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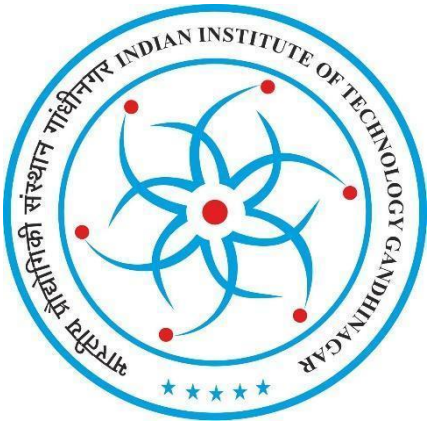


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# Project - 18 : Scattering of a Quantum Mechanical Wavepacket by a Potential in 1 - Dimension

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**MA202 Project Report**

**Group 14**

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# Contents

# Summary

Scattering of a quantum mechanical wavepacket by a potential in 1-dimension is a problem that involves solving the Schrödinger equation for a wavefunction that represents a particle with a certain energy and momentum encountering a potential barrier or well. The wave function can be decomposed into an incoming plane wave and an outgoing spherical wave. The scattering amplitude and cross-section can be calculated from the boundary conditions at the potential region. The scattering process can exhibit phenomena such as reflection, transmission, resonance and tunnelling, depending on the energy of the particle and the shape and height of the potential.

The Runge-Kutta method is a numerical technique for solving ordinary differential equations, such as the Schrödinger equation. It involves using a series of intermediate steps to approximate the solution at each time step based on the slope or derivative of the function at different points. The method can have different orders of accuracy, depending on how many evaluations of the function are used. The most common one is the fourth-order Runge-Kutta method, which uses four evaluations of the function at each step. The Runge-Kutta method can be applied to solve the Schrödinger equation for various potentials and initial conditions and compare the numerical results with analytical solutions or experimental data.

# Introduction

Quantum mechanics is the branch of physics that describes the behaviour of matter and energy at the smallest scales.

One of the fundamental concepts of quantum mechanics is wave-particle duality, which states that every physical entity, such as an electron or a photon, can exhibit both wave-like and particle-like properties, depending on the experimental situation. For example, an electron can behave like a particle when it collides with another electron, but it can also behave like a wave when it passes through a slit or a barrier.

A quantum mechanical wavepacket is a mathematical construct that represents a superposition of plane waves with different wavelengths and amplitudes. A wavepacket can be used to model the state of a quantum particle that has a well-defined position and momentum within some uncertainty. A wavepacket can also evolve in time according to the Schrödinger equation, which is the fundamental equation of motion for quantum systems.

Scattering is a physical process in which a particle interacts with another particle or a potential field and changes its direction or energy. Scattering is ubiquitous in nature and plays an important role in many phenomena, such as light reflection, diffraction, refraction, absorption, emission, etc. Scattering can also reveal information about the structure and properties of the scatterer, such as its shape, size, charge, spin, etc.

In this project, we will study the scattering of a quantum mechanical wavepacket by a potential in 1 - dimension. This is a simplified model that captures some essential features of quantum scattering phenomena. We will consider different types of potentials, such as step, barrier, well, delta-function, etc., and investigate how they affect the behaviour of the wavepacket. We will also compare the quantum results with the classical ones and explore some quantum effects, such as reflection, transmission, interference, tunnelling, resonance, etc.

To solve the scattering problem numerically, we will use the Runge-Kutta method, which is a widely used technique for solving differential equations. The Runge-Kutta method approximates the solution as a series of steps, each of which involves evaluating the derivative of the function at some intermediate points. The Runge-Kutta method can achieve high accuracy without requiring high-order derivatives of the function.

# Equations to be Solved

***One Dimensional time-dependent Schrodinger Equation (1)***

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

***Another format for one-dimensional time-dependant Schrodinger Equation (2)***

$$\imath\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\,\psi$$

***Splitting Equation into Real and Imaginary Parts (3)***

$$\psi(x,t) = R(x,t) + \imath\, I(x,t)$$

***Time-Derivative of Real and Imaginary Part (4)***

$$\frac{\partial R}{\partial t} = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)\right) I$$
$$\frac{\partial I}{\partial t} = \left(\frac{1}{2}\frac{\partial^2}{\partial x^2} - V(x)\right) R\,,$$

***Expressing the second partial derivative in the usual finite-difference form (5)***

$$\psi(m,n+1) \approx \psi(m,n) + \frac{\imath\,\Delta t}{2}\left[\frac{\psi(m+1,n)+\psi(m-1,n)-2\,\psi(m,n)}{(\Delta x)^2}\right] - \imath\,\Delta t\,V(m)\,\psi(m,n)$$

***Wave Function at t = 0 (6)***

$$\psi(x,t=0) = C\,\exp[-(x-x_0)^2/\sigma^2]\,\exp[\imath\,k_0\,x]$$

# The Runge-Kutta Method

The Runge-Kutta method is a family of numerical methods for solving differential equations by approximating the solution as a series of steps based on the derivatives of the function at different points. The most common version of the Runge-Kutta method is the fourth-order one, which has a local truncation error of order h^5 and a global truncation error of order h^4, where h is the step size. The fourth-order Runge-Kutta method works as follows:

- Given an initial value problem of the form y' = f(x,y), $y(x_0) = y_0$, choose a step size h and define

$$x_n = x_0 + nh \text{ for } n = 0, 1, 2, ...$$

- To find the approximate value of y at $x_{n+1}$, use the following formula:

$$y_{n+1} = y_n + (1/6)(k_1 + 2k_2 + 2k_3 + k_4)$$

where

$$k_1 = hf(x_n,y_n)$$

$$k_2 = hf(x_n + h/2, y_n + k_1/2)$$

$$k_3 = hf(x_n + h/2, y_n + k_2/2)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

- Repeat this process until the desired value of x is reached.

The idea behind this method is to use a weighted average of four slopes at different points within each step to estimate the change in y. The slopes are computed using the function f and the previous values of y. The weights are chosen to match the Taylor series expansion of the exact solution up to the fourth order. This method is more accurate and stable than lower-order methods such as Euler's method or Heun's method.

Scattering of a quantum mechanical wavepacket by a potential in 1-dimension is a problem that involves solving the Schrödinger equation with an ingoing plane wave and finding the scattering amplitude and the differential cross section for different directions. The Runge-Kutta method can be used to approximate the solution of the Schrödinger equation by discretising the time variable and applying the formula for the fourth-order Runge-Kutta methods. The use of this method in this project may depend on the specific form of the potential function and the initial conditions of the wavepacket.

# Central Difference Double Derivative method

- Central difference double derivative method is a numerical method used to approximate the second derivative of a function.
- The method uses the values of the function at x + $i$, x, and x - $i$ to calculate the approximation of the second derivative at x.
- The formula for the central difference double derivative method is :

  $f''(x) \approx [f(x + i) - 2f(x) + f(x - i)] / [\Delta i^2]$, where $i$ is a small number called the grid size. The truncation error is found to be a function of $O(\boldsymbol{i^2})$ which is approximated to the above equation.
- The method is relatively easy to implement and requires knowledge of the function values at only three points.
- The choice of an appropriate step size is crucial in achieving accurate results while maintaining numerical stability.

# Methodology

To use the Runge-Kutta method to solve for the scattering of a quantum mechanical wavepacket by a potential in 1-dimension, the following needs to be done:

- The Schrödinger equation for the wave function of the particle is written in terms of its position and time. This will be a partial differential equation of the form $\partial\psi/\partial t = iH\psi$, where $H$ is the Hamiltonian operator that depends on the potential and the kinetic energy of the particle.

- An initial condition for the wave function at $t = 0$ is chosen. This will be a function of x that represents the shape and momentum of the wavepacket before it encounters the potential.

- A boundary condition for the wave function at $x = \pm\infty$ is chosen. This will be a function of t that represents the asymptotic behaviour of the wave function far away from the potential.

- The position and time domains are discretised into small intervals of size $\Delta x$ and $\Delta t$. Choose values that are small enough to capture the features of the wavefunction and the potential, but not too small to cause numerical instability or overflow.

- The Runge-Kutta method is used to approximate the solution of the Schrödinger equation at each grid point (x, t) using the values of the wavefunction and its derivatives at neighbouring points. We updated the value of wave function at each time step.
- The result that we get from this analyzed by plotting probability density function with respect to x with different values of t to show propagation.

- We apply central difference double differentiation method to numerically calculate value of double derivative function and approximate the value of wave function from Schrödinger equation at different time while propagation towards potential and after reflecting from it.

- We plot the graph of probability density reflecting from potential wall at different time .

# Code Description

[1] : In file name (WaveFunction(t = 0).py) we plot the probability density and wave function real and Imaginary part in eq(3) by simply taking wave function as gaussian wave function at t=0. By putting parameters in it we plot the graph of it at difference value of x.

[2] : In file name (Probabilitydensitydifferenttime.py) we evaluate the wave function with runge kutta method and use central difference method to find double derivative of wave function with respect to x . we give input as parameters of gaussian wave function, time intervals and we get the output of a plot between probability density v/s x with different values of time.

[3] : In file Name(Probabilitydensitywithpotential.py) we evaluate the propagation of wave with time interval and presence of potential wall. We provide input as parameter of gaussian wave function and potential wall location and value we get output as plot between probability density v/s x with different time during and after the reflection.

# Conclusion

In conclusion, the scattering of a quantum mechanical wavepacket by a potential in 1-dimension is a fundamental problem in quantum mechanics that involves solving the Schrödinger equation for a wavefunction that describes the behaviour of a particle encountering a potential barrier or well. The wave function can be decomposed into an incoming plane wave, and an outgoing spherical wave, and the scattering process can exhibit various phenomena such as reflection, transmission, resonance and tunnelling, depending on the energy of the particle and the shape and height of the potential. To solve the Schrödinger equation numerically, the Runge-Kutta method is a widely used technique that involves approximating the solution at each time step based on the slope or derivative of the function at different points. The method can have different orders of accuracy, with the fourth-order Runge-Kutta method being the most common one that uses four evaluations of the function at each step.By applying the Runge-Kutta method to various potentials and initial conditions, researchers can compare the numerical results with analytical solutions or experimental data, and gain insights into the behavior of quantum particles in different physical scenarios. This problem has wide applications in fields such as materials science, atomic physics, and quantum computing. Further research on this topic can lead to the development of new quantum technologies and a better understanding of the fundamental principles of quantum mechanics.

# Sources :

(1) Lecture 2 Quantum mechanics in one dimension - University of Cambridge. https://www.tcm.phy.cam.ac.uk/~bds10/aqp/lec2_compressed.pdf.

(2) 11.4: Scattering in one dimension - Square Well - Physics LibreTexts. https://phys.libretexts.org/Bookshelves/Quantum_Mechanics/Quantum_Physics_(Ackland)/11%3A_Fundamentals_of_Quantum_Scattering_Theory/11.04%3A_Scattering_in_one_dimension_-_Square_Well.

(3) Runge-Kutta Methods - Massachusetts Institute of Technology. https://web.mit.edu/10.001/Web/Course_Notes/Differential_Equations_Notes/node5.html.