PHAS1202 - Atoms, Stars and The Universe
Problem Solving Tutorial Sheet 2
Model Answers

Objectives:

1. Perform a dimensional analysis on Planck's constant.
2. Gain practise with normalising wave-functions and calculating their properties, including expectation values.
3. Practise using the TISE to calculate energies for an unfamiliar potential.
4. Get a practise with the integration and differentiation which arises very often in problems of this kind.

Useful definitions

Planck's constant h is 6.6×10^{-34} Js (2 s.f.).

The time-independent Schrödinger equation (TISE) for a particle in one-dimensional potential $V(x)$ with mass m, energy E with wave-function $\psi(x)$ is

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

1: The dimensions of h

In Physics, studying the dimensions of quantities can be a very important way of discovering relationships (or potential relationships) between them. Here we will consider the dimensions arising in Planck-Einstein's photon energy law and Bohr's atomic model.

1.a) Write down the dimensions of Planck's constant h in terms of the fundamental quantities of mass M, length L and time T, taking the definition of h to be through Planck and Einsteins relationship $E = hf$. Why does $\hbar$ have the same dimensions as h?

1.b) Find the dimensions (in terms of mass M, length L and time T) of angular momentum and show that these are the same as those of Plancks constant h. Hence show that Bohrs quantisation assumption $L = n\hbar$ (where L is the angular momentum and n is an integer) is dimensionally consistent.

We shall use square brackets to denote units, e.g. $[h]$ refers to the units of h.

1.a) From Planck-Einstein's formula:

$$[h] = \frac{[E]}{[f]}$$

The units of frequency are Hz or s^-1, hence

$$[f] = [T]^{-1}$$

To express the units of energy in terms of mass $[M]$, length $[L]$ and time $[T]$ we can refer to any equation for energy which contains only these quantities. Kinetic energy will do:

$$\text{K.E} = \frac{1}{2}mv^2$$

and hence

$$[E] = [M][L]^2[T]^{-2}$$

Thus

$$[h] = \frac{[E]}{[f]} = [M][L]^2[T]^{-1}.$$

$\hbar$ has the same dimensions as h since $\hbar = h/2\pi$ and 2π is dimensionless.

1.b) To find the dimensions of angular momentum we can use

$$l = rp$$

where p is momentum. The dimensions of momentum are $[M][L][T]^{-1}$ from $p = mv$.

Hence

$$[l] = [L][M][L][T]^{-1} = [M][L]^2[T]^{-1}$$

Therefore the left-handside and the right-handside of Bohr's angular momentum assumption are both equal, and $\hbar$ has the same dimension as angular momentum.

2: Calculating properties of wave-functions

Normalise the following wave-functions; sketch the normalised wave-function and the corresponding probability density; use the normalised function to calculate the probability of finding a particle in region $0 \leq x \leq 1$; and compute the expectation value of position $\langle x \rangle$.

2a)

$$\psi_1(x) = \begin{cases} \cos(\pi x) & \text{if } -1.5 \leq x \leq 1.5 \\ 0 & \text{otherwise} \end{cases}$$

We need to find a new wavefunction

$$\tilde{\psi}_1(x) = a\psi_1(x)$$

such that

$$\int_{-\infty}^{\infty} a^2 \psi_1(x)^2 dx = 1$$

Thus

$$\int_{-1.5}^{1.5} a^2 \cos^2(\pi x) dx = 1$$

Use the trig identity:

$$\cos^2(x) = (1/2)(1 + \cos(2x))$$

and thus our integral is

$$\frac{a^2}{2} \int_{-1.5}^{1.5} (1 + \cos(2\pi x)) dx = \frac{a^2}{2} \left(\Big[x \Big]_{-1.5}^{1.5} + \frac{1}{2\pi} \Big[\sin(2\pi x) \Big]_{-1.5}^{1.5} \right)$$

$$= \frac{a^2}{2}((1.5 - (-1.5)) + \frac{1}{2\pi}(\sin(3\pi) - \sin(-3\pi)) = \frac{3a^2}{2} = 1$$

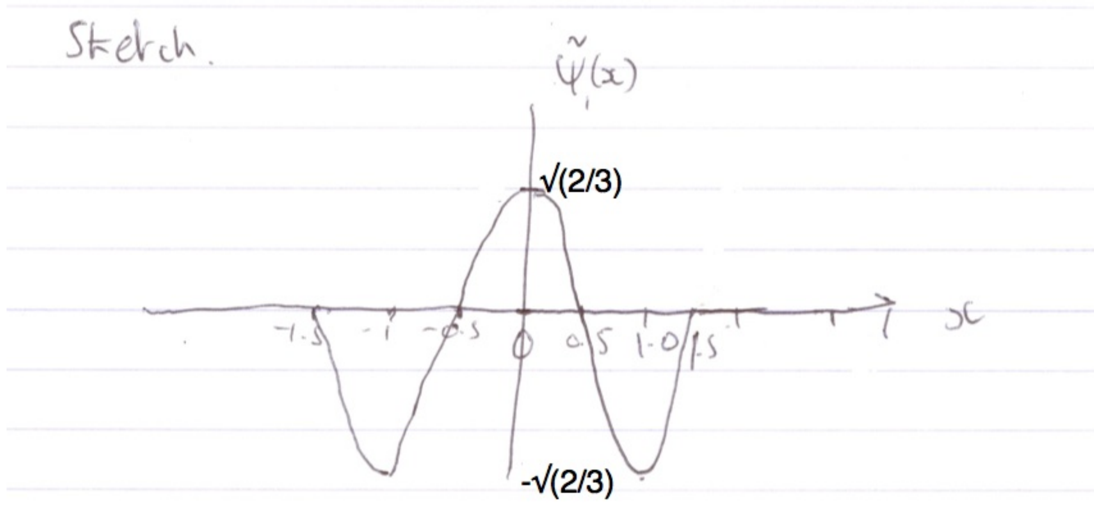
Hence

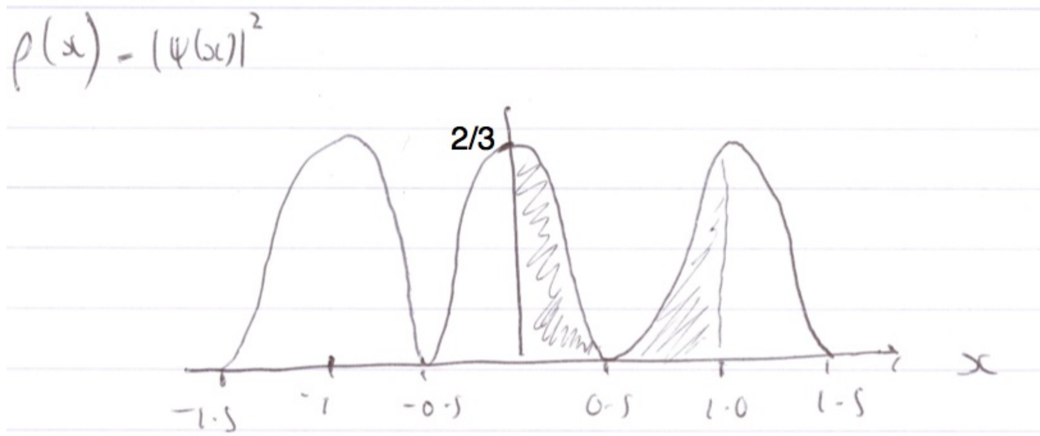
$$a = \sqrt{\frac{2}{3}}$$

and the normalised wave-function is:

$$\tilde{\psi}_1(x) = \begin{cases} \sqrt{\frac{2}{3}} \cos(\pi x) & \text{if } -1.5 \le x \le 1.5 \\ 0 & \text{otherwise} \end{cases}$$

Sketches:





To calculate the probability of finding the particle between $x = 0$ and $x = 1$ we use the normalised wavefunction and Born's rule:

$$\int_0^1 \tilde{\psi}_1(x)^2 dx = \frac{2}{3} \int_0^1 \cos^2(\pi x) dx$$

$$= \frac{2}{3} \int_0^1 \frac{1}{2} \left(1 + \cos(2\pi x)\right) dx = \frac{1}{3} \left(1 - 0 + 0 - 0\right) = \frac{1}{3}$$

As a visual check, the area is shaded in the sketch above, and indeed, corresponds to a third of the area under the graph.

Finally, we compute the expectation value of position $\langle x \rangle$

$$\langle x \rangle = \int_{-\infty}^{\infty} x \tilde{\psi}_1(x)^2 dx$$

$$= \frac{2}{3} \int_{-1.5}^{1.5} x \cos^2(\pi x) dx$$

This integral can be computed by integrating by parts, but there is a shortcut. $f(x) = x$ is an odd function, whereas $f(x) = \cos^2(\pi x)$ is an even function. Therefore $x\cos^2(\pi x)$ is an odd function. Given any odd function $f(x)$

$$\int_{-a}^{a} f(x) = 0$$

Since the area on each side of the x=0 line is exactly equal and opposite and cancels out and thus

$$\langle x \rangle = 0$$

2b)

$$\psi_2(x) = \begin{cases} \sin(2\pi x) & \text{if } -2 \le x \le 0 \\ \sin(\pi x) & \text{if } 0 \le x \le 2 \\ 0 & \text{otherwise} \end{cases}$$

Wave-functions can have different functional forms in different regions. This is an example of this. Let the normalised wavefunction be:

$$\tilde{\psi}_2(x) = a\psi_2(x) = \begin{cases} a\sin(2\pi x) & \text{if } -2 \le x \le 0 \\ a\sin(\pi x) & \text{if } 0 \le x \le 2 \\ 0 & \text{otherwise} \end{cases}$$

Note the same constant multiplies both sides. We are rescaling the entire function by the same factor.

The normalisation condition thus splits into two integrals:

$$a^2 \int_{-2}^{0} \sin^2(2\pi x)dx + a^2 \int_{0}^{2} \sin^2(\pi x)dx = 1$$

Let us consider the first integral and use a similar method as in part 3a:

$$\int_{-2}^{0} \sin^2(2\pi x)dx = \frac{1}{2}\int_{-2} (1 + \cos(4\pi x))dx$$
$$= \frac{1}{2}\left(\Big[x\Big]_{-2}^{0} + \frac{1}{4\pi}\Big[\sin(4\pi x)\Big]_{-2}^{0}\right) = \frac{0-(-2)}{2} + \frac{0-0}{8\pi} = 1$$

We integrate the second integral via a nearly identical calcuation and put it all together to find:

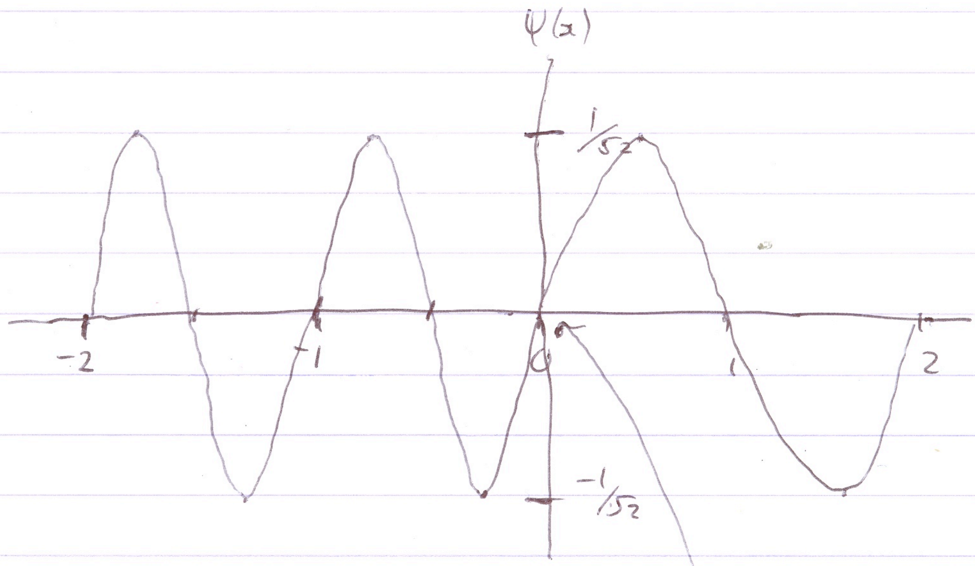
$$a^2 \int_{-2}^{0} \sin^2(2\pi x)dx + a^2 \int_{0}^{2} \sin^2(\pi x)dx = a^2(1+1) = 2a^2$$

and so $a = 1/\sqrt{2}$.

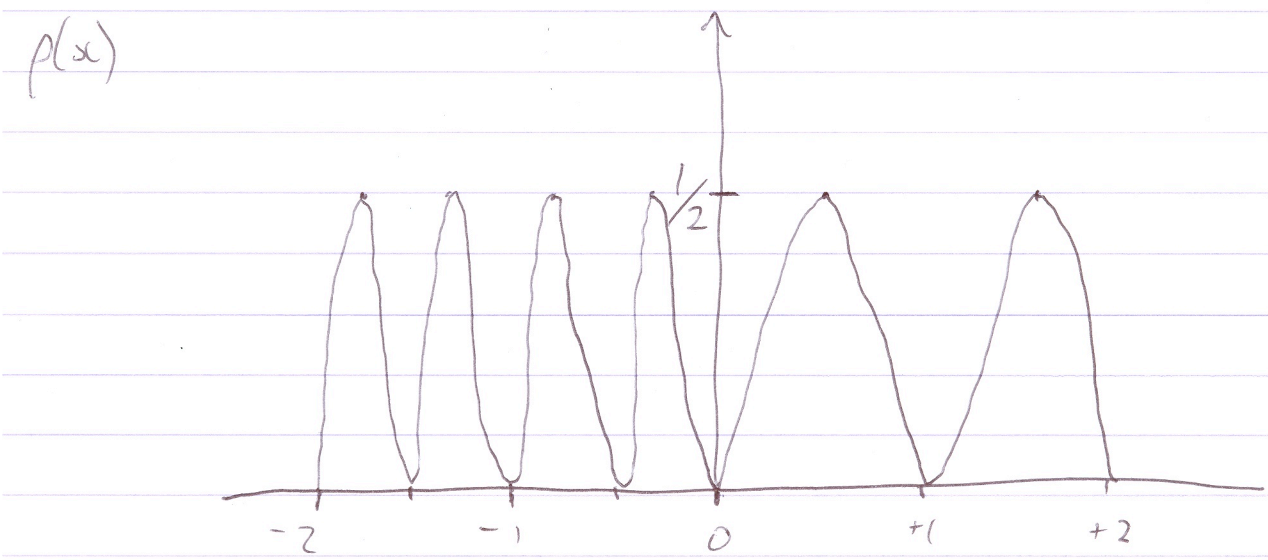
The normalised wavefunction is thus:

$$\tilde{\psi}_2(x) = \begin{cases} \frac{1}{\sqrt{2}} \sin(2\pi x) & \text{if } -2 \leq x \leq 0 \\ \frac{1}{\sqrt{2}} \sin(\pi x) & \text{if } 0 \leq x \leq 2 \\ 0 & \text{otherwise} \end{cases}$$

Sketch.



NB Here is a kink, a discontinuity in $\frac{d\psi}{dx}$ so this is not a physical wave function!



The probability that the particle is between 0 and 1 is:

$$\int_0^1 \tilde{\psi}_2(x)^2 dx = \frac{1}{2}\int_0^1 \sin^2(\pi x)dx = \frac{1}{4}.$$

The expectation value is $\langle x \rangle = 0$. We can calculate this via integration by parts over each region of the wavefunction. This is probably the most lengthy calculation of the PST but there are some tricks we can use to simplify it.

Let's start with the definition of expectation value:

$$\langle x \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 x dx$$

For the wavefunction in this question, this becomes:

$$\langle x \rangle = \frac{1}{2}\left(\int_{-2}^{0} x\sin^2(2\pi x)dx + \int_0^2 x\sin^2(\pi x)dx\right)$$

We use our trig identity for $\sin^2(x)$ to rewrite this:

$$\langle x \rangle = \frac{1}{4}\left(\int_{-2}^{0} x(1-\cos(4\pi x)dx + \int_0^2 x(1-\cos(2\pi x)dx\right)$$

Part of that integral is easy to evaluate, so let's do so:

$$\langle x \rangle = \frac{1}{4}\left(\int_{-2}^{0} xdx + \int_0^2 xdx - \int_{-2}^{0} x\cos(4\pi x)dx - \int_0^2 x\cos(2\pi x)dx\right)$$

We can solve the first two integrals using symmetry:

$$\int_{-2}^{0} xdx + \int_{0}^{2} xdx = \int_{-2}^{2} xdx$$

This is an integral over an odd function between limits symmetric about $x = 0$. It therefore evaluates to zero.

Therefore we can set that to zero in our expression. We now have:

$$\langle x \rangle = -\frac{1}{4}\left(\int_{-2}^{0} x\cos(4\pi x)dx + \int_{0}^{2} x\cos(2\pi x)dx\right)$$

Note that the two remaining terms have the form:

$$\int_{a}^{b} x\cos(n\pi x)dx$$

for integers a, b and n. So let's solve this general case. We use integration by parts:

$$\int_{a}^{b} uv'dx = [uv]_{x=a}^{x=b} - \int_{a}^{b} vu'dx$$

We can let $u = x$ and $v' = \cos(n\pi x)$. Then $u' = 1$ and $v = (1/n\pi)\sin(n\pi x)$.

Then

$$\int_{a}^{b} x\cos(n\pi x)dx = [x(1/n\pi)\sin(n\pi x)]_{x=a}^{x=b} - \int_{a}^{b} (1/n\pi)\sin(n\pi x)dx$$

If a and b are integers (as in our case) the first term is zero, since $\sin(n\pi = 0$ for any integer n. We then have

$$-\int_{a}^{b} (1/n\pi)\sin(n\pi x)dx = (1/n\pi)^2[\cos(n\pi x)]_{x=a}^{x=b}$$

In our case, a and b are *even* integers. $\cos(n\pi x) = 1$ if n is an even integer. Therefore,

$$\langle x \rangle = -\frac{1}{4}\left(\int_{-2}^{0} x\cos(4\pi x)dx + \int_{0}^{2} x\cos(2\pi x)dx\right) = -\frac{1}{4}(0+0) = 0$$

3: Which functions are valid wave-functions? (seen)

To represent a physical particle, wave-functions must be continuous and normalisable. Consider the following functions. Can they represent a wave-function for a physical system? If not, explain why.

3a)

$$f_1(x) = \sin(px/\hbar)$$

As we saw in lectures,

$$\int_{-\infty}^{\infty} \sin^2(px/\hbar)dx$$

diverges to infinity, and therefore this function cannot be normalised and cannot represent a physical state.

3b)

$$f_2(x) = \begin{cases} \cos(2\pi x) - \cos(\pi x) & \text{if } 0 \leq x \leq 2 \\ 0 & \text{otherwise} \end{cases}$$

Yes - this is a physical wavefunction. It is continuous, and normalisable, and so satisfies the criteria in the question.

Give yourself a bonus mark if you noted that this wavefunction is also continuous in its first derivative. Since in the middle region,

$$\frac{df_3(x)}{dx} = -2\pi \sin(2\pi x) + \pi \sin(\pi x)$$

which at $x = 0$ is equal to 0 and at $x = 2$ is also equal to 0, matching the zero first derivative of the constant wavefunction outside this region.

3c)

$$f_3(x) = \begin{cases} \cos(\pi x) & x \leq 0 \\ \sin(\pi x) & x > 0 \end{cases}$$

This is not a valid wave-function since it is *not continuous*. $\sin(0) = 0$ but $\cos(0) = 1$ hence there is a discontinuity at $x = 0$.

3d)

$$f_4(x) = e^x$$

This wave-function blows up to infinity as x gets large, and thus the normalisation integral also blows up to infinity. This wavefunction cannot be normalised and is unphysical.

4: Ground state of a chemical bond

A chemical bond can be approximated by a simple spring between two masses (which represent the atoms), the potential energy of which depends on their separation x, according to:

$$V(x) = \frac{1}{2}kx^2$$

where k is the spring constant. If we solve the TISE for such a potential, the lowest energy state has a wave function of the form:

$$\psi(x) = A\exp[-\alpha^2 x^2/2]$$

where $\alpha = \sqrt{m\omega/\hbar}$ and $\omega = \sqrt{k/m}$.

4a) Use the TISE to compute the energy of wavefunction $\psi(x)$.

The TISE for this potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

We know that $\psi(x)$ is a solution to this, so by substituting it into the TISE we can compute the energy.

We need to compute

$$\frac{d^2\psi(x)}{dx^2} = \frac{d}{dx}A\left(\frac{-2x\alpha^2}{2}\right)\exp[-\alpha^2x^2/2] = -A\alpha^2\frac{d}{dx}\left(x\exp[-\alpha^2x^2/2]\right)$$

$$= -A\alpha^2\left(\exp[-\alpha^2x^2/2] + \frac{-2\alpha^2}{2}x^2\exp[-\alpha^2x^2/2]\right) = A(\alpha^4x^2 - \alpha^2)\exp[-\alpha^2x^2/2]$$

where we used the chain rule and the product rule.

Hence we obtain:

$$-\frac{\hbar^2}{2m}A(\alpha^4x^2-\alpha^2)\exp[-\alpha^2x^2/2]+\frac{1}{2}kx^2A\exp[-\alpha^2x^2/2]=EA\exp[-\alpha^2x^2/2]$$

and after cancellations

$$-\frac{\hbar^2}{2m}(\alpha^4x^2-\alpha^2)+\frac{1}{2}kx^2=E$$

$$\left(-\frac{\hbar^2}{2m}\alpha^4+\frac{1}{2}k\right)x^2=(E-\frac{\hbar^2}{2m}\alpha^2)$$

When we substitute for the values of α and ω given above the LHS cancels to zero. Hence

$$(E-\frac{\hbar^2}{2m}\alpha^2)=0$$

$$E=\frac{\hbar^2\alpha^2}{2m}=\frac{\hbar^2 m\omega}{2m\hbar}=\frac{\hbar\omega}{2}$$

4b) Use the symmetry of the wave-function to determine the expectation value for separation x.

$\langle x\rangle=0$. The wavefunction $\psi(x)$ is an even function. Therefore the probability density $|\psi(x)|^2$ is also even. The integral:

$$\langle x\rangle=\int_{-\infty}^{\infty}x|\psi(x)|^2dx.$$

is an integral over the odd function $x|\psi(x)|^2$ which evaluates to zero.

4c) Find the value of A which normalises this wavefunction, and calculate the expectation value of separation x.

You may find the following integral useful

$$\int_{-\infty}^{\infty}e^{-y^2}dy=\sqrt{\pi}$$

To find A we solve:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Hence

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = A^2 \int_{-\infty}^{\infty} \exp[-\alpha^2 x^2] dx$$

To use the given integral I need to change variables: $y = \alpha x$ and hence $dy = \alpha dx$.

$$A^2 \int_{-\infty}^{\infty} \exp[-\alpha^2 x^2] dx = \frac{A^2}{\alpha} \int_{-\infty}^{\infty} \exp[-y^2] dy = \frac{A^2}{\alpha} \sqrt{\pi}.$$

Hence

$$A = \frac{\sqrt{\alpha}}{\pi^{1/4}}.$$

Now we need to compute $\langle x \rangle$ via:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = A^2 \int_{-\infty}^{\infty} x \exp[-\alpha^2 x^2] dx.$$

You are not given an identity to solve this equation, instead you can solve it from its structure. x is an odd function, while $\exp[-\alpha^2 x^2]$ is even. Hence the integrand is odd, and thus the integral is zero. Hence $\langle x \rangle = 0$.
