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Eigen Energy Values and Eigen Functions of a Particle in an Infinite Square Well Potential by Laplace Transforms

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Abstract- ***Quantum mechanics is one of the branches of physics and is a fundamental theory which explains the nature of atoms and subatomic particles at the smallest scale of energy. In this mechanics, physical problems are solved by algebraic and analytic methods. By applying Laplace Transforms we can find the general solutions of one dimensional Schrodinger's time-independent wave equation for a particle in an infinite square well potential. In this paper, we will discuss the Eigen energy values and Eigen functions of a particle in an infinite square well potential. We will find that general solutions (Eigen functions) of one dimensional Schrodinger's time- independent wave equation for a particle in an infinite square well potential have very interesting characteristics that each Eigen function is associated with a particular value of energy (Eigen energy value) of the particle confined inside an infinite square well potential.***

Keywords: Eigen functions, Eigen values, Infinite square well, Laplace Transforms.

I. INTRODUCTION

In Quantum mechanics, physical problems are solved by algebraic and analytic methods. By applying Laplace Transforms to the one dimensional Schrodinger's time-independent wave equation, we can obtain the Eigenenergy values and Eigenfunctions of a particle in a square well potential of infinite height. To define Eigenvalues and Eigenfunctions, suppose that an operator Ô is operated on the function g and resultsthe same function g multiplied by some constant α i.e. Ô g = α g. In this equation, g is the Eigenfunction of operator Ô and the constant α is the Eigen value of the operator Ô related with the Eigenfunction g and the equation is known as Eigen value equation. The Eigenfunctions are selected from a special class of functions. For example, in bound state problem, all wave functions and their derivatives must be continuous, single valued and finite everywhere. They must also vanish at infinity. Such functions are called as well-behaved functions[1-4]. As an example, to illustrate the Eigen value of an operator, consider the operator $\left(\frac{d}{dz}\right)$ operating on a well – behaved function e^{-6z}. The result is

$$\frac{d}{dz}(e^{-6z}) = -6e^{-6z}.$$

Comparing this equation with standard Eigen value equation Ô g = α g, we find that (-6) is the Eigen value of operator$\left(\frac{d}{dz}\right)$ associated with the Eigen functione^{-6z}.

II. DEFINITION OF LAPLACE TRANSFORMATIONS

Let F (t) is a well-defined function of real numbers t ≥ 0. The Laplace transformations of F (t), denoted by f (p) or L {F (t)}, is defined as

L {F (t)} $=\int_0^\infty e^{-pt}F(t)dt = f(p)$, provided that the integral exists, i.e. convergent. If the integral is convergent for some value of p, then the Laplace transformations of F (t) exists otherwise not. Where p *is* the parameter which may be real or complex number and L isthe Laplace transformations operator [1-3].

A. Laplace Transformations of Elementary Functions

1. $L\{1\} = \frac{1}{p},\ p > 0$
2. $L\{t^n\} = \frac{n!}{p^{n+1}},$ $\quad where\ n = 0,1,2,3 \ldots$
3. $L\{e^{bt}\} = \frac{1}{p-b},\ p > b$
4. $L\{sinbt\} = \frac{b}{p^2+b^2},\ p > 0$
5. $L\{sinhbt\} = \frac{b}{p^2-b^2},\ p > |b|$
6. $L\{cosbt\} = \frac{p}{p^2+b^2},\ p > 0$
7. $L\{coshbt\} = \frac{p}{p^2-b^2},\ p > |b|$

B. Proof of Laplace Transformations of Some Elementary Functions

According to the definition of Laplace transformations,

1. L {F (t)} $=\int_0^\infty e^{-pt}F(t)dt$, then

$$L\{1\} = \int_0^\infty e^{-pt}\,1\,dt$$

$$= -\frac{1}{p}(e^{-\infty} - e^{-0})$$

$$= -\frac{1}{p}(0-1)$$

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$$= \frac{1}{p} = f(p)\ \ , p > 1$$

2. $L\ \{F\ (t)\} = \int_0^\infty e^{-pt}\, F(t) dt$, then

$L\ \{\ sinhbt\ \} = \int_0^\infty e^{-pt}\ sinhbt\ dt$

$= \int_0^\infty e^{-pt} \left(\frac{e^{bt} - e^{-bt}}{2}\right) dt$

$= \int_0^\infty \left(\frac{e^{-(p-b)t} - e^{-(p+b)t}}{2}\right) dt$

$$= -\frac{1}{2(p-b)}\ (\ e^{-\infty} - \ e^{-0})$$

$$+ \frac{1}{2(p+b)}\ (\ e^{-\infty} - \ e^{-0})$$

$= \frac{1}{2(p-b)} - \frac{1}{2(p+b)}$

$= \frac{1}{2} \cdot \frac{2b}{p^2-b^2}$

Therefore, $L\ \{sinhbt\} = \frac{b}{p^2-b^2}\ ,\ \ p > |b|$

C. Laplace Transformations of derivatives

Let the function F is having exponential order, that is F is continuous function and is piecewise continuous function on any interval, then the Laplace transforms of derivative of F (t), denoted by $L\ \{F'(t)\}$, is given by

$$L\ \{F'(t)\} = \int_0^\infty e^{-pt}\ F'(t) dt$$

Integrating by parts and using the condition that, $e^{-pt} F(t) = 0\ when\ t = \ \infty$, we get

$L\ \{F'(t)\} = [0 - F(0)] - \int_0^\infty -pe^{-pt}\ F(t)\ dt$

$L\ \{F'(t)\} = -F(0) + p\int_0^\infty e^{-pt}\ F(t) dt$

$L\ \{F'(t)\} = \ \ \ pL\{F(t)\} - F(0)$

$L\ \{F'(t)\} = \ \ \ \ pf(p) - F(0)$

Now, since $\ \ L\{F'(t)\} = pL\{F(t)\} - F(0),$

Therefore, $L\{F''(t)\} = pL\{F'(t)\} - F'(0)$

$L\{F''(t)\} = p\{pL\{F(t)\} - F(0)\} - F'(0)$

$L\{F''(t)\} = p^2L\{F(t)\} - \mathrm{p}F(0) - F'(0)$

$L\{F''(t)\} = p^2f(p) - \mathrm{p}F(0) - F'(0)$

Similarly, $L\{F'''(t)\} = p^3f(p) - p^2F(0) - pF'(0) - F''(0)$ and so on.

D. Inverse Laplace Transformations

The inverse Laplace transformsof the function f(p) is L^{-1}[f (p)] =F (t). If we write L [F(t)] = f(p), then L^{-1}[f(p)] = F (t), where L^{-1} is called the inverse Laplace transforms operator [1-3].

E. Inverse Laplace Transformations of Some Functions

1. $L^{-1}\{\frac{1}{p}\} = 1$
2. $L^{-1}\{\frac{1}{(p-b)}\} = e^{bt}$
3. $L^{-1}\{\frac{1}{p^2+b^2}\} = \frac{1}{b}$ sinbt
4. $L^{-1}\{\frac{p}{p^2+b^2}\}$ = cosbt
5. $L^{-1}\{\frac{p}{p^2-b^2}\}$ = coshbt
6. $L^{-1}\{\frac{1}{p^2-b^2}\} = \frac{1}{b}$sinhbt
7. $L^{-1}\{\frac{1}{p^n}\} = \frac{t^{n-1}}{(n-1)!}$

III. FORMULATION

A. Infinite Square Well Potential

A potential well is a potential energy function with a minimum. If a particle is left in the well and the total energy of the particle is less than the height of the potential well, we can say that the particle is trapped in the well. In classical mechanics, a particle trapped in the potential well can vibrate back and forth but cannot leave the well. In quantum mechanics, such a trapped particle is called bound state [4-6]. Considering a particle confined to the region 0 < z < a. it can move freely with in the region 0 < z < a, but subject to strong forces at z = 0 and z = a. Therefore, the particle never cross to the right to the regionz > a, or to the left of z < 0. It means V = 0 in the region 0 < z < a, and rises to infinity at z = 0 and z = a. This situation is called one dimensional potential box. Therefore, an infinite square well potential V (z) (shown in figure 1) is defined as

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

= ∞ for z ≤ 0 and z ≥ a.

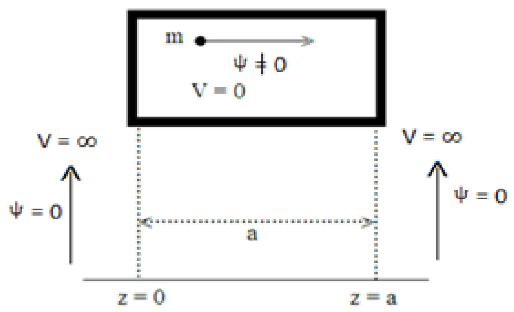

Figure 1: infinite square well potential

The time - independent Schrodinger'sequation in one dimension is written as[7-8]:

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

$$D_z \equiv \frac{\partial}{\partial z}$$

This equation is second-order linear differential equation. In equation (1), ψ(z) is probability wave function of the particle and V (z) is the potential energy. Now we will solve equation (1) to obtain Eigenenergy values and Eigenfunctions of a particle in an infinite square well potential.

For a particle inside an infinite square well potential,

V(z) = 0.

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Substitute this value of potential in equation (1), we get

$D_z^2\psi(z) + \frac{2m}{\hbar^2}E\,\psi(z) = 0$ (2)

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

For convenience, let us substitute

$\frac{2m}{\hbar^2}E = k^2$(3)

Therefore, equation (2) becomes

$D_z^2\psi(z) + k^2\psi(z) = 0$ (4)

Taking Laplace Transform of equation (4), we get

$L[D_z^2\psi(z)] + k^2L[\psi(z)] = 0$

This equation gives

$p^2\bar{\psi}(p) - p\psi(0) - D_z\psi(0) + k^2\bar{\psi}(p) = 0$ (5)

Applying boundary condition: $\psi(0) = 0$, equation (5) becomes,

$p^2\bar{\psi}(p) - D_z\psi(0) + k^2\bar{\psi}(p) = 0$

Or $p^2\bar{\psi}(p) + k^2\bar{\psi}(p) = D_z\psi(0)$ (6)

In this equation, $D_z\psi(0)$ is some constant.

Let us substitute $D_z\psi(0) = A,$

Equation (6) becomes

$p^2\bar{\psi}(p) + k^2\bar{\psi}(p) = A$

Or $\bar{\psi}(p) = \frac{A}{(p^2+k^2)}$ (7)

Taking inverse Laplace transforms of equation (7), we get

$\psi(z) = \frac{A}{k}\sin(k\,z)$ (8)

Applying boundary condition: $\psi(a) = 0$, equation (8) gives $\frac{A}{k}\sin(k\,a) = 0$

Since A cannot be equal to zero because for A = 0, $\psi(z) = 0$. This means that particle is not present inside the infinite square well potential which is not possible.

Therefore, sin (k a) = 0

Or ka = n π, where n is a positive integer.

Or $k = \frac{n\pi}{a}$ (9)

Substitute the value of k from equation (9) in equation (8), we get

$\psi(z) = \frac{A}{\frac{n\pi}{a}}\sin\left(\frac{n\pi}{a}z\right)$(10)

Where A is normalization constant.

B. Eigenenergy Values

Substitute the value of k from equation (9) in equation (3), we get

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

Solving, we get $E = \frac{n^2\pi^2\hbar^2}{2ma^2}$

Replacing E by E_n for different values of quantum number n, we have

$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$(11)

This equation gives the Eigenenergy values of the particle in an infinite square well potential. The above equation indicates that a particle confined in a certain region can have only certain values of energy. In other words energy quantization is a consequence of restricting a micro particle to a certain region. The minimum possible energy possessed by the particle inside the infinite square well potential is called Ground State or Zero Point Energy. The energy of the particle inside the infinite square well potential will be minimum at n = 1. This is because if n = 0, then $\psi_0(z) = 0$ everywhere inside the infinite square well potential and then probability density inside the infinite square well potential, $|\psi_0(z)|^2 = 0$, which means that particle is not present inside the infinite square well potential. Hence E = 0 is not allowed. This means that the particle cannot have zero total energy inside the infinite square well potential, so it cannot be at rest inside the infinite square well potential quantum mechanically.

For n=1, $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$

This gives the Ground State or Zero Point Energy of particle in an infinite square well potential.

C. Determination of constant A

Since the probability density between z = 0 and z = a, is one, because the particle is somewhere within this boundary, that is inside the infinite square well potential. Hence applying normalization condition, we can write

$\int_{z=0}^{z=a}\psi(z)\,\psi(z)^*dz = 1$ (12)

Here $\psi(z)^*$ is the complex conjugate of $\psi(z)$.

Using equation (10) in equation (12), we can write

$\left(\frac{A}{\frac{n\pi}{a}}\right)^2\int_{z=0}^{z=a}\sin^2\left(\frac{n\pi}{a}z\right)\,dz = 1$

Or $\left(\frac{A}{\frac{n\pi}{a}}\right)^2\int_{z=0}^{z=a}\frac{1}{2}\left[1-\cos\left(\frac{2n\pi}{a}z\right)\right]dz = 1$

Solving the integration and arranging, we get

$A = \frac{n\pi}{a}\left(\frac{2}{a}\right)^{\frac{1}{2}}$ (13)

D. Normalized Wave function (Eigen functions)

Substitute the value of A from equation (13) in equation (10), we get

$\psi(z) = \left(\frac{2}{a}\right)^{\frac{1}{2}}\sin\left(\frac{n\pi}{a}z\right)$

Replacing $\psi(z)$ by $\psi_n(z)$ for different values of quantum number n, we can write

$\psi_n(z) = \left(\frac{2}{a}\right)^{\frac{1}{2}}\sin\left(\frac{n\pi}{a}z\right)$(14)

This equation gives the Eigenfunctions or normalized wavefunction of the particle in an infinite square well potential. Since $\psi_n(z)$ is normalized, therefore the value of $|\psi_n(z)|^2$ is always positive and at a given z is equal to the probability density of finding the particle there. At z = 0 and z = a, the boundaries of the infinite square well potential, $|\psi_n(z)|^2 = 0$. The probability density of the particle being present inside the infinite square well potential may be different for different quantum numbers. For example, $\left|\psi_1\left(\frac{a}{2}\right)\right|^2 = \frac{a}{2}$, maximum in the middle of the box and $\left|\psi_2\left(\frac{a}{2}\right)\right|^2 = 0$, minimum in the middle of the box. This means that a particle in the lowest energy state at n = 1 is most likely to be in the middle of the box while a particle in the next higher energy state at n = 2 is never there quantum mechanically. Classical physics, of course, suggests the same probability for the particle being anywhere inside the infinite square well potential.

For n = 1, $\psi_1(z) = \left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{\pi}{a}z\right)$…….. (15)

This equation (15) gives the ground state wave function of the particle in an infinite square well potential.

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IV. CONCLUSION

In this paper an attempt is made to find the Eigenenergy values and Eigenfunctions of the particle in an infinite square well potential via solving Schrodinger time-independent equation for the particle in an infinite square well potential via Laplace transforms. This method can be an effective method as through simple computation we have obtained Eigenenergy values and Eigenfunctions of the particle in an infinite square well potential. We have found a remarkable characteristic of the Eigenfunctions of one dimensional Schrodinger's time-independent wave equation for a particle in an infinite square well potential that each Eigenfunctionis associated with a particular Eigenenergy value of the particle confined inside an infinite square well potential.

REFERENCES

1. Advanced Engineering Mathematics by Erwin Kreysig 10th edition, 2014
2. Higher Engineering Mathematics byDr.B.S.Grewal 43rd edition 2015.
3. Advanced engineering mathematics by H.K. Dass. Edition: Reprint, 2014.
4. Quantum mechanics by Satya Parkash. Edition: Reprint, 2016.
5. A text book of Engineering Physics by M.N. Avadhanulu. Revised edition 2014.
6. Introduction to Quantum mechanics by David j. Griffiths. Edition 2nd, 2017.
7. Principles of quantum mechanics by P.A.M. Dirac. Edition: Reprint, 2016.
8. Quantum Mechanics and Path Integralsby Richard P. Feynman, Albert R. Hibbs, Daniel F. Styer
9. Quantum mechanics by B.N. Srivastava, R.M. Richaria. 16th edition, 2017.
10. An introduction to Laplace transforms and Fourier series by Dyke and Phil.

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