PHAS0004 - Atoms, Stars and The Universe
Problem Solving Tutorial Sheet 2 - 2018

All questions (or variations of them) may appear in the In-Course-Assessment test. Questions are made available approximately one week before the PST. Please attempt the problem sheet in advance of the PST class. A solution sheet will be made available after all PSTs have taken place. **Please bring an electronic copy of this question sheet to the PST.**

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 practise with the integration and differentiation which arises very often in problems of this kind.

5. Gain practise in solving the TISE for different trial solutions and showing that certain functions are not solutions.

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 Einstein's 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 Plank's constant h. Hence show that Bohr's quantisation assumption $L = n\hbar$ (where L is the angular momentum and n is an integer) is dimensionally consistent.

2: Calculating properties of wave-functions

Consider a particle with the wavefunction $\psi(x)$

$$\psi(x) = \begin{cases} Ae^{-x}\left(1 - e^{-x}\right) & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$$

2a) Sketch this wavefunction and show that $A = \sqrt{12}$ normalises the wavefunction $\psi(x)$.

2b) Calculate the expectation value $\langle x \rangle$ for the position of the particle .

2c) Use the probability distribution function to determine the most probable position of the particle. Explain the difference between the most probable position and the expectation value.

2d) Sketch a potential which could give rise to a wavefunction with the form above.

3: Which functions are valid wave-functions?

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)

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

3b)

$$f_2(x) = \begin{cases} \cos(4\pi x) - \cos(2\pi x) & \text{if } 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

3c)

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

3d)

$$f_4(x) = e^{-x}$$

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 $\psi(x)$.

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

4c) Using the method of integration by substitution, and the definite integral given below, calculate the value of constant A which ensures that the wavefunction is normalised.

You may find the following integral useful

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

5: Solving the Time Independent Schrödinger Equation for a free particle

In lectures we saw that a general sinusoidal function:

$$\psi(x) = A\sin\left(\frac{2\pi(x-\phi)}{\lambda}\right)$$

was a solution of the TISE for a free particle, and we calculated the associated energy. In this question, you are going to attempt to solve the TISE for a free particle yourselves, using a variety of trial functions.

The TISE for a free particle is:

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

5a) In lectures you heard that the only classes of functions which are proportional to their second derivative have sine-like and exponential-like forms. Let's look at some other functions and see how they fail. First let's consider

$$\psi(x) = x^2$$

Show that this function is *not* a solution to the free particle TISE.

5b) Is there any (finite) value of n for which

$$\psi(x) = x^n$$

could be a solution to the TISE for a free particle?

5c) Now consider the following function:

$$\psi(x) = A\sin(ax) + B\cos(bx)$$

Find an expression for the ratio

$$\frac{d^2\psi(x)}{dx^2} \div \psi(x).$$

Show that if $b = a$ this ratio is a constant, and that the wavefunction is solution to the TISE and calculate the energy of the particle as a function of parameters a, A and B.

(NB. In general, if $b \neq a$ then $\psi(x)$ above is not a solution to the free-particle TISE. You can convince yourself of this by plotting $\psi(x)$ and $d^2\psi/dx^2$ for $a \neq b$, e.g. on a graphical calculator or using Python or Mathematica.)

Ryan Nichol, October 2018