

# 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.

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**Abstract:** Quantum mechanics is one of the fundamental theories of physics which explains the nature of atoms and subatomic particles at least possible energy scale. In this mechanics, we solve physical problems by algebraic and analytic methods. The general solutions of Schrodinger's time - independent one dimensional equation for a particle restricted to move inside the infinite square well potential can be obtained by solving the Schrodinger's equation via matrix method. In this paper, we will discuss the Eigen energy values and Eigen functions of a particle restricted to move inside the infinite square well potential by solving Schrodinger's time-independent one dimensional equation by matrix method. We will conclude that the Eigen functions obtained by solving the Schrodinger's time - independent one dimensional equation for a particle restricted to move inside the infinite square well potential have a very interesting property that each Eigen function is linked with a particular Eigen energy value of the particle inside the infinite square well potential.

**Key Words:** Eigen functions, Eigen values, infinite square well, particle.

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## I. Introduction

Quantum mechanics is one of the fundamental theories of physics which explains the nature of atoms and subatomic particles at least possible energy scale and also describes the behavior of matter and energy on the scale of atoms and subatomic particles or waves. In this mechanics, we solve physical problems by algebraic and analytic methods. By solving Schrodinger's time- independent one dimensional equation via matrix method, we can obtain the Eigen energy values and Eigen functions of a particle restricted to move in an infinite square well potential. The general solutions of Schrodinger's time- independent one dimensional equation for a particle restricted to move inside the infinite square well potential have a very interesting property that each Eigen function is linked with a particular Eigen energy value of the particle inside the infinite square well potential. To define Eigen values and Eigen functions, suppose that an operator  $\hat{O}$  is operated on the function  $g$  and results the same function  $g$  multiplied by some constant  $\alpha$  i.e.  $\hat{O} g = \alpha g$ . In this equation,  $g$  is the Eigen function of operator  $\hat{O}$  and the constant  $\alpha$  is the Eigen value of the operator  $\hat{O}$  related with the Eigen function  $g$  and the equation is known as Eigen value equation. The Eigen functions 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. As an example, to illustrate the Eigen value of an operator, consider the operator  $(\frac{d^2}{dz^2})$  operating on a well-behaved function  $\sin 5z$ . The result is

$$\frac{d^2}{dz^2}(\sin 5z) = -25 \sin 5z$$

Comparing this equation with standard Eigen value equation  $\hat{O} g = \alpha g$ , we find that (-25) is the Eigen value of operator  $(\frac{d^2}{dz^2})$  associated with the Eigen function  $\sin 5z$ .

### Eigen values and Eigen vectors:

If  $B$  is any square matrix of order  $n$  with elements  $b_{ij}$ , we can find a column matrix  $Y$  and a constant  $\lambda$  such that  $BY = \lambda Y$  or  $BY - \lambda Y = 0$  or  $(B - \lambda I)Y = 0$

This matrix equation represents  $n$  homogeneous linear equations:

$$\begin{aligned}(b_{11} - \lambda) y_1 + b_{12} y_2 + b_{13} y_3 + \dots + b_{1n} y_n &= 0 \\ b_{21} y_1 + (b_{22} - \lambda) y_2 + b_{23} y_3 + \dots + b_{2n} y_n &= 0\end{aligned}$$

..... $b_{n1} y_1 + b_{n2} y_2 + b_{n3} y_3 + \dots + (b_{nn} - \lambda) y_n = 0$ ,  
 which will have a non - trivial solution only if the determinant of the coefficients vanishes i.e.

$$\begin{vmatrix} (b_{11} - \lambda) & b_{12} & \dots & b_{1n} \\ b_{21} & (b_{22} - \lambda) & \dots & b_{2n} \\ \dots & \dots & \dots & \dots \\ b_{n1} & b_{n2} & \dots & (b_{nn} - \lambda) \end{vmatrix} = 0$$

When we expand the determinant we will get  $n^{\text{th}}$  degree equation in  $\lambda$ , which is known as characteristic equation of the matrix B. The roots of the characteristic equation of matrix B i.e.  $\lambda_i$  (where  $i = 1, 2, 3, \dots, n$ ) are called Eigen values or latent roots. Corresponding to each Eigen value, the characteristic equation of matrix B will

have a non-zero solution  $Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$  (a column matrix), which is known as Eigen vector.

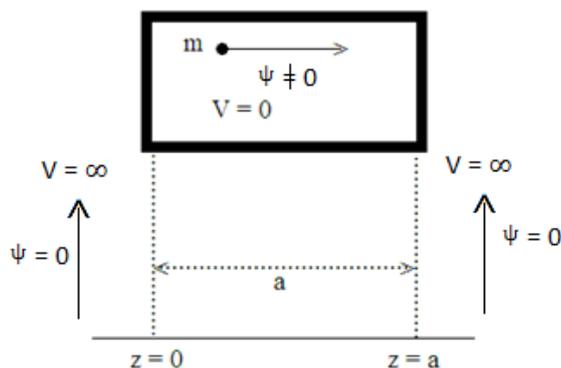
**Formulation:**

**Infinite Square well potential:**

A potential well is a potential energy function with a minimum. If a particle is left in this potential well and the total energy of the particle is less than the height of the potential well, then we can say that the particle is confined inside the potential well. In classical mechanics, a particle confined inside the potential well can vibrate to and fro but cannot leave the well. In quantum mechanics, such a confined particle is called a bound state. Considering a particle restricted to move in the region  $0 < z < a$ . It can move freely within the region  $0 < z < a$ , but acted upon by strong forces at  $z = 0$  and  $z = a$ . Therefore, the particle never crosses to the right to the region  $z > a$ , or to the left of the region  $z < 0$ . It means that the potential energy of the particle is zero in the region  $0 < z < a$ , and rises to infinity at  $z = 0$  and  $z = a$ . Such a situation is called one - dimensional potential box. Therefore, a square well potential  $V(z)$  of infinite height (shown in figure 1) is defined as

$$V(z) = 0 \text{ for } 0 < z < a$$

$$= \infty \text{ for } z \leq 0 \text{ and } z \geq a.$$



**Figure 1: infinite square well potential**

The time - independent Schrodinger's equation in one dimension is written as:

$$D_z^2 \psi(z) + \frac{2m}{\hbar^2} \{E - V(z)\} \psi(z) = 0 \dots \dots \dots (1) \quad D_z \equiv \frac{\partial}{\partial z}$$

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

For a particle inside the infinite square well potential,  $V(z) = 0$

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

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

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

For convenience, let us substitute

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

Therefore, equation (2) becomes

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

Let us substitute

$$\psi(z) = \psi_1(z) \text{ and}$$

$$D_z \psi_1(z) = \psi_2(z) \dots \dots \dots (5)$$

We can rewrite equation (4) as

$$D_z \psi_2(z) + k^2 \psi_1(z) = 0$$

Or  $D_z \psi_2(z) = -k^2 \psi_1(z) \dots \dots \dots (6)$

Differential equations (5) and (6) can be written in single matrix formas

$$D_z \begin{bmatrix} \psi_1(z) \\ \psi_2(z) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k^2 & 0 \end{bmatrix} \begin{bmatrix} \psi_1(z) \\ \psi_2(z) \end{bmatrix}$$

The characteristic equation of  $\begin{bmatrix} 0 & 1 \\ -k^2 & 0 \end{bmatrix}$  is

$$\begin{vmatrix} 0 - \lambda & 1 \\ -k^2 & 0 - \lambda \end{vmatrix} = 0$$

Solving the determinant, we get

$$\lambda^2 + k^2 = 0$$

Or  $\lambda = \pm i k$

Now the Eigen vector for  $\lambda = i k$  is given by  $\begin{bmatrix} 0 - i k & 1 \\ -k^2 & 0 - i k \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

Applying elementary transformation  $R_2 \rightarrow R_2 + i k R_1$ , we can write

$$\begin{bmatrix} -i k & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

This results

$$-i k z_1 + z_2 = 0$$

Or  $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ i k \end{bmatrix}$

And the Eigen vector for  $\lambda = -i k$  is given by

$$\begin{bmatrix} 0 + i k & 1 \\ -k^2 & 0 + i k \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Applying elementary transformation  $R_2 \rightarrow R_2 - i k R_1$ , we can write

$$\begin{bmatrix} i k & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

This results

$$i k z_1 + z_2 = 0$$

Or  $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -i k \end{bmatrix}$

The matrix of Eigen vectors is  $\begin{bmatrix} 1 & 1 \\ i k & -i k \end{bmatrix}$ .

Let  $P = \begin{bmatrix} 1 & 1 \\ i k & -i k \end{bmatrix}$ , then the inverse matrix of P is given by  $P^{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2ik} \\ \frac{1}{2} & \frac{-1}{2ik} \end{bmatrix}$ .

Now we have to find  $P e^{\lambda z} P^{-1}$ .

$$\begin{aligned} P e^{\lambda z} P^{-1} &= \begin{bmatrix} 1 & 1 \\ i k & -i k \end{bmatrix} \begin{bmatrix} e^{i k z} & 0 \\ 0 & e^{-i k z} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2ik} \\ \frac{1}{2} & \frac{-1}{2ik} \end{bmatrix} \\ &= \begin{bmatrix} e^{i k z} & e^{-i k z} \\ i k e^{i k z} & -i k e^{-i k z} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2ik} \\ \frac{1}{2} & \frac{-1}{2ik} \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{2}(e^{i k z} + e^{-i k z}) & \frac{1}{2ik}(e^{i k z} - e^{-i k z}) \\ \frac{ik}{2}(e^{i k z} - e^{-i k z}) & \frac{1}{2}(e^{i k z} + e^{-i k z}) \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{2}(e^{i k z} + e^{-i k z}) & \frac{1}{2ik}(e^{i k z} - e^{-i k z}) \\ \frac{-k}{2i}(e^{i k z} - e^{-i k z}) & \frac{1}{2}(e^{i k z} + e^{-i k z}) \end{bmatrix} \\ &= \begin{bmatrix} \cos k z & \frac{1}{k} \sin k z \\ -k \sin k z & \cos k z \end{bmatrix} \end{aligned}$$

Applying initial condition i.e.  $\psi_1(0) = \psi(0) = 0$  and since  $\psi_2(0) = D_z \psi(0)$  is constant, therefore substituting  $\psi_2(0) = D_z \psi(0) = C$  (a constant), we can write

$$\begin{bmatrix} \psi_1(z) \\ \psi_2(z) \end{bmatrix} = \begin{bmatrix} \cos k z & \frac{1}{k} \sin k z \\ -k \sin k z & \cos k z \end{bmatrix} \begin{bmatrix} 0 \\ C \end{bmatrix}$$

$$\text{Or } \begin{bmatrix} \psi_1(z) \\ \psi_2(z) \end{bmatrix} = \begin{bmatrix} \frac{C}{k} \sin kz \\ C \cos kz \end{bmatrix}$$

This equation results

$$\psi_1(z) = \frac{C}{k} \sin kz$$

$$\text{Or } \psi(z) = \frac{C}{k} \sin kz \dots\dots\dots (7)$$

$$\text{And } \psi_2(z) = C \cos kz$$

$$\text{Or } D_z \psi(z) = C \cos kz \dots\dots\dots (8)$$

Applying boundary condition:  $\psi(a) = 0$ , equation (7) gives  $\frac{C}{k} \sin(ka) = 0$

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

Therefore,  $\sin(ka) = 0$

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

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

Substitute the value of k from equation (9) in equation (7), we get

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

Where C is normalization constant.

**Eigen energy values:**

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

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

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

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

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

This equation provides the Eigen Energy values of the particle in an infinite square well potential. The above equation indicates that a particle restricted to move inside 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.

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

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

**Determination of constant normalization constant C:**

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

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

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

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

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

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

Solving the integration and rearranging, we get

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

**Normalized wave function (Eigen Functions):**

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

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

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

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

This equation provides the Eigen functions or normalized wave function 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 the boundaries of the square well potential of infinite height i.e. at  $z = 0$  and  $z = a$ ,  $|\psi_n(z)|^2 = 0$ . The probability density of the particle being present inside the infinite square well potential may be different for different quantum numbers. For example,  $|\psi_1(z)|^2 = \frac{a}{2}$ , which is maximum in the middle of the infinite square well potential and  $|\psi_2(z)|^2 = 0$ , which is minimum in the middle of the infinite square well potential. This means that a particle in the lowest energy state at  $n = 1$  is most likely to be in the middle of the infinite square well potential 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 square well potential of infinite height.

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

This equation provides the ground state or lowest energy state wave function of the particle restricted to move inside the infinite square well potential.

## II. Conclusions

In this paper an attempt is made to find the Eigen energy values and Eigen functions of the particle inside the infinite square well potential by solving Schrodinger time - independent equation for the particle in an infinite square well potential via matrix method. We have found a remarkable property of the Eigen functions that each Eigen function is linked with a particular Eigen energy value of the particle which is restricted to move inside the infinite square well potential.

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