

A Cavendish Quantum Mechanics Primer

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University of Cambridge

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PREFACE

This primer, starting with a platform of school mathematics, treats quantum mechanics “properly”. You will calculate deep and mysterious effects for yourself. It is decidedly not a layman’s account that describes quantum mechanical phenomena qualitatively, explaining them by analogy where all attempts at analogy must fail. Nor is it an exhaustive textbook; rather this brief student guide explains the fundamental principles of quantum mechanics by solving phenomena such as how quantum particles penetrate classically forbidden regions of space, how particle motion is quantised, how particles interfere as waves, and many other completely non-intuitive effects that underpin the quantum world. The mathematics needed is mostly covered in the AS (penultimate) year at school. So take heart! The quantum mechanics you will see may look formidable, but it is all accessible with your existing skills and with practice.

Chapters 1–3 require differentiation, integration, trigonometry and the solution of two types of differential equations met at school. The only special function that arises is the exponential, which is also at the core of school mathematics. We review this material. In these chapters we cover quantisation, confinement to potential wells, penetration into forbidden regions, localisation energy, atoms, relativistic pair production, and the fundamental lengths of physics. Exercises appear throughout the notes. It is vital to solve them as you proceed. They will make physics an active subject for you, rather than the passive knowledge gained from popular science books. Such problem solving will transform your fluency and competence in all of the mathematics and physics you study at school and the first years at university. Especially, the gained confidence in mathematics will underpin further studies in any science; in any event, mathematics is the natural language of physics.

Chapter 4 needs complex numbers. It introduces the imaginary number $i = \sqrt{-1}$, something often done in the last year at school. Armed with i , you will see that quantum mechanics is essentially complex, that is, it involves both real and imaginary numbers. Waves, so central to quantum mechanics, also require recalling. We shall then deal with free particles and their currents, reflection from and penetration of steps and barriers, flow of electrons along nano-wires and related problems. Calculating these phenomena precisely will consolidate your feeling for i , and for the complex exponentials that arise, or introduce you first to the ideas and practice in advance, if you are reading them a few months early. Finally, Chapter 5 introduces partial derivatives which are not generally done at school, but

which are central to the whole of physics. They are a modest generalisation of ordinary derivatives to many variables. Chapter 5 opens the way to quantum dynamics and to quantum problems in higher dimensions. We revisit quantum dots and nano wires more quantitatively. Chapters 4 and 5 are more advanced and will take you well into a second-year university quantum mechanics course.

Some readers will find Chapters 4 and 5 challenging at first. Physics is an intellectually deep and difficult subject, wherein rests its attraction to the ambitious student. While moving from exposure-level treatments to the real edifice of physics, think of Alexander Pope

A little learning is a dangerous thing;
drink deep, or taste not the Pierian spring:
there shallow draughts intoxicate the brain,
and drinking largely sobers us again.

Alexander Pope (1688–1744)
from “An Essay on Criticism”, 1709

Physics is a linear subject; you will need the building blocks of mechanics and mathematics to advance to quantum mechanics, statistical mechanics, electromagnetism, fluid mechanics, relativity, high energy physics and cosmology. This book takes serious steps along this path of university physics. Towards the end of school, you already have the techniques needed to start this journey; their practice here will help you in much of your higher mathematics and physics. We hope you enjoy a concluding exercise, quantising the string — a first step towards quantum electrodynamics.

Mark Warner & Anson Cheung
Cavendish Laboratory, University of Cambridge.
June, 2012

PREFACE TO THE SECOND EDITION

We have corrected several typographical and also some consequent errors, and thank the several readers who have pointed these out. Readers should consult the Primer’s website for errata and for additional materials that are appearing. Many exercises have been added throughout this new edition.

MW & ACHC
March, 2013

ACKNOWLEDGEMENTS

We owe a large debt to Robin Hughes, with whom we have extensively discussed this book. Robin has read the text very closely, making great improvements to both the content and its presentation. He suggested much of the challenging physics preparation of chapter 1. Robin and Peter Sammut have been close colleagues in The Senior Physics Challenge, from which this primer has evolved. Peter too made very helpful suggestions and was also most encouraging over several months. Both delivered some quantum mechanics to advanced classes in their schools, using our text. We would be lost without their generosity and without their deep knowledge of both physics and of school students. Peter also shaped ACHC's early physics experiences.

Quantum mechanics is a counter-intuitive subject and we would like to thank Professor David Khmelnitskii for stimulating discussions and for clarification of confusions; MW also acknowledges similar discussions with Professor J.M.F. Gunn, Birmingham University. We are most grateful to Dr Michael Rutter for his indispensable computing expertise. Dr Dave Green has been invaluable in his support of our pedagogical aims with the SPC and this book, where he has assisted in clarifying our exposition. We also thank colleagues and students who read our notes critically: Dr Michael Sutherland, Dr Michael Rutter; Georgina Scarles and Avrish Gooranah. Generations of our departmental colleagues have refined many of the problems we have drawn upon in this primer. We mention particularly the work of Professor Bryan Webber. Of course, any slips in our new problems are purely our responsibility.

ACHC thanks Trinity College for a Fellowship.

The Ogden Trust was a major benefactor of the SPC over many years of the project. The wider provision of these kinds of notes for able and ambitious school students is one of our goals that has been generously supported by the Trust throughout.

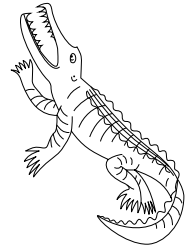
TEACHING RESOURCES

This primer grew from lecture notes written for the Senior Physics Challenge (SPC), the schools physics development project of the Cavendish Laboratory, University of Cambridge. We aim to make it as widely available as possible to school and university students alike: chapter 1 can be seen as a resource of problems and as an assembly of skills needed for Oxbridge entry tests and interviews¹. The Primer's function of preparing both for admissions and for university level quantum mechanics is not accidental — fluency and confidence in its material is also needed for continuing study. Practice over a period will be required for the mastery of chapter 1, but the material is not advanced. The skills acquired are then required for the remainder of the book and in all higher physics. Chapters 2 and 3 offer further practice for fluency while exploring the wonders of quantum mechanics. Chapters 2–5 are core to our first two years of quantum mechanics teaching in Cambridge.

Chapter 1 is freely downloadable at this Primer's website² and at the Senior Physics Challenge website³.

Please consult THE PERIPHYSEOS PRESS⁴ or the Primer's site for *very* substantial price reductions for group or bulk orders of this primer.

THE PERIPHYSEOS PRESS derives its name from Greek “peri” = “about, concerning”, and “physeos” = “(of) nature” — the same root as physics itself. The Press aims to make texts on natural sciences easily and cheaply available to students. The crocodile symbol (© M.J. Rutter), commissioned for the Cavendish Laboratory by the great Russian physicist Kapitza, is thought to be a reference to Lord Rutherford, the then Cavendish Professor.



ADDITIONAL RESOURCES will be available to students and teachers as a companion to the Primer; please check our website².

We would be grateful for suggestions for further material, or being made aware of typographical and other errors that readers might find in the text. Please contact us via the Primer's website, where accumulated errata are also presented.

¹Differential equations are typically not required.

²www.cavendish-quantum.org.uk

³www-spc.phy.cam.ac.uk

⁴www.periphyseos.org.uk

Mathematical symbols and notation; Physical quantities

Greek symbols with a few capital forms (alphabetical order is left to right, then top to bottom):

α	alpha	β	beta	γ Γ	gamma	δ Δ	delta	ϵ	epsilon
ζ	zeta	η	eta	θ Θ	theta	ι	iota	κ	kappa
λ	lambda	μ	mu	ν	nu	ξ Ξ	xi	\omicron	omicron
π Π	pi	ρ	rho	σ Σ	sigma	τ	tau	υ Υ	upsilon
ϕ Φ	phi	χ	chi	ψ Ψ	psi	ω Ω	omega	∇	nabla

Miscellaneous symbols and notation:

For (real) numbers a and b with $a < b$, the *open* interval (a, b) is the set of (real) numbers satisfying $a < x < b$. The corresponding *closed* interval is denoted $[a, b]$, that is, $a \leq x \leq b$.

\in means “in” or “belonging to”, for example, the values of $x \in (a, b)$.

\sim means “of the general order of” and “having the functional dependence of”, for instance $f(x, y) \sim x \sin(y)$.

\propto means “proportional to” $f(x, y) \propto x$ in the above example (there is more behaviour not necessarily displayed in a \propto relation).

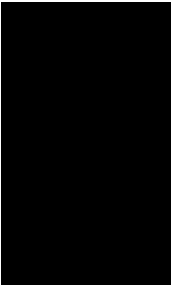
$\langle (\dots) \rangle$ means the average of the quantity (\dots) ; see Section 1.2.

$\partial/\partial x$ means the partial derivative (of a function) with respect to x , other independent variables being held constant; see Section 5.1.

$|\dots|$ means “the absolute value of”. For complex numbers, it is more usual to say “modulus of”.

Physical quantities:

Constant	Symbol	Magnitude	Unit
Planck's constant/ 2π	\hbar	1.05×10^{-34}	J s
Charge on electron	e	1.6×10^{-19}	C
Mass of electron	m_e	9.11×10^{-31}	kg
Mass of proton	m_p	1.67×10^{-27}	kg
Speed of light	c	3.00×10^8	m s^{-1}
Bohr radius	$a_B = 4\pi\epsilon_0\hbar^2/(m_e e^2)$	53.0×10^{-12}	m
Permittivity free space	ϵ_0	8.85×10^{-12}	F m^{-1}



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Preliminaries — some underlying quantum ideas and mathematical tools

1.1 Moving from classical to quantum

Wavefunctions, probability, uncertainty, wave-particle duality, measurement

Quantum mechanics describes phenomena from the subatomic to the macroscopic, where it reduces to Newtonian mechanics. However, quantum mechanics is constructed on the basis of mathematical and physical ideas different to those of Newton. We shall gradually introduce the ideas of quantum mechanics, largely by example and calculation and, in Chapter 4 of this primer, reconcile them with each other and with the mathematical techniques thus far employed. Initially, we deal with uncertainty and its dynamical consequences, and introduce the idea that a quantum mechanical system can be described in its entirety by a wavefunction. We shall also re-familiarise ourselves with the necessary mathematical tools. Our treatment starts in Chapter 2 with the Schrödinger equation and with illustrative calculations of the properties of simple potentials. In Chapter 3, we deal with more advanced potentials and penetration of quantum particles into classically forbidden regions. Later we introduce the momentum operator, free particle states, expectation values and dynamics. We remain within the Schrödinger “wave mechanics” approach of differential equations and wavefunctions, rather than adopting operators and abstract spaces.

Quantum mechanics and probability in 1-D

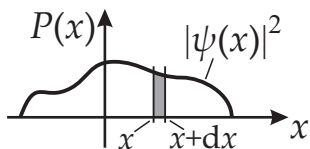


Figure 1.1: A quantum probability density $P(x)$.

A quantum mechanical system, for instance a single particle such as an electron, can be completely described by a *wavefunction*. We call this function $\psi(x)$, which is a function of position x along one dimension. Later we treat higher dimensions and time. It is denoted by the Greek letter “psi”, which is pronounced as in the word “psychology”. ψ has the interpretation of, when squared, giving the probability density $P(x)$ of finding the particle at the position x ; see Fig. 1.1. Density in this case means “the probability per unit length”, that is, we multiply by a short length dx to get the probability $P(x)dx$ that the particle is in the interval x to $x + dx$. As always the total probability, here $\int P(x)dx$, must be 1. Most of this book is concerned with real wavefunctions and we have in effect $P(x) = \psi^2(x)$. However quantum mechanics is an intrinsically *complex* subject, that is, its quantities in general involve both the usual real numbers and imaginary numbers. Chapters 4 and 5 address quantum mechanical phenomena that need $i = \sqrt{-1}$, whereupon the probability becomes $P(x) = |\psi(x)|^2$, where $|\dots|$ means “the absolute value of”. For complex numbers, it is more usual to say “modulus of”. To be unambiguous we shall write $|\psi(x)|^2$, though the simple square is mostly all we mean.

Uncertainty in quantum mechanics

Knowing the wavefunction (the aim of much of this book) evidently only tells us the probability of finding the particle at a position x . To this extent quantum mechanics is not certain — we can only say that the outcome of many measurements of position would be distributed as $P(x)$ as in, for example, Fig. 1.1. We shall see, however, at the end that $\psi(x)$ evolves deterministically in time. We shall also encounter the celebrated Heisenberg uncertainty principle:

$$\Delta x \cdot \Delta p \geq \frac{1}{2} \hbar, \quad (1.1)$$

where Δx denotes the standard deviation (uncertainty) of x , and equivalently Δp for the momentum p in the x -direction. The quantity \hbar is Planck’s constant divided by 2π and is one of the fundamental constants of nature: $\hbar = 1.05 \times 10^{-34}$ J s. Rearranging gives us $\Delta p \geq \frac{1}{2} \hbar / \Delta x$, an inverse relation which says that as the uncertainty in position becomes small ($\Delta x \rightarrow 0$),

then the uncertainty in momentum, Δp , gets very large. Speaking loosely, if we confine a quantum particle in space it moves about violently. We cannot know both spatial and motional information at the same time beyond a certain limit.

There is another important consequence of uncertainty. For wavefunctions with small average momentum $\langle p \rangle$, Δp is a rough measure of the magnitude of the momentum p of the particle¹. Given that $p = mv$, with m the mass and v the speed, and that the kinetic energy is $T = \frac{1}{2}mv^2 = p^2/2m$, then

$$T \geq \frac{\hbar^2}{2m} \frac{1}{(\Delta x)^2}, \quad (1.2)$$

where in this qualitative discussion we discard the $\frac{1}{2}$ in Eq. (1.1). As we confine a particle, its energy rises. This “kinetic energy of confinement”, as it is known, gives rise, for instance, to atomic structure when the confining agent is electromagnetic attraction and to relativistic particle/anti-particle pair production when the energy scale of T is $\geq 2mc^2$, that is, more than twice the Einsteinian rest mass energy equivalent.

Measurement and wave–particle duality in quantum mechanics

Quantum mechanical particles having a probability $P(x)$ of being found at x , means that the outcomes of many measurements are distributed in this way. Any given measurement has a definite result that localises the particle to the particular position in question. We say that the wavefunction collapses on measurement. Knowing the position exactly removes any knowledge we might have had about the momentum, as we have seen above. In quantum mechanics physical variables appear in *conjugate pairs*, in fact the combinations that appear together in the uncertainty principle. Position and momentum are a basic pair, of which we cannot be simultaneously certain. Another pair we meet is time² and energy. Measurement of one gives a definite result and renders the other uncertain. Notice that momentum is the fundamental quantity, not velocity.

It will turn out that the wavefunction ψ will indeed describe waves, and thus also the fundamentally wave-like phenomena such as diffraction

¹Consider for instance a particle where the momentum takes the values $+p$ or $-p$. So $\langle p \rangle = 0$. The mean square of the momentum is clearly p^2 , and the root mean square, that is, the standard deviation, $\Delta p = p$ simply. If p takes a spread of values, then Δp is not so precisely related to any of the individual p values, but it still gives an idea of the typical size of the momentum.

²Time is special as it is not a true dynamical variable.

and interference that quantum mechanical particles exhibit. For electrons the appropriate “slits” leading to diffraction and then interference are actually the atoms or molecules in a crystal. They have a characteristic spacing matched to the wavelength of electrons of modest energy. A probability $P(x)$ of finding diffracted particles, for instance, on a plane behind a crystal is reminiscent of the interference patterns developed by light behind a screen with slits. However the detection of a particle falling on this plane will localise it to the specific point of detection — particles are not individually smeared out once measured. Thus a wave-like aspect is required to get a $P(x)$ characteristic of interference, and a particle-like result is observed in individual measurements; this is the celebrated wave–particle duality. In Chapter 4 we show pictures of particles landing on a screen, but distributed as if they were waves!

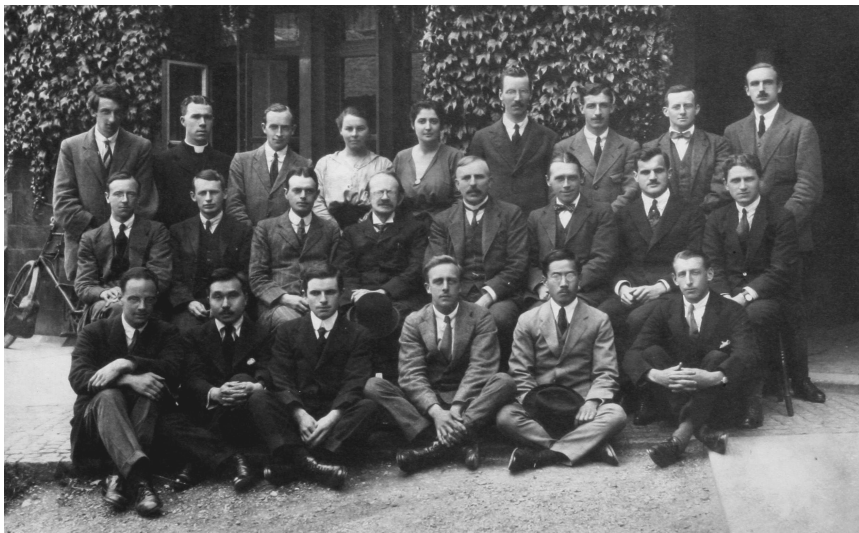


Figure 1.2: G.P. Thomson — Nobel Prize (1937; with Davisson) for diffraction of electrons as quantum mechanical waves, and J.J. Thomson — Nobel Prize (1906) for work “on conduction of electricity by gases”, middle row, 2nd and 4th from left respectively. In this class photo of Cavendish Laboratory research students in 1920 there are four other Nobel prize winners to be identified — see this book’s web site for answers.

The electron was discovered as a fundamental particle by J.J. Thomson

using apparatus reminiscent of the cathode ray tube as in an old fashioned TV. His son, G.P. Thomson, a generation later discovered the electron as a wave using diffraction (through celluloid); see Fig. 1.2. Both the father and son separately received Nobel Prizes in physics for discovering the opposite of each other! J.J. was Cavendish Professor in Cambridge (the supervisor and predecessor of Rutherford), and was Master of Trinity College, Cambridge. G.P. made his Nobel discovery in Aberdeen, did further fundamental work at Imperial College, and was Master of Corpus Christi College, Cambridge.

Potentials, potential energies and forces

Unlike the standard treatments of classical mechanics in terms of forces, quantum mechanics deals more naturally with energies. In particular, the role of a force is replaced by its potential energy. Forces due to fields between particles, charges etc., or for instance those exerted by a spring, do work when the particles or charges move, or the spring changes length. The energy stored in the field or spring is potential energy $V(x)$, a function of separation, extension, etc. x . Movement of the point of application of the force, f , *against* its direction by $-dx$ gives an *increase* in the stored energy $dV = -f dx$ (“force times distance”), that is, force is given by $f = -dV/dx$. Note the $-$ sign. Associated with a field is normally a potential³, $U(x)$ say, that may be a function of position. For instance associated with a charge Q_2 is a Coulomb potential with the value $U(x) = Q_2/(4\pi\epsilon_0 x)$ a distance x away from Q_2 . Another charge Q_1 feels this potential and as a result has a potential energy $V(x) = Q_1 U(x)$. We can, using the previous result for f , calculate the force felt by Q_1 from Q_2 ; see Ex. 1.1 below. One speaks of Q_1 being at a potential $U(x)$ when at x . In quantum mechanics potential energy is generally denoted by $V(x)$ and is loosely referred to simply as potential. We follow these two conventions — the meaning is generally clear, especially if one is consistent with the notation.

Three most well-known potentials, giving rise to potential energies $V(x)$, are

$$\begin{aligned} V(x) &= +\frac{Q_1 Q_2}{4\pi\epsilon_0 x} && \text{(Coulomb/electric)} \\ &= -\frac{Gm_1 m_2}{x} && \text{(gravitation)} \\ &= +\frac{1}{2}qx^2. && \text{(harmonic)} \end{aligned}$$

³Fields with an associated potential are known as conservative.

The second gives the gravitational attractive force between two masses m_1 and m_2 , the masses being a distance x apart. The third potential gives the harmonic potential energy leading to a retractive force $-qx$ when, for instance, a spring is stretched by x away from its natural length. The constants that determine the energy scale, ϵ_0 , G and q are the permittivity of free space, the gravitational constant and the spring constant, respectively.

A potential with an attractive region can confine particles in its vicinity if they do not have sufficient energy to free themselves. Such particles are often referred to as being in a “bound state”, and the potential energy landscape known as a “potential well”. We shall explore quantum motion and energies in potentials of various shapes.

It is important to think about and solve the problems posed in the text. Mostly they will have at least some hint to their solution. The problems in part illustrate the principles under discussion. But physics and maths are subjects only really understood when one can “do”. Problems are the only route to this understanding, and also give fluency in the core (mathematical) skills of physics. So repeat for yourself even the problems where complete or partial solutions have been given.

Exercise 1.1: Derive from the electric, gravitational and harmonic potentials their force laws. Explain the sign of the forces — is it what you expect? Take care over the definition of the zero of potential. Does the position where the potential is zero matter?

Because quantum mechanics deals with energies, rather than forces, we now explore the shift from using forces to potentials in analysing dynamics problems. For instance, to calculate the change in speed of a particle, you might have considered a force-displacement curve. This is a diagram which tells you what forces are acting as a function of the position of the particle. In fact, one would need to know the area under the curve, which amounts to the change of energy of the particle (from potential energy to kinetic energy or vice versa). We can avoid having to know such detail by simply using the potential energy graph. These ideas are best illustrated by the following examples.

Exercise 1.2: Consider a particle of mass m passing a potential well of width a , as shown in Fig. 1.3. The particle has total energy $E > V_0$, the depth of the well. Calculate the time taken by the particle to traverse the figure.

Solution: First, we note that the well is a schematic of the energies and we

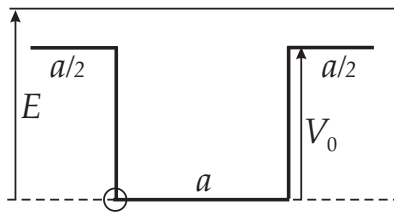


Figure 1.3: A finite square well potential of depth V_0 .

are asked to use energies directly rather than forces. Secondly, the nature of the forces is irrelevant — this is the advantage of an energy approach. The diagram is not describing a dip in a physical landscape.

In the regions outside the well, the kinetic energy is the difference between the total energy E and the potential energy V_0

$$\frac{1}{2}mv^2 = E - V_0. \quad (1.3)$$

So the speed is given by $v = \sqrt{\frac{2(E-V_0)}{m}}$. Inside the well, all the energy is entirely kinetic and so the speed is $v' = \sqrt{\frac{2E}{m}}$. Making use of the definition of speed, we find the total time

$$t = \sqrt{\frac{ma^2}{2}} \left(\frac{1}{\sqrt{E}} + \frac{1}{\sqrt{E - V_0}} \right). \quad (1.4)$$

Exercise 1.3: A particle of mass m slides down, under gravity, a smooth ramp which is inclined at angle θ to the horizontal. At the bottom, it is joined smoothly to a similar ramp rising at the same angle θ to the horizontal to form a V-shaped surface. If the particle slides smoothly around the join, determine the period of oscillation, T , in terms of the initial horizontal displacement x_0 from the centre join. Note the shape of the potential well.

Hint: We see that the potential well appears as a sloping line similar to the one along which the particle is constrained to move. It is only this linear slope at angle θ to the horizontal, that happens to resemble the potential energy graph of the same shape, which misleads us into thinking that we can see the potential energy. The potential energy is a concept, represented

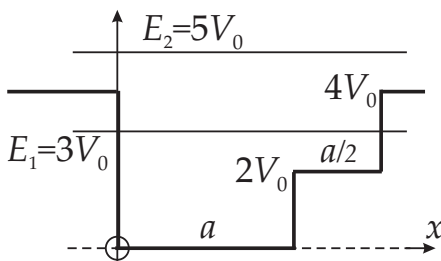


Figure 1.4: A stepped rectangular potential well

pictorially by a graph and the shape of the graph happens, in some cases, to resemble the mechanical system.

The distinction between the actual landscape (flat) and the potential is clear in the case of a quadratic potential. See Fig. 3.4 on page 59.

Exercise 1.4: A particle moves in a potential $V(x) = \frac{1}{2}qx^2$. If it has total energy $E = E_0$ give an expression for its velocity as a function of position $v(x)$. What is the amplitude of its motion?

Exercise 1.5: The potential energy of a particle of mass m as a function of its position along the x axis is as shown in Fig. 1.4.

(a) Sketch a graph of the force versus position in the x direction which acts on a particle moving in this potential well with its vertical steps. Why is this potential unphysical?

(b) Sketch a more realistic force versus position curve for a particle in this potential well. For a particle moving from $x = 0$ to $x = \frac{3a}{2}$, which way does the force act on the particle? If the particle was moving in the opposite direction, which way would the force be acting on the particle?

Hint: Take care over the physical meaning of the potential energy. It can look misleadingly like the physical picture of a particle sliding off a high shelf, down a very steep slope and then sliding along the floor, reflecting off the left hand wall and then back up the slope. This is too literal an interpretation since, for example, the potential change might be due to an electrostatic effect rather than a gravitational one, and the time spent moving up or down the slope is due to artificially putting in an extra vertical

dimension in a problem which is simply about motion in only one dimension. An example of where there is literally motion vertically as well as horizontally, is that of a frictionless bead threaded on a parabolic wire. The motion is not the same as in the one-dimensional simple harmonic motion of Ex. 1.4. Although the potential energy is expressible in the form $\frac{1}{2}qx^2$ due to the constraint of the wire, the kinetic energy involves both the x and y variables.

Exercise 1.6: Consider again the particle in Ex. 1.5. If it has a total mechanical energy E equal to $3V_0$, calculate the period for a complete oscillation.

Quantum mechanics in the world around us

Quantum effects are mostly manifested on a length scale much smaller than we can observe with light and hence are not directly part of our everyday world. Indeed we shall see that quantum mechanics takes us far from our common experience. A particle can be in two places at the same time — it must pass through at least two slits for interference to occur — and we shall see the need to think of them as having a wave–particle duality of character. But our world is dominated by the macroscopic effects of quanta. The conductivity of metals and semiconductors is entirely dominated by quantum effects and without them there would be no semiconductor age with computers, consumer electronics, digital cameras, telecommunications, modern medical equipment, or lasers with which to read digital discs. Atomic and molecular physics, chemistry, superconductivity and superfluidity, electron transfer in biology are all dominated by quantum mechanics. It is with quantum mechanical waves, in an electron microscope, that we first saw the atomic world. The ability of quantum particles to tunnel through classically forbidden regions is exploited in the scanning tunnelling microscope to see individual atoms.

We shall explore such fundamental effects. For instance, we shall see how quantum particles explore classically forbidden regions where they have negative kinetic energy and should really not venture. We shall even at the end quantise a model of electromagnetic standing waves and see how photons and phonons arise. However fundamental the phenomena we examine, and those that more advanced courses deal with, these effects have all had a revolutionary influence in the last century through their applications to technology, and have fashioned the world in which we live.

1.2 Mathematical preliminaries for quantum mechanics

Probability, trigonometric and exponential functions, calculus, differential equations, plotting functions and qualitative solutions to transcendental equations

Mathematics suffuses all of physics. Indeed some of the most important mathematics was developed to describe physical problems: for example Newton's description of gravitational attraction and motion required his invention of calculus. If you are good at maths, and especially if you enjoy using it (for instance in mechanics), then higher physics is probably for you even if this is not yet clear to you from school physics. This book depends on maths largely established by the end of the penultimate year at school. We simply sketch what you have learned more thoroughly already, but might not yet have practised much or used in real problems. So we assume exposure to trigonometric and exponential functions, and to differentiation and integration in calculus. We later introduce some more elaborate forms of what you know already — for instance the extension of algebra to the imaginary number i and its use in the exponential function, and differentiation with respect to one variable while keeping another independent variables constant (partial differentiation).

Probability

Wavefunctions generate probabilities, for instance that of finding a particle in a particular position. We shall use probabilities throughout these notes, taking averages, variances etc. Familiar averages over a discrete set of outcomes i are written, for instance:

$$\langle x \rangle = \sum_i x_i p_i \quad \text{and} \quad \langle f(x) \rangle = \sum_i f(x_i) p_i. \quad (1.5)$$

Here $\langle \rangle$ around a quantity means its average over the probabilities p_i . This is called the *expectation value* of the quantity. When outcomes are continuously distributed, we replace the p_i by a probability density (probability per unit length) $P(x)$ which gives a probability $P(x)dx$ that an outcome falls in the interval x to $x + dx$. Just as the discrete probabilities must add up to 1, so do the continuous probabilities:

$$\sum_i p_i = 1 \rightarrow \int P(x)dx = 1. \quad (1.6)$$

Such probabilities are said to be normalised. If the probability is not yet normalised, we can still use it but we must divide our averages by $\int P(x)dx$,

which is in effect just performing the normalisation. You will see that in some problems it pays to delay this normalisation process in the hope that it eventually cancels between numerator and denominator. Thus averages (1.5) become

$$\langle x \rangle = \int xP(x)dx \quad \text{and} \quad \langle f(x) \rangle = \int f(x)P(x)dx. \quad (1.7)$$

Exercise 1.7: The variance σ^2 in the values of x is the average of the square of the deviations of x from its mean, that is,

$$\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle.$$

Prove the above agrees with the standard result $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$ for both discrete and continuous x .

Essential functions for quantum mechanics

We shall see that a particle in a constant potential $V(x) = V_0$, say, is represented by a wavefunction $\psi \propto \sin(kx)$, where \propto means “proportional to” (that is, we have left off the constant of proportionality between ψ and $\sin(kx)$). The argument of the sine function, the combination kx , can be thought of as an angle, say $\theta = kx$. It must be dimensionless, as the argument for all functions must be — this is a good physics check of algebra! Hence k must have the dimensions of 1/length and we shall return to its meaning in Chapter 2.3. ψ could equally be represented by $\cos(kx)$ with a change of phase. We shall constantly use properties of trigonometric functions, among the simplest being:

$$\sin^2 \theta = 1 - \cos^2 \theta \quad (1.8)$$

$$\cos(2\theta) = 2 \cos^2 \theta - 1 = 1 - 2 \sin^2 \theta \quad (1.9)$$

$$\sin(2\theta) = 2 \sin \theta \cos \theta \quad (1.10)$$

$$\tan \theta = \sin \theta / \cos \theta \quad (1.11)$$

$$\sin(\theta + \phi) = \sin(\theta) \cos(\phi) + \sin(\phi) \cos(\theta) \quad (1.12)$$

$$\cos(\theta + \phi) = \cos(\theta) \cos(\phi) - \sin(\theta) \sin(\phi) \quad (1.13)$$

$$\sin \theta + \sin \phi = 2 \sin \left(\frac{\theta + \phi}{2} \right) \cos \left(\frac{\theta - \phi}{2} \right) \quad (1.14)$$

$$\cos \theta + \cos \phi = 2 \cos \left(\frac{\theta + \phi}{2} \right) \cos \left(\frac{\theta - \phi}{2} \right) \quad (1.15)$$

The double angle relations (1.9) and (1.10) are sometimes used in integrals in rearranged form, e.g. $\sin^2 \theta = \frac{1}{2}(1 - \cos(2\theta))$. The addition formulae (1.14) and (1.15) are used when adding waves together, and are simply derived by adding and subtracting results like (1.12) and (1.12).

Exercise 1.8: Prove that $\tan 2\theta = 2 \tan \theta / (1 - \tan^2 \theta)$ and $\tan 4\theta = 4 \tan \theta (1 - \tan^2 \theta) / (1 - 6 \tan^2 \theta + \tan^4 \theta)$. If $t = \tan(\theta/2)$, then show that $\sin \theta = 2t / (1 + t^2)$ and $\cos \theta = (1 - t^2) / (1 + t^2)$, while $\tan \theta = 2t / (1 - t^2)$ is also a special form of the $\tan 2\theta$ identity. Prove that $1 + \tan^2 \theta = \sec^2 \theta$ where $\sec \theta = 1 / \cos \theta$. These relations are useful in integration by substitution.

In quantum mechanics it is possible to have negative kinetic energy, something that is classically forbidden since clearly our familiar form is $T = p^2/2m \geq 0$. If while $T < 0$ the potential is also constant, $V(x) = V_0$, then the wavefunction will have the exponential form $\psi \propto e^{-kx}$ or $\propto e^{kx}$. We shall find sin, cos and exp as wavefunctions whose oscillations in wells, and decay away from wells, describe localised quantum mechanical particles. See Chapt. 4, page 73, for hyperbolic functions, the equivalents of trig functions but based upon e^{kx} and e^{-kx} .

The *Gaussian* function $e^{-x^2/2\sigma^2}$ has a very special place in the whole of physics. The form given is the standard form complete with the factor of 2 and its characteristic width σ for reasons made clear in Ex. 1.16. It is the wavefunction for the quantum simple harmonic oscillator in its ground state and is also the wavefunction with the minimal uncertainty. We return to it at the end of Chapter 3.

Exercise 1.9: Plot $e^{-x^2/2\sigma^2}$ for a range of positive and negative x . Label important points on the x axis (including where the function is $1/e$) and the y axis. Pay special attention to $x = 0$, including slope and curvature there. What is the effect on the graph of varying σ ?

A little calculus — differentiation

The first derivative of the function $f(x)$, denoted by df/dx , is the slope of f . Figure 1.5 shows the tangent to the curve $f(x)$ and, in a triangle, how the limit as $\delta x \rightarrow 0$ of the ratio of the infinitesimal rise δf to the increment δx along the x axis gives $\tan \theta$ and hence the slope of $f(x)$ at a point. Vitally important is the second derivative d^2f/dx^2 since this leads to the quantum mechanical kinetic energy, T . It is the rate of change of the slope.

Figure 1.5 shows regions of increasing/decreasing slopes and hence positive/negative second derivatives. The second derivative is in effect the rate

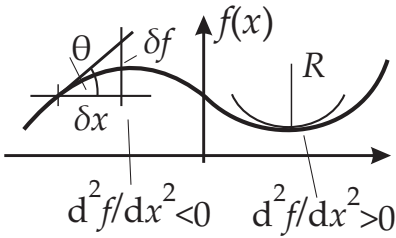


Figure 1.5: The gradient $df/dx = \tan \theta$ of the function $f(x)$. The second derivative $d^2 f/dx^2$ is positive at the minimum where the slope is increasing with x . The curvature, $1/R$, derives from the circular arc, of radius R , fitted to $f(x)$ at x .

at which the curve deviates from its local tangent. We shall also loosely refer to it as the “curvature”. Figure 1.5 shows an arc of a circle of radius R fitted to a minimal point, a point of zero slope where the second derivative is exactly $d^2 f/dx^2 = 1/R$. Away from minima or maxima, but for not too great a slope, the curvature is approximately the second derivative⁴.

We require derivatives of the most common functions encountered in quantum mechanics:

$$\frac{d}{dx} \sin(kx) = k \cos(kx) \quad (1.16)$$

$$\frac{d}{dx} \cos(kx) = -k \sin(kx) \quad (1.17)$$

$$\frac{d}{dx} e^{kx} = k e^{kx}. \quad (1.18)$$

The latter is a definition of the exponential function — the function that is its own derivative. To see this relation, we make the substitution $u = kx$ into Eq. (1.18). The derivatives become $\frac{d}{dx} = \frac{du}{dx} \frac{d}{du} = k \frac{d}{du}$ and so we find that $\frac{d}{du} e^u = e^u$.

Exercise 1.10: Show that $\frac{d}{dx} (\tan x) = \sec^2 x$.

Another common function in physics is the inverse function to the exponential — the natural logarithm. Consider the curve $y = e^x$. The inverse function is

$$x = e^y. \quad (1.19)$$

To see this we sketch both functions on the same axes, Fig. 1.6. We write the

⁴A precise definition for the curvature is $1/R = d^2 f/dx^2 / (1 + (df/dx)^2)^{3/2}$ which takes account of an increment δx not being the same as an increment of length along the curve.

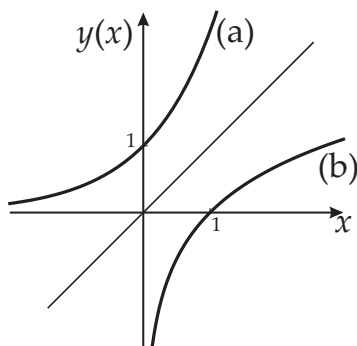


Figure 1.6: Plots of (a) $y(x) = e^x$ and (b) $y(x) = \ln(x)$. They are reflections of each other in the line $y = x$ and thus one can think of (b) as $x = e^y$.

solution to Eq. (1.19) as $y = \ln x$. The derivative may be found by making use of the result for derivatives of inverse functions, viz. $\frac{dy}{dx} = 1 / (\frac{dx}{dy})$. Since $\frac{dx}{dy} = e^y = x$ we have

$$\frac{d}{dx} \ln x = \frac{1}{x}. \quad (1.20)$$

Exercise 1.11: Plot $\sin(kx)$, $\cos(kx)$, and $e^{\pm kx}$ for positive and negative x , and plot $\ln(kx)$ for positive x . Label important points (e.g. intersections with axes, maxima and minima) on the x and y axes. What happens to these points and the graph if you change k ? Revise elementary properties of the exponential and logarithmic functions. What are $(e^x)^2$, e^x / e^y , $a \ln x$ and $\ln x + \ln y$?

We often need to differentiate the product of two functions:

$$\frac{d}{dx} (g(x).h(x)) = \frac{dg(x)}{dx}.h(x) + g(x).\frac{dh(x)}{dx}, \quad (1.21)$$

which is the *product rule*.

Sometimes we shall differentiate a function of a function for which one requires the *chain rule*.

Exercise 1.12: Use the chain rule to show that $\frac{d}{dx}e^{-x^2/2\sigma^2} = -\frac{x}{\sigma^2}e^{-x^2/2\sigma^2}$. Plot the derivative of the Gaussian on the same graph as the Gaussian you plotted in Ex. 1.9. This result helps in the integration by parts in Ex. 1.16.

Solution: The chain rule allows us to differentiate a function of a function, that is $\frac{d}{dx}f(g(x))$. Differentiate the function $f(g)$ with respect to its argument g , and then differentiate g with respect to its argument x , thus getting $\frac{d}{dx}f(g(x)) = \frac{df}{dg} \cdot \frac{dg}{dx}$, both parts of the right hand side being functions ultimately of x . Here f is the exponential function e^g , and $g(x) = -x^2/2\sigma^2$, whence $df/dg = f$ and $dg/dx = -x/\sigma^2$ and we obtain the desired result. Plot the graph.

A little calculus — integration

Integration is the reverse operation to differentiation. Geometrically, it gives the area, A , under a curve between the points $x = a$ and b in Fig. 1.7. We write the integral as $A(a,b) = \int_a^b f(x)dx$ and can think of it as the limit of the sum (Σ) of infinitesimal component areas. $A(a,b)$ can be divided into a very large number of very thin rectangular slices of width dx and height $f(x)$. Each element in the sum $A = \sum_a^b f(x)dx$ is one of the infinitesimal areas shown in Fig. 1.7. It is clear that since areas add,

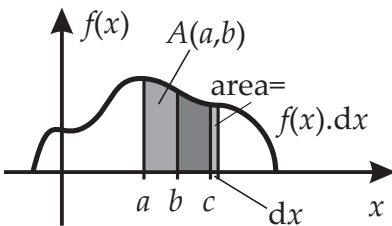


Figure 1.7: Integration gives the area under a curve of the function. Integrals can be added, thus $A(a,b) + A(b,c) = A(a,c)$.

then $\int_a^b f(x)dx + \int_b^c f(x)dx = \int_a^c f(x)dx$. These are examples of *definite* integrals, that is with definite limits specified. Where the limits are not given these integrals are termed *indefinite*. Commonly, there is no distinction made between independent and dummy variables. For example, $\int e^x dx = e^x$ has x as the same variable for both sides. We shall not abuse

this notation. For instance,

$$\int^x \sin(kz) dz = -\frac{1}{k} \cos(kx) + c_1 \quad (1.22)$$

$$\int^x \cos(kz) dz = \frac{1}{k} \sin(kx) + c_2 \quad (1.23)$$

$$\int^x e^{kz} dz = \frac{1}{k} e^{kx} + c_3. \quad (1.24)$$

Note that an arbitrary constant (c_1, c_2, c_3 in the above) then arises in each integration. It can be thought of related to the starting point of the integration which has been left indefinite. To reconcile the absent lower limit to the appearance of an arbitrary constant, consider as an example $\int_a^x e^z dz = e^x - e^a$. If a is an arbitrary constant, then so is the constant e^a . Upon differentiation these constants are removed. The variable of integration, z , is a dummy variable — any symbol can be used. This is identical to the dummy index used in discrete sums. For instance, the sum $\sum_i x_i$ is the same as $\sum_j x_j$. The only difference is that z in the former example is a continuous variable whereas i and j are discrete.

Exercise 1.13: Confirm by differentiation of the right hand sides of Eqs. (1.22–1.24) that, in these cases at least, differentiation is indeed the reverse process from integration; that is, $\frac{d}{dx} \int^x f(z) dz = f(x)$ in the above examples.

The result is generally true; take $I(x + dx) = \int^{x+dx} f(z) dz$ and subtract from it $I(x) = \int^x f(z) dz$. Use the ideas in Fig. 1.7 of adding or subtracting integrals to construct $\frac{dI}{dx} = \lim_{dx \rightarrow 0} \frac{I(x+dx) - I(x)}{dx}$. The numerator is clearly $A(x, x + dx)$ which, from the definition of integration, is in this limit $f(x) \cdot dx$. Putting this result in and cancelling the dx factors top and bottom, one obtains $\frac{dI}{dx} = f(x)$.

Integration by parts

Integration by parts is frequently useful in quantum mechanics. It can be thought of as the reverse of differentiation of a product. Integrating Eq. (1.21) gives

$$\int_a^b \frac{d}{dx} [g(x) \cdot h(x)] dx = \int_a^b \frac{dg(x)}{dx} \cdot h(x) dx + \int_a^b g(x) \cdot \frac{dh(x)}{dx} dx. \quad (1.25)$$

Rearranging we find that

$$\int_a^b g(x) \cdot \frac{dh(x)}{dx} dx = [g(x) \cdot h(x)]_a^b - \int_a^b \frac{dg(x)}{dx} \cdot h(x) dx. \quad (1.26)$$

Notice that h on the right hand side can be regarded as the indefinite integral of the dh/dx factor on the left hand side, that is $h(x) = \int^x \frac{dh}{dz} dz$. For clarity rewriting g as $u(x)$ and dh/dx as $v(x)$, one can rewrite in a form easier to remember and apply:

$$\int_a^b u(x) \cdot v(x) dx = \left[u(x) \cdot \left(\int_a^x v(z) dz \right) \right]_a^b - \int_a^b \left(\frac{du}{dx} \right) \cdot \left(\int_a^x v(z) dz \right) dx. \quad (1.27)$$

Be fluent with the use of the result. Our experience shows that it is best to remember it for use directly along the lines of

“to integrate a product (uv), integrate one part (v) and evaluate this integral times the other function between the given limits, that is giving the first term on the right. Take away the integral of [(the integral already done) \times (the derivative of the other factor)], giving the second term on the right.”

Judiciously choose the easier of u and v to integrate. For instance,

$$\int_0^{\infty} x e^{-kx} dx = \left[-x \frac{1}{k} e^{-kx} \right]_0^{\infty} + \int_0^{\infty} \frac{1}{k} e^{-kx} dx, \quad (1.28)$$

where $u(x) = x$ and $v(x) = e^{-kx}$, with $du/dx = 1$ and $\int^x v(z) dz = -\frac{1}{k} e^{-kx}$. The first term of the right hand side of (1.28) is zero since it vanishes at both limits, and the second term is $1/k^2$ on doing the exponential integral a second time, and this is the answer.

Exercise 1.14: Integrate $\int_0^{\infty} x^n e^{-x} dx$ once by parts. For n an integer, the result suggests repetition until a final result. What well-known function then results?

Exercise 1.15: Integrate $\int_0^{\pi/2} x^2 \sin x dx$ and $\int_0^{\pi/2} x^2 \cos x dx$.

The split into u and v can require delicacy! For example, the integral $\int_{-\infty}^{\infty} x^2 e^{-x^2/2\sigma^2} dx$ can be written as $\int u \cdot v dx = \int (-\sigma^2 x) \cdot \left(-\frac{x}{\sigma^2} e^{-x^2/2\sigma^2} \right) dx$.

Identifying $v(x)$ as the second factor, the integral $\int^x v(z)dz = e^{-x^2/2\sigma^2}$ is easy; see in Ex. 1.12 the differentiation of this answer back to the starting point, and $du/dx = -\sigma^2$ is also easy. The integral has been reduced to another one which does not have a simple answer, but that itself is not necessarily a difficulty — a problem delayed is sometimes a problem solved!

Exercise 1.16: If $P(x) \propto e^{-x^2/2\sigma^2}$, show that the average $\langle x^2 \rangle = \sigma^2$.

Hint: The average is the integral over x^2 times $e^{-x^2/2\sigma^2}$, divided by the integral of $e^{-x^2/2\sigma^2}$ (why?). The integral of the Gaussian by itself is rather difficult, but the numerator can be done by parts and then much of it cancels with the denominator. So avoiding hard integrals is a common technique in quantum mechanics.

This Gaussian result is found throughout physics and is worth remembering:

“From a Gaussian probability written in its standard form $P(x) \propto e^{-x^2/2\sigma^2}$, one reads off the mean square value of x as being σ^2 , that is, the number appearing in the denominator of the exponent, taking care to re-arrange slightly if the required factor of two is not directly apparent.”

What would be the mean square value of x be if the probability were $P(x) \propto e^{-2x^2/b^2}$? Answer: $\langle x^2 \rangle = b^2/4$.

The reader eager to get on to quantum mechanics could skip the next problems, quickly revise differential equations, and jump to Chapter 2. It will be obvious to you when it is to your advantage to return to this exercise.

Exercise 1.17: Evaluate $N = \int_0^L \sin^2(\frac{\pi x}{L})dx$ and $\frac{1}{N} \int_0^L x^2 \sin^2(\frac{\pi x}{L})dx$.

Hint: Use a double angle result and integration by parts. $N = L/2$, a result that is rather general for the integration of squares of sine and cosine through intervals that defined as being between various of their nodes. After studying quantum wells you might like to return to the choice π/L for the coefficient of x in the argument of sine. The second result is $L^2 \left(\frac{1}{3} - \frac{1}{2\pi^2} \right)$. Given your result for N , then $\frac{1}{N} \int_0^L x^2 \sin^2(\pi x/L)$ would be an acceptable probability $P(x)$. What is $\langle x \rangle$? What is the variance of x ?

Exercise 1.18: Integrate the functions $\ln x$, $\frac{\ln x}{x^2}$ and $\frac{\ln(\sin x)}{\cos^2 x}$.

Integration by substitution

In some integrals $\int dx f(x)$ it is advantageous to substitute trig functions for x , for instance $x \rightarrow \sin \theta$ or $\cos \theta$, or sometimes $x \rightarrow \sin^2 \theta$ or $\cos^2 \theta$, depending on the form of $f(x)$ to be integrated. Remember that as well as changing the x where ever it appears in f , one has to change the differential. For instance when $x = \sin^2 \theta$ is chosen as a substitution, the dx becomes $d\theta 2 \sin \theta \cos \theta$. Sometimes to eliminate trig functions in integrals $\int d\phi f(\phi)$, one can use $t = \tan(\phi/2)$ where $dt = \frac{1}{2}d\phi \sec^2 \phi$.

Exercise 1.19: Show that $\int \frac{dx}{\sqrt{1-x^2}} = \sin^{-1} x$, and $\int \frac{dx}{1+x^2} = \tan^{-1} x$. Show that $\int \frac{d\phi}{\cos \phi} = \ln \left(\frac{1+\tan \theta/2}{1-\tan \theta/2} \right)$. Thence show that $\int \frac{dx}{\sqrt{1+x^2}} = \ln \left(\frac{x+\sqrt{1+x^2-1}}{x-\sqrt{1+x^2+1}} \right)$. See Ex. 4.10 for a method using hyperbolic functions.

Differential equations

Most of physics involves differential equations and they certainly underpin quantum mechanics. Such equations involve the derivatives of functions as well or instead of the usual familiar algebraic operators in simple equations such as powers. The first differential equations we meet are those of free motion, or motion with constant acceleration, such as free fall with g . Thus force = mass times acceleration is the differential equation $mdv/dt = mg$. It is easily integrated once with respect to time t : the right hand side is constant in time and gives $mg t$. The left hand side has the derivative nullified by integration to give $mv + \text{constant}$. Cancelling the masses, gives $v = v_0 + gt$. We have taken the initial speed (at $t = 0$) as v_0 , that is, we have fixed the constant of integration by using an initial condition. More generally, these are termed *boundary conditions*. Rewriting the answer as $dz/dt = v_0 + gt$, where z is the distance fallen down, we can integrate both sides again to yield $z = v_0 t + \frac{1}{2}gt^2$, where we have taken the next constant of integration, the position z_0 at $t = 0$, to be zero. This familiar result of kinematics is actually the result of solving a differential equation with a second order derivative since we could have written our starting equation as $d^2z/dt^2 = g$.

Exercise 1.20: For the mass under free fall described above, sketch on the same axes the acceleration $\frac{dv}{dt}$, velocity v and displacement z as a function of time.

Simple harmonic motion

Ubiquitous throughout physics is simple harmonic motion (SHM) or the simple harmonic oscillator (SHO) which for instance in dynamics results when a particle of mass m is acted on by a spring exerting a force $-qz$ where now z denotes the particle's displacement from the origin. The corresponding potential giving rise to the force is harmonic — see the discussion of potentials on page 5. The $-$ sign indicates that the force is restoring, that is, opposite in direction to the displacement, and q is Hooke's constant. Newton's second law is $f = ma$ with the acceleration $a = \frac{dv}{dt}$ being the time derivative of the velocity, that is, of $v = \frac{dz}{dt}$. Using the Hookean force, one obtains the equation of motion

$$m \frac{d^2z}{dt^2} = -qz \quad \text{or} \quad \frac{d^2z}{dt^2} = -\omega^2 z, \quad (1.29)$$

where the angular frequency, ω , will be discussed below and is clearly $\omega = \sqrt{q/m}$. This equation describes oscillations of the particle here, but in a general form also those of an electric field in electromagnetic radiation, or the quantum fields in quantum electrodynamics. Thus differential equations differ from the usual kinds of algebraic equations since they involve derivatives of the function. The highest derivative in (1.29) is a second derivative and so (1.29) is called a second order (ordinary) differential equation. The "ordinary" means there is only one independent variable, t here. We shall later meet cases of more than one independent variable which give rise to "partial" differential equations.

An honourable and perfectly legitimate method of solving differential equations is to guess a solution and try it out. Guesses can often be very well informed and hence this is not entirely magic!

Exercise 1.21: Inspect Eqs. (1.16–1.18) and differentiate each side again. Confirm that for $f = \sin(kx)$ and $\cos(kx)$, and separately for $f = e^{\pm kx}$, one has respectively the similar results:

$$\frac{d^2f}{dx^2} = -k^2 f \quad \text{and} \quad \frac{d^2f}{dx^2} = k^2 f. \quad (1.30)$$

In a mysterious way e^{kx} is like $\sin(kx)$ or $\cos(kx)$, but with k^2 replaced by $-k^2$. This turns out to be true, but there is the little matter of a squared number becoming negative! ($5^2 = 25$ and $(-5)^2 = 25$ too; how would one get a result of -25 ?) We treat imaginary and complex numbers in Chapter 4.1 which could also be read now if desired.

Considering time t rather than x as the independent variable, one can confirm that two solutions for SHM (Eq. (1.29)) are

$$z(t) = z_s \sin(\omega t), \quad z(t) = z_c \cos(\omega t). \quad (1.31)$$

Since sine and cosine repeat when $\omega t = 2\pi$, that is, after a period $t = T = 2\pi/\omega$, then rearrangement shows that $\omega = 2\pi/T \equiv 2\pi\nu$ — the angular frequency where $\nu = 1/T$ is the usual frequency. The amplitudes z_s and z_c of oscillation are arbitrary and indeed the general solution would be $z(t) = z_s \sin(\omega t) + z_c \cos(\omega t)$, which is an arbitrary combination of the oscillatory components differing in phase by $\pi/2$ or 90 degrees.

We have seen in the second order differential equation (1.29), a constant is introduced every time we integrate. Two integrations and thus two constants are required to get a general solution. How do we fix these constants? “Boundary conditions”, in this case two, and in general as many as the order of the equation, are required to fully solve differential equations. Here for instance, at $t = 0$ we have $z(t = 0) = 0$ and $dz/dt = v_0$ (the particle is initially at the origin with velocity v_0). The first condition demands that $z_c = 0$ (recall what $\sin(0)$ and $\cos(0)$ are). The second condition gives

$$v_0 = \left. \frac{dz}{dt} \right|_{t=0} = \omega z_s \cos(\omega t)|_{t=0} = \omega z_s,$$

that is $z_s = v_0/\omega$. See also the simple example above of integrating the differential equation of free fall. Note that the period ($T = 2\pi/\omega$) is independent of the amplitude: only the ratio between the inertia factor (the mass) and the elasticity factor (the spring constant) matters. This is generally not true. See Ex. 1.3 where the period increases with amplitude and Ex. 1.36 for more exotic behaviour. Consult Sect. 3.2 for further discussion of classical SHM.

Exercise 1.22: A mass m , attached to a light spring of constant q , slides on a horizontal surface of negligible friction, as shown in Figure 1.8. The mass is displaced through a distance x_0 from the equilibrium position and released. Write down Newton’s 2nd law as applied to the displaced mass.

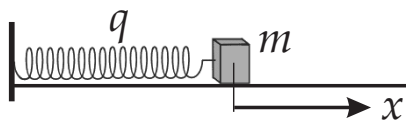


Figure 1.8: A mass on a light spring.

A clock is started at some later time and the dependence of the displacement on time is given by $x(t) = x_0 \sin(\omega t + \phi)$. Act on the time dependent displacement $x(t)$ with the operator $\frac{d^2}{dt^2}$. You will see that the same function is obtained up to a multiplicative constant. Obtain the constant and relate it to the result of Newton's 2nd Law.

Sketch a graph of the system's potential energy versus displacement.

Exponentially decaying motion

If friction dominates, that is, if there is no or insufficient restoring force, we have exponential instead of sinusoidal motion.

Exercise 1.23: A block sliding on a surface suffers a retarding force proportional to its velocity, $f = -\mu v$, where μ is a constant. Show that $dv/dt = -(\mu/m)v$ and solve the equation subject to $v(t=0) = v_0$. What is the displacement as a function of time? Sketch the block's displacement, velocity and acceleration as a function of time on the same axes.

Solution: Applying Newton II gives $m \frac{dv}{dt} = -\mu v$. This is a first order separable differential equation. The solution can be found by either comparison with radioactive decay or by separating variables. Performing the latter yields $\frac{dv}{v} = -\frac{\mu}{m} dt$. Integrating and inserting the boundary condition gives

$$\int_{v_0}^v \frac{dv}{v} = -\frac{\mu}{m} \int_0^t dt \quad (1.32)$$

$$\ln \left(\frac{v}{v_0} \right) = -\frac{\mu}{m} t \quad (1.33)$$

$$v = v_0 e^{-\frac{\mu}{m} t}. \quad (1.34)$$

Note that there is only one boundary condition since it is a first order differential equation. Check that this is indeed a solution to the differential

equation (and the initial condition) by direct substitution. A further integration produces the displacement $\frac{mv_0}{\mu} \left(1 - e^{-\frac{\mu}{m}t}\right)$ at time t .

Exercise 1.24: A model for a parachutist's downward speed $v(t)$ at time t in free fall after jumping out is given by

$$m \frac{dv}{dt} = mg - kv. \quad (1.35)$$

Explain the physical origin of each of the terms. Solve the differential equation (1.35) given his initial speed is zero when he jumps out. What is his terminal velocity?

We return to very general and important aspects of differential equations in Sect. 2.3 on Sturm–Liouville theory.

Interference of waves

We have seen that the general solution to the SHM equation (1.29) is $z(t) = z_s \sin(\omega t) + z_c \cos(\omega t)$. That is, any sum or linear combination of $z(t) = \sin(\omega t)$ and $z(t) = \cos(\omega t)$ is also a solution. This is a general property of linear differential equations. Linear means that there are no powers in the derivatives or the function z . The differential equation governing waves is also linear in the same way. And thus waves can add or superpose to give other composite waves that are also solutions of the same equation.

When we superpose two waves, in some places the disturbances add, in other places they subtract, depending on the relative phase of the two quantities being added. The phase might depend on position such as in the two slit experiment. Here we have two separated but identical sources of waves which travel to an observation screen. At a general point on the screen the distances travelled by the two sets of waves will be different. Let us take two extremal examples. First, if the path difference between waves from the double slits to a given observation point is exactly a wavelength, the waves add in phase and give a maximum of intensity (known as constructive interference). Conversely, if the path difference is a half wavelength, one has destructive interference and thus a node, a position of zero intensity, on the observation screen. This process of wave interference occurs for any waves travelling in any direction through the same region of space. See the 2-slit experiment of Fig. 4.3 on page 76. An-

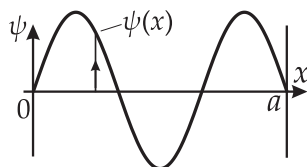
other example is standing waves which are produced by the interference of two identical counterpropagating waves:

Exercise 1.25: Show that the waves $\sin(kx + \phi/2)$ and $\sin(kx - \phi/2)$, differing in phase by ϕ , add to give a resultant wave $2 \sin(kx) \cos(\phi/2)$. Consider the cases of being in phase ($\phi = 0$) and in anti-phase ($\phi = \pi$) when these two waves interfere.

Waves on a stretched string

Consider a string under tension T and of mass per unit length μ . It is anchored at $x = 0$ and $x = a$; see Fig. 1.9. For small sideways displacements

Figure 1.9: A snapshot of standing waves on a stretched string at a particular time. For snapshots of the string at other times, see Fig. 5.6. The transverse displacement is $\psi(x)$.



$\psi(x)$ at the position x the length changes little and the tension remains T . One can show that the envelope $\psi(x)$ of standing or stationary waves obeys the equation

$$\frac{d^2\psi}{dx^2} = -\frac{\mu}{T}\omega^2\psi. \quad (1.36)$$

See Sect. 5.3 for a derivation of the full motion, of which this is one limit. For standing sound waves in a tube, $\psi(x)$ would be the pressure that varies with position x along the tube. The wave speed is $c = \sqrt{T/\mu}$ and $\omega = 2\pi\nu$ connects the angular and conventional frequencies, ω and ν . Thus in the above equation

$$\frac{\omega}{c} = \frac{2\pi\nu}{c} = \frac{2\pi}{\lambda} = k, \quad (1.37)$$

where these rearrangements employ $\nu\lambda = c$ with λ the wavelength. The final definition $k = 2\pi/\lambda$ introduces the wavevector that is so ubiquitous in quantum mechanics and optics. Thus the standing wave equation becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad (1.38)$$

which is the form of Eq. (1.30). Its solutions are $\sin(kx)$ and $\cos(kx)$. Figure 1.9 shows that since $\psi(0) = 0$ we have to discard the $\cos(kx)$ solutions,

since they are non-zero at $x = 0$, in favour of $\sin(kx)$ solutions that naturally vanish at $x = 0$. Equally in Fig. 1.9, to ensure $\psi(x = a) = 0$, it is necessary for an integer number of half wavelengths to be fitted between $x = 0$ and $x = a$. So

$$n \cdot \frac{\lambda}{2} = a \Rightarrow \lambda = \frac{2a}{n}$$

whence

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{a}. \quad (1.39)$$

Only discrete choices of λ , or equivalently k , corresponding to integer n are permitted. Only certain waves are possible. In fitting waves into this interval with its boundary conditions, we have our first encounter with what we later see is quantisation!

Qualitative understanding of functions

We shall meet equations we cannot solve exactly. For instance, they can involve transcendental functions⁵ such as trigonometric and exponential functions. However, a deep understanding of the behaviour of quantum systems emerges from plotting the functions, as well as from using calculus and a knowledge of their asymptotes and zeros. For instance Fig. 1.10 shows the two functions $y = \sqrt{x}$ and $y = \tan(x^2)$. Explain the behaviour

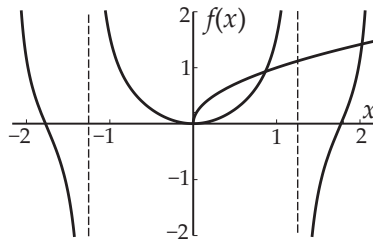


Figure 1.10: A plot of the functions \sqrt{x} and $\tan(x^2)$.

of each function at important points such as the origin and at nodes (zeros) of the somewhat unusual tangent function. Why at one node is the slope zero, and why is it finite at others? Where are the nodes in general? Where the two functions cross are the solutions of the equation $\tan(x^2) = \sqrt{x}$.

⁵That is, functions that return values that can be transcendental numbers. Such numbers are not roots of polynomial equations, as algebraic numbers (both rational and irrational) are. For example π and e are transcendentals.

Exercise 1.26: Plot the functions $y = \sqrt{x_0 - x}$ and $\tan(\sqrt{x})$ on the same graph for positive x , taking the former function up to x_0 (a constant). Identify the zeros of each function and give their locations. What is the behaviour of the functions around these zeros, in particular their slopes there? How many solutions does the equation $\tan(\sqrt{x}) = \sqrt{x_0 - x}$ possess. What about the equation $\tan(\sqrt{x}) = -\sqrt{x_0 - x}$? Precise location of the solutions requires numerics. Discuss their approximate locations. Similar analysis will be important for quantum wells of finite depth; see Sect. 3.1.

Hint: It might be helpful to differentiate or use the approximation that $\tan x \approx x$ for small x .

We later solve a slightly more complicated version of this problem to find the characteristic states of a quantum particle found in a finite square well; see Eq. (3.8).

A little calculus is sometimes helpful in analysing equations. Another transcendental equation is $e^x = kx$; see Fig. 1.11.

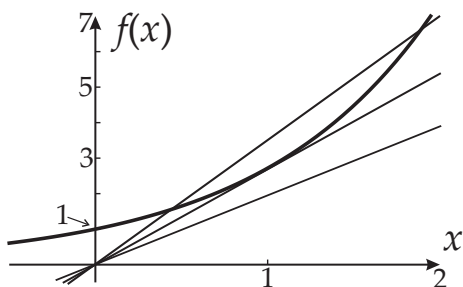


Figure 1.11: Plots of e^x , and of kx for various values of k .

Exercise 1.27: For what values of k do there exist solutions of the equation $e^x = kx$? What is the solution at the k , say k_c , where solutions first appear?

Hint: Consider the case where the line first touches the exponential. What two conditions are required there? Solve them simultaneously.

Exercise 1.28: Consider the equation $e^x = \frac{1}{2}ax^2$, for $a > 0$. For what ranges of a are there 1, 2, or 3 solutions to this equation?

It is very helpful to know the power series expansions of functions for small values of their arguments, and how in general to expand functions

about an arbitrary point in their range. To get a first approximation recall that the derivative is the limiting ratio as $\delta x \rightarrow 0$

$$\frac{dy}{dx} \simeq \frac{\delta y}{\delta x} \simeq \frac{y(x_0 + \delta x) - y(x_0)}{\delta x}. \quad (1.40)$$

Rearranging we find that

$$y(x_0 + \delta x) \simeq y(x_0) + \delta x \cdot \left. \frac{dy}{dx} \right|_{x_0}, \quad (1.41)$$

so we have some knowledge of y at another point $(x_0 + \delta x)$ if we know $y(x_0)$ and the first derivative at x_0 . We shall use a rearrangement of the first of Eq. (1.41) to get the difference of the values of a function evaluated at two different points: $y(x_0 + \delta x) - y(x_0) \simeq \delta x \cdot \frac{dy}{dx}$.

Repeated application of this procedure gives us better knowledge further away, at the expense of needing higher derivatives. So we may write in terms of derivatives evaluated at $x = x_0$, the *Taylor expansion*

$$y(x_0 + \delta x) = y(x_0) + \delta x \frac{dy}{dx} + \frac{(\delta x)^2}{2!} \frac{d^2 y}{dx^2} + \frac{(\delta x)^3}{3!} \frac{d^3 y}{dx^3} + \dots \quad (1.42)$$

For instance, some familiar functions expanded about $x_0 = 0$ while calling δx simply x :

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots \quad (1.43)$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots \quad (1.44)$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \quad (1.45)$$

$$\frac{1}{1-x} = 1 + x + x^2 + \dots \quad (1.46)$$

$$\tan x = x + \frac{x^3}{3} + \frac{2x^5}{15} + \dots \quad (1.47)$$

Exercise 1.29: Confirm the expansions $(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \dots + x^n$, terminating at x^n for positive integer n , and $\tan(x) = x + x^3/3 + \dots$

Hint: Recall that $\tan(x) = \sin(x)/\cos(x)$ and expand the denominator up into the numerator using (1.46) with a more complicated “ x ”.

Exercise 1.30: For each of the functions in Eqns. (1.43–1.45), sketch the function, the separate terms in the approximation, and finally the sum of those terms on the same diagram.

Hint: Note how each successive term builds up to form a better approximation to the true function.

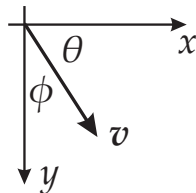
Vectors

In Sect. 1.2 and Ex. 1.20, we analysed the downwards motion of a falling particle. Suppose we had fired the mass horizontally with speed v_0 at time $t = 0$. What is the subsequent motion of the mass? The horizontal and vertical motions are independent from each other. The vertical motion is as described previously. Since we have assumed no frictional forces, the horizontal speed remains constant.

Exercise 1.31: Show that the motion of the mass is parabolic with equation $y = (g/2v_0^2)x^2$, adopting the coordinates of Fig. 1.12.

The motion of the projectile is decoupled into horizontal and vertical directions, Newton's laws of course applying in both directions. However, we need not have chosen horizontal and vertical axes for Newton's laws to apply. We expect that the laws of physics are independent of our particular choice of co-ordinates. The mathematical way of expressing such laws is in terms of vectors.

Figure 1.12: A vector v has magnitude and direction. It has an identity independent of a particular representation. It can be resolved into the x and y directions of a particular coordinate system.



A scalar quantity, such as the mass of the projectile, can be represented by a single number. A vector, such as velocity, by contrast possesses both magnitude and direction. The mass travels in a particular direction at a certain rate. We represent vectors in boldface or they are underlined in handwriting. Referred to a particular co-ordinate system, say, the usual x and y axes, the vector v of length v , has v_x and v_y components in x and y

directions respectively,

$$v_x = v \cos \theta, \quad (1.48)$$

$$v_y = v \cos \phi, \quad (1.49)$$

where angles θ and ϕ are between v and the x and y axes respectively (see Fig. 1.12). Note that $\phi = \frac{\pi}{2} - \theta$. Written in components explicitly, v can be written as a row or column or numbers. Hence, we may write $v = (v_x, v_y)$ or $v = \begin{pmatrix} v_x \\ v_y \end{pmatrix}$. Squaring and adding the components, we find that

$$\begin{aligned} v_x^2 + v_y^2 &= v^2 \cos^2 \theta + v^2 \cos^2 \phi \\ &= v^2 (\cos^2 \theta + \sin^2 \theta) \\ &= v^2 \end{aligned} \quad (1.50)$$

is independent of angle θ and thus of co-ordinate choice. Rotating our choice of axes does not change the length v of the vector; but it does change the components. It is the same object from different viewpoints.

More generally, the *scalar product* of vectors \mathbf{a} and \mathbf{b} , defined by

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z, \quad (1.51)$$

is a co-ordinate independent scalar quantity. If $\mathbf{b} = \mathbf{a}$, then $\mathbf{a} \cdot \mathbf{a} = |\mathbf{a}|^2 = a^2$ is called the modulus squared of vector \mathbf{a} . The modulus is the length of the vector. An important scalar for our later work is that of the particle's kinetic energy $T = \frac{1}{2} m \mathbf{v} \cdot \mathbf{v} = \frac{1}{2} m (v_x^2 + v_y^2 + v_z^2)$. The meaning of this expression is that the kinetic energies in the different perpendicular directions add to give the total.

Exercise 1.32: Write the kinetic energy in terms of the components of the momentum \mathbf{p} .

Exercise 1.33: By considering $\mathbf{c} = \mathbf{a} + \mathbf{b}$ or otherwise, show that $\mathbf{a} \cdot \mathbf{b}$ is independent of the choice of co-ordinates.

Solution: Use the result that $|\mathbf{a}|^2$, $|\mathbf{b}|^2$ and $|\mathbf{c}|^2$ are invariant upon co-ordinate rotation together with the definition of scalar product, in particular applying it to $\mathbf{c} \cdot \mathbf{c}$.

Exercise 1.34: By appropriate choice of axes or otherwise, show that

$$\mathbf{a} \cdot \mathbf{b} = ab \cos \theta, \quad (1.52)$$

where $\theta \in [0, \pi)$ is the angle between vectors \mathbf{a} and \mathbf{b} . If $\mathbf{a} \cdot \mathbf{b} = 0$ then \mathbf{a} and \mathbf{b} are perpendicular or *orthogonal* to each other. In general, the trigonometric factor $\cos \theta$ shows the dot product has the meaning of the projection of \mathbf{b} along \mathbf{a} times the length of \mathbf{a} or equivalently *vice versa*. We use this in analysing 2-D waves in Sect. 5.3.

If the unit vectors⁶ in the x , y and z directions are \mathbf{i} , \mathbf{j} and \mathbf{k} respectively, then a vector can be written as

$$\begin{aligned} \mathbf{v} &= v_x \mathbf{i} + v_y \mathbf{j} + v_z \mathbf{k} \\ &= (\mathbf{v} \cdot \mathbf{i}) \mathbf{i} + (\mathbf{v} \cdot \mathbf{j}) \mathbf{j} + (\mathbf{v} \cdot \mathbf{k}) \mathbf{k}, \end{aligned} \quad (1.53)$$

where we have made use of the result of Ex. 1.34. This way of expressing the vector is called resolving or expanding into basis vectors.

1.3 Summary

To gain a deep understanding of physics, including quantum mechanics, one requires mathematical fluency. We have revised the essentials of probability, algebra and calculus, and derived results which will be used in later chapters, particularly those of the harmonic oscillator and waves on a string. More mathematical material and practice is in Chapter 4.1 where \mathbf{i} , that is $\sqrt{-1}$, is introduced.

Quantum mechanics is founded on different physical concepts from classical physics. Central is the idea of a wavefunction from which we can derive the probability of finding a particle in a given position.

Adopting a theory based on probability, we found that it is impossible to determine simultaneously the position and momentum of particles beyond a certain accuracy (Heisenberg's uncertainty principle). We shall explore the ramifications of this in later chapters. To describe the motion of quantum particles, we use the idea of potential energy rather than forces. The classical potential problems we give are important practice for this new approach.

⁶Conventionally in vector analysis, these are denoted with a hat above the vector, e.g. $\hat{\mathbf{i}}$. However, we shall reserve the hat for use with quantum mechanical operators.

1.4 Additional problems

Exercise 1.35: A particle of energy $E_2 = 5V_0$ approaches the potential of Fig. 1.4. How long does it take to travel from $-a$ to $+2a$?

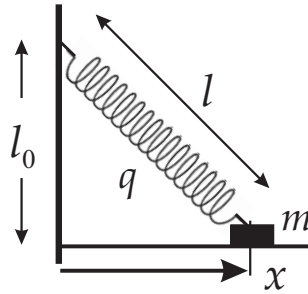


Figure 1.13: A constrained mass on a spring

Exercise 1.36: A particle of mass m is constrained to slide along a smooth wire lying along the x axis, as shown in Figure 1.13. The particle is attached to a spring of natural length l_0 and spring constant q which has its other end fixed at $x = 0, y = l_0$.

- Obtain an expression for the force exerted on m in the x direction.
- For small displacements ($x \ll l_0$), how does the force depend upon displacement x ?
- The potential $U(x)$ depends upon x in the form of $U \simeq Ax^n$ for small x . What are the values of n and A in terms of the constants given?
- Find the exact potential.
- By sketching a graph of the potential energy, suggest qualitatively how the period of oscillation of the object will depend on the amplitude.
- For $n = 4$ and amplitude x_0 , show that the period is

$$\tau = 4 \frac{1}{x_0} \sqrt{\frac{m}{2A}} \int_0^1 \frac{du}{\sqrt{1-u^4}}.$$

Exercise 1.37: An ideal spring obeying a linear force-extension law will store elastic potential energy when stretched or compressed. A real spring will often have other (smaller) force-extension terms included, and can be used as a model for the attractive and repulsive forces in other systems. In this

example we add to the force a quadratic repulsive term, q_2x^2 , to the linear attractive term, the restoring force eventually becoming repulsive at large enough x values.

$$F(x) = -q_1x + q_2x^2.$$

(a) Calculate the potential energy, $U(x)$, stored in the spring for a displacement x . Take $U = 0$ at $x = 0$.

(b) It is found that the stored energy for $x = -a$ is twice the stored energy for $x = +a$. What is q_2 in terms of q_1 and a ?

(c) Sketch the potential energy diagram for the spring.

(d) Consider a particle attached to the end of this spring. At what amplitude of motion in the $x > 0$ region does the particle cease to oscillate? At what $x < 0$ would we release the particle from rest in order to start seeing this failure to oscillate? Describe the motion.

Exercise 1.38: A particle with energy E incident from $x < 0$ on a potential ramp of the form $V(x) = 0$ for $x < 0$ and $V(x) = V_0x/d$ for $x \in (0, d)$ and $V = V_0$ for $x > d$. For $E < V_0$ give the x value of the classical turning point, x_{ctp} , where the particle briefly stops⁷. Show that the time taken to travel from $x = 0$ to a point x_0 on the ramp ($x_0 \leq x_{\text{ctp}}$) is $t_0 \propto (1 - \cos \theta_0)$, where $\cos \theta_0 = (1 - \frac{V_0x_0}{Ed})^{1/2}$. Give the constant of proportionality. What is the time taken to reach the classical turning point?

Hint: the form of the answer is a steer to the calculus involved.

What is the form of the force implied by this potential? Solve this elementary problem instead by integration of Newton's Second Law and show that the answer is the same as above.

Exercise 1.39: Consider a particle with energy E incident from $x < 0$ on a potential $V(x) = 0$ for $x < 0$ and $V(x) = \frac{1}{2}V_0(x/d)^2$ for $x > 0$. Again calculate x_{ctp} . Show that the time taken to reach a position $0 < x_0 \leq x_{\text{ctp}}$ from $x = 0$ is $t_0 \propto \sin^{-1} \left(\sqrt{\frac{V_0}{2E}} \frac{x_0}{d} \right)$, and give the constant of proportionality.

What is important about the E -dependence of the time taken to reach the classical turning point? Evaluate and interpret this time.

Exercise 1.40: Functions ψ_0 and ψ_1 describing the first two quantum states of the harmonic oscillator are $\psi_0(u) = A_0e^{-u^2/2}$ and $\psi_1(u) = A_12ue^{-u^2/2}$

⁷A classical, i.e. non quantum, particle cannot proceed further than this point, hence the name.

where A_0 and A_1 are normalisations that ensure $\int_{-\infty}^{\infty} \psi^2 du = 1$. The variable u is related to the displacement from the minimum of the quadratic potential, see page 62. Show that $A_1 = A_0/\sqrt{2}$. Do not evaluate A_0 , but give a value for the particle's mean square position when in the second quantum state: $\langle u^2 \rangle = \int_{-\infty}^{\infty} u^2 \psi_1^2 du$.

Exercise 1.41: Show that $\int_0^a x \sin^2(kx) dx = \frac{a^2}{4} \left[1 - \frac{\sin(2ka)}{ka} + \frac{\sin^2(ka)}{(ka)^2} \right]$.