

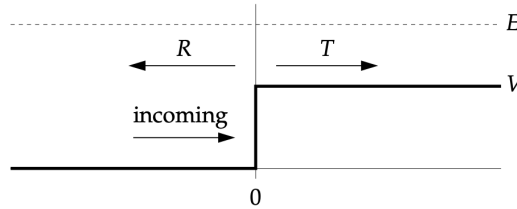
# Lab Assignment-1

## PHY617/PHY473-Computational Physics

9th Jan, 2025

Explain the algorithm you are using for each question.

**Question 1.** A well-known quantum mechanics problem involves a particle of mass  $m$  that encounters a one-dimensional potential step, like this:



The particle with initial kinetic energy  $E$  and wavevector  $k_1 = \sqrt{2mE}/\hbar$  enters from the left and encounters a sudden jump in potential energy of height  $V$  at position  $x = 0$ . By solving the Schrödinger equation, one can show that when  $E > V$  the particle may either (a) pass the step, in which case it has a lower kinetic energy of  $E - V$  on the other side and a correspondingly smaller wavevector of  $k_2 = \sqrt{2m(E - V)}/\hbar$ , or (b) it may be reflected, keeping all of its kinetic energy and an unchanged wavevector but moving in the opposite direction. The probabilities  $T$  and  $R$  for transmission and reflection are given by

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}, \quad R = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2.$$

Suppose we have a particle with mass equal to the electron mass  $m = 9.11 \times 10^{-31}$  kg and energy 10 eV encountering a potential step of height 9 eV. Write a Python program to compute and print out the transmission and reflection probabilities using the formulas above.

**Question 2.** Write a python program to perform a co-ordinate transformation from cartesian to polar co-ordinate. That is, ask the user for the Cartesian coordinates  $x, y$  of a point in two-dimensional space, and calculate and print the corresponding polar coordinates, with the angle  $\theta$  given in degrees.

**Question 3.** The orbit in space of one body around another, such as a planet around the Sun, need not be circular. In general it takes the form of an ellipse, with the body sometimes closer in and sometimes further out. If you are given the distance  $\ell_1$  of closest approach that a planet makes to the Sun, also called its perihelion, and its linear velocity  $v_1$  at perihelion, then any other property of the orbit can be calculated from these two as follows.

Kepler's second law tells us that the distance  $\ell_2$  and velocity  $v_2$  of the planet at its most distant point, or aphelion, satisfy  $\ell_2 v_2 = \ell_1 v_1$ . At the same time the total energy, kinetic plus gravitational, of a planet with velocity  $v$  and distance  $r$  from the Sun is given by

$$E = \frac{1}{2}mv^2 - \frac{GmM}{r},$$

where  $m$  is the planet's mass,  $M = 1.9891 \times 10^{30} \text{ kg}$  is the mass of the Sun, and  $G = 6.6738 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$  is Newton's gravitational constant. Given that energy must be conserved, we can calculate  $v_2$  as the smaller root of the quadratic equation

$$v_2^2 - \frac{2GM}{v_1 \ell_1} v_2 - \left[ v_1^2 - \frac{2GM}{\ell_1} \right] = 0.$$

Once we have  $v_2$  we can calculate  $\ell_2$  using the relation  $\ell_2 = \ell_1 v_1 / v_2$ .

1. Given the values of  $v_1$ ,  $\ell_1$ , and  $\ell_2$ , other parameters of the orbit are given by simple formulas that can be derived from Kepler's laws and the fact that the orbit is an ellipse:

$$\begin{aligned} \text{Semi-major axis:} \quad a &= (\ell_1 + \ell_2), \\ \text{Semi-minor axis:} \quad b &= \sqrt{\ell_1 \ell_2}, \\ \text{Orbital period:} \quad T &= \frac{2\pi ab}{\ell_1 v_1}, \\ \text{Orbital eccentricity:} \quad e &= \frac{\ell_2 - \ell_1}{\ell_2 + \ell_1}. \end{aligned}$$

Write a program that asks the user to enter the distance to the Sun and velocity at perihelion, then calculates and prints the quantities  $\ell_2$ ,  $v_2$ ,  $T$ , and  $e$ .

2. Test your program by having it calculate the properties of the orbits of the Earth (for which  $\ell_1 = 1.4710 \times 10^{11} \text{ m}$  and  $v_1 = 3.0287 \times 10^4 \text{ m s}^{-1}$ ) and Halley's comet ( $\ell_1 = 8.7830 \times 10^{10} \text{ m}$  and  $v_1 = 5.4529 \times 10^4 \text{ m s}^{-1}$ ). Among other things, you should find that the orbital period of the Earth is one year and that of Halley's comet is about 76 years.