## Second Year Quantum Mechanics

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## Michaelmas Term Problems

These problems cover all the material we will be studying in the lectures this term. The **Synopsis** tells you approximately which problems are associated with which lectures.

Some of the problems have a double dagger ††; they are a bit more challenging but if you can do them you're really on top of the subject. Some of the problems have a single dagger †. They are straightforward extensions and applications of things we will do in the lectures; first time round they will take you some time and may raise difficulties that you'll need to discuss with your tutor but in a couple of years time they'll seem really easy. Finally there are problems with no daggers; these are either really easy or pretty much the same as problems we've done in the lectures. If you're paying attention you should be able to do them.

There are quite a lot of these problems, more than most of you will manage to do by the end of term, and your tutor may well tell you to do just a subset of them to start with. However, **in the end you should try them all**, perhaps over the vacation, as you will learn a great deal.

# 1 Photons, Matter Waves, and Orders of Magnitude

1. **The Photoelectric Effect**

   A beam of ultraviolet light of wavelength $\lambda = 124$ nm and intensity $1.6 \times 10^{-12}$ $W/m^2$ is suddenly turned on and falls on a metal surface, ejecting electrons through the photo-electric effect. The beam has a cross-sectional area of $10^{-4}\text{m}^2$ and the work function of the metal is 5 eV. Estimate the time delay before the first photoelectron appears by the following approaches:

   (i) A crude estimate using classical physics is to calculate the time needed for the work function energy to be accumulated over the area of one atom (radius $\approx 10^{-10}$ m).

   (ii) Lord Rayleigh showed that this is a bit pessimistic and that a better estimate of the effective area (or *scattering cross section*) that the atom presents is $\lambda^2$. Use this to revise your estimate of the time delay.

   (iii) In the quantum approach, emission can occur as soon as the first photon arrives (why?). To obtain a time delay that can be compared to these classical estimates, calculate the average time interval between arrival of successive photons.

2. **Generalized energy-frequency relation for photons**

Einstein brilliantly hypothesised the existence of quanta (photons) of light together with the energy-frequency relation $E = hf$. In a theory consistent with special relativity this should be generalized to a relation between the energy-momentum four-vector $(E, \mathbf{p})$ and another four-vector with first component $hf$. The relation is

$$(E, \mathbf{p}) = (hf, h\mathbf{k}) \tag{1}$$

where $\mathbf{k}$ is the wavevector of the electromagnetic radiation. Note that the magnitude of the momentum part of the generalized energy-frequency relation can be rewritten as

$$\lambda = \frac{h}{|\mathbf{p}|} \tag{2}$$

which motivated de Broglie in his definition of 'matter waves'.

(i) Verify that the relation (1) is consistent with the constant velocity of light being $c$. [Hint: the relativistic energy-momentum relation for a particle of rest mass $m_0$ is $E^2 = (m_0c^2)^2 + (pc)^2$. What rest mass must the photon have given that the relativistic expression for the velocity is $v = dE/dp$?]

(ii) The wavelength of visible light from the sun is roughly in the band 390 to 780 nm. What is the momentum of a single photon of wavelength 600nm? What is it's energy? Given that the intensity of midday solar radiation impinging on the Earth is roughly $1\text{kW/m}^2$, estimate how many photons per second your eye sees. How far away, in light years, would a sun-like star have to be for you to see only 100 photons/second from such a star? [You may be amused to learn that the sensors in the retina are just able to detect single photons. However, apparently neural filters only allow a signal to pass to the brain to trigger a conscious response when about five to ten or more arrive within less than 0.1s. This seems to be a necessary adaptation – if we could consciously see single photons we would experience too much visual 'noise' in very low light. I am told that frogs are different!]

3. †**The Compton Effect**

The experiment that provide the most direct evidence for the existence of the photon as a quanta of light is the Compton effect. Compton discovered that EM (X-ray) radiation scattered off the electrons in a graphite crystal in a fashion that was not consistent with classical electromagnetic theory. In particular not only was there a scattered component with the same wavelength as the incomming radiation, but in addition a second component with a shifted wavelength, with the amount of the shift depending upon scattering angle.

Following Compton we can explain the second shifted component by treating the incomming beam of radiation as a beam of individual photons, each with energy-momentum given by (1), and with each photon elastically scattering off an (approximately stationary and lightly bound) target electron, with energy and momentum seperately conserved *as in a normal particle scattering process.*

Thus consider a photon of initial momentum $\mathbf{p}$ incident upon an electron at *rest*. After the collision let the photon and electon momenta be $\mathbf{p}'$ and $\mathbf{q}$ respectively.

(i) Write down the equations for conservation of momentum and energy and show that the equation for the conservation of momentum may be written as

$$\mathbf{q}^2 = \left(\frac{hf}{c}\right)^2 + \left(\frac{hf'}{c}\right)^2 - 2\frac{hf}{c}\frac{hf'}{c}\cos(\theta) \tag{3}$$

where $f$ and $f'$ are the frequencies of the initial and scattered photons respectively, and $\theta$ is the angle between them.

(ii) Show that the equation for the conservation of energy may be written as

$$q^2c^2 = (hf - hf')^2 + 2m_ec^2(hf - hf') \tag{4}$$

where $m_e$ is the electron mass, and combine with the above equation to show that

$$f' = \frac{f}{1 + (hf/m_ec^2)(1 - \cos\theta)}. \tag{5}$$

From this form we see that for initial photon energies $hf \ll m_ec^2$ the scattering does not, to a good approximation, change the frequency of the radiation. In this regime the scattering is well described by the classical electromagnetic 'Thomson scattering' process. Show that an alternate form of the previous equation is

$$\lambda' - \lambda = \frac{h}{m_ec}(1 - \cos\theta), \tag{6}$$

where $\lambda'$ and $\lambda$ are the wavelengths of the initial and final photons. These formulae agree very well with the measurements of the shift in wavelength or frequency of the second component of the scattered radiation. [Roughly speaking the unmodified component is due to scattering by the entire atom; more precisely the electrons that are tightly bound to the atoms in the material of the crystal.] Is the energy of the scattered photon always reduced, increased, or neither? Physically why?

(iii) The quantity $h/(m_ec)$ has the dimensions of a length, and is known as the Compton length of the electron. Evaluate this length. Similarly we may define the Compton wavelength $\lambda_c$ of any *massive* particle (or bound system) of mass $M$ to be $\lambda_c = h/(Mc)$. Evaluate this length for carbon, the atomic constituent of graphite. Given that Compton used X-rays of wavelength 0.71 Angstrom, what are, at $\theta = 90^o$, the relative shifts $(\lambda' - \lambda)/\lambda$ in the wavelength of the incoming X-rays in the two cases of scattering off a single electron, and scattering off a carbon atom?

4. **Matter waves**

The single-slit diffraction pattern for a monochromatic wave of wavelength $\lambda$ incident normally on a narrow slit of width $a$ is described (in the "Fraunhofer region") by the intensity

$$I(\theta) = I_0 \frac{\sin^2[(\pi a/\lambda)\sin\theta]}{[(\pi a/\lambda)\sin\theta]^2} \tag{7}$$

where $\theta$ is the deflection angle perpendicular to the incident wavefront. (We'll see how to derive this later in Question 5.4.)

(i) What is the value of $I(\theta)$ as $\theta \to 0$?

(ii) Sketch the form of $I(\theta)$ versus $\theta$ for the particular case $\lambda = a/2$. How does the sketch change as $\lambda$ decreases? Show that the intensity peak centred on $\theta = 0$ falls to half its central intensity at

$$\theta = \sin^{-1}(0.443\lambda/a). \tag{8}$$

(iii) Nuclear reactors provide high fluxes of neutrons with energies $\sim 10^{-2}$ or $10^{-3} eV$. For neutrons with an energy of 4.18 x $10^{-3}$ eV, what is (a) their speed, (b) their wavelength?

(iv) In an experiment (C. G. Schull, Physical Review 179 (1969) 752-754) neutrons of energy 4.18 x $10^{-3}$ eV were incident on a slit of width 5.6 $\mu$m. It was found that the full width at half maximum of the central intensity peak (measured downstream from the slit) was 15.4 arc seconds. Is this consistent with the above diffraction formula $I(\theta)$?

5. **The importance of $\hbar$**

Planck's constant $\hbar$ is equal to $1.0 \times 10^{-34}$ Js, to two significant figures. A system (e.g. a mechanical watch) has moving parts of size $d$ and mass $m$, and the movement occurs on a characteristic timescale $\tau$.

(i) Construct a quantity, call it $S$, having the same dimensions as $\hbar$ from $d$, $m$ and $\tau$ (such quantities are said to have the dimensions of *action*). The rule of thumb is that if $S$ has numerical value much bigger than $\hbar$ then quantum effects are negligible.

(ii) Evaluate your $S$ and compare it to $\hbar$ for
a) The final stage of a turbofan engine (the thing that makes an aircraft fly; typically the final stage turbine rotates at an incredible 30,000 rpm!).
b) The motion of a mechanical wristwatch.
c) A bacteria "swimming".

(iii) Now take $d$ to be a typical atomic size, and $m$ to be the electron mass. Find $\tau$ such that your action quantity is equal to $\hbar$ in this case. Defining an average velocity by $v = d/\tau$ , calculate the corresponding kinetic energy of the electron, in eV.

6. Microscopes using waves with wavelength $\lambda$ can resolve objects roughly as small as $\lambda$ but no smaller. Determine the kinetic energy of electrons in an electron microscope needed to resolve

   (i) a DNA molecule ( $10^{-8}$m )

   (ii) a proton ($10^{-15}$m).

   [Use the de Broglie relation $\lambda = h/p$; in each case consider whether you should use the non-relativistic expression $T = p^2/2m$ for the kinetic energy $T$, or the relativistic one $T + mc^2 = [m^2c^4 + c^2p^2]^{1/2}$.

7. (i) Calculate the de Broglie wavelength of a non-interacting gas of particles of mass $m$ at temperature $T$. Assume that $T$ is low enough so that the non-relativistic form of kinetic energy applies, and recall that the mean linear KE of a particle at temperature $T$ is $3k_BT/2$ where $k_B$ is Boltzmann's constant. Note that this wavelength $\lambda_{TdB}$ (known as the 'thermal de Broglie wavelength') grows as $T$ decreases.

   (ii) Evaluate $\lambda_{TdB}$ for Helium gas at room temperature (300K). Estimate the mean spacing between He atoms in such a gas at atmospheric pressure. Do you expect quantum effects to be important for this gas?

   (iii) Estimate the mean interparticle spacing for liquid Helium near its boiling point (4.2K with density 125 kg/m$^3$). What is the thermal de Broglie wavelength? Do you expect quantum effects to be important for liquid Helium?

# 2 Time Dependent Schrödinger Equation

The 1-D TDSE is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t). \tag{9}$$

1. **Einstein - de Broglie - Schrödinger waves**

   A plane wave solution of the time-dependent Schrödinger equation in one dimension is given by

   $$\psi(x,t) = Ae^{ikx-i\omega t}. \tag{10}$$

   (i) By substituting this solution into the TDSE for the case that $V(x) = 0$ find the relation between $\omega$ and $k$ for such waves.

   (ii) The "phase velocity" $v_p$ is defined to be $\omega/k$ and the "group velocity" $v_g$ is defined to be $d\omega/dk$. Find expressions for $v_p$ and $v_g$ in terms of the "particle velocity" defined by $v = p/m$. Are the results what you expect, and why?

2. **Probability interpretation of the wavefunction**

   In Max Born's original paper (Zeitschrift für Physik <u>37</u> 863-67 (1926)) the sentences proposing the probability interpretation of the wavefunction read as follows (quoting from the English translation, printed in "Quantum Theory and Measurement", Edited by J A Wheeler and W H Zurek, Princeton University Press, 1983, pages 52-55):

"If one translates this result into terms of particles, only one interpretation is possible. $\Phi_{\eta\tau m}(\alpha, \beta, \gamma)$ [the wavefunction for the particular problem he is considering] gives the probability *for the electron, arriving from the z-direction, to be thrown out into the direction designated by the angles $\alpha, \beta, \gamma$ ... .

* Addition in proof: More careful considerations show that the probability is proportional to the square of the quantity $\Phi_{\eta\tau m}$. "

Give as many "considerations" as you can why a general wavefunction $\psi$ does **not** have suitable properties to be interpreted as a probability density, but the square modulus $|\psi|^2$ does.

3. **Continuous probability distributions**

For a certain continuous variable $x$, the probability that it has a value lying between $x$ and $x + dx$ is $\rho(x)dx$. The possible values of $x$ range from $a$ to $b$.

(i) What conditions must $\rho(x)$ satisfy?

(ii) Define the average value $\langle f(x) \rangle$ of a function of $x$, $f(x)$.

(iii) The *variance* of the distribution is $\sigma^2$, defined by $\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle$. Show that $\sigma^2 = \langle x^2 \rangle - (\langle x \rangle)^2$. (A customary measure of the "spread" of a distribution is $\sigma$, which by the above result is equal to $[\langle x^2 \rangle - (\langle x \rangle)^2]^{1/2}$. Frequently this may be written as $\Delta x$.)

4. **Solutions of the TDSE separated in $x$ and $t$**

Consider solutions in which the $x$- and $t$- dependence is *separated* ie we write $\psi(x, t) = \phi(x) \times T(t)$.

(i) Show that

$$\frac{1}{T(t)} i\hbar \frac{dT(t)}{dt} = \frac{1}{\phi(x)} \left( -\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} \right) + V(x) \tag{11}$$

and explain why each side of this equation must equal the same constant "$A$".

(ii) Solve the $T$-equation for $T(t)$ given that $T(0) = 1$. Show that if $A$ is real, $| \psi(x, t) |^2$ is independent of $t$. What is the frequency $\omega$ of the wave in terms of $A$? Assuming the Einstein relation $E = \hbar\omega$, find $E$ in terms of $A$, and obtain an expression for the average value of $x$. Such solutions are called *stationary state solutions*: why? Do all wavefunctions have to satisfy the TISE?

(iii) Suppose $V$ depends on $t$ as well as on $x$: $V(x, t)$. Will such a separation of the $x$ and $t$ variables be possible, in general? Can you invent a $V(x, t)$ for which it would be mathematically possible (even if not physically sensible)?

(iv) Returning to the case $V(x)$, suppose $A$ is in fact complex, $A = E - i\Gamma/2$. Show that the total (integrated over $x$) probability decays exponentially with a half-life of $(\hbar \ln 2)/\Gamma$. Suggest a physical problem in which such a solution might be useful.

# 3 Particle in a Box

1. **Necessary integrals**

   You will need certain integrals repeatedly over the next few weeks. They are given here; make sure that you can do them and then keep this piece of paper handy.

   $$\int_0^a \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{a}{2}, & \text{if } n = m; \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

   $$\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{2an}{\pi(n^2-m^2)}, & \text{if } n+m \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \tag{13}$$

2. **Particle in a box: average values**

   Consider the particle in the infinitely deep square well potential ($V = 0$ for $0 < x < a$, $V = \infty$ for $x \leq 0, x \geq a$).

   (i) Show that the allowed energy values are $E_n = \hbar^2 n^2 \pi^2 / 2ma^2$ for $n = 1, 2, \ldots$ and that the associated normalised eigenfunctions are

   $$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{14}$$

   Why is there no state with $E = 0$? What does it mean to say that the $\phi_n$ are orthogonal?

   (ii) Show qualitatively by means of a sketch that the eigenfunctions $\phi_1(x)$ and $\phi_2(x)$ are orthogonal.

   (iii) For a particle with energy $E_1$, calculate the quantum-mechanical expectation value of $x$, denoted by $\langle x \rangle$.

   (iv) Without working out any integrals, show that $\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - a^2/4$. Hence find $\langle (x - \langle x \rangle)^2 \rangle$ using the result

   $$\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}. \tag{15}$$

   (v) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical averages values $\langle x \rangle_c$ and $\langle (x - \langle x \rangle_c)^2 \rangle_c$, and show that for high values of $n$ the quantum and classical results tend to each other.

3. **†Superposition of eigenfunctions**

   Suppose the state is described at time $t = 0$ by the wavefunction

   $$\psi(x, t = 0) = \frac{1}{\sqrt{2}} (\phi_1(x) + \phi_2(x)) \tag{16}$$

   i) Show that $\psi$ is correctly normalized.

ii) Show that this is not an energy eigenfunction. What are the possible results of a measurement of the energy of the particle, what are the corresponding amplitudes, and what are the corresponding probabilities? What do you expect the expectation value of the energy to be?

iii) Repeat (ii) but with the wavefunction

$$\psi'(x, t=0) = \frac{1}{\sqrt{2}}\left(\phi_1(x) + e^{i\theta}\phi_2(x)\right) \tag{17}$$

iv) Reverting to $\psi$, explain why at subsequent times the wavefunction is given by

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\phi_1(x)e^{-iE_1t/\hbar} + \phi_2(x)e^{-iE_2t/\hbar}\right) \tag{18}$$

Does the outcome of a measurement of the energy of the particle depend on when the measurement is made?

v) Show that

$$|\psi(x,t)|^2 = \frac{1}{a}\left\{\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos\omega t\right\} \tag{19}$$

where $\omega = (E_2 - E_1)/\hbar = 3E_1/\hbar$. Make rough sketches of $|\psi|^2$ for $t = 0$, $t = h/12E_1$, $t = h/6E_1$, $t = h/4E_1$. Does the outcome of a measurement of the position of the particle depend on when the measurement is made?

vi) Given that

$$\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx = -\frac{8a^2}{9\pi^2}, \tag{20}$$

show that a particle with this wavefunction has $\langle x\rangle = a/2$ - $(16a/9\pi^2)\cos\omega t$. Discuss the connection between this result and the sketches of $|\psi|^2$.

vii) What is the value of $\omega$ for an electron confined to a distance comparable to the size of an atom (say $10^{-10}$ m)? What is the wavelength of radiation having this (circular) frequency?

# 4 Operators, Expectation Values, Conservation Laws

1. **Hermitian Operators**

   Why are dynamical quantities (energy, momentum ...) represented by Hermitian operators in quantum mechanics?

   The Hermitian conjugate $A^\dagger$ of a differential operator $A$ is defined via its matrix elements between arbitrary wavefunctions $\phi_1$ and $\phi_2$,

$$\int_{-\infty}^{\infty}\phi_1^*(x)A^\dagger\phi_2(x)dx \stackrel{def}{=} \int_{-\infty}^{\infty}\left(A\phi_1(x)\right)^*\phi_2(x)dx \tag{21}$$

provided $\phi_1$ and $\phi_2$ vanish at $x = \pm\ \infty$. Show that

$$\left(\frac{\partial}{\partial x}\right)^{\dagger} = -\frac{\partial}{\partial x} \tag{22}$$

(you will need to do an integration by parts - see Rae p67,68) and

$$\left(\frac{\partial^2}{\partial x^2}\right)^{\dagger} = \frac{\partial^2}{\partial x^2} \tag{23}$$

Deduce from (22) that the momentum operator $-i\hbar(\partial/\partial x)$ is Hermitian and from (23) that the kinetic energy operator is Hermitian.

2. **Eigenfunctions**

   (i) Is $e^{ipx/\hbar} + e^{-ipx/\hbar}$ an eigenfunction of momentum? Is it an eigenfunction of kinetic energy?

   (ii) Is $\mathrm{e}^{-|x|/a}$ an eigenfunction of momentum? (Careful: a sketch and some thought is the best approach).

3. **†Probability current density and the 1-D barrier**

   Derive the continuity equation relating the rate of change of probability density $\psi^*\psi$ to the gradient of a probability current density $j$, and find the expression for $j$. Find $j$ for the plane wave solution $\psi(x,t) = A\ e^{ikx-i\omega t}$ and express your answer in terms of the particle velocity $p/m$. [Note: $A$ is in general complex].

   Particles of mass $m$ and energy $E$ are incident from the region $x < 0$ on the "finite step" potential $V(x) = 0$ for $x \leq 0$, $V(x) = V_0$ for $x > 0$, with $V_0 > E$.

   (i) Explain why the solution of the time independent Schrodinger equation in the region $x \leq 0$ may be taken to have the form $\phi_1(x) = e^{ikx} + re^{-ikx}$ where $k = (2mE/\hbar^2)^{\frac{1}{2}}$, and why the solution in the region $x > 0$ has the form $\phi_2(x) = ae^{-Kx}$ where $K = [2m(V_0 - E)/\hbar^2]^{\frac{1}{2}}$.

   (ii) By imposing suitable boundary conditions at $x = 0$ show that

$$r = \frac{k - iK}{k + iK}, \quad a = \frac{2k}{k + iK}. \tag{24}$$

   (iii) Is your solution for the wavefunction an energy eigenstate? Is it a momentum eigenstate?

   (iv) Compute the probability current density in the two regions. Discuss your result.

   (v) Show that $r$ can be written as $e^{-2i\alpha}$ where $\alpha = \tan^{-1}(K/k)$, and hence show that

$$|\phi_1(x)|^2 = 4\cos^2(kx + \alpha). \tag{25}$$

   Make two separate sketches, for the special cases $E = V_0/2$ and $E = V_0$, of $|\phi_1|^2$, and of $|\phi_2|^2$, showing how they match at $x = 0$.

   (vi) Estimate the penetration distance into the region $x > 0$ for an electron with $V_0 - E = 1eV$.

4. †**Equations of motion for expectation values**

Prove that

$$\frac{d}{dt}\langle\psi|A|\psi\rangle = \frac{i}{\hbar}\langle\psi|[H,A]|\psi\rangle \tag{26}$$

where $A$ is any operator (not explicitly depending on $t$) representing an observable dynamical quantity. You can do this either by writing out $\langle\psi|A|\psi\rangle$ as an integral, and differentiating with respect to time or directly in the Dirac notation by using

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi\rangle &= H|\psi\rangle \\ -i\hbar\frac{\partial}{\partial t}\langle\psi| &= \langle\psi|H \end{aligned} \tag{27}$$

What is the corresponding result if the operator $A$ does depend explicitly on $t$?

5. †**Commutators and Consequences**

i) Verify that if the momentum operator $p$ is represented by $-i\hbar(\partial/\partial x)$ (in one dimension) acting on wavefunctions, then

$$[p,x]\phi(x) = -i\hbar\phi(x) \tag{28}$$

for any differentiable wavefunction $\phi(x)$, where $[A,B]$ means $AB - BA$.

ii) Find $[p, V(x)]$.

iii) For any operators $A, B$, verify that

$$[A, B^2] = [A,B]B + B[A,B] \tag{29}$$

For $H = \frac{p^2}{2m} + V(x)$ use (29) together with your results for i) and ii) to show that

$$\begin{aligned} [H,x] &= -i\hbar\frac{p}{m} \\ [H,p] &= i\hbar\frac{dV}{dx} \end{aligned} \tag{30}$$

iiiA) Alternatively, if you're not happy with iii) use the differential operator representation $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ to calculate the commutators (30) directly.

iv) Use the commutators (30) and the equation of motion (26) to show that

$$\begin{aligned} \frac{d}{dt}\langle x\rangle &= \langle\frac{p}{m}\rangle \\ \frac{d}{dt}\langle p\rangle &= -\langle\frac{dV}{dx}\rangle. \end{aligned} \tag{31}$$

v) Let $V(x) = \frac{1}{2}m\omega^2 x^2$ (ie the S.H.O. potential). Plug this into (31), solve the resulting differential equations and show that $\langle x\rangle$ has the same time dependent behaviour as $x$ does classically.

6. ††**Relation to Classical Eqns of Motion**

   What is the relationship between the results (31) and the classical equations of motion? In the classical mechanics of one particle in a potential what information do we need to specify at time $t = 0$ to have a well-defined problem (recall, in classical physics the equations of motion are second order in time dervatives)? Are the equations of motion of classical mechanics deterministic? In the quantum physics of one particle in a potential how much initial information do you have to give to have a well-defined problem? Do we have to specify less or more initial information in the quantum case? Is the time-dependent Schrodinger equation a deterministic equation? Why is this consistent with the probabalistic nature of QM?

7. ††**Two Particles**

   The Hamiltonian for two particles of mass $m$ moving in one dimension interacting via their mutual potential energy $V(x_1 - x_2)$ is given by

   $$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_1 - x_2) \tag{32}$$

   where $x_1$ and $x_2$ are the coordinates of the two particles. Show that the total momentum of the two particles is conserved. [Hint: the total momentum operator $P$ is $P = p_1 + p_2$ where $p_1 = -i\hbar\frac{\partial}{\partial x_1}$ and similarly for $p_2$.]

8. ††**Eigenvalues and Eigenfunctions of Hermitian Operators**

   In Dirac's notation if $Q$ is a Hermitian operator then $|v\rangle = Q|u\rangle$ implies $\langle v| = \langle u|Q$. Eigenstates of $Q$ are labelled by their eigenvalues $q_1, \ldots$ and satisfy $Q|q_n\rangle = q_n|q_n\rangle$.

   Show that $\langle u|Q|v\rangle = (\langle v|Q|u\rangle)^*$ and hence that the eigenvalues of $Q$ must be real.

   Show that when $q_n \neq q_m$ then $\langle q_n|q_m\rangle = 0$.

   Suppose that $|a\rangle$ and $|b\rangle$ are eigenstates of $Q$ with the *same* eigenvalue; then the previous proof of orthogonality fails. However it is always possible to construct linear combinations of $|a\rangle$ and $|b\rangle$, let's call them $|\tilde{a}\rangle$ and $|\tilde{b}\rangle$, which *are* orthogonal. Do it.

# 5 Measurement

1. **Change of state following a measurement**

   A particle in the infinite-sided box has the wavefunction (16). At a certain instant, its energy is measured and found to have the value $h^2/2ma^2$. What is the probability of finding the particle in the region $0 \leq x \leq a/2$ (i) before the energy measurement? (ii) after it? Explain the answers qualitatively, with the aid of a sketch.

2. **Compatibility**

Explain why it is possible to have quantum states for a particle in which the momentum and the kinetic energy both have well-defined values, but that this is possible for the momentum and the total energy only if the potential energy is a constant.

Find a wavefunction (not normalised) such that $p_x = -i\hbar\frac{\partial}{dx}, p_y = -i\hbar\frac{\partial}{\partial y}$ and $p_z = -i\hbar\frac{\partial}{\partial z}$ all have well-defined values, say $\hbar k_x, \hbar k_y$, and $\hbar k_z$ (i.e. you are looking for a wavefunction for a particle with definite momentum (vector) $\hbar\mathbf{k}$). Why can all three components of momentum have well-defined values?

Two operators $A$ and $B$ do not commute. Is it true that

$$[A, B]|\psi\rangle \neq 0 \tag{33}$$

for any state $\psi$?

3. **Uncertainty relations**

As a simple example of a time-independent wavepacket, consider the function

$$\phi(x) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx}dk \tag{34}$$

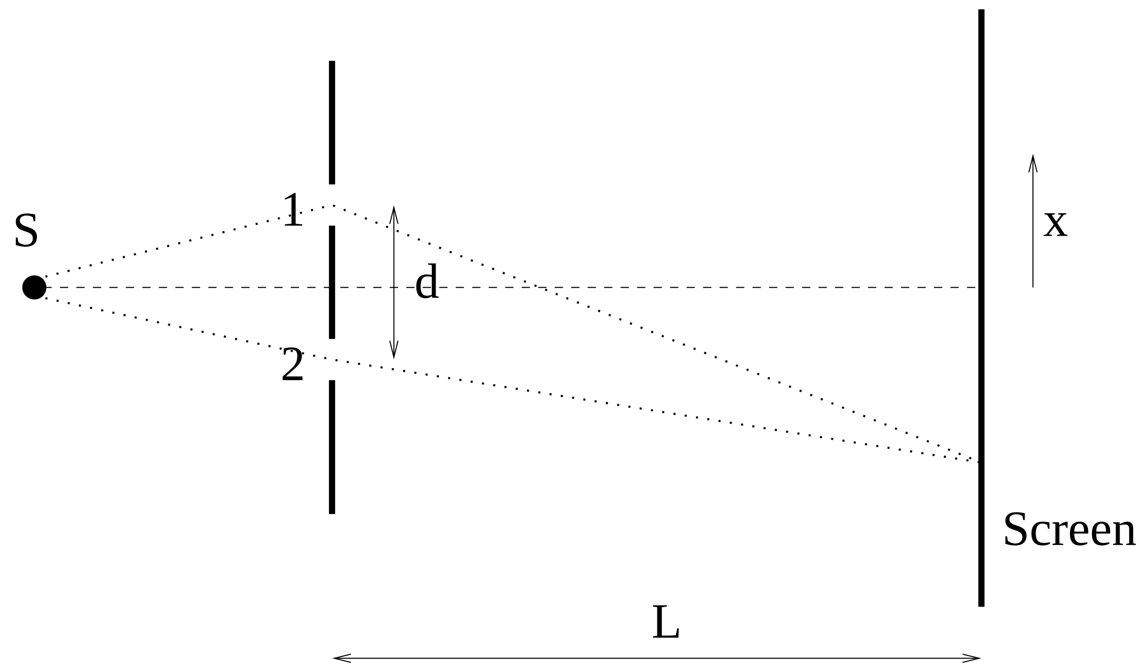
which may be regarded as a superposition of (complex) waves $e^{ikx}$ with different $k$'s, lying within $\Delta k$ on either side of a central value $k_0$. Evaluate this integral and show that

$$|\phi(x)|^2 = \frac{\sin^2(\Delta k.x)}{(\Delta k.x)^2}. \tag{35}$$

Sketch $|\phi(x)|^2$ versus $x$ (recall that $\Delta k$ is the spread in the wavenumbers of the packet). $|\phi(x)|^2$ is mostly concentrated in the region bounded by its first zeros on either side of the origin; if the size of this region is denoted by "$\Delta x$", show that "$\Delta x$" $\Delta k = 2\pi$. Relate this to the uncertainty relation $\Delta x\Delta p \geq \frac{1}{2}\hbar$.

[The reason we used quotes in "$\Delta x$" is that it is not quite the same as the mathematically precise definition $\Delta x = [\langle(x - \langle x\rangle)^2\rangle]^{\frac{1}{2}}$].

4. †**Two-Slit Interference**




Let the amplitude for a particle from source $S$ to reach slit 1 be $\langle 1|S\rangle$, to get from slit 1 to point $x$ on the screen $\langle x|1\rangle$ etc. Assume each slit is infinitely narrow but that if a particle hits the slit it goes through with amplitude 1.

i) Write down expressions for the amplitude for a particle to leave $S$ and reach the point $x$ via slit 1, via slit 2, and via both slits. Explain why the result of measuring the number of particles arriving at the screen qualitatively differs for two open slits compared to one open slit. What happens to the distribution of particles on the screen if both slits are open but there is a measuring device on the slits detecting which slit the particle goes through? Does the distribution on the screen depend on whether we read the output of the measuring device or not? Why? When no such measuring device is present is it correct to say that particles go through either slit 1 or slit 2? (You are **strongly** advised to read Chapter 1 of Feynman's *Lectures on Physics, Vol III.*)

ii) Now assume that the source $S$ is infinitely far away from the slits (so that the probability amplitudes for the particles at slits 1 and 2 are equal and in phase). Given that the amplitude for a particle of momentum $\mathbf{p}$ starting at $\mathbf{y}$ to end at $\mathbf{x}$ is

$$\langle \mathbf{x}|\mathbf{y}\rangle = \frac{1}{|\mathbf{x}-\mathbf{y}|}e^{i\mathbf{p}.(\mathbf{x}-\mathbf{y})/\hbar}. \tag{36}$$

compute exactly the *probability distribution* $P(x)$ for particles arriving at the screen when both slits are open.

iii) Now simplify $P(x)$ in the regime $L \gg d$ and $L \gg x$.

5. †The eigenstates of two commuting operators $A$ and $B$ are denoted $|a,b\rangle$ and satisfy the eigenvalue equations $A|a,b\rangle = a|a,b\rangle$ and $B|a,b\rangle = b|a,b\rangle$. A system is set up in the state

$$|\psi\rangle = N\left(|1,2\rangle + |2,2\rangle + |1,3\rangle\right) \tag{37}$$

What is the value of the normalization constant $N$?

A measurement of the value of $A$ yields the result 1. What is the probability of this happening? What is the new state $|\psi'\rangle$ of the system?

Then a measurement of the value of $B$ yields the result 2. What is the probability of this happening? What is the new state $|\psi''\rangle$ of the system?

Given that the system starts in the state $|\psi\rangle$ and then $A$ is measured and then $B$ is measured what is the probability that it ends up in the state $|\psi''\rangle$?

Repeat the above but measure $B$ first and then $A$. Comment on your results.

6. ††The operators $A$ and $B$ do not commute. The eigenstates of $A$ are $|0\rangle$ and $|1\rangle$ and satisfy $A|a\rangle = a|a\rangle$. The eigenstates of $B$ are

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle) \tag{38}$$

with eigenvalues $\pm 1$ respectively.

A system starts in the state $|0\rangle$. A measurement of $B$ yields the value $+1$. What is the probability of this and what is now the state of the system?

Now a measurement of $A$ is made. What are the possible outcomes and what state will the system be in afterwards?

Suppose the measurements of $A$ and $B$ are made in the opposite order. Discuss what happens.

Suppose alternating measurements of $A$ and $B$ are made *ad infinitum*. Discuss what happens.

7. ††**Meaning of the Uncertainty Relations**

One of the most important ideas in quantum mechanics is Heisenberg's uncertainty relation (HUR) between the position and momentum of a particle $\Delta x \Delta p \geq \hbar/2$. Some of the most popular of the many interpretations of this inequality are

(a) Position and momentum cannot be *measured* simultaneously to an arbitrary degree of accuracy.

(b) The exact position and momentum cannot be *known* simultaneously, with the HUR indicating the degree to which prior knowledge of one observable is lost in the act of measuring the conjugate quantity.

(c) The essentially classical concepts of position and momentum cannot be simultaneously *defined* in quantum mechanics.

(d) A particle cannot simultaneously *possess* an exact value for momentum and position.

(e) The results of a collection of position and momentum measurements have *statistical dispersions* which satisfy the HUR.

Think about the meaning and interconnection of these various statements and discuss with your peers and tutor!

8. †**The energy-time uncertainty relation**

In many books on Quantum Mechanics ones sees quoted without much discussion an uncertainty relation (UR) between energy and time of the form

$$\Delta E \Delta t \geq \hbar/2. \tag{39}$$

But there is a sublety with this in QM. In class we derived the general uncertainty relation which follows from the non-commutativity $[\hat{A}, \hat{B}] \neq 0$ of the two hermitian operators $\hat{A}$ and $\hat{B}$ which represent the physical observables $A$ and $B$. In QM we certainly have an energy operator – it's just the Hamiltonian $H$ – but we *do not have an operator for time*. Indeed time in QM is *just a parameter* and not an observable. Thus the status of the energy-time UR differs from that of other UR's.

One way to derive a well-defined form of the energy-time UR involves the general relation $\Delta A \Delta B \geq \frac{1}{2}|\langle [A, B] \rangle|$ derived in lectures. By taking $B = H$, the Hamiltonian of the system, but keeping $A$ arbitrary (apart from the assumption that both $A$ and $H$ have no *explicit* time dependence), show that the above equation together with Eqn.(26) of the problem set implies

$$\frac{\Delta A}{|d\langle A \rangle/dt|} \Delta H \geq \hbar/2. \tag{40}$$

*Defining* the uncertainty in time as

$$\Delta t = \frac{\Delta A}{|d\langle A \rangle/dt|}, \tag{41}$$

then leads to the $\Delta E \Delta t \geq \hbar/2$ relation. (The interpretation of (41) is that the "uncertainty in time" is expressed as the average time taken for the expectation of some operator $A$ to change by its standard deviation, and is physically reasonable as it gives the shortest time scale on which we will be able to notice changes by using $A$ in state $|\psi\rangle$.)

As an application of the energy-time UR, consider the excited '2p' state in hydrogen which decays to the ground state with lifetime $1.6 \times 10^{-9} s$. Approximately what value do you expect for the intrinsic uncertainty in the energy of the emitted photon (the so-called 'natural width' of the emission)?

[††There is another useful way of thinking about the meaning of the energy-time uncertainty relation involving Fourier transforms which is well covered in Question 5 of Problem Set 5 of the 2nd year Mathematical Methods course. Make sure you understand this problem.]

# 6 The Simple Harmonic Oscillator

1. †**Eigenfunctions, eigenvalues**

   The eigenvalue equation for the SHO is

   $$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\phi = E\phi \tag{42}$$

   where $\omega$ is the classical frequency of the oscillator.

   i) Show that by making the change of variables $x = y\sqrt{\frac{\hbar}{m\omega}}$ (42) becomes

   $$\frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial y^2} + y^2\right)\phi = E\phi \tag{43}$$

   ii) Show that $\phi(y) = e^{-\frac{y^2}{2}}$ satisfies the eigenvalue equation for the SHO and find $E$. In fact this is the ground state. Show that the correctly normalized wavefunction is

   $$\phi_0(x) = \left(\frac{1}{\pi a^2}\right)^{\frac{1}{4}}\exp(-x^2/2a^2) \quad \text{where} \quad a^2 = \hbar/m\omega. \tag{44}$$

   iii) Find the expectation values of $x$, $x^2$, $p$ and $p^2$ for a particle in the ground state. [Hint: for $\langle p^2\rangle$ use $p^2/2m + \frac{1}{2}m\omega^2x^2 = E$].

   iv) Defining $\Delta x = [\langle(x - \langle x\rangle)^2\rangle]^{\frac{1}{2}}$, $\Delta p = [\langle(p - \langle p\rangle)^2\rangle]^{1/2}$ show that in this case $\Delta x\Delta p = \frac{1}{2}\hbar$. Comment on this result.

   You will need the integrals

   $$\int_{-\infty}^{\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}; \qquad \int_{-\infty}^{\infty} x^2e^{-\alpha x^2}dx = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}. \tag{45}$$

2. **Pictures**

   On the same diagram, plot carefully (paying particular attention to the points of intersection of the various curves)

   i) $\phi_0(x)$ from 44 versus $x$, indicating where $\frac{d^2\phi_0}{dx^2} = 0$

   ii) the potential energy $\frac{1}{2}m\omega^2x^2$ versus $x$

   iii) the total energy $E = \frac{1}{2}\hbar\omega$ versus $x$

   iv) the region in $x$ to which the particle would be confined according to classical mechanics.

   Why do the $x$-values such that $\frac{d^2\phi_0}{dx^2} = 0$ lie at the limits of the classically allowed region?

3. †**Spectrum**

   The form (43) strongly suggests that we should try factorizing the differential operator. So define

$$
\begin{aligned}
D^\dagger &= \frac{1}{\sqrt{2}}\left(-\frac{d}{dy}+y\right) \\
D &= \frac{1}{\sqrt{2}}\left(\frac{d}{dy}+y\right)
\end{aligned}
\tag{46}
$$

   i) Show that

$$
\begin{aligned}
D^\dagger D f &= \frac{1}{2}\left(-\frac{d^2 f}{dy}+y^2 f-f\right) \\
D\,D^\dagger f &= \frac{1}{2}\left(-\frac{d^2 f}{dy}+y^2 f+f\right)
\end{aligned}
\tag{47}
$$

   and hence that (43) may be written

$$
\hbar\omega\left(D^\dagger D+\frac{1}{2}\right)\phi = E\phi \tag{48}
$$

   and that

$$
D^\dagger D - D\,D^\dagger = -1 \tag{49}
$$

   ii) Now *assume* that $\phi$ satisfies (48). Show that $\phi' = D\,\phi$ also satisfies (48) but with $E$ replaced by $E' = E - \hbar\omega$. (Most easily done by acting on (48) with $D$ and then using the commutator to reverse the order of $D$ and $D^\dagger$.)

   iii) Explain why there must be a $\phi_0$ satisfying $D\,\phi_0 = 0$. Writing this condition out explicitly gives a first order differential equation for $\phi_0$; solve it. To what value of $E$ does $\phi_0$ correspond?

   iv) Now show that if $\phi$ satisfies (48) then $\phi' = D^\dagger\phi$ also satisfies (48) but with $E$ replaced by $E' = E + \hbar\omega$.

   v) Now assemble everything to give the spectrum $E_n$ and a recipe for generating the eigenfunctions $\phi_n$. Write out the first three eigenfunctions explicitly and plot them on a graph.

   vi) Is the ground state wavefunction an even or odd function of $x$? How do the excited states behave under $x \to -x$? (This property is called the *parity* of the state.)

4. ††**A slicker way**

   Of course what we did in the previous question didn't really depend on a differential equation; just on the properties of some operators. So actually it can be done at a more abstract level without reference to differential operators at all. So let

$$
H = \frac{p^2}{2m}+\frac{m\omega^2 x^2}{2}
$$

$$
\begin{aligned}
A &= \sqrt{\frac{m\omega}{2}}x + i\frac{p}{\sqrt{2m\omega}} \\
A^\dagger &= \sqrt{\frac{m\omega}{2}}x - i\frac{p}{\sqrt{2m\omega}}
\end{aligned} \tag{50}
$$

i) Show that $[A, A^\dagger] = \hbar$ and $H = \omega A^\dagger A + \hbar\omega/2$.

ii) Show that $[H, A] = -\hbar\omega A$ and $[H, A^\dagger] = \hbar\omega A^\dagger$

iii) Assume that $H|\psi\rangle = E|\psi\rangle$; show that $|\psi'\rangle = A|\psi\rangle$ satisfies $H|\psi'\rangle = (E - \hbar\omega)|\psi'\rangle$. Deduce that there must be a state $|0\rangle$ satisfying $A|0\rangle = 0$ and give its energy.

iv) Show that $|\psi'\rangle = A^\dagger|\psi\rangle$ satisfies $H|\psi'\rangle = (E + \hbar\omega)|\psi'\rangle$. Now you can deduce the spectrum $E_n$ and how the corresponding states $|n\rangle$ are related to $|0\rangle$.

v) It's easy to compute the correct normalization too. Being careful we have

$$
|n+1\rangle = C_n A^\dagger |n\rangle \tag{51}
$$

where the states are all normalised and $C_n$ is a constant. Show that

$$
1 = \langle n+1|n+1\rangle = |C_n|^2\hbar(n+1). \tag{52}
$$

This tells you $C_n$; find the constant $N_n$ such that

$$
|n\rangle = N_n (A^\dagger)^n |0\rangle \tag{53}
$$

is correctly normalized.

# 7 Barriers and Wavepackets

1. †**Momentum probability distribution I**

   Consider the following two normalised wavefunctions

   $$
   \phi_1(x) = \frac{1}{\sqrt{a}}\exp(-|x|/a), \quad \phi_2(x) = e^{ikx}\frac{1}{\sqrt{a}}\exp(-|x|/a). \tag{54}
   $$

   Calculate $\langle x\rangle$ and $\langle p\rangle$ for both of these wavefunctions.

   Sketch $|\phi_1|^2$ and $|\phi_2|^2$ versus $x$ for fixed $a$.

   The momentum probability amplitude corresponding to a position probability amplitude $\phi(x)$ is (see Question 7.2)

   $$
   \tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\phi(x)dx \tag{55}
   $$

   Evaluate $\tilde{\phi}_1(p)$ and $\tilde{\phi}_2(p)$ and sketch both as a function of $p$, for fixed $a$. Give an informal (qualitative) definition of the "spreads" of $|\phi_1(x)|^2$ in $x$ and of $|\tilde{\phi}_1(p)|^2$ in $p$. Show that their product is of order $\hbar$.

2. ††**Momentum probability distribution II**

   A particle is in the state $|\psi\rangle$. Describe in words what information the amplitude $\langle x|\psi\rangle$ contains; what do we usually call this amplitude?

   Let $|p\rangle$ be an eigenstate of the *momentum* operator $\hat{p}$ (contrary to our usual practice we need a hat on the operator here to avoid getting confused) so that $\hat{p}|p\rangle = p|p\rangle$. Describe in words what information the amplitude $\langle x|p\rangle$ contains. Explain why $\langle x|p\rangle \propto \exp(ipx/\hbar)$.

   Describe in words what information the amplitude $\langle p|x\rangle$ contains and give its form as a function of $p$ and $x$.

   Describe in words what information the amplitude $\langle p|\psi\rangle$ contains and explain why
$$\langle p|\psi\rangle \propto \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\psi\rangle, \tag{56}$$
   which, up to a constant factor, is (55). Confirm that the factor $1/\sqrt{2\pi\hbar}$ ensures that
$$\int_{-\infty}^{\infty} |\tilde{\phi}(p)|^2 dp = 1 \tag{57}$$
   if $\phi(x)$ is normalised. (You'll need to use the Dirac delta function covered in the Mathematical Physics lectures.)

3. †**The 1-D finite well**

   A particle of mass $m$ is in a "finite well" potential
$$\begin{aligned} V(x) &= V_0 \quad \text{for} \quad |x| > a \\ &= 0 \quad \text{for} \quad |x| \leq a \end{aligned} \tag{58}$$
   where $V_0$ is positive. It may be shown that for such a potential, which satisfies the condition $V(-x) = V(x)$, each energy eigenfunction has a definite parity, which can be either *even* ($\psi(-x) = \psi(x)$) or *odd* ($\psi(-x) = -\psi(x)$). (We'll meet parity again next term.)

   (i) Assuming that the well parameters $V_0$ and $a$ are such that these bound states are possible, sketch the form of the wavefunctions for the first two bound states ($E < V_0$) of even parity, and for the first two bound states of odd parity (*not* exact wavefunctions; just the right number of wiggles, the right parity, and the right behaviour at the edge of the well and as $x \to \pm\infty$).

   (ii) The bound state wavefunction for even parity states has the form
$$\psi(x) = A\cos kx \quad \text{for} \quad 0 \leq x \leq a \tag{59}$$
$$\phantom{\psi(x)} = Be^{-Kx} \quad \text{for} \quad x \geq a, \tag{60}$$
   where $k = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$ and $K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$. Write down $\psi(x)$ for $-a \leq x \leq 0$ and for $x \leq -a$. By applying the boundary condition at $x = a$, show that the allowed $k$ (i.e. $E$) values are determined by the roots of the equation
$$(v^2 - s^2)^{\frac{1}{2}} = s\tan s \tag{61}$$

where $v = [2mV_0a^2/\hbar^2]^{\frac{1}{2}}$ and $s = ka$. Check that $v$ and $s$ are dimensionless. Why is it not necessary to consider the boundary condition at $x = -a$ as well? This equation (61) can be solved for $s$, given $v$, by a graphical method. For positive $s$, sketch the function $s \tan s$ versus $s$, and the function $(v^2 - s^2)^{\frac{1}{2}}$ versus $s$. Where these curves meet, you have a solution for $s$. Show (a) that there is always *one* solution, whatever the value of $v$; (b) that a second "even" bound state is possible as soon as $v$ becomes greater than $\pi$.

(iii) Write down a similar form of the wavefunction for odd-parity states, and show that the energy eigenvalue condition is

$$(v^2 - s^2)^{\frac{1}{2}} = -s \cot s \tag{62}$$

Sketch both sides of (62) as a function of $s$, and show that there is no odd-parity bound state if $v < \pi/2$.

(iv) Explain why the number of bound states (even + odd) is given by the next integer greater than the value of $2v/\pi$ (which is called the "well parameter").

(v) The roots of (61) and (62) can be found by (for example) using the Find Root command on Mathematica - or by trial and error. Take $m$ = electron mass, $a = 0.5$ nm and $V_0 = 20$ eV. How many bound states are there?

Verify that the two lowest roots for $s$ are $s = 1.44438$ and $s = 2.88685$ and find the corresponding eigenvalues in eV.

4. **†Barrier penetration and transmission**

A particle of mass $m$ is incident with energy $E < V_0$ from the region $x < 0$ on the finite potential barrier

$$\begin{aligned} V(x) &= 0 \quad \text{for} \quad x < 0, x > a \\ &= V_0 \quad \text{for} \quad 0 \le x \le a. \end{aligned} \tag{63}$$

Take the wavefunction in $x < 0$ to be

$$\psi_1 = e^{ikx} + Re^{-ikx}, \tag{64}$$

in $0 \le x \le a$ to be

$$\psi_2 = Ae^{Kx} + Be^{-Kx} \tag{65}$$

and in $x > a$ to be

$$\psi_3 = Ce^{ikx} \tag{66}$$

where $K^2 = \frac{2m}{\hbar^2}(V_0 - E), k^2 = 2mE/\hbar^2$.
i) Is the wavefunction an energy eigenstate?
ii) Is the wavefunction a momentum eigenstate?
iii) From the boundary conditions at $x = 0$ deduce that

$$2 = A(1 - \frac{iK}{k}) + B(1 + \frac{iK}{k}) \tag{67}$$

and from the boundary conditions at $x = a$ deduce that

$$A = \frac{1}{2}e^{-Ka}(1 + \frac{ik}{K})e^{ika}C \tag{68}$$

and

$$B = \frac{1}{2}e^{Ka}(1 - \frac{ik}{K})e^{ika}C. \tag{69}$$

Substitute these expressions for $A$ and $B$ into the previous equation to show that

$$C = \frac{2e^{-ika}}{\left[2\cosh Ka - i\left(\frac{k}{K} - \frac{K}{k}\right)\sinh Ka\right]} \tag{70}$$

Hence show that the transmission coefficient (defined as the transmitted flux divided by the incident flux) is

$$|C|^2 = \left(1 + \frac{(K^2 + k^2)^2}{4K^2k^2}\sinh^2 Ka\right)^{-1}, \tag{71}$$

which can also be written as

$$|C|^2 = \left(1 + \frac{\sinh^2[v^2(1 - E/V_0)]^{\frac{1}{2}}}{4(E/V_0)(1 - E/V_0)}\right)^{-1} \tag{72}$$

where $v$ is as defined in Q 1, $v = (2mV_0a^2/\hbar^2)^{\frac{1}{2}}$.

iv) Compute the probability flux *inside* the barrier, ie from $\psi_2$. [Hint: caution - $A$ and $B$ are complex!] Compare your result with part iii).

v) Show that if $E/V_0 \ll 1$ and $v \gg 1$, $|C|^2$ is given approximately by

$$|C|^2 \approx \frac{16E}{V_0}e^{-2v}. \tag{73}$$

This shows the characteristic *exponential tunnelling probability*: the amplitude for waves with $E < V_0$ is exponentially attenuated by the barrier (though of course classical particles wouldn't get through at all); it is analogous to the evanescent waves in optics (e.g. in total internal reflection).

Suppose $E = 1eV, V_0 = 6eV$ and $a = 1$nm. By what factor will $|C|^2$ change if $a$ increases to 1.1 nm?

The "Scanning Tunnelling Microscope" is just one application of quantum tunnelling - see G. Binnig and H. Rohrer Reviews of Modern Physics **59** (1987) 615 (their Nobel lecture).

5. ††**Transmission resonances**

In Question 4 above, imagine the energy gradually increasing until it becomes equal to $V_0$. What is $|C|^2$ when $E = V_0$? Now suppose $E$ becomes greater than $V_0$. Then $K^2$ becomes negative, $K \to i|K|$ (or maybe $-i|K|$?) and $\sinh^2 Ka \to (i \sin|K|a)^2$, so

$$|C|^2 \to \left(1 + \frac{\sin^2[v^2(E/V_0 - 1)]^{\frac{1}{2}}}{4(E/V_0)(E/V_0 - 1)}\right)^{-1} \tag{74}$$

(if you don't like this, you can of course repeat the whole calculation from scratch ...).

Show that this new $|C|^2$ is equal to unity when $\left[\frac{2m}{\hbar^2}(E - V_0)\right]^{\frac{1}{2}} = n\pi/a$. What does the wave in the region $0 \leq x \leq a$ look like at these values of $E$?

6. ††**Time dependent packets; dispersion**

A simple example of a time-dependent wave packet is provided by a superposition of waves for which the *frequency is proportional to the wavenumber*: $\omega = ck$. Light, of course, is such a wave. Consider the packet

$$\phi(x,t) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_o+\Delta k} e^{ik(x-ct)}dk \tag{75}$$

(Note that $\phi(x,0)$ is the packet in Question 5.3).

(i) Evaluate the integral and show that

$$|\phi(x,t)|^2 = \frac{\sin^2[\Delta k(x-ct)]}{[\Delta k(x-ct)]^2} \tag{76}$$

(as in Q5.3). For fixed $t$, at what $x$ is $|\phi(x,t)|^2$ a maximum, and at what values of $x$ do the first zeros of $|\phi(x,t)|^2$ away from the maximum occur? Sketch $|\phi(x,t)|^2$ for fixed $t$ versus $x$. Describe how the packet moves along in $x$ as $t$ varies. Does the *shape* of the function $|\phi(x,t)|^2$ change?

Consider now the packet for fixed $x$, as $t$ varies. Where is the maximum as a function of $t$ for fixed $x$, and where do the first minima on either side of it occur? If the spread in the packet in time, "$\Delta t$", is defined as the distance between the first minima on either side of the central maximum, show that $\Delta\omega$ "$\Delta t$" $= 2\pi$, where $\Delta\omega = c\Delta k$. Relate this to $\Delta E\ \Delta t\ \geq \frac{1}{2}\hbar$.

(ii) A time-dependent free-particle (plane wave) solution of the 1-D Schrödinger equation is $\psi(x,t) = N\exp(ikx - iEt/\hbar)$ where $N$ is a normalization constant and $E = p^2/2m = \hbar^2k^2/2m = \hbar\omega$. It follows that for these waves the frequency $\omega$ is *not* proportional to $k$ but to $k^2$: $\omega = \hbar k^2/2m$. This makes a dramatic difference to the way a packet of these waves evolves with time: the packet does *not* maintain its shape, but "flattens out", a phenomenon called *dispersion* (of the packet). Consider the packet

$$\psi(x,t) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx - i\hbar k^2 t/2m}dk \tag{77}$$

(note that $\psi(x,0)$ is again the packet from Q5.3). This time the integral can *not* be done in terms of elementary functions. However, if $k_0 \gg \Delta k$ and the $t$-term in the exponent is "not too big" we can expand "$k^2$" about the point $k = k_0$ by a Taylor series: $k^2 = k_0^2 + (k - k_0).2k_0$, and we are back to only a *linear* term in the exponent, which can be integrated exactly. Show that in this approximation

$$|\psi(x,t)|^2 = \frac{\sin^2[\Delta k(x - vt)]}{[\Delta k(x - vt)]^2} \tag{78}$$

where $v = \hbar k_0/m$, and describe how this packet moves as $t$ varies.