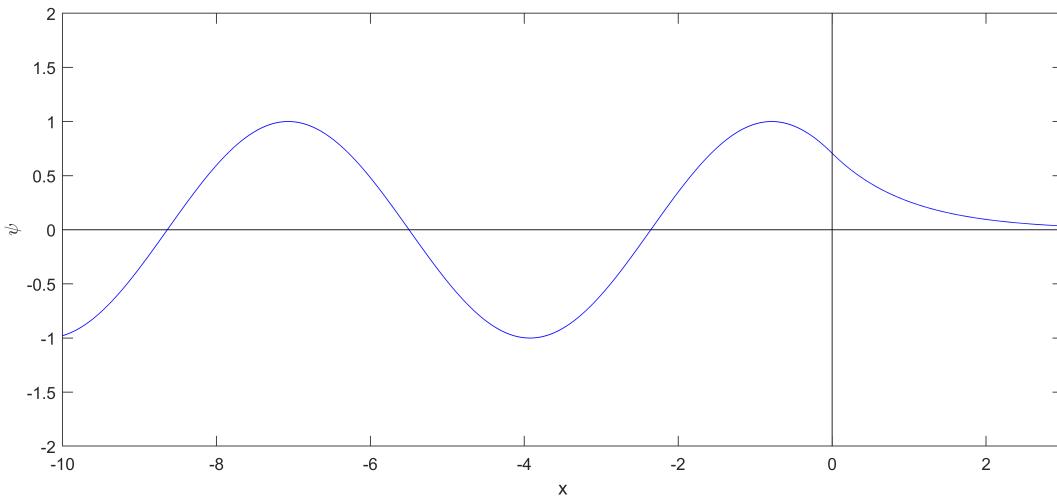


Figure 4.9: A particle beam impinging on a step barrier.

#### 4.5.4 The Parabolic Well

The final potential we will discuss in this section is that of the so called quantum harmonic oscillator. That is to say that, we will be looking at the quantum mechanical equivalent of a mass on a spring. Although this is by far the hardest system to solve out of those we have looked at so far, it is definitely the most useful. First of all, most potentials can be reasonably well approximated by a parabola, for small deviations from equilibrium, which gives this potential tremendous utility as a quick approximation to systems like vibrating molecules or phonons in a crystalline solid. In addition to this, quantum field theory is actually based on harmonic oscillator potentials, so it really is a crucial one to understand. We are going to be considering potentials of the form:

$$V(x) = \frac{m\omega^2}{2}x^2 \quad (4.72)$$

If we substitute this into the time independent Schrödinger equation we obtain the following eigenvalue problem:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{m\omega^2}{2}x^2\psi(x) = E\psi(x) \quad (4.73)$$

To simplify the algebra somewhat, we can use the process of nondimensionalisation to reduce equation (4.73) into a more usable form. First we divide through by  $\hbar\omega$ , and then we introduce the constant  $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ , in order to create the dimensionless variable  $u = \frac{x}{x_0}$ . Finally, we introduce the new function  $\xi(u) = \psi(ux_0)$  to rewrite the equation as:

$$-\frac{1}{2}\frac{\partial^2\xi}{\partial u^2} + \frac{1}{2}u^2\xi(u) = \frac{E}{\hbar\omega}\xi(u) \quad (4.74)$$

One of the neatest ways of solving this equation is by ‘factorising’ the operator on the left hand side into two separate operators, which are called ladder operators. Based on the form of the equation we might think to try and use the difference of two squares, which gives us:

$$\left(u + \frac{\partial}{\partial u}\right)\left(u - \frac{\partial}{\partial u}\right) = -\frac{\partial^2}{\partial u^2} + u^2 + 1 \quad (4.75)$$

$$\left(u - \frac{\partial}{\partial u}\right)\left(u + \frac{\partial}{\partial u}\right) = -\frac{\partial^2}{\partial u^2} + u^2 - 1 \quad (4.76)$$

If we now introduce the following operators, we can use these results to obtain the commutation relations:

$$\begin{aligned} \hat{H} &= \frac{1}{2} \left[ u^2 - \frac{\partial^2}{\partial u^2} \right] & \hat{A} &= u + \frac{\partial}{\partial u} & \hat{A}^\dagger &= u - \frac{\partial}{\partial u} \\ [\hat{A}, \hat{A}^\dagger] &= 2 & [\hat{H}, \hat{A}] &= -\hat{A} & [\hat{H}, \hat{A}^\dagger] &= \hat{A}^\dagger \end{aligned} \quad (4.77)$$

Let us now consider the effect of these operators on the eigenfunctions. If  $\xi(u)$  is an eigenfunction of  $\hat{H}$  with eigenvalue  $N$ , then we must have:

$$\hat{H}\xi(u) = N\xi(u) \quad (4.78)$$

If we multiply this by  $\hat{A}$ , and then apply the commutation relations in (4.77) we obtain the result that:

$$\hat{H}\hat{A}\xi(u) = (N - 1)\hat{A}\xi(u) \quad (4.79)$$

Therefore, we can conclude that  $\hat{A}\xi(u)$  is also an eigenfunction of the Hamiltonian, but with an eigenvalue that is lower by one. For this reason,  $\hat{A}$  is called a lowering operator. Physically, we would not expect there to exist an infinite number of negative energy states, which is a statement that can be proven mathematically as follows. If we wish for our function to be normalisable, then its derivative must tend towards 0 at  $\pm\infty$ . It therefore follows from the mean value theorem that, there exists a point at which  $\frac{\partial^2\xi}{\partial u^2} = 0$ . At this point,  $\hat{H}\xi(u) = u^2\xi(u)$ , and so if this is an eigenfunction, the eigenvalue must always be positive, since  $u^2 \geq 0$  for all  $u$ . The only way this can be the case, with the existence of  $\hat{A}^\dagger$ , is if there is some ground state  $\xi_0(u)$ , which is mapped to 0 by the lowering operator. This gives us the reasonably simple differential equation:

$$\frac{\partial\xi_0}{\partial u} + u\xi_0(u) = 0 \implies \xi_0(u) = Ce^{-\frac{u^2}{2}} \quad (4.80)$$

We can fairly easily plug this solution back into our eigenvalue equation to confirm that it is, in fact, an eigenfunction with an eigenvalue of  $\frac{1}{2}$ . We can now perform a similar style of analysis for the operator  $\hat{A}^\dagger$ . If, once again, we let  $\xi(u)$  be an eigenfunction we find that:

$$\hat{H}\xi(u) = N\xi(u) \implies \hat{H}\hat{A}^\dagger\xi(u) = (N + 1)\hat{A}^\dagger\xi(u) \quad (4.81)$$

For this reason,  $\hat{A}^\dagger$  is referred to as a raising operator. In order to avoid creating an infinite set of negative eigenstates, which we have shown to be impossible, all of the eigenfunctions must be generated by the repeated application of the raising operator on the ground state. Thus, we can give the  $n$ th eigenfunction, which has an eigenvalue of  $n + \frac{1}{2}$  with the general form:

$$\xi_n(u) = C_n\hat{A}^{\dagger n}\xi_0(u) \quad (4.82)$$

Where  $C_n$  is simply a normalisation constant. We can express this in a nicer analytic form by noting the following property of the raising operator:

$$u\xi(u) - \frac{\partial\xi(u)}{\partial u} = -e^{\frac{u^2}{2}}\frac{\partial}{\partial u}\left[e^{-\frac{u^2}{2}}\xi(u)\right] \quad (4.83)$$

Therefore, we obtain the result that:

$$\xi_n(u) = C_n e^{\frac{u^2}{2}} \frac{\partial^n e^{-u^2}}{\partial u^n} \quad (4.84)$$

We can now redimensionalise our solution, in order to obtain an expression for the energy of the  $n$ th eigenstate:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n \in \mathbb{Z}^{>0} \quad (4.85)$$

A few of these eigenstates are shown on the next page.

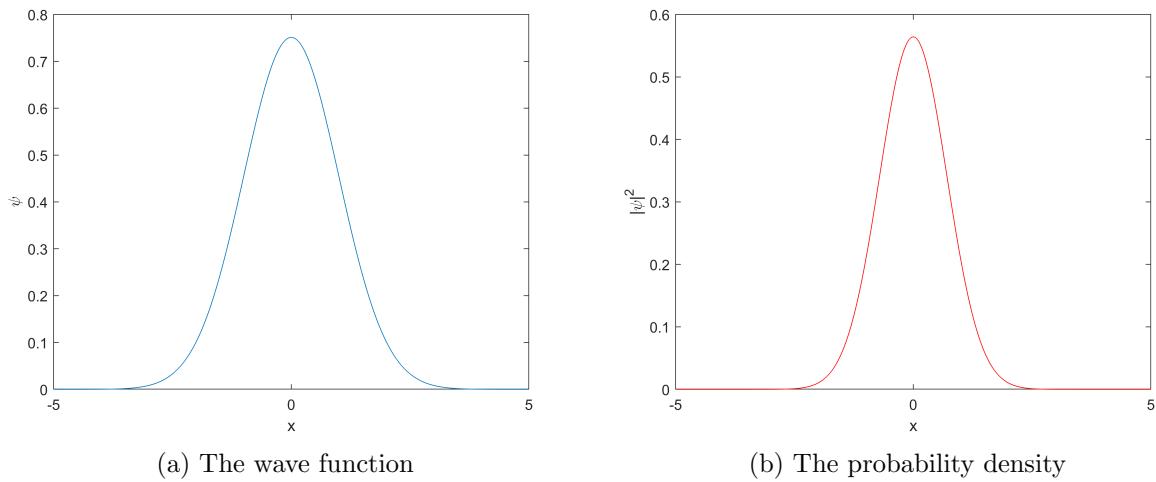


Figure 4.10: The ground state of a quantum harmonic oscillator.

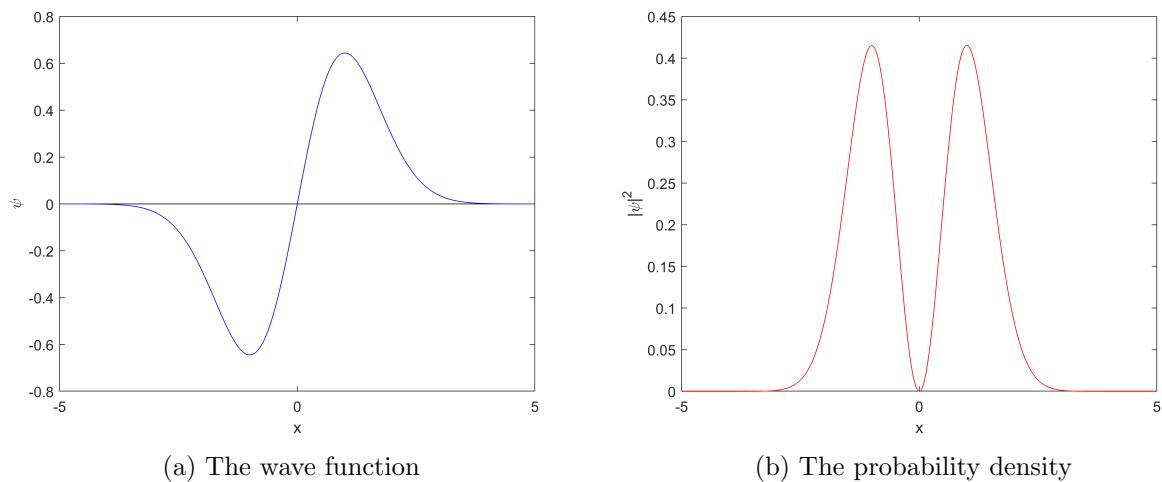


Figure 4.11: The first excited state of a quantum harmonic oscillator.

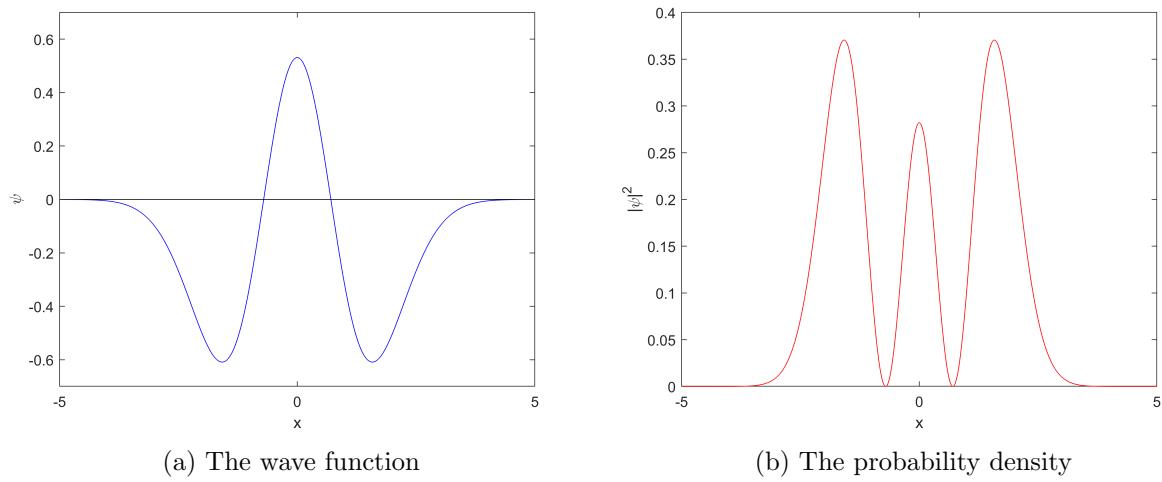


Figure 4.12: The second excited state of a quantum harmonic oscillator

# 5 Rotational Dynamics

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## 5.1 Angular Motion

Rotational mechanics is, in many ways, less of an exercise in understanding the underlying physics behind a system's behaviour, and more an exercise in mathematical manipulations. Everything that we shall discuss in this chapter follows directly from Newton's laws of motion, and as such, we are not really introducing any new physical principles. Nonetheless, the techniques that we shall develop for analysing rotating systems, are truly invaluable in our description of classical dynamics.

### 5.1.1 Angular Momentum

We shall begin our discussion of angular motion by introducing the concept of an angular momentum. As we shall see, many of the laws of rotational motion take essentially the same form as those of linear motion that we have already encountered, with every linear quantity having a corresponding angular equivalent. Perhaps unsurprisingly, the angular momentum, serves as the rotational equivalent to the linear momentum. By definition, the angular momentum of a point mass, with position  $\mathbf{r}$  and momentum  $\mathbf{p}$ , relative to some specified origin, is given by:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad (5.1)$$

We should note that there is an inherent ambiguity in this definition, since the actual value of  $\mathbf{L}$  is dependent on exactly which point in space we choose to be our origin. In fact, this is nothing new, we have already seen how the velocity of a frame of reference can impact the value of the linear momentum, it simply turns out that the angular momentum is sensitive to both the position and velocity of a coordinate system's origin.

We can now extend this definition to an arbitrary system of masses in motion, by simply summing up the contributions to the total angular momentum from each individual mass element. In the case of a continuous system, this summation then becomes an integral over all of the systems mass. This gives us:

$$\mathbf{L}_{\text{tot}} = \sum_{i=1}^n \mathbf{r}_i \times \mathbf{p}_i = \sum_{i=1}^n m_i (\mathbf{r}_i \times \dot{\mathbf{r}}_i) = \int_V \rho(\mathbf{r} \times \mathbf{v}) dV \quad (5.2)$$

Where  $\mathbf{r}_i$  and  $\mathbf{p}_i$  are the position and momentum of the  $i$ th mass respectively, and  $\rho$  represents the density of our continuous body at position  $\mathbf{r}$ . The region of integration  $M$  implies that the integral is to be evaluated over the region of space, which contains all the mass of the system in question. It follows directly from these expressions, that the angular momentum can be given by:

$$\mathbf{L}_{\text{tot}} = \mathbf{L}^* + \mathbf{r}_{\text{CM}} \times \mathbf{p}_{\text{tot}} \quad (5.3)$$

Where the quantity  $\mathbf{L}^*$  represents the angular momentum of the system about its centre of mass, and  $\mathbf{r}_{\text{CM}}$  is the position of the system's centre of mass. This is a consequence of the fact that, by definition:

$$\int_M \rho(\mathbf{r} - \mathbf{r}_{\text{CM}}) dV = \mathbf{0} \quad \int_M \rho(\mathbf{v} - \dot{\mathbf{r}}_{\text{CM}}) dV = \mathbf{0} \quad (5.4)$$

### 5.1.2 Torque

Let us now consider how the angular momentum varies with time. Just as before, we shall start by considering a single point mass, with angular momentum given by  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ . We can differentiate with respect to time in order to obtain:

$$\dot{\mathbf{L}} = \mathbf{r} \times \dot{\mathbf{p}} + \dot{\mathbf{r}} \times \mathbf{p} \quad (5.5)$$

Now since  $\mathbf{p} = m\dot{\mathbf{r}}$ , we can say that the cross product of velocity with momentum will always be identically zero. If we then substitute in Newton's second law,  $\mathbf{F} = \dot{\mathbf{p}}$  we can obtain the result:

$$\dot{\mathbf{L}} = \mathbf{r} \times \mathbf{F} \quad (5.6)$$

This quantity  $\mathbf{r} \times \mathbf{F}$  is referred to as the torque produced by  $\mathbf{F}$ , and is often denoted by  $\mathbf{G}$ . This relationship is at the heart of the similarities between angular and linear motion, since it is directly analogous to Newton's second law. As we might expect, there is an inherent ambiguity in the torque, dependent on the location of the origin. Luckily, this does not cause any problems, since the angular momentum possesses exactly the same ambiguity. This can be generalised to composite or continuous systems through a sum, or an integral respectively.

$$\mathbf{G}_{\text{tot}} = \dot{\mathbf{L}}_{\text{tot}} = \sum_{i=1}^n \mathbf{r}_i \times \mathbf{F}_i = \int_V \mathbf{r} \times \mathbf{f} dV \quad (5.7)$$

Where  $\mathbf{r}_i$  is the position through which the  $i$ th force  $\mathbf{F}_i$  acts, and  $\mathbf{f}$  represents the force per unit volume experienced by the body.

The torque transformation law for converting between different origins is given by equation (5.10) below:

$$\mathbf{G}_{\text{tot}} = \mathbf{G}^* + \mathbf{r}_{\text{CM}} \times \mathbf{F}_{\text{tot}} \quad (5.8)$$

Where  $\mathbf{G}^*$  is the total torque acting on the system, evaluated about its centre of mass. This result implies that, if there is no resultant force acting on an object, the torque it experiences will be the same, independent of our choice of origin.

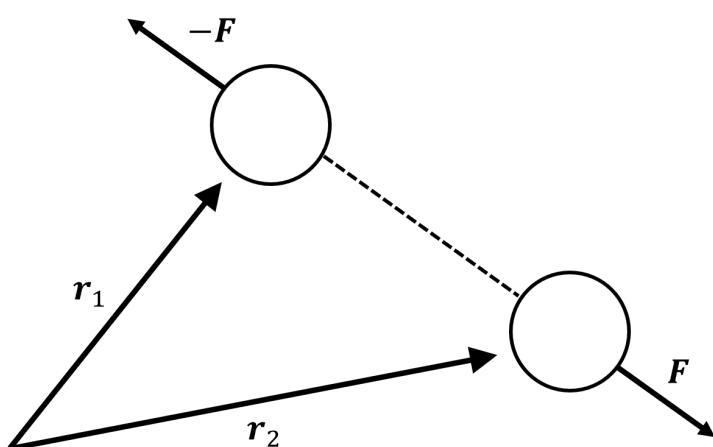


Figure 5.1: The pairwise interaction between two bodies.

Let us now consider the interaction between two isolated bodies, as shown in figure 5.1. If we assume that the force between the two bodies depends only on their positions, then it follows from symmetry that the forces acting on each of them must be parallel to  $\mathbf{r}_2 - \mathbf{r}_1$ . This, together with Newton's third law leads to the conclusion that:

$$\mathbf{G}_1 = -\mathbf{G}_2 \quad (5.9)$$

Thus, for an isolated system, which experiences no external torques, its total angular momentum must be a conserved quantity.

### 5.1.3 Circular Motion

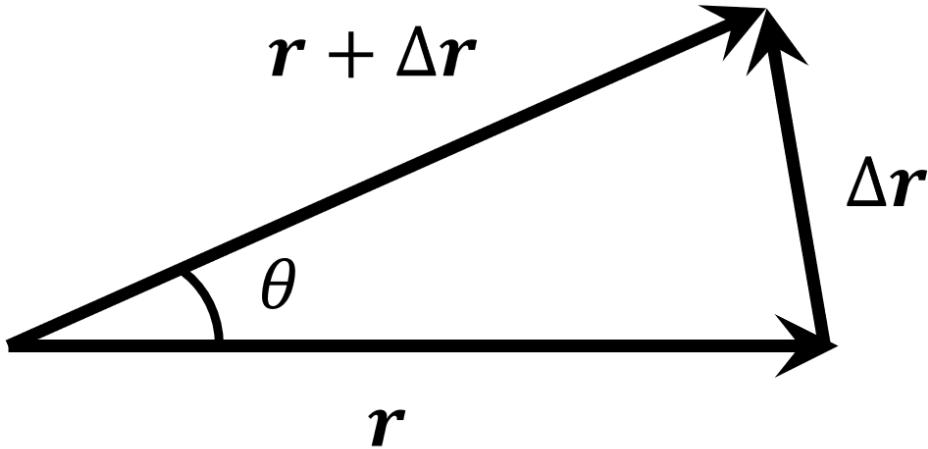


Figure 5.2: A vector  $\mathbf{r}$  being rotated through an angle  $\theta$  about an axis that emerges perpendicularly from the page.

Circular motion is the description given to any extended body rotating about some fixed axis. As we can see from figure 5.2, rotating an arbitrary vector  $\mathbf{r}$  through an angle  $\theta$  will give us a new vector  $\mathbf{r} + \Delta\mathbf{r}$ , where the displacement is given by:

$$\Delta\mathbf{r} = (\cos \theta - 1)(\mathbf{r} - (\hat{\mathbf{n}} \cdot \mathbf{r})\hat{\mathbf{n}}) + (\sin \theta)\hat{\mathbf{n}} \times \mathbf{r} \quad (5.10)$$

Where  $\hat{\mathbf{n}}$  is the unit vector along the axis of rotation. There is a sign ambiguity in the direction of  $\hat{\mathbf{n}}$ , since it could point in either direction along this axis, as such, we adopt a right handed convention, meaning that the direction of rotation is determined by a right handed corkscrew rule. To extract something useful from these equations, let us consider the limit as  $\theta$  becomes infinitesimally small. In this limit we find that, to first order:

$$d\mathbf{r} = d\theta \times \mathbf{r} \quad (5.11)$$

Where  $d\theta = \hat{\mathbf{n}}d\theta$ . If we identify the angular velocity of this motion to be given by  $\boldsymbol{\omega} = \frac{d\theta}{dt}$ , we obtain the defining equation of circular motion:

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r} \quad (5.12)$$

Implicitly in this equation, we have assumed that the axis of rotation passes through the origin, since only an on axis position can have zero velocity. Modifying this equation to allow for an arbitrary origin is reasonably straightforward, and gives us:

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r} + \boldsymbol{\omega} \times \mathbf{R} \quad (5.13)$$

Where  $\mathbf{R}$  represents the position of the origin relative to some point on the axis of rotation. Physically, we can interpret this result to mean that any extended body undergoing circular motion, is simply rotating about its centre of mass, whilst the centre of mass itself is performing circular motion about the axis of rotation.

### 5.1.4 The Moment of Inertia

Let us now consider the angular momentum of a rigid body undergoing rotational motion, in the manner we have just described. We know that the total angular momentum can be calculated by evaluating the integral:

$$\mathbf{L} = \int_V \rho[\mathbf{r} \times \mathbf{v}]dV = - \int_V \rho[\mathbf{r} \times (\mathbf{r} \times \boldsymbol{\omega})]dV \quad (5.14)$$

In order for us to analyse this integral, we are first going to consider the different ways in which we can represent the action of the vector cross product. It turns out that, in this case, the best representation is to use matrix multiplication for each of the components. We can do this by noting that:

$$\mathbf{r} \times \boldsymbol{\omega} = [\mathbf{r}]\boldsymbol{\omega} = \begin{pmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix} \quad (5.15)$$

The skew symmetric matrix  $[\mathbf{r}]$  is known as the Hodge dual of  $\mathbf{r}$ . Although the concept of the Hodge dual can be generalised, this specific relationship between a vector and a matrix only exists in three dimensional space, which is why the cross product only applies to three dimensional vectors. Since matrix multiplication is associative, it follows that we can represent the vector triple product in (5.14) with:

$$\mathbf{r} \times (\mathbf{r} \times \boldsymbol{\omega}) = [\mathbf{r}]^2 \boldsymbol{\omega} \quad (5.16)$$

Where  $[\mathbf{r}]^2$  is the symmetric matrix that is produced when  $[\mathbf{r}]$  is multiplied by itself. Furthermore, since matrix multiplication is distributive over addition, we can factor  $\boldsymbol{\omega}$  out of the integral, and rewrite equation (5.14) in the form:

$$\mathbf{L} = \left( - \int \rho[\mathbf{r}]^2 dV \right) \boldsymbol{\omega} = \mathcal{I}\boldsymbol{\omega} \quad (5.17)$$

Where  $\mathcal{I}$  is referred to as the body's moment of inertia, and is given by equation (5.18) below. This gives the rather unintuitive result that the angular momentum and angular velocity are not necessarily parallel to one another, in stark contrast to their linear equivalents.

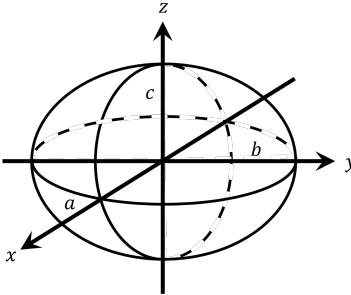
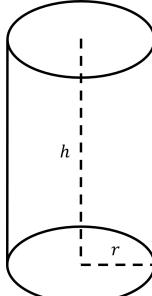
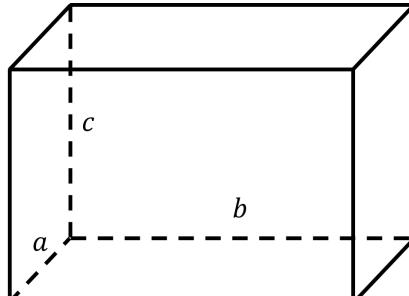
$$\mathcal{I} = - \int \rho[\mathbf{r}]^2 dV = \int \rho \begin{pmatrix} y^2 + z^2 & -xy & -xz \\ -xy & x^2 + z^2 & -yz \\ -xz & -yz & x^2 + y^2 \end{pmatrix} dV \quad (5.18)$$

Due to the symmetry of the inertia matrix, it will always be possible to pick a set of coordinate axes that diagonalize the inertia matrix, as shown below. These are referred to as the principal axes of the body and represent axes of rotation for which the angular momentum does align with the angular velocity. For this reason, the principle axes often tend to have symmetry operations associated with them, since this often helps the off axis contributions to the angular momentum to cancel out.

$$\mathcal{I} = \begin{pmatrix} I_x & 0 & 0 \\ 0 & I_y & 0 \\ 0 & 0 & I_z \end{pmatrix} \quad (5.19)$$

Table 5.1 below provides a few simple geometric shapes together with their corresponding inertia matrices. For simplicity, these moments of inertia are all evaluated with respect to the shape's principle axes and with the origin located at the centre of mass.

Table 5.1: The moments of inertia for common geometric shapes.

	$\mathcal{I} = \frac{m}{5} \begin{pmatrix} b^2 + c^2 & 0 & 0 \\ 0 & a^2 + c^2 & 0 \\ 0 & 0 & a^2 + b^2 \end{pmatrix}$
	$\mathcal{I} = \frac{m}{12} \begin{pmatrix} 3r^2 + h^2 & 0 & 0 \\ 0 & 3r^2 + h^2 & 0 \\ 0 & 0 & 6r^2 \end{pmatrix}$
	$\mathcal{I} = \frac{m}{12} \begin{pmatrix} b^2 + c^2 & 0 & 0 \\ 0 & a^2 + b^2 & 0 \\ 0 & 0 & a^2 + b^2 \end{pmatrix}$

One important fact to note is that, if all three of the principle axes have equivalent components in the inertia matrix, the moment of inertia will be completely isotropic, and thus, the angular momentum will always be parallel to the angular velocity. In the case of a sphere this is not really surprising, since we know that every axis through the centre of a sphere must be identical; however, it is not immediately obvious that the same should hold true for a cube.

### 5.1.5 The Parallel Axis Theorem

It should not come as a surprise to us that a system's moment of inertia depends on the origin which it is measured with respect to. As such, we shall now derive a result known as the parallel axis theorem, which allows us to convert the moment of inertia from one origin to another. Let us start by considering the moment of inertia evaluated about the system's centre of mass:

$$\mathcal{I}^* = - \int_V \rho[\mathbf{r} - \mathbf{r}_{CM}]^2 dV \quad (5.20)$$

Since the mapping between a vector and its Hodge dual is linear, it follows directly from the definition of the centre of mass, that we must have:

$$\int_V \rho[\mathbf{r}]dV = [\mathbf{r}_{CM}] \int_V \rho dV = M_{tot}[\mathbf{r}_{CM}] \quad (5.21)$$

We can now expand out the matrix multiplication in equation (5.20), and substitute in this result, to deduce that the moment of inertia about an arbitrary origin is given by:

$$\mathcal{I} = - \int_V \rho[\mathbf{r}]^2 dV = \mathcal{I}^* - M_{tot}[\mathbf{r}_{CM}]^2 \quad (5.22)$$

Where  $\mathbf{r}_{CM}$  is the position of the body's centre of mass, and  $M_{tot}$  is its total mass. This result is known as the parallel axis theorem, because while we may have shifted the origin of our coordinate system, the directions of the axes remain unchanged. As such, it will also be necessary to perform an additional rotation of the coordinate axes, if we wish to keep them aligned with the principle axes of the system.

The parallel axis theorem is in keeping with the general trend we have been seeing, that the motion of a system can always be split into the motion of its centre of mass and its own motion about its centre of mass.

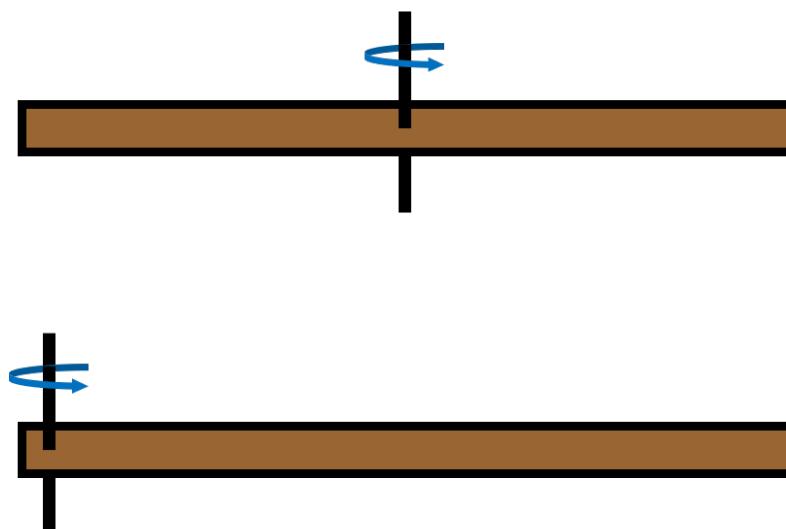


Figure 5.3: A shift in the origin in the case of a rotating rod.

### 5.1.6 Work and Energy

We are now going to consider how work and energy can be calculated for a rotating system. As it turns out, the expressions we shall arrive at are very similar in form to those in linear mechanics, with all of the linear quantities exchanged for their angular equivalents.

#### 5.1.6.1 Work Done by a Torque

We already know that the work done by a force when it moves through an infinitesimal displacement  $d\mathbf{r}$ , is given by:

$$dW = \mathbf{F} \cdot d\mathbf{r} \quad (5.23)$$

Now we can recall from section 5.1.3 that, when an object undergoing circular motion rotates through an infinitesimal angle  $d\theta$ , the displacement of any given point is  $d\mathbf{r} = d\theta \times \mathbf{r}$ . If we substitute this into equation (5.23), and apply the scalar triple product identity, we obtain:

$$dW = \mathbf{F} \cdot (d\theta \times \mathbf{r}) = (\mathbf{r} \times \mathbf{F}) \cdot d\theta \quad (5.24)$$

If we recognise that  $\mathbf{r} \times \mathbf{F}$  is, in fact, nothing more than the torque produced by that force, we can express the work done in the form:

$$dW = \mathbf{G} \cdot d\theta \quad (5.25)$$

#### 5.1.6.2 Kinetic Energy

Let us consider a rigid body undergoing circular motion in the manner we have just been describing. The total kinetic energy of the rotating body will then be given by:

$$T = \frac{1}{2} \int_V \rho(\mathbf{v} \cdot \mathbf{v}) dV = \frac{1}{2} \int_V \rho(\boldsymbol{\omega} \times \mathbf{r}) \cdot (\boldsymbol{\omega} \times \mathbf{r}) dV \quad (5.26)$$

We can now apply the scalar triple product identity to the integrand in equation (5.23), in order to obtain:

$$T = -\frac{\boldsymbol{\omega}}{2} \cdot \int_V \rho[\mathbf{r} \times (\mathbf{r} \times \boldsymbol{\omega})] dV = \frac{\boldsymbol{\omega} \cdot \mathcal{I}\boldsymbol{\omega}}{2} = \frac{\boldsymbol{\omega} \cdot \mathbf{L}}{2} \quad (5.27)$$

If we now consider the general case of a rigid body, moving with a centre of mass velocity  $\mathbf{v}_{CM}$ , and rotating about its centre of mass with an angular velocity of  $\boldsymbol{\omega}$ , we find that since any object's total momentum about its centre of mass is zero, the total kinetic energy is given by:

$$T = \frac{\mathbf{v}_{CM} \cdot \mathbf{p}_{tot} + \boldsymbol{\omega} \cdot \mathbf{L}^*}{2} \quad (5.28)$$

Where as before  $\mathbf{L}^*$  represents the angular momentum, measured about the system's centre of mass. Once again, we can see that the motion of an object's centre of mass, and its rotation about that centre of mass, are entirely separable.

## 5.2 Rotating Frames

In this section, we are going to be discussing non-inertial reference frames, with a particular emphasis on frames which are undergoing circular motion. A frame of reference is nothing more than a set of axes with which we can measure the coordinates of any given point in space. In an inertial frame, these axes remain fixed in place, although the origin may move at some fixed velocity. In a rotating frame however, the axes themselves move around the origin, in such a way that the coordinates of any objects undergoing circular motion about that origin remain fixed. Adopting a rotating frame can be particularly useful for a variety of reasons, not least of which is that as a consequence of the Earth's rotation, we actually live our lives in a rotating frame of reference.

### 5.2.1 Fictitious Forces

In any frame of reference, we must have a set of basis vectors  $\vec{e}_i$ , with which we can measure the coordinates of any given vector. In addition to this, we must have some origin  $\vec{o}$ , which all positions are measured relative to. That is to say that the position vector  $\mathbf{x}$  can be expressed in terms of its components as:

$$\mathbf{x} = \vec{o} + x_1\vec{e}_1 + x_2\vec{e}_2 + x_3\vec{e}_3 \quad (5.29)$$

From here, it is important that we establish the existence of two distinct ways in which we can differentiate the vector  $\mathbf{x}$ , with respect to time. The first is the coordinate derivative, denoted by  $\mathbf{x}'$ , which represents the velocity of  $\mathbf{x}$  relative to the frame in question. The second, denoted by  $\dot{\mathbf{x}}$ , is the coordinate free derivative, which represents the actual velocity of the vector. Since this derivative is independent of the reference frame, it is in terms of this derivative that physical laws, such as  $\mathbf{F} = m\mathbf{a}$ , must be expressed. In terms of the components, the derivatives are given by:

$$\begin{aligned} \mathbf{x}' &= \frac{dx_1}{dt}\vec{e}_1 + \frac{dx_2}{dt}\vec{e}_2 + \frac{dx_3}{dt}\vec{e}_3 \\ \dot{\mathbf{x}} &= \frac{d\vec{o}}{dt} + \frac{dx_1}{dt}\vec{e}_1 + x_1\frac{d\vec{e}_1}{dt} + \frac{dx_2}{dt}\vec{e}_2 + x_2\frac{d\vec{e}_2}{dt} + \frac{dx_3}{dt}\vec{e}_3 + x_3\frac{d\vec{e}_3}{dt} \end{aligned} \quad (5.30)$$

In a rotating frame, with angular velocity  $\boldsymbol{\omega}$ , the time derivatives of the basis vectors are simply given by:

$$\frac{d\vec{e}_i}{dt} = \boldsymbol{\omega} \times \vec{e}_i \quad (5.31)$$

Thus, it follows that the true velocity of an object can be expressed in terms of its coordinate velocity and position by:

$$\dot{\mathbf{x}} = \frac{d\vec{o}}{dt} + \mathbf{x}' + \boldsymbol{\omega} \times (\mathbf{x} - \vec{o}) \quad (5.32)$$

If we differentiate (5.32) again to obtain the acceleration, and also restrict ourselves to frames in which the origin is inertial, meaning that  $\frac{d^2\vec{o}}{dt^2} = \mathbf{0}$ , we obtain the following expression:

$$\ddot{\mathbf{x}} = \mathbf{x}'' + 2\boldsymbol{\omega} \times \mathbf{x}' + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times (\mathbf{x} - \vec{o})) + \frac{d\boldsymbol{\omega}}{dt} \times (\mathbf{x} - \vec{o}) \quad (5.33)$$

Substituting this into Newton's second law, and introducing the vector  $\mathbf{r} = \mathbf{x} - \vec{\mathbf{o}}$ , which represents the object's displacement from the origin, we obtain:

$$\mathbf{F} - m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) - 2m\boldsymbol{\omega} \times \mathbf{r}' - m \frac{d\boldsymbol{\omega}}{dt} \times \mathbf{r} = m\mathbf{r}'' \quad (5.34)$$

The additional terms on the left hand side of the equation are known as fictitious forces, because they do not arise from any physical interaction, whilst they still cause a coordinate acceleration that can be measured in the rotating frame. It is worth remembering that although, in principle, we could always describe a system in terms of an inertial frame, which does not feature any fictitious forces, it can often be easier to use a rotating frame instead. We can separate out the fictitious forces into three distinct components, which are summarised below:

$$\mathbf{F}_{\text{centrifugal}} = -m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) \quad \mathbf{F}_{\text{Coriolis}} = -2m\boldsymbol{\omega} \times \mathbf{r}' \quad \mathbf{F}_{\text{Euler}} = -m \frac{d\boldsymbol{\omega}}{dt} \times \mathbf{r} \quad (5.35)$$

The dynamics of an object in a rotating frame can then be analysed in exactly the same manner as they would be in an inertial frame, by replacing the resultant force with the sum of all the physical and fictitious forces acting on the object.

The first fictitious force in (5.34) is called the centrifugal force and it represents the fact that, an inwards centripetal force is required to keep an object moving in a circular path instead of flying off in a straight line. The centrifugal force manifests itself in a variety of ways. One such example is the shape of the Earth; although gravity tries to compact the Earth into a sphere, the centrifugal force causes it to bulge outwards around the equator, thus making the Earth an oblate spheroid. This is the same effect that is utilised in a centrifuge, which uses the dependence of the centrifugal force on an object's mass to separate mixtures by their density.

The second is the fictitious Coriolis force, which depends on the velocity of an object relative to the rotating frame. This effect arises to compensate for the fact that a constant velocity in the rotating frame is constantly accelerating when measured in an inertial frame. The Coriolis effect can be seen when a ball is dropped at the equator, it will appear to be deflected eastwards, in the direction of the Earth's rotation, as it falls to the ground. We can understand this by noting that in an inertial frame, the ball was already undergoing circular motion in order to keep up with the Earth's rotation. Then as it fell, the ball's angular velocity must have increased in order to conserve angular momentum. As such, it would land ahead of the point it was dropped from, in the direction of the rotation.

The final inertial effect is the Euler force, which only comes into play if the angular velocity of the rotating frame is itself accelerating. This effect represents the fact that an object would need to experience a tangential force in order to increase its angular velocity and keep pace with the accelerating frame. The Euler force is no different in origin to the fictitious force that throws passengers forwards when a car brakes suddenly, and like all fictitious forces, arises a consequence of an object's inertia.

### 5.2.2 Euler's Equations

One of the major sources of difficulty when analysing the behaviour of a rigid body is that in general, the moment of inertia changes as the body rotates. This can be avoided by adopting the rotating frame of the body itself, in which the components of the inertia matrix remain constant. If we take the derivative of the angular momentum we obtain:

$$\mathbf{G} = \dot{\mathbf{L}} = \mathbf{L}' + \boldsymbol{\omega} \times \mathbf{L} \quad (5.36)$$

If we now substitute in  $\mathbf{L} = \mathcal{I}\boldsymbol{\omega}$ , and recall that, in this frame,  $\mathcal{I}' = \mathbf{0}$ , we obtain the following equation:

$$\mathbf{G} = \mathcal{I}\boldsymbol{\omega}' + \boldsymbol{\omega} \times \mathcal{I}\boldsymbol{\omega} \quad (5.37)$$

If we now express this in component form, with respect to the principle axes of the body, we obtain Euler's equations for the motion of a rigid body:

$$\begin{aligned} G_1 &= I_1\dot{\omega}_1 + (I_3 - I_2)\omega_2\omega_3 \\ G_2 &= I_2\dot{\omega}_2 + (I_1 - I_3)\omega_3\omega_1 \\ G_3 &= I_3\dot{\omega}_3 + (I_2 - I_1)\omega_1\omega_2 \end{aligned} \quad (5.38)$$

Where  $I_1, I_2$  and  $I_3$  are the diagonal components of the moment of inertia along each of the principle axes.

### 5.2.3 Stability of Rotation Axes

One important consequence of these equations is the existence of stable and unstable axes of rotation. To see this, let us consider a rigid body, which is primarily rotating about its first principle axis, that is to say that  $\omega_2, \omega_3 \ll \omega_1$ . Furthermore, let us suppose that there are no external torques acting on the body. We can now differentiate the second Euler equation and substitute in the first and third to obtain:

$$I_2\ddot{\omega}_2 + (I_1 - I_3)(I_1 - I_2)\omega_1^2\omega_2 + (I_1 - I_3)(I_2 - I_3)\omega_3^2\omega_2 = 0 \quad (5.39)$$

If we consider the limiting case as  $\omega_2, \omega_3 \rightarrow 0$ , we can see from the first Euler equation that  $\omega_1$  will become approximately constant. Furthermore, we can see that the third term in equation (5.39) will be dominated by the second, leading us to the result:

$$\ddot{\omega}_2 + \frac{(I_1 - I_3)(I_1 - I_2)\omega_1^2}{I_2} \omega_2 \approx 0 \quad (5.40)$$

If  $I_1$  is either the largest or smallest out of  $I_1, I_2$  and  $I_3$ , then this will be nothing more than the fundamental equation of simple harmonic motion, and so  $\omega_2$  will simply oscillate about zero, whilst remaining very small, and the same will also be true of  $\omega_3$ . However, if  $I_1$  is intermediate in size,  $\omega_2$  will grow exponentially, and the motion will become much more complicated. As such, any object with three different components in its diagonalised inertia matrix, will have two stable axes of rotation, and one unstable axis. Rotations about the stable axes will not be interrupted by small perturbations to the other axes, whereas rotation about the unstable axis will rapidly degenerate into a much more complicated form.

## 5.3 Gyroscopes

A gyroscope typically consists of a rapidly rotating flywheel, mounted in a set of gimbals, which allow it to freely rotate about either axis perpendicular to the axis of its internal rotation; however, in practice any object with a movable axis of rotation can act as a gyroscope. Gyroscopes are well known for their unintuitive behaviour, which is what we shall be investigating here.



Figure 5.4: A typical example of a gyroscope.

### 5.3.1 Response to a Couple

When considering the behaviour of a gyroscope, it can often be helpful to realise that different sets of forces have equivalent effects. For a rigid body, two sets of forces are equivalent, if and only if, they produce the same resultant force and the same resultant torque. For example, the two couples shown below, both produce the same force ( $\mathbf{0}$ ) and the same torque (pointing into the page).

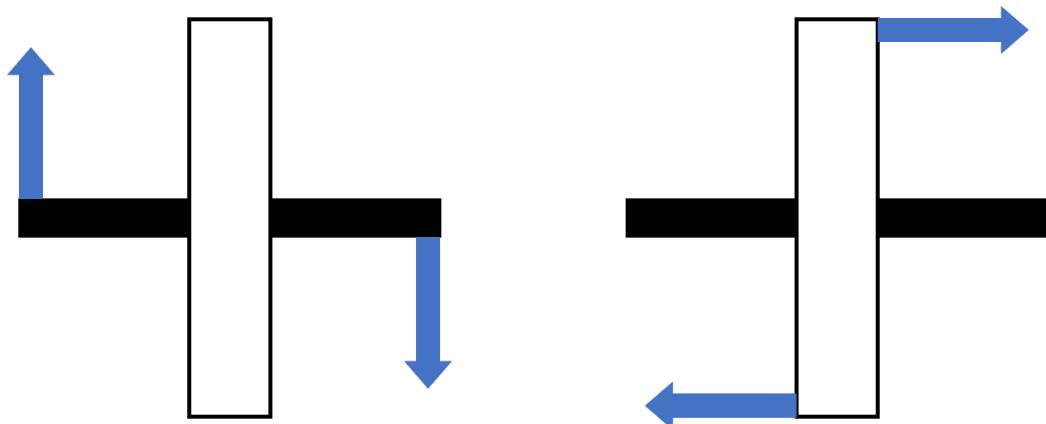


Figure 5.5: Two equivalent couples, applied to a simple gyroscope.

Intuitively, we know that, if the wheel isn't spinning, the application of either couple would cause the wheel to rotate clockwise in the plane of the page. To understand what happens when the wheel is spinning, let us consider the individual elements of the wheel, as shown in figure 5.6 (a). The green arrows represent the velocity of the wheel, while the blue arrows represent the forces due to the applied couple. We can see that, since the vertical sections of the wheel are separated from the centre of mass in the direction of the applied torque, they feel no force, and thus, their upwards velocity must remain constant. Furthermore, we can see that the top of the wheel is accelerating into the page, while the bottom of the wheel is accelerating out of the page. However, since the gyroscope is a rigid body, the only way that the velocities can change direction, is for the whole wheel to rotate about its vertical axis. This is shown by the red arrow in figure 5.6 (b).

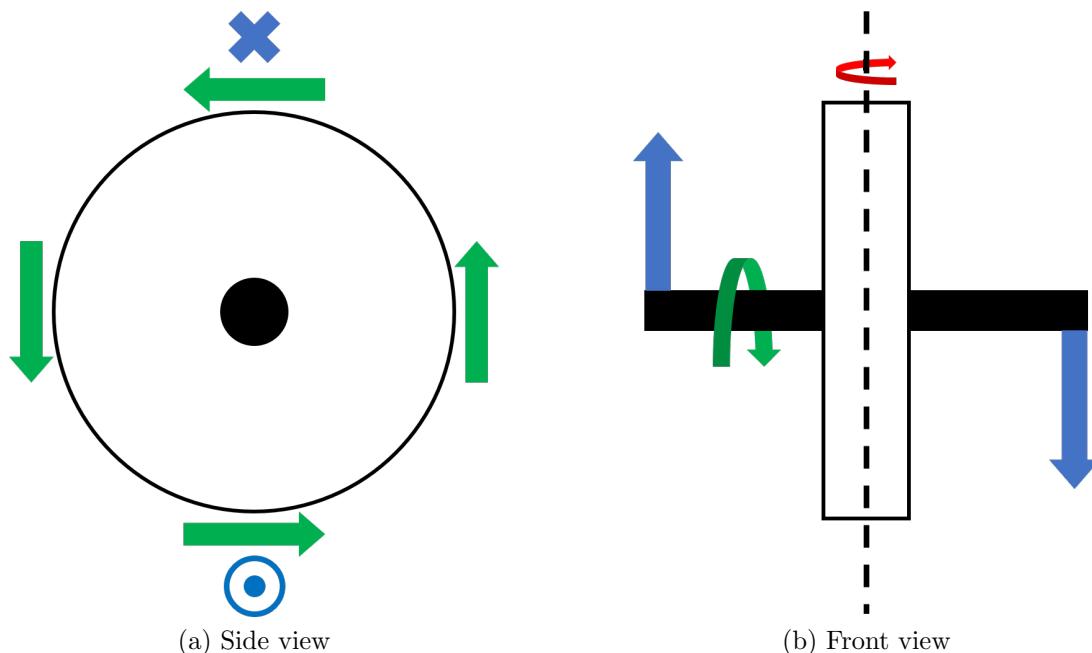


Figure 5.6: The effect of a couple on a gyroscope.

This phenomenon can be described mathematically, by noting that the applied torque is always perpendicular to the angular momentum of the wheel. As such, we can express the torque in terms of the vector cross product:

$$\mathbf{G} = \dot{\mathbf{L}} = \boldsymbol{\Omega} \times \mathbf{L} \quad (5.41)$$

This is exactly the same differential equation that we used to describe circular motion in section 5.1.3, which implies that under the action of the torque, the angular momentum vector must trace out a circle. Since the angular momentum of the gyroscope is primarily generated by the spinning of the wheel, this change in the angular momentum requires the wheel to rotate about its axis.

### 5.3.2 Precession

Arguably, the phenomenon that gyroscopes are best known for is precession. This is essentially the same effect that we have already been considering, only in this case the gyroscope is responding to the torque produced by its own weight. For example, consider a spinning top as shown in figure 5.7 below. The top's weight and it's reaction with the ground form a couple, and produce a torque of magnitude  $mgl \sin \theta$ . Since this torque is always perpendicular to both the vertical axis, and the angular momentum of the top, it follows that  $\mathbf{G} = \boldsymbol{\Omega} \times \mathbf{L}$ , where  $\boldsymbol{\Omega}$  is a vertical vector with magnitude  $\frac{mgl}{L}$ . Therefore, the top will precess with an angular frequency of  $\frac{mgl}{L}$ .

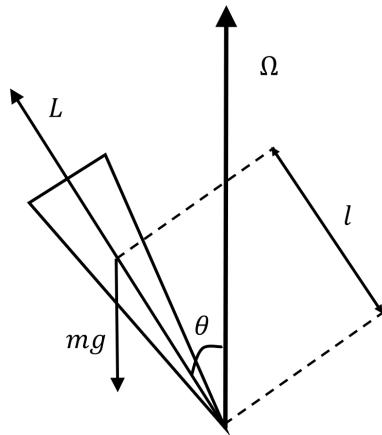


Figure 5.7: A spinning top.

However, we can see that, in order for the gyroscope to precess in this manner, it will need to have some vertical component to its angular momentum. The origin of this momentum lies in the fact that the gyroscope does not begin precessing immediately, instead it first falls down a little in the 'intuitive' direction. This causes a change in the vertical component of the gyroscope's angular momentum, which is counter-acted by the angular momentum of the precession.

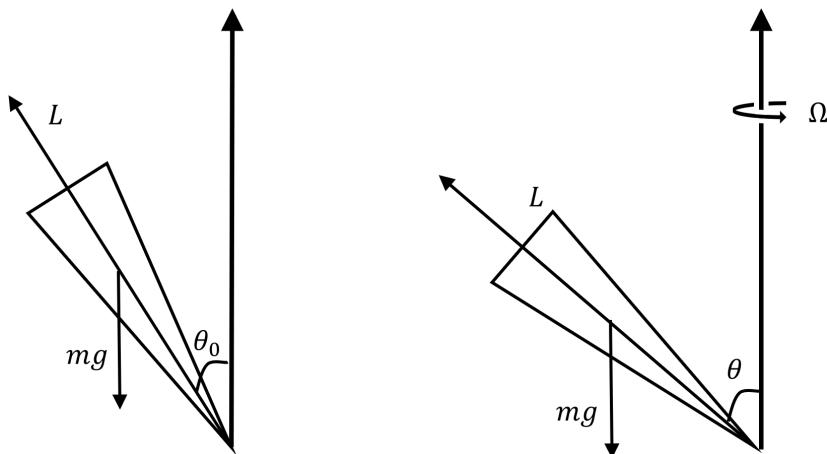


Figure 5.8: A spinning top falling over, and then beginning to precess.

### 5.3.3 Nutation

While gyroscopes are best known for precession, their motion can be characterised by several more complicated phenomena, of which nutation is a prime example. When a gyroscope is released under its own weight, it will initially fall down and begin precession. However, due to the gyroscope's inertia, it will overshoot the position at which it could precess in a steady state. The gyroscope will then rebound back upwards, and will oscillate about this optimal position, in the process known as nutation. To demonstrate this, let us consider a gyroscope such as the one shown in figure 5.9, which is released from a horizontal position.

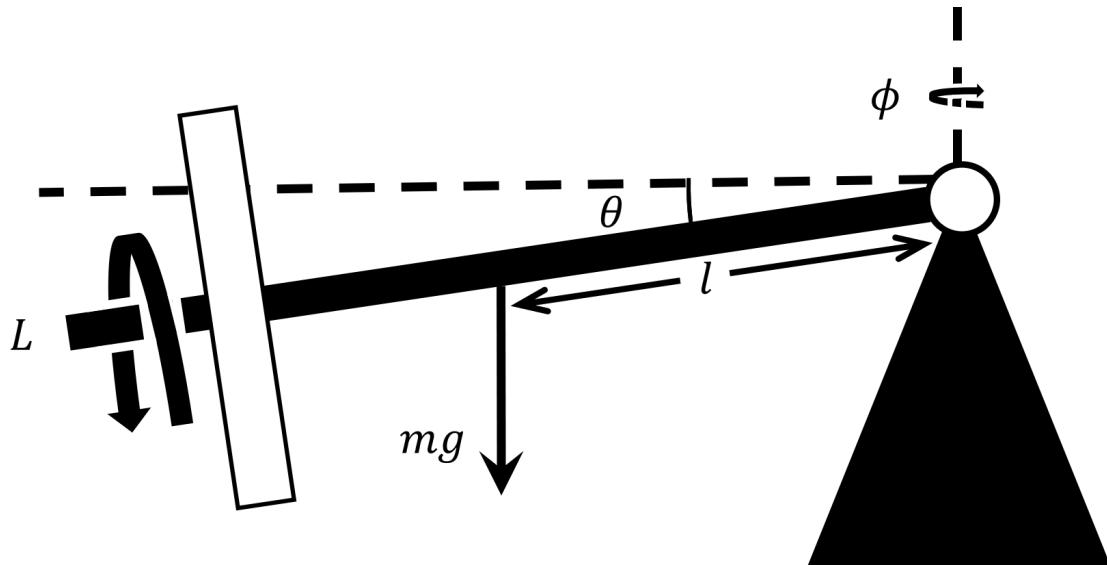


Figure 5.9: A simple gyroscope moving under the torque of its own weight.

We shall let  $\theta$  represent the inclination of the gyroscope to the horizontal,  $\phi$  the angle that the gyroscope has rotated about the vertical axis,  $m$  the mass of the gyroscope,  $l$  the position of the centre of mass along the axle, and  $L$  the magnitude of the angular momentum stored in the flywheel. If we equate the rate of change of the gyroscope's angular momentum to the torque acting on it, we obtain:

$$I_1 \ddot{\phi} - L \dot{\theta} \cos \theta = 0 \quad I_2 \ddot{\theta} + L \dot{\phi} \cos \theta = mgl \cos \theta \quad (5.42)$$

Where  $I_1$  and  $I_2$  are the components of the gyroscope's moment of inertia along the vertical and azimuthal axes respectively (we shall take these to be principle axes). The radial component of the angular momentum has not been accounted for, because the friction at the joint will provide a non-trivial torque in order to prevent the axle from rotating with the flywheel. If we now integrate the first of these equations to obtain a conserved component of the angular momentum and then substitute in the second, we can obtain the following equations of motion:

$$I_1 \dot{\phi} = L \sin \theta \quad \ddot{\theta} + \frac{L^2}{2I_1 I_2} \sin 2\theta = \frac{mgl}{I_2} \cos \theta \quad (5.43)$$

Unfortunately, these equations do not possess an analytic solution, for precisely the same reasons that one cannot solve the motion of a simple pendulum. As such, we can only obtain an approximate solution by assuming that  $\theta$  is very small, which will be the case if  $L$  is sufficiently large. Discarding terms of order  $\theta^2$  and higher, we obtain:

$$\dot{\phi} = \frac{L}{I_1}\theta \quad \ddot{\theta} + \xi^2(\theta - \theta_0) = 0 \quad (5.44)$$

Where the constants  $\xi$  and  $\theta_0$  are given by:

$$\xi = \frac{L}{\sqrt{I_1 I_2}} \quad \theta_0 = \frac{I_1 m g l}{L^2} \quad (5.45)$$

Since (5.32) is nothing more than the fundamental equation of simple harmonic motion, we can immediately solve for  $\theta$  and  $\phi$  in order to obtain:

$$\phi = \Omega(t - \sin \xi t) \quad \theta = \theta_0(1 - \cos \xi t) \quad (5.46)$$

Where  $\Omega = \frac{mgl}{L}$ , just as it was in section 5.3.2. As we can see, the gyroscope will precess about its vertical axis, with an average angular velocity of  $\Omega$ , whilst the axle oscillates up and down. The curve traced out by the gyroscope's motion is the same as that traced out by a point on a rolling wheel, a cycloid.

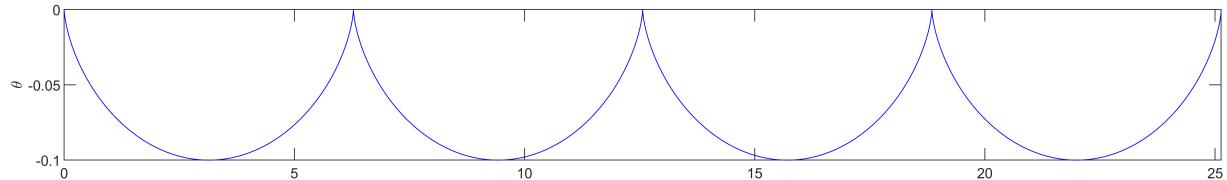


Figure 5.10: A cycloid curve.

In practice however, dissipative forces tend to damp out this oscillatory motion rather quickly, leading the gyroscope to settle into a steady precession about its axis. This damping will lead to a curve of the form shown in figure 5.11.

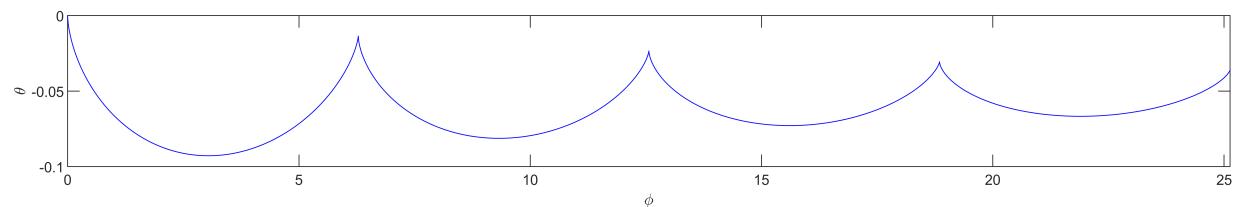


Figure 5.11: A cycloid curve with a decaying amplitude.

Of course this analysis was only valid so long as  $\theta$  was always much smaller than one. It follows from equation (5.33) that this assumption is valid, if  $L$  is much larger than  $\sqrt{I_1 m g l}$ . This should not come as a surprise to us, since we know that when  $L = 0$ , the gyroscope does not precess at all, and instead simply falls over immediately.

# 6 Special Relativity

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## 6.1 The Postulates of Special Relativity

Any physical theory is fundamentally rooted in its postulates. These are the initial statements that the theory assumes to be true, from which everything else can be derived. There can be no theoretical basis for why one set of postulates should be preferred over the other, unless of course one is contradictory, and thus the strength of a postulate can only be measured by how well its predictions compare to experiment. In his theory of special relativity, Einstein made two key postulates about the nature of the universe, and then simply proceeded to examine the consequences of these assumptions. At this point, the experimental evidence for the theory is so overwhelming, that it seems nearly impossible that they are wrong, so we are definitely justified in making these assumptions.

Einstein's first postulate is that the laws of physics must be the same for all inertial observers. That is to say that the universe has no concept of absolute speed, and so no observer could make a measurement to determine how fast they were going, only how fast they are going relative to something else. This principle has its origins long before Einstein, and is unlikely to be overturned any time soon. Although it seems quite abstract in its current form, the first postulate can be presented rather elegantly by understanding the underlying geometry behind time and space. Put simply, the first postulate is really nothing more than a generalisation of the idea that any physical laws should not be dependent on the coordinate system we use to measure them.

Einstein's second postulate is that the speed of light in a vacuum  $c$ , is a fundamental constant of the universe, and as such, must be the same for all inertial observers. This postulate arises from Maxwell's equations of electromagnetism, and their fundamental incompatibility with Galilean relativity, which was the established framework for converting between reference frames before the development of special relativity. As we shall see in chapter 8, Maxwell's equations introduce the constant  $c$  as the phase velocity of perturbations within an electromagnetic field, without ever specifying that this velocity is relative to some physical body. This leads to one of two conclusions, either Maxwell's equations do not hold true in all inertial frames, or space and time must be arranged in such a way, that this speed  $c$  takes the same value in all reference frames. It is this second postulate that acts as the source of all the unusual seeming results of special relativity; however, at this point, experiments such as those by Michelson and Morley have more than demonstrated its validity.

In addition to this, Einstein assumed the homogeneity and isotropy of space. That is to say he assumed that, in the absence of any matter to break symmetry, space must have the same fundamental character everywhere, and it must be the same in all directions. While these statements may seem obvious, and indeed we assume them implicitly all the time, there is no reason why this must be true. In fact, there are those who believe that experimental data shows that the fine structure constant ( $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$ ) actually varies across space. Only time will tell the validity of this belief.

## 6.2 The Space-Time Metric

We are going to start our exploration of special relativity, by examining what it is that Einstein's postulates imply about the geometric structure of space and time. To do this, we are going to forgo any additional assumptions that we may be tempted to make, such as the uniformity of time between inertial frames, and simply regard everything as existing within a 4-dimensional space-time. To describe any given time and place, we will require 4 coordinates, of the form  $(t, x, y, z)$ , measured relative to some set of axes. As a general rule, if we wanted to express the coordinates of the same point in space-time measured relative to a different set of axes, we would use primed coordinates  $(t', x', y', z')$  to make it clear that we were using a different coordinate system, even if some of the coordinates haven't changed.

### 6.2.1 Definitions

In order to help with clarity in the subsequent discussion, a list of a few fundamental definitions is provided below.

**An event** is a single point in space-time, which usually corresponds to some specific thing occurring. Examples of events include an atom spontaneously emitting a photon, two particles colliding, or a spaceship taking off from earth.

**Coordinates** are a set of labels used to identify an event's position in space-time. As far as we can tell, four coordinates are needed to do this, one time coordinate and three spatial ones. Different observers may or may not use the same coordinates to describe a given event.

**A frame** or an observer is essentially a set of axes with which the coordinates of an event can be measured. An inertial frame is one in which a particle experiencing no net force moves in a straight line. We often talk about the frame of a given observer, when we say this, we really mean the frame in which that observer is at rest. Thus, an inertial frame can also be viewed as the rest frame of a non-accelerating particle.

**A world line** is a particle's path through space-time. That is to say that it represents the locus of all the events for which that particle was present. The world lines of non-accelerating particles are straight lines in all inertial reference frames.

**The time** between two events is equal to the difference in their time coordinates in the frame of the observer in question. Importantly, although space and time are fundamentally intertwined, any given observer can always identify which is their time coordinate. For an observer, their time coordinate has the special property that increasing it will always generate an event somewhere else along their world line.

**The displacement** between two events, as measured in the frame of a given observer, can be expressed as the difference in three linearly independent coordinates, all of which are orthogonal to the observers time coordinate. Here orthogonality means that increasing one of the spatial coordinates by  $\delta$  and the time coordinate by  $\frac{\delta}{c}$  must always generate an event separated from the original by the path of a light ray.

### 6.2.2 The Interval

We are now going to consider the space-time interval, or metric, which separates two events. What we want to do is find some function of the coordinates between two events, which will generate an output that all inertial observers can agree on. To achieve this, let us consider two frames  $S$  and  $S'$ , which measure the coordinates separating two points on the path of a light ray to be  $(t, x, y, z)$  and  $(t', x', y', z')$ . Thus, it follows from Einstein's second postulate that:

$$c^2 t^2 - x^2 - y^2 - z^2 = 0 \iff c^2 t'^2 - x'^2 - y'^2 - z'^2 = 0 \quad (6.1)$$

We can compactly write equation (6.1) in matrix form as shown below. Since we will be dealing with matrices of this nature quite a lot, we shall adopt index notation, together with the Einstein summation convention, to represent matrix equations in component form. In special relativity, we number the components of matrices from zero to three, with zero representing the time-like component of the entity. So for example, the 4-position would have components  $(X^0, X^1, X^2, X^3) = (ct, x, y, z)$ . For now, we shall not worry too much about whether an index should be raised or lowered, this is a distinction we shall return to in a later section.

$$c^2 t^2 - x^2 - y^2 - z^2 = X^\mu \eta_{\mu\nu} X^\nu = 0 \quad (6.2)$$

Here the matrix  $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$  is known as the Minkowski metric tensor, and its form is one of the most fundamental results in special relativity. As long as space is homogeneous and isotropic, it follows that the coordinates of an event in the frame  $S'$  must be linearly dependent on the coordinates of that event in  $S$  (assuming that the two frames share a common origin). As such, we can very generally express the coordinates  $X'^\mu$  in the form:

$$X'^\mu = \Lambda_\nu^\mu X^\nu \quad (6.3)$$

For some matrix  $\Lambda_\nu^\mu$ . If we substitute this expression for the primed coordinates into equation (6.2), we obtain the following useful relationship that must be obeyed by  $\Lambda_\nu^\mu$ :

$$X'^\mu \eta_{\mu\nu} X'^\nu = X^\rho \Lambda_\nu^\mu \eta_{\mu\nu} \Lambda_\sigma^\nu X^\sigma = X^\rho \xi_{\rho\sigma} X^\sigma = 0 \quad (6.4)$$

Where we have defined the matrix  $\xi_{\rho\sigma} = \Lambda_\rho^\mu \eta_{\mu\nu} \Lambda_\sigma^\nu$ . Since equation (6.4) must hold for all light-separated events, we can make some useful conclusions about  $\xi_{\rho\sigma}$ . Firstly, we can see that, by definition,  $\xi_{\rho\sigma}$  must be a symmetric matrix, meaning that  $\xi_{\rho\sigma} = \xi_{\sigma\rho}$ . Thus, it follows that the partial derivative of  $X^\rho \xi_{\rho\sigma} X^\sigma$ , with respect to the coordinate  $X^\sigma$ , must be equal to  $2X^\rho \xi_{\rho\sigma}$ . It follows that, if (6.2) and (6.4) define the same hyper-surface in space-time, their partial derivatives must be proportional to one another, which implies that  $\xi_{\rho\sigma} = a \eta_{\rho\sigma}$ , for some constant  $a$ . Finally, we can employ some physical reasoning and argue that, since space is isotropic, this constant can only depend on the relative speed between frames  $S$  and  $S'$ . If we now introduce a third frame  $S''$ , such that all three frames have the same relative speed to one another, then it follows that, because the transformations  $S \mapsto S' \mapsto S'' \equiv S \mapsto S''$  are equivalent, we must have  $a^2 = a \implies a = 1$ . Thus, for any valid transformation between inertial frames, we have:

$$\Lambda_\rho^\mu \eta_{\mu\nu} \Lambda_\sigma^\nu = \eta_{\rho\sigma} \quad (6.5)$$

The matrices which satisfy equation (6.5) are referred to as the Lorentz transformations, and they map coordinates from one inertial frame to another. We can utilise equation (6.5) to generalise Einstein's second postulate slightly, by noting that, for any two frames  $S$  and  $S'$ , which share a common origin, we must have:

$$X^\mu \eta_{\mu\nu} X^\nu = X'^\mu \eta_{\mu\nu} X'^\nu \quad (6.6)$$

The ultimate consequence of all this is that we can define an interval  $\Delta s$  between any two events in space-time, such that all inertial observers will agree on its value. Having a frame invariant way to quantify the separation between two events is obviously exceptionally useful, since it allows us to transfer information between different frames without having to wade through a lot of algebra. The definition of the interval follows directly from (6.6):

$$(\Delta s)^2 = (c\Delta t)^2 - (\Delta x)^2 - (\Delta y)^2 - (\Delta z)^2 \quad (6.7)$$

The invariance of the interval serves as a generalisation of the idea from classical geometry that the distance between two points should not depend on the coordinate axes used to measure it.

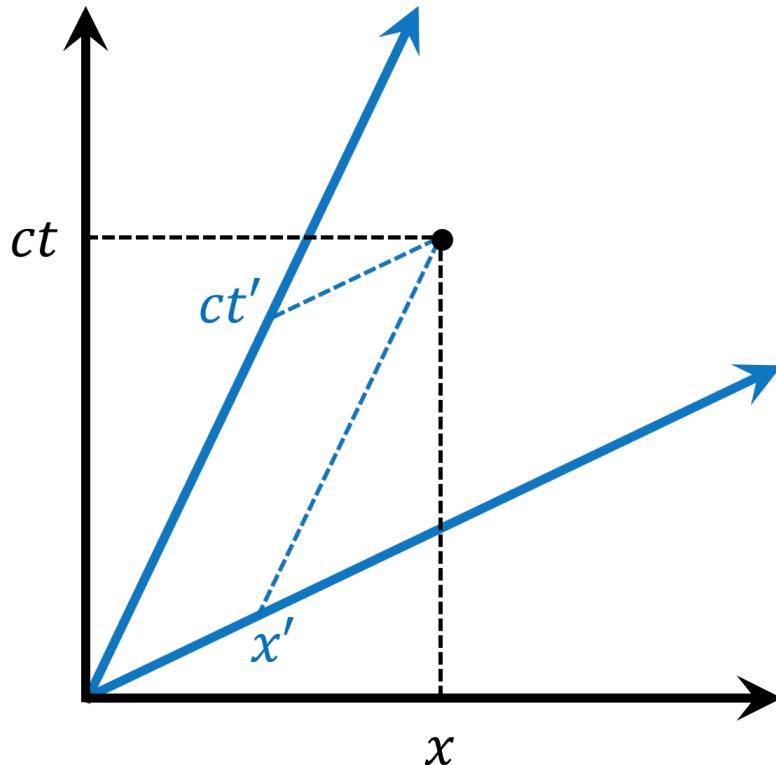


Figure 6.1: A graphical view of different reference frames. The blue axes represent the frame  $S'$  which has a velocity in the positive  $x$  direction with respect to the black axes of the frame  $S$ . The general property to note is that both sets of axes are bisected by a light ray, which is precisely what we would expect given Einstein's second postulate.

### 6.2.3 The Lorentz Transformations

We have seen that in order to convert between two inertial frames, a Lorentz transform must leave the Minkowski metric unchanged. This is equivalent to stating that a Lorentz transform must preserve the invariance of the space-time interval  $s$ . One trivial example of a Lorentz transform is a rotation of the spatial coordinates. Since this rotation preserves the distance between two points, without affecting the time coordinate, it must automatically preserve the interval. Another reasonably straightforward example is to perform a boost along the  $x$  axis. A boost is a mixing of the time coordinate with one of the spatial coordinates, and serves as the equivalent of rotating the time axis into one of the spatial axes.

Since we are only boosting along the  $x$  axis, the coordinates  $y$  and  $z$  will be unchanged by this transformation. Thus we need only ensure that the quantity  $s^2 + y^2 + z^2 = c^2t^2 - x^2$  is preserved by our transformation. If we write out the transformation in component form, we obtain:

$$\begin{pmatrix} ct \\ x \end{pmatrix} \mapsto \begin{pmatrix} ct' \\ x' \end{pmatrix} = \begin{pmatrix} \Lambda_{tt}ct + \Lambda_{tx}x \\ \Lambda_{xx}x + \Lambda_{xt}ct \end{pmatrix} \quad (6.8)$$

Substituting this into the equation for  $s$  yields the following relationships between the coefficients.

$$\Lambda_{tt}^2 - \Lambda_{xt}^2 = 1 \quad \Lambda_{xx}^2 - \Lambda_{tx}^2 = 1 \quad \Lambda_{tt}\Lambda_{tx} = \Lambda_{xx}\Lambda_{xt} \quad (6.9)$$

We can represent the general solution to this system of equations in terms of the parameter  $\theta$ , known as the rapidity of the boost. This result does not look at all dissimilar to a rotation, with the major distinction being the use of hyperbolic trigonometric functions instead of the normal sines and cosines. This should not come as a shock, since after all, the quantity we were trying to keep constant  $c^2t^2 - x^2$  traces out a hyperbola in the  $x$ - $t$  plane, as opposed to the normal circle, which would be generated by a rotation.

$$\begin{pmatrix} \Lambda_{tt} & \Lambda_{tx} \\ \Lambda_{xt} & \Lambda_{xx} \end{pmatrix} = \begin{pmatrix} \cosh \theta & -\sinh \theta \\ -\sinh \theta & \cosh \theta \end{pmatrix} \quad (6.10)$$

This is all well and good; however, it would be useful if we could express the transformation not in terms of the rapidity, but instead in terms of the velocity between the two frames. If the velocity of the frame  $S'$  is  $v$  relative to the frame  $S$ , then it follows that any particle at rest in  $S'$  would have a velocity  $v$  in  $S$ . A particle at rest in  $S'$  would have a world line described by  $x' = \text{const.}$ , which when expressed in our original coordinates gives us:

$$x \cosh \theta - ct \sinh \theta = \text{const.} \implies v = \frac{dx}{dt} = c \tanh \theta \quad (6.11)$$

We can now use trigonometric identities to determine  $\cosh \theta$  and  $\sinh \theta$  in terms of  $v$ . When working in special relativity it becomes convenient to define the quantities  $\beta$  and  $\gamma$  such that:

$$\tanh \theta = \beta = \frac{v}{c} \quad \cosh \theta = \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \sinh \theta = \beta \gamma = \frac{v}{\sqrt{c^2 - v^2}} \quad (6.12)$$

### 6.2.4 Time dilation and Length Contraction

Time dilation and length contraction are two of the most famous consequences of special relativity. All we need to understand these phenomena are the Lorentz transforms, which we derived earlier.

$$\begin{aligned}\Delta t' &= \gamma (\Delta t - \frac{v\Delta x}{c^2}) & \Delta x' &= \gamma (\Delta x - v\Delta t) \\ \Delta t &= \gamma (\Delta t' + \frac{v\Delta x'}{c^2}) & \Delta x &= \gamma (\Delta x' + v\Delta t')\end{aligned}\tag{6.13}$$

We have explicitly written in the  $\Delta$  to show that we are really considering the differences in the coordinates between two events. The main thing we need to be careful of here is making sure that we clearly define the events we are interested in.

#### 6.2.4.1 Time Dilation

Consider two events A and B in space-time. Let the separation between the events be such that they both lie on the time axis of the frame  $S'$ . Thus,  $\Delta x'_{AB}$  must be zero by definition. In addition, we now define  $\Delta t'_{AB}$  to be the proper time between the events, given the symbol  $\tau$ . Substituting these into our Lorentz transforms give us the following results:

$$\Delta t_{AB} = \gamma\tau \quad \Delta x_{AB} = v\gamma\tau\tag{6.14}$$

From the definition of  $\gamma$ , we can see that it must always be greater than or equal to one, and hence, the time between A and B must always be greater than or equal to the proper time. Thus,  $\tau$  represents the minimum time between two events. This phenomenon of the time between events being larger, for observers moving relative to those events, is known as time dilation.

#### 6.2.4.2 Length Contraction

Let us now consider a rigid rod aligned along the  $x$  axis, such that it is at rest in the frame  $S'$ . That is to say that the rod is moving with a constant velocity  $v$  in the  $x$  direction, when measured by an observer in  $S$ . Suppose that some observer in  $S$  wanted to measure the length of this rod, to do this they would find the separation between two events A and B, which occur simultaneously on either end of the rod. Thus, by definition of A and B,  $\Delta t_{AB} = 0$ . We can substitute this into our Lorentz transforms to obtain the results below:

$$\Delta x'_{AB} = \gamma\Delta x_{AB} \quad \Delta t'_{AB} = -\frac{v\gamma}{c^2}\Delta x_{AB}\tag{6.15}$$

Now, since the rod is at rest in  $S'$ , it follows that the length of the rod, as measured in  $S'$  must be equal to  $\Delta x'_{AB}$ . If we define  $l_0$  to be the length of the rod in its rest frame, then we must have  $\Delta x'_{AB} = l_0$ . Thus, we can conclude that the length of the rod measured in  $S$  must be shorter than its natural length. This phenomenon is referred to as length contraction.

$$l = \frac{l_0}{\gamma}\tag{6.16}$$

Importantly, both length contraction and time dilation act in opposite directions, such that both frames  $S$  and  $S'$  agree on their relative velocity. This makes sense, because if the two frames disagreed on their relative velocities, this would be a clear violation of spatial isotropy.

## 6.3 4-Vectors

When it comes to describing the behaviour of any mathematical entity in special relativity, the most important factor is always how it behaves under Lorentz transformation. When we construct physical laws, the principle of relativity implies that we must be able to do so in a coordinate independent way, so, in a sense, all physical laws are Lorentz invariant. Now the simplest example of such a quantity is a so called Lorentz scalar, which is the same in all inertial frames, and obeys the simple transformation law:

$$\Phi' = \Phi \quad (6.17)$$

We have already met a Lorentz scalar in the form of the interval  $\Delta s$ , which we defined to have precisely this property. Another common example is the phase of a wave, since the phase is a property of a single point in space-time, all observers must agree on its value at any given event. Finally, the mass of a particle is also a scalar. Now the treatment of mass in relativity is something that can often get confused, and so warrants a discussion here. In some places, especially introductions to the subject, one encounters the concept of a relativistic mass, which changes with velocity. However, the convention that we shall adopt here, which is the one consistently used by practising physicists, is to define the mass of an object as being measured in that objects rest frame. It follows from this definition that the mass must be Lorentz invariant, because the frame in which it must be measured is already specified.

In addition to scalars, there is another class of mathematical object which does not change with the reference frame. This object is a vector, or to distinguish it from the vectors we might encounter in classical mechanics, a 4-vector. Now it is important here that we understand exactly what is meant by the statement that a 4-vector is invariant under a Lorentz transformation. What we are saying is that there is some underlying physical quantity, represented by this vector, and that this quantity does not change when we choose a different set of axes to describe it. However, unlike a scalar, which can simply be given as a number without need for a coordinate system, we can not simply state the value of a vector, and instead must expand it in some basis relative to a given coordinate system. That is to say that an arbitrary 4-vector  $\mathbf{V}$  can be written as the summation:

$$\mathbf{V} = V^0 \vec{\mathbf{e}}_0 + V^1 \vec{\mathbf{e}}_1 + V^2 \vec{\mathbf{e}}_2 + V^3 \vec{\mathbf{e}}_3 = V^\mu \vec{\mathbf{e}}_\mu \quad (6.18)$$

Where the  $\vec{\mathbf{e}}_\mu$  are our basis vectors, representing unit displacements along each of our coordinate axes. Importantly, while the underlying vector  $\mathbf{V}$  does not change under Lorentz transformation, the basis vectors must necessarily change, because they are defined in terms of the coordinate axes. As a result, the components  $V^\mu$  must change with the inverse transformation of the basis vectors, such that the overall sum remains the same. As it happens, we have already encountered an example of a 4-vector, when we considered the 4-position of an event in space-time. This example also helps to capture precisely what a 4-vector is. The actual position of an event in space-time does not change, when we apply a Lorentz transform, instead the axes that we are using to measure it, and hence its coordinates change. Written in vector form the 4-position is:

$$\mathbf{X} = ct \vec{\mathbf{e}}_0 + x \vec{\mathbf{e}}_1 + y \vec{\mathbf{e}}_2 + z \vec{\mathbf{e}}_3 \quad (6.19)$$

Luckily, since the components of all 4-vectors must transform in the same way (this is because they are all measured with respect to the same set of basis vectors) and we already know how the components of the 4-position behave under a Lorentz transformation, we immediately obtain the transformation law:

$$V'^\mu = \Lambda_\nu^\mu V^\nu \quad (6.20)$$

Where  $V^\nu$  and  $V'^\mu$  are the components of  $\mathbf{V}$  in the frames  $S$  and  $S'$  respectively, while  $\Lambda_\nu^\mu$  is one of the Lorentz matrices we have previously discussed. It follows from this that, if we define the dot product of any two 4-vectors  $\mathbf{V}$  and  $\mathbf{U}$  to be given by equation (6.21) below, then the result must be a Lorentz scalar.

$$\mathbf{V} \cdot \mathbf{U} = V^\mu \eta_{\mu\nu} U^\nu \quad (6.21)$$

A useful idea to consider when thinking about the dot product, is the concept of a covector. Formally, a 4-covector exists as a linear mapping between the space of 4-vectors and the real numbers. That is to say that if  $\omega$  is a covector:

$$\omega(\mathbf{V}) \mapsto \mathbb{R} \quad \text{such that} \quad \omega(a\mathbf{V} + b\mathbf{U}) = a\omega(\mathbf{V}) + b\omega(\mathbf{U}) \quad (6.22)$$

Just as it is possible to expand a 4-vector in terms of a basis set, it is also possible to do the same for a 4-covector. To do this, we need to have some definition of what it means to add two covectors together. The most sensible way to do this is to make the definition:

$$\omega = \chi + \zeta \implies \omega(\mathbf{V}) = \chi(\mathbf{V}) + \zeta(\mathbf{V}) \quad (6.23)$$

In principle, we could expand a covector in any basis we desired; however, it turns out that the most useful basis to use is one that derives from the coordinate axes and their associated basis vectors. If we define the basis  $\tilde{\mathbf{e}}^\mu$ , such that  $\tilde{\mathbf{e}}^\mu(\tilde{\mathbf{e}}_\nu) = \delta_\nu^\mu$ , where  $\delta_\nu^\mu$  is the Kronecker delta, we can say:

$$\omega = \omega_0 \tilde{\mathbf{e}}^0 + \omega_1 \tilde{\mathbf{e}}^1 + \omega_2 \tilde{\mathbf{e}}^2 + \omega_3 \tilde{\mathbf{e}}^3 = \omega_\mu \tilde{\mathbf{e}}^\mu \implies \omega(\mathbf{V}) = \omega_\mu V^\mu \quad (6.24)$$

Since the action of a covector on a vector yields a scalar, it immediately follows that the components of a covector must change with the inverse transformation to those of a vector. This is the reason why the components of a covector are denoted with lowered indices, while those of a vector are raised.

This is all relevant because the existence of the dot product implies that every 4-vector  $\mathbf{V} = V^\mu \tilde{\mathbf{e}}_\mu$ , has an associated 4-covector  $\mathbf{V}^* = V_\nu \tilde{\mathbf{e}}^\nu$ , defined by the relationship that  $\mathbf{V}^*(\mathbf{U}) = \mathbf{V} \cdot \mathbf{U}$ . Thus, it follows that the components of the covector are given by:

$$V_\nu = V^\mu \eta_{\mu\nu} \quad (6.25)$$

Similarly, it is possible to associate a 4-vector to every 4-covector, by applying the inverse transformation. This process is known as index juggling because the indices of the components swap from being raised to lowered each time.

A common notation used for a 4-vector is to say that  $V^\mu = (V^0, \mathbf{v})$ , where  $\mathbf{v}$  is a normal 3-vector with components  $V^1, V^2$  and  $V^3$ . Using this notation, the 4-position, which we encountered earlier, can be represented by  $\mathbf{X} = (ct, \mathbf{x})$ , where  $\mathbf{x}$  is simply the normal three dimensional, spatial position.

### 6.3.1 4-Velocity and 4-Momentum

Let us consider a particle whose 4-position world line can be described by  $\mathbf{X}(\tau)$ , where  $\tau$  is the proper time, measured along the particle's word line. We can define the particle's 4-velocity to be given by:

$$\mathbf{U} = \frac{d}{d\tau} \mathbf{X}(\tau) \quad (6.26)$$

Since the proper time  $\tau$  is a frame invariant quantity the 4-velocity must behave in exactly the same way as the 4-position under Lorentz transformation, and thus, it fulfils the necessary criteria to be a 4-vector. We can calculate the components of  $\mathbf{U}$  by using the chain rule to generate the expression:

$$\mathbf{U} = \frac{dt}{d\tau} \frac{d}{dt} \mathbf{X} \quad (6.27)$$

If we then recognise that  $\frac{dt}{d\tau} = \gamma$ , which follows from our discussion of time dilation in section 6.2.4, and substitute in  $X^\mu = (ct, \mathbf{x})$ , we can obtain:

$$U^\mu = \gamma_u(c, \mathbf{u}) \quad (6.28)$$

Where  $\mathbf{u}$  is the particle's velocity, as measured by the frame in question. We can easily see from this expression that  $\mathbf{U} \cdot \mathbf{U} = c^2$  in all frames of reference, just as we would expect for a 4-vector dot product. This fact gives us an interesting way of interpreting the 4-velocity, in reality all it represents is a 4-vector that is instantaneously tangential to the particle's world line, that has been normalised to have a magnitude of  $c$ .

Since we know how the components of the 4-velocity change under Lorentz transformation, we can now derive a relativistic velocity addition formula. Let us consider a particle that, in the frame  $S'$ , has a 4-velocity  $U'^\mu = \gamma_{u'}(c, \mathbf{u}')$ . We now wish to determine the components of the particle's 4-velocity in the frame  $S$ , which is moving relative to  $S'$  with a speed  $v$  in the negative  $x$  direction. If we apply the appropriate Lorentz transformations to the 4-velocity, we obtain:

$$\begin{aligned} \gamma_u &= \gamma_{u'} \gamma_v \left( 1 + \frac{vu'_x}{c^2} \right) & u_x &= \frac{u'_x + v}{1 + \frac{vu'_x}{c^2}} \\ u_y &= \frac{u'_y}{\gamma_v \left( 1 + \frac{vu'_x}{c^2} \right)} & u_z &= \frac{u'_z}{\gamma_v \left( 1 + \frac{vu'_x}{c^2} \right)} \end{aligned} \quad (6.29)$$

For convenience, it is often more elegant to express the velocity addition formulae in vector form, as shown in equation (6.30) below:

$$\mathbf{u} = \frac{1}{1 + \frac{\mathbf{v} \cdot \mathbf{u}'}{c^2}} \left[ \mathbf{v} + \frac{\mathbf{u}'}{\gamma_{\mathbf{v}}} + \frac{1}{c^2} \frac{\gamma_{\mathbf{v}}}{1 + \gamma_{\mathbf{v}}} (\mathbf{u}' \cdot \mathbf{v}) \mathbf{v} \right] \quad (6.30)$$

Interestingly, we can see that the velocity addition formula is only symmetric in  $\mathbf{u}'$  and  $\mathbf{v}$ , if they are travelling in the same direction. This is actually a very general statement about the Lorentz transforms, since they are represented by matrices, there is no reason why we should expect them to commute in the general case.

Once we have the 4-velocity of a particle, the 4-momentum of the particle is trivially defined as the particle's rest mass multiplied by this 4-velocity. Here we have to be careful about the notion of mass in relativity. As we shall go on to see, one consequence of special relativity is mass energy equivalence, which is expressed by Einstein's famous equation  $E = mc^2$ . This leads to the idea of a relativistic mass, which increases as a particle speeds up. However, if we take this view, with mass and energy being entirely equivalent, we have a redundancy; we have two words describing precisely the same thing. Thus, by convention, whenever we say mass, we are referring to the mass of that object as measured in its rest frame, and when we say energy, we are indeed referring to the energy of the object in a given frame. Thus,  $m$  is frame invariant, and so  $\mathbf{P}$  must also be a 4-vector.

$$\mathbf{P} = m\mathbf{U} \iff P^\mu = \gamma_{\mathbf{u}}(mc, m\mathbf{u}) \quad (6.31)$$

An interesting consequence of Einstein's first postulate is that, in order for the laws of physics to be the same in all reference frames, they must be written in a manifestly Lorentz covariant form. That is to say that, they must be written in terms of 4-vectors, since these are the only things that transform consistently upon a change of reference frame. For example, the law of conservation of momentum states that  $\Delta\mathbf{p} = \mathbf{0}$ , for any isolated system. In order for this to be written in a relativistic manner we must replace  $\mathbf{p}$  with a 4-vector of some kind. Since in the limit as  $|\mathbf{u}| \rightarrow 0$ , the spatial components of the 4-momentum tends towards the classical momentum, it makes sense to choose this as our 4-vector. Thus, we obtain the law of conservation of 4-momentum  $\Delta\mathbf{P} = \mathbf{0}$ . In accordance, we identify the relativistic expression for the 3-momentum as  $\mathbf{p} = \gamma_{\mathbf{u}}m\mathbf{u}$ . In addition to this, the time component of the 4-momentum must also be a conserved, so it would be nice if we could relate this to some other well known property of the system.

### 6.3.1.3 Energy in Special Relativity

Let us identify a 3-force in terms of our newly defined 3-momentum as:

$$\mathbf{f} = \frac{d\mathbf{p}}{dt} \quad (6.32)$$

Note that this is most certainly not a frame invariant quantity; however, since we are aiming to determine an expression for energy, which is not itself frame invariant, this is not create a problem. Just as in classical mechanics we can identify the work done by this force as:

$$dW = \mathbf{f} \cdot d\mathbf{x} \quad (6.33)$$

Substituting in our expression for  $\mathbf{f}$  we can rearrange this to obtain:

$$dW = d(m\gamma_{\mathbf{u}}\mathbf{u}) \cdot \mathbf{u} = m(u^2 d\gamma_u + \gamma_u u du) \quad (6.34)$$

If we recall the definition of the Lorentz factor,  $\gamma_u = \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}}$ , we can express its differential in the form  $d\gamma_u = \gamma_u^3 \frac{u du}{c^2}$ . Substituting this into equation (6.34), and then rearranging, yields the relatively simple expression:

$$dW = m\gamma_u u \left( \gamma_u^2 \frac{u^2}{c^2} + 1 \right) du = m\gamma_u^3 u du \quad (6.35)$$

The kinetic energy of a particle is defined to be the total work that must be done in order to accelerate it from rest up to its current velocity. As such, the relativistic expression for the kinetic energy is given by the integral:

$$T = \int_0^u m\gamma^3 u du = mc^2 \int_1^\gamma d\gamma \quad (6.36)$$

This then yields the expression for the relativistic kinetic energy of a particle,  $T = (\gamma - 1)mc^2$ . One can perform a Taylor series expansion of  $\gamma$  to demonstrate that, in the low velocity limit, this reduces to the classical expression for kinetic energy,  $T \approx \frac{1}{2}mu^2$ . While this formula for the energy is certainly useful, Einstein's true breakthrough was realising that the laws of special relativity implied that every object has a rest energy, an energy which it possesses just by virtue of existing.

Let us consider a body of mass  $m$  moving at a velocity  $u$  along the  $x$  axis in a frame  $S$ , and at rest in a frame  $S'$ . In  $S'$ , the body spontaneously emits two pulses of light, each with energy  $\frac{\Delta E}{2}$ , that travel in opposite directions along the  $y$  axis. By symmetry, the body must therefore remain at rest in  $S'$ , and thus it directly follows from the Lorentz transformations, that in  $S$  the particle's velocity also remains unchanged.

If we now consider the pulses of light, we encounter a problem. When we substitute a velocity of  $c$  into our expression for kinetic energy, we find that the Lorentz factor  $\gamma$  diverges to infinity. As such the only sensible way for us to consider light is in the limit that  $u \rightarrow c, m \rightarrow 0$ , such that  $\gamma_u m$  is finite. In this limit, we find that the energy and momentum of a particle must be related by  $E = pc$ . Returning to the light in question, since the  $x$  coordinates of the light pulses and the body were the same for all time in  $S$ , it follows that the same must be true in  $S'$ . We can then use the constancy of  $c$  to deduce that the components of the light's velocity along the  $x$  and  $y$  axes are given by  $u$  and  $\pm\sqrt{c^2 - u^2}$  respectively. Since the  $y$  component of the light's momentum should be unchanged by the Lorentz transformation  $S' \mapsto S$ , we can conclude that in the frame  $S$ , the body lost a total momentum of  $\frac{\gamma\Delta Eu}{c^2}$  along the  $x$  axis. Since its velocity has not changed, the only conclusion we can reach is that its mass must have changed. This gives us equation (6.37) for the change in mass of the body, after it has emitted the radiation.

$$\Delta p = \gamma\Delta mu = \frac{\gamma\Delta Eu}{c^2} \implies \Delta m = \frac{\Delta E}{c^2} \quad (6.37)$$

Therefore, if we wish for the body to have zero energy when it does not exist (i.e it has zero mass), we obtain Einstein's famous equation, where  $E^*$  is the energy of the body in its rest frame. If we recall that the particle's kinetic energy was given by  $T = (\gamma_u - 1)mc^2$ , we can express the total energy as:

$$E^* = mc^2 \implies E = \gamma_u mc^2 \quad (6.38)$$

This differs from the time component of the 4-momentum by nothing more than a factor of  $c$ , and so we can say that  $P^\mu = (\frac{E}{c}, \mathbf{p})$ . This means that the conservation of 4-momentum accounts for the conservation of both energy and momentum. If we consider the dot product of the 4-momentum with itself, we obtain the so called E-P invariant, shown below:

$$\mathbf{P} \cdot \mathbf{P} = \frac{E^2}{c^2} - |\mathbf{p}|^2 = m^2 c^2 \quad (6.39)$$

### 6.3.2 The 4-Wave Vector

In special relativity, our interpretation of what a wave is changes somewhat. Since we are now thinking about a unified space-time, a wave is nothing more than a field defined everywhere on that space-time. From the perspective of an observer moving along their world line, the wave will appear to oscillate over time in the way that we would expect. Let us now consider a wave  $\psi$ , given by equation (6.59) in a frame  $S$ .

$$\psi = \psi_0 e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} \quad (6.40)$$

We can rewrite this in 4-vector notation as follows:

$$\psi = \psi_0 e^{i\mathbf{K} \cdot \mathbf{X}} \quad (6.41)$$

Where  $\mathbf{K}$  is 4-wave vector given by:

$$K^\mu = \left( \frac{\omega}{c}, \mathbf{k} \right) \quad (6.42)$$

Since each value of  $\psi$  is assigned to a point in space-time, all observers must agree on its value at any given event. That is to say that, our choice of coordinate system used to describe 4-position in space-time, should not affect the value of  $\psi$  at any given event. Thus, the dot product  $\mathbf{K} \cdot \mathbf{X}$  must be a Lorentz scalar, and thus, we must find that the components of  $\mathbf{K}$  transform as those of a 4-vector. Applying the Lorentz transformations to  $\mathbf{K}$  allows us to determine how the frequency and wavelength of a wave change when we change reference frame, a phenomenon known as the Doppler effect.

To demonstrate this, let us consider a wave with phase velocity  $c$  (the obvious example being light itself). For such a wave, the frequency and wave vector are related by  $\omega = c|\mathbf{k}|$ , and so our 4-wave vector can be given by  $K^\mu = (|\mathbf{k}|, \mathbf{k})$ . This means that  $\mathbf{K} \cdot \mathbf{K} = 0$ , which as a Lorentz scalar must be frame invariant. This is really just a statement of the second postulate that a wave moving at speed  $c$  in one frame must also move at speed  $c$  in all other inertial frames. If we now transform to a frame  $S'$ , moving with a velocity  $v$  along the  $x$  axis in  $S$ , the new components of the 4-wave vector can be obtained by applying the Lorentz transformations, as shown below:

$$K'^\mu = (|\mathbf{k}'|, \mathbf{k}') = \left( \gamma(|\mathbf{k}| - \beta k_x), \mathbf{k} + \left[ (\gamma - 1)k_x - \beta|\mathbf{k}|\right] \hat{\mathbf{x}} \right) \quad (6.43)$$

Let us now consider the special case that occurs, when the observer is moving in the direction of the wave, that is to say that the wave vector points along the  $x$  axis. In this case, we find that  $k_x = |\mathbf{k}|$  and  $k_y = k_z = 0$ . Substituting this into equation (6.62) yields the commonly seen formula for the relativistic Doppler shift:

$$\omega' = \omega \gamma(1 - \beta) = \omega \sqrt{\frac{1 - \beta}{1 + \beta}} \quad (6.44)$$

An interesting point to note about the 4-wave vector is that, together with the 4-momentum, it satisfies the relativistic form of de Broglie's equation,  $\mathbf{P} = \hbar\mathbf{K}$ . If we apply this to a single photon, it follows that since  $\mathbf{K} \cdot \mathbf{K} = 0$ , the E-P invariant  $\mathbf{P} \cdot \mathbf{P} = m^2c^2$  must also be equal to zero. This is fully consistent with the concept of a photon as a massless particle.

### 6.3.3 The 4-Gradient

Let us now consider a Lorentz scalar field  $\Phi$ , defined across space-time. Examples of such a field could include, but are not limited to, the rest density<sup>4</sup> of a dust in space, the pressure of some gas, or even a scalar wave such as the one we described in section 6.3.2. In any given frame of reference, we can always expand the differential of  $\Phi$  to obtain:

$$d\Phi = \frac{\partial\Phi}{\partial t}dt + \frac{\partial\Phi}{\partial x}dx + \frac{\partial\Phi}{\partial y}dy + \frac{\partial\Phi}{\partial z}dz \quad (6.45)$$

Since  $\Phi$  is a scalar field, we must find that  $d\Phi$  is invariant under Lorentz transformation. Since the infinitesimal displacement  $dX^\mu = (cdt, d\mathbf{x})$ , derives entirely from the 4-position, it must itself be a 4-vector. Thus it follows that the gradient of  $\Phi$  defines a 4-covector, such that:

$$\partial\Phi(d\mathbf{X}) = d\Phi \iff \partial_\mu\Phi = \frac{\partial\Phi}{\partial X^\mu} \quad (6.46)$$

We can verify that the 4-gradient as defined in this way obeys the correct transformation law by utilising the chain rule of partial differentiation. Expanding one of the derivatives in a primed reference frame and substituting in  $X'^\mu = \Lambda_\nu^\mu X^\nu$ , yields the following transformation law:

$$\frac{\partial\Phi}{\partial X^\nu} = \frac{\partial\Phi}{\partial X'^\mu} \frac{\partial X'^\mu}{\partial X^\nu} \implies \partial_\nu\Phi = \Lambda_\nu^\mu \partial'_\mu\Phi \quad (6.47)$$

As such, we can see that the components of  $\partial\Phi$  will transform with the inverse Lorentz matrix, just as we would expect for a 4-covector. If we refer back to the introduction of section 6.3, we can now use the Minkowski metric to generate an associated 4-vector,  $\partial^\mu\Phi = (\frac{1}{c}\frac{\partial\Phi}{\partial t}, -\nabla\Phi)$ , which will transform in the traditional manner.

All of the transformation laws we have established are not properties of  $\Phi$ , but are instead a consequence of the way in which the partial derivatives relate to the coordinate system. As such, we can generalise these ideas somewhat, by introducing the 4-vector and 4-covector operators:  $\partial^\mu = (\frac{1}{c}\frac{\partial}{\partial t}, -\nabla)$  and  $\partial_\mu = (\frac{1}{c}\frac{\partial}{\partial t}, \nabla)$  respectively. This now gives us a way in which we can apply derivatives to 4-vectors, for example the 4-divergence of the 4-vector  $\mathbf{V}$ , which has components  $V^\mu = (V^0, \mathbf{v})$ , is given below.

$$\boldsymbol{\partial} \cdot \mathbf{V} = \partial_\mu V^\mu = \frac{1}{c} \frac{\partial V^0}{\partial t} + \nabla \cdot \mathbf{v} \quad (6.48)$$

It follows that since  $\partial_\mu$  varies with the inverse Lorentz matrix and  $V^\mu$  transforms with the regular matrix, the 4-divergence, as defined above, must be a Lorentz scalar. This is particularly important when it comes to the concept of a conserved quantity in special relativity. If we have some continuous scalar quantity, we can define its 4-flux  $\mathbf{J}$ , such that its components are  $J^\mu = (\rho c, \mathbf{j})$ , where  $\rho$  is the density of that quantity and  $\mathbf{j}$  is its regular 3-flux (we can see that this must be a 4-vector by noting that for a quantity with rest density  $\rho_0$  and a flow 4-velocity  $\mathbf{U}$ ,  $\mathbf{J} = \rho_0 \mathbf{U}$ ). If that quantity is conserved, it must obey the Lorentz invariant continuity equation:

$$\boldsymbol{\partial} \cdot \mathbf{J} = \partial_\mu J^\mu = \frac{\partial\rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (6.49)$$

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<sup>4</sup>Since as a result of length contraction, density is not itself Lorentz invariant, we often tend to describe the rest density of a fluid, which is the density the fluid in its local rest frame

## 6.4 Relativistic Collisions

In principle, there is nothing more to collisions than conserving relativistic 4-momentum (which ensures the conservation of both energy and momentum). Many of the same ideas that we would use in classical mechanics apply here too. For example, it can often be helpful, when interpreting a collision, to transform into the zero momentum frame of the system. This ensures that all of the spatial components of the total 4-momentum are zero, and thus, helps to simplify any algebra involved.

### 6.4.1 A Two Body Collision

We can put the ideas we have been developing to use by analysing a simple two body collision. The general method for approaching a relativistic collision is to first calculate the total 4-momentum from the initial conditions, and call it  $\mathbf{P}_0$ . If we now suppose that the result of the collision is two particles with 4-momenta  $\mathbf{P}_1$  and  $\mathbf{P}_2$  respectively, we can apply conservation of 4-momentum:

$$\mathbf{P}_1 + \mathbf{P}_2 = \mathbf{P}_0 \quad (6.50)$$

Now if we assume that the identities of the particles are known (and hence so are their masses, which we shall call  $m_1$  and  $m_2$ ), we can use equation (6.50) to say that:

$$\mathbf{P}_2 \cdot \mathbf{P}_2 = \mathbf{P}_0 \cdot \mathbf{P}_0 + \mathbf{P}_1 \cdot \mathbf{P}_1 - 2\mathbf{P}_0 \cdot \mathbf{P}_1 \quad (6.51)$$

Rearranging this and substituting in  $\mathbf{P}_i \cdot \mathbf{P}_i = m_i^2 c^2$  we obtain the following result:

$$2\mathbf{P}_0 \cdot \mathbf{P}_1 = [m_0^2 + m_1^2 - m_2^2] c^2 \quad (6.52)$$

From here, the best way to proceed is to shift into the zero momentum frame of the system (denoted by a  $\star$ ), where  $P_0^{\star\mu} = (m_0 c, \mathbf{0})$ . This then allows us to determine the energy of the first particle in this frame:

$$E_1^\star = \frac{m_0^2 + m_1^2 - m_2^2}{2m_0} c^2 \quad (6.53)$$

We can then use the known mass of particle 1 in order to find the magnitude of its momentum in the zero momentum frame:

$$|\mathbf{p}_1^\star|^2 = \frac{m_0^4 + m_1^4 + m_2^4 - 2m_0^2 m_1^2 - 2m_0^2 m_2^2 - 2m_1^2 m_2^2}{4m_0^2} c^2 \quad (6.54)$$

If we then chose our axes, such that particle 1 was emitted in the positive  $x$  direction, this would be sufficient to fully reconstruct the 4-momentum  $\mathbf{P}_1$  in the zero momentum frame, and then, by appropriate use of Lorentz transformation, we can determine the components of  $\mathbf{P}_1$  in any frame we desire. Importantly, if  $m_0 = 0$ , meaning that we started with a single photon, these equations break down completely. It is for this reason that pair production can not occur in a vacuum, it is impossible to conserve energy and momentum while producing massive particles from a photon. We can see this very intuitively as follows, suppose a single photon spontaneously produces a positron and an electron. There will always be a frame of reference in which the total momentum of the two particles is zero, and as such in this frame the photon must have had zero momentum. However, since a photon must always move at speed  $c$ , it can only have zero momentum if it has zero energy, or in other words, it doesn't exist. Thus, the original event could not possibly have happened.

### 6.4.2 Compton Scattering

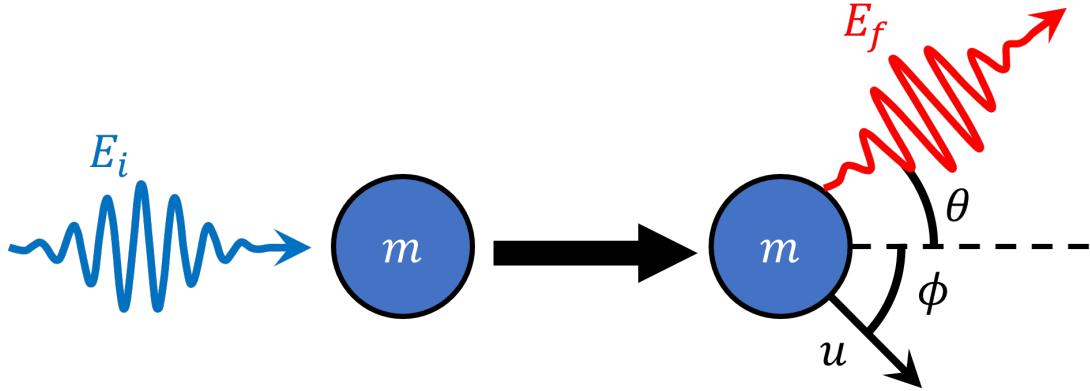


Figure 6.2: An example of Compton Scattering.

Compton scattering is, in its most general sense, a collision between a massless particle and a massive particle. In practice, the only common example of this occurs between photons and electrons. Now in principle, we could always analyse this collision using the procedure outlined in section 6.4.1; however, since it turns out that the most useful case to consider starts with the electron at rest, we shall simply perform all of our analysis in this frame. If we choose our axes such that the particles move in the  $x$ - $y$  plane, then our 4-momenta become:

$$\begin{aligned} P_{pi}^\mu &= \frac{E_i}{c}(1, 1, 0, 0) & P_{ei}^\mu &= m_e c(1, 0, 0, 0) \\ P_{pf}^\mu &= \frac{E_f}{c}(1, \cos \theta, \sin \theta, 0) & P_{ef}^\mu &= \frac{E_e}{c}(1, \beta_u \cos \phi, -\beta_u \sin \phi, 0) \end{aligned} \quad (6.55)$$

Where  $pi$ ,  $pf$ , and  $ef$  refer to the initial and final values for the photon and electron respectively. If we now apply the conservation of 4-momentum, and evaluate the dot product  $(P_{pi} + P_{ei} - P_{pf}) \cdot (P_{pi} + P_{ei} - P_{pf}) = P_{ef} \cdot P_{ef}$ , we obtain:

$$m_e^2 c^2 + 2m_e E_i - 2m_e E_f - \frac{2E_i E_f (1 - \cos \theta)}{c^2} = m_e^2 c^2 \quad (6.56)$$

Rearranging this gives us a formula for the energy of the outbound photon as a function of the scattering angle. It is then a simple matter to apply conservation of energy, and obtain a corresponding formula for the energy of the electron.

$$E_f = \frac{m_e c^2 E_i}{m_e c^2 + E_i (1 - \cos \theta)} \quad E_e = m_e c^2 + \frac{E_i^2 (1 - \cos \theta)}{m_e c^2 + E_i (1 - \cos \theta)} \quad (6.57)$$

By equating the components of the momenta along both axes, one can then arrive at the following formula for the recoil angle of the electron. It is worth noting that, this implies the existence of a maximum recoil angle of  $\frac{\pi}{2}$ .

$$\cot \phi = \left(1 + \frac{E_i}{mc^2}\right) \tan\left(\frac{\theta}{2}\right) \quad (6.58)$$

## 6.5 Tensors

We are going to finish our discussion of special relativity, by briefly commenting on tensors, and how they relate to the Lorentz transforms. If we recall the introduction to section 6.3, we established that there are different ways in which an object can be Lorentz invariant. It could simply be a scalar, and so remain completely unaffected by a change in reference frames, or it could be a 4-vector, in which case its components will change in such a way that the underlying mathematical object remains the same. There is however, no reason why we have to stop at a 4-vector, in principle we could generate objects with an arbitrarily large number of components, and this is the central idea behind a tensor. However, for the sake of simplicity, we shall restrict our considerations to rank two tensors, which have a total of 16 components, in four dimensional space-time. One way for us to think about tensors of this type is as a linear mapping between any two 4-covectors and the real numbers. That is to say that, for a tensor  $\mathbf{T}$ :

$$\begin{aligned} \mathbf{T}(\boldsymbol{\omega}, \boldsymbol{\chi}) \mapsto \mathbb{R} \quad \text{such that} \quad & \mathbf{T}(a\boldsymbol{\chi} + b\boldsymbol{\omega}, \boldsymbol{\zeta}) = a\mathbf{T}(\boldsymbol{\chi}, \boldsymbol{\zeta}) + b\mathbf{T}(\boldsymbol{\omega}, \boldsymbol{\zeta}) \\ & \mathbf{T}(\boldsymbol{\zeta}, a\boldsymbol{\omega} + b\boldsymbol{\chi}) = a\mathbf{T}(\boldsymbol{\zeta}, \boldsymbol{\omega}) + b\mathbf{T}(\boldsymbol{\zeta}, \boldsymbol{\chi}) \end{aligned} \quad (6.59)$$

Just as we have done before, we can utilise the linearity of the tensor's mapping to expand it out in a set of basis tensors. If we define the basis  $\vec{\mathbf{e}}_\mu \otimes \vec{\mathbf{e}}_\nu (\tilde{\mathbf{e}}^\rho, \tilde{\mathbf{e}}^\sigma) = \delta_{\mu\rho}\delta_{\nu\sigma}$  we can express an arbitrary tensor as:

$$\mathbf{T} = T^{\mu\nu} \vec{\mathbf{e}}_\mu \otimes \vec{\mathbf{e}}_\nu \iff \mathbf{T}(\boldsymbol{\omega}, \boldsymbol{\chi}) = T^{\mu\nu} \omega_\mu \chi_\nu \quad (6.60)$$

Where the interpretation of tensor addition is much the same as the interpretation of covector addition, that we developed in section 6.3. Formally speaking, what we have described here is a twice contravariant tensor, because it has two raised indices, the validity of which can be readily checked by considering that the summation of  $T^{\mu\nu} \omega_\mu \chi_\nu$  must be Lorentz invariant, which leads us to obtain the transformation law:

$$T'^{\rho\sigma} = \Lambda_\mu^\rho T^{\mu\nu} \Lambda_\nu^\sigma \quad (6.61)$$

We can, in much the same way, go about introducing a twice covariant tensor, which acts as a mapping between two 4-vectors and the real numbers. In fact we have already met one such tensor, the Minkowski metric  $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ , which maps two 4-vectors onto their dot product. Just as before, it is possible to juggle the indices of a tensor by contracting it with the metric to obtain:

$$T_{\rho\sigma} = \eta_{\rho\mu} T^{\mu\nu} \eta_{\nu\sigma} \quad (6.62)$$

Finally, we can construct tensors from 4-vectors, through the use of the so called tensor product. This product is defined, such that:

$$\mathbf{T} = \mathbf{V} \otimes \mathbf{U} \iff T^{\mu\nu} = V^\mu U^\nu \iff \mathbf{T}(\boldsymbol{\omega}, \boldsymbol{\chi}) = \boldsymbol{\omega}(\mathbf{V}) \boldsymbol{\chi}(\mathbf{U}) \quad (6.63)$$

### 6.5.1 The Stress-Energy Tensor

In section 6.3.3, we briefly encountered the idea of a 4-flux, which describes how some physical quantity, such as electric charge, is distributed throughout space time. The stress-energy tensor captures this same idea, but represents the flux of a 4-vector, the 4-momentum to be precise. To understand this, let us consider the energy density of some region in space. When we apply a Lorentz transform to change reference frames, we would expect that as the time-like component of a 4-vector the energy would increase by a factor of  $\gamma$ , with some additional correction if there was already momentum present in that region of space. However, because of length contraction, the Lorentz transformation will also decrease the volume that this energy occupies by a factor of  $\gamma$ . As such, the energy density must scale with  $\gamma^2$ , which would be typical for the time-like component of a rank two 4-tensor. The tensor in question turns out to be the stress-energy tensor, which can be interpreted by noting that the element  $T^{\mu\nu}$  represents the flux of the  $P^\mu$  component of the 4-momentum, through a surface of constant  $X^\nu$ .

To demonstrate the principles behind the stress-energy tensor, we shall determine its form, in the case of an ideal fluid, which is in thermal equilibrium. If we consider an element of fluid in its rest frame, then its energy density must be equal to  $\rho_0 c^2$ , where  $\rho_0$  is its rest density. Since we are in the rest frame, the momentum density must be zero ,and because there is no flow of energy through conduction, the energy flux must also be zero. If we note that force is the rate of change of momentum, then we can conclude that the hydrostatic pressure  $p$ , must be contributing a force, which is equivalent to a flow of momentum, normal to any given surface. As such, in the local rest frame we have:

$$T^{*\mu\nu} = \begin{pmatrix} \rho_0 c^2 & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix} \quad (6.64)$$

If we note that, in this rest frame, the tensor product of the fluid's flow 4-velocity, with itself, can be simply given by  $U^\mu U^\nu = \text{diag}(c^2, 0, 0, 0)$ , we can express the stress energy tensor as:

$$T^{\mu\nu} = \left( \rho_0 + \frac{p}{c^2} \right) U^\mu U^\nu - p \eta^{\mu\nu} \iff \mathbf{T} = \left( \rho_0 + \frac{p}{c^2} \right) \mathbf{U} \otimes \mathbf{U} - p \boldsymbol{\eta} \quad (6.65)$$

Where  $\eta^{\mu\nu} = \text{diag}(1, -1, -1, -1)$  is the inverse metric tensor, which maps any two covectors to the dot product of their associated vectors. Since this tensor equation holds true in one reference frame, it must hold true in all inertial frames. Hence, we have arrived at a general expression for the stress-energy tensor of an ideal fluid. One important point to note here is that  $T^{\mu\nu} = T^{\nu\mu}$ . This symmetry turns out to be a very general property of the stress energy tensor and is of crucial importance in general relativity.

Just as we saw in section 6.3.3, we can express 4-momentum conservation in terms of the 4-divergence of the stress energy tensor. That is to say that, if the rate of change of 4-momentum in a given volume is to be exactly equal to the 4-momentum flowing out of it, we must have:

$$\boldsymbol{\partial} \cdot \mathbf{T} = \mathbf{0} \iff \partial_\nu T^{\mu\nu} = 0 \quad (6.66)$$

### 6.5.2 Angular Momentum

The final tensor that we are going to consider represents an object's angular momentum, within the framework of 4-dimensional space time. Naively we might expect that, just as the linear momentum morphed into the 4-momentum, when extended to special relativity, the angular momentum would have an associated 4-vector as well. However, it quickly becomes apparent from the definition of the classical angular momentum,  $\mathbf{l} = \mathbf{x} \times \mathbf{p}$ , that since the components of both  $\mathbf{x}$  and  $\mathbf{p}$  transform with the Lorentz matrices, the transformation law for the components of  $\mathbf{l}$  must be more complicated. The reason for this discrepancy ultimately lies in the non-generality of the cross product, since the cross product of two vectors can only be well defined in a three dimensional space, it clearly isn't going to translate directly into four dimensional space-time. Instead, we are going to consider a generalisation of the cross product, known as the exterior, or wedge product of two vectors. This is another way of combining two vectors to generate a tensor, and is defined as:

$$\mathbf{V} \wedge \mathbf{U} = \mathbf{V} \otimes \mathbf{U} - \mathbf{U} \otimes \mathbf{V} \iff (\mathbf{V} \wedge \mathbf{U})^{\mu\nu} = V^\mu U^\nu - V^\nu U^\mu \quad (6.67)$$

In general, the exterior product of two vectors is an antisymmetric ( $T^{\mu\nu} = -T^{\nu\mu}$ ) rank two tensor, which in three dimensions can be uniquely associated to a vector, through a process known as Hodge conjugation. In four dimensions however, we simply have to make do with leaving our answer in tensor form. As such, we define the relativistic angular momentum to be given by the exterior product:

$$\mathbf{L} = \mathbf{X} \wedge \mathbf{P} \iff L^{\mu\nu} = X^\mu P^\nu - X^\nu P^\mu \quad (6.68)$$

As an antisymmetric, 4-dimensional, second rank tensor, it follows that  $\mathbf{L}$  only has six independent components (the diagonal components are all necessarily zero and the antisymmetry relation means that the remaining twelve components are split into pairs), three of which correspond directly to the components of the classical angular momentum. The remaining three components relate to the additional 3-vector quantity  $\mathbf{n} = c^2 t \mathbf{p} - E \mathbf{x}$ , which must also be conserved, if we wish to maintain consistency with the conservation of  $\mathbf{l}$ , in all inertial frames.

As it happens, the conservation of angular momentum follows directly from the symmetry of the stress-energy tensor. To see this, let us consider the flux of the angular momentum, which will be given by  $M^{\mu\nu\rho} = X^\mu T^{\nu\rho} - X^\nu T^{\mu\rho}$ , as per the definition of the stress energy tensor. Thus, the 4-divergence of this flux is given by:

$$\partial_\rho M^{\mu\nu\rho} = X^\mu (\partial_\rho T^{\nu\rho}) - X^\nu (\partial_\rho T^{\mu\rho}) + T^{\nu\mu} - T^{\mu\nu} \quad (6.69)$$

If we substitute in the stress-energy continuity equation (6.66), this expression reduces to simply give  $\partial_\rho M^{\mu\nu\rho} = T^{\nu\mu} - T^{\mu\nu}$ . As such, we obtain the result that, whenever the stress-energy tensor is symmetric, the angular momentum must satisfy the continuity equation:

$$\boldsymbol{\partial} \cdot \mathbf{M} = \mathbf{0} \iff \partial_\rho M^{\mu\nu\rho} = 0 \quad (6.70)$$

# 7 Gravitation

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## 7.1 The Gravitational Field

Field theories have historically been some of the most successful models in all of physics. Understanding fields really is integral to understanding modern physics, and for that matter large chunks of classical physics as well. For that reason, we are going to look at the first field theory, that of Newtonian Gravity. Before we get started, we should quickly explain exactly what a field is, and then specifically what is meant by a gravitational field. A field is simply any function of both position and time, which has some kind of physical effect. In particular, we often think about force fields, where the value of the field at a given point is related to the force felt by an object at that point in space. This is the case for the gravitational field  $\mathbf{g}(\mathbf{r})$ , which is defined such that the force felt by a mass  $m$  at position  $\mathbf{r}$  is given by:

$$\mathbf{F}(\mathbf{r}) = m\mathbf{g}(\mathbf{r}) \quad (7.1)$$

This highlights one of the most important properties of gravity, any object will accelerate at exactly the same rate in a gravitational field, irrespective of its mass, precisely because the force scales linearly with the mass. In fact, it was this observation which was key in Einstein's discovery of general relativity; however, for our purposes we shall just consider it as part of the definition of gravity.

### 7.1.1 Newton's Universal Law of Gravitation

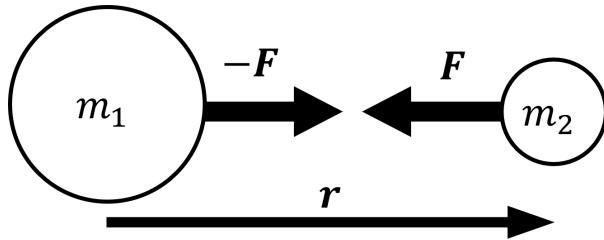


Figure 7.1: Two gravitationally interacting masses.

bold face to specify a vector's magnitude throughout this chapter. Note that the minus sign is put in place since gravity is a purely attractive interaction, meaning that the force must act in the opposite direction to the separation. If we compare this to equation (7.1), we can see that the gravitational field generated by a point mass  $M$  located at position  $\mathbf{r}'$  is quite simply:

$$\mathbf{g}(\mathbf{r}) = -\frac{GM}{|\mathbf{r} - \mathbf{r}'|^3}(\mathbf{r} - \mathbf{r}') \quad (7.3)$$

Now we are going to consider the gravitational field that is generated by a system of several point masses. It is implicitly stated in Newton's law that the pairwise forces are independent of each other, and as such, the force on any given body is simply the sum of all the forces acting on it from other masses.

This is really a statement of the fact that the gravitational field is linearly related to the presence of masses, and as such the field produced by a set of  $n$  masses, with masses  $m_i$  and positions  $\mathbf{r}_i$  is given by:

$$\mathbf{g}(\mathbf{r}) = - \sum_{i=1}^n \frac{Gm_i}{|\mathbf{r} - \mathbf{r}_i|^3} (\mathbf{r} - \mathbf{r}_i) \quad (7.4)$$

If we wish to extend this to continuous mass distributions, then we model every mass element  $dm = \rho dV$  as an infinitesimal point mass. As such, we can say that the field is given by the integral:

$$\mathbf{g}(\mathbf{r}) = - \int_{\mathbb{R}^3} \frac{G\rho(\mathbf{r}') (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} dV' \quad (7.5)$$

Where  $\rho(\mathbf{r}')$  represents the mass density at position  $r'$ . The interesting thing about this result is that, unlike equation (7.4), which diverges whenever  $\mathbf{r} = \mathbf{r}_i$ , this expression for the gravitational field will converge everywhere, as long as  $\rho(\mathbf{r})$  is finite. The reason for this is that although the field follows an inverse square law, the volume and hence mass of a small element is proportional to its size cubed and thus the field produced by an infinitesimal mass element is still itself infinitesimal. In a sense, we are actually evaluating an improper integral which takes the range of integration to be all space except position  $\mathbf{r}$ , in the same way that one can evaluate the integral  $\int_0^a \frac{dx}{\sqrt{x}}$  despite the integrand's divergence at the origin. It is for this reason that, when using equation (7.4), we have to make sure to ignore the field produced by the mass we are calculating the force on, whereas in equation (7.5) we do not<sup>5</sup>. If we are dealing with a continuous mass system, then we also need to evaluate an integral to determine the total gravitational force acting on a body. This is given by:

$$\mathbf{F} = \int_V \rho(\mathbf{r}) \mathbf{g}(\mathbf{r}) dV \quad (7.6)$$

Where the range of interaction  $V$  is the full volume of the object in question. It follows from considerations of symmetry that any isolated system will experience no resultant gravitational force acting on it, which is in keeping with the principle of momentum conservation. Similarly, one can compute the torque acting on a body due to gravity, which will give an analogous result for an isolated system, by evaluating the integral:

$$\mathbf{G} = \int_V \rho(\mathbf{r}) \mathbf{r} \times \mathbf{g}(\mathbf{r}) dV \quad (7.7)$$

The fact that gravity can produce a torque on an extended body is actually very important for explaining phenomena such as the tidal locking, which is what keeps one side of the Moon facing the Earth. Furthermore, we should notice that unless  $\mathbf{g}$  is approximately uniform, which is the case on the surface of the earth, this does not necessarily imply that a gravitational force acts through an object's centre of mass.

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<sup>5</sup>Assuming that  $\rho(\mathbf{r})$  is finite. It is possible to gain equation (7.4) from (5) through use of the Dirac delta function and obviously in this case we must apply the same principle to obtain a finite result.

### 7.1.2 Gravitational Potential

Although the gravitational field is conceptually easier to understand, in the sense that it represents something manifestly physical, the acceleration felt by a body at a given point in space, mathematically it is convenient to formulate everything in terms of a scalar potential. This formalism arises from the fact that the gravitational field is conservative, that is to say that no work is done on a body moving in a closed loop. Mathematically we can express this by saying that:

$$\nabla \times \mathbf{g}(\mathbf{r}) = \mathbf{0} \implies \mathbf{g}(\mathbf{r}) = -\nabla\Phi(\mathbf{r}) \quad (7.8)$$

The scalar field  $\Phi(\mathbf{r})$  is referred to as the gravitational potential, and is defined by the above relationship to the gravitational field. However, this definition is not unique, something which is not in and of itself a problem so long as any ambiguities do not have physical consequences, but for simplicity we often impose the restriction that  $\Phi \rightarrow 0$  as  $|\mathbf{r}| \rightarrow \infty$ , which is sufficient to uniquely define the potential. If we apply this definition to equation (7.5), we obtain the following general form of the potential:

$$\Phi(\mathbf{r}) = - \int_{\mathbb{R}^3} \frac{G\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' \quad (7.9)$$

The benefits of this approach are twofold: firstly, as a scalar field  $\Phi$  is simply easier to manipulate and visualise than the vector field  $\mathbf{g}$ , and secondly, we can use the potential to construct a conserved quantity, which is always useful in physics. If we note that for a particle with position  $\mathbf{r}$ , its acceleration is described by  $\ddot{\mathbf{r}} = \mathbf{g}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$ , we can say that:

$$\frac{d}{dt} \left[ \frac{1}{2} \dot{\mathbf{r}} \cdot \dot{\mathbf{r}} + \Phi(\mathbf{r}) \right] = \dot{\mathbf{r}} \cdot \ddot{\mathbf{r}} + \nabla\Phi(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0 \quad (7.10)$$

Physically, we interpret this by identifying the particle's conserved total energy  $E$  to be given by its mass  $m$  multiplied by the conserved quantity above. Since we identify the first term as the particle's kinetic energy, we can conclude that the potential represents the work done per unit mass when moving an object from infinity (where  $\Phi$  is defined to be zero) to its current position.

$$E = \frac{m}{2} \dot{\mathbf{r}} \cdot \dot{\mathbf{r}} + m\Phi(\mathbf{r}) \quad (7.11)$$

One way to conceptualise this gravitational potential is to think of each mass as a sort of potential well. When lots of mass is concentrated together, it forms a fairly deep and reasonably steep well, which other nearby masses fall into. This gives rise to the phenomenon of gravitational attraction as discussed in section 1.1.

It is worth taking the opportunity here to briefly remark on the exact nature of energy. Simply put, energy is defined in such a way that, it must necessarily be conserved, when an experiment is found that appears to violate conservation of energy (for example near light speed collisions) we simply develop a new physical theory which defines the energy in a slightly different way, such that it is conserved. The assertion that it is even possible construct such a conserved quantity is one of the most fundamental postulates of physics and is supported not by theoretical considerations but by an overwhelming amount of empirical evidence.

### 7.1.3 Poisson's Equation and Gauss' Law

Since we want to start working in terms of the potential field, it would be helpful if we could reformulate Newton's law of gravitation into a more convenient representation. As it turns out, the way to do this is by considering the Laplacian of the potential. If we take the Laplacian of equation (7.9) we determine that:

$$\nabla^2 \Phi(\mathbf{r}) = - \int_{\mathbb{R}^3} G\rho(\mathbf{r}') \nabla^2 \frac{1}{|\mathbf{r} - \mathbf{r}'|} dV' = \int_{\mathbb{R}^3} G\rho(\mathbf{r}') \nabla \cdot \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} dV' \quad (7.12)$$

Evaluating this divergence turns out to require some slightly subtle manipulation. We can use the vector calculus identity that  $\nabla \cdot (\psi \mathbf{F}) = \nabla\psi \cdot \mathbf{F} + \psi \nabla \cdot \mathbf{F}$  to say that:

$$\nabla \cdot \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} = -\frac{3(\mathbf{r} - \mathbf{r}') \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^5} + \frac{3}{|\mathbf{r} - \mathbf{r}'|^3} \quad (7.13)$$

That is to say that,  $\forall \mathbf{r} \neq \mathbf{r}'$  the divergence is well defined and equal to zero. However, when  $\mathbf{r} = \mathbf{r}'$ , the field is not differentiable and so the divergence does not have a finite value. However we can still gain an insight into the function's behaviour by utilising Gauss' theorem:

$$\int_V \nabla \cdot \mathbf{A} dV = \oint_{\partial V} \mathbf{A} \cdot d\mathbf{S} \quad (7.14)$$

Now technically this result is only valid everywhere that the field  $\mathbf{A}$  is differentiable, such that  $\nabla \cdot \mathbf{A}$  is well defined. However, what we can do is evaluate the surface integral in the simple case of a unit sphere centred on  $\mathbf{r}'$  and then use Gauss' theorem to relate this surface integral to any other we may wish to consider. This gives us the result:

$$\oint_{\partial V} \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \cdot d\mathbf{S} = \begin{cases} 4\pi & \mathbf{r}' \in V \\ 0 & \mathbf{r}' \notin V \end{cases} \quad (7.15)$$

If we note that the Dirac delta function (which in truth is not a function but a distribution, although the distinction is only really important to mathematicians) is defined by:

$$\int_V \delta(\mathbf{r}) dV = \begin{cases} 1 & \mathbf{0} \in V \\ 0 & \mathbf{0} \notin V \end{cases} \quad (7.16)$$

It is apparent that we could achieve a full consistency with Gauss' theorem by stating that:

$$\nabla \cdot \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} = 4\pi\delta(\mathbf{r} - \mathbf{r}') \quad (7.17)$$

Substituting this into equation (7.12) then yields Poisson's equation:

$$\nabla^2 \Phi(\mathbf{r}) - 4\pi G\rho(\mathbf{r}) = 0 \quad (7.18)$$

A more elegant formulation of gravitational theory is, to take Poisson's equation as a fundamental physical postulate, along with the definition that  $\mathbf{g}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$ , in order to derive all of our previous results.

This also gives rise to another incredibly useful principle, Gauss' law (not to be confused with Gauss' theorem, despite the similarities between the two), which allows us to calculate gravitational fields fairly quickly in high symmetry situations. Gauss' law is obtained by first rewriting Poisson's equation (7.18) in terms of the gravitational field and then applying Gauss' theorem:

$$\nabla \cdot \mathbf{g}(\mathbf{r}) = -4\pi G\rho(\mathbf{r}) \implies \oint_{\partial V} \mathbf{g}(\mathbf{r}) \cdot d\mathbf{S} = -4\pi GM_V \quad (7.19)$$

Where  $M_V$  is the total mass contained within the volume  $V$ . To demonstrate the utility of this law, we shall calculate the gravitational field produced by a uniform solid sphere of mass  $M$  and radius  $a$ . Given the symmetry of the situation, it makes sense for us to adopt a spherical polar coordinate system concentric with the massive sphere. We can then consider the case where the volume  $V$  is the interior of a sphere of radius  $r$ :

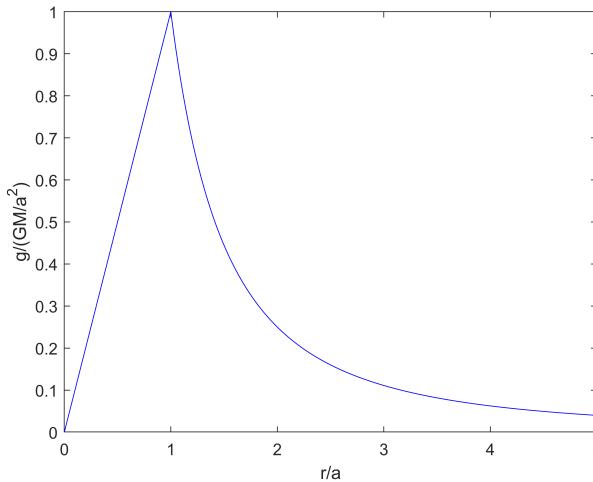
$$M_V = \begin{cases} \frac{Mr^3}{a^3} & r \leq a \\ M & r > a \end{cases} \quad (7.20)$$

By symmetry, the gravitational field must be radially outwards from the sphere, and must have a constant magnitude everywhere on the surface of a sphere with radius  $r$ . As such we can conclude that:

$$\oint_{\partial V} \mathbf{g}(\mathbf{r}) \cdot d\mathbf{S} = 4\pi r^2 g(r) \quad (7.21)$$

Where  $\mathbf{g}(\mathbf{r}) = g(r)\frac{\mathbf{r}}{r}$ . Applying Gauss's law then allows us to calculate the gravitational field everywhere:

$$\mathbf{g}(\mathbf{r}) = \begin{cases} -\frac{GM}{a^3}\mathbf{r} & r \leq a \\ -\frac{GM}{r^3}\mathbf{r} & r > a \end{cases} \quad (7.22)$$



What we are actually seeing here is a consequence of Newton's shell theorem, which states that a spherical shell of mass produces no field in its interior and produces a field identical to that of a point mass in its exterior. Newton derived this from purely geometric arguments; however, a worthwhile exercise for the reader would be to derive it by explicitly evaluating the integral in equation (7.5).

Figure 7.2: The gravitational field strength produced by a uniform sphere.

## 7.2 Gravitational Energy

We are now going to discuss the concept of gravitational potential energy, that is the energy stored by the gravitational interactions of different masses. As such, we need a working definition for the gravitational potential energy of a system. Thus, we define the total gravitational energy to be the work that must be done in order to construct the system in its given state, by bringing all of the masses together from an infinite separation (where they have no interaction). Since gravity is always an attractive force, this energy will always be negative, since work will always be required to separate the masses.

### 7.2.1 Potential Energy

Let us start with the simplest example of two interacting point masses. If we neglect the self energy of the masses, that is to say that we define a point mass in isolation to have zero potential energy, then the total gravitational potential energy is given by:

$$U(\mathbf{r}_1, \mathbf{r}_2) = -\frac{Gm_1m_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (7.23)$$

Where  $m_1, m_2, \mathbf{r}_1, \mathbf{r}_2$  are the masses and positions of the two bodies respectively. It is important to bear in mind that this energy is not attributed to any one of the masses, but is instead a general property of the entire system. To see why this is the case we can simply consider the time derivative of the total energy  $E = \frac{1}{2}(m_1|\dot{\mathbf{r}}_1|^2 + m_2|\dot{\mathbf{r}}_2|^2) + U(\mathbf{r}_1, \mathbf{r}_2)$ .

$$\dot{E} = \left[ m_1 \ddot{\mathbf{r}}_1 + \frac{Gm_1m_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3} (\mathbf{r}_1 - \mathbf{r}_2) \right] \cdot \dot{\mathbf{r}}_1 + \left[ m_2 \ddot{\mathbf{r}}_2 + \frac{Gm_1m_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3} (\mathbf{r}_2 - \mathbf{r}_1) \right] \cdot \dot{\mathbf{r}}_2 \quad (7.24)$$

If we were to substitute in Newton's Law of gravitation from section 1.1, we would find that in the absence of any external forces  $\dot{E} = 0$  exactly as it should be in order to maintain consistency with the principle of conservation of energy.

We can now try to apply this principle to an arbitrary mass distribution  $\rho(\mathbf{r})$  that has a velocity field  $\mathbf{v}(\mathbf{r})$ . If we calculate the total kinetic energy of this mass distribution, we obtain:

$$T = \frac{1}{2} \int_{\mathbb{R}^3} \rho(\mathbf{r}) \mathbf{v}(\mathbf{r}) \cdot \mathbf{v}(\mathbf{r}) dV \quad (7.25)$$

Differentiating this integral, then substituting in the results that  $\dot{\rho} = -\nabla \cdot (\rho \mathbf{v})$  and  $\dot{\mathbf{v}} = \mathbf{g} - (\mathbf{v} \cdot \nabla) \mathbf{v}$ , we obtain:

$$\dot{T} = \int_{\mathbb{R}^3} \rho(\mathbf{r}) \mathbf{v}(\mathbf{r}) \cdot \mathbf{g}(\mathbf{r}) - \frac{1}{2} \nabla \cdot (\rho(\mathbf{r}) (\mathbf{v}(\mathbf{r}) \cdot \mathbf{v}(\mathbf{r})) \mathbf{v}(\mathbf{r})) dV \quad (7.26)$$

Where we have used the result that  $\nabla \cdot (\rho(\mathbf{v} \cdot \mathbf{v}) \mathbf{v}) = \nabla \cdot (\rho \mathbf{v}) \mathbf{v} \cdot \mathbf{v} + 2\rho \mathbf{v} \cdot (\mathbf{v} \cdot \nabla) \mathbf{v}$ , to collect up some of the additional terms. If the mass distribution is localised, then  $\rho(\mathbf{r})$  must tend towards zero at infinity, and thus, the integral of the divergence must vanish. As such, we can say that:

$$\dot{T} = \int_{\mathbb{R}^3} \rho(\mathbf{r}) \mathbf{v}(\mathbf{r}) \cdot \mathbf{g}(\mathbf{r}) dV \quad (7.27)$$

We can now use the identity  $\nabla \cdot (\psi \mathbf{F}) = \psi \nabla \cdot \mathbf{F} + \mathbf{F} \cdot \nabla \psi$  to evaluate this integral by parts, with the substitutions  $\mathbf{g} = -\nabla \Phi$  and  $\dot{\rho} = -\nabla \cdot (\rho \mathbf{v})$ , to obtain:

$$\dot{T} = - \int_{\mathbb{R}^3} \dot{\rho}(\mathbf{r}) \Phi(\mathbf{r}) dV = \iint_{\mathbb{R}^3 \mathbb{R}^3} \frac{G \dot{\rho}(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' dV \quad (7.28)$$

If we note that in this expression  $\mathbf{r}$  and  $\mathbf{r}'$  are completely interchangeable, we can separate the integrand out into two distinct terms, yielding the result:

$$\dot{T} = -\frac{1}{2} \int_{\mathbb{R}^3} \dot{\rho}(\mathbf{r}) \Phi(\mathbf{r}) + \rho(\mathbf{r}) \dot{\Phi}(\mathbf{r}) dV \quad (7.29)$$

It therefore follows that, if we wish for our total energy  $E = T + U$  to be conserved, we require  $\dot{U} = -\dot{T}$ , which we can then integrate to find an expression for the potential energy. Of course, there is always an ambiguity of an arbitrary additive constant in the potential energy, so we utilise the definition that  $U = 0$ , when all of the masses are infinitely separated, which implies the potential energy should be zero, when the density is equal to zero.

$$U = \frac{1}{2} \int_{\mathbb{R}^3} \rho(\mathbf{r}) \Phi(\mathbf{r}) dV \quad (7.30)$$

There are a great many ways of arriving at equation (7.30), such as considering all of the pairwise interactions of the individual mass elements, which is essentially what we did with equation (7.23), and then adding in a factor of  $\frac{1}{2}$  to account for double counting. Another method is to explicitly calculate the work done in building up the mass distribution, by considering the case when the density is  $\alpha \rho(\mathbf{r})$  and then increasing  $\alpha$  from 0 to 1. This is the method that we shall employ in chapter 8, when we derive similar results; however, the above derivation is presented to provide some variety.

Let us now apply this result, to determine the gravitational potential energy stored in a uniformly dense sphere of mass  $M$  and radius  $a$ , such as the one we considered at the end of section 1.3. Using the results we derived earlier, the potential inside the sphere is:

$$\Phi(\mathbf{r}) = \frac{GM(r^2 - 3a^2)}{2a^3} \quad (7.31)$$

Substituting this, along with the density  $\rho = \frac{3M}{4\pi a^3}$ , into equation (7.30) gives us:

$$U = -\frac{3GM^2}{4a^6} \int_0^a (3a^2 - r^2)r^2 dr = -\frac{3GM^2}{2a^6} \left[ a^2 r^3 - \frac{r^5}{5} \right]_0^a = -\frac{3GM^2}{5a} \quad (7.32)$$

The release of this potential energy, when a low density cloud of dust collapses into a protostar, is one of the key mechanisms by which the core temperature is raised high enough to begin fusion. An interesting thing to note about this expression is that, it implies point masses have an infinite internal potential energy. Luckily however, this is not something we have to worry about, since point masses do not really exist in nature, and even if they did, that kind of length scale would be beyond the scope of classical Newtonian gravity anyway.

It would have also been possible to arrive at this result by explicitly building up the sphere with concentric shells of mass, and calculating the work done on each shell as it is brought in from infinity. Although methods such as this can often be quicker in simple, high symmetry examples like a sphere, the generality of equation (7.30) means that it is typically the easiest approach.

### 7.2.2 Energy Density of the Field

As we discussed, the potential energy of a system is not a property of the individual masses, but instead simply a property of the system itself. As a result, while we can always use equation (7.30) to calculate the total potential energy, there is always an ambiguity in the physical location of that energy. The most obvious, and most intuitive approach is to associate the potential energy with the masses in the system, which gives would give a potential energy density of  $\frac{\rho\Phi}{2}$ . However, there is another interpretation, which associates all of the energy with the gravitational field itself. To see how this result can be obtained, let us start with equation (7.30) for the total gravitational potential energy stored in a system. We can then use Poisson's equation from section 7.1.3 to express the density in terms of the potential:

$$U = \frac{1}{8\pi G} \int_{\mathbb{R}^3} \Phi(\mathbf{r}) \nabla^2 \Phi(\mathbf{r}) dV \quad (7.33)$$

If we recall the identity  $\nabla \cdot (\psi \mathbf{F}) = \psi \nabla \cdot \mathbf{F} + \mathbf{F} \cdot \nabla \psi$ , we can rewrite the integrand to give us the expression:

$$U = \frac{1}{8\pi G} \int_{\mathbb{R}^3} \nabla \cdot (\Phi(\mathbf{r}) \nabla \Phi(\mathbf{r})) - \nabla \Phi(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}) dV \quad (7.34)$$

It follows from Gauss' theorem that, since  $\Phi \rightarrow 0$  at infinity, the integral of the first term over all space vanishes. To see this, let us consider what would happen, if we carry the integration out over a volume bounded by a surface of constant  $\Phi$ . We can then apply Gauss' theorem to convert this into an integral over the equipotential surface. It then follows from Gauss' law that this surface integral will be equal to  $\Phi$  multiplied by a fixed constant (assuming that our region of integration always encompasses all of the present masses). Thus, if we let the size of this region tend to infinity,  $\Phi$  and hence the value of the integral will tend to zero. Finally, we can tidy up the second term somewhat by substituting in  $\mathbf{g}(\mathbf{r}) = -\nabla \Phi(\mathbf{r})$ , in order to obtain:

$$U = -\frac{1}{8\pi G} \int_{\mathbb{R}^3} \mathbf{g}(\mathbf{r}) \cdot \mathbf{g}(\mathbf{r}) dV \quad (7.35)$$

For this reason, the quantity  $\mathcal{G} = -\frac{\mathbf{g} \cdot \mathbf{g}}{8\pi G}$  is referred to as the energy density of the gravitational field. Of course, this result is far from unique; any function of the density, potential, and the field, which differs from  $\mathcal{G}$  by the divergence of a field that tends to zero sufficiently quickly, could also act as our energy density. However, the two results that we have encountered already,  $\frac{\rho\Phi}{2}$  and  $\mathcal{G}$ , are by far the simplest options, and as such, are the most commonly encountered. Luckily, the question of where energy is located only really becomes important in general relativity, which supersedes Newtonian gravitation anyway.

Interestingly, there is a way for us to formulate our theory of gravitation to remove this ambiguity. If we were to reformulate our model such that the fundamental postulates are Poisson's equation and the form of the potential energy density, we could then, in principle, derive all of the results that we have discussed already, such as Newton's universal law of gravitation. Of course, this only removes the ambiguity as a matter of definition, which is not particularly helpful, since we still need to know what the correct expression for the energy density is. The value of this approach would be that, if we were able to determine experimentally which form was correct, we could keep the number of postulates in our theory to a minimum, since the energy density would replace the now redundant force law  $\mathbf{F} = mg$ .

## 7.3 Conic Sections

Before we move on to discuss orbits in Newtonian gravity, we need to first take some time to examine some geometry. As it turns out, the solutions to the equation of motion for a body moving in the gravitational field of a point mass, all trace out trajectories in the form of conic sections. As such we should take the opportunity to cover the geometric properties of these shapes.

There exists a wide variety of ways to arrive at the properties of the conic sections, as the name implies they were originally discovered by considering the shapes generated at the intersection of a plane with a cone. However, for our purposes, the most useful and most general description of a conic section is in terms of focus-directrix properties. That is to say that, any conic section can be described as the locus of points such that the distance to a fixed point, the focus, is proportional to the distance from a fixed straight line, the directrix. The constant of proportionality for this relationship is known as the eccentricity  $e$ .

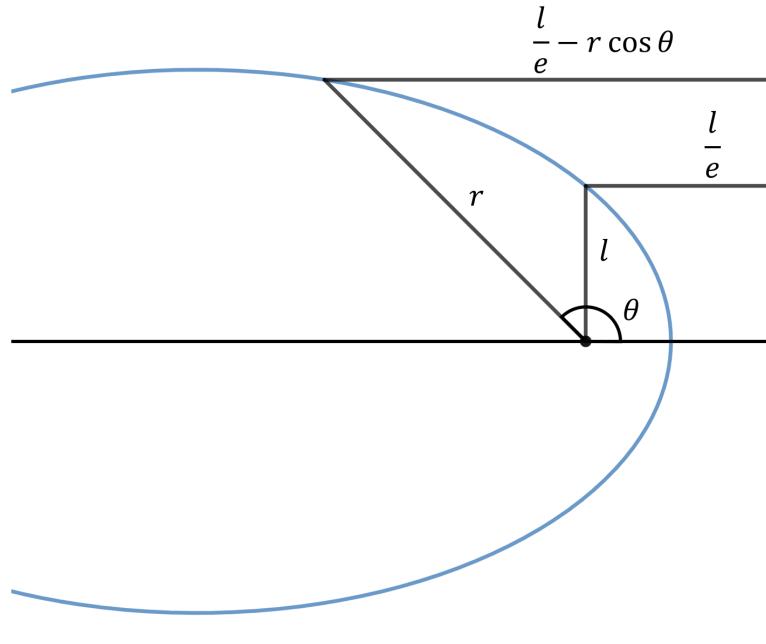


Figure 7.3: A general conic section.

Figure 7.3 shows an arbitrary conic section defined in this way. The semi-latus rectum  $l$  of the conic is defined to be the distance of the curve from the focus in the direction parallel to the directrix. It therefore follows that, by definition, the distance from the focus to the directrix must be  $\frac{l}{e}$ . Thus, if we consider an arbitrary point  $(r, \theta)$ , given in polar coordinates centred on the focus, we find that it must satisfy  $r = e \left( \frac{l}{e} - r \cos \theta \right)$ . We can rearrange this slightly to obtain the general form of a conic section:

$$\frac{l}{r} = 1 + e \cos \theta \quad (7.36)$$

The value of  $e$  then gives rise to several distinct cases, each of which has its own unique properties. We shall examine each of these in turn, in the following sections.

### 7.3.1 Circles

The simplest case to consider is that of a circle, which occurs when the eccentricity is equal to zero. In this case, the conic section traces out the locus of points a distance  $l$  from the focus, which is precisely the definition of a circle with a radius of  $l$ . Since circles are fairly well known shapes, we shall not spend a lot of time discussing their properties in detail, and instead we shall simply quote the important results. A circle of radius  $r$ , centred on the origin can be described by the Cartesian equation  $x^2 + y^2 = r^2$ , which follows directly from the Pythagorean theorem. By definition, the circumference of such a circle is given by  $2\pi r$ , which then implies that its area must be given by  $\pi r^2$ .

### 7.3.2 Ellipses

The next case that occurs is when the eccentricity is between zero and one, and is called an ellipse. It can be shown that, an equivalent description of an ellipse is in terms of two distinct foci, with the ellipse being the locus of all points such that the sum of the distances to each focus is the same. This description gives rise to a natural parametrisation of the ellipse in terms of its semi-major and semi-minor axes  $a$  and  $b$ . The semi-major axis  $a$  is equal to one half the length of the ellipse perpendicular to the directrix, and is related to the semi-latus rectum and eccentricity by:  $a(1 - e^2) = l$ . Both foci lie along this long axis of an ellipse, having a separation of  $2ae$  with the ellipse being the locus of points such that the sum of the distances to the foci equals  $2a$ . The semi-minor axis  $b$  is defined as one half the length of the ellipse parallel to the directrix and is given by  $b^2 = a^2(1 - e^2) = l^2(1 - e^2)^{-1}$ . From this definition of an ellipse, one can arrive at the Cartesian equation  $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$ , which implies that an ellipse is nothing more than a circle that has been stretched in one direction. Thus it follows that the area of an ellipse is simply given by  $\pi ab = \pi l^2(1 - e^2)^{-\frac{3}{2}}$ . The circumference of an ellipse is a rather non trivial matter, and as it turns out, can only be expressed as the result of an infinite series, or as the result of a special class of integral with no analytic solution, known as elliptic integrals.

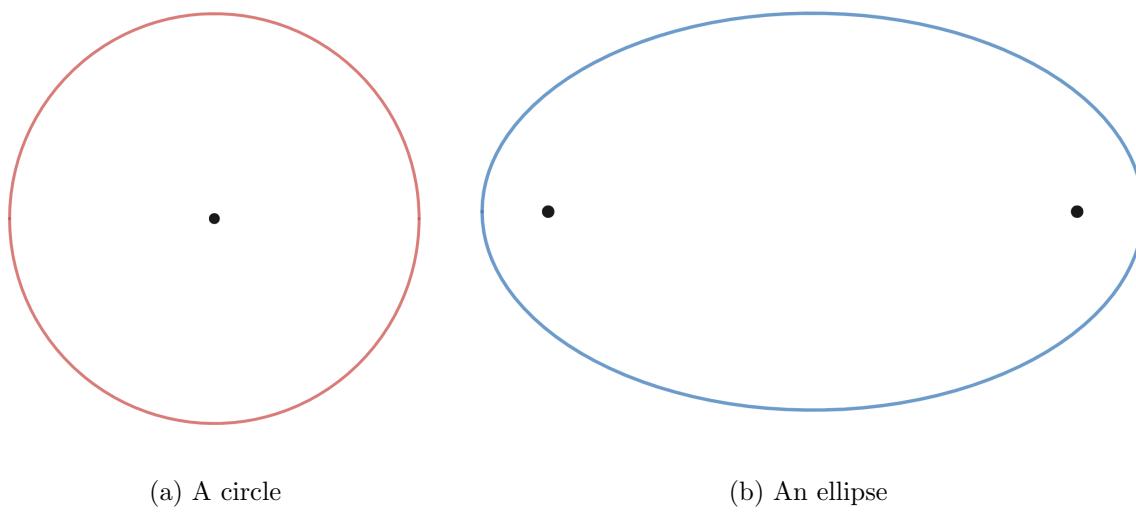


Figure 7.4: The two closed form conic sections.

### 7.3.3 Parabola

A parabola is the shape obtained in the special case that the eccentricity is precisely equal to one, and as such, it describes the locus of all points that are equidistant from the focus and the directrix. The most well known example of a parabola is the curve traced out by a quadratic function, such as  $y = x^2$ . For this parabola, the focus is located at the point  $(0, \frac{1}{4})$  with the directrix being the line  $y = -\frac{1}{4}$ . One can show, by simple rearrangement, that any general quadratic function  $y = ax^2 + bx + c$  will produce a version of this parabola that has been stretched and translated. As it happens, stretching a parabola in any direction, produces another parabola, and as such all quadratic functions must produce parabolic curves, when graphed. Perhaps the most useful property of a parabola is the fact that, if a mirror is constructed in the shape of a parabolic surface (technically in 3D this would be called a paraboloid), it will reflect any incoming parallel rays in such a way that they meet on its focal plane. It is for this reason that telescopes typically use parabolic collecting dishes.

### 7.3.4 Hyperbola

A hyperbola describes any conic section that has an eccentricity greater than one. In many ways a hyperbola is similar to an ellipse, as it too can be described in terms of two foci. However, the hyperbola represents the locus of points, such that the difference between the distances to each focus is a constant. If we centre our hyperbola on the origin, and set the distance between opposite vertices to be  $2a$  where  $a(e^2 - 1) = l$ , then the foci become positioned at  $(\pm ea, 0)$ . In order to draw analogy to an ellipse, we can define  $b$  such that  $b^2 = a^2(e^2 - 1)$ , and obtain the Cartesian equation of a hyperbola  $\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1$ . It follows from this equation that, at large distances from the foci, every hyperbola asymptotically approaches a pair of straight lines. Interestingly, this is precisely the behaviour displayed by the graph of  $y = \frac{1}{x}$ , which asymptotically approaches both the  $x$  and  $y$  axes. This is because, the curve is in fact a rectangular hyperbola, so called because its eccentricity of  $\sqrt{2}$  causes the two asymptotes to intersect at right angles.

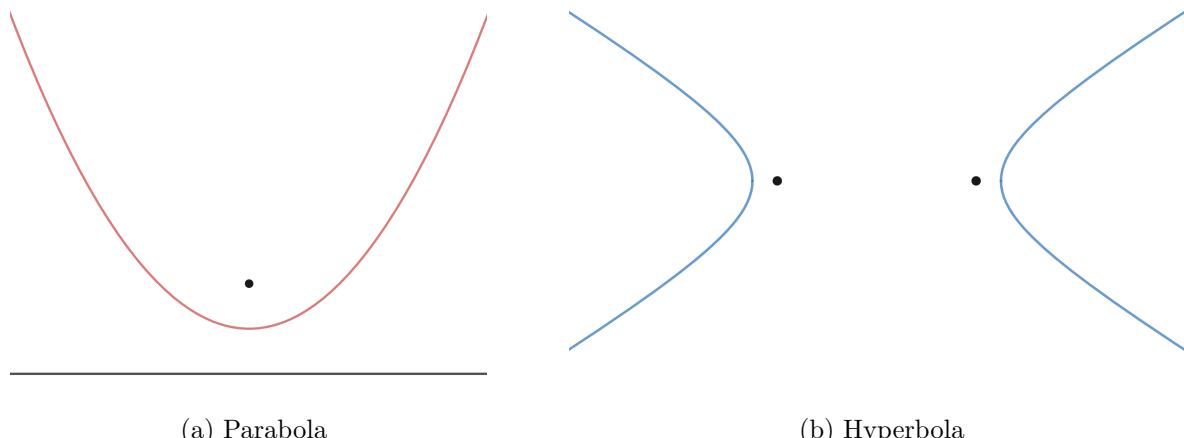


Figure 7.5: The two open conic sections.

## 7.4 Orbits

Now that we have established the basic geometry required to describe an orbit, we can actually go ahead and solve the equation of motion. To begin with, we shall consider the so called one body problem, which describes an infinitesimal test mass orbiting a much larger fixed mass. Despite the fact that the one body problem only really represents the limiting case of the more realistic two body problem, we shall see that Kepler's laws are all formulated in terms of this one body problem, because the sun is so massive that the solar system is fairly well described by this approximation. If we place our fixed mass  $M$  at the origin, then the equation of motion we need to solve is simply obtained from Newton's law:

$$\ddot{\mathbf{r}} + \frac{GM}{r^3}\mathbf{r} = \mathbf{0} \quad (7.37)$$

Even in this simplest of cases, there is no analytic form for the position of an orbiting body as a function of time. However, despite this, we can obtain a few, relatively simple laws, which describe the motion and trajectory of an orbiting body.

### 7.4.1 Kepler's Laws

Kepler's Laws are a set of rules which can be used to describe the solutions of equation (7.37). Kepler himself derived these laws by purely empirical means, and it was not until Newton that they were able to be understood in terms of any kind of theoretical model. In keeping with this, we shall first state the three laws before we go on to actually derive them in the later sections. Kepler's laws are as follows:

Kepler's first law states that all bound orbits take the form of ellipses, with one focus at the sun. More generally, we can take the first law to state that the trajectory of any body, moving in the Sun's gravitational field, will be a conic section focused on the Sun.

Kepler's second law states that the line joining the Sun to a planet will sweep out equal areas in equal times. This law describes how an orbiting body will speed up as it gets closer to the sun, and slow down as it gets farther away. This is actually a consequence of the conservation of angular momentum, as opposed to unique property of gravitation.

Kepler's third law states that the period of an orbit squared is proportional to the cube of its semi-major axis. More precisely, it states that the period of an orbit with semi-major axis  $a$  about a body of mass  $M$  is given by  $T^2 = \frac{4\pi^2}{GM}a^3$ .

Since it is the easiest to derive we shall start by considering Kepler's second law. It follows from simple geometry that if a body at position  $\mathbf{r}$  moves through an infinitesimal displacement  $d\mathbf{r}$ , it shall sweep out an area given by  $d\mathbf{A} = \frac{1}{2}\mathbf{r} \times d\mathbf{r}$ , and therefore the rate at which this area is swept out is given by:

$$\dot{\mathbf{A}} = \frac{1}{2}\mathbf{r} \times \dot{\mathbf{r}} = \frac{1}{2m}\mathbf{L} \quad (7.38)$$

Where  $m$  is the mass of the orbiting body, and  $\mathbf{L}$  is its angular momentum, defined to be  $\mathbf{L} = \mathbf{r} \times \mathbf{p} = m\mathbf{r} \times \dot{\mathbf{r}}$ . To see that the angular momentum is conserved we can simply note that  $\dot{\mathbf{L}} = m[\mathbf{r} \times \ddot{\mathbf{r}} + \dot{\mathbf{r}} \times \dot{\mathbf{r}}]$ , then substituting in equation (7.37) and recalling that any vector crossed with itself is  $\mathbf{0}$ , we find that  $\dot{\mathbf{L}} = \mathbf{0}$ , which directly implies Kepler's second law.

### 7.4.2 The Laplace-Runge-Lenz Vector

When solving differential equations, it is often helpful for us to find quantities that remain constant, throughout the system's motion. This is typically done by manipulating the original differential equation, such that we can equate the derivative of some quantity to zero. In the case of a Newtonian orbit, we can see, from equation (7.37), that we must have:

$$\dot{\mathbf{r}}(\mathbf{r} \cdot \ddot{\mathbf{r}}) - \mathbf{r}(\dot{\mathbf{r}} \cdot \ddot{\mathbf{r}}) + \frac{GM}{r}\dot{\mathbf{r}} - \frac{GM(\mathbf{r} \cdot \dot{\mathbf{r}})}{r^3}\mathbf{r} = 0 \quad (7.39)$$

If we multiply this equation by  $m^2$ , and then tidy up the first two terms with the vector triple product identity, we obtain the following result:

$$\mathbf{L} \times \dot{\mathbf{p}} + \frac{d}{dt} \left[ \frac{GMm^2}{r} \mathbf{r} \right] = 0 \quad (7.40)$$

Since we know that angular momentum is conserved, we can integrate equation (7.40) to find the following conserved quantity, known as the Laplace-Runge-Lenz vector:

$$\mathbf{K} = \mathbf{L} \times \mathbf{p} + \frac{GMm^2}{r}\mathbf{r} \quad (7.41)$$

If we now choose our axes, such that  $\mathbf{K}$  is aligned with the negative  $x$  direction, and take the dot product  $\mathbf{K} \cdot \mathbf{r}$ , we find that, after some rearrangement, (7.41) implies that:

$$\frac{L^2/GMm^2}{r} = 1 + \frac{K}{GMm^2} \cos \theta \quad (7.42)$$

This describes a general conic section, with semi-latus rectum  $l = \frac{L^2}{GMm^2}$ , and eccentricity  $e = \frac{K}{GMm^2}$ . Thus we have derived Kepler's first law. It can often be helpful to define an eccentricity vector  $\mathbf{e}$ , whose magnitude is the eccentricity of the orbit and which points in the direction of aphelion, the furthest point in the orbit from the Sun. This eccentricity vector is simply given by:

$$\mathbf{e} = \frac{\mathbf{K}}{GMm^2} = \frac{\mathbf{L} \times \mathbf{p}}{GMm^2} + \frac{\mathbf{r}}{r} \quad (7.43)$$

If we take the dot product of this vector with itself we find that:

$$e^2 = \mathbf{e} \cdot \mathbf{e} = \frac{L^2 p^2}{G^2 M^2 m^4} - \frac{2L^2}{GMm^2 r} + 1 = 1 + \frac{2L^2 E}{G^2 M^2 m^3} \quad (7.44)$$

Where  $E = \frac{p^2}{2m} - \frac{GMm}{r}$  is the total energy of the orbit, and for a bound orbit must be a negative quantity. We can use this result, along with the relation  $a(1 - e^2) = l$ , to obtain an expression for the semi-major axis of the orbit:

$$l = \frac{L^2}{GMm^2} \quad e = \sqrt{1 + \frac{2L^2 E}{G^2 M^2 m^3}} \implies a = -\frac{GMm}{2E} \quad (7.45)$$

In order to find the period of an orbit, we can use equation (7.38), which gives the rate at which area is swept out, together with the total area of an ellipse  $A = \pi a^2 \sqrt{1 - e^2}$ , which yields Kepler's third law:

$$T = \frac{2m\pi}{L} a^2 \sqrt{-\frac{2L^2 E}{G^2 M^2 m^3}} = \frac{2\pi a^{\frac{3}{2}}}{\sqrt{GM}} \quad (7.46)$$

### 7.4.3 The Two Body Problem

As it turns out, everything that we have discussed above, can be fairly easily extended to the two body problem. Given two gravitationally interacting point masses  $m_1$  and  $m_2$ , with positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$  respectively, the equations of motion become:

$$\ddot{\mathbf{r}}_1 = \frac{Gm_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3}(\mathbf{r}_2 - \mathbf{r}_1) \quad \ddot{\mathbf{r}}_2 = \frac{Gm_1}{|\mathbf{r}_1 - \mathbf{r}_2|^3}(\mathbf{r}_1 - \mathbf{r}_2) \quad (7.47)$$

To analyse these equations, it is helpful or us to describe the system in terms of two new variables:  $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$ , which represents the position of  $m_1$  as measured by  $m_2$ , and  $\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}$ , which represents the position of the centre of mass. If we differentiate the definitions of these new variables, and then substitute in (7.47), we obtain the two decoupled equations of motion:

$$\ddot{\mathbf{s}} + \frac{G(m_1 + m_2)}{s^3}\mathbf{s} = \mathbf{0} \quad \ddot{\mathbf{R}} = \mathbf{0} \quad (7.48)$$

Firstly, we can see that, as we would expect, the centre of mass is not accelerating, and therefore simply moves through space, with a constant velocity. Furthermore, the equation for  $\mathbf{s}$  is equivalent to a single body orbiting a mass of  $m_1 + m_2$ , just as we described in section 7.4.2. Once we have solved for  $\mathbf{s}$  and  $\mathbf{R}$ , we can then recover our original variables via the coordinate transformation:

$$\mathbf{r}_1 = \mathbf{R} + \frac{m_2\mathbf{s}}{m_1 + m_2} \quad \mathbf{r}_2 = \mathbf{R} - \frac{m_1\mathbf{s}}{m_1 + m_2} \quad (7.49)$$

Relative to the centre of mass, the two bodies must trace out oppositely oriented elliptical orbits, sharing a focus at their combined barycentre. If we wish to apply Kepler's third law to this system, then we simply take the sum of the two semi-major axes, which represents the average of the minimum and maximum separations of the two bodies. In the limit as one body becomes more massive than the other, the size of the more massive body's orbit will shrink, and we shall regenerate all of our results from section 7.4.2. In the case of the Earth-Sun system, the combined centre of mass lies inside the surface of the Sun, and so the deviation from the limit is incredibly small, giving the Sun only a slight gravitational wobble. Figure 7.6 shows an example of the trajectories one would see in a binary star system.

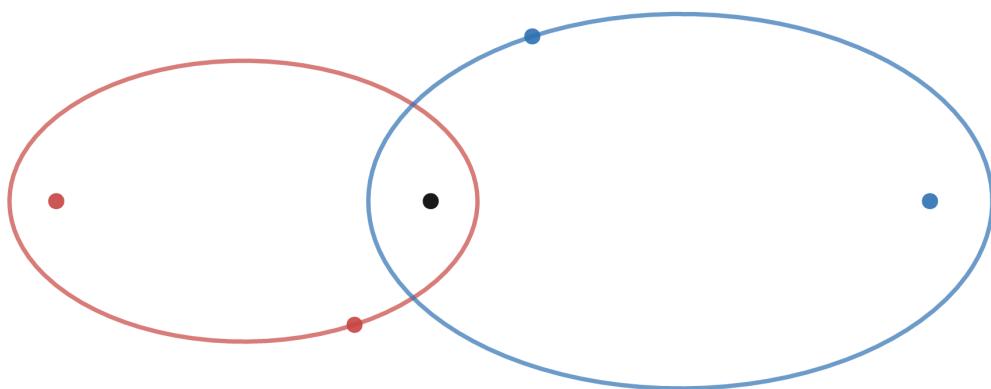


Figure 7.6: The trajectories of a binary star system.

### 7.4.4 Lagrange Points

Unfortunately, there is no general solution to the three body problem, and in fact, three gravitationally interacting masses form a chaotic system. However, there is one special case which is reasonably straightforward, whilst still being fairly useful. Let us first consider a binary system which consists of two bodies in circular orbits about their combined barycentre. We wish to find the positions where an infinitesimal test mass could be placed, such that it remains at rest, with respect to the two bodies. These are the so called Lagrange points. There are two cases to consider, the first is when the test mass is collinear with the orbiting bodies. In this case, there are three points known as  $L_1, L_2$  and  $L_3$ , which sit between the two masses, and on either side, respectively. As it turns out, the positions of these points arise as the solutions of quintic equations, and so no analytic form exists. The more interesting case arises, when the test mass is elsewhere on the plane of the orbit.

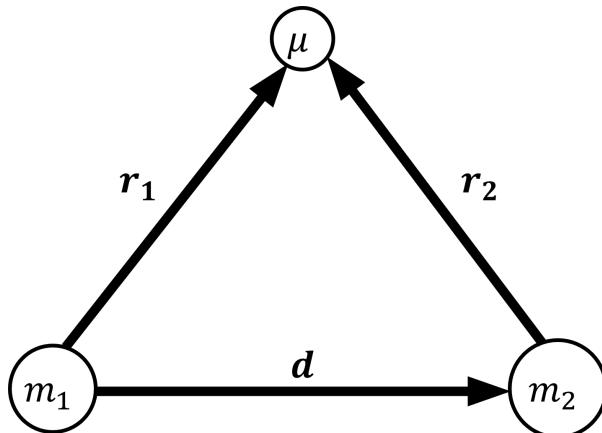


Figure 7.7: A Lagrange point.

give the following expression for the centripetal acceleration required to keep  $\mu$  in the desired circular orbit:

$$\mathbf{a}_{\text{cent}} = - \left[ \frac{Gm_1}{d^3} \mathbf{r}_1 + \frac{Gm_2}{d^3} \mathbf{r}_2 \right] \quad (7.51)$$

We can calculate the gravitational field generated by the two masses, using Newton's law, as outlined in section 7.1.1. This then allows us to deduce the acceleration that the test mass  $\mu$  will experience:

$$\mathbf{a}_{\text{grav}} = - \left[ \frac{Gm_1}{r_1^3} \mathbf{r}_1 + \frac{Gm_2}{r_2^3} \mathbf{r}_2 \right] \quad (7.52)$$

Since we have assumed that  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are not collinear, they must form a basis for every point in the plane of the orbit. As such, if two vectors are expressed as a linear combination of  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , they can only be equal if the coefficients of each vector are the same. Thus, by equating the centripetal and gravitational accelerations, we obtain:

$$r_1 = r_2 = d \quad (7.53)$$

This allows us to conclude that, when  $\mu$  is located in either of the two remaining Lagrange points,  $L_4$  and  $L_5$ , the three masses must form the vertices of an equilateral triangle.

# 8 Electromagnetism

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## 8.1 Maxwell's Equations

We are going to begin our study of classical electromagnetism with the fundamental equations that govern all electromagnetic phenomena. These physical laws describe the dynamical behaviour of two fields  $\mathbf{E}$  and  $\mathbf{B}$ , known as the electric and magnetic fields respectively, and how the fields are generated by charged particles. The Lorentz force law then tells us how charged particles respond in the presence of these fields, which will then in turn cause the fields to change and so on. Before we do however, it is worth taking a moment to consider exactly what is meant when we say an object possesses a certain charge. In truth the existence of electric charge is simply an empirical finding, and as far as we can tell it is a fundamental property of the universe that some matter has it. All we can say is that, when we perform experiments there are certain forces we detect (those that we would now identify as electromagnetic in origin) that always affect different bodies in the same ratio. When we measure this ratio relative to some fixed standard, we call it electric charge. There are several different unit systems that are often used to measure charge; however, throughout this chapter, we shall be using the SI conventions, and thus, our equations shall be formulated in keeping with this.

### 8.1.1 The Lorentz Force Law

The first law we shall look at is not considered to be one of Maxwell's equations, although it is just as important. The Lorentz force law describes the force felt by a particle with charge  $q$ , in the presence of electromagnetic fields  $\mathbf{E}$  and  $\mathbf{B}$  and can be taken as the physical definition of these fields. The law states that:

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (8.1)$$

Where  $\mathbf{v}$  is the velocity of the charged particle.

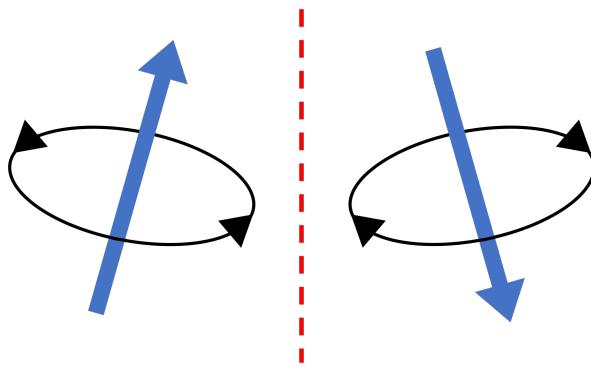


Figure 8.1: The effect of reflection on the magnetic field.

One of the most important things to note about this law is the presence of the vector cross product, and hence, an implied right handed convention. This has very important consequences when one wishes to consider the symmetry of a magnetic field. Normally, if a physical system has a plane of symmetry, we would expect any fields generated by that system to maintain that symmetry, which is indeed the case for the electric field. However, since the action of reflection in the plane of symmetry would convert a right handed convention into a left handed one, the magnetic field acquires a sign change upon reflection.

Formally, this is because  $\mathbf{B}$  is not actually a vector field, but instead a pseudo-vector field, a distinction which is often overlooked. Figure 8.1 attempts to show this visually with the magnetic field of two opposite current loops.

### 8.1.2 Gauss' Law

As with all of the Maxwell equations, Gauss' law has both an integral and a differential representation. Perhaps unsurprisingly, in this case the two forms are related by Gauss' theorem for the divergence of a vector field. The equation is:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \iff \oint_{\partial V} \mathbf{E} \cdot d\mathbf{S} = \frac{Q_V}{\epsilon_0} \quad (8.2)$$

Where  $\rho$  is the charge density,  $Q_V$  is the total charge enclosed within the volume  $V$ , and  $\epsilon_0$  is the permittivity of free space which takes the value  $\epsilon_0 = 8.854\,187\,8\dots \times 10^{-12} \text{ F m}^{-1}$ . Gauss' law is referred to as one of the inhomogeneous Maxwell equations, since it relates one of the fields to the external charges. We shall study some important solutions of Gauss' law later, when we discuss electrostatics; however, for now we shall simply note the implication that positive charges act as sources for the electric field, while negative charges are sinks. In fact, it can sometimes be helpful to think of the electric field as a kind of fluid, that comes flowing out of positive charges, and then draining away at negative charges, pulling any charged particles along with it. It is by drawing analogy to the fluid flow picture, that the integral of  $\mathbf{E}$  through the surface  $\partial V$  is referred to as the flux of  $\mathbf{E}$  through that surface. Confusingly, in other areas of physics, a flux is taken to mean a flow per unit area e.g a heat flux or particle flux, which in the contexts of electromagnetism we would refer to as a flux density. This discrepancy is purely historical in nature and does not carry any significance about the nature of the fields themselves.

### 8.1.3 Gauss' Law for Magnetism

Gauss' Law for magnetism is very similar to his law for the electric field, except this is one of the homogeneous Maxwell equations, that is to say it describes the behaviour of one of the fields independent of any external charges. Gauss' Law for magnetism states that:

$$\nabla \cdot \mathbf{B} = 0 \iff \oint_{\partial V} \mathbf{B} \cdot d\mathbf{S} = 0 \quad (8.3)$$

Physically, we can interpret this equation as a statement that there are no magnetic monopoles, that is to say that, if you were to break a bar magnet in half you would simply obtain two smaller bar magnets, instead of isolated North and South poles. It is this property that fundamentally drives all of the asymmetry between the electric and magnetic fields, and if someone were to ever discover magnetic monopoles, Maxwell's equations could be modified to make them entirely symmetric in  $\mathbf{E}$  and  $\mathbf{B}$ . We can also interpret this law in terms of the fluid flow analogy that we described earlier. If the magnetic field represented the velocity of a fluid, the fact that it has zero divergence would imply that the fluid in question was incompressible, since the net flow of the fluid into any given volume would be zero. Interestingly, we can see that, in the vacuum (where  $\rho = 0$ ), both the electric and magnetic fields obey the same condition of having zero divergence, a fact that is worth bearing in mind as it can sometimes help to spot the general shape of the fields in slightly unconventional situations.

### 8.1.4 The Maxwell-Faraday Law

The Maxwell-Faraday equation is the second of the homogeneous Maxwell equations, and describes how the electric field is effected by changes in the magnetic field. This law states that:

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = \mathbf{0} \iff \oint_{\partial S} \mathbf{E} \cdot d\mathbf{l} + \frac{d}{dt} \int_S \mathbf{B} \cdot d\mathbf{S} \quad (8.4)$$

This equation suggests that, if the magnetic field is changing in time, the electric field has a tendency to circulate around it. In terms of our fluid flow analogy, the changing magnetic field encourages the fluid to flow in closed loops, which when combined with its natural tendency to flow from positive to negative charges, will give rise to the overall form of the field. An important consequence of this is that the electric field is not necessarily a conservative field (which would require  $\nabla \times \mathbf{E}$  to be identically zero), meaning that there is no well defined potential energy associated with it. This has a very interesting consequence, which shall be explored in depth in the later sections, that in order for energy to be conserved, the fields themselves must possess some form of energy. The idea that something as seemingly abstract as a field can carry something as physical as energy is rather strange indeed. As it happens, this is a special case where quantum mechanics appears to help mitigate the confusion, by explaining that the fields are really nothing more than a large ensemble of photons, each carrying its own energy, which seems to make more intuitive sense.

### 8.1.5 The Maxwell-Ampere Law

The Maxwell-Ampere Law is the second inhomogeneous Maxwell equation, and it describes how the electromagnetic fields respond to an electric current, which is just another word for moving charges. In some sense, it is the magnetic equivalent to the Maxwell-Faraday law, with the added bonus that it contains a source for the magnetic field. The Law is as follows:

$$\nabla \times \mathbf{B} - \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{j} \iff \oint_{\partial S} \mathbf{B} \cdot d\mathbf{l} - \mu_0 \epsilon_0 \frac{d}{dt} \int_S \mathbf{E} \cdot d\mathbf{S} = \mu_0 I_S \quad (8.5)$$

Here  $\mu_0$  is the vacuum permeability and takes a value of  $\mu_0 = 1.256\,637\dots \times 10^{-6} \text{ H m}^{-1}$ .<sup>6</sup> In this equation  $\mathbf{j}$  is the current density, that is to say the current flowing per unit area, and is given by  $\mathbf{j} = \rho \mathbf{v}$ , where  $\mathbf{v}$  is the velocity of the charges at that point (assuming all the charges have the same velocity). This then means that  $I_S$  must be the current flowing through the surface  $S$ .

One interesting implication of this law arises, if we take the divergence of equation (8.5). Substituting in Gauss' law from equation (8.1), and rearranging, then gives us:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (8.6)$$

This is called a continuity equation, and it implies the conservation of electric charge. It was actually the desire to achieve charge continuity that motivated Maxwell to add the time derivative term into Ampere's existing law, which simply related the force between circuits to the currents flowing through them.

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<sup>6</sup>Until recently the value of  $\mu_0$  was fixed by definition as  $4\pi \times 10^{-7} \text{ H m}^{-1}$ ; however, this was changed with the 20 May 2019 redefinitions.

## 8.2 Electrostatics

In general, solving Maxwell's equations can be quite complicated, and so we are going to spend most of our time focusing on a variety of special cases. The first of these is to operate under electrostatic assumptions, that is to say, we assume that all charges are immobile. From this, we can make several deductions. Firstly, since the sources for the fields are not changing in time, all of the time derivatives of the fields must vanish. Strictly speaking this is not quite true, as electromagnetic waves could still propagate; however, for the purposes of electrostatics, they are often ignored, since under most circumstances they would cause any present charges to move, destroying our assumptions anyway. Furthermore, since all the charges are stationary, we must have  $\mathbf{j} = \mathbf{0}$ , and hence there is no source for the magnetic field. In mathematical terms, we now have  $\nabla \cdot \mathbf{B} = 0$  and  $\nabla \times \mathbf{B} = \mathbf{0}$ , which together with the requirement that  $\mathbf{B}$  vanishes at infinity, implies that  $\mathbf{B} = \mathbf{0}$  everywhere. The remaining two Maxwell equations now state that:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \nabla \times \mathbf{E} = \mathbf{0} \quad (8.7)$$

### 8.2.1 The Electric Potential

The two equations in (8.7) can be quite cumbersome to use, so a common approach in electrostatics is to introduce an auxiliary scalar field  $\Phi$ , called the electrostatic potential, which allows to combine both laws into a single equation. To do this we can use the Helmholtz decomposition theorem to state that, if a vector field has zero curl, it must be conservative. In mathematical terms:

$$\nabla \times \mathbf{E} = \mathbf{0} \implies \exists \Phi \text{ such that } \mathbf{E} = -\nabla\Phi \quad (8.8)$$

If we then substitute the definition that  $\mathbf{E} = -\nabla\Phi$  into Gauss' law, we obtain Poisson's equation for the electric potential:

$$\nabla^2\Phi + \frac{\rho}{\epsilon_0} = 0 \quad (8.9)$$

One of the most useful consequences of this approach is that, if a charged particle is allowed to move in an electrostatic field (meaning that all the other charges are kept stationary), then the quantity<sup>7</sup>:

$$\mathfrak{Z} = \frac{mv^2}{2} + q\Phi \quad (8.10)$$

Will remain constant throughout its motion. For this reason, the electrostatic potential can often be thought of as a potential energy per unit charge, a quantity which we would refer to as voltage, in the context of an electric circuit. We shall return to the idea of  $\Phi$  and energy in section 8.2.6. As it turns out, measuring potential differences is quite easy to do, using a device like a voltmeter, which is one of the major benefits of thinking in terms of the potential instead of the field.

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<sup>7</sup>The potential  $\Phi$  in this equation does not include any contribution from the dynamic charge, since it can't interact with itself.

### 8.2.2 Coulomb's Law

We are now going to discuss the solutions to Poisson's equation, which we derived in section 8.2.1. One of the most elegant ways of solving the equation is by finding the Green's function, which satisfies the equation  $\nabla^2 G(\mathbf{r}) = \delta(\mathbf{r})$ , where  $\delta(\mathbf{r})$  is the Dirac delta function. Now as it happens the Green's function is not unique, a fact that can actually be very useful; however, for our purposes we shall ensure uniqueness by imposing the boundary condition  $G \rightarrow 0$  as  $r \rightarrow \infty$ . To find the Green's function let us consider the limit  $G(\mathbf{r}) = \lim_{R \rightarrow 0} G^*(\mathbf{r})$ , where:

$$\nabla^2 G^*(\mathbf{r}) = \begin{cases} 0 & r > R \\ \frac{3}{4\pi R^3} & r \leq R \end{cases} \quad (8.11)$$

Since both our boundary condition, and the inhomogeneous part of equation (8.11) are spherically symmetric,  $G^*(\mathbf{r})$  must possess the same symmetry. As such, we can express the Laplacian in spherical polar coordinates, and discard the angular derivatives, to obtain:

$$\frac{1}{r^2} \frac{d}{dr} \left[ r^2 \frac{dG^*(\mathbf{r})}{dr} \right] = \begin{cases} 0 & r > R \\ \frac{3}{4\pi R^3} & r \leq R \end{cases} \quad (8.12)$$

Rearranging, integrating, and then applying our boundary conditions to this equation yields the following expression for  $G^*$ . If we then take the limit as  $R \rightarrow 0$ , this expression holds over all space, to give us:

$$G^*(\mathbf{r}) = -\frac{1}{4\pi r} \quad r > R \implies G(\mathbf{r}) = -\frac{1}{4\pi r} \quad (8.13)$$

We can then solve Poisson's equation, by convolving the Green's function with the charge density, to obtain an expression for the potential. Taking the gradient of that then gives us an expression for the field:

$$\Phi = \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}'|} dV' \implies \mathbf{E} = \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}'|^3} dV' \quad (8.14)$$

This result is called Coulomb's law, although it is conventionally expressed in terms of the force between two point charges, which decays with the square of their separation. For this reason, Coulomb's law is often referred to as an example of an inverse square law, a phenomenon that often arises when dealing with dispersion in 3D space. It is worth taking a moment to discuss the motivation behind the boundary conditions imposed on  $G(\mathbf{r})$ . In essence, because Maxwell's equations are all partial differential equations, there is always an ambiguity in the electric and magnetic fields that can not be resolved by the source terms  $\rho$  and  $\mathbf{j}$ . In its most general form, this ambiguity manifests as electromagnetic wave solutions, in particular a wave with an infinite wavelength, which is simply a uniform field. However, since we would not physically expect to find waves like this, that exist throughout all space without a source, we impose the boundary condition on our fields that they must vanish at infinity. Of course, this still allows  $\Phi$  to vary by some constant term, which has no physical meaning, since we can only ever measure potential differences, and is conventionally dealt with, by also defining  $\Phi$  to be 0 at infinity. This then gives rise to the boundary conditions on the Green's function.

### 8.2.3 Dipole Moment

Unfortunately, the integral in equation (8.14) can be quite computationally difficult to evaluate for arbitrary charge distributions. As such, it can often be useful to develop approximations for the field of an object, which are much simpler to compute. In the case of a charge distribution that is localised around the origin, a good approximation to the field at large distances away comes from a multipole expansion. In this text, we shall only use the first two terms of the expansion, the monopole and dipole moments; however, higher order terms can be derived in a similar manner. First, let us take a Taylor series expansion of  $\frac{1}{|\mathbf{r}-\mathbf{r}'|}$ , as follows:

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r} + \frac{\mathbf{r} \cdot \mathbf{r}'}{r^3} + \frac{3(\mathbf{r} \cdot \mathbf{r}')^2 - r^2 r'^2}{2r^5} + \mathcal{O}\left(\frac{1}{r^4}\right) \quad (8.15)$$

If we discard terms of order  $\frac{1}{r^3}$  or higher and substitute this into equation (8.14), we obtain:

$$\Phi \approx \frac{Q}{4\pi\epsilon_0 r} + \frac{\mathbf{p} \cdot \mathbf{r}}{4\pi\epsilon_0 r^3} \quad (8.16)$$

Where  $Q$  and  $\mathbf{p}$  are the total charge and dipole moment respectively, defined as:

$$Q = \int_{\mathbb{R}^3} \rho dV \quad \mathbf{p} = \int_{\mathbb{R}^3} \mathbf{r} \rho dV \quad (8.17)$$

Obviously, in order for this approximation to be valid, all of the charge needs to be localised into a small volume  $V$  around the origin, such that  $r$  is much larger than any linear dimension of  $V$ . Furthermore, we can note that, since displacing the origin by a vector  $\mathbf{a}$  will result in the dipole moment being altered by a vector  $-Q\mathbf{a}$ , unless  $Q = 0$ , it will always be possible to choose an origin such that  $\mathbf{p} = \mathbf{0}$ . However, in the case that the net charge is zero, the dipole moment is invariant under a change of origin, and thus has a much greater physical significance. If we take the gradient of equation (8.16), we can obtain the first two terms in the multipole expansion of the electric field:

$$\mathbf{E} = -\nabla\Phi \approx \frac{Q}{4\pi\epsilon_0 r^3} \mathbf{r} + \frac{3(\mathbf{p} \cdot \mathbf{r})\mathbf{r} - r^2 \mathbf{p}}{4\pi\epsilon_0 r^5} \quad (8.18)$$

The concept of a dipole moment can be used for more than just determining the field, we can use essentially the same technique to approximate the forces felt by a charged object, when it is placed in an electric field. By taking a Taylor series expansion of the field about the centre of the charged body, we can say that to first order:

$$\mathbf{F} \approx Q\mathbf{E} + (\mathbf{p} \cdot \nabla)\mathbf{E} \quad \mathbf{G} \approx \mathbf{p} \times \mathbf{E} \quad (8.19)$$

Where  $\mathbf{F}$  is the resultant force acting on the body, and  $\mathbf{G}$  is the torque on the object, evaluated about the same origin as the dipole moment. If one wishes to obtain the torque about an arbitrary origin, then they can just add on  $\mathbf{r} \times \mathbf{F}$ , where  $\mathbf{r}$  is the position of the old origin relative to the new one. We can see from these results that, when a dipole is placed in an electric field, it will rotate into alignment with the field, and since the field strength decreases with distance from the source, it will be attracted towards the source.

### 8.2.4 Conductors

A conductor is any material within which charges are free to flow, or equivalently a material with a finite resistivity. There are two key properties of conductors that define their behaviour, within the framework of electrostatics. Firstly, if the electric field is ever non-zero inside a conductor, it will accelerate the mobile charges within, which would violate our electrostatic assumptions, and therefore no field can exist within a conductor. Secondly, if there is any component of the field parallel to the surface of a conductor, this too will cause the free charges to accelerate and violate the electrostatic assumptions. Another way of phrasing this is to note that  $\Phi$  must be constant everywhere within a conductor, which makes sense since if there was a potential difference, we would expect a current to flow as per Ohm's Law. Now it is important to note that it is not physically impossible for a field to exist within a conductor, it is merely impossible whilst maintaining electrostatics. As a result, these assumptions will only be valid if the conductor is given sufficient time to redistribute charges among itself, and equilibrate with an applied field.

We can use these properties of conductors to make several useful statements. Firstly, the absence of any field within the conductor, together with Gauss' law, directly implies that  $\rho = 0$  everywhere except the surface of the conductor. Since all of the charge is localised on the surface of the conductor, we would normally describe it with a surface density  $\sigma$  instead of the volume density  $\rho$ , which is technically infinite. It also follows from Gauss' law that directly above the surface of a conductor the field is given by:

$$\mathbf{E} = \frac{\sigma}{\epsilon_0} \hat{\mathbf{n}} \quad (8.20)$$

Where  $\hat{\mathbf{n}}$  is the unit normal to the surface at that point. An interesting consequence of this build up of charge is that the surface of the conductor feels an outward pressure, due to the repulsion of all the surface charges. To calculate this pressure we consider an infinitesimal area element, with surface charge density  $\sigma$ . If this charge was in isolation, then it would produce a local field of magnitude  $\frac{\sigma}{2\epsilon_0}$  in both directions from the surface. However, we know that the interior field must be zero, and so all of the remaining charges must produce a field of  $\frac{\sigma}{2\epsilon_0} \hat{\mathbf{n}}$  to cancel out the inward component of the field. As such, the total force per unit area on the surface is given by:

$$P = \frac{\sigma^2}{2\epsilon_0} = \frac{\epsilon_0 E^2}{2} \quad (8.21)$$



Figure 8.2: The charged surface of a conductor.

### 8.2.5 Image Charges

Now that we have examined the properties of conductors, we are going to take the opportunity to discuss one of the methods that can be employed to calculate the fields they produce. This is the so called method of image charges, which relies on the uniqueness of solutions to Poisson's equation. Let us consider some region of space  $V$  over which the charge density  $\rho$  is known. If we suppose that there are two solutions to Poisson's equation  $\Phi_1$  and  $\Phi_2$  within this region, then they both must satisfy:

$$\nabla^2 \Phi_1 = \nabla^2 \Phi_2 = -\frac{\rho}{\varepsilon_0} \quad (8.22)$$

Since the Laplacian is a linear operator, we can introduce a new field  $\Psi = \Phi_1 - \Phi_2$ , which must obey Laplace's equation over the entire region  $V$ :

$$\nabla^2 \Psi = 0 \quad (8.23)$$

If we now substitute this into the vector calculus identity  $\nabla \cdot (\Psi \nabla \Psi) = \Psi \nabla^2 \Psi + |\nabla \Psi|^2$ , and integrate both sides of the equation over  $V$  with Gauss' theorem, we obtain:

$$\int_V |\nabla \Psi|^2 dV = \oint_{\partial V} \Psi \nabla \Psi \cdot d\mathbf{S} \quad (8.24)$$

Importantly, if equation (8.24) is equal to zero, we must have  $\nabla \Psi = \mathbf{0} \implies \nabla \Phi_1 = \nabla \Phi_2$  everywhere within  $V$ , because the integrand  $|\nabla \Psi|^2 \geq 0$ . Therefore, it follows that, if either the potential or the field is specified everywhere on the boundary  $\partial V$ , the field must be uniquely determined throughout the whole region. The method of image charges then utilises this result by finding arrangements of charge outside the region  $V$  that match the boundary conditions and thus must produce the same internal field.

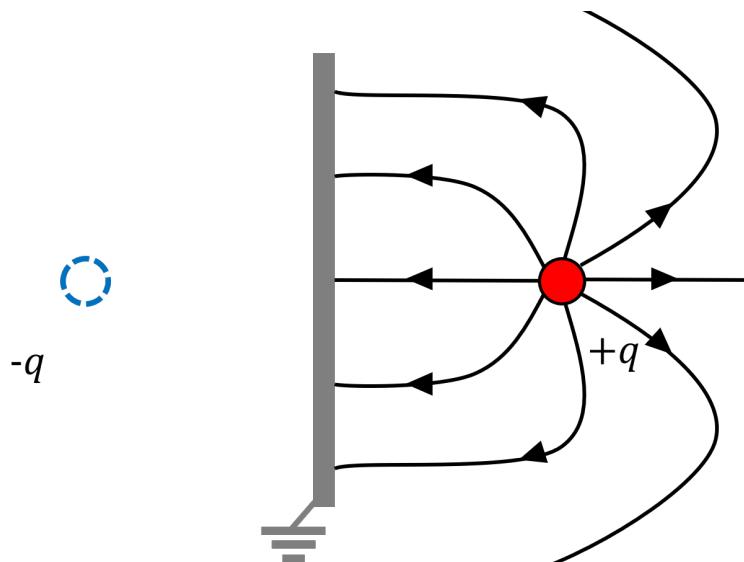


Figure 8.3: A point charge next to an infinite, earthed plate.

We shall now demonstrate this principle by considering a few simple examples. First let us consider the situation shown in figure 8.3 of a point charge  $q$ , which is held in position relative to an infinite, earthed, metal plate. Since the plate is a conductor, we know that it must have a uniform potential across it, and furthermore, earthing the plate ensures that this potential is zero (if we adopt the definition that  $\Phi \rightarrow 0$  as  $r \rightarrow \infty$ ). We can now split space into two distinct regions on either side of the plate, and apply the method of images to each. The region that does not contain the charge is bounded on all sides by a surface of  $\Phi = 0$  and since  $\rho = 0$  everywhere in this region, the only solution is for the potential to be identically zero everywhere. As such, the field produced by the charge distribution on the plate must be exactly equal and opposite to that of the point charge  $q$ , in order to completely cancel it out. Since all of the charge lies on the surface of the plate, it must be unchanged by a reflection in that plane. Thus, by symmetry, we would expect the field of the plate in the second region to be exactly that of a charge  $-q$  reflected in the plane of the plate. We can easily verify that this image charge produces the correct potential on the surface of the plate, and so must give the correct field. Similar analyses can be carried out for different shapes of plate, for example a right angled L shape.

Another useful case to analyse is that of a grounded spherical shell of radius  $R$ . Let us place a point charge  $q$  at a position  $\mathbf{r}$ , relative to the centre of the sphere, such that  $r > R$ . We are going to look for an image charge  $q'$  at position  $\mathbf{r}'$  inside the sphere, that can replicate the potential along the surface of the sphere.

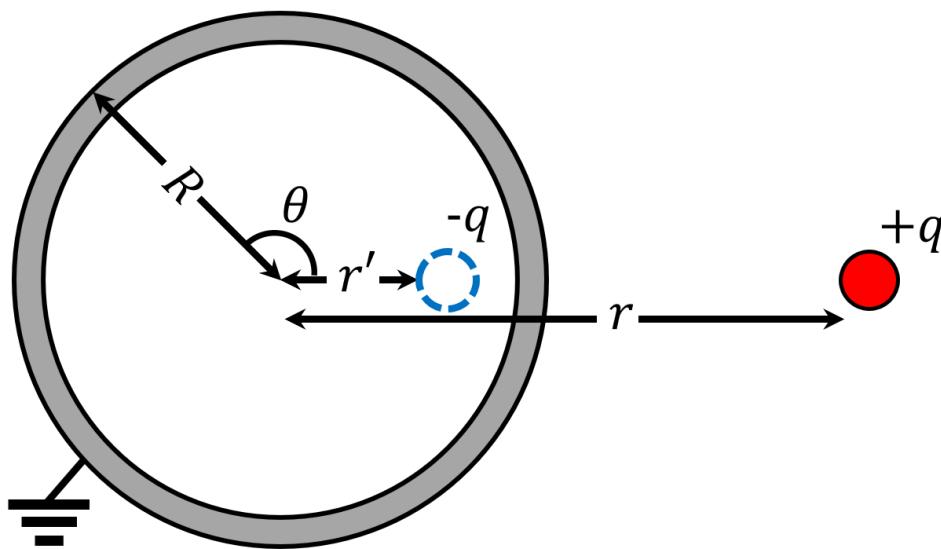


Figure 8.4: A point charge next to an earthed conducting sphere.

By symmetry, we require that  $\mathbf{r}'$  be parallel to  $\mathbf{r}$ . Thus, in order to obtain the correct potential we must have:

$$\frac{q}{\sqrt{R^2 + r^2 - 2rR \cos \theta}} + \frac{q'}{\sqrt{R^2 + r'^2 - 2r'R \cos \theta}} = 0 \quad (8.25)$$

For all values of the polar angle  $\theta$  between 0 and  $\pi$ . The only way this can hold true for all the possible angles is if the  $\cos \theta$  terms and the angle independent terms are both separately proportional to the squares of the charges. As such, the following condition must be satisfied:

$$\frac{R^2 + r'^2}{R^2 + r^2} = \frac{r'}{r} = \frac{q'^2}{q^2} \quad (8.26)$$

We can expand equation (8.26) to obtain the quadratic equation in  $r'$  below. Trivially, we can see that one solution to this equation will always be to set  $\mathbf{r}' = \mathbf{r}$  and  $q' = -q$ , which is not particularly useful because we want our image charge to be inside the sphere. However, this does allow us to easily factorise the quadratic equation and quickly obtain the useful solution:

$$r'^2 - \frac{R^2 + r^2}{r} r' + R^2 = (r' - r) \left( r' - \frac{R^2}{r} \right) = 0 \quad (8.27)$$

Thus, we can conclude that the image charge is given by:

$$\mathbf{r}' = \frac{R^2}{r^2} \mathbf{r} \quad q' = -\frac{R}{r} q \quad (8.28)$$

While this approach is very useful for an earthed conductor, we can also extend it to deal with an isolated sphere. In this case the potential is not held at zero but instead at some fixed constant  $V$ , which we have to determine. The simplest way of achieving this is to start with our previous solution and then place an additional image charge  $Q$  at the centre of the sphere, such that  $V = \frac{Q}{4\pi\epsilon_0 R}$ . We can determine  $Q$  by noting that, if the sphere is electrically neutral, meaning that it carries no net charge, Gauss' law implies that  $Q + q' = 0$ . Since Maxwell's equations are all linear, this result is not limited to a single point charge and can be used to determine a general expression for the field produced around the sphere (assuming that  $\rho = 0$  inside the sphere):

$$\mathbf{E} = \begin{cases} \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}') dV'}{4\pi\epsilon_0} \left[ \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3} - R r'^3 \frac{(r'^2 \mathbf{r} - R^2 \mathbf{r}')}{|r'^2 \mathbf{r} - R^2 \mathbf{r}'|^3} + \frac{R \mathbf{r}}{r^4} \right] & r \geq R \\ \mathbf{0} & r < R \end{cases} \quad (8.29)$$

Here we are seeing the very important result, that the field inside a conducting surface is independent of the external charge distribution. This is the principle behind a Faraday cage, which can be used to shield sensitive equipment from external electromagnetic fields, and is also the reason why you are safe from a lightning strike in a car. Of course, if there are any charges inside the sphere, they will produce their own internal field, which can be calculated using exactly the same image charge formula applied in reverse. However, it is worth noting that, while the interior of the sphere is completely shielded from the exterior charges, any charges inside the sphere will produce a field equivalent to that of a central point charge in the exterior region. The reason for this is simple; whilst the interior is completely bounded by the sphere, and thus unaffected by the absolute potential of the surface (since a constant offset in  $\Phi$  vanishes from  $\mathbf{E}$ ), the exterior is bounded by the sphere and infinity, meaning it is sensitive to the potential difference between the surface of the sphere and infinity.

### 8.2.6 Energy Density

We are now going to spend some time discussing the concept of electrostatic potential energy. We already saw in section 8.2.1 that, the quantity  $q\Phi$  acts as a form of potential energy for a particle in an electrostatic field, an idea which we shall now explore in greater detail. If we define the electrostatic potential energy of a system as the work done against electrostatic forces to assemble the charges from infinity (which would have to be done infinitely slowly so as to preserve the electrostatic assumptions), then we can calculate it as follows. Since  $\mathbf{E} = -\nabla\Phi$  we can say that the work that must be done to move an infinitesimal charge  $dq$  from infinity to position  $\mathbf{r}$  is given by  $dW = [\Phi(\mathbf{r}) - \Phi(\infty)] dq = \Phi(\mathbf{r}) dq$ . It therefore follows that, if we build up a charge distribution  $\rho$  by setting the instantaneous density to be  $\alpha\rho$ , and varying  $\alpha$  from zero to one, the potential energy must be given by:

$$U = \int_0^1 \alpha \int_{\mathbb{R}^3} \rho \Phi dV d\alpha \quad (8.30)$$

Where we have used the expression for the potential in section 8.2.2 to conclude that, if the instantaneous charge distribution is  $\alpha\rho$ , the instantaneous potential must be  $\alpha\Phi$ . Furthermore, we have utilised the fact that, when  $\alpha$  is increased slightly, infinitesimal change in charge at each point in space is  $\rho dV d\alpha$ . Evaluating this integral yields:

$$U = \frac{1}{2} \int_{\mathbb{R}^3} \rho \Phi dV \quad (8.31)$$

We can manipulate this expression by substituting in Poisson's equation for  $\rho = -\varepsilon_0 \nabla^2 \Phi$ . We can then evaluate the integral in equation (8.31) by parts, using the vector calculus identity  $\nabla \cdot (\psi \mathbf{F}) = \psi \nabla \cdot \mathbf{F} + \nabla \psi \cdot \mathbf{F}$ , to imply that:

$$U = -\frac{\varepsilon_0}{2} \int_{\mathbb{R}^3} \Phi \nabla^2 \Phi dV = \frac{\varepsilon_0}{2} \int_{\mathbb{R}^3} \nabla \Phi \cdot \nabla \Phi dV - \frac{\varepsilon_0}{2} \int_{\mathbb{R}^3} \nabla \cdot (\Phi \nabla \Phi) dV \quad (8.32)$$

Since the product of  $\Phi$  and  $\nabla\Phi$  decays with  $r^{-3}$ , and the surface area of  $\partial V$  only grows with  $r^2$ , as  $V \rightarrow \mathbb{R}^3$ , Gauss' theorem implies that the second integral on the right hand side must vanish. Therefore, we can obtain a new expression for the potential energy as:

$$U = \frac{\varepsilon_0}{2} \int_{\mathbb{R}^3} \mathbf{E} \cdot \mathbf{E} dV = \int_{\mathbb{R}^3} \mathcal{E}_E dV \quad (8.33)$$

Where  $\mathcal{E}_E$  is the energy density of the electric field, given in equation (8.34) below. As we shall see later, this expression turns out to be applicable in much broader situations than just electrostatics. We can also note that it is equal to the electrostatic pressure we derived in section 8.2.4, which makes sense if one considers the work done during the expansion of a conductor.

$$\mathcal{E}_E = \frac{\varepsilon_0 E^2}{2} \quad (8.34)$$

This inherent ambiguity in the actual location of the energy, is typical for continuous systems. This is simply because, the existence of boundary conditions makes it possible to vary the integrand by a derivative without changing the value of the overall energy.

## 8.3 Magnetostatics

We are now going to begin our consideration of magnetostatics, where just as in electrostatics, the fields are assumed to be in a steady state, such that the time derivatives vanish from Maxwell's equations. However, for the purposes of magnetostatics, we relax the restriction that charges must be stationary, and instead impose that both  $\rho$  and  $\mathbf{j}$  must not change with time. Under these assumptions, the equations for the electric field remain the same as they were in section 8.2, and so much of what we have already discussed still applies. The remaining two of Maxwell's equations become:

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \times \mathbf{B} = \mu_0 \mathbf{j} \quad (8.35)$$

### 8.3.1 The Magnetic Vector Potential

Once again, we are going to find that it is easier to work in terms of an auxiliary field; however, in the case of magnetism we introduce a vector potential field  $\mathbf{A}$ . It follows from the Helmholtz decomposition theorem and Gauss' law for magnetism that,  $\mathbf{B}$  can be expressed as the curl of a vector field:

$$\nabla \cdot \mathbf{B} = 0 \implies \exists \mathbf{A} \text{ such that } \mathbf{B} = \nabla \times \mathbf{A} \quad (8.36)$$

If we substitute this into Ampere's law (the name given to the Maxwell-Ampere equation when the time derivative term is neglected), and apply the vector calculus identity for the curl of the curl, we obtain:

$$\nabla^2 \mathbf{A} - \nabla(\nabla \cdot \mathbf{A}) + \mu_0 \mathbf{j} = \mathbf{0} \quad (8.37)$$

Now it is worth noting that, just as before, the potential field is not unique. However, unlike the electrostatic potential, imposing the restriction that  $\mathbf{A} \rightarrow \mathbf{0}$  at infinity is not enough to give a single unique field. This gives us the freedom to impose another restriction on  $\mathbf{A}$ , known as a gauge condition. For magnetostatics the most common choice is to adopt Coulomb gauge, which requires that  $\nabla \cdot \mathbf{A} = 0$ . To verify that this is always possible, we simply note that the potential  $\mathbf{A}' = \mathbf{A} + \nabla \lambda$  will always give rise to the same magnetic field, and thus, fixing the divergence of  $\mathbf{A}$  is simply a matter of solving Poisson's equation for  $\lambda$ . In Coulomb gauge, equation (8.37) reduces down to the vector form of Poisson's equation.

$$\nabla^2 \mathbf{A} + \mu_0 \mathbf{j} = \mathbf{0} \quad (8.38)$$

We already determined the solution to the scalar form of Poisson's equation in section 8.2.2, and since the vector form is nothing more than the scalar form for all three components separately, we can immediately say that:

$$\mathbf{A} = \int_{\mathbb{R}^3} \frac{\mu_0 \mathbf{j}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} dV' \quad (8.39)$$

The similarity of this expression to that in equation (8.14) for the electrostatic potential is one of the great benefits of Coulomb gauge. For this reason, we shall implicitly use Coulomb gauge throughout the rest of this section.

### 8.3.2 The Biot-Savart Law

If we wish to obtain an expression for the magnetic field, then all we need to do is take the curl of equation (8.39). This yields the Biot-Savart law for the magnetic field:

$$\mathbf{B} = \int_{\mathbb{R}^3} \frac{\mu_0 \mathbf{j}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|^3} dV' \quad (8.40)$$

Just as we should expect, given the pseudo-vector nature of the magnetic field, this expression features the cross product of two true vectors. Another fairly elegant method to arrive at this result is to directly take the curl of Ampere's law, and substitute in Gauss' law for magnetism, which yields:

$$\nabla^2 \mathbf{B} + \mu_0 \nabla \times \mathbf{j} = \mathbf{0} \implies \mathbf{B} = \int_{\mathbb{R}^3} \frac{\mu_0 \nabla' \times \mathbf{j}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} dV' \quad (8.41)$$

Evaluating this integral by parts with the identity  $\nabla \times (\psi \mathbf{F}) = \psi \nabla \times \mathbf{F} + \nabla \psi \times \mathbf{F}$ , and using Gauss' theorem to verify that the integral of the left hand side vanishes, also produces the Biot-Savart law. Care must be taken when using this law, since it appears to imply pairwise interactions between current elements; however, these seemingly pairwise interactions are in direct violation of Newton's third law. This problem arises, because it is impossible to have individual current elements interacting, without violating the magnetostatic assumptions. We shall explore this idea more fully in section 8.5; however, for now we should just note that, in magnetostatics, the Biot-Savart Law should only be applied to complete circuits. When calculating the magnetic field produced by a closed circuit  $C$ , with wires of negligible thickness, we can simplify the Biot-Savart law to the loop integral:

$$\mathbf{B} = \frac{\mu_0 I}{4\pi} \oint_C \frac{d\mathbf{l}' \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \quad (8.42)$$

### 8.3.3 Current Loops

We are now going to examine one of the most important building blocks of magnetic systems, current loops. Current loops can be found in a variety of circumstances, from the rotation of a charged object about its axis to more familiar examples in terms of wire coils. Unfortunately, there is no analytic form for the full magnetic field field of even a simple circular current loop, so we are reduced to employing a number of approximations. Firstly, while we may not be able to evaluate the whole field of a circular loop, the Biot-Savart law does allow us to calculate the field along the axis of the ring. If a loop of radius  $r$ , carrying a current  $I$ , lies in the  $x$ - $y$  plane, with its centre at the origin, then the field along the  $z$  axis is given by:

$$\mathbf{B}(z) = \frac{\mu_0 I r^2}{2(r^2 + z^2)^{\frac{3}{2}}} \hat{\mathbf{z}} \quad (8.43)$$

Where  $\hat{\mathbf{z}}$  is a unit vector along the  $z$ -axis. It is important to note here that the positive direction of the current flow is defined in a right handed sense about the  $z$  axis. Interestingly enough, we can notice that as  $z \rightarrow \pm\infty$ , this field asymptotically approaches that of a dipole.

If we want the field produced by a more general current loop, we can once again utilise a multipole expansion. Let us start by converting equation (8.39) for the vector potential into a path integral around the current loop. We can then apply a Taylor series expansion to obtain:

$$\mathbf{A} = \frac{\mu_0 I}{4\pi r} \oint_C \frac{1}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{l}' \approx \frac{\mu_0 I}{4\pi r^3} \oint_C r^2 + \mathbf{r} \cdot \mathbf{r}' d\mathbf{l}' \quad (8.44)$$

This integral can be evaluated using a corollary of Stoke's theorem, which states that for any scalar field  $\psi$  and any surface  $S$ :

$$\oint_{\partial S} \psi d\mathbf{l} = - \int_S \nabla \psi \times d\mathbf{S} \quad (8.45)$$

This theorem can be proven quite easily by taking the dot product of the left hand side with an arbitrary constant vector, and then applying Stoke's theorem. Thus, it follows that the vector potential is given by:

$$\mathbf{A} \approx \frac{\mu_0 \mathbf{m} \times \mathbf{r}}{4\pi r^3} \quad (8.46)$$

Where  $\mathbf{m}$  is the magnetic dipole moment defined as  $\mathbf{m} = IS$ , with  $\mathbf{S}$  being the total vector area enclosed by the current loop. Evaluating the curl of the potential then gives us an expression for the magnetic field, directly analogous to equation (8.18) for a dipolar field.

$$\mathbf{B} \approx \frac{\mu_0 [3(\mathbf{m} \cdot \mathbf{r})\mathbf{r} - r^2 \mathbf{m}]}{4\pi r^5} \quad (8.47)$$

Now it is interesting that this same expression arises in both electrostatics and magnetostatics. This is because, with the exception of the origin, which is undefined, the dipolar field is both irrotational and incompressible everywhere. Of course, since the dipole field only ever arises as a far field approximation, what happens at the origin is neither here nor there.

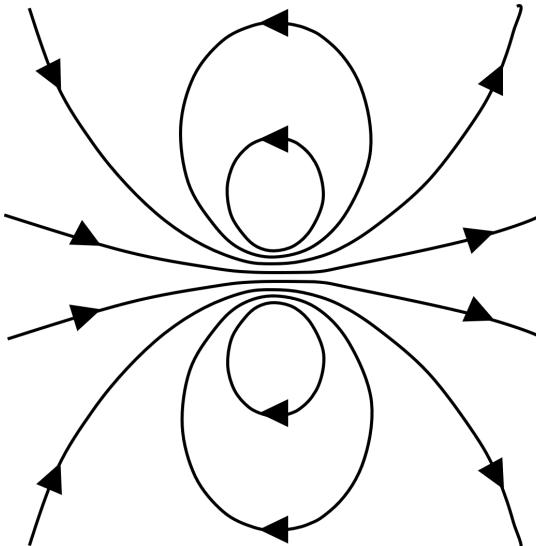


Figure 8.5: The field of a magnetic dipole.

### 8.3.4 Solenoids

Now that we have an appreciation of the behaviour displayed by current loops, we can discuss the related concept of a solenoid. A solenoid is formed by tightly winding a wire around some kind of core, and can be treated as a stack of current loops, one on top of another. The most useful property of a solenoid is that it produces a fairly uniform magnetic field in its centre. We can see this by noting that halfway along the solenoid, symmetry implies that there can be no component of  $\mathbf{B}$  perpendicular to the central axis. Furthermore, if the solenoid is long, then these components must be vanishingly small in the vicinity of the halfway point. If two components of the field are uniform, then the only way that we can have both  $\nabla \cdot \mathbf{B} = 0$  and  $\nabla \times \mathbf{B} = \mathbf{0}$  is if the third and final component is also uniform. The same argument applies to the field outside the solenoid, it must also be approximately constant in the solenoid's plane of symmetry, and thus, must be vanishingly small due to the restriction that  $\mathbf{B} \rightarrow \mathbf{0}$  at infinity. This allows us to determine the field inside the centre of a long solenoid using Ampere's law.

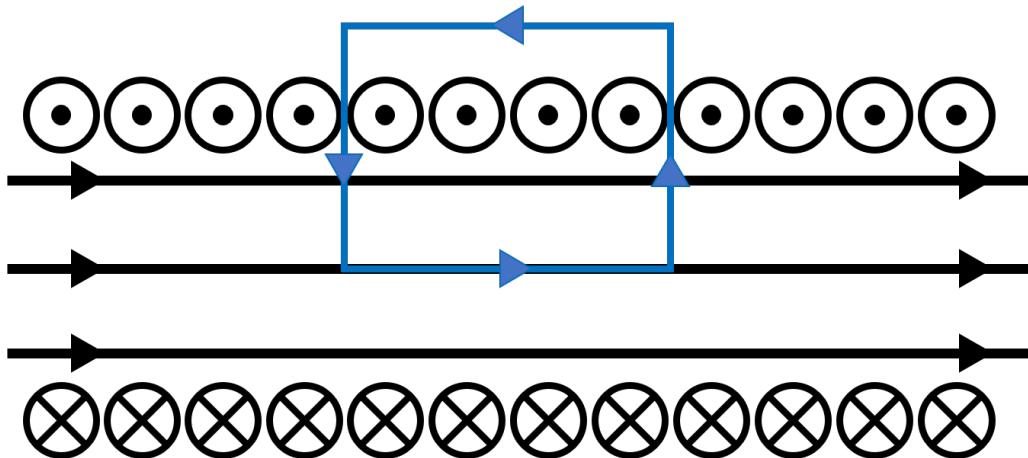


Figure 8.6: Ampere's law applied to a long solenoid.

If we integrate along the Amperian loop shown in figure 8.6, we can obtain an expression for the magnetic field strength in terms of the current  $I$  flowing through the solenoid, the number of turns per unit length  $n$ , and the unit vector along the axis of the solenoid  $\hat{\mathbf{z}}$ . Once again, the positive direction of current is taken in a right handed sense about the  $\hat{\mathbf{z}}$  axis.

$$\mathbf{B} = \mu_0 n I \hat{\mathbf{z}} \quad (8.48)$$

We could always verify this result in the case of a cylindrical solenoid, by stacking circular current loops on top of each other, and integrating equation (8.43) along the full range of  $z$ . It also follows from equation (8.48) that, since the middle of a solenoid is equivalent to the ends of two equivalent solenoids which have been pushed together, the axial component of the magnetic field at the end of a long solenoid is  $\frac{\mu_0 n I}{2}$ .

## 8.4 Induction

This brings us nicely onto our next topic: induction. Broadly speaking, electromagnetic induction refers to the general phenomenon of a time dependent interaction with a magnetic field giving rise to an electromotive force (referred to as an emf for the sake of brevity) around a closed circuital loop. The easiest way to get a handle on these phenomena is to start with the simple case of a perfectly conducting rod, with length  $l$ , moving through a uniform magnetic field  $\mathbf{B}$ , at velocity  $\mathbf{v}$ . This is shown in figure 8.7 on the right. If we consider a charged particle within the rod, it feels a force due to moving through the magnetic field of  $\mathbf{F} = q\mathbf{v} \times \mathbf{B}$ . If we define the emf  $\xi$  to be the work done per unit charge, when a charge moves through  $\mathbf{l}$  from one end of the rod to another, we find that  $\xi = \mathbf{l} \cdot (\mathbf{v} \times \mathbf{B})$ .

Now if the rod is left in isolation, then there is no way for this emf to manifest itself in any meaningful way. In fact, what happens is that charges build up on the ends of the rod, such that the resultant electric field exactly cancels out the force from the magnetic field. In this case, the emf represents the difference in the potential  $\Phi$  (which is well defined because  $\frac{\partial \mathbf{B}}{\partial t} = \mathbf{0}$ ) between the ends of the rod. However, if we connect the ends of the rod to an external circuit, it can act as a battery, and the emf will cause a current to flow. Care must be taken here, as it is quite easy to get confused. The way that we have presented the expression for the emf seems to imply that work is being done by the magnetic field; however, since the magnetic force is always perpendicular to a particles' velocity this should be impossible. What we have to realise is that once a current begins to flow, this new component to the velocities of the charges will result in a new component to the magnetic force on the rod. As such if we want to maintain the rod at a constant velocity, we will need to apply an external force given by:

$$\mathbf{F}_{\text{ext}} = -I\mathbf{l} \times \mathbf{B} \implies P = -I\mathbf{v} \cdot (\mathbf{l} \times \mathbf{B}) = \xi I \quad (8.49)$$

We can see from the scalar triple product identity that, the power of this external force is precisely equal to the power that would be dissipated in an external circuit,  $\xi I$ . As such, we can see that the work is done not by the magnetic field, but instead by this external force.

This simple example is really helpful to hold in the back of our minds moving forwards, as it encapsulates the key principles of induction, without being bogged down in any particularly complicated algebra.

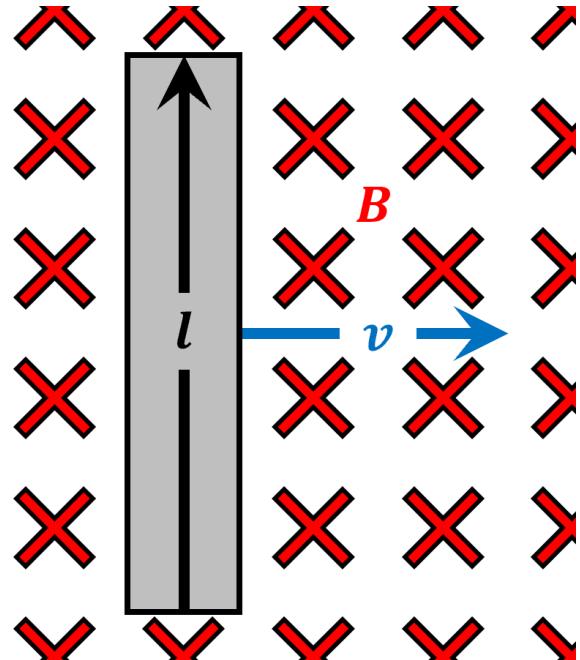


Figure 8.7: A rod being pulled through a magnetic field

### 8.4.1 Faraday's Law of Induction

We are now going to generalise the results of the previous example into a more mathematically concise form (although perhaps a less intuitive one). We are going to consider the total emf acting around an arbitrary closed loop  $C(t)$ , which bounds a surface  $\Sigma(t)$ . Figure 8.8 below shows the two components of the velocity that a charged particle would have as it circulates the curve  $C(t)$ . The flow velocity  $\mathbf{v}_I$  is related to the current in the loop, whereas the outwards velocity  $\mathbf{v}_C$  is determined by the evolution of  $C(t)$  in time.

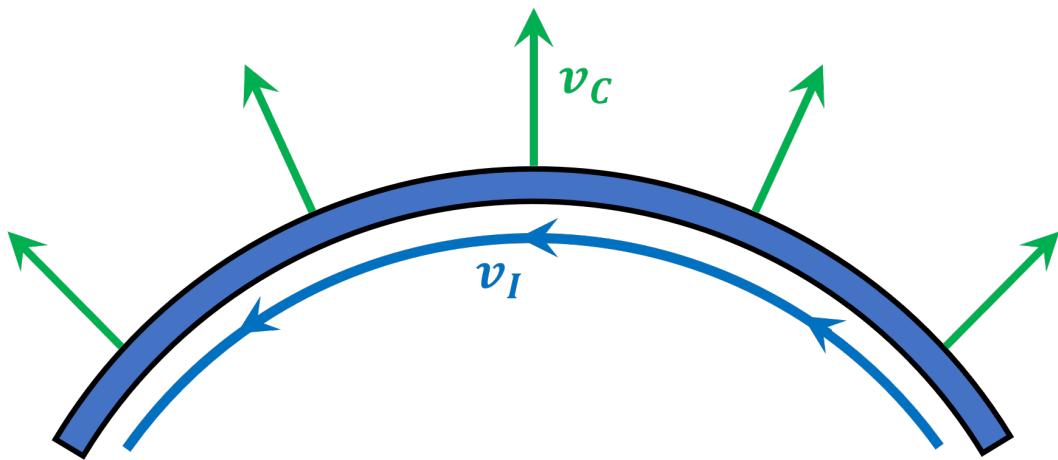


Figure 8.8: The velocities of particles circulating a loop.

Now we can determine the total work done per unit charge, which is the definition of the emf, when travelling once around the loop by evaluating the following integral:

$$\xi = \oint_{C(t)} \left[ \mathbf{E} + (\mathbf{v}_C + \mathbf{v}_I) \times \mathbf{B} + \frac{1}{q} \mathbf{F}_{\text{ext}} \right] \cdot d\mathbf{l} \quad (8.50)$$

We can simplify things slightly by noting that the external force  $\mathbf{F}_{\text{ext}}$  is the force required to counterbalance the magnetic force on the particle, that arises due to its circulation, in order to prevent  $\mathbf{v}_I$  from interfering with  $C(t)$ . As such, the force must satisfy  $\mathbf{F}_{\text{ext}} = -q(\mathbf{v}_I \times \mathbf{B})$ , everywhere along the loop. We can then tidy up the integral by using the Maxwell-Faraday equation  $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ , followed by Stokes' theorem, in addition to the scalar triple product identity for the second term.

$$\xi = \oint_{C(t)} (\mathbf{E} + \mathbf{v}_C \times \mathbf{B}) \cdot d\mathbf{l} = - \left[ \int_{\Sigma(t)} \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{S} + \int_{C(t)} \mathbf{B} \cdot (\mathbf{v}_C \times d\mathbf{l}) \right] \quad (8.51)$$

By considering the geometrical interpretation of the vector cross product, we can see that the right hand side of this equation is actually the time derivative of the magnetic flux through  $\Sigma(t)$ , which yields Faraday's law of induction:

$$\xi = -\frac{d}{dt} \int_{\Sigma(t)} \mathbf{B} \cdot d\mathbf{S} \quad (8.52)$$

As we noted before, the integral of a field through a surface, such as that in equation (8.52), is known as a flux. So Faraday's law takes a particularly simple form when expressed in terms of the magnetic flux, which is denoted by  $\Phi_B$  and should not be confused with the electrostatic scalar potential, through  $C(t)$  as follows:

$$\Phi_B = \int_{\Sigma(t)} \mathbf{B} \cdot d\mathbf{S} \implies \xi = -\frac{d\Phi_B}{dt} \quad (8.53)$$

Of course, everything that we have just been discussing is all framed within the context of a single current carrying loop. If we wish to extend these ideas to a tightly wound coil of wire, such as a solenoid, then we use the same trick as we did in section 8.3.4 to approximate the coil as a series of loops stacked on top of one another. However, since all of the turns are connected, the total emf induced in the coil is the sum of the emfs induced in each loop. This leads us to the concept of a flux linkage, given by  $N\Phi_B$ , where  $N$  is the number of turns in the coil and  $\Phi_B$  is the magnetic flux through the surface bounded by the coil. We can then express the total emf as the rate of change of the coil's flux linkage:

$$\xi = -\frac{dN\Phi_B}{dt} \quad (8.54)$$

A very important property of electromagnetic induction is summarised in Lenz's law, which states that when a changing magnetic flux induces an emf, that emf always acts in a direction such that if current were to flow, the flux produced by the induced current would act to oppose the change that created it. This is essentially the reason that the minus sign appears in Faraday's law of induction, and it follows quite simply from the principle of conservation of energy. If Lenz's law were to be violated, and an induced current reinforced the change that was creating it, this would lead to an even greater induced current, and thus, an even greater reinforcement, and so on ad infinitum. Clearly, it would be physically unacceptable if our equations permitted such a solution, so it is a good thing that Lenz's law holds true.

The final question that we should consider, concerns where exactly the energy comes from during induction. We have already invested a considerable amount of effort in establishing that during motional induction, such as the example in the introduction, and more generally any emf that arises due to the deformation of  $C(t)$  over time, the energy is supplied by the external forces, which are responsible for the deformation, doing work on the charges as they move. However transformer induction, when  $C(t)$  remains constant and the magnetic field changes, is slightly more complicated. The first thing that we need to realise is that the difference between motional and transformer induction is merely a frame of reference. For any wire in motion there exists an inertial frame, in which it is instantaneously at rest. That is to say that if a wire moves through a magnetic field to us it may appear to be experiencing motional induction, but from the perspective of the wire, it is stationary, whilst the magnetic field is changing. Thus the existence of transformer induction is simply a necessary part of maintaining the equivalence of inertial frames. This is as much detail as we can actually give, since induction is fundamentally built in to the definition of magnetic energy, as we shall see later. This reminds us of an important point, energy is defined such that it is conserved, and so, if a new phenomenon like induction appears to violate this conservation law, we simply need a new definition of energy.

### 8.4.2 Self Inductance

The next logical extension of our study into electromagnetic induction is to consider the phenomenon of self inductance. Let us consider an isolated electrical circuit, carrying a steady current  $I$ , which forms a fixed loop  $C$ . If we recall the Biot-Savart law from section 8.3.2, then it follows that the magnetic field produced by the circuit must be linearly related to the current flowing through it. Since the geometry of the circuit is fixed, this directly implies that the flux through the circuit varies according to  $\Phi_B = LI$ , where the self inductance  $L$  is a geometrical property of the system. To calculate  $L$ , we can first use Stokes' theorem to express the magnetic flux as:

$$\Phi_B = \int_{\Sigma} \mathbf{B} \cdot d\mathbf{S} = \oint_C \mathbf{A} \cdot d\mathbf{l} \quad (8.55)$$

This is a very useful equation to have at our disposal, because not only have we simplified our surface integral into a path integral, we have also expressed the flux in terms of the vector potential, which is typically a simpler function than the field itself. If we then substitute in equation (8.39) for the vector potential, we obtain the following integral expression for the self inductance.

$$L = \frac{\mu_0}{4\pi} \iint_{C^2} \frac{d\mathbf{l} \cdot d\mathbf{l}'}{|\mathbf{r} - \mathbf{r}'|} \quad (8.56)$$

It follows that, if the current through the circuit is changing over time, a back emf  $\xi = -L\dot{I}$  will be induced in the circuit. Thus, in order to maintain an accelerating current, we need to apply an external voltage of at least  $L\dot{I}$  across the circuit. In practice the circuit will also have resistive components, which will require an additional voltage in order to maintain the current in the circuit.

This result is particularly useful, because it gives us a way of understanding the magnetostatic potential energy stored in a current distribution. We can define this potential energy to be the total work that has to be done against emfs induced by self inductances when turning on a current network. We do not need to account for any Ohmic losses in resistive parts of the circuit, because we already know that energy has been dissipated as heat. If we wish to model the behaviour of a circuit as it turns on, we should let the instantaneous current in the circuit be  $i(t)$ , which satisfies the following conditions:  $i(0) = 0$  and  $i(\tau) = I$  for some sufficiently large time  $\tau$ . In principle, we can make  $\tau$  arbitrarily large, such that at all times the system is well approximated by the magnetostatic equilibrium we used to justify the self inductance in the first place. Since the power that must be supplied to combat back emfs in a current loop is given by  $P = -\xi I$ , we must have:

$$U = - \int_0^\tau \xi(t)i(t)dt = \int_0^\tau L \frac{di(t)}{dt} i(t)dt = \int_0^I Lidi = \frac{LI^2}{2} \quad (8.57)$$

While equation (8.57) is quite useful, it is limited in its scope, because strictly speaking it only applies in the case where our current distribution forms a single closed loop. Nonetheless, it is still a useful result to have, since often the magnetic fields produced by a current will be sufficiently weak at long ranges, that we can neglect interactions between different circuits.

In order to determine the magnetostatic energy in a more general case, we simply need to extend the same principles to a more arbitrary current distribution. The only restriction we shall apply is that our final current distribution must be consistent with the magnetostatic assumptions. Interestingly, this implies that the current density must be an incompressible field, that is to say that  $\nabla \cdot \mathbf{j} = 0$ , otherwise charge density and thus an electric field would build up in certain locations. We are going to use a similar technique to the one we employed in section 8.2.3, building up our current distribution by setting the instantaneous current density  $\mathbf{j}^* = \alpha \mathbf{j}$  and then increasing  $\alpha$  from zero to one. If we do this, then the instantaneous power required to oppose the back emfs is:

$$P(t) = - \int_{\mathbb{R}^3} \mathbf{E}^* \cdot \mathbf{j}^* dV = -\alpha(t) \int_{\mathbb{R}^3} \mathbf{E}^* \cdot \mathbf{j} dV \quad (8.58)$$

With  $\mathbf{E}^*$  being the instantaneous electric field. Rewriting the Maxwell-Faraday equation in terms of  $\mathbf{E}^*$  and  $\mathbf{A}^*$ , and then utilising the symmetry of mixed partial derivatives to reorder the curl in the second term, we find that:

$$\nabla \times \left( \mathbf{E}^* + \frac{\partial \mathbf{A}^*}{\partial t} \right) = \nabla \times \left( \mathbf{E}^* + \frac{d\alpha}{dt} \mathbf{A} \right) = \mathbf{0} \quad (8.59)$$

It is worth noting that the vector calculus identity  $\nabla \cdot (\psi \nabla \times \mathbf{F}) = (\nabla \psi) \cdot (\nabla \times \mathbf{F})$ , implies that for any two fields, such that one is irrotational and the other is solenoidal, the integral of their dot product over all space will be zero, provided that the fields vanish at infinity (a necessary condition for the integral to converge). If we employ this theorem, we can rewrite the integral in equation (8.58) as:

$$P(t) = \int_{\mathbb{R}^3} \frac{\partial \mathbf{A}^*}{\partial t} \cdot \mathbf{j}^* dV = \alpha(t) \frac{d\alpha}{dt} \int_{\mathbb{R}^3} \mathbf{A} \cdot \mathbf{j} dV \quad (8.60)$$

We can now work out the total work done in setting up the currents, and hence the total magnetostatic potential energy, in precisely the same way that we did before. If we set  $\alpha(0) = 0$  and  $\alpha(\tau) = 1$ , with  $\tau$  sufficiently large that the magnetostatic approximation to the behaviour is valid throughout the time interval, the energy is given by:

$$U = \int_0^\tau \alpha(t) \frac{d\alpha}{dt} dt \int_{\mathbb{R}^3} \mathbf{A} \cdot \mathbf{j} dV = \int_0^1 \alpha d\alpha \int_{\mathbb{R}^3} \mathbf{A} \cdot \mathbf{j} dV \quad (8.61)$$

Finally, we can evaluate the integral over  $\alpha$  to obtain the standard expression for the magnetostatic potential energy of a current distribution.

$$U = \frac{1}{2} \int_{\mathbb{R}^3} \mathbf{A} \cdot \mathbf{j} dV \quad (8.62)$$

The striking similarity between this result and equation (8.31) in section 8.2.6, tells us that, although it does not relate to the energy quite so obviously as  $\Phi$ , we were still very much justified in calling  $\mathbf{A}$  a potential. Another interesting facet to this equation is that, nowhere in our derivation did we specify a gauge condition for  $\mathbf{A}$ . This must mean that equation (8.62) holds true in all gauges, which is indeed the case. To see why this is the case we simply need to note that the only gauge freedom available to  $\mathbf{A}$  is for it to vary by an irrotational field, since this will not actually effect the magnetic field. We can then simply refer back to our previous theorem about the scalar product of an irrotational and a incompressible field, to see why this will have no effect on the energy.

### 8.4.3 Energy Density

Since our expressions for the magnetostatic and electrostatic potential energies are so similar, it does not seem unreasonable for us to assume that we can find an energy density for the magnetic field, just as we did for the electric field in section 8.2.6. Indeed this assumption turns out to be correct, and furthermore, the process by which we arrive at the result is more or less the same. The first thing we can do is use Ampere's law to rewrite equation (8.62) in the form:

$$U = \frac{1}{2\mu_0} \int_{\mathbb{R}^3} \mathbf{A} \cdot \nabla \times (\nabla \times \mathbf{A}) dV \quad (8.63)$$

Just as we have done several times already, we wish to evaluate this integral by parts. As it turns out, the identity that we want here, is a variation on the classic vector calculus identity  $\nabla \cdot (\mathbf{F} \times \mathbf{G}) = \mathbf{G} \cdot \nabla \times \mathbf{F} - \mathbf{F} \cdot \nabla \times \mathbf{G}$ . If we substitute in  $\mathbf{F} = \mathbf{A}$  and  $\mathbf{G} = \nabla \times \mathbf{A}$ , we obtain a useful identity. We can then evaluate integral (8.63) using this identity, to obtain:

$$U = \frac{1}{2\mu_0} \int_{\mathbb{R}^3} |\nabla \times \mathbf{A}|^2 dV - \frac{1}{2\mu_0} \int_{\mathbb{R}^3} \nabla \cdot (\mathbf{A} \times \nabla \times \mathbf{A}) dV \quad (8.64)$$

It follows from Gauss' theorem that the second integral in this expression will be vanishingly small, and thus, the energy reduces to the simple expression:

$$U = \frac{1}{2\mu_0} \int_{\mathbb{R}^3} \mathbf{B} \cdot \mathbf{B} dV = \int_{\mathbb{R}^3} \mathcal{E}_B dV \quad (8.65)$$

Here  $\mathcal{E}_B$  represents the magnetostatic energy density, and is given by equation (8.66) below.

$$\mathcal{E}_B = \frac{B^2}{2\mu_0} \quad (8.66)$$

We can now use this result to try understand why it is magnets behave in the ways that they do. As an example, we can use the energy density of the field to justify the formation of domains within a magnetic material. The fact that a material is magnetic, means that the most favourable arrangement of its internal dipoles is to have them all aligned parallel to each other. However, if too many of the dipoles are aligned in the same direction, they will produce a considerable stray field outside the material, which has an associated energy cost. If the stray field gets too large, it becomes favourable for the material to split into several distinct domains, which cancel out the stray field at the expense of unfavourable domain wall interactions.

Equation (8.65) also offers us a different way of calculating the self inductance of a circuit. Instead of evaluating it directly, we can integrate the magnetic field it produces over all of space, before comparing this against the known result that  $U = \frac{1}{2}LI^2$ . To demonstrate this let us consider a long solenoid of length  $l$ , cross sectional area  $A$ , and containing  $N$  turns of wire. If the solenoid is sufficiently long, then to a reasonable approximation, we can treat the field as  $\frac{\mu_0 NI}{l}$  everywhere inside the solenoid and 0 everywhere outside. This then yields

$$U = \frac{\mu_0 N^2 I^2 A}{2l} \implies L = \frac{\mu_0 N^2 A}{l} \quad (8.67)$$

## 8.5 Electrodynamics

Up until this point we have always been considering the fields within the framework of certain simplifying assumptions. However, in many ways, the most significant theoretical consequence of Maxwell's equation was the prediction of electromagnetic waves, something which can only be possible if we consider the full dynamical nature of the fields. As such, this section is dedicated to providing a reasonably detailed discussion of how Maxwell's equations can be solved in their most general form. For convenience, all four equations, which we introduced in section 8.1, have been reproduced below.

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{\rho}{\epsilon_0} & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= \mathbf{0} & \nabla \times \mathbf{B} - \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} &= \mu_0 \mathbf{j} \end{aligned} \quad (8.68)$$

### 8.5.1 Dynamic Potentials and Gauge Fixing

At this point, it should not come as a surprise that our first step in solving these equations is to introduce some auxiliary potential fields. Since Gauss' law for magnetism is just as true here as it was in section 8.3, we are free to continue using our vector potential  $\mathbf{A}$  in the same way that we have been doing already. Substituting this into the Maxwell-Faraday law then allows us to introduce a scalar potential such that  $\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \Phi$ , this is simply an extension of the electrostatic potential, from section 8.2, into the realm of electrodynamics. Collecting these results together, we can now express our fields in terms of the potentials:

$$\mathbf{E} = -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \quad \mathbf{B} = \nabla \times \mathbf{A} \quad (8.69)$$

Just as we found before, there is an inherent ambiguity in the potentials, which allows us to make certain alterations without affecting the fields. We can see that, for any two potentials  $\Phi$  and  $\mathbf{A}$ , the new potentials  $\Phi'$  and  $\mathbf{A}'$ , which are related by the gauge transformation below, will give rise to the exactly the same electric and magnetic fields.

$$\Phi' = \Phi - \frac{\partial \lambda}{\partial t} \quad \mathbf{A}' = \mathbf{A} + \nabla \lambda \quad (8.70)$$

Where  $\lambda$  is any arbitrary scalar field. With an appropriate choice of  $\lambda$ , it is possible to enforce a wide variety of gauge conditions. However, the restriction that is of the most interest to us is known as Lorentz gauge, which requires that:

$$\mu_0 \epsilon_0 \frac{\partial \Phi}{\partial t} + \nabla \cdot \mathbf{A} = 0 \quad (8.71)$$

We can see from this equation that, if the fields are static, the Lorentz gauge condition is equivalent to the Coulomb gauge condition, that we applied in our study of magnetostatics. Since our definitions of  $\mathbf{E}$  and  $\mathbf{B}$ , in terms of the potentials, automatically satisfy the homogeneous Maxwell's equations, we simply need to substitute equation (8.69) into Gauss' law and the Maxwell-Ampere equation. Doing so and then applying the Lorentz gauge condition, yields the following equations for  $\Phi$  and  $\mathbf{A}$ :

$$\mu_0 \epsilon_0 \frac{\partial^2 \Phi}{\partial t^2} - \nabla^2 \Phi = \frac{\rho}{\epsilon_0} \quad \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mu_0 \mathbf{j} \quad (8.72)$$

### 8.5.2 Electromagnetic Waves

In free space, Maxwell's equations adopt a simpler form, because the source terms,  $\rho$  and  $\mathbf{j}$ , are identically equal to zero. If we substitute these conditions into equation (8.72), from the previous section, then we can immediately see that we obtain 3 dimensional wave equations for  $\Phi$  and  $\mathbf{A}$ . It then directly follows from the symmetry of mixed partial derivatives, that the electric and magnetic fields must also obey the wave equations:

$$\frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} - \nabla^2 \mathbf{E} = \mathbf{0} \quad \frac{1}{c^2} \frac{\partial^2 \mathbf{B}}{\partial t^2} - \nabla^2 \mathbf{B} = \mathbf{0} \quad (8.73)$$

Where we have made the substitution  $c^2 = \frac{1}{\mu_0 \epsilon_0}$ . Obviously, when Maxwell first discovered these wave equations for the electromagnetic field, it was not understood that light itself was an example of electromagnetic radiation, and one of the principle sources of evidence was the strong agreement between the phase velocity that we have defined here, and the experimentally measured speed of light. Of course, nowadays the nature of light is well understood, and so this fact is often built into the formulation of Maxwell's equations by substituting in  $\mu_0 = \frac{1}{c^2 \epsilon_0}$ , for simplicity.

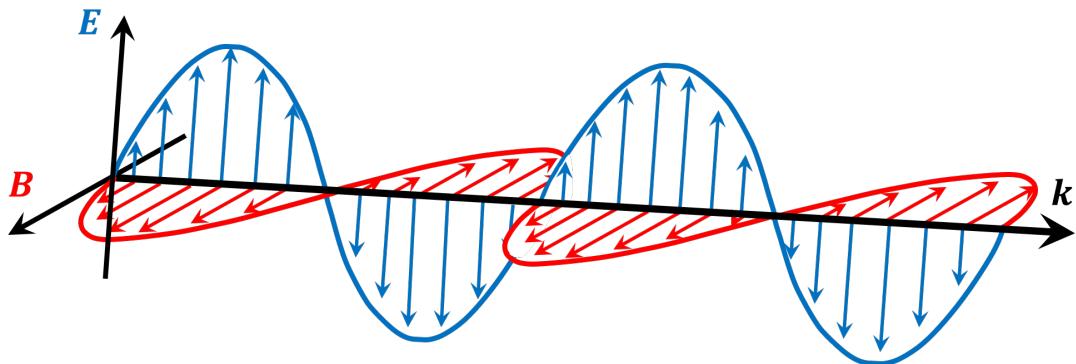


Figure 8.9: An electromagnetic plane wave.

Whilst there exists an infinite variety of possible solutions to the wave equations in (8.73), one of the most useful to consider is that of a plane wave. In general terms, any set of fields of the form below will satisfy the wave equations, provided that the wave vector and frequency  $\omega$  are related by  $\omega = |\mathbf{k}|c$ .

$$\mathbf{E} = \mathbf{E}_0 \cos(\omega t - \mathbf{k} \cdot \mathbf{r} + \phi) \quad \mathbf{B} = \mathbf{B}_0 \cos(\omega t - \mathbf{k} \cdot \mathbf{r} + \phi) \quad (8.74)$$

One of the nice properties of such a plane wave, is that we can always reconstruct the magnetic field from the electric and vice versa. If we suppose that both  $\mathbf{E}$  and  $\mathbf{B}$  take the form presented in equation (8.74), then it follows from the Maxwell-Faraday and Maxwell-Ampere laws, that  $\phi$ ,  $\omega$  and  $\mathbf{k}$  must be the same for both fields. In addition to this, we can also obtain the following restrictions on the allowed values of  $\mathbf{E}_0$  and  $\mathbf{B}_0$ :

$$\omega \mathbf{B}_0 = \mathbf{k} \times \mathbf{E}_0 \quad \mathbf{k} \cdot \mathbf{E}_0 = 0 \quad (8.75)$$

As such, we can conclude that at any point on an electromagnetic plane wave, the electric and magnetic fields are orthogonal to both the direction of propagation, and each other, as shown in figure 8.9. Thus, we can conclude that light is a transverse wave.

This principle of only needing to specify one field, applies quite generally to all forms of electromagnetic radiation, and not just to plane waves. To see this, let us suppose that the electric field  $\mathbf{E}$  has been specified over all space and time (by the symmetry of Maxwell's equations, all of the same arguments apply if the magnetic field is specified). Furthermore, let us suppose that there are two possible solutions for the magnetic field,  $\mathbf{B}_1$  and  $\mathbf{B}_2$ . If we now define the field  $\mathbf{B} = \mathbf{B}_1 - \mathbf{B}_2$ , it follows directly from Maxwell's equations that:

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \times \mathbf{B} = \mathbf{0} \quad \frac{\partial \mathbf{B}}{\partial t} = \mathbf{0} \quad (8.76)$$

Firstly, since  $\mathbf{B}$  is constant in time, it doesn't really make sense to describe this discrepancy as part of the wave, which is a dynamic object. However, it turns out that we can make an even stronger statement that the magnetic field must be unique, provided that certain boundary conditions are met. To see this let us first note that  $\mathbf{B}$  being irrotational implies that there exists some scalar field, such that  $\mathbf{B} = \nabla \mathcal{A}$ . Furthermore, the incompressibility of  $\mathbf{B}$  implies that  $\nabla \cdot (\mathcal{A}\mathbf{B}) = \mathbf{B} \cdot \nabla \mathcal{A}$ . If we now consider the integral of  $\mathbf{B} \cdot \mathbf{B}$  over some region of space  $V$ , we can use Gauss' theorem to state that:

$$\int_V \mathbf{B} \cdot \mathbf{B} dV = \oint_{\partial V} \mathcal{A}\mathbf{B} \cdot d\mathbf{S} \quad (8.77)$$

We can see from equation (8.77) that, if a suitable boundary condition is imposed on  $\mathbf{B}$ , the integral must be equal to zero. Since the integrand, which is equal to  $|\mathbf{B}|^2$ , can never be negative, this being the case implies that  $\mathbf{B} = \mathbf{0}$  everywhere, and thus, the magnetic field must be unique. If we consider the limit as  $V \rightarrow \mathbb{R}^3$ , then the boundary condition that the magnetic field vanishes at infinity will be sufficient to make it unique. Interestingly however, we may note that the plane wave solution from earlier does not satisfy this boundary condition, which seems to defeat our entire argument. However, what we must realise is that a true plane wave extending over all space, while useful for its simplicity, is in a sense unphysical. However, this does not stop the plane wave from being a useful description, since it offers a good approximation to the behaviour of a more realistic beam of radiation, so long as sufficient care is taken at the edges of the beam.

We can understand the origin of this seeming lack of freedom in the fields, by returning to our description in terms of the potentials  $\Phi$  and  $\mathbf{A}$ . Between the two potentials, there are only four components that can be varied, since  $\Phi$  is a scalar. Furthermore, it makes sense that the imposition of a gauge condition on the potentials, reduces the number of available degrees of freedom to three, all of which would be uniquely determined by specifying all three components of one of the fields.

Considering the behaviour of the fields in a vacuum is all well and good; however, in reality, we know that space does not provide an infinite vacuum in all directions. As such, if we wish to apply these principles to the real world, we will have to develop a sense for the boundary conditions that will be applied to our fields. The simplest example of this occurs when the fields are confined by a conductor. Assuming the material is perfectly conducting, charge will always flow, in such a way that it opposes any forces acting parallel to the surface. As such, both of the parallel components of  $\mathbf{E}$  and the normal component of  $\mathbf{B}$  must vanish at the surface of the conductor. This is nothing more than a generalisation of the electrostatic boundary conditions that we encountered in section 8.2.5.

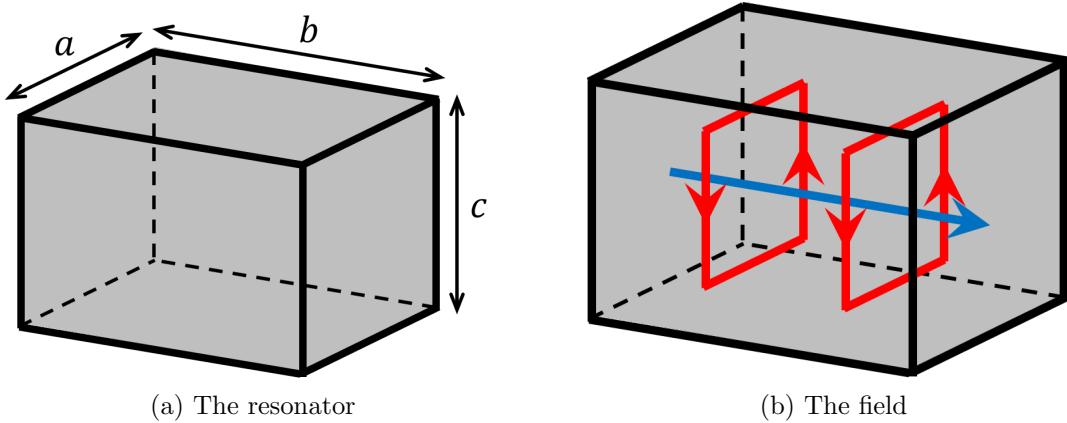


Figure 8.10: A simple cavity resonator and the field produced within it.

To demonstrate this principle in action, let us consider a simple cavity resonator, which consists of a hollow, conducting box, of side lengths  $a, b$  and  $c$  respectively. The simplest choice of coordinate system for this problem, is to place the origin at one of the corners of the box and then orient the axes with its edges. If we now consider the electric field, we can write the boundary conditions in terms of its components as:

$$\begin{aligned} E_x(x, 0, z, t) &= E_x(x, y, 0, t) = E_x(x, b, z, t) = E_x(x, y, c, t) = 0 \\ E_y(x, y, 0, t) &= E_y(0, y, z, t) = E_y(x, y, c, t) = E_y(a, y, z, t) = 0 \\ E_z(0, y, z, t) &= E_z(x, 0, z, t) = E_z(a, y, z, t) = E_z(x, b, z, t) = 0 \end{aligned} \quad (8.78)$$

In addition, we can use Gauss' law that  $\nabla \cdot \mathbf{E} = 0$  (the inside of the cavity is taken to be a vacuum), to generate an additional set of boundary conditions for the first derivatives of  $\mathbf{E}$ :

$$\begin{aligned} \frac{\partial E_x}{\partial x}(0, y, z, t) &= \frac{\partial E_x}{\partial x}(a, y, z, t) = 0 \\ \frac{\partial E_y}{\partial y}(x, 0, z, t) &= \frac{\partial E_y}{\partial y}(x, b, z, t) = 0 \\ \frac{\partial E_z}{\partial z}(x, y, 0, t) &= \frac{\partial E_z}{\partial z}(x, y, c, t) = 0 \end{aligned} \quad (8.79)$$

As is typical for problems such as this, we are now going to employ Fourier's method of separating the variables. That is to say that, we will be looking for solutions of the separable form  $E_x(x, y, z, t) = E_{x,0}X_x(x)Y_x(y)Z_x(z)T_x(t)$ , with equivalent expressions for both  $E_y$  and  $E_z$ . For convenience we have added in the scaling constant  $E_{x,0}$ , such that all of the separated functions have a maximum value of 1. Substituting this solution into Gauss' law gives us:

$$X'_x(x)Y_x(y)Z_x(z)T_x(t) + X_y(x)Y'_y(y)Z_y(z)T_y(t) + X_z(x)Y_z(y)Z'_z(z)T_z(t) = 0 \quad (8.80)$$

The only way that this can hold true for all  $x, y, z$  and  $t$  is, if all of the following conditions are met, for some constants  $\alpha, \beta$  and  $\gamma$ :

$$\begin{aligned} \alpha X'_x(x) &= X_y(x) = X_z(x) & Y_x(y) &= \beta Y'_y(y) = Y_z(y) \\ Z_x(z) &= Z_y(z) = \gamma Z'_z(z) & T_x(x) &= T_y(y) = T_z(z) \end{aligned} \quad (8.81)$$

To find the general form of the separable functions, we can substitute them into the wave equation (8.73), which after some rearrangement gives us:

$$\frac{X''_x(x)}{X_x(x)} + \frac{Y''_x(y)}{Y_x(y)} + \frac{Z''_x(z)}{Z_x(z)} = \frac{1}{c^2} \frac{T''_x(t)}{T_x(t)} \quad (8.82)$$

Since each term in this equation is a function of a different variable, they must each be equal to some constant. This implies that each of the separate functions must either be some kind of exponential function, or a sinusoidal function. If we then apply all of our boundary conditions from the previous page, we can narrow this down to give solutions of the general form:

$$\mathbf{E} = \begin{pmatrix} E_{x,0} \cos(k_x x) \sin(k_y y) \sin(k_z z) \\ E_{y,0} \sin(k_x x) \cos(k_y y) \sin(k_z z) \\ E_{z,0} \sin(k_x x) \sin(k_y y) \cos(k_z z) \end{pmatrix} \sin(\omega t + \phi) \quad (8.83)$$

Subject to the conditions that:

$$k_x = \frac{\pi n}{a}, \quad k_y = \frac{\pi m}{b}, \quad k_z = \frac{\pi l}{c} \quad n, m, l \in \mathbb{Z}^+ \text{ and } \omega = c \sqrt{k_x^2 + k_y^2 + k_z^2} \quad (8.84)$$

We can now establish if there are any restrictions on the allowed values of the constants  $E_{x,0}$ ,  $E_{y,0}$  and  $E_{z,0}$ . By applying Gauss' law, we can conclude that the only allowed amplitudes satisfy  $\mathbf{E}_0 \cdot \mathbf{k} = 0$ , where  $\mathbf{E}_0$  is the vector formed from the components  $E_{x,0}$ ,  $E_{y,0}$ ,  $E_{z,0}$ , and  $\mathbf{k}$  is the vector formed from the components  $k_x$ ,  $k_y$ ,  $k_z$ . Since this condition describes a plane in  $\mathbf{E}_0$  space, it follows that for each set of the wave numbers  $n, m, l$ , there will be two linearly independent modes of oscillation. Finally, we can note that by using a three dimensional Fourier series, it would be possible to reproduce any set of initial conditions by taking linear combinations of solutions in the form of (8.83). Thus, it follows that the general solution to the wave equation in the cavity can be represented as a superposition of the standing waves we have just described.

If we so desired, we could repeat this whole procedure to obtain the solutions for the magnetic field; however, as per our considerations earlier in this section, this is unnecessary. If the electric field is given by equation (8.83), then the corresponding magnetic field is given by:

$$\mathbf{B} = \begin{pmatrix} B_{x,0} \sin(k_x x) \cos(k_y y) \cos(k_z z) \\ B_{y,0} \cos(k_x x) \sin(k_y y) \cos(k_z z) \\ B_{z,0} \cos(k_x x) \cos(k_y y) \sin(k_z z) \end{pmatrix} \cos(\omega t + \phi) \quad (8.85)$$

Where the vector  $\mathbf{B}_0$ , which is formed from the components  $B_{x,0}$ ,  $B_{y,0}$ ,  $B_{z,0}$ , is given by the vector equation  $\omega \mathbf{B}_0 = \mathbf{k} \times \mathbf{E}_0$ .

It is worth taking a moment to comment on the significance of the two independent modes at each set of wave numbers. What we are actually seeing here is, that as a transverse wave, light has two distinct polarisations available to it. This property manifests in a lot of optical phenomena, and together with the theoretical prediction of the speed of light, was a key piece of evidence suggesting that light was, in fact, a form of electromagnetic radiation. The polarisation of light also has an interesting interpretation within the framework of quantum mechanics. Here, the polarisation is a property of each individual photon, related to its spin, and can be considered as analogous to the spin pairing of electrons in atomic orbitals.

### 8.5.3 The Jefimenko Equations

Now that we have studied the solutions to the sourceless Maxwell's equations in a significant amount of depth, it is high time that we return to the full formulation of electrodynamics, with the source terms included once again. We can start by recalling from section 8.5.1 that, in Lorentz gauge, the dynamics of the fields are governed by the equations:

$$\frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} - \nabla^2 \Phi = \frac{\rho}{\varepsilon_0} \quad \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mu_0 \mathbf{j} \quad (8.86)$$

Solving these equations is achieved using exactly the same principles that we employed before, when we solved Poisson's equation in electrostatics. Just as we did for the Laplacian, we now wish to find the Green's function of the d'Alembertian wave operator  $\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right]$ . The fundamental definition of the Green's function is that:

$$\frac{1}{c^2} \frac{\partial^2 G}{\partial t^2} - \nabla^2 G = \delta(\mathbf{r}, t) \quad (8.87)$$

Where  $\delta(\mathbf{r}, t) = \delta(\mathbf{r})\delta(t)$  is the 4-dimensional Dirac delta function. Just as before, the Green's function is not unique, and so we have some freedom in exactly what function we end up using. Physically, the option that makes the most sense is to set  $G = 0$  for all  $t < 0$ , since before this point there have been no sources to interact with the field. Under this restriction solving equation (8.87) simply becomes a matter of solving the wave equation subject to the initial conditions:

$$G(\mathbf{r}, 0) = 0 \quad \frac{\partial G(\mathbf{r}, 0)}{\partial t} = c^2 \delta(\mathbf{r}) \quad (8.88)$$

Since the general solution to the wave equation is well known, we can immediately proceed to give the Green's function as:

$$G(\mathbf{r}, t) = \begin{cases} \frac{\delta(r-ct)}{4\pi t} & t > 0 \\ 0 & t \leq 0 \end{cases} \quad (8.89)$$

It therefore follows, by the linearity of the d'Alembertian operator, that equation (8.86) can be solved by convolving the charge/current density with the Green's function. If we do this and then evaluate the integral over time, we obtain:

$$\Phi = \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}', t_r)}{4\pi\varepsilon_0 |\mathbf{r} - \mathbf{r}'|} dV' \quad \mathbf{A} = \int_{\mathbb{R}^3} \frac{\mu_0 \mathbf{j}(\mathbf{r}', t_r)}{4\pi |\mathbf{r} - \mathbf{r}'|} dV' \quad (8.90)$$

Where  $t_r$  is the retarded time, given by  $t_r = t - \frac{1}{c}|\mathbf{r} - \mathbf{r}'|$ . Importantly, the addition of the retarded time implies that any changes to the fields must propagate at speed  $c$  through space. This should not surprise us at all, since this is a very general feature of the solutions to inhomogeneous wave equations. We can now evaluate the derivatives of the potentials to obtain Jefimenko's equations:

$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0} \int_{\mathbb{R}^3} \left[ \left( \frac{\rho(\mathbf{r}', t_r)}{|\mathbf{r} - \mathbf{r}'|^3} + \frac{1}{c|\mathbf{r} - \mathbf{r}'|^2} \frac{\partial \rho(\mathbf{r}', t_r)}{\partial t} \right) (\mathbf{r} - \mathbf{r}') - \frac{1}{c^2 |\mathbf{r} - \mathbf{r}'|} \frac{\partial \mathbf{j}(\mathbf{r}', t_r)}{\partial t} \right] dV' \quad (8.91)$$

$$\mathbf{B} = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \left[ \left( \frac{\mathbf{j}(\mathbf{r}', t_r)}{|\mathbf{r} - \mathbf{r}'|^3} + \frac{1}{c|\mathbf{r} - \mathbf{r}'|^2} \frac{\partial \mathbf{j}(\mathbf{r}', t_r)}{\partial t} \right) \times (\mathbf{r} - \mathbf{r}') \right] dV' \quad (8.92)$$

### 8.5.4 Field Energy and Momentum

Having just derived the Jefimenko equations, we are in a prime position to consider one of their most important consequences. Let us perform a thought experiment in which we have a single charged particle, isolated in a vacuum. Let us now apply some external force to the particle so that it begins to accelerate. As its velocity increases, it will produce an electromagnetic field around itself, which will in turn lead to a force that opposes the acceleration. However, this has the rather alarming consequence that the energy and momentum of the particle are increasing at a slower rate than we are supplying them through our external force. The only conclusion that we can draw is that the fields themselves must carry some energy and momentum.

Let us start by considering the energy stored in an electromagnetic field. In order for the total energy to be conserved, the rate at which the field energy is lost must be identically equal to the rate at which the fields do work. As such we must have:

$$\frac{dU}{dt} = - \int_{\mathbb{R}^3} \mathbf{E} \cdot \mathbf{j} dV \quad (8.93)$$

We can now substitute in the Maxwell-Ampere equation, in order to rewrite this integral purely in terms of the fields. We can further manipulate the integral by utilising the vector calculus identity  $\nabla \cdot (\mathbf{F} \times \mathbf{G}) = \mathbf{G} \cdot \nabla \times \mathbf{F} - \mathbf{F} \cdot \nabla \times \mathbf{G}$ , which allows us to obtain:

$$\frac{dU}{dt} = \int_{\mathbb{R}^3} \varepsilon_0 \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} - \frac{1}{\mu_0} \mathbf{B} \cdot \nabla \times \mathbf{E} + \frac{1}{\mu_0} \nabla \cdot (\mathbf{E} \times \mathbf{B}) dV \quad (8.94)$$

From here, the first step is to simply note that, provided the fields vanish at infinity, Gauss' theorem implies that the integral of  $\nabla \cdot (\mathbf{E} \times \mathbf{B})$  must be equal to zero. Furthermore, if we use the Maxwell-Faraday equation to substitute for  $\nabla \times \mathbf{E}$ , we find the rather elegant result:

$$\frac{dU}{dt} = \frac{d}{dt} \int_{\mathbb{R}^3} \frac{\varepsilon_0 E^2}{2} + \frac{B^2}{2\mu_0} dV \implies U = \int_{\mathbb{R}^3} \frac{\varepsilon_0 E^2}{2} + \frac{B^2}{2\mu_0} dV \quad (8.95)$$

We have neglected to include a constant of integration in equation (8.95), since the zero point of energy is, outside of general relativity, an arbitrary definition. In addition to this, it seems that defining a complete absence of any fields as having zero energy, is a fairly sensible working definition.

This result is fully consistent with the work we have already completed in sections 8.2.6 and 8.4.3, establishing energy densities in electrostatic and magnetostatic systems respectively. As far as the energy density goes, equation (8.95) seems to be implying that the energy density takes the form of equation (8.96) below; however, it could always vary by some derivative that vanishes at our boundary conditions, thus not affecting the total field energy. Within the context of electrodynamics, we have no way of verifying which of the possible expressions for the energy density is correct and so we shall adopt the logic of Occam's razor and assume the simplest answer to be true.

$$\mathcal{E} = \frac{\varepsilon_0 E^2}{2} + \frac{B^2}{2\mu_0} \quad (8.96)$$

Now that we have established the energy density of the electromagnetic fields, it would be useful if we could find an expression for the flux of the field energy at a given point. That is to say that, we would like to find some vector  $\mathbf{S}$  such that the following continuity equation, which is known as Poynting's theorem, is obeyed.

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \mathbf{S} + \mathbf{E} \cdot \mathbf{j} = 0 \quad (8.97)$$

In fact, we have already come across one such vector, since we used this very fact in our derivation of the energy density. However, just as with the energy density, this single expression is not unique, after all we could always vary  $\mathbf{S}$  by any incompressible combination of the fields, without violating Poynting's theorem. Just as before, we shall choose the simplest example to deduce that the Poynting vector is given by:

$$\nabla \cdot \mathbf{S} = \frac{1}{\mu_0} \nabla \cdot (\mathbf{E} \times \mathbf{B}) \implies \mathbf{S} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} \quad (8.98)$$

Of course, the fields do not just possess their own energy, indeed the fields also possess a form of momentum. We shall find an expression for the field momentum in exactly the same way as we found the field energy. It follows from the Lorentz force law, that the rate at which the fields loose momentum to charged particles is given by:

$$\frac{d\mathbf{p}}{dt} = - \int_{\mathbb{R}^3} \mathbf{E}\rho + \mathbf{j} \times \mathbf{B} dV \quad (8.99)$$

Substituting in the relevant Maxwell's equations allows us to eliminate the source terms  $\rho$  and  $\mathbf{j}$  to express the integral entirely in terms of the fields:

$$\frac{d\mathbf{p}}{dt} = \epsilon_0 \int_{\mathbb{R}^3} \frac{\partial \mathbf{E}}{\partial t} \times \mathbf{B} + c^2 \mathbf{B} \times \nabla \times \mathbf{B} - (\nabla \cdot \mathbf{E}) \mathbf{E} dV \quad (8.100)$$

Before we can proceed any farther on this integral, we need to first consider how exactly we can deal with the  $(\nabla \cdot \mathbf{E})\mathbf{E}$  term in our integral, since it is not something that arises in very many vector calculus identities at all. The most elegant way to deal with it is to consider the divergence of the tensor:

$$\nabla \cdot (\mathbf{E} \otimes \mathbf{E}) = (\nabla \cdot \mathbf{E})\mathbf{E} + (\mathbf{E} \cdot \nabla)\mathbf{E} \quad (8.101)$$

It then follows from the tensor form of Gauss' theorem, that since  $\mathbf{E}$  is vanishingly small at infinity, we must have:

$$\int_{\mathbb{R}^3} (\nabla \cdot \mathbf{E})\mathbf{E} dV = - \int_{\mathbb{R}^3} (\mathbf{E} \cdot \nabla)\mathbf{E} dV \quad (8.102)$$

If we wished to avoid utilising the tensor product, as used here, this same result can be achieved using the normal Gauss' theorem, by splitting the integrand up into its components, this is simply a more concise notation. Returning to integral (8.100), we can now use this identity, together with the corresponding one for  $\mathbf{B}$ , which must vanish due to Gass' law for magnetism, to rewrite the integral in terms of the gradient:

$$\nabla \left( \frac{E^2}{2} + \frac{c^2 B^2}{2} \right) = \mathbf{E} \times \nabla \times \mathbf{E} + (\mathbf{E} \cdot \nabla)\mathbf{E} + c^2 [\mathbf{B} \times \nabla \times \mathbf{B} + (\mathbf{B} \cdot \nabla)\mathbf{B}] \quad (8.103)$$

If we now apply the Maxwell-Faraday law, to express  $\nabla \times \mathbf{E}$  in terms of the magnetic field, we can express (8.100) as the following integral:

$$\frac{d\mathbf{p}}{dt} = \varepsilon_0 \int_{\mathbb{R}^3} \frac{\partial \mathbf{E}}{\partial t} \times \mathbf{B} + \mathbf{E} \times \frac{\partial \mathbf{B}}{\partial t} + \nabla \left( \frac{E^2}{2} + \frac{c^2 B^2}{2} \right) dV \quad (8.104)$$

A corollary of Gauss' law tells us that the integral of the gradient term is vanishingly small, provided the fields tend to zero at infinity, which allows us to express (8.104) in the very simple form:

$$\frac{d\mathbf{p}}{dt} = \frac{1}{c^2} \frac{d}{dt} \int_{\mathbb{R}^3} \mathcal{S} dV \quad (8.105)$$

Just as we found before, while this does not allow us to uniquely determine an expression for the momentum density of the fields, in the absence of a better option, we shall simply adopt the simplest expression that seems to work. Thus, we can conclude that the electromagnetic fields have a momentum density of:

$$\mathcal{P} = \varepsilon_0 (\mathbf{E} \times \mathbf{B}) = \frac{\mathcal{S}}{c^2} \quad (8.106)$$

This relationship between the Poynting vector, which represents a flux of energy, and the momentum density of the field, is not merely a coincidence, and is a necessary condition in order to be consistent with the symmetry of the stress-energy tensor in special relativity. Interestingly, since we have already established that the electromagnetic fields propagate through space with a phase velocity of  $c$ , this equation implies that the energy carried by a propagating field is equal to  $c$  times its momentum, just as it should be for a massless particle such as the photon, within the framework of special relativity.

As we conclude this section, it is worth noting that in the formulation of electromagnetism we have employed, where we have started by assuming the truth of Maxwell's equations, these results about field energy and momenta arise in a seemingly incidental fashion. These ideas actually follow much more naturally from a Lagrangian formulation, and Noether's theorem. While we shall not spend any significant time on the matter, it is worth being aware that the fields can be described by the Lagrangian density:

$$\mathcal{L} = \frac{\varepsilon_0 E^2}{2} - \frac{B^2}{2\mu_0} - \rho\Phi + \mathbf{j} \cdot \mathbf{A} \quad (8.107)$$

We can also give the Lagrangian function for a single charged particle moving in the electromagnetic fields as:

$$L = \frac{mv^2}{2} - q[\Phi - \mathbf{v} \times \mathbf{A}] \quad (8.108)$$

Everything that we have discussed throughout this entire chapter actually follows from just these two definitions, and the principle of least action, which just goes to show why variational principles are considered to be such a powerful technique.

# 9 Thermodynamics

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## 9.1 The Laws of Thermodynamics

Thermodynamics, or statistical mechanics as it is often referred to in its modern form, is one of the most powerful parts of modern physical theory. While it initially began as a purely empirical discipline, with the principle goal of maximising the efficiency of steam engines, thermodynamics has since evolved into a broad theoretical discipline, that is essential in any description of a macroscopic system. Central to any physical theory are its postulates, and, in the case of thermodynamics, these take the form of the four fundamental laws, which are the topic of this section. While some of these laws may seem obvious, we should remember that, it is still important for us to present them in a rigorous manner. As such, we shall discuss these laws, without assuming anything about the nature of quantities such as temperature.

### 9.1.1 The Zeroth Law

The zeroth law of thermodynamics states that, if two bodies  $A$  and  $B$  are in thermal equilibrium with each other, and  $B$  is also in thermal equilibrium with some third body  $C$ , then  $A$  and  $C$  must also be in thermal equilibrium with one another, even if there exists no direct thermal contact between them.

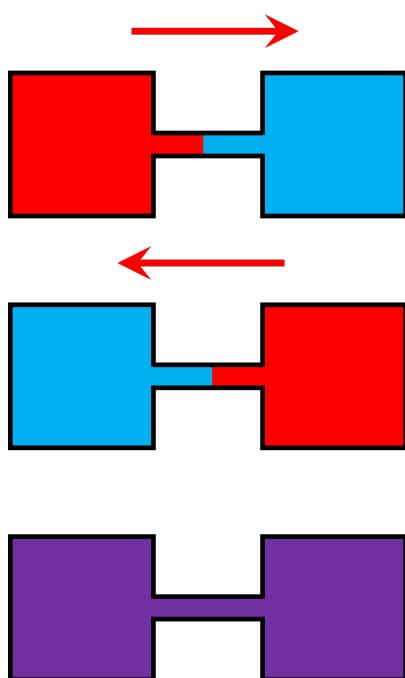


Figure 9.1: Heat flowing between bodies.

To understand this law, we should first unpack precisely what is meant by the terminology used to express it. Two bodies are considered to be in thermal contact, if they are capable of exchanging heat with one another. Here heat is used to describe the flow of energy from one body to another, by a mechanism other than mechanical work. At the present moment, we have not established how to determine in which direction heat flows between the two bodies, although intuitively we know that this will happen down a temperature gradient. Two bodies can then be described as being in thermal equilibrium, if they are in thermal contact, but no heat flows between them.

Figure 9.1 shows the different ways heat can flow between two bodies in thermal contact. In the final case, when no heat flows, they are in equilibrium. The zeroth law tells us that, determining whether or not two objects are in thermal equilibrium is not simply a pairwise process. Instead, we can assign some quantity, called temperature, to an object, and determine the nature of the thermal contact between two bodies, by comparing their temperatures.

It is worth highlighting that, for two bodies to be in thermal contact, they do not necessarily have to be physically touching each other. Instead, all that is required is a conductive pathway, through which heat can flow, from one body to the other. As such, every element of an extended body must be in thermal contact with every other element. Thus, if the body is in thermodynamic equilibrium, its temperature must be uniform, throughout its volume.

### 9.1.2 The First Law

The first law of thermodynamics relates changes in the internal energy of a system, to the heat and work transferred to that system. As such, it states that:

$$dU = \delta q + \delta w \quad (9.1)$$

Where  $dU$  represents the infinitesimal change in internal energy of a system, over some infinitesimal time interval. The terms  $\delta q$  and  $\delta w$ , then represent the infinitesimal heat and work transferred to the system, over that same interval. Since we defined heat to be any transfer of energy to a system other than mechanical work, this is simply a statement of the conservation of energy. Importantly, the work referred to in the context of thermodynamics is subtly different from the work we discussed in chapter 1. The thermodynamic work done on a system is equal to the work done, against the macroscopic forces produced by the system, when changing its state. This does not include any work done by forces, which accelerate the system's centre of mass, or forces, which change the system's total potential energy arising from external force fields. Thus, when we talk about a system's internal energy, we are discussing the component of that system's energy, which is not affected by either the system's position or motion through space.

It is worth noting the choice to represent the change in the internal energy with a differential  $d$ , while we represented the heat and work with a  $\delta$ . This is because the internal energy is a state function, for any change in the system, it can be assigned a value at the initial state, the final state, and at every moment in between. As such, we can meaningfully take the differential of the internal energy, by considering the difference in its value, between two subsequent moments. Conversely, the heat and work are not state functions, since the values they take depend on what process is used to convert the system from one state to another. Thus, we use a  $\delta$  to indicate that that we are not taking the differential of a function of the system's variables.

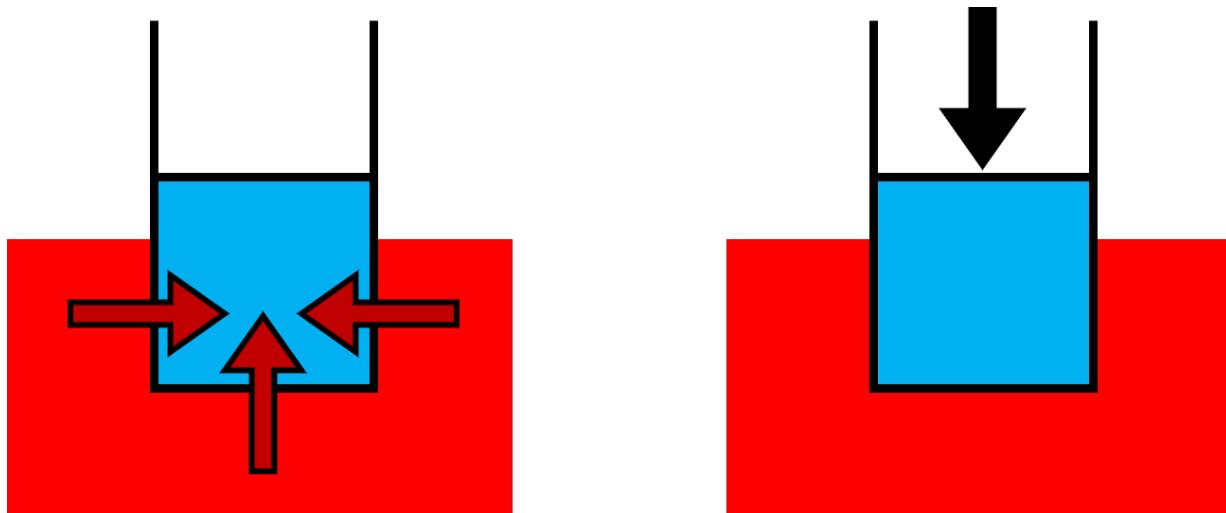


Figure 9.2: The two different methods of energy transfer.

### 9.1.3 The Second Law

The second law of thermodynamics states that, for any closed system, the change in entropy  $S$  must always be positive. That is to say that:

$$dS \geq 0 \quad (9.2)$$

Since, ultimately, the universe is a closed system, this implies that the total entropy of the universe must always increase. Although we shall provide a definition of the entropy later, we can already appreciate the value of this law. Once we find an expression for  $S$ , it would enable us to predict in which direction any given process would occur. For example, on an atomic scale, there is no reason why any given chemical reaction could not occur in both the forwards and backwards directions. However, with the second law, we can explain why it is that macroscopic reactions, typically only proceed in one direction. Like the internal energy, entropy is a state function, hence the use of a  $d$  to denote the differential of a function. Processes which convert a system between states of equal entropy are referred to as being reversible, since they are the only processes for which, both the forwards and backwards directions satisfy the second law. Such reversible processes can only occur infinitely slowly, since if the change in entropy is zero, there is no driving force for the process to occur at all. Nonetheless, they are still useful to consider, and can offer a very good approximation for a process carried out slowly.

We shall establish a formal definition for the entropy soon, but for now we can consider it to be a measure of the disorder within a system. In this way the second law makes a degree of intuitive sense, assuming that nature has no reason (for example an energetic barrier) to prefer one state over another, it will naturally tend to find itself in progressively more disordered states over time. This can be thought of by analogy to something simple, such as a Rubik's cube. The ordered, solved state can only be achieved in one very specific configuration, whereas the disordered, unsolved state has thousands of essentially equivalent configurations. Thus, if a blindfolded player were to randomly turn the Rubik's cube, they would essentially never be able to return to the solved state, and the cube would rapidly degenerate into a completely chaotic unsolved state.

### 9.1.4 The 3rd Law

The third law of thermodynamics states that, the entropy of a system tends to a fixed positive constant, as its temperature tends towards absolute zero. In the case of a perfect crystal this constant entropy is in fact zero.

Although we do not currently have a formal definition for thermodynamic temperature, we can use our intuition that it represents a system's ability to reject heat into the surroundings, in order to gain some insight into the concept of absolute zero. If a system has lost all of its internal energy, then it can not transfer any more heat to its surroundings, and thus its temperature could not be any lower. We call this minimum possible temperature absolute zero. At this point, the system has its minimum possible internal energy, and so, irrespective of other properties, can only be found in its lowest energy, ground state(s). As such, the disorder, and hence entropy, of the system is fixed to take a certain value, which can not be influenced by other factors, such as pressure, or external force fields.

## 9.2 Thermodynamic Quantities

We are now going to discuss some important thermodynamic quantities, and also establish rigorous definitions for quantities, such as thermodynamic temperature and pressure. For the sake of simplicity, we shall be exploring these concepts within the framework of a fairly idealised system, that of a homogeneous material containing a fixed number of particles. For such a simple system, it turns out that, only two thermodynamic state functions are required, in order to uniquely define the macroscopic state of the system.

### 9.2.1 Entropy

The Boltzmann definition of entropy is that:

$$S = k \ln \Omega \quad (9.3)$$

Where  $k$  is Boltzmann's constant, taking a value of  $k = 1.380\,649 \times 10^{-23} \text{ J K}^{-1}$  by definition<sup>8</sup>. Technically speaking, the Boltzmann constant is not necessary in a formulation of thermodynamics, since it simply serves the purpose of relating the units of energy and the units of temperature. If we were to measure temperature in units of energy, then the Boltzmann constant would become unity, and the entropy would become a dimensionless physical quantity. Although this is certainly the more natural way to work, we shall stick to the standard SI convention, throughout this chapter, since this allows us to keep quantities like temperature in familiar units.

Of greater importance is the meaning of  $\Omega$ , since this is the physical basis for the entropy.  $\Omega$  represents the number of micro-states of the system, which are equivalent to the observed macro-state. We can understand what this means by returning to the Rubik's cube analogy of section 9.1.3. For simplicity, let us suppose that the Rubik's cube has three distinguishable macroscopic states: solved, partially solved and unsolved. There is only one configuration of the cube that would be considered solved, and so, for this state,  $\Omega = 1$ , which implies that  $S = 0$ . Thus, the solved state represents a perfect crystal at absolute zero. Depending on how one defines a partially solved cube, there are about  $\Omega = 750000$  different configurations, giving an entropy of  $S \approx 14k$ . For an unsolved cube, there are about  $\Omega = 4.3 \times 10^{19}$  possible configurations, to give a total entropy of  $S \approx 45k$ . We can see immediately from this example that due to the logarithmic nature of the entropy, small changes in  $S$  correspond to overwhelmingly large increases in  $\Omega$ , and thus, the second law of thermodynamics follows from simply considering the probabilities of the system being in each state. We can see that, since  $\Omega$  depends only on the current state of the system,  $S$  must be a state function

As it turns out, the Boltzmann entropy is a simplification of a more fundamental definition of entropy. For a system that has many micro-states available to it, such that the probability of the system being in the  $i$ th state at any given time is  $p_i$ , we can express the entropy as:

$$S = -k \sum_i p_i \ln p_i \quad (9.4)$$

---

<sup>8</sup>As of 20 May 2019, the Kelvin is defined such that the Boltzmann constant takes precisely this value.

Luckily, for large systems, the overwhelming majority of the micro-states are those that have the same total energy, and are thus equally probable (as we shall see later), meaning that these contributions dominate the value of the entropy. If all the micro-states are equally probable, then all of the probabilities must be  $p_i = \frac{1}{\Omega}$ , and thus, the Boltzmann entropy is restored. We can now use equation (9.4) to find the differential of  $S$ , upon small changes to the probabilities of each micro-state:

$$dS = -k \sum_i \ln(Zp_i) dp_i \quad (9.5)$$

Where  $Z$  is some property of the system that we have yet to determine. This factor of  $Z$  arises from the restriction on the sum of all the probabilities. Since the total probability of finding the system in some state is always one, we must have:

$$\sum_i p_i = 1 \implies \sum_i dp_i = 0 \quad (9.6)$$

Therefore, the factor of  $Z$  in equation (9.5) will always cancel from the overall differential, leaving an ambiguity in the exact values of each of the terms. Although the value of  $Z$  does not affect the value of  $dS$ , it does have an impact on the individual partial derivatives of  $S$ , which according to equation (9.5) must be:

$$\frac{\partial S}{\partial p_i} = -k \ln(Zp_i) \quad (9.7)$$

Of course, this definition of entropy is not the only one that would satisfy the second law, for example the quantity  $e^S$ , must also increase in any physical process. The value of the entropy defined in this way, is that it possesses a very useful property known as extensivity. That is to say that, the total entropy of two identical systems is equal to precisely twice the entropy of one of the systems in isolation. This is a highly desirable property, since it makes calculations a lot quicker, and more intuitive. As we shall see, the vast majority of thermodynamic functions are either extensive, or intensive, which means that the value does not scale at all with the size of the system. To see the extensivity of the entropy we simply note that, given two identical systems, the probability of the first being in the  $i$ th state, and the second in the  $j$ th, is simply  $p_i p_j$ . Therefore:

$$S_2 = -k \sum_i \sum_j p_i p_j \ln(p_i p_j) \quad (9.8)$$

If we then split the logarithm, and note that the sum of all the probabilities must equal one, we conclude that:

$$S_2 = -k \sum_i p_i \ln p_i \sum_j p_j - k \sum_j p_j \ln p_j \sum_i p_i = -2k \sum_i p_i \ln p_i = 2S_1 \quad (9.9)$$

Importantly, the two sub-systems are distinguishable, meaning that the state  $i, j$  is distinct from the state  $j, i$ . In this example the distinguishability most likely arises from the systems having different physical locations in space. Properly accounting for distinguishability is very important in thermodynamics, and helps to explain why mixing two containers of the same gas has a much lower entropy change than mixing two different gases.

### 9.2.2 Internal Energy

The internal energy of a system represents the total non-macroscopic energy stored within that system. As such, the internal energy does not include any contributions from the kinetic energy associated with the system's centre of mass motion, or from the potential energy of the system's position in an external force field. That is to say that, the internal energy is the component of the system's energy, which will remain the same, wherever it is in space, and in whatever reference frame it is observed. This distinction is important to bear in mind, when we start discussing the work done on a system. When we are talking in the context of thermodynamics, that work does not include work done in accelerating the centre of mass of the system, and instead solely refers to any work done on the internal components of the system.

For the physical system that we have been considering so far, we can express the internal energy as:

$$U = \sum_i p_i E_i \quad (9.10)$$

Where  $E_i$  represents the energy of the  $i$ th micro-state available to the system. Since the  $E_i$  are determined by the physical parameters of the system, such as its volume, and the  $p_i$  are used to describe the state of the system,  $U$  must also be a state function. Furthermore, since energies add linearly, in the same way that  $\ln p_i p_j = \ln p_i + \ln p_j$ , we can use a similar argument to the one in section 9.2.1, in order to say that  $U$  must also be extensive. Just as we did with the entropy earlier, we can take the differential of  $U$  to obtain:

$$dU = \sum_i E_i dp_i + \sum_i p_i dE_i \quad (9.11)$$

Technically, we could add an extra constant to the  $E_i$  terms, since the sum of all the  $dp_i$  must be zero, in the same way that we added  $Z$  to equation (9.5). However, the freedom of energy to differ by an arbitrary additive constant is nothing new, and this ambiguity can simply be absorbed by the ambiguity in the zero point of energy. By comparing this to the first law in section 9.1.2, we can see that:

$$\delta q + \delta w = \sum_i E_i dp_i + \sum_i p_i dE_i \quad (9.12)$$

A particular special case of this arises, when these changes are carried out reversibly. Since reversible changes require that the entropy change of the entire universe is zero, they must always be carried out at equilibrium, and thus, happen infinitely slowly. If work is done by such a slow, continuous process, the adiabatic theorem of quantum mechanics tells us that the probabilities must remain fixed. This result is a consequence of the way time dependence is introduced into quantum mechanics, through the Schrödinger equation, and for our purposes we can simply accept it as true. Intuitively however, it makes a degree of sense, that physical work actually changes the states available to the system, whereas the more abstract heat simply allows the system to access higher energy states. This allows us to say that for a reversible process:

$$\delta w_{\text{rev}} = \sum_i p_i dE_i \quad \delta q_{\text{rev}} = \sum_i E_i dp_i \quad (9.13)$$

### 9.2.3 Temperature

We now come to define thermodynamic temperature. In principle, all that we need to measure an object's temperature is some definition, which relates a specific physical system to a specific temperature. In the past, this was done by using the thermal expansion of different materials, or the pressure and volume of a gas. We could then find an object's temperature by bringing it into thermal contact with such a test system until they reach equilibrium. In our more theoretical formulation, we can instead define the temperature directly from state functions we have already introduced.

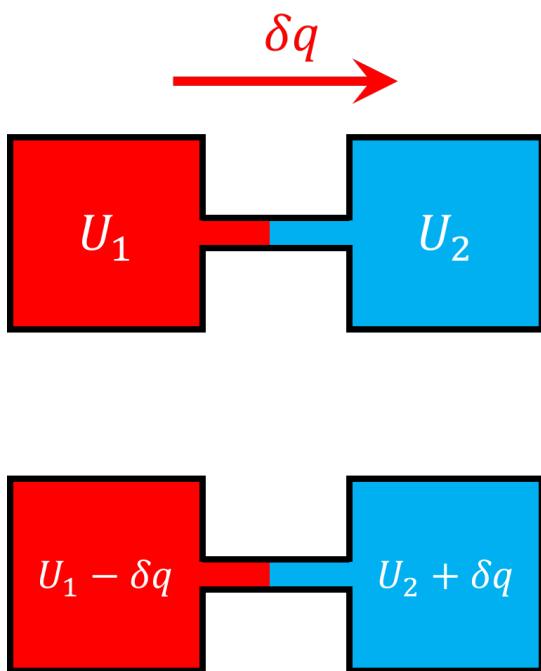


Figure 9.3: Heat flowing from a hotter body to a cooler one.

Let us bring two systems with internal energies  $U_1, U_2$  and entropies  $S_1, S_2$  into thermal contact. If we now suppose that a small amount of heat  $\delta q$  flows from system 1 into system 2, we can write the overall change in entropy of the combined system as:

$$dS = \left[ \left( \frac{\partial S_2}{\partial U_2} \right)_{V_2} - \left( \frac{\partial S_1}{\partial U_1} \right)_{V_1} \right] \delta q \quad (9.14)$$

The partial derivatives are evaluated at constant volume, because no work is being done on either system. Now by considering the second law that  $dS \geq 0$  we must conclude the following about the sign of  $\delta q$ :

$$\left( \frac{\partial S_2}{\partial U_2} \right)_{V_2} - \left( \frac{\partial S_1}{\partial U_1} \right)_{V_1} \gtrless 0 \implies \delta q \gtrless 0 \quad (9.15)$$

Thus, the derivative of entropy with respect to energy acts as a measure of how easily a system can accept heat from its surroundings.

In other words, systems with a larger value of  $(\frac{\partial S}{\partial U})_V$  will be better at absorbing heat from other systems. Since we want low temperature systems to be good at absorbing heat, we choose to define the temperature as:

$$\frac{1}{T} = \left( \frac{\partial S}{\partial U} \right)_V \iff T = \left( \frac{\partial U}{\partial S} \right)_V \quad (9.16)$$

No matter what configuration a system is in, supplying it with more energy will always allow it to spread out over a wider range of the available energy states. As such, the entropy of a system must always increase with its internal energy, and thus, the thermodynamic temperature of the system must always be positive. This is fully in keeping with our discussion of an absolute zero temperature, from section 9.1.4. In addition to this, we can note that, since both  $S$  and  $U$  are extensive properties of a system, the temperature must itself be intensive. Furthermore, it immediately follows from this definition that, two objects can only be in thermal equilibrium, if the both have the same temperature, which is fully consistent with the zeroth law.

We can now use some of the results derived in previous sections, to gain a greater understanding of how exactly temperature affects a thermodynamic system. Since under constant volume conditions the geometry of a system, and hence its energy levels, do not change, we can use equation (9.11) to say that:

$$dU_{\text{const.}V} = \sum_i E_i dp_i \quad (9.17)$$

By equating this result to the standard first order expansion of a multi variable function, we can conclude that the partial derivatives of the internal energy are given by:

$$\left( \frac{\partial U}{\partial p_i} \right)_V = E_i \quad (9.18)$$

We can compare these results to our th derivatives of the entropy from section 9.2.1, by utilising the chain rule of partial differentiation:

$$\frac{\partial S}{\partial p_i} = \left( \frac{\partial S}{\partial U} \right)_V \left( \frac{\partial U}{\partial p_i} \right)_V = \frac{E_i}{T} \quad (9.19)$$

If we now substitute in the results from equation (9.7), we arrive at the following expression for the probabilities of each state:

$$\ln(Zp_i) = -\frac{E_i}{kT} \quad (9.20)$$

By requiring that the sum of the probabilities must be equal to one, we can determine the value of  $Z$ , and thus, derive an expression for all of the probabilities at a given temperature:

$$p_i = \frac{e^{-\beta E_i}}{Z} \quad Z = \sum_i e^{-\beta E_i} \quad (9.21)$$

Where  $\beta = \frac{1}{kT}$  is a fairly common piece of notation, that we shall consistently use, in order to help simplify our algebra. Interestingly, we can note that our expression for the change in the internal energy  $U$ , under constant volume conditions, is precisely the same as our expression for  $\delta q_{\text{rev}}$ , and furthermore, if we substitute equation (9.20) into equation (9.5), we find that:

$$dS = \frac{\delta q_{\text{rev}}}{T} \quad (9.22)$$

This result is often referred to as the classical definition of entropy, although, in our formulation of thermodynamics, it is merely a consequence of the way in which we have defined the temperature. Nonetheless, this macroscopic definition is, in many cases, more convenient to use, since actually calculating all of the different states available to a system can be quite time consuming. In addition to this, macroscopic quantities, such as heat and temperature, also have the advantage of being much easier to measure experimentally. This result shall be particularly useful, when it comes time for us to consider extracting work from a thermodynamic system, since it relates the entropy, which is what limits the efficiency of a system, to the macroscopic quantities.

### 9.2.4 Pressure

Classically, we can think of pressure as representing a force acting per unit area. Since we know that the work done by a force  $\mathbf{F}$ , when it moves through a displacement  $d\mathbf{r}$ , is given by the dot product  $\mathbf{F} \cdot \mathbf{x}$ , it follows that the work done by an external pressure, when it changes the volume of a system by  $dV$ , is given by:

$$\delta w = -P_{\text{ext}} dV \quad (9.23)$$

The minus sign here arises, because  $\delta w$  represents the work done on the system, which is positive if the system is being forcibly compressed. For a reversible process, the system must always be in equilibrium with the external pressure, and so the resultant force on any given area must be zero. Thus, the internal pressure  $P$  must be equal to the external pressure  $P_{\text{ext}}$ . As such, we can conclude that the reversible work done on a system is given by:

$$\delta w_{\text{rev}} = -P dV \quad (9.24)$$

If we consider the first law of thermodynamics for a reversible process, and then substitute in equation (9.22) for the heat, and (9.24) for the work, we obtain the following result, often referred to as the fundamental thermodynamic relation:

$$dU = T dS - P dV \quad (9.25)$$

The standard expression for the differential of  $U$  is given by the first order Taylor series expansion:

$$dU = \left( \frac{\partial U}{\partial S} \right)_V dS + \left( \frac{\partial U}{\partial V} \right)_S dV \quad (9.26)$$

By comparing this result to the fundamental thermodynamic relation, we can conclude that the internal pressure must be given by the partial derivative:

$$P = - \left( \frac{\partial U}{\partial V} \right)_S \quad (9.27)$$

Since both  $U$  and  $V$  are extensive state functions, this equation implies that pressure is itself an intensive state function. There are several properties of the pressure, which make it a particularly useful variable to consider. Firstly, since the pressure is related to macroscopic effects, such as the force a system exerts on its surroundings, it is significantly easier to measure than a quantity like entropy. Additionally, since a lot of systems are in mechanical equilibrium with the atmosphere, they are maintained at a constant pressure, which can help to simplify our calculations, by essentially reducing our thermodynamic quantities to functions of a single variable.

There are a number of different mechanisms, by which a system can generate an internal pressure. In solid systems, the principle source of the internal pressure is the strain stored in the bonds between the atoms and molecules, while in liquids it arises from the collisions between molecules and the walls of their container. Pressure can also arise as a consequence of other less intuitive mechanisms, such as the absorption and re-emission of light, a phenomenon known as radiation pressure.

### 9.2.5 Enthalpy, Free Energy and Free Enthalpy

When working with thermodynamic systems, it can often be useful to define new state functions, which enable us to deal with certain situations more easily. We shall examine three such functions: enthalpy, Helmholtz free energy, and Gibbs free energy, which is also known as free enthalpy. To understand the motivation behind these quantities, we shall start by considering the fundamental thermodynamic relation from equation (9.25).

$$dU = TdS - PdV \quad (9.28)$$

It follows from this equation, and the symmetry of mixed partial derivatives that:

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V \quad (9.29)$$

This is known as a Maxwell relation, and as we shall see, we can obtain a similar relationship between thermodynamic variables, from the differentials of each of the state functions we shall introduce in this section.

The first quantity for us to introduce is the enthalpy  $H$ , which is defined as the Legendre transformation:

$$H = U + PV \quad (9.30)$$

Taking the differential of the enthalpy, and substituting in (9.28), we obtain:

$$dH = TdS + VdP \quad (9.31)$$

Which implies the Maxwell relation:

$$\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P \quad (9.32)$$

In a similar manner, we can introduce the Helmholtz free energy  $F$ , defined to be:

$$F = U - TS \quad (9.33)$$

Evaluating the differential of the free energy gives us:

$$dF = -PdV - SdT \quad (9.34)$$

Which gives rise to the Maxwell relation:

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T \quad (9.35)$$

Finally, if we combine the enthalpy and free energy transformations, we obtain the Gibbs free energy, also known as the free enthalpy, which is defined by:

$$G = U + PV - TS = H - TS = F + PV \quad (9.36)$$

Once again, we can take the differential to obtain:

$$dG = VdP - SdT \quad (9.37)$$

Which gives us the corresponding Maxwell relation:

$$\left(\frac{\partial V}{\partial T}\right)_P = -\left(\frac{\partial S}{\partial P}\right)_T \quad (9.38)$$

## 9.3 Distributions

Thermodynamic distributions are very useful tools in the statistical description of large systems. A distribution is used to describe the probability that a microscopic subsystem of the macro-system in question finds itself in a given state. This can also be very useful for determining the bulk properties of the system, since the numbers involved are so large that the deviations of the actual system from the average of its distribution is essentially negligible.

### 9.3.1 Boltzmann Distribution

The Boltzmann distribution is the simplest, and most fundamental distribution we will encounter. In fact, we already encountered the Boltzmann distribution in section 2.3, when we determined that the probability of finding a system in the  $i$ th energy level was:

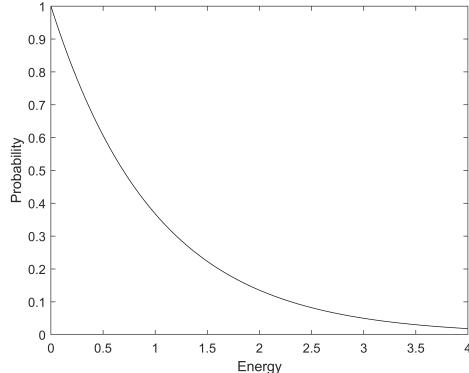


Figure 9.4: The Boltzmann distribution.

$$p_i = \frac{e^{-\beta E_i}}{Z}$$

This result can be understood fairly nicely by considering our system to be in contact with a large heat bath. Often our system is itself a subsystem of a larger system, and then the remainder of the system can perform the role of heat bath. If our system is brought into contact with the heat bath, and reaches an energy  $E$ , which by virtue of the bath's size is much smaller than the total energy  $U$ , the first law implies that the energy of the bath will be  $U - E$ . If we then calculate the entropy of the bath, we find that:

$$S(U - E) = S(U) - \frac{\partial S}{\partial U}E = S(U) - \frac{E}{T} \quad (9.39)$$

If the heat bath is large, then we can use the Boltzmann entropy, and thus, the total number of micro-states of the bath is given by  $\Omega(E) = e^{\frac{S(U)}{k} - \frac{E}{kT}}$ . Assuming that every micro-state of the bath is equally likely, the probability of finding the system in any given state must be proportional to the corresponding number of bath micro-states. Thus, we obtain:

$$p_E \propto e^{\frac{S(U)}{k} - \frac{E}{kT}} \propto e^{-\beta E} \quad (9.40)$$

This is essentially the same result that we derived in section 9.2.3. Just as we did then, we can introduce a quantity  $Z$ , which is known as the partition function of the system, to act as a normalisation constant for the probabilities. That is to say that:

$$Z = \sum_i e^{-\beta E_i} \implies p_E = \frac{1}{Z} e^{-\beta E} \quad (9.41)$$

As it turns out, this partition function is actually a very convenient way to describe a thermodynamic system, and shall form the basis for a lot of the results in later chapters.

To see the value of the partition function, we can first substitute the Boltzmann probabilities into equation (9.4) for the entropy, which yields:

$$S = -k \sum_i p_i \ln p_i = k \sum_i p_i(\beta E_i + \ln Z) = \frac{U}{T} + k \ln Z \quad (9.42)$$

By substituting this result into the definition of the Helmholtz free energy, we obtain the incredibly useful relationship:

$$F = -kT \ln Z \iff Z = e^{-\beta F} \quad (9.43)$$

Since the free energy is an extensive quantity, the partition function is neither intensive or extensive, instead when combining different systems we multiply their partition functions together. This is because, we can factorise the overall partition function to give:

$$\sum_i \sum_j \dots e^{-\beta E_i + E_j + \dots} = \left( \sum_i e^{\beta E_i} \right) \left( \sum_j e^{\beta E_j} \right) \dots \implies Z = \prod_k z_k \quad (9.44)$$

Where  $z_k$  is the partition function of the  $k$ th subsystem. However, we should bear in mind that, this is only the case for distinguishable subsystems. If the different subsystems are truly indistinguishable from one another, such as gas molecules in the same container, equation (9.44) above will have massively over counted the number of states available to the system. We can compensate for this by dividing by the combinatorial factor  $N!$ , where  $N$  is the number of subsystems, to obtain:

$$Z = \frac{z^N}{N!} \quad (9.45)$$

When modelling large systems, the summations used to generate quantities such as the partition function, are often carried out over such a large number of terms, that they can be approximated by converting them into an integral. This gives us the expression:

$$Z = \frac{1}{h^{\mathcal{F}}} \int e^{-\beta E} d\Gamma \quad (9.46)$$

Where  $h$  is Planck's constant, representing the typical volume of a state in phase space,  $d\Gamma$  is a phase space volume element, and  $\mathcal{F}$  is equal to the number of position-momentum coordinate pairs that define the phase space. This equation implies that the available states are uniformly distributed in phase space, which is reasonable because, in the classical limit, every point in phase space represents a distinct state of the system. Thus, if we are close enough to the classical limit to apply the integral approximation, the number of states in a region of phase space must be proportional to its volume. If we evaluate this integral over all but one of the phase space coordinates, and evaluate the final integral by parts, we obtain the equipartition theorem:

$$\left\langle x_i \frac{\partial E}{\partial x_i} \right\rangle = \frac{\int x_i \frac{\partial E}{\partial x_i} e^{-\beta E} dx_i}{\int e^{-\beta E} dx_i} = kT \quad (9.47)$$

In order for this result to hold, we require that either  $x_i$  is zero, or  $E$  is infinite, at both limits of the integral. This tends to be the case, since it is precisely this energy barrier that confines the coordinates to the region of integration in the first place.

### 9.3.2 Maxwell-Boltzmann Distribution

The Maxwell-Boltzmann distribution is used to describe the momenta of the molecules which make up a gas. Since the components of any particle's momentum are phase space coordinates, the probability that the magnitude of a molecule's momentum is between  $p_1$  and  $p_2$  will be given by:

$$P(p_1 \leq p \leq p_2) \propto \iiint_{p_1 \leq \sqrt{p_x^2 + p_y^2 + p_z^2} \leq p_2} e^{-\frac{\beta}{2m}[p_x^2 + p_y^2 + p_z^2]} dp_x dp_y dp_z \quad (9.48)$$

We can simplify this integral by expressing the momentum in spherical polar coordinates. If we then evaluate the integral over the angular coordinates, and utilise the normalisation condition to determine the constant of proportionality, we obtain:

$$P(p_1 \leq p \leq p_2) = \sqrt{\frac{2\beta^3}{m^3\pi}} \int_{p_1}^{p_2} p^2 e^{-\frac{\beta p^2}{2m}} dp \quad (9.49)$$

Therefore, the magnitude of the momentum has a probability density function  $\sqrt{\frac{2\beta^3}{m^3\pi}} p^2 e^{-\frac{\beta p^2}{2m}}$ , which is shown in figure 9.5.

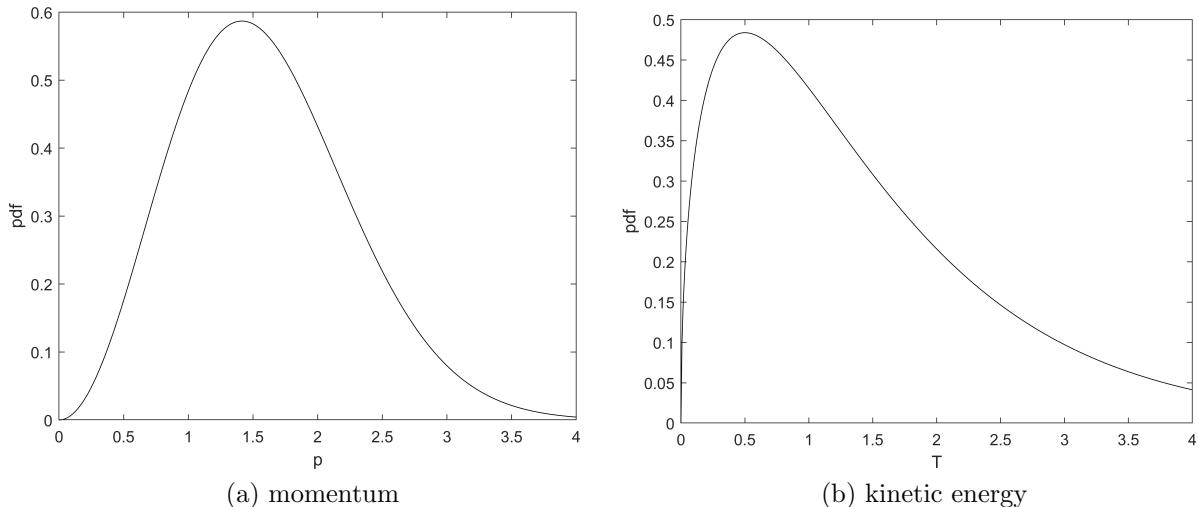


Figure 9.5: The Maxwell-Boltzmann distribution.

We can use a similar argument to calculate the partition function of a Maxwell-Boltzmann gas. For a single molecule of a structureless gas, confined to a volume  $V$ , the partition function is given by:

$$z = \frac{1}{h^3} \iiint_V \iiint_{\mathbb{R}^3} e^{-\frac{\beta}{2m}[p_x^2 + p_y^2 + p_z^2]} dp_x dp_y dp_z dx dy dz \quad (9.50)$$

This integral can be evaluated to give:

$$Z = \frac{V}{\Lambda^3} \quad \Lambda = \sqrt{\frac{h^2\beta}{2\pi m}} \quad (9.51)$$

The use of Planck's constant to define the density of states in position-momentum phase space is motivated by the application of quantum mechanics and the Heisenberg uncertainty principle. This result follows from the quantum mechanical particle in a box, which we discussed in chapter 4.

### 9.3.3 Fermi-Dirac Distribution

We now come to the Fermi-Dirac distribution. This distribution is used to describe the behaviour of a particular class of indistinguishable particles, fermions. In quantum mechanics, indistinguishable particles can be classed as either fermions, which obey the Pauli exclusion principle, or bosons, which do not. To analyse a system of fermions, we treat each available energy level as a subsystem that can have one of the two possible states: occupied or unoccupied. For an energy level with energy  $\varepsilon$ , the partition function is therefore:

$$Z_\varepsilon = \sum_i e^{-\beta E_i} = 1 + e^{\beta(\mu-\varepsilon)} \quad (9.52)$$

Where  $\mu$  represents the energy required to add another particle to the rest of the system. If we define the unoccupied state to have zero energy, it follows that, since we are removing a particle from the system, and placing it into a level with energy  $\varepsilon$ , the energy of the occupied state must be  $\varepsilon - \mu$ . The value of  $\mu$  will be determined by the total number of Fermions in the system. We can use this partition function to find the expected occupancy of the state:

$$\bar{n}(\varepsilon) = \frac{e^{\beta(\mu-\varepsilon)}}{1 + e^{\beta(\mu-\varepsilon)}} = \frac{1}{1 + e^{\beta(\varepsilon-\mu)}} \quad (9.53)$$

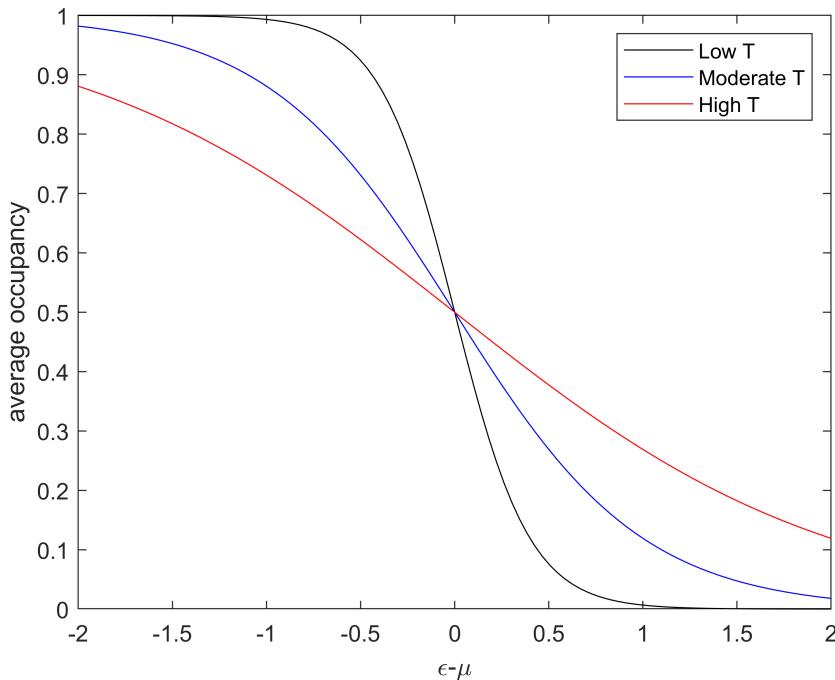


Figure 9.6: The Fermi-Dirac distribution.

This inability of fermions to occupy the same energy level has some very important consequences on their properties. One such example is the ability to exert a pressure, even as their temperature approaches absolute zero. We have already seen that, since reducing the volume of a system, increases the separation of its energy levels, work has to be done in the process. However, in a classical gas, this pressure would tend towards zero with the temperature, because all of the molecules would collapse into the lowest energy state. In a fermion gas, many of the higher energy states are occupied, even at absolute zero, and so a substantial pressure is exerted, even at low temperatures

### 9.3.4 Bose-Einstein Distribution

The Bose Einstein distribution is used to describe Bosons, particles which are capable of occupying the same energy level as each other. We shall take the same approach as we did for fermions, and treat each energy level as a subsystem; however, the difference here is that there is no limit on the occupation number of each level. Thus, the partition function is given by the geometric progression:

$$Z_\varepsilon = \sum_{n=0}^{\infty} e^{n\beta(\mu-\varepsilon)} = \frac{1}{1 - e^{\beta(\mu-\varepsilon)}} \quad (9.54)$$

If we now calculate the expected occupation number, we find that:

$$\bar{n}(\varepsilon) = \frac{1}{Z_\varepsilon} \sum_{n=1}^{\infty} n e^{n\beta(\mu-\varepsilon)} \quad (9.55)$$

The simplest way to evaluate this sum is to recognise that it can be rewritten in terms of the partition function, which gives us:

$$\bar{n}(\varepsilon) = \frac{\partial \ln Z_\varepsilon}{\partial \beta(\mu-\varepsilon)} = \frac{e^{\beta(\mu-\varepsilon)}}{1 - e^{\beta(\mu-\varepsilon)}} = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} \quad (9.56)$$

Where  $\mu$  is playing exactly the same role as it was in section 9.3.3.

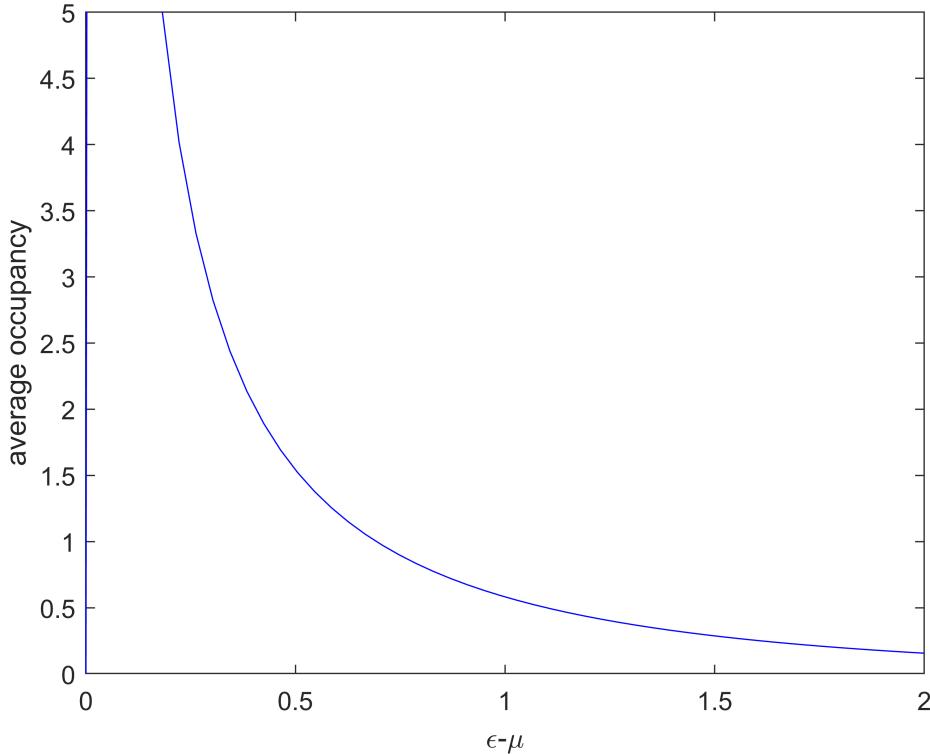


Figure 9.7: The Bose-Einstein distribution.

An interesting consequence of Bose-Einstein statistics is that, at very low temperatures, nearly all of the bosons collapse into the lowest energy state available. This is known as Bose-Einstein condensation, and is responsible for phenomena such as the formation of Helium super-fluid.

## 9.4 Gases

Gases are very useful thermodynamic systems to consider. Firstly, unlike solids and liquids, the weak nature of the interactions between gas molecules makes them significantly easier to model. Secondly, gases are some of the only thermodynamic systems which are capable of undergoing major volume changes, and thus, are capable of doing work on their environment. Finally, gases simply occur very often in nature, from the gases in our atmosphere which we are fairly familiar with, to more abstract gases, such as the electron gas which supports stars against gravitational collapse, gases appear nearly everywhere.

### 9.4.1 The Ideal Gas

An ideal gas is a simplified model of a gas, which can give a remarkable amount of insight into the behaviour of more general real systems. In practice, there is actually no such thing as an ideal gas, since it represents the limiting behaviour of a gas as its density tends to zero. Nonetheless, it does give a pretty good description of the behaviour of gases under most conditions that we would encounter on Earth, and even when it does deviate from reality, the ideal gas model allows us to highlight some key principles, without being distracted by complicated mathematics.

#### 9.4.1.1 Assumptions

**There are no long range interactions between gas molecules.** That is to say that, other than random collisions, which serve to redistribute energy throughout the system, and maintain thermodynamic equilibrium, the gas molecules can be treated as entirely independent. This means that, when we come to model an ideal gas, all we need to do is model a single molecule, and then use the relevant rules for combining the thermodynamic properties of different sub-systems.

**The gas molecules have negligible volume.** The ideal gas model does not account for the non-zero volume actually occupied by the gas molecules, and so is only a valid approximation when the volume of the molecules is much smaller than the volume of the actual container. As we shall see, correcting for this volume is one of the simple alterations that gives rise to the slightly more sophisticated Van der Waals gas model.

**The gas molecules are all sufficiently energetic that quantum effects are negligible.** When we model an ideal gas, we approximate the energy states as being essentially continuous, as we saw in section 9.3.1. As such, the molecules must possess energies much larger than the typical separation of their quantum energy levels, in order for our results to be valid. Furthermore, we need the molecules to be sufficiently spread out across the available energy levels, such that we would expect very few states to be occupied by more than one particle. This means that we do not have to worry about the differences between bosons and fermions, and instead, we can simply use Maxwell-Boltzmann statistics, which represents the limiting case of both distributions.

**The gas contains a large number of molecules.** This assumption is often implicit in thermodynamics, since it is the sheer size of macroscopic systems which makes many of our conclusions valid in the first place.

### 9.4.1.2 Equation of State

We already briefly mentioned in equation (9.50) of section 9.3.2 that the partition function for a single, structureless molecule of an ideal gas, confined to a volume  $V$ , is given by:

$$z = \frac{1}{h^3} \iiint_V dx dy dz \iiint_{\mathbb{R}^3} e^{-\frac{\beta}{2m}[p_x^2 + p_y^2 + p_z^2]} dp_x dp_y dp_z \quad (9.57)$$

If we consider this in more detail, we can see that what we are doing is constructing a 6-dimensional position momentum phase space, which completely describes the state of the molecule. That is to say that, in order to uniquely define the state of the molecule, we need to specify three position coordinates  $x, y, z$ , and three momentum coordinates  $p_x, p_y, p_z$ . We then treat each 6-cube in this phase space with volume  $h^3$ , as a distinct state available to the particle. The appearance of  $h$  here is a direct consequence of the Heisenberg uncertainty principle, although for our purposes the only thing that matters is that  $h$  is small. We then generate the partition function in the usual way by summing up the Boltzmann factors  $e^{-\beta E}$  for each state, where we are approximating the discrete sum to a continuous integral because  $h$  is small. Since there are no interactions between the molecules,  $E$  must be equal to the molecule's kinetic energy. Evaluating these integrals gives us:

$$z = \frac{V}{\Lambda^3} \quad (9.58)$$

Where  $\Lambda$  is a quantity referred to as the thermal de Broglie wavelength, although in actuality it is equal to half the expected de Broglie wavelength of the molecule, and takes the value:

$$\Lambda = \sqrt{\frac{h^2 \beta}{2\pi m}} \quad (9.59)$$

To deduce the overall partition function for an  $N$  particle ideal gas we simply use the relation that  $Z = \frac{z^N}{N!}$  to obtain:

$$Z = \frac{V^N}{\Lambda^{3N} N!} \implies \ln Z = N \ln V - 3N \ln \Lambda + N - N \ln N \quad (9.60)$$

If we now recall equation (9.43) from section 9.3.1, it follows that the pressure of the gas is given by  $P = kT \left( \frac{\partial \ln Z}{\partial V} \right)_T$ . Substituting in our expression for the partition function yields:

$$P = \frac{NkT}{V} \implies PV = NkT \quad (9.61)$$

This result is known as the ideal gas law, and it can be thought of as describing the limiting behaviour of a rarefied gas. Historically, this result was actually taken to be a postulate of thermodynamics, since it was used as the definition of temperature. The ideal gas law is the simplest example of what we call an equation of state, some physical law relating the pressure, volume, and temperature of a system to one another. We can see that, for any gas with a fixed particle number  $N$ , the existence of the ideal gas law implies that, if any two of  $P$ ,  $V$ , or  $T$  are known, the other can be uniquely determined. As such, we would describe an ideal gas as being defined by only two macroscopic state variables.

In addition to the ideal gas law, there is another very useful equation in the description of an ideal gas. This relates the internal energy of the gas and its temperature. To find this result, let us first consider the energy of a single molecule. We shall model the energy of the molecule as taking the form:

$$E = \sum_{i=1}^{\nu} a_i x_i^2 \quad (9.62)$$

Where  $a_i$  is just some constant, and  $x_i$  is one of the molecule's phase space coordinates. As such,  $x_i$  could be one of the components of the particles momentum, a coordinate describing the rotation of the molecule, or even the vibration of an atomic bond within the molecule. We should note that, although our earlier derivation of the ideal gas law did not account for the effect of these latter two variables, since, in essence, we restricted ourselves to a monatomic gas, they do not impact the ideal gas law, because they only effect the temperature dependence of the partition function. The average energy of a molecule can now be calculated from the equipartition theorem (equation (9.47) section 9.3.1), to give:

$$\langle E \rangle = \sum_{i=1}^{\nu} \langle a_i x_i^2 \rangle = \frac{1}{2} \sum_{i=1}^{\nu} \left\langle x_i \frac{\partial E}{\partial x_i} \right\rangle = \frac{\nu kT}{2} \quad (9.63)$$

If our gas contains a sufficiently large number of molecules  $N$ , then its total energy will simply be given by  $N\langle E \rangle$ , and as such, the internal energy of an ideal gas with  $\nu$  quadratic degrees of freedom is:

$$U = \frac{\nu}{2} N kT = \frac{\nu}{2} P V \quad (9.64)$$

For a monatomic gas,  $\nu$  is always equal to three, since all the molecule can do is move through space. Diatomic molecules can be significantly more complicated. At sufficiently low temperatures,  $kT$  is small enough that there is no significant population of the excited rotational and vibrational energy levels, which means equipartition does not apply, because the energy spectrum can not be approximated as continuous. Thus, at low temperatures  $\nu = 3$ . At room temperature, we typically find that rotational energy levels are active and continuous, while the vibrations are still frozen out. Since a diatomic molecule has 2 distinct axes it can rotate about (the internuclear axis does not count as the moment of inertia is 0), we would see  $\nu = 5$ . At high temperatures, the vibrational energy levels become active, contributing two additional degrees of freedom, one for kinetic energy, and one for potential energy. Thus, the maximum value of  $\nu$  is 7. For any molecule larger than a diatomic, the internal structure is too complicated for us to predict, and so we can use tabulated values of  $\nu$ . Figure 9.8 on the next page shows how the effective number of degrees of freedom for a diatomic gas varies with temperature. At room temperature pretty much all diatomics will have  $\nu = 5$ , so when dealing with the atmosphere (primarily  $N_2$  and  $O_2$ ) this is the value of choice.

It is also worth mentioning how equation (9.64) can be used to determine other thermodynamic functions. As an example, if we wish to determine the enthalpy of the gas, we can substitute (9.64) into the definition of enthalpy,  $H = U + PV$ , along with the ideal gas law to obtain:

$$H = \frac{\nu + 2}{2} N kT = \frac{\nu + 2}{2} P V \quad (9.65)$$

### 9.4.1.3 Heat Capacity

We are now in a position to determine quite a lot about the properties of an ideal gas. We shall start by considering heat capacity. In general terms, the heat capacity of a system represents the ratio between the heat transferred to that system, and the increase in the system's temperature. That is to say that, if a given process can be described by:

$$\delta q = C dT \quad (9.66)$$

The heat capacity for that process is  $C$ . It is important to note here that since the heat  $q$  is not a state function, the heat capacity of a system must inherently depend on the nature in which the process is carried out. For a gas, there are two heat capacities which are typically of interest, which are the constant volume heat capacity  $C_V$ , and the constant pressure heat capacity  $C_P$ . The first thing that will greatly simplify this analysis is to note that, since no work can possibly be done under constant volume conditions, it follows immediately from the first law that:

$$\delta q_{\text{const.}V} = dU_{\text{const.}V} = \left( \frac{\partial U}{\partial T} \right)_V dT \quad (9.67)$$

We can use our previous expression for the internal energy to determine that:

$$C_V = \left( \frac{\partial U}{\partial T} \right)_V = \frac{\nu}{2} N k \quad (9.68)$$

Figure 9.8 shows a plot of the degrees of freedom  $\nu$  (which is proportional to  $C_V$ ) in a diatomic gas, against temperature.

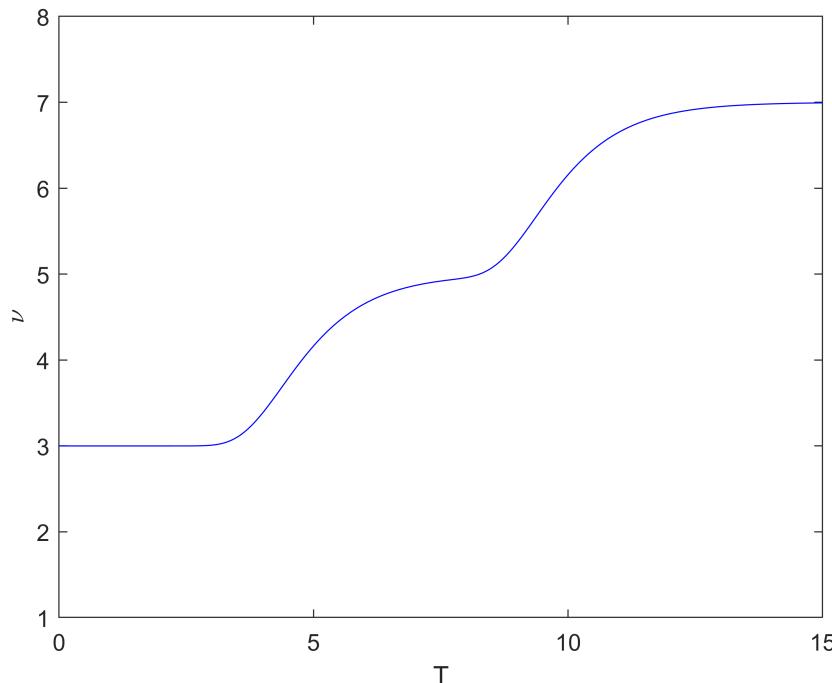


Figure 9.8: The degrees of freedom in a diatomic gas, as a function of temperature.

Heat capacities are fairly easy to measure, which is how we were able to obtain data on the variation of  $\nu$  with temperature. If we now move on to consider the constant pressure heat capacity, we should note that we are implicitly taking both the internal pressure and the external pressure to be constant. This makes sense, since we would not expect what we are doing to the system to affect the external pressure. Since the external and internal pressures will be equal throughout the heating, any work done must be reversible, which means that we can use the first law, and the definition of enthalpy, to say that:

$$\delta q_{\text{const.}P} = dU_{\text{const.}P} + PdV = dH_{\text{const.}P} = \left(\frac{\partial H}{\partial T}\right)_P dT \quad (9.69)$$

Therefore, the constant pressure heat capacity is given by:

$$C_P = \left(\frac{\partial H}{\partial T}\right)_P = \frac{\nu + 2}{2} kT \quad (9.70)$$

Often, a useful quantity to consider is the heat capacity ratio  $\gamma$ , which is defined as the ratio between  $C_P$  and  $C_V$ :

$$\gamma = \frac{C_P}{C_V} = \frac{\nu + 2}{\nu} \quad (9.71)$$

This heat capacity ratio is particularly useful for discussing adiabatic processes, those which occur without any exchange of heat, as we shall see in section 6.2. For now, it is just something for us to keep in the back of our minds.

Unfortunately however, some systems just can't be evaluated in terms of constant pressure and volume. For example, let us consider a thin, spherical soap bubble, containing an ideal gas. For simplicity, let us assume that the bubble is placed in vacuum such that the only external pressure acting on the gas arises as a result of the surface tension of the soap. Since the pressure due to surface tension scales inversely with the radius, we find that:

$$P = \frac{\alpha}{r}$$

Where  $\alpha$  is some constant of proportionality. If we take the differential of this, and then multiply by the volume, we find that:

$$dP = -\frac{\alpha}{r^2} dr \implies VdP = -\frac{4\pi}{3} \alpha r dr = -\frac{1}{3} PdV$$

Taking the differential of the ideal gas law, and substituting in our previous result, leads to the helpful relationship:

$$PdV + VdP = NkdT \implies PdV = \frac{3}{2} NkdT$$

Finally, if we assume that the heating is carried out reversibly, we can use equation (9.64) for the internal energy to deduce that  $dU = \frac{\nu}{2} NkdT$ . Substituting this into the first law  $\delta q = dU + PdV$ , we obtain:

$$\delta q = \frac{\nu + 3}{2} NkdT \implies C = \frac{\nu + 3}{2} Nk$$

#### 9.4.1.4 Entropy

One thing that we have not yet tackled is the entropy of an ideal gas. One way in which we can achieve our desired result is from the partition function. In section 4.1 we established that the partition function of a structureless, ideal gas is given by:

$$Z = \frac{V^N}{\Lambda^{3N} N!} \implies \ln Z = N \ln V - 3N \ln \Lambda + N - N \ln N \quad (9.72)$$

Where we have assumed that  $N$  is very large, and utilised Stirling's approximation for  $N!$ , when taking the logarithm. In addition to this, if we recall equation (9.43) in section 9.3.1, we can calculate the entropy of the gas from its partition function by evaluating:

$$S = k \ln Z + kT \left( \frac{\partial \ln Z}{\partial T} \right)_V = k \left[ N \ln \left( \frac{V}{N} \right) + \frac{3N}{2} \ln \left( \frac{mkT}{2\pi\hbar^2} \right) + \frac{5N}{2} \right] \quad (9.73)$$

Converting this result to the general case of a gas with  $\nu$  degrees of freedom is fairly straightforward, and yields more or less the same expression, with slight adjustments to some of the coefficients. These changes all follow from replacing  $\Lambda^3$  in equation 9.58 with the more general  $\Lambda^\nu$ . In principle, this expression is all we need to calculate the entropy change for any given process, although there are elegant ways in which we can handle certain special cases.

One common process, which a gas might undergo, is an isothermal expansion, where the system does work by expanding against an external pressure, whilst simultaneously absorbing heat from its surroundings, such that its temperature remains constant. In this case, we can use one of the Maxwell relations in section 9.2.5, which states that  $(\frac{\partial S}{\partial V})_T = (\frac{\partial P}{\partial T})_V$ , together with the ideal gas law, to determine that  $(\frac{\partial S}{\partial V})_T = \frac{Nk}{V}$ .

Conversely, we may also wish to consider the process of isochoric heating, where heat is supplied to the gas in order to raise its temperature, without allowing it to expand. Here, we can use both the chain rule of partial differentiation, which states that  $(\frac{\partial S}{\partial T})_V = (\frac{\partial S}{\partial U})_V (\frac{\partial U}{\partial T})_V$ , and the definitions of both  $C_V$  and  $T$ , to deduce that  $(\frac{\partial S}{\partial T})_V = \frac{C_V}{T}$ . Combining both of these results yields the differential:

$$dS = \frac{NkdV}{V} + \frac{C_VdT}{T} \quad (9.74)$$

Alternatively, if we wish to consider a macroscopic change of gas, from an initial volume and temperature of  $V_1, T_1$ , to final conditions of  $V_2, T_2$ , we can integrate (9.74) to obtain:

$$\Delta S = Nk \ln \left( \frac{V_2}{V_1} \right) + \frac{\nu}{2} Nk \ln \left( \frac{T_2}{T_1} \right) \quad (9.75)$$

This result, along with the second law, allows us to explain why it is that gases behave in the way that they do. A gas will expand to fill any available space because the increase in volume will lead to an increase in its entropy. This principle also applies to the mixing of different ideal gases, since if the molecules do not interact with one another, there should be no difference between a gas expanding into empty space and it expanding into, and mixing with another gas.

### 9.4.2 Van der Waals Gas

This brings us on to a Van der Waals gas. The Van der Waals model corrects the ideal gas model, by first allowing the molecules to have non-zero volume, and then attempting to account for the long range interactions between them. In order to apply these corrections let us return to the single particle partition function.

$$z = \iiint_{V-Nb} e^{\frac{\beta a N}{V}} dx dy dz \iiint_{\mathbb{R}^3} e^{-\frac{\beta}{2m}[p_x^2 + p_y^2 + p_z^2]} dp_x dp_y dp_z \quad (9.76)$$

Firstly, the integration over position  $x, y, z$  is no longer carried out over the full volume of the container, but instead over the available volume, which is not occupied by other molecules. Each molecule will have a volume  $b$  around it, within which another molecule can not exist. The exact size of this volume is difficult to calculate, since atoms are not hard spheres, and as a result will allow significant interpenetration of their electron clouds.

There is also an additional factor  $e^{-\beta\phi}$  to account for the favourable interactions between molecules, with  $\phi$  representing the average energy drop experienced by a molecule due to these forces. Since the strength of these interactions decays fairly rapidly with distance (the London dispersion force decays with  $\frac{1}{r^7}$ ),  $\phi$  will be dominated by the nearby particles, and so should not depend on the volume of the container. In addition,  $\phi$  must scale with the number density of molecules, because this will be directly proportional to the number of interactions one molecule experiences. Thus, we can write  $\phi$  as  $\phi = -\frac{aN}{V}$  where  $a$  is some constant of proportionality that will depend on the polarisability of the gas molecules. The minus sign here arises from the fact that the intermolecular forces are attractive. Evaluating this integral, and using equation (9.45) for the  $N$  particle partition function, gives us:

$$z = \frac{(V - Nb)}{\Lambda^3} e^{\frac{N\beta a}{V}} \implies Z = \frac{(V - Nb)^N}{\Lambda^{3N} N!} e^{\frac{N^2 \beta a}{V}} \quad (9.77)$$

Once again, recalling that  $P = kT \left( \frac{\partial \ln Z}{\partial V} \right)_T$ , we obtain the equation of state:

$$P = \frac{NkT}{V - Nb} - \frac{N^2 a}{V^2} \implies \left( P + \frac{aN^2}{V^2} \right) (V - Nb) = NkT \quad (9.78)$$

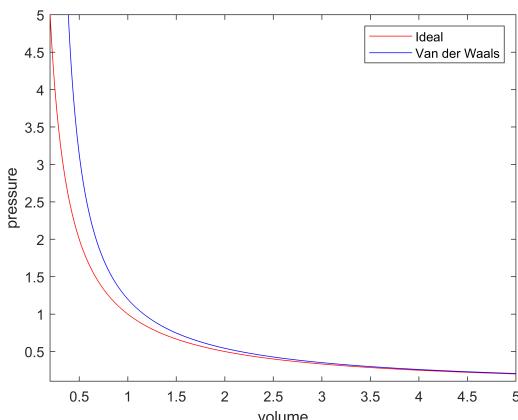


Figure 9.9: PV curve for a VdW gas compared to that of an ideal gas.

We can see that, at low particle densities, the Van der Waals equation tends towards the ideal gas law, which is precisely what we would expect since, both molecular volume and intermolecular forces, would become less significant as the particle density decreases. We can clearly see from Figure 9.10, that the two models are asymptotically the same at low pressures, with the deviations becoming increasingly more significant at high pressure. For typical atmospheric gases, under standard conditions, the deviation from that of an ideal gas is less than 1 part in 1000.

## 9.5 Variable Particle Number

We are now going to discuss the ways in which we can adjust our thermodynamic tools, to describe systems, where the particle number is allowed to vary. Clearly, this is of huge benefit to us, since one of the most useful thermodynamic systems for us to describe is that of a chemical reaction, which must involve changes in particle number, by definition. Furthermore, the technique we shall employ in this section in order to adapt our state functions for an additional variable, is a very general method for dealing with more complicated systems. In addition to all of this, we are going to understand why a chemists' thermodynamic variable of choice is always the Gibbs free energy, which makes a degree of sense since most chemical reactions are carried out under controlled temperatures and pressures.

### 9.5.1 Chemical Potential

The first thing we need to do in order to accommodate changes in particle number, is to adjust our fundamental equations, such that our thermodynamic state functions become functions of more than just two variables. The way we do this is by introducing the idea of a chemical potential. For a system that contains multiple types of particles we can let the number of the  $i$ th type of particle be  $n_i$ , in which case our fundamental thermodynamic relation becomes:

$$dU = TdS - PdV + \sum_i \mu_i dn_i \quad (9.79)$$

Where  $\mu_i$  is referred to as the chemical potential of species  $i$ , and is actually defined by this equation. This means that, by definition,  $\mu_i$  is given by:

$$\mu_i = \left( \frac{\partial U}{\partial n_i} \right)_{S,V} \quad (9.80)$$

We can then propagate these changes throughout our other thermodynamic state functions, although two that are of particular importance are the entropy, and the free enthalpy:

$$\begin{aligned} dS &= \frac{1}{T} \left[ dU + PdV - \sum_i \mu_i dn_i \right] \\ dG &= VdP - SdT + \sum_i \mu_i dn_i \end{aligned} \quad (9.81)$$

Since conditions of constant temperature and pressure (for example a system open to the atmosphere that is being heated in a controlled manner) arise more naturally, and are easier to imagine than conditions of constant entropy and volume, the equivalent definition of the chemical potential in terms of the Gibbs energy is often preferred:

$$\mu_i = \left( \frac{\partial G}{\partial n_i} \right)_{P,T} \quad (9.82)$$

Equivalent statements can be made relating the chemical potential to both the enthalpy and the Helmholtz free energy of the system. The Gibbs free energy formulation does, however, have the major advantage, that both of the natural variables  $P$  and  $T$  are intensive properties, which is very useful, when the size of your system is changing due to a chemical reaction.

Let us consider a system that has fixed temperature  $T$  and pressure  $P$ , and as such we, can drop these variables as arguments of the function  $G$ . We can now note that our new function is homogeneous of order one, since the Gibb's energy is an extensive property. That is to say that:

$$G_{P,T}(\alpha n_1, \alpha n_2, \dots) = \alpha G_{P,T}(n_1, n_2, \dots) \quad (9.83)$$

The subscripts here are added to simply remind ourselves that this analysis is being carried out at fixed values of  $P$  and  $T$ . If we now note the existence of Euler's theorem of homogeneous functions, which states that:

$$f(\alpha x_1, \alpha x_2, \dots) = \alpha^k f(x_1, x_2, \dots) \implies \sum_i x_i \frac{\partial f}{\partial x_i} = k f(x_1, x_2, \dots) \quad (9.84)$$

We can apply this to our own homogeneous function, to deduce that:

$$G_{PT} = \sum_i \mu_i n_i \quad (9.85)$$

Thus, we can understand the chemical potential as the Gibbs free energy per molecule of species  $i$ . We can use this fact to help us calculate chemical potentials of a mixture of different ideal gases. The overall partition function for the mixture is given by:

$$Z = \prod_i \frac{V^{n_i}}{\Lambda_i^{3n_i} n_i!} \implies \ln Z = \sum_i n_i \ln \left( \frac{V}{n_i} \right) + n_i - 3n_i \ln \Lambda_i \quad (9.86)$$

Note that since the different gases are distinguishable, there is no need to divide by a combinatorial factor, when combining their partition functions. If we now wish to calculate the Gibbs energy of the mixture, we can use the relationship  $G = kTV \left( \frac{\partial \ln Z}{\partial V} \right)_T - kT \ln Z$ , which follows from equation (9.43) in section 9.3.1. This gives us:

$$G = kT \sum_i n_i \ln \left( \frac{n_i}{V} \right) + 3n_i \ln \Lambda_i \quad (9.87)$$

By noting that since these are ideal gases, the volume is given by  $V = \frac{NkT}{P}$ , where  $N$  is the total number of gas molecules, which is equal to the sum of all the  $n_i$ , and further defining the value of  $\mu_i$  at temperature  $T$  and some standard pressure  $P^\circ$  to be  $\mu_i^\circ$  we arrive at the conclusion that:

$$\mu_i = \mu_i^\circ + \ln \left( \frac{n_i P}{N P^\circ} \right) \quad (9.88)$$

This form of expression for the chemical potential is so common that we define a quantity known as the activity of species  $i$ , such that:

$$\mu_i = \mu_i^\circ + \ln(a_i) \quad (9.89)$$

Where  $\mu_i^\circ$  is just the chemical potential measured in a certain set of standard conditions, which are specified. For non interacting systems, such as ideal gases and dilute solutions, the activity is approximated reasonably well as being proportional to the partial pressure/concentration, which we can see in equation (9.88). For systems which remain in essentially the same state, such as solvents, which are always approximately pure, provided the solution is dilute enough, and solids which do not mix together, the activity can just be approximated as one.

### 9.5.2 Chemical Reactions

We are now going to examine how the chemical potential can be used to explain chemical reactions. Firstly, since most chemical reactions are carried out at constant temperature and pressure, we shall restrict our considerations to reactions of this nature. Under these conditions, it turns out that the Gibbs free energy is the most useful state function for us to consider. It follows from the equations in (9.81) that:

$$dS_{\text{sys}} - \frac{dU + PdV}{T} = -\frac{1}{T}dG \quad \text{const. } P, T. \quad (9.90)$$

The 'sys' subscript has been added to highlight that this is the change in entropy of the system, and not the total change in entropy of the universe. Helpfully however, it follows from the first law that  $dU + PdV$  is the heat absorbed from the surroundings by the system. If we assume that the surroundings are maintained at the same constant temperature as the system, which is reasonable because otherwise there would be a tendency for the temperatures to equalise and thus change, then the entropy change of the surroundings is simply  $-\frac{\delta q}{T}$ , with the minus sign arising because heat is flowing from the surroundings. Thus, we can rewrite equation (9.90) as:

$$dG = -TdS_{\text{tot}} \quad \text{const. } P, T. \quad (9.91)$$

Since the thermodynamic temperature is always positive, it follows from the second law that the only processes that will be observed at constant temperature and pressure, are those which reduce the Gibbs energy of the system.

We are now going to put this to use in modelling an actual chemical reaction. Let us consider a general reaction which takes the form:



Here we have used the convention for the Stoichiometric coefficients  $\nu_i$  that, for products the coefficient is positive, and for reactants it is negative, which explains the presence of the minus signs on the left hand side. Now although we have multiple different particle numbers that can change, since they can only change through this chemical reaction, there is only one degree of freedom in the state of the system, once the initial amount of each species is specified. If we let  $x$  be a variable that represents how much of the reaction has gone to completion, we find that:

$$\frac{dG}{dx} = \sum_i \nu_i \mu_i \quad (9.92)$$

If we now substitute in equation (9.80) for the chemical potential, and rearrange (9.92) a bit, we can obtain:

$$\frac{dG}{dx} = \Delta_r G^\circ - kT \ln(Q) \quad (9.93)$$

Where  $\Delta_r G^\circ$  is the standard Gibbs free energy change of the reaction, which represents the change in Gibbs energy, if the reaction were to proceed from pure reactants to pure products,

all in their standard states.  $Q$  is referred to as the reaction quotient, and it measures the activities of all of the species present.

$$\Delta_r G^\circ = \sum_i \nu_i \mu_i^\circ \quad Q = \prod_i a_i^{\nu_i} \quad (9.94)$$

Figure 9.11 shows an example of how the Gibbs energy might vary with  $x$  for a reaction of this nature. We can note the presence of a clear minimum at an intermediate value of  $x$ .

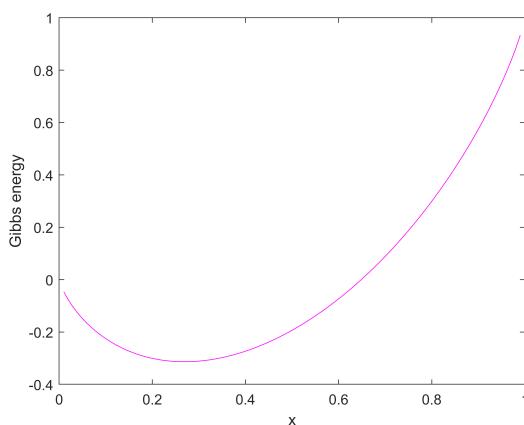


Figure 9.10: The Gibbs curve of a reaction.

equilibrated. Equation (9.95) is arguably the most important result in chemical thermodynamics, as it is often the centrepiece of any analysis that is carried out. One particularly nice feature of the equilibrium constant arises in the Van't Hoff isochore, which is derived as follows. Firstly, we take the derivative of  $\ln K$  with respect to temperature at constant pressure:

$$\left( \frac{\partial \ln K}{\partial T} \right)_P = -\frac{1}{kT} \left( \frac{\partial \Delta_r G^\circ}{\partial T} \right)_P + \frac{\Delta_r G^\circ}{kT^2}$$

We can now use the result, which follows immediately from the differential (9.37) in section 9.2.5, that  $\left( \frac{\partial \Delta_r G^\circ}{\partial T} \right)_P = -\Delta_r S^\circ$  and the definition that  $\Delta_r G^\circ = \Delta_r H^\circ - T\Delta_r S^\circ$  to obtain:

$$\left( \frac{\partial \ln K}{\partial T} \right)_P = \frac{\Delta_r H^\circ}{T^2} \quad (9.96)$$

Perhaps surprisingly, this result tells us that the temperature dependence of an equilibrium depends only on the enthalpy change for that reaction. Furthermore, we can see that, for exothermic reactions ( $\Delta_r H^\circ < 0$ ), the equilibrium constant will decrease with temperature, and thus the equilibrium will lie closer to the reactants. The opposite is true for endothermic reactions. This aligns perfectly with what we would predict using Le'Chatelier's principle.

A useful experimental trick that we can employ to find  $\Delta_r H^\circ$  is to plot  $\ln K$  against  $\frac{1}{T}$ . We can see that this will give a straight line of gradient  $-\Delta_r H^\circ$ , as follows:

$$\left( \frac{\partial \ln K}{\partial T^{-1}} \right)_P = \left( \frac{\partial \ln K}{\partial T} \right)_P \frac{dT}{dT^{-1}} = -T^2 \left( \frac{\partial \ln K}{\partial T} \right)_P = -\Delta_r H^\circ \quad (9.97)$$

### 9.5.3 Black Body Radiation

We are going to analyse the radiation emitted from a black body, by considering the thermodynamic properties of a photon gas. Inside a black body, photons are continuously being absorbed and re-emitted with different energies, which from a thermodynamic perspective, is essentially equivalent to the collisions between molecules of a material gas. If we confine our photons to a volume  $V$ , we can determine the number of states with frequencies between  $\nu$  and  $\nu + d\nu$ , by evaluating the integral over phase space:

$$N(\nu, \nu + d\nu) = \frac{2}{h^3} \iiint_V dx dy dz \iiint_{h\nu \leq pc \leq h(\nu + d\nu)} dp_x dp_y dp_z \quad (9.98)$$

Where we have used the fact that a photon's energy can be given by either of the two expressions  $h\nu$  or  $pc$ . Furthermore, the additional factor of two in front of the integral arises from the fact that, for each combination of position and momentum, there are two polarisation states available to each photon. Evaluating the integral gives us:

$$N(\nu, \nu + d\nu) = \frac{8\pi V}{c^3} \nu^2 d\nu \quad (9.99)$$

We can now use this expression, along with equation (9.56) for the average occupancy of a state in a boson gas, which we derived in section 3.4, and Planck's formula  $E = h\nu$ , to determine the spectral energy density of photons with frequency  $\nu$ . That is to say that, we wish to find the function  $\mathcal{E}_\nu(\nu)$ , such that, the energy stored in photons with frequencies between  $\nu$  and  $\nu + d\nu$  is given by  $\mathcal{E}_\nu(\nu)d\nu$ .

$$\mathcal{E}_\nu(\nu)d\nu = N(\nu, \nu + d\nu)\bar{n}(h\nu)h\nu \implies \mathcal{E}_\nu(\nu) = \frac{8\pi hV}{c^3} \frac{\nu^3}{e^{\beta h\nu} - 1} \quad (9.100)$$

Since the black body can always emit a photon of arbitrarily small energy, the  $\mu$  term in the Bose-Einstein distribution is equal to zero. We can also express this result in terms of the energy stored by photons of wavelength  $\lambda$ . Importantly, we should be aware that, since these results give a spectral energy density (energy per unit frequency or per unit wavelength), we can not simply substitute  $\nu\lambda = c$  into (9.100).

$$\mathcal{E}_\nu\left(\frac{c}{\lambda}\right)d\left(\frac{c}{\lambda}\right) = \mathcal{E}_\lambda(\lambda)d\lambda \implies \mathcal{E}_\lambda(\lambda) = 8\pi hcV \frac{\lambda^{-5}}{e^{\frac{\beta hc}{\lambda}} - 1} \quad (9.101)$$

Using this result it is possible for us to derive a formula for the wavelength of photon with the maximum intensity within a black body gas. It is worth making it clear now that, if we were to perform this same analysis for the frequency, we would not obtain  $\nu_{\max}\lambda_{\max} = c$ . This is because the spectral energy density that we are maximising also depends on the density of photon states, which grows with frequency, but decays with wavelength.

$$\begin{aligned} \frac{d\mathcal{E}_\lambda}{d\lambda} &= 8\pi hcV \left[ \frac{\beta hc}{\lambda^7} \frac{e^{\frac{\beta hc}{\lambda}}}{(e^{\frac{\beta hc}{\lambda}} - 1)^2} - \frac{5}{\lambda^6} \frac{1}{e^{\frac{\beta hc}{\lambda}} - 1} \right] \\ \frac{d\mathcal{E}_\lambda}{d\lambda} = 0 &\implies \left( \frac{\beta hc}{\lambda} - 5 \right) e^{\frac{\beta hc}{\lambda}} + 5 = 0 \end{aligned} \quad (9.102)$$

The equation  $(x - 5)e^x + 5 = 0$  is transcendental in  $x$ , but can be solved numerically using the Newton-Raphson method, to find that  $x = 4.96511423174\dots$ . This actually brings up an interesting point about solving equations numerically. Even though, in this case, there is no analytic solution for  $x$ , with modern computers we can so easily, and so quickly, find it to within an error so much smaller than any observation we could ever make, that for all intents and purposes we know the number exactly. Using this numerical value for  $x$ , we obtain Wien's displacement law:

$$\lambda_{\max} = \frac{\alpha}{T} \quad \alpha = 2.89777\dots \times 10^{-3} \text{ K m} \quad (9.103)$$

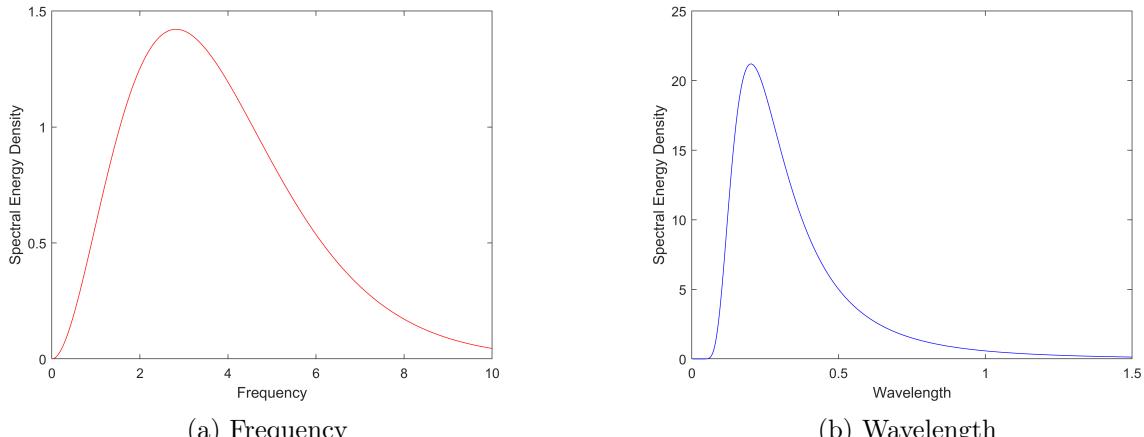


Figure 9.11: Spectral energy density in a black body gas.

This is all well and good, but it would also be useful if we could calculate the values of thermodynamic state functions for the black body gas. The easiest to evaluate is the internal energy, which will simply be the sum of the energy stored in each frequency:

$$U = \int_0^\infty E(\nu)d\nu = \frac{8\pi hV}{c^3} \int_0^\infty \frac{\nu^3 d\nu}{e^{\beta h\nu} - 1} \quad (9.104)$$

This integral is an example of a standard form, known as a Bose integral, which can be evaluated by taking a Taylor series expansion of the denominator, and then integrating by parts to obtain a convergent infinite series. In this case, the standard result that is of use to us is:

$$\int_0^\infty \frac{u^3 du}{e^u - 1} = \frac{\pi^4}{15} \quad (9.105)$$

From here, we obtain the result that:

$$U = \frac{8\pi^5 k^4 V T^4}{15 c^3 h^3} = \frac{4V\sigma T^4}{c} \quad (9.106)$$

Where  $\sigma$  is the Stefan-Boltzmann constant, which takes a value of  $\sigma = \frac{2\pi^5 k^4}{15c^2 h^3}$ . Although it is not clear now, why this was the constant we chose to factorise out, we shall see that this was the sensible choice, when we consider the power radiated away from a black body.

Once we have determined the internal energy as a function of both volume and temperature, we can calculate the entropy of the photon gas by evaluating the partial derivative:

$$\left(\frac{\partial S}{\partial T}\right)_V = \left(\frac{\partial S}{\partial U}\right)_V \left(\frac{\partial U}{\partial T}\right)_V = \frac{1}{T} \frac{16V\sigma T^3}{c} \implies S = \frac{16V\sigma T^3}{3c} = \frac{4U}{3} \quad (9.107)$$

We do not need to worry about the arbitrary function of  $V$  that arises from the integration because we know that  $S$  must be zero at absolute zero, since there will be no photons, and thus only one micro-state. From here, we can go on to calculate all of the thermodynamic state functions, which are listed in table 9.1 below:

Table 9.1: Thermodynamic properties of a black body gas.

State Function	$U$	$S$	$P$	$F$	$H$	$G$
Value	$\frac{4V\sigma T^4}{c}$	$\frac{16V\sigma T^3}{3c}$	$\frac{4\sigma T^4}{3c}$	$-\frac{4V\sigma T^4}{3c}$	$\frac{16V\sigma T^4}{3c}$	0

The thing we notice about all of the state functions is that, with the obvious exception of the Gibbs free energy, they all depend very strongly on the temperature. This is a consequence of the variable photon number of the gas. When the temperature rises, the equilibrium occupation of every single state rises with it, and thus in order to raise the temperature of a photon gas, one has to produce a lot of new photons. This becomes increasingly true at higher temperatures, because the number of states with significant occupation rises even more rapidly, since there are more photon states at higher energies.

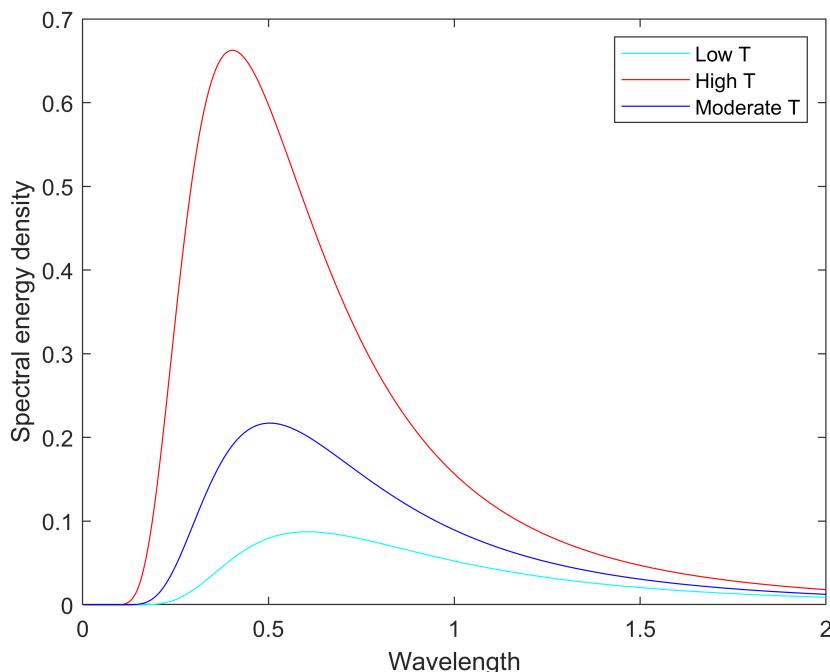


Figure 9.12: Black body curves at a range of temperatures.

We can use the black body photon gas to predict the power radiated away by an object. At the surface of the black body, any photons which scatter in the outwards direction, run the risk of leaving the body entirely. Once the photon leaves the surface, there will be no more matter for it to be absorbed and remitted by, and so it will simply continue on a straight line path indefinitely, permanently removing it from the system. We can calculate the rate at which energy is dissipated as follows. The energy density of the photon gas is simply  $u = \frac{4\sigma T^4}{c}$ , and thus the energy flux in its direction of motion is  $uc = 4\sigma T^4$ .

However, since the photons are all moving in random directions only some fraction of this energy flux will actually be leaving the surface. To find this fraction, we can first note that half of the photons will be moving inwards, away from the boundary, and so can be discounted.

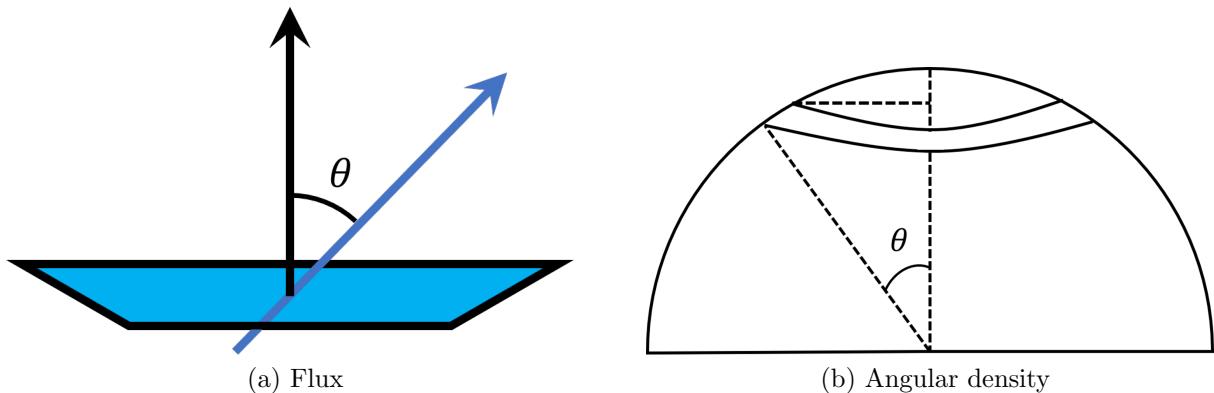


Figure 9.13: Diagrams to show the photon flux through a surface.

Furthermore, of the remaining photons moving in the right direction, most will be exiting the surface at some kind of angle. If the photons leave at an angle  $\theta$  to the surface normal, then they were only able to flow through the component of the surface projected in their direction of motion. As such, the contribution to the total radiated flux by photons at angle  $\theta$  to the normal, is simply:

$$dJ = 2\sigma T^4 \cos \theta g(\theta) d\theta \quad (9.108)$$

Where  $g(\theta)$  is the angular probability density function. As we can see from figure 9.14 (b), the total solid angle between the angles  $\theta$  and  $\theta + d\theta$  is given by  $2\pi \sin \theta d\theta$ . To obtain the angular probability density we simply divide this by the total solid angle on the hemisphere  $2\pi$ . Thus, we obtain:

$$J = 2\sigma T^4 \int_0^{\frac{\pi}{2}} \cos \theta \sin \theta d\theta \quad (9.109)$$

We can evaluate this integral by simply noting that  $d(\sin \theta) = \cos \theta d\theta$ , and then evaluating  $\frac{\sin^2 \theta}{2}$  at each of the limits. Doing this gives us the Stefan-Boltzmann law:

$$J = \sigma T^4 \quad (9.110)$$

This result is particularly useful in astrophysics, because it can allow us to work out the radiance of a star, and hence by comparing this to its measured intensity, we can determine how far away the star is.

## 9.6 Extracting Work

Finally, we shall cover the topic that was, arguably, the most important in the development of thermodynamics, extracting work from a heat engine. Obviously, maximising the efficiency of a heat engine would have been of great interest during the heart of the industrial revolution, and so, many of the first developments in thermodynamics were based on these principles. Let us first begin by considering what exactly a heat engine is. In general terms, a heat engine is any device which transfers energy across a temperature difference, and in the process, does some mechanical work.

### 9.6.1 Reversible and Irreversible Processes

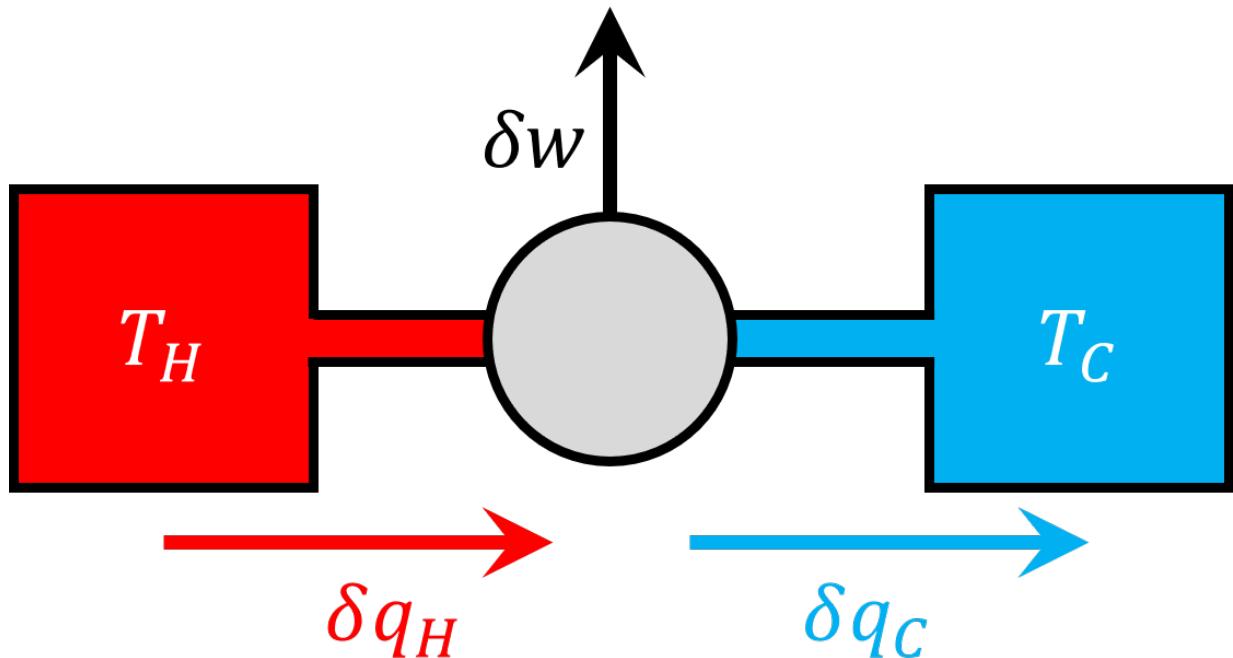


Figure 9.14: A thermodynamic heat engine.

Figure 9.15 shows a simple description of a heat engine. Some heat  $\delta q_H$  is absorbed from the heat source at temperature  $T_H$ , then passed through the heat engine and in the process some work  $\delta w$  is done. The remaining heat  $\delta q_C$  is then rejected into the cold sink at a temperature  $T_C$ . There are two important relationships we can derive about this heat engine by applying the first and second laws respectively.

$$\delta w = \delta q_H - \delta q_C \quad dS = \frac{\delta q_C}{T_C} - \frac{\delta q_H}{T_H} \geq 0 \quad (9.111)$$

Note that the heat flow is not necessarily reversible, but since the change in state of the heat source is the same as it would be, if the heat was flowing reversibly, we can use the classical equation for the entropy change. Combining the two results, then allows us to deduce the maximum work that can be done by the heat engine:

$$\delta w \leq \left(1 - \frac{T_C}{T_H}\right) \delta q_H \quad (9.112)$$

The ratio between the work extracted, and the heat absorbed is called the efficiency of the engine, and, as we have shown, the second law imposes a restriction on the maximum efficiency attainable. This maximum efficiency is referred to as the Carnot efficiency, and importantly we can see that the hotter the source is, the more efficient the engine. It is this reason why there is a huge drive for engines to operate economically at higher and higher temperatures, in order to reduce fuel costs and emissions as much as possible. Another interesting thing for us to notice is that the maximum work is extracted, when the engine is operating reversibly. This turns out to be a very general result, and is the reason why there is so much interest in reversible processes.

### 9.6.2 The Carnot Cycle

We shall conclude our discussion of heat engines with one of the most famous, and simplest, heat engines possible, the Carnot cycle. This engine features an ideal gas, which is cycled between temperatures  $T_H$  and  $T_C$ , whilst doing work in the process. There are four stages in the cycle; first the gas isothermally absorbs heat from the heat source at a temperature  $T_H$ . The gas is then allowed to expand adiabatically (no heat exchange with the environment), until it reaches a temperature  $T_C$ . The gas then isothermally rejects heat into the sink, before being adiabatically compressed back to a temperature  $T_H$ . Figure 9.16 shows the cycle on both a pressure-volume graph, and a temperature-entropy graph. In both cases, the work done is represented by the area inside the graph. As we can see, the efficiency of a perfect Carnot cycle is the ideal  $1 - \frac{T_C}{T_H}$ .

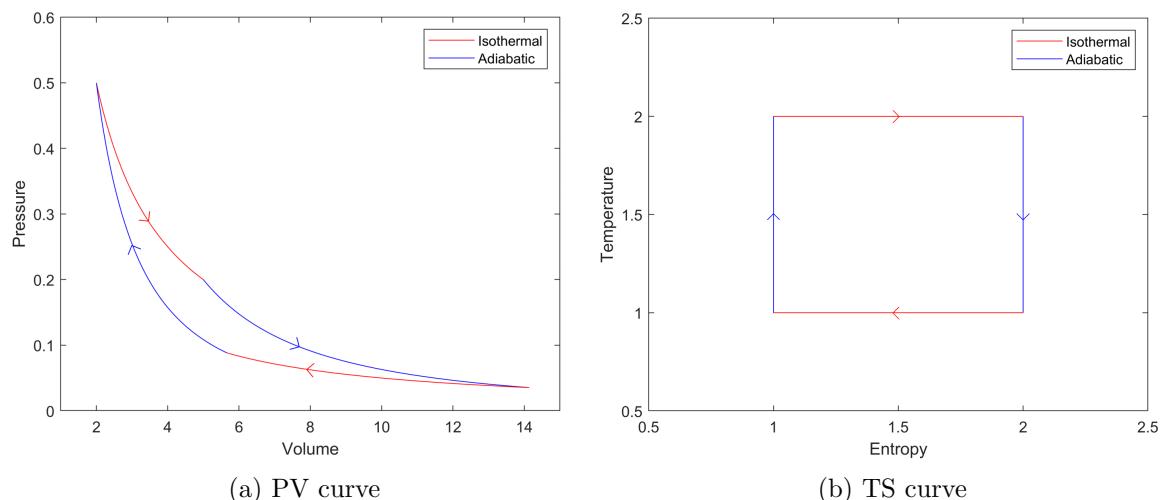


Figure 9.15: The Carnot cycle.

We are going to finish our discussion of the Carnot cycle by taking the opportunity to describe what happens to a gas during reversible, adiabatic compressions and expansions. An adiabatic process is one, which does not involve any heat exchange with the surroundings, and as such, it follows directly from the classical definition of entropy that, for a reversible, adiabatic process,  $\delta q_{\text{rev}} = 0 \implies dS = 0$ . It is for this reason that reversible, adiabatic processes are often referred to as isentropic. If we take the differential of equation (9.64) for the internal energy of an ideal gas, we find that:

$$dU = TdS - PdV = \frac{\nu}{2} [PdV + VdP] \quad (9.113)$$

For an isentropic process  $dS = 0$ , and so we obtain the relationship that:

$$\frac{\nu+2}{2} PdV + \frac{\nu}{2} VdP = 0 \quad \text{const. } S \quad (9.114)$$

Dividing through by  $\frac{\nu}{2}$  and multiplying by  $V^{\gamma-1}$  gives us the following equation, where  $\gamma = \frac{\nu+2}{\nu}$  is the heat capacity ratio we defined in section 9.4.1.

$$d(PV^\gamma) = \gamma PV^{\gamma-1}dV + V^\gamma dP = 0 \quad (9.115)$$

By integrating this differential and then substituting in the ideal gas law we can conclude that all three of the following quantities are conserved in an isentropic process:

$$PV^\gamma = \text{const.} \quad (9.116)$$

$$P^{1-\gamma}T^\gamma = \text{const.} \quad (9.117)$$

$$V^{\gamma-1}T = \text{const.} \quad (9.118)$$

One application of these results is to model the temperature of the atmosphere. As is typical for gases, the atmosphere has a fairly low thermal conductivity, which is a consequence of the reasonably low particle density. As such, the principle method of heat transfer within the atmosphere is convection, where parcels of air will rise and fall redistributing the thermal energy in the process. Therefore, the atmosphere will reach a thermal equilibrium, when the temperature of a rising air parcel changes at the same rate as the surrounding atmosphere. As the thermal conductivity of the air is so low, we can essentially model the expansion of the air parcel as adiabatic. Thus, when we differentiate equation (9.118), we must obtain:

$$(1 - \gamma)P^\gamma T^\gamma \frac{dP}{dh} + \gamma P^{1-\gamma} T^\gamma \frac{dT}{dh} = 0 \quad (9.119)$$

Furthermore, in order for the atmosphere to remain in mechanical equilibrium, the atmospheric pressure gradient must be sufficient to support the atmosphere against its own weight. If we set up this equality, and then use the ideal gas law to express the density in terms of the pressure and temperature, we obtain:

$$\frac{dP}{dh} = -\rho g = -\frac{\mu g P}{kT} \quad (9.120)$$

Where  $\rho$  is the density if the air, and  $\mu$  is the average mass of an air molecule. Combining these, we can see that the temperature varies linearly with height:

$$\frac{dT}{dh} = -\frac{(\gamma - 1)\mu g}{k\gamma} \quad (9.121)$$