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SOLVING SCHRODINGER EQUATION FOR A QUANTUM MECHANICAL PARTICLE BY A NEW INTEGRAL TRANSFORM: ROHIT TRANSFORM

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ABSTRACT

Quantum mechanics explains the nature of atomic particles at the small scale of energy and most of the boundary value problems in this mechanics are generally solved by ordinary algebraic or analytical methods or calculus approach or by Fourier Transform. In this paper, a new approach is presented to solve the one-dimensional time-independent Schrodinger's equation for a particle inside the one-dimensional infinitely high potential box and for a particle impinging on the vertical potential step by applying a new integral transform called Rohit Transform (RT) and demonstrated it to find the eigen values and eigen functions for a particle inside the one-dimensional infinitely high potential box and for a particle impinging on the vertical potential step to find the reflection and transmission coefficients.

Keywords: Rohit Transform (RT), Schrodinger Equation, Vertical Potential Step, and Infinitely high Potential Box.

I. INTRODUCTION

This paper discusses the application of a new integral transform called Rohit Transform to the one-dimensional time-independent Schrodinger's equation to obtain the eigen values and eigen functions for a particle inside the one-dimensional infinitely high potential box and for a particle impinging on the vertical potential step to obtain the reflection and transmission coefficients. Generally, such boundary value problems have been solved by ordinary algebraic or analytical methods or by calculus approach or Fourier Transform [1-4]. The Rohit Transform (RT) was proposed by the author Rohit Gupta in recent years and generally, it has been applied in different areas of science and engineering and is not widely known as it has composed recently [5]. Suppose an operator Ô operates on the function g and gives the same function g multiplied by constant α i.e. Ô g = α g. In this equation, g is the Eigen function of the Ô and α is the Eigen value of the Ô and the equation is known as Eigen value equation [6-9].

II. BASIC DEFINITION

Rohit Transform (RT)

The Rohit Transform [5] of g(y), y ≥ 0 is defined as $R\{g(y)\} = r^3\int_0^\infty e^{-ry}\, g(y)\,dy = G(r)$, provided that the integral is convergent, where r may be a real or complex parameter.

The Rohit Transform (RT) of some derivatives [5] of g(y) are given by

$R\{g'(y)\} = rR\{g(y)\} - r^3 g(0)$

Or

$R\{g'(y)\} = rG(r) - r^3 g(0)$,

$R\{g''(y)\} = r^2 G(r) - r^4 g(0) - r^3 g'(0)$,

And so on.

III. MATERIAL AND METHOD

The one-dimensional time-independent Schrodinger's equation [7-8] is given by

$\psi''(z) + \frac{2m}{\hbar^2}\{E - V(z)\}\psi(z) = 0$ ... (1)

In this equation, $\psi(z)$ is the probability wave function and $V(z)$ is the potential energy function.

Infinite potential well

Consider a particle confined to the region 0 < z < a. It can move freely in this but subject to strong forces at z = 0 and z = a. The one-dimensional infinitely high potential box (shown in figure 1) is defined as [6, 7]

V (z) = 0 for 0 < z <a

= ∞ for z ≤ 0 and z ≥ a.

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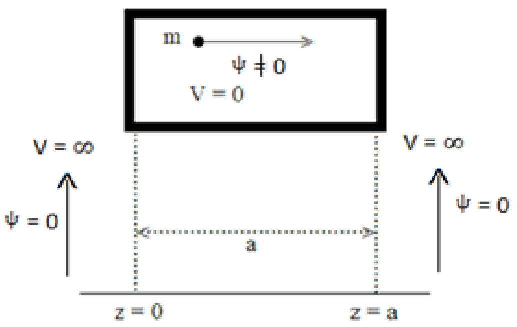

Figure 1: infinite square well potential

For a particle inside the one-dimensional infinitely high potential box, $V(z) = 0$

From (1), it can be written

$\psi''(z) + k^2\psi(z) = 0$ ...... (2); $k = \sqrt{\frac{2mE}{\hbar^2}}$

where z belongs to [0, a] with $\psi(0) = \psi(a) = 0$.

The Rohit Transform [5] of (2) provides

$p^2\bar{\psi}(p) - p^4\psi(0) - p^3\psi'(0) + k^2\bar{\psi}(p) = 0$... (3)

Put $\psi(0) = 0$ and $\psi'(0) = A$, (3) becomes

$\bar{\psi}(p) = \frac{Ap^3}{(p^2+k^2)}$ .... (4)

The inverse RT [5] of (4) provides

$\psi(z) = \frac{A}{k}\sin(kz)$ ..... (5)

Put $\psi(a) = 0$, (5) gives

$\sin(ka) = 0$

Or

$ka = n\pi$, where n is a positive integer.

Or

$k = \frac{n\pi}{a}$ ----- (6)

Comparing the values of k, it can be written

$\frac{2mE}{\hbar^2} = (\frac{n\pi}{a})^2$

Solving and rearranging, it can be written

$E = \frac{n^2\pi^2\hbar^2}{2ma^2}$....... (7)

Substitute (6) in (5),

$\psi(z) = \frac{A}{\frac{n\pi}{a}}\sin(\frac{n\pi}{a}z)$ .... (8)

Applying normalization condition, it can be written

$\int_{z=0}^{z=a}\psi(z)\ \psi(z)^*dz = 1$ .... (9)

Using (8) in (9) and simplifying, it can be written

$A = \frac{n\pi}{a}.\sqrt{\frac{2}{a}}$ ...... (10)

Using (10) in (8), it can be written

$\psi(z) = \sqrt{\frac{2}{a}}\ \sin(\frac{n\pi}{a}z)$....... (11)

Vertical Potential Step

Consider a particle of mass m and total energy E moving from a region of zero potential to a region of constant potential, then the vertical potential function (as shown in figure 2) is represented as [8]

V (z) = 0 for z < 0 and V (z) = for z > 0.

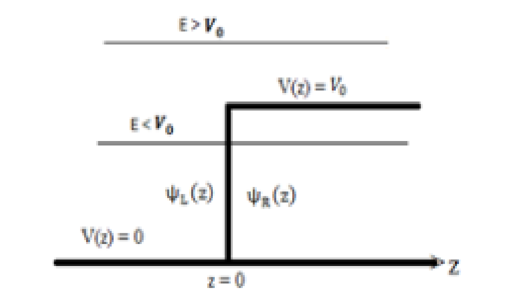

Figure 2: Representation of one-dimensional vertical potential step.

If $\psi_L(z)$ and $\psi_R(z)$ are the wave functions to the left and the right side of the vertical potential step at z = 0, then at z = 0,

$\psi_L(0) = \psi_R(0) = A$ (say)

and $\psi_L'(0) = \psi_R'(0) = B$ (say),

where A and B are constants.

In the region, z < 0, V (z) = 0, therefore, the one-dimensional time-independent Schrodinger equation, in this region is written as

$\psi_L''(z) + k_1^2\psi_L(z) = 0$ ...... (12),

$where\ k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

The RT [5] of (12) provides

$p^2\bar{\psi}_L(p) - p^4\psi_L(0) - p^3\psi_L'(0) + k_1^2\bar{\psi}_L(p) = 0$

Or

$p^2\ \bar{\psi}_L\ (p) - p^4\ A\ - p^3 B + k_1^2\bar{\psi}_L\ (p) = 0.$

Rearranging, it can be written

$\bar{\psi}_L\ (p) = \frac{p^4 A + p^3 B}{p^2 + k_1^2}$

Or

$\bar{\psi}_L\ (p) = \frac{p^4 A}{p^2+k_1^2} + \frac{p^3 B}{p^2+k_1^2}$

Taking inverse RT [5], it can be written

$\psi_L(z) = A\ \cos k_1 z + \frac{B}{k_1}\ \sin k_1 z$.... (13)

Writing $\cos k_1 z\ and\ \sin k_1 z$ in terms of exponentials, we get

$$\psi_L(z) = A\ \frac{e^{ik_1 z} + e^{-ik_1 z}}{2} + \frac{B}{k_1}\ \frac{e^{ik_1 z} - e^{-ik_1 z}}{2i}$$

Or

$\psi_L(z) = (\frac{A}{2} - i\frac{B}{2k_1})\ e^{ik_1 z} + (\frac{A}{2} + i\frac{B}{2k_1})e^{-ik_1 z}$... (14)

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In (14), the terms on R.H.S $i.e.$

$(\frac{A}{2} - i\frac{B}{2k_1})\, e^{ik_1z}$ and $(\frac{A}{2} + i\frac{B}{2k_1})\, e^{-ik_1z}$ represent the incident and the reflected waves in the region z < 0 i.e.

$$\psi_{in}(z) = (\frac{A}{2} - i\frac{B}{2k_1})\, e^{ik_1z}$$

and

$$\psi_{re}(z) = (\frac{A}{2} + i\frac{B}{2k_1})e^{-ik_1z}.$$

Now, in the region, z > 0, two possibilities arise: either V (z) = $V_0 < E$ or V (z) = $V_0 > E$.

Case I: E > V_0

In this case, in the region, z > 0, V (z) = $V_0 < E$, therefore, the Schrodinger equation is written as

$[\psi_R''(z)] + k_2^2[\psi_R(z)] = 0$ …. (15), where $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ *is real.*

Taking (RT) of (15), it can be written

$p^2\bar{\psi}_R(p) - p^4\psi_R(0) - p^3\psi_R'(0) + k_2^2\bar{\psi}_R(p) = 0$

Or

$$p^2\,\bar{\psi}_R(p) - p^4 A - p^3 B + k_2^2\bar{\psi}_R(p) = 0.$$

Rearranging, it can be written

$$\bar{\psi}_R(p) = \frac{p^4 A}{p^2 + k_2^2} + \frac{p^3 B}{p^2 + k_2^2}$$

Taking inverse (RT), it can be written

$$\psi_R(z) = A\cos k_2 z + \frac{B}{k_2}\sin k_2 z \quad \text{.... (16)}$$

Writing $\cos k_2 z$ *and* $\sin k_2 z$ in terms of exponentials, it can be written

$$\psi_R(z) = A\,\frac{e^{ik_2z} + e^{-ik_2z}}{2} + \frac{B}{k_2}\,\frac{e^{ik_2z} - e^{-ik_2z}}{2i}$$

Or

$$\psi_L(z) = (\frac{A}{2} - i\frac{B}{2k_2})e^{ik_2z} + (\frac{A}{2} + i\frac{B}{2k_2})e^{-ik_2z} \quad \text{... (17)}$$

In (17), the first term on R.H.S. $i.e.$

$(\frac{A}{2} - i\frac{B}{2k_2})\, e^{ik_2z}$ represents the transmitted wave in the region z > 0 i.e.

$$\psi_{tr}(z) = (\frac{A}{2} - i\frac{B}{2k_2})\, e^{ik_2z}.$$

Since $(\frac{A}{2} + i\frac{B}{2k_2})$ represents the coefficient of a beam incident from right on the potential step, which is not physical, therefore,

$$(\frac{A}{2} + i\frac{B}{2k_2}) = 0$$

Or $B = ik_2A$…… (18)

Using (18), it can be written

$$\psi_{in}(z) = \frac{A}{2}(1 + \frac{k_2}{k_1})\, e^{ik_1z} \quad \text{... (19),}$$

$$\psi_{re}(z) = \frac{A}{2}(1 - \frac{k_2}{k_1})\, e^{-ik_1z} \quad \text{.... (20)}$$

and

$$\psi_{tr}(z) = Ae^{ik_2z} \quad \text{... (21)}$$

The quantum mechanical reflection coefficient R is given by

$R = \frac{v_1\psi_{re}\psi_{re}^*}{v_1\psi_{in}\psi_{in}^*}$, where v_1 is the velocity in z < 0 and ψ_{in}^* and ψ_{re}^* are the complex conjugates.

Using (19) and (20) and simplifying, it can be written

$$R = [\frac{k_1 - k_2}{k_1 + k_2}]^2 \quad \text{...... (22)}$$

The quantum mechanical transmission coefficient T is given by

$T = \frac{v_2\psi_{tr}\psi_{tr}^*}{v_1\psi_{in}\psi_{in}^*}$, where v_2 is the velocity in z < 0 and ψ_{tr}^* is the complex conjugate.

Using (19) and (21) and simplifying, it can be written

$$T = \frac{4v_2}{v_1\left(1 + \frac{k_2}{k_1}\right)^2} \quad \text{........ (23)}$$

Using the relation $\frac{p_2}{p_1} = \frac{mv_2}{mv_1} = \frac{\hbar k_2}{\hbar k_1}$,

Or

$\frac{v_2}{v_1} = \frac{k_2}{k_1}$ and simplifying, it can be written

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \quad \text{..... (24)}$$

On adding equations, (22) and (24), it has been found that the sum of R and T is one.

Case II: E < V_0

In this case, in the region, z < 0, the solution remains the same.

In the region, z > 0, V (z) = $V_0 < E$, therefore, the Schrodinger equation is written as

$[\psi_R''(z)] + k_3^2[\psi_R(z)] = 0$.. (25),

Where,

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$k_3 = i\sqrt{\frac{2m(V_0-E)}{\hbar^2}} = ik$ *is complex*; $k = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$.

Taking RT of (25), it can be written

$p^2\bar{\psi}_R(p) - p^4\psi_R(0) - p^3\psi_R{}'(0) + k_3{}^2\bar{\psi}_R(p) = 0$

Or

$$p^2\,\bar{\psi}_R(p) - p^4 A - p^3 B + k_3{}^2\bar{\psi}_R(p) = 0.$$

Rearranging the equation, it can be written

$$\bar{\psi}_R(p) = \frac{p^4 A + p^3 B}{p^2 + k_3{}^2}$$

Or $\bar{\psi}_R(p) = \frac{p^4 A}{p^2+k_3{}^2} + \frac{p^3 B}{p^2+k_3{}^2}$

Taking inverse RT [5], it can be written

$$\psi_R(z) = A\cos k_3 z + \frac{B}{k_2}\sin k_3 z \;\ldots.\; (26)$$

Writing $\cos k_3 z$ *and* $\sin k_3 z$ in terms of exponentials, it can be written

$$\psi_R(z) = A\,\frac{e^{ik_3z} + e^{-ik_3z}}{2} + \frac{B}{k_3}\,\frac{e^{ik_3z} - e^{-ik_3z}}{2i}$$

Or

$$\psi_R(z) = \left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3z} + \left(\frac{A}{2} + i\frac{B}{2k_3}\right)e^{-ik_3z} \ldots (27)$$

In (27), $\left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3z}$ represents the transmitted wave in the region z > 0 i.e.

$$\psi_{tr}(z) = \left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3z} \ldots. (28)$$

Since $\left(\frac{A}{2} + i\frac{B}{2k_3}\right)$ represents the coefficient of a beam incident from right on the potential step, which is not physical, therefore,

$$\left(\frac{A}{2} + i\frac{B}{2k_3}\right) = 0$$

Or $B = ik_3 A \ldots\ldots (29)$

Using (29), it can be written

$$\psi_{in}(z) = \frac{A}{2}\left(1 + \frac{k_3}{k_1}\right)e^{ik_1z} \ldots (30)$$

$$\psi_{re}(z) = \frac{A}{2}\left(1 - \frac{k_3}{k_1}\right)e^{-ik_1z} \ldots.. (31)$$

and

$$\psi_{tr}(z) = Ae^{ik_3z} \ldots\ldots (32)$$

The quantum mechanical reflection coefficient R is given by

$$R = \frac{v_1\psi_{re}\psi_{re}^*}{v_1\psi_{in}\psi_{in}^*}$$

Using (30) and (31) and simplifying, it can be written

R = 1 …… (33)

The quantum mechanical transmission coefficient T is given by

$$T = \frac{v_2\psi_{tr}\psi_{tr}^*}{v_1\psi_{in}\psi_{in}^*}$$

Using (30) and (32) and simplifying, it can be written

$$T = \frac{4v_2}{v_1\left[1+\left(\frac{k}{k_1}\right)^2\right]} \ldots.. (34)$$

Using the relation $\frac{v_2}{v_1} = \frac{k_3}{k_1}$ or $\frac{v_2}{v_1} = i\frac{k}{k_1}$ and simplifying, it can be written

$$T = \frac{4ik}{k_1\left[1+\left(\frac{k}{k_1}\right)^2\right]}$$

Or

$$Real(T) = 0 \ldots.. (35)$$

On adding (33) and (35), it has been found that that R + T = 1.

IV. CONCLUSION

In this paper, the Rohit Transform has been applied successfully to solve the one-dimensional time-independent Schrodinger's equation to find the eigen energy values and eigen functions for a particle inside the infinitely high potential well and for a particle impinging on vertical potential step to find the reflection and transmission coefficients and revealed that the application of Rohit Transform to solve the one-dimensional time-independent Schrodinger's equation is effective and simple.

REFERENCES

[1] Introduction to Quantum mechanics by David j. Griffiths. Publisher: Cambridge University Press. 2nd edition.

[2] Quantum mechanics by B.N. Srivastava, R.M. Richaria. Publisher: Pragati Prakashan Meerut. 16th edition.

[3] Principles of quantum mechanics by P.A.M. Dirac. Publisher: Oxford University Press. Edition: Reprint, 2016.

Doi: 10.2016-53692176; DOI Link :: http://doi-ds.org/doilink/10.2020-36786965/

[4] Nouredine Zettili, Quantum Mechanics: Concepts and Applications. Publisher: John Wiley and Sons. 2nd edition.

[5] Rohit Gupta, "On novel integral transform: Rohit Transform and its application to boundary value problems", ASIO Journal of Chemistry, Physics, Mathematics and Applied Sciences (ASIO-JCPMAS), Volume 4, Issue 1, 2020, PP. 08-13.

[6] Rohit Gupta, Rahul Gupta, Dinesh Verma, Eigen Energy Values and Eigen Functions of a Particle in an Infinite Square Well Potential by Laplace Transforms, International Journal of Innovative Technology and Exploring Engineering, Volume 8 Issue 3, January 2019, PP 6-9.

[7] Rohit Gupta, Rahul Gupta, Matrix Method For Solving The Schrodinger's Time - Independent Equation To Obtain The Eigen Functions And Eigen Energy Values of A Particle Inside The Infinite Square Well Potential, IOSR Journal of Applied Physics (IOSR-JAP), Volume 10, Issue 5 Ver. I (Sep. – Oct. 2018), PP 01-05.

[8] Rohit Gupta, Tarun Singhal, Dinesh Verma, Quantum mechanical reflection and transmission coefficients for a particle through a one-dimensional vertical step potential, International Journal of Innovative Technology and Exploring Engineering, Volume-8 Issue-11, September 2019, PP 2882-2886.

[9] Rohit Gupta, Rahul Gupta, Dr. Dinesh Verma, Eigenenergy values and Eigenfunctions of one dimensional quantum mechanical harmonic oscillator, IOSR Journal of Engineering (IOSRJEN), Vol. 09, Issue 1 (January. 2019),V (III), PP 17-21.

Doi: 10.2016-53692176; DOI Link :: http://doi-ds.org/doilink/10.2020-36786965/