IIT GANDHINAGAR
MA 203: NUMERICAL METHODS

NUMERICAL ANALYSIS OF SCHRODINGER EQUATION FOR A PARTICLE IN A DOUBLE – WELL POTENTIAL CURVE

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INTRODUCTION

1) The goal of this project is to solve the one-dimensional time-independent Schrödinger equation using Finite Difference Method (FDM).

2) We applied this approach to study the superposition of a particle in a double well potential.

3) We also extended this result to explain the Umbrella inversion in ammonia molecules.

EQUATIONS

1) Function For Double Well Potential

$$V(x) = (x^2 - a^2)^2$$

2) Potential Energy Curve For Ammonia Molecule

$$V(x) = V_o e^{(-Ax^2)} + Bx^0 + Cx^2 + Dx^4 + Ex^6$$

$V_o = 17683.5627\ eV$ $A = 3.6530\ \dot{A}^{-2}$ $B =$ -15661.4233 eV

C = 35750.2356 eV $- \dot{A}^{-2}$ D = 3417.3434 $eV - \dot{A}^{-4}$ E = -88.7202 $eV - \dot{A}^{-6}$

3) One Dimensional Time Independent Schrodinger Equation

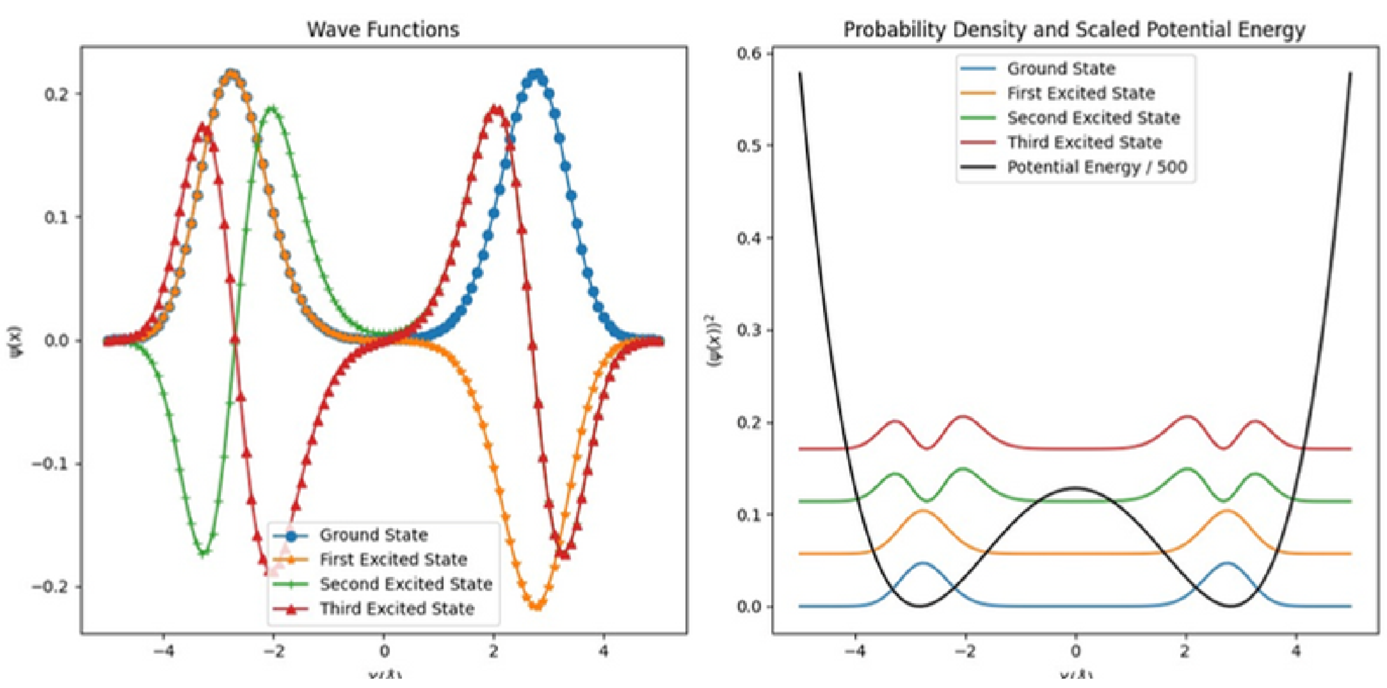
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(\vec{x})\right)\psi(x) = E\,\psi(x)$$

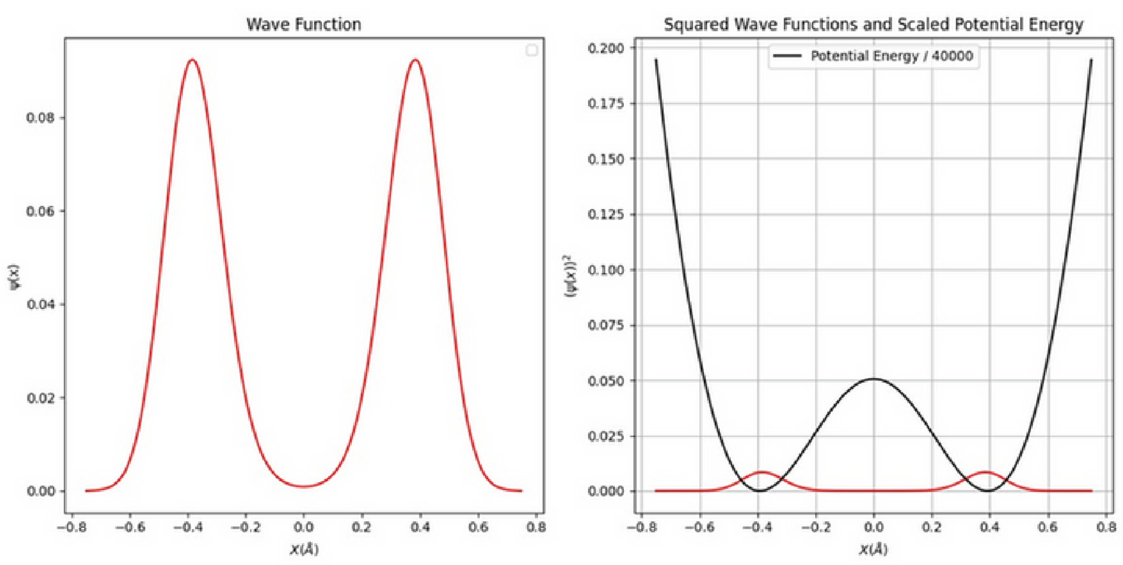
4) Final Equation After Applying Finite Difference Method

$$-\psi(x)_{i+1} + \left(2 + \frac{2m}{\hbar^2}(\Delta x)^2(V(x)_i)\right)\psi(x)_i - \psi(x)_{i-1} = \frac{2m}{\hbar^2}(\Delta x)^2 E\,\psi(x)_i$$

RESULTS

1) From the Figure, We can observe that there is an equal and non-zero probability of finding a particle in both the wells of the double well potential curve as per the principles of quantum superposition.





2) The figure shows that the ammonia molecule is in superposition between the two states